



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:57 PM UTC

PDB ID : 7OUI / pdb_00007oui
EMDB ID : EMD-13078
Title : Structure of C2S2M2-type Photosystem supercomplex from Arabidopsis thaliana (digitonin-extracted)
Authors : Graca, A.T.; Hall, M.; Persson, K.; Schroder, W.P.
Deposited on : 2021-06-11
Resolution : 2.79 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

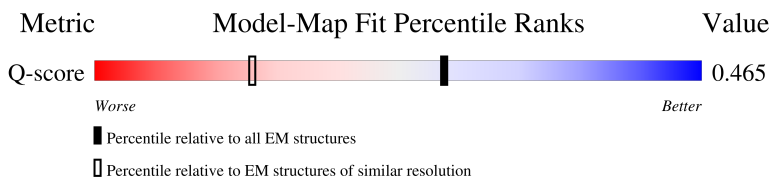
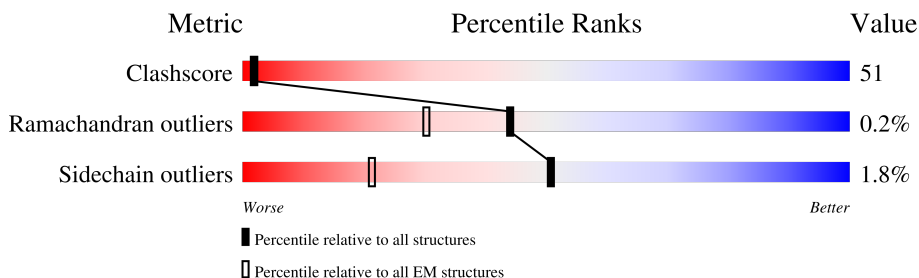
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	266	76% 30% 43% 24%
1	3	266	76% 30% 43% 24%
1	5	266	76% 30% 43% 24%
1	7	266	76% 30% 43% 24%

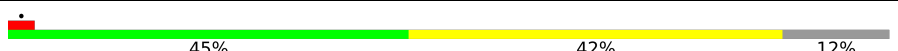
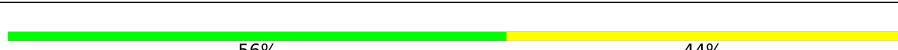
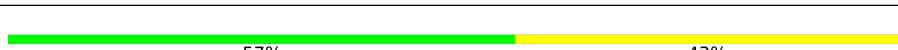
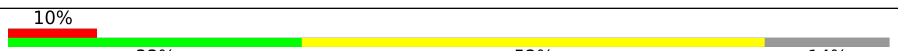
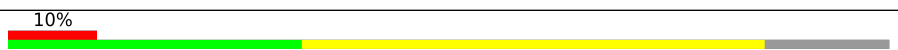
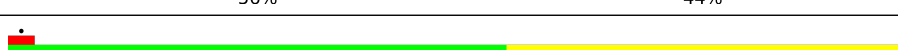
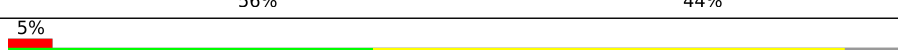
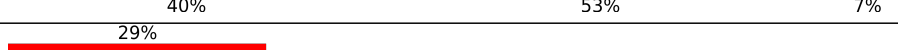
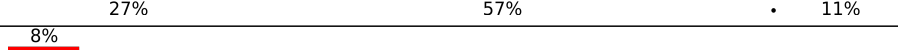
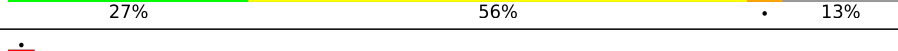
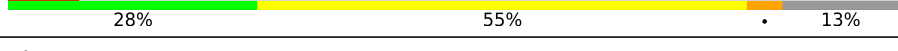
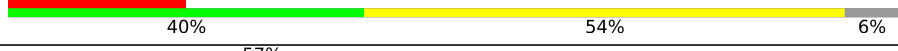
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Mol	Chain	Length	Quality of chain
2	2	243	
2	6	243	
3	4	212	
3	8	212	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	459	
6	c	459	
7	D	352	
7	d	352	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	72	
10	h	72	
11	I	36	
11	i	36	
12	K	37	
12	k	37	
13	L	38	
13	l	38	
14	M	34	

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Mol	Chain	Length	Quality of chain
14	m	34	
15	O	247	
15	o	247	
16	T	33	
16	t	33	
17	W	54	
17	w	54	
18	X	42	
18	x	42	
19	Z	62	
19	z	62	
20	S	232	
20	s	232	
21	G	232	
21	N	232	
21	Y	232	
21	g	232	
21	n	232	
21	y	232	
22	R	250	
22	r	250	
23	U	28	
23	u	28	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	1	301	X	-	-	-
24	CHL	1	302	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	603	X	-	X	-
24	CHL	5	301	X	-	-	-
24	CHL	5	302	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	603	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	X	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	X	-
24	CHL	R	605	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	613	X	-	-	-
24	CHL	S	302	X	-	-	-
24	CHL	S	306	X	-	-	-
24	CHL	S	307	X	-	-	-
24	CHL	S	308	X	-	-	-
24	CHL	Y	302	X	-	X	-
24	CHL	Y	306	X	-	-	-
24	CHL	Y	307	X	-	-	-
24	CHL	Y	308	X	-	-	-
24	CHL	Y	309	X	-	-	-
24	CHL	Y	310	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	n	607	X	-	X	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	X	-
24	CHL	r	605	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	613	X	-	-	-
24	CHL	s	302	X	-	-	-
24	CHL	s	306	X	-	-	-
24	CHL	s	307	X	-	-	-
24	CHL	s	308	X	-	-	-
24	CHL	y	302	X	-	X	-
24	CHL	y	306	X	-	-	-
24	CHL	y	307	X	-	-	-
24	CHL	y	308	X	-	-	-
24	CHL	y	309	X	-	-	-
24	CHL	y	310	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	A	401	X	-	-	-
25	CLA	A	402	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	X	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	X	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	X	-
25	CLA	N	603	X	-	X	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	X	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	X	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	608	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	303	X	-	-	-
25	CLA	S	304	X	-	-	-
25	CLA	S	305	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	S	314	X	-	-	-
25	CLA	Y	303	X	-	X	-
25	CLA	Y	304	X	-	X	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	311	X	-	X	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	X	-
25	CLA	c	511	X	-	X	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	610	X	-	X	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	X	-
25	CLA	n	603	X	-	X	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	X	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	X	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	608	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	614	X	-	-	-
25	CLA	s	303	X	-	-	-
25	CLA	s	304	X	-	-	-
25	CLA	s	305	X	-	-	-
25	CLA	s	309	X	-	-	-
25	CLA	s	310	X	-	-	-
25	CLA	s	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	s	312	X	-	-	-
25	CLA	s	313	X	-	-	-
25	CLA	s	314	X	-	-	-
25	CLA	y	303	X	-	X	-
25	CLA	y	304	X	-	-	-
25	CLA	y	305	X	-	-	-
25	CLA	y	311	X	-	X	-
25	CLA	y	312	X	-	-	-
25	CLA	y	313	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-
28	BCR	t	101	-	-	X	-
32	AJP	A	412	X	-	-	-
32	AJP	B	624	X	-	-	-
32	AJP	G	618	X	-	-	-
32	AJP	N	619	X	-	-	-
32	AJP	N	620	X	-	-	-
32	AJP	S	319	X	-	-	-
32	AJP	Y	320	X	-	-	-
32	AJP	Y	321	X	-	-	-
32	AJP	Y	322	X	-	-	-
32	AJP	Y	323	X	-	-	-
32	AJP	Y	324	X	-	-	-
32	AJP	a	413	X	-	-	-
32	AJP	b	624	X	-	-	-
32	AJP	g	618	X	-	-	-
32	AJP	n	619	X	-	-	-
32	AJP	n	620	X	-	-	-
32	AJP	s	319	X	-	-	-
32	AJP	y	320	X	-	-	-
32	AJP	y	321	X	-	-	-
32	AJP	y	322	X	-	-	-
32	AJP	y	323	X	-	-	-
32	AJP	y	324	X	-	-	-
33	BCT	A	413	-	-	X	-
39	LUT	s	316	-	-	X	-
41	XAT	r	616	-	-	X	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 85897 atoms, of which 1470 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	3	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	5	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	7	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		
2	6	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
3	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		
4	a	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		
5	b	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
6	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		
7	d	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	66	Total	C	N	O	0	0
			543	357	88	98		
8	e	66	Total	C	N	O	0	0
			543	357	88	98		

- Molecule 9 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
9	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

- Molecule 10 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			446	293	70	81	2		
10	h	60	Total	C	N	O	S	0	0
			446	293	70	81	2		

- Molecule 11 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
11	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

- Molecule 12 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	37	Total	C	N	O	S	0	0
			301	211	44	45	1		
12	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

- Molecule 13 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	36	Total	C	N	O	S	0	0
			302	200	47	55			
13	l	36	Total	C	N	O	S	0	0
			302	200	47	55			

- Molecule 14 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	32	Total	C	N	O	S	0	0
			250	173	35	41	1		
14	m	32	Total	C	N	O	S	0	0
			250	173	35	41	1		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	197	Total	C	N	O	S	0	0
			1516	969	241	302	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	197	Total	C	N	O	S	0	0
			1516	969	241	302	4		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
17	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 18 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	36	Total	C	N	O		0	0
			248	162	39	47			
18	x	36	Total	C	N	O		0	0
			248	162	39	47			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			464	313	69	81	1		
19	z	62	Total	C	N	O	S	0	0
			464	313	69	81	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
20	s	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		

- Molecule 21 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
21	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	Y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
21	g	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
21	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		

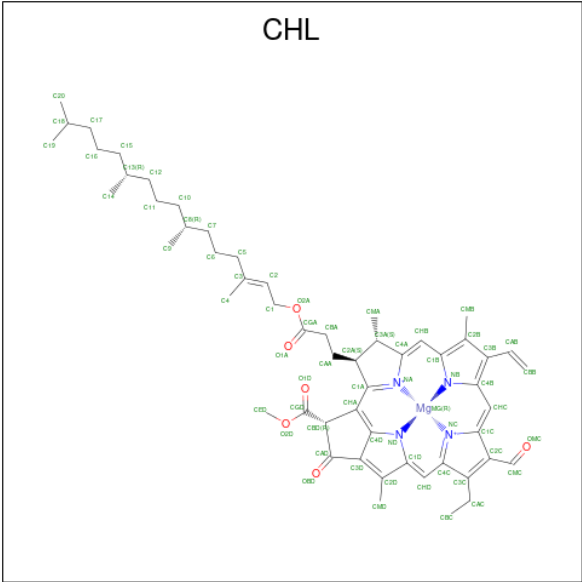
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	235	Total	C	N	O	S	0	0
			1827	1183	298	343	3		
22	r	235	Total	C	N	O	S	0	0
			1827	1183	298	343	3		

- Molecule 23 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	25	Total	C	N	O	S	0	0
			194	122	36	33	3		
23	u	25	Total	C	N	O	S	0	0
			194	122	36	33	3		

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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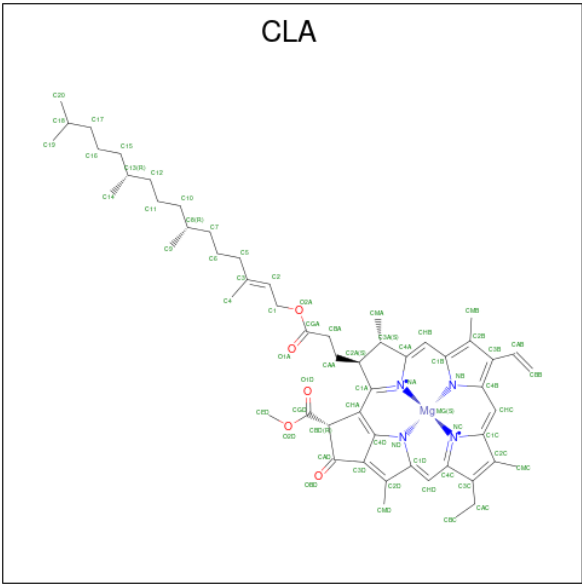
Mol	Chain	Residues	Atoms					AltConf
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0

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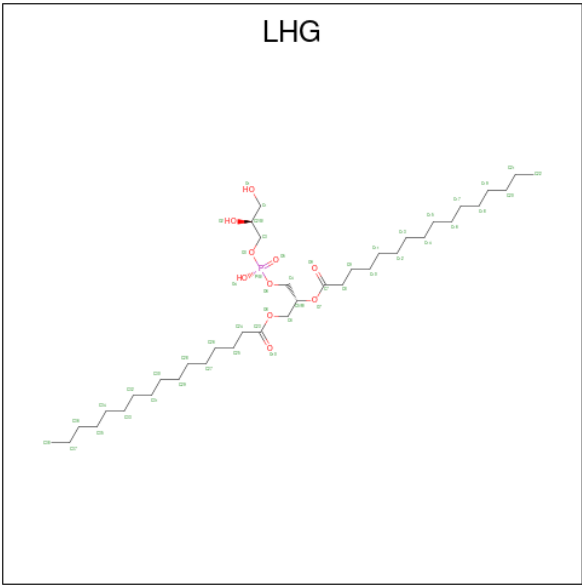
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			49	38	10	1	

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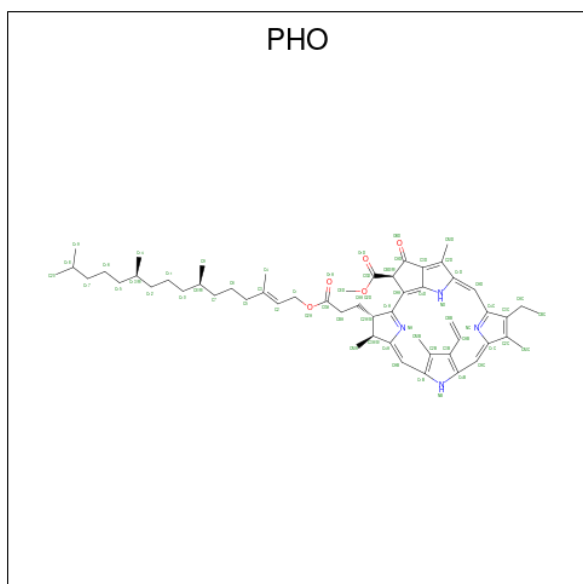
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 46	C 35	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 123	C 38	H 74	O 10 P 1	0	
26	D	1	Total 49	C 38	O 10	P 1	0	
26	L	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	N	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	R	1	Total 42	C 31	O 10	P 1	0	
26	6	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 49	C 38	O 10	P 1	0	
26	b	1	Total 46	C 35	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 123	C 38	H 74	O 10 P 1	0	
26	d	1	Total 49	C 38	O 10	P 1	0	
26	l	1	Total 49	C 38	O 10	P 1	0	

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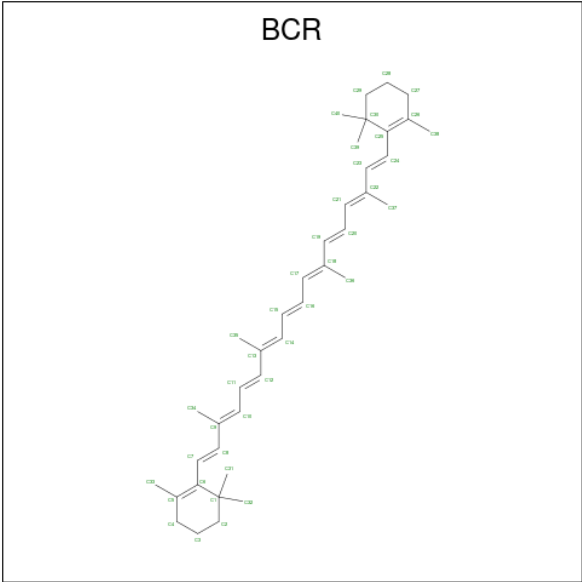
Mol	Chain	Residues	Atoms				AltConf
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	r	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



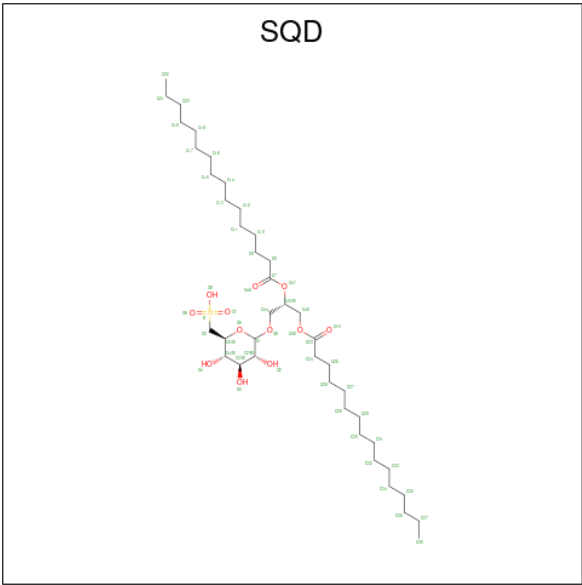
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	H	1	Total C 40 40	0
28	I	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	T	1	Total C 40 40	0
28	Z	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	i	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0
28	z	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



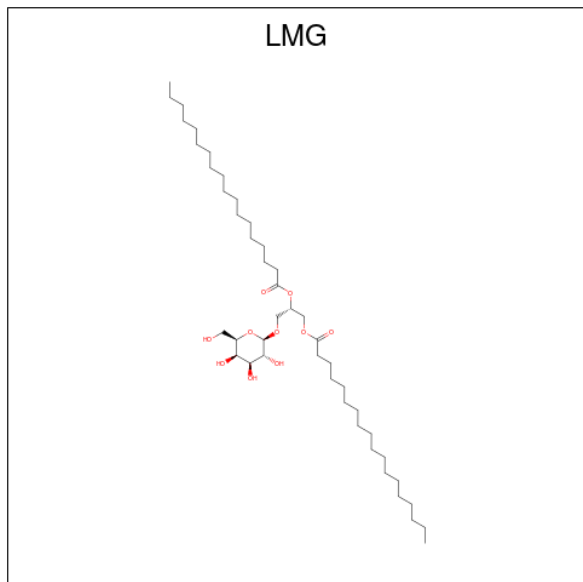
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O S 50 37 12 1	0
29	A	1	Total C O S 54 41 12 1	0
29	L	1	Total C O S 42 29 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	L	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



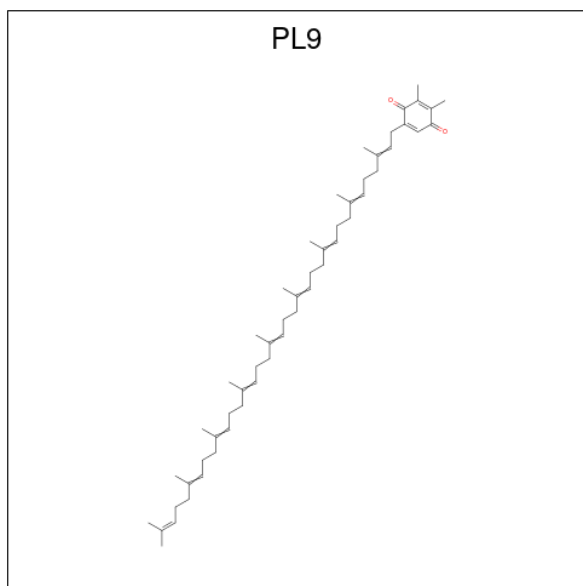
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O		0
			48	38	10		
30	A	1	Total	C	O		0
			40	30	10		
30	B	1	Total	C	O		0
			51	41	10		
30	B	1	Total	C	O		0
			55	45	10		
30	C	1	Total	C	O		0
			51	41	10		
30	D	1	Total	C	O		0
			46	36	10		

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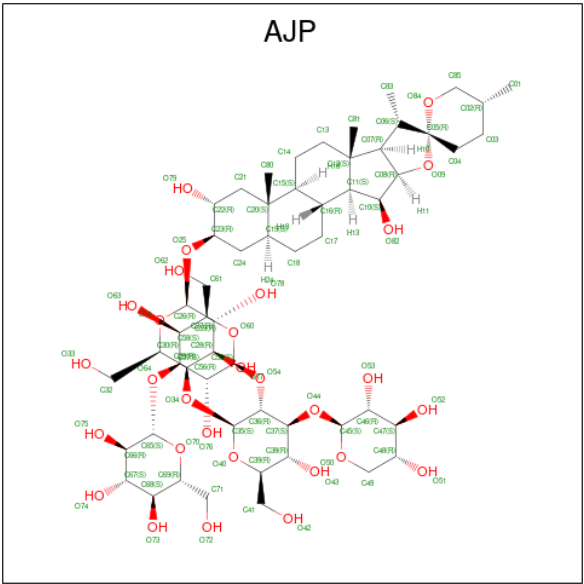
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			48	38	10	
30	a	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			55	45	10	
30	c	1	Total	C	O	0
			51	41	10	
30	d	1	Total	C	O	0
			46	36	10	

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			13	11	2	
31	D	1	Total	C	O	0
			55	53	2	
31	a	1	Total	C	O	0
			13	11	2	
31	d	1	Total	C	O	0
			55	53	2	

- Molecule 32 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉) (labeled as "Ligand of Interest" by depositor).



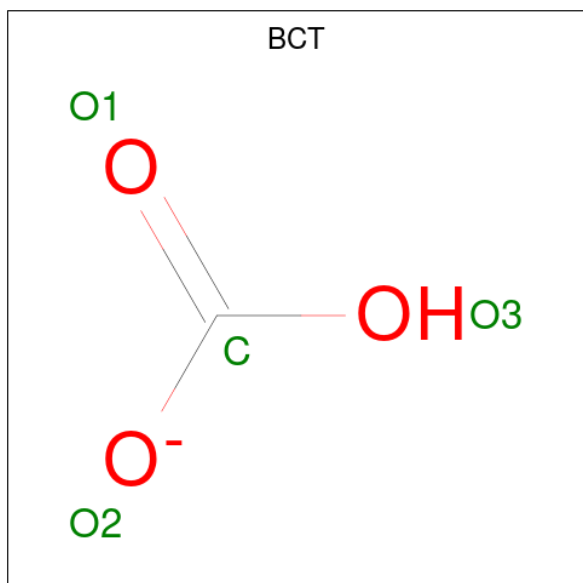
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	H	O	0
			177	56	92	29	
32	B	1	Total	C	H	O	0
			177	56	92	29	
32	S	1	Total	C	H	O	0
			95	33	53	9	
32	G	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	a	1	Total	C	H	O	0
			177	56	92	29	

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Mol	Chain	Residues	Atoms				AltConf
32	b	1	Total	C	H	O	0
			177	56	92	29	
32	s	1	Total	C	H	O	0
			95	33	53	9	
32	g	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			4	1	3	

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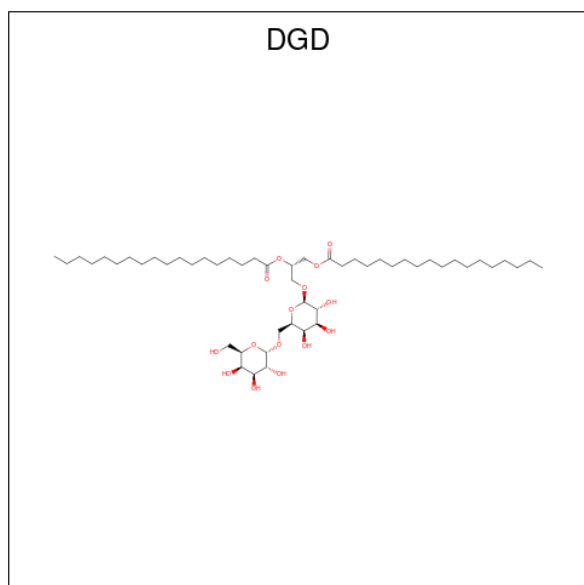
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Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	C	O	0
			4	1	3	

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe		0
			1	1		
34	a	1	Total	Fe		0
			1	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			59	44	15	
35	B	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	a	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			62	47	15	

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Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	

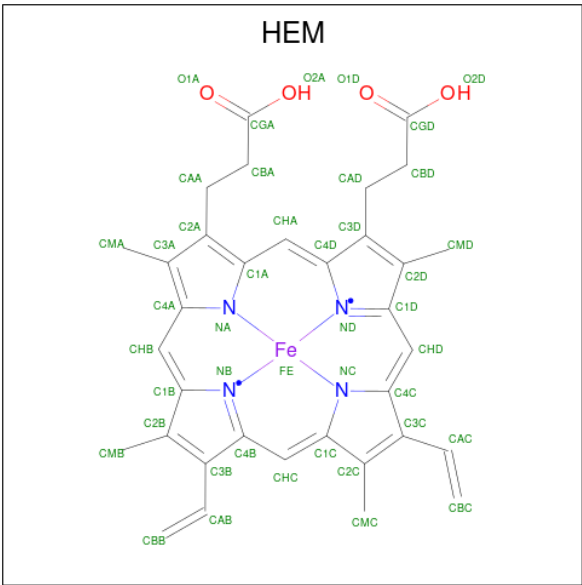
- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Ca	0
			1	1	
36	B	1	Total	Ca	0
			1	1	
36	a	1	Total	Ca	0
			1	1	
36	b	1	Total	Ca	0
			1	1	

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

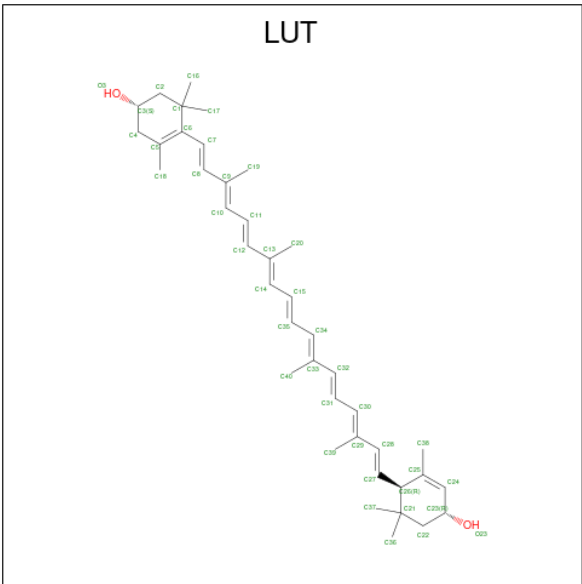
Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Cl	0
			1	1	
37	d	1	Total	Cl	0
			1	1	

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
38	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



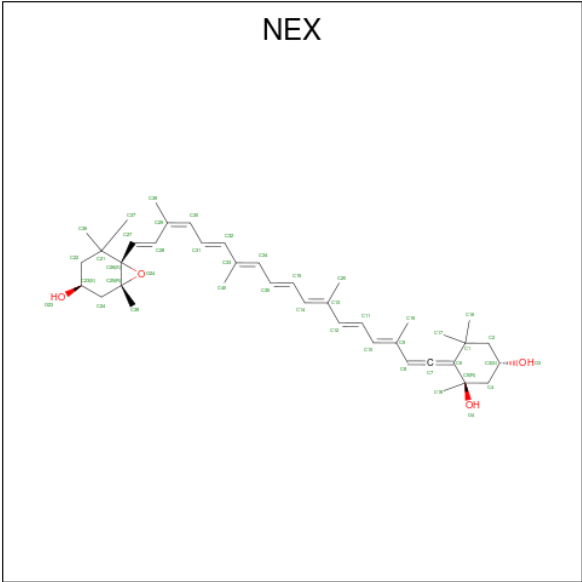
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	

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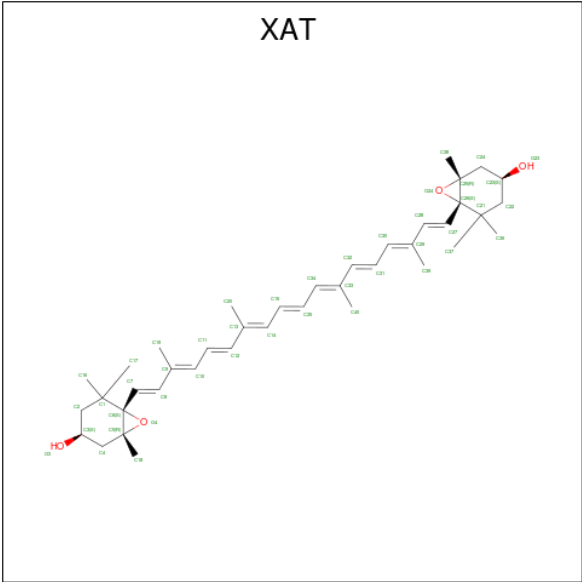
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	s	1	Total	C	O	0
			42	40	2	
39	s	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	y	1	Total	C	O	0
			42	40	2	
39	y	1	Total	C	O	0
			42	40	2	
39	r	1	Total	C	O	0
			42	40	2	

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
40	S	1	Total	C	O	0
			44	40	4	
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	R	1	Total	C	O	0
			44	40	4	
40	s	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	y	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
41	R	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	23	Total	O	0
			23	23	
42	B	10	Total	O	0
			10	10	
42	C	14	Total	O	0
			14	14	
42	D	14	Total	O	0
			14	14	
42	H	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	L	3	Total	O	0
			3	3	
42	M	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	W	1	Total	O	0
			1	1	

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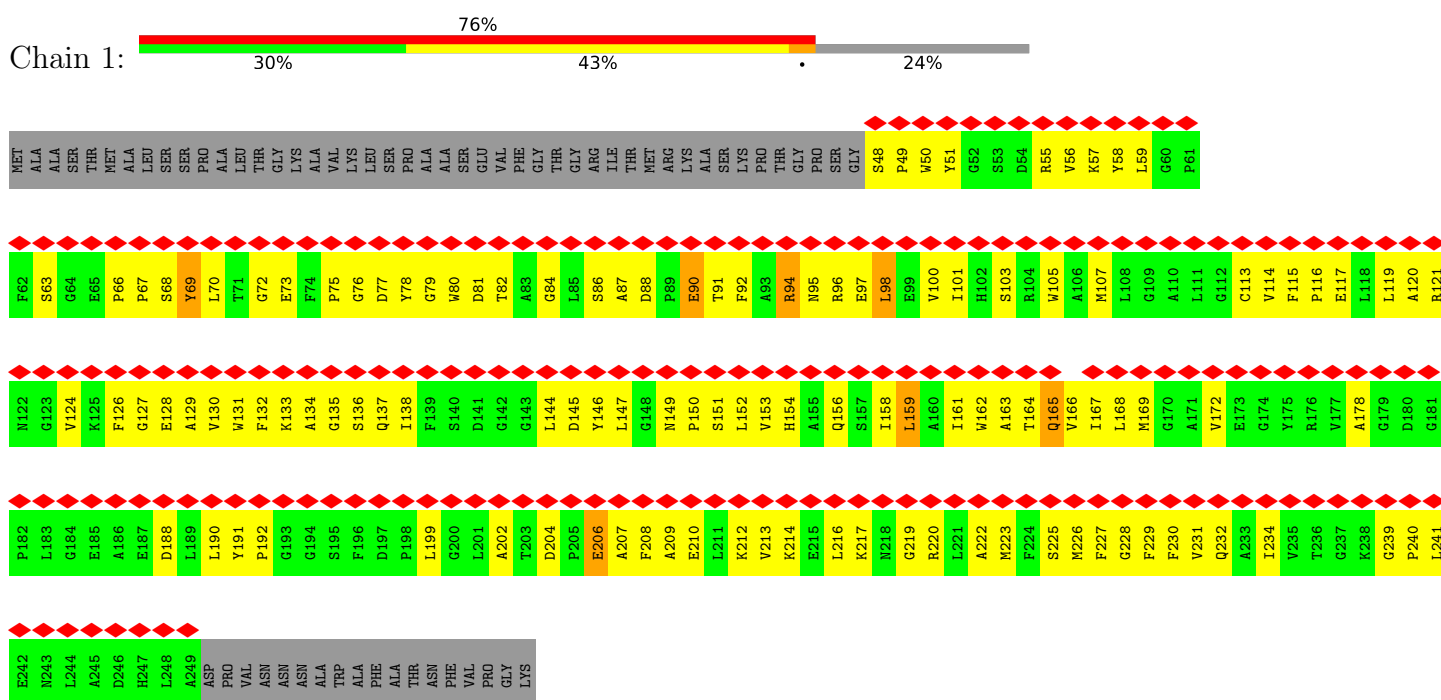
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Mol	Chain	Residues	Atoms		AltConf
42	a	23	Total 23	O 23	0
42	b	10	Total 10	O 10	0
42	c	14	Total 14	O 14	0
42	d	14	Total 14	O 14	0
42	h	1	Total 1	O 1	0
42	i	1	Total 1	O 1	0
42	l	3	Total 3	O 3	0
42	m	2	Total 2	O 2	0
42	t	1	Total 1	O 1	0
42	w	1	Total 1	O 1	0

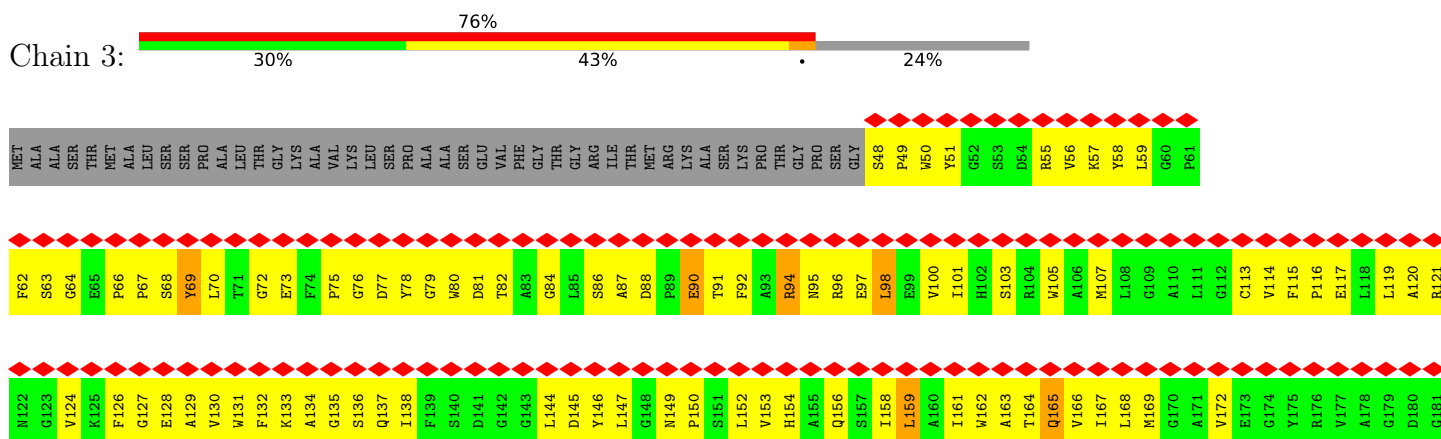
3 Residue-property plots

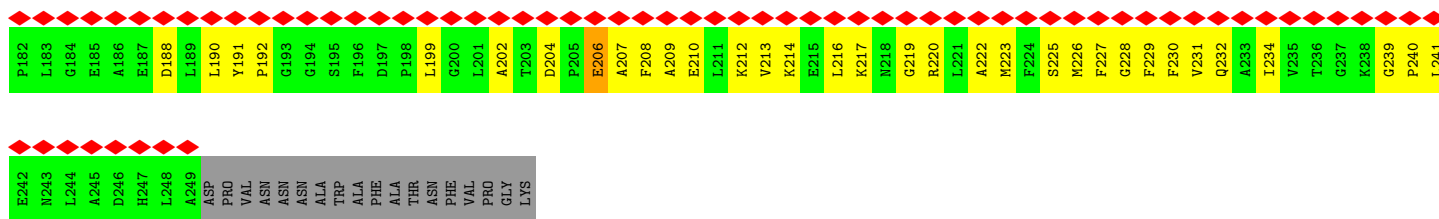
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

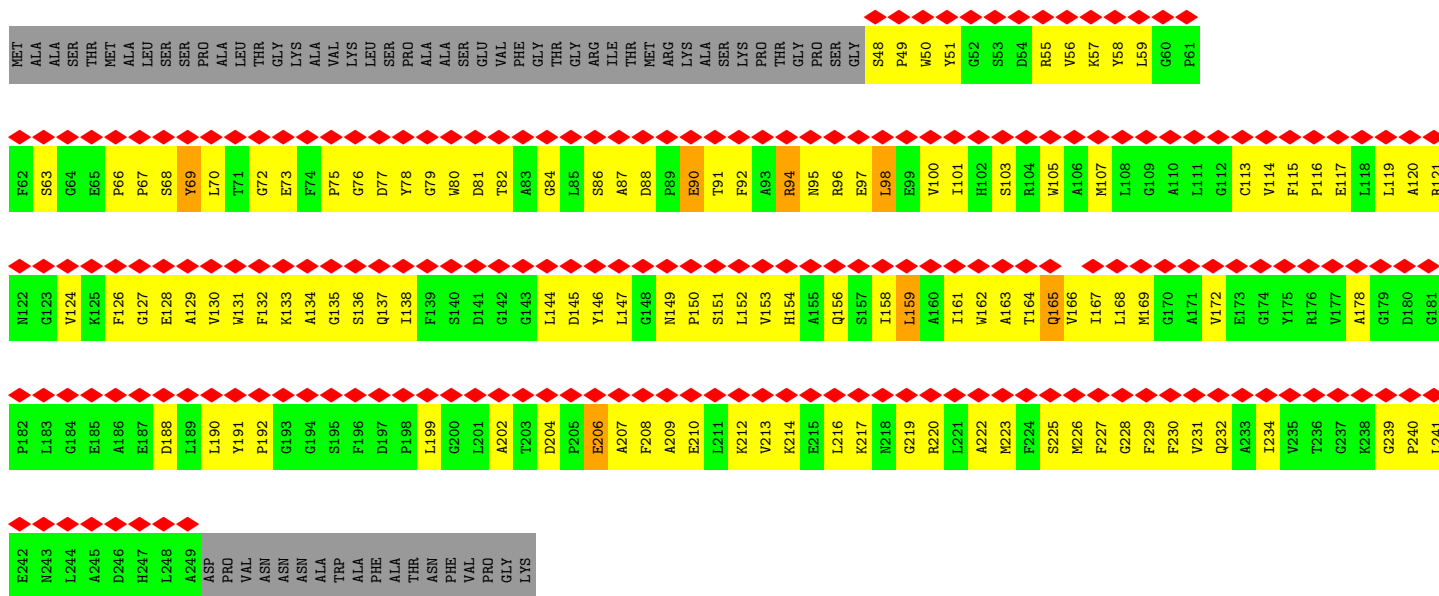
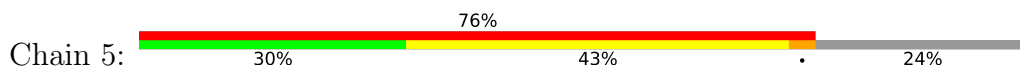


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

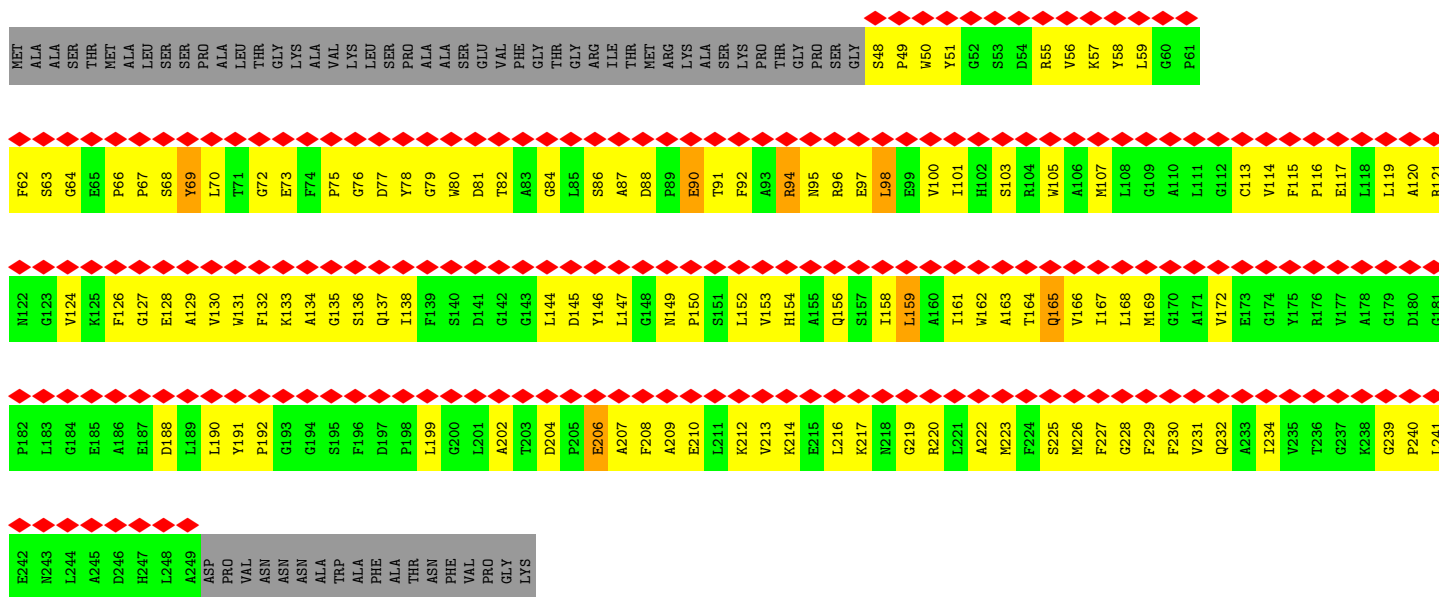
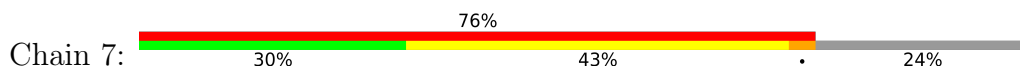




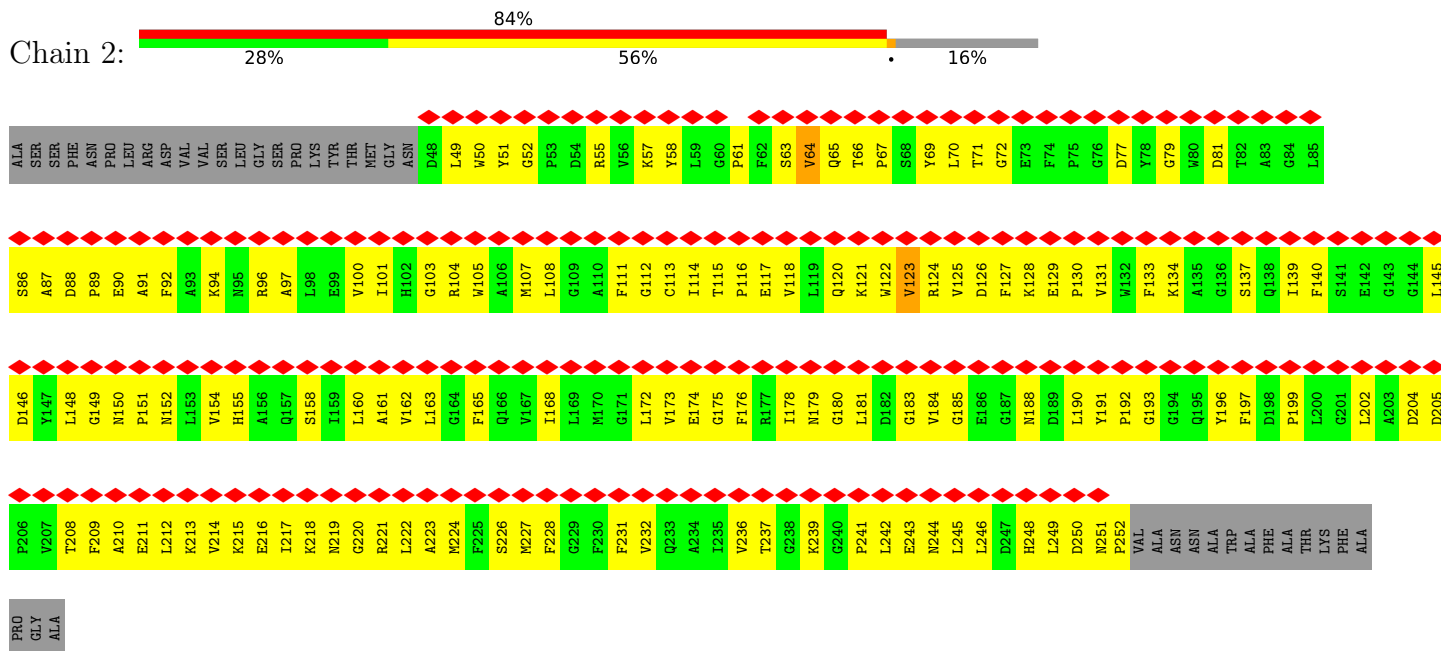
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



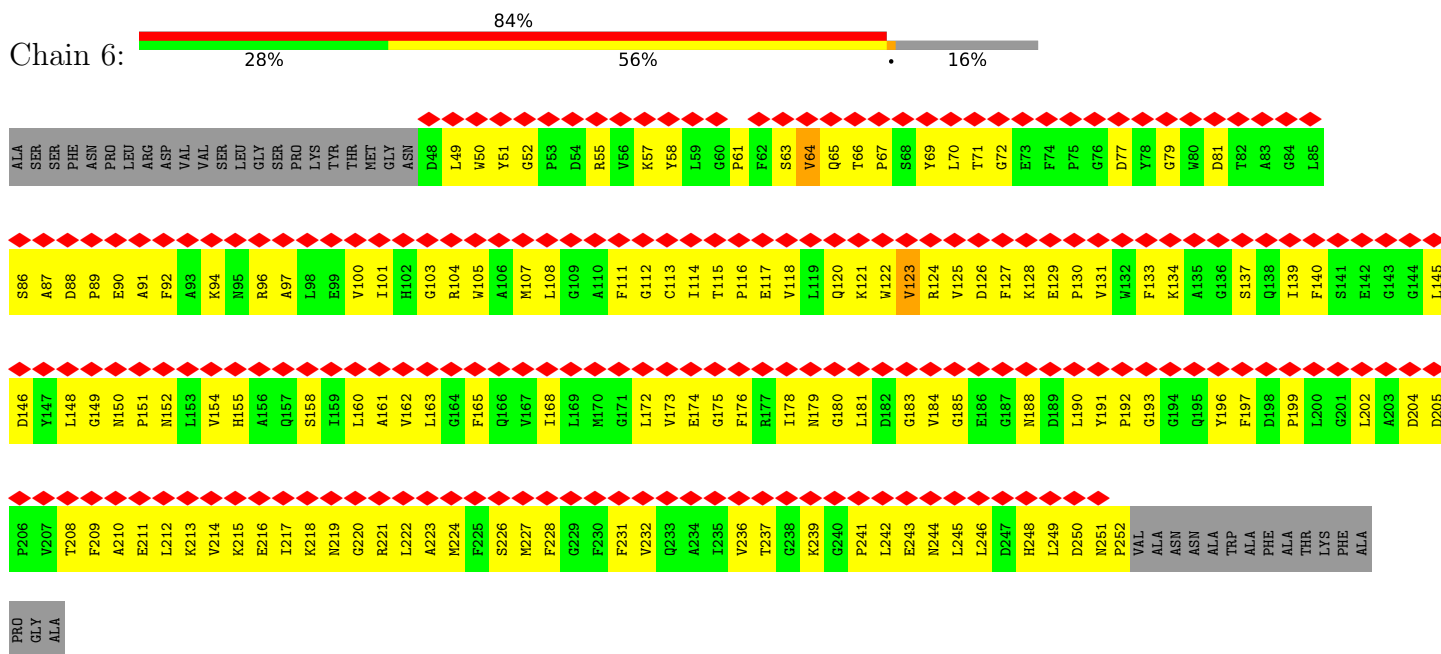
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



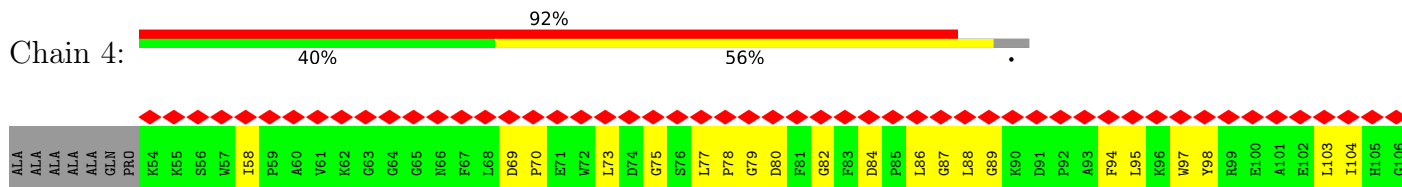
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

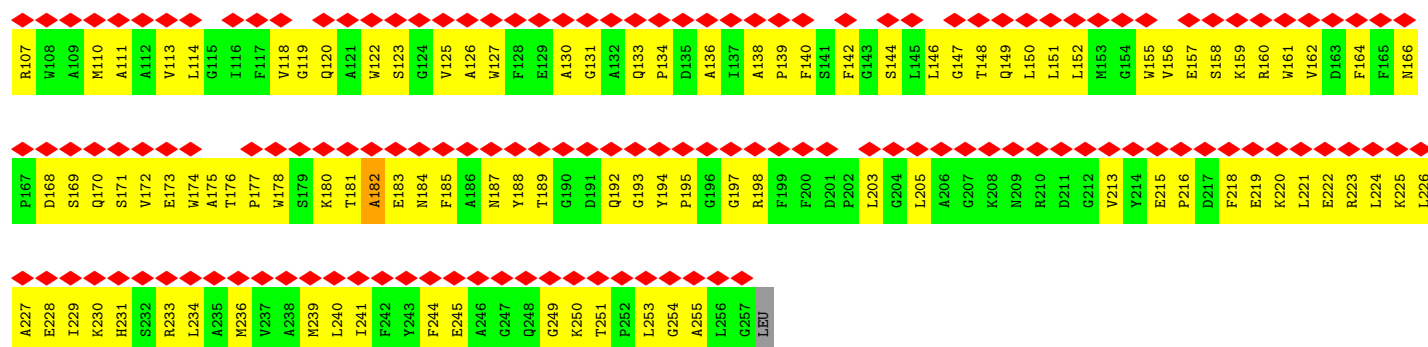


- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

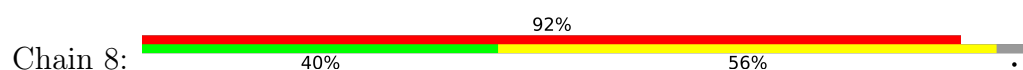


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

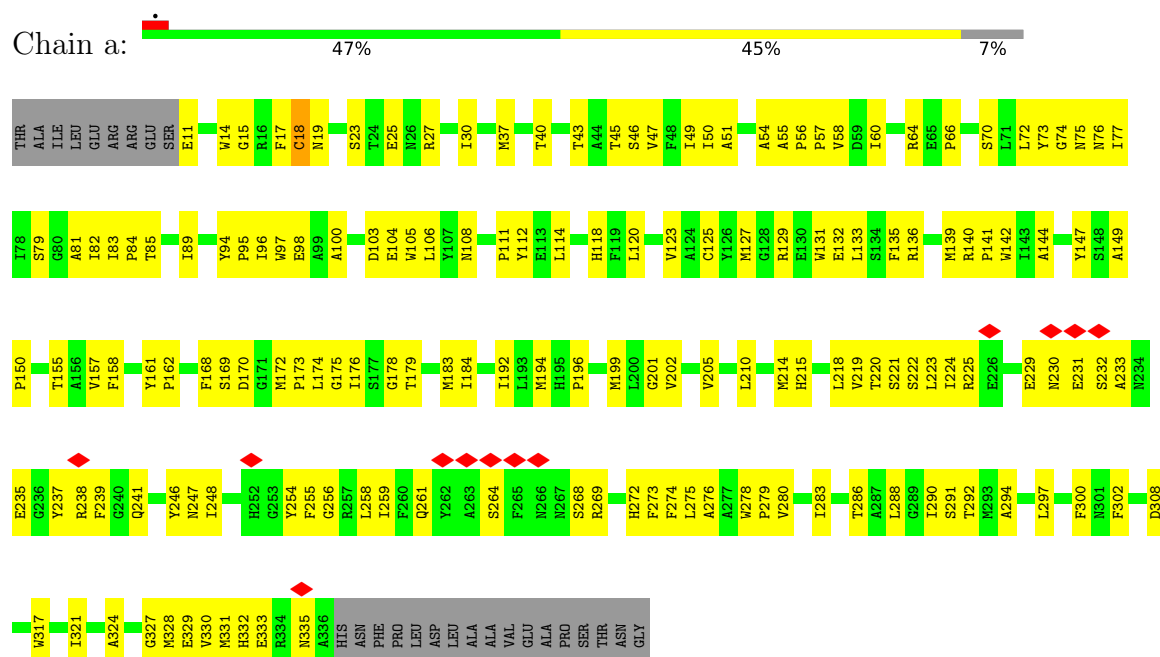




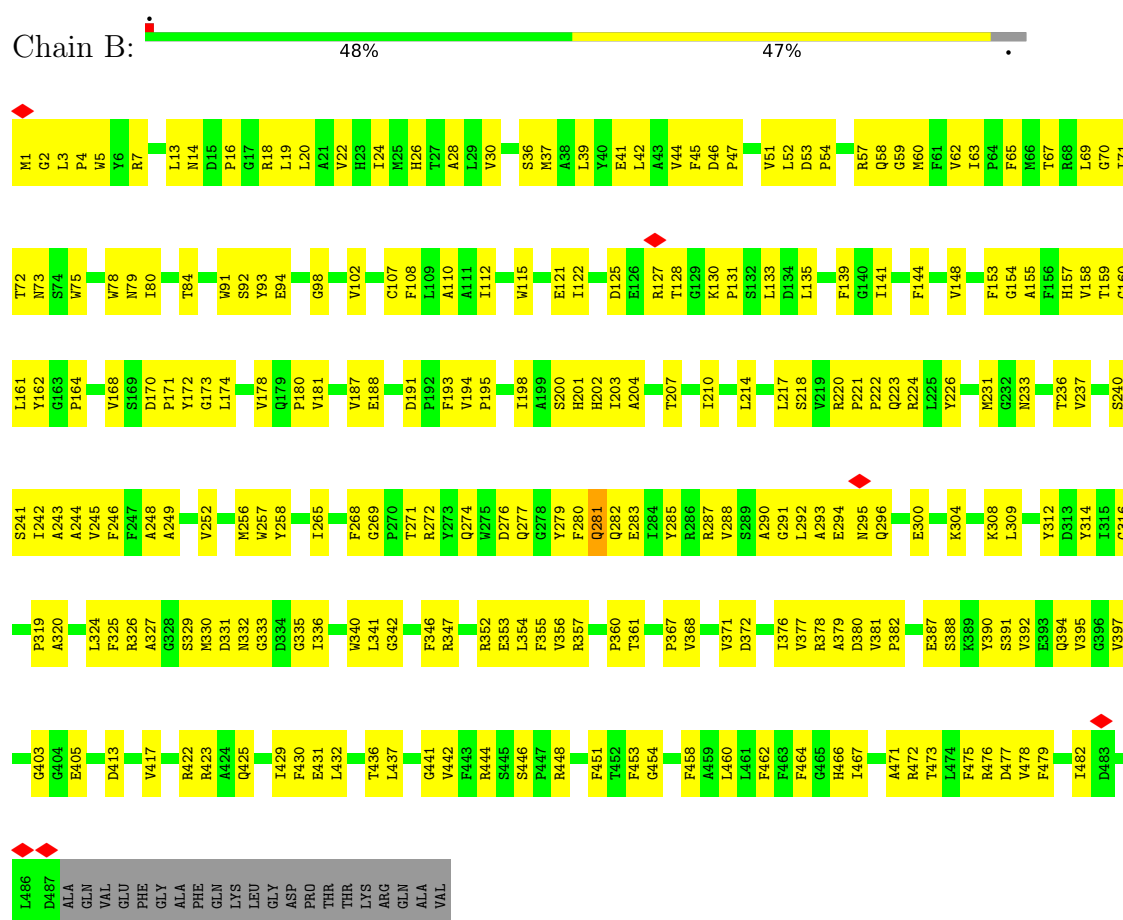
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic



- Molecule 4: Photosystem II protein D1

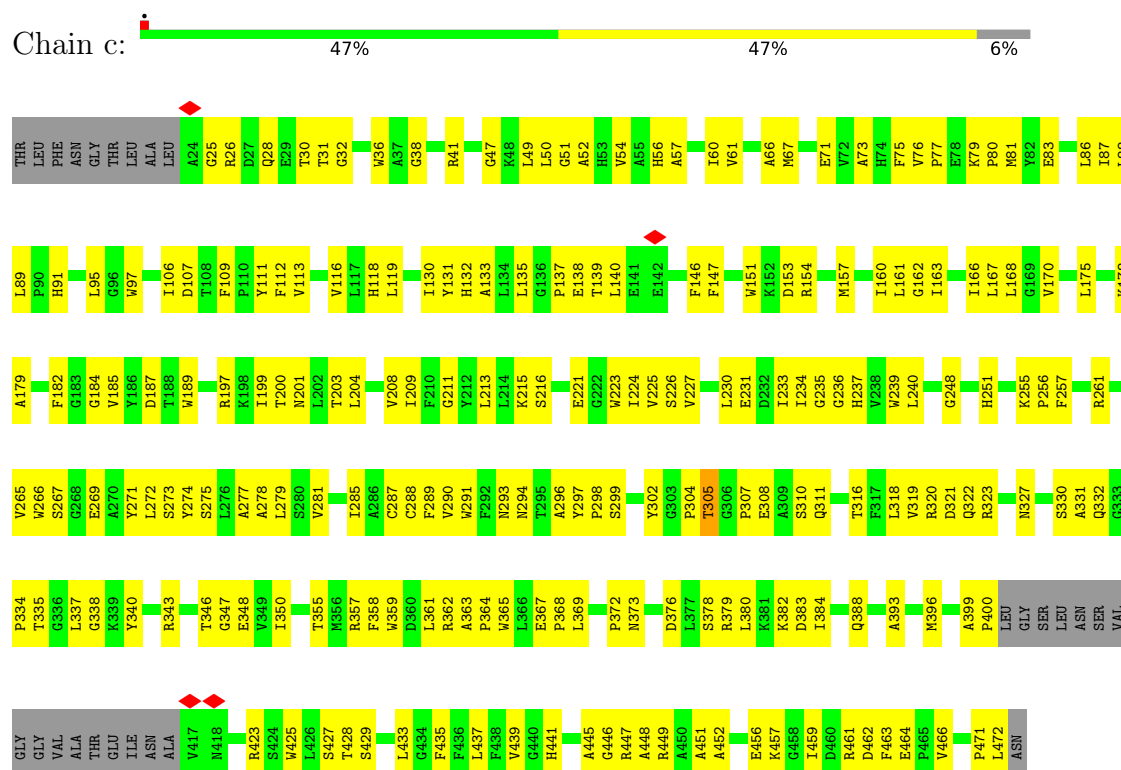


- Molecule 5: Photosystem II CP47 reaction center protein

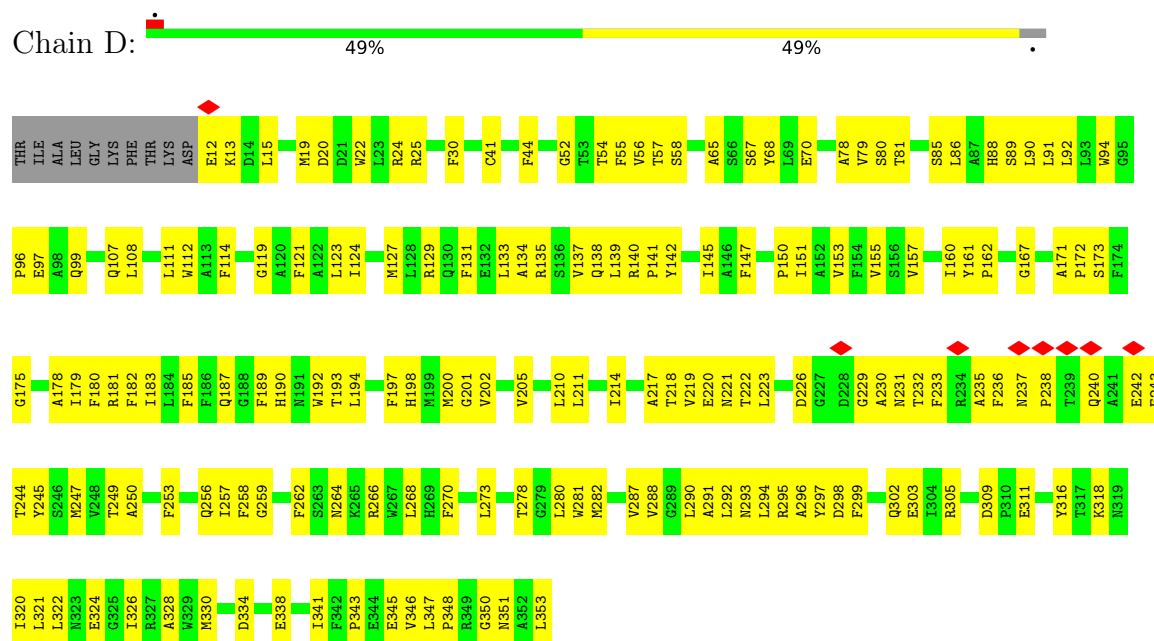


- Molecule 5: Photosystem II CP47 reaction center protein

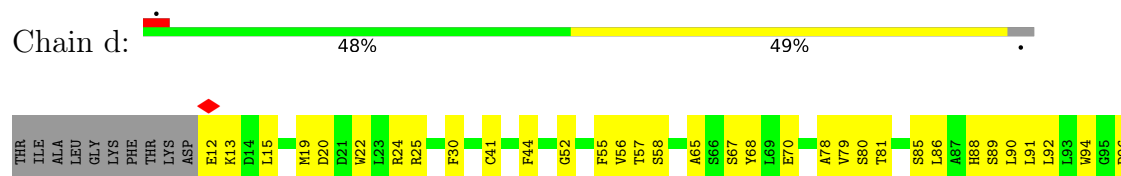


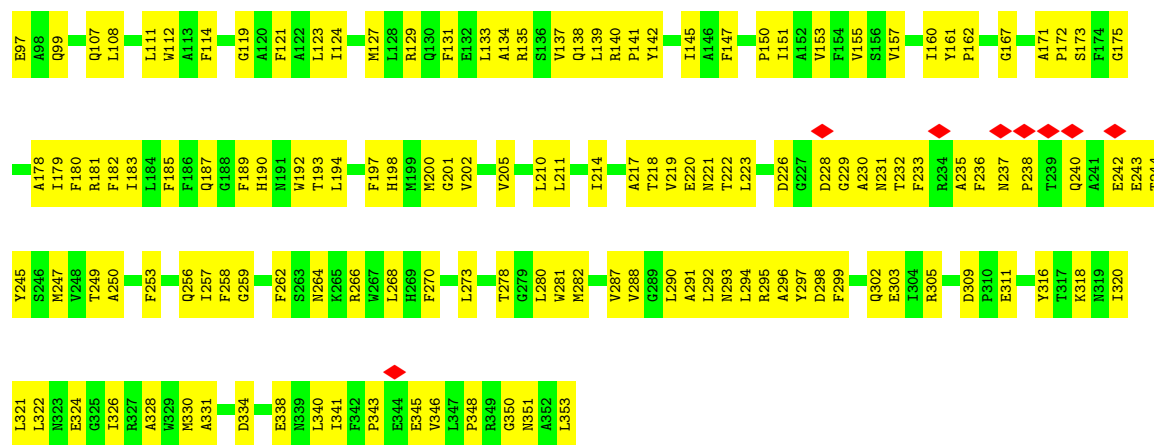


• Molecule 7: Photosystem II D2 protein

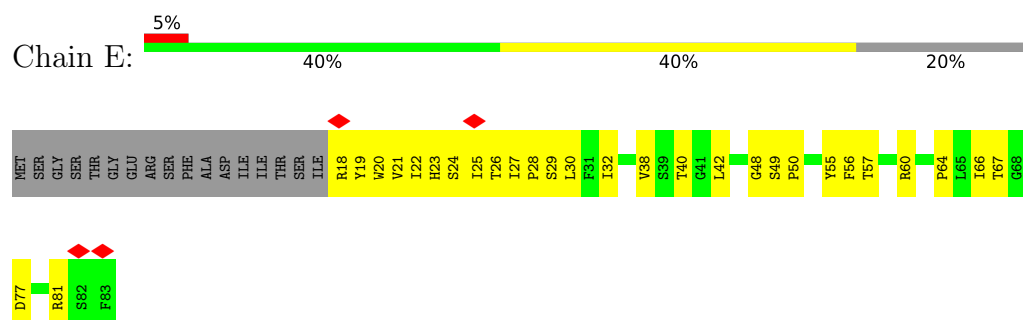


• Molecule 7: Photosystem II D2 protein

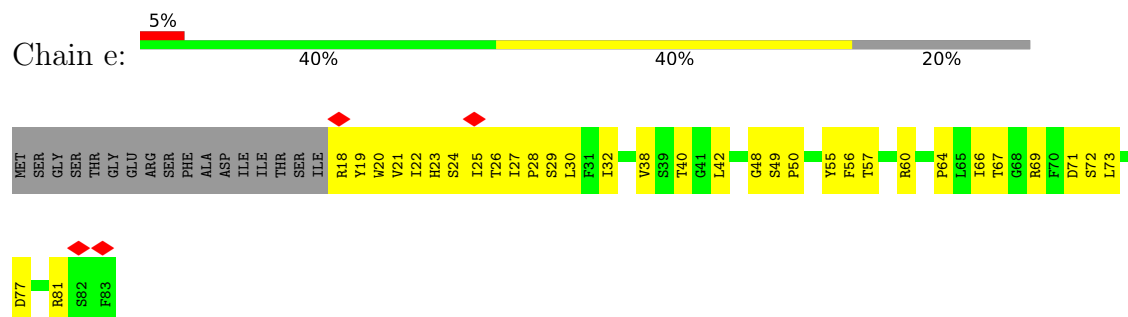




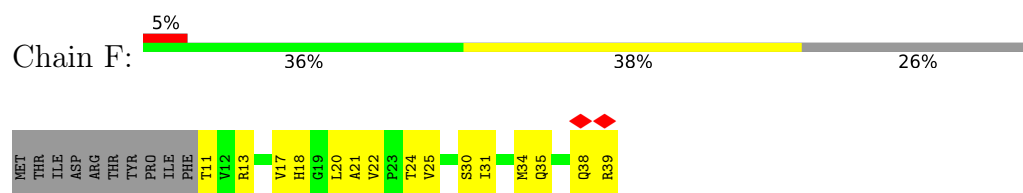
• Molecule 8: Cytochrome b559 subunit alpha



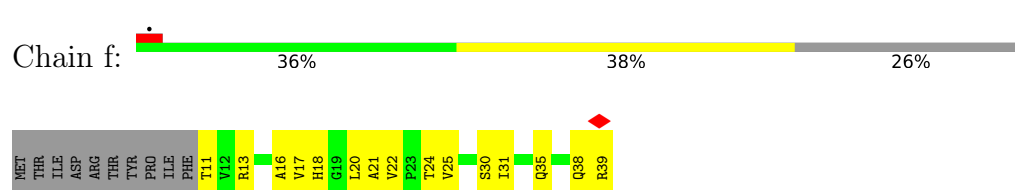
• Molecule 8: Cytochrome b559 subunit alpha



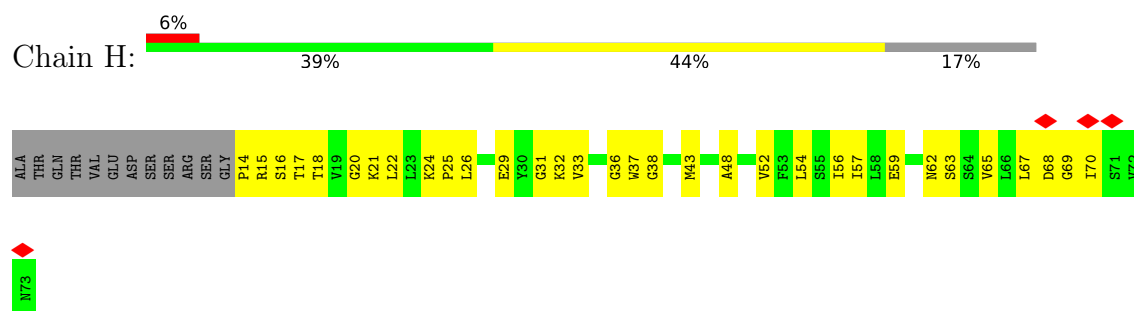
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



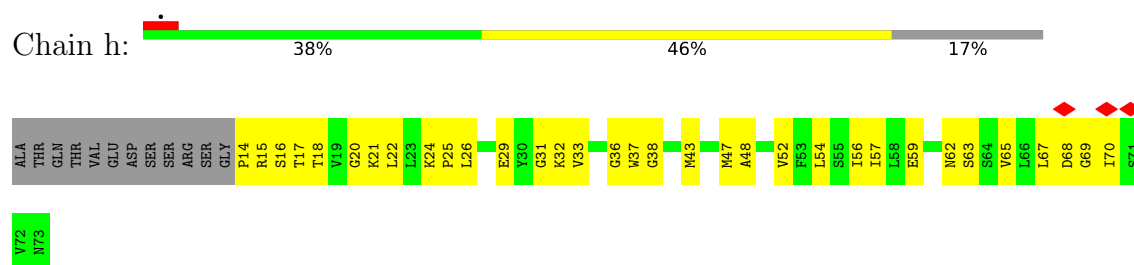
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



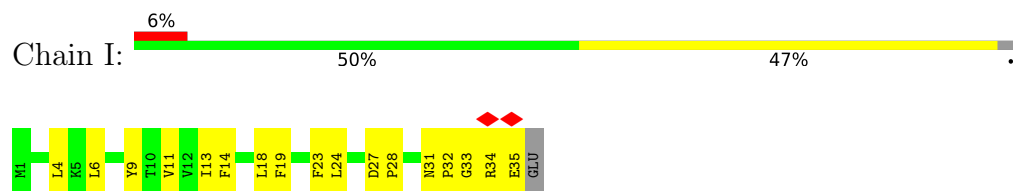
- Molecule 10: Photosystem II reaction center protein H



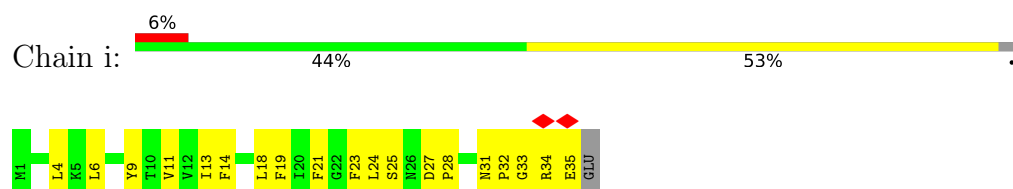
- Molecule 10: Photosystem II reaction center protein H



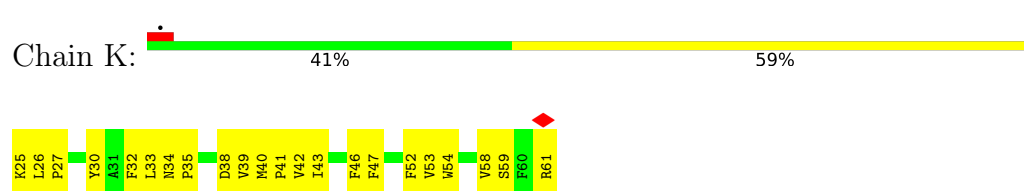
- Molecule 11: Photosystem II reaction center protein I



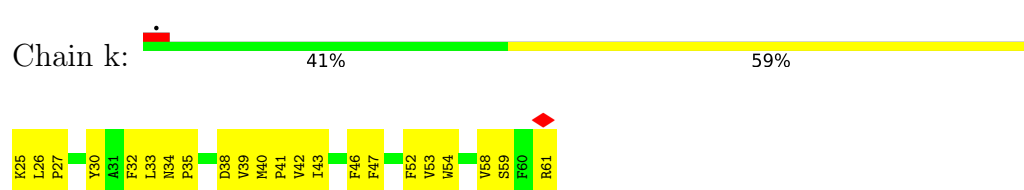
- Molecule 11: Photosystem II reaction center protein I



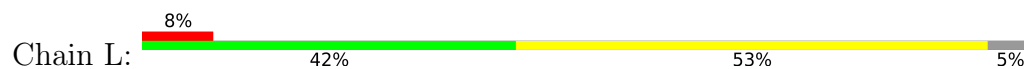
- Molecule 12: Photosystem II reaction center protein K



- Molecule 12: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein L



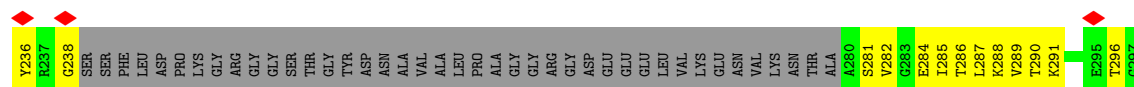
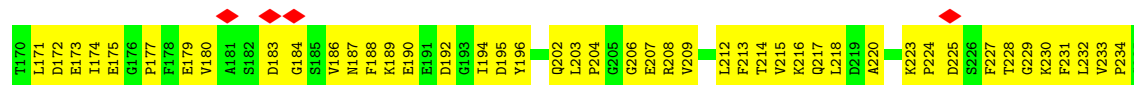
- Molecule 14: Photosystem II reaction center protein M



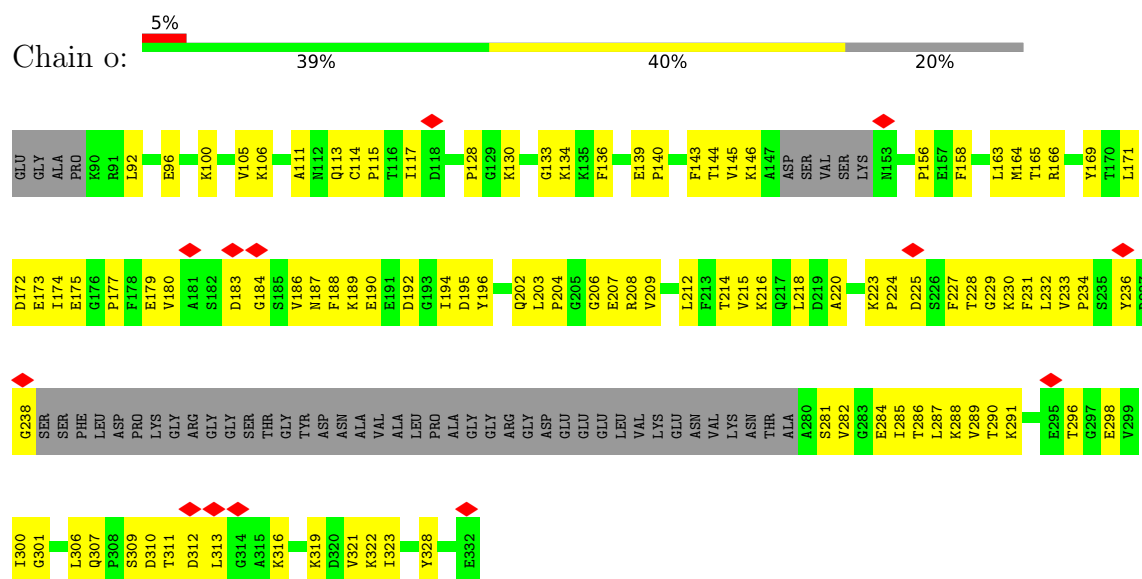
- Molecule 14: Photosystem II reaction center protein M



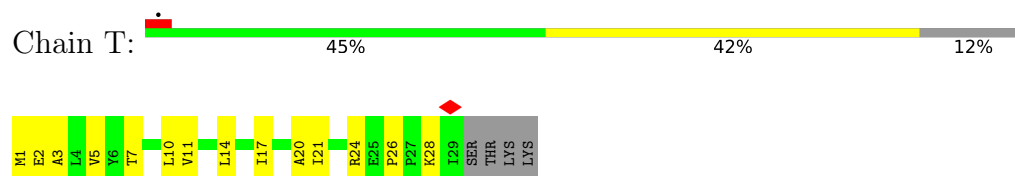
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



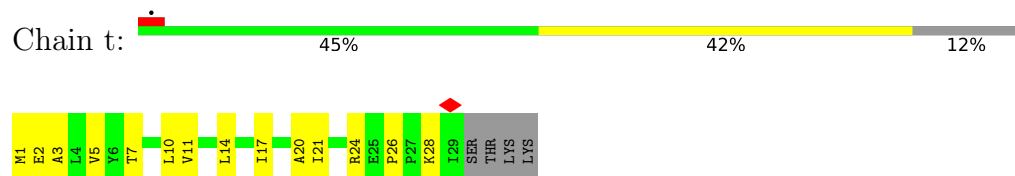
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



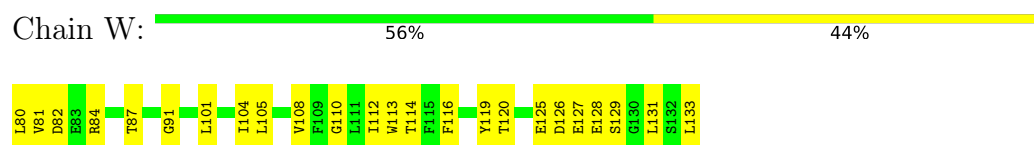
- Molecule 16: Photosystem II reaction center protein T



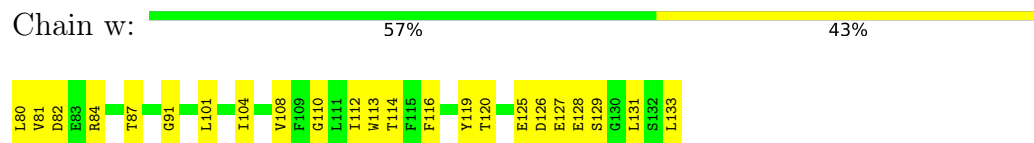
- Molecule 16: Photosystem II reaction center protein T



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



- Molecule 18: (thale cress) hypothetical protein





- Molecule 18: (thale cress) hypothetical protein



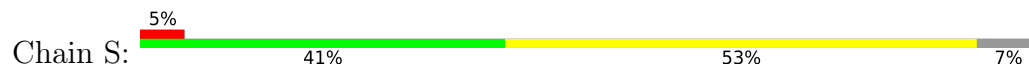
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

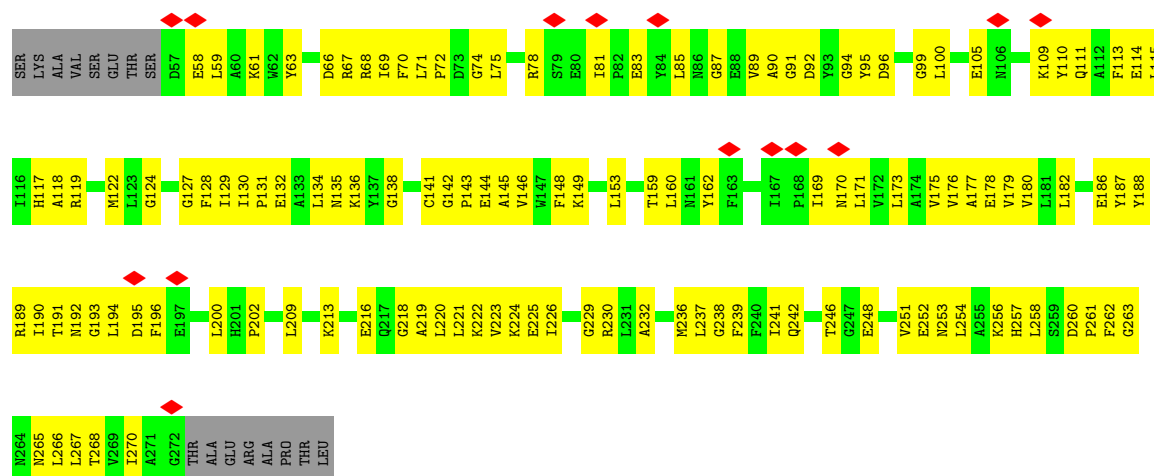


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

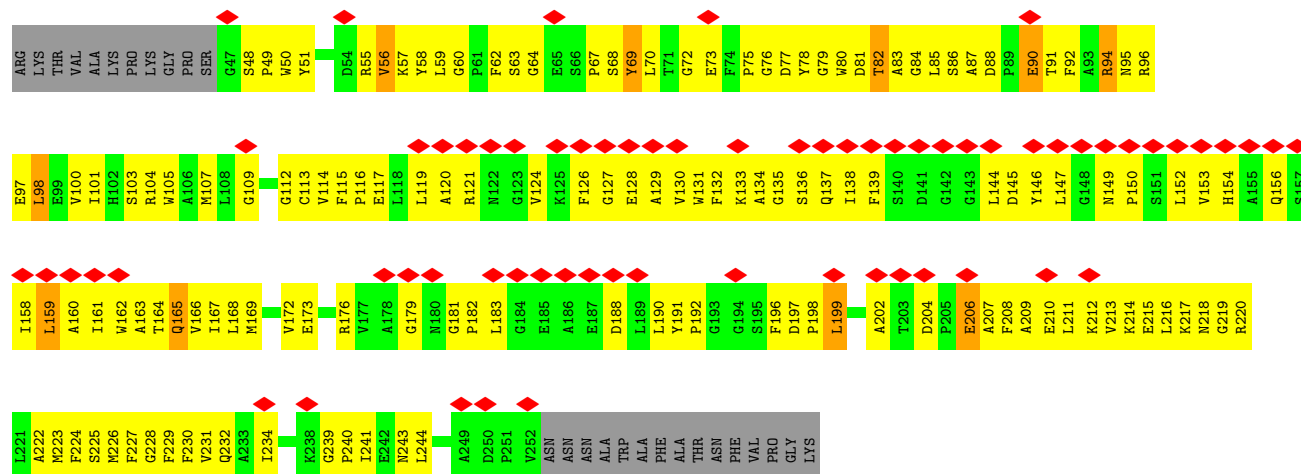


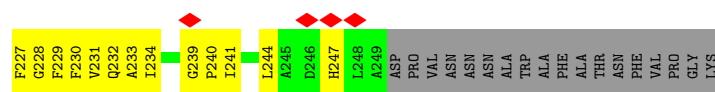
- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic



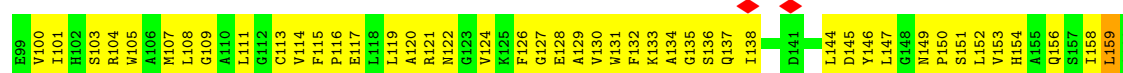
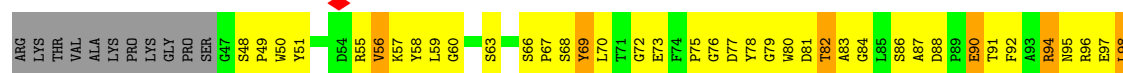
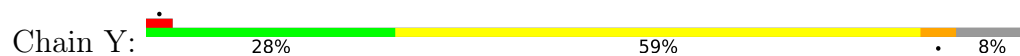


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

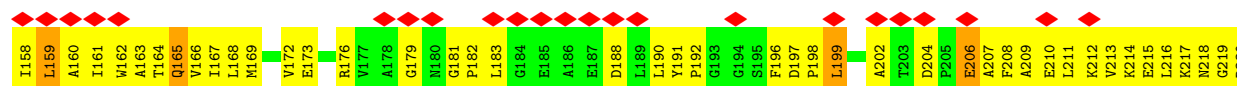
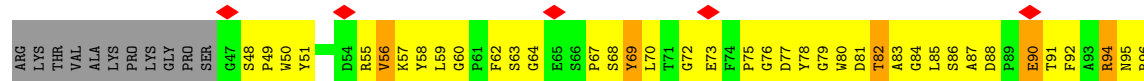




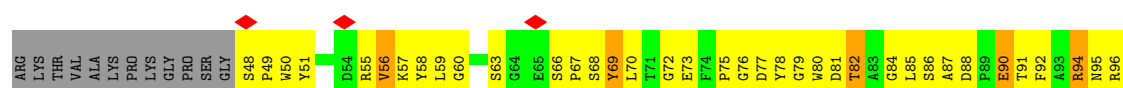
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

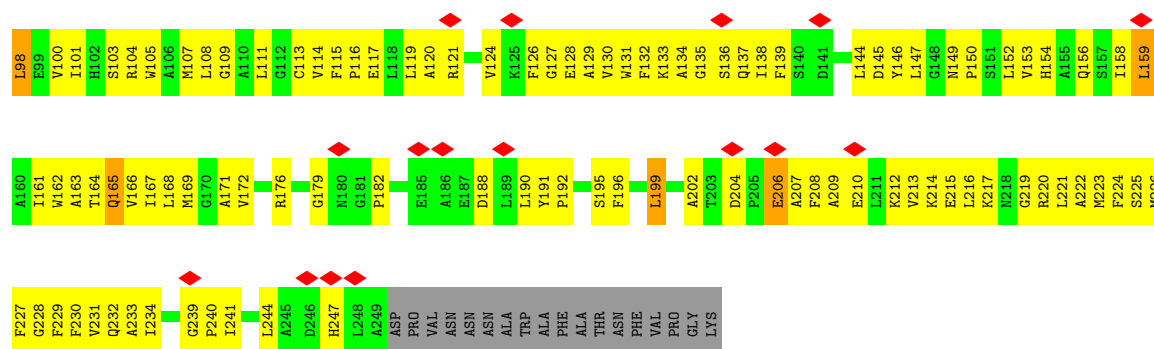


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



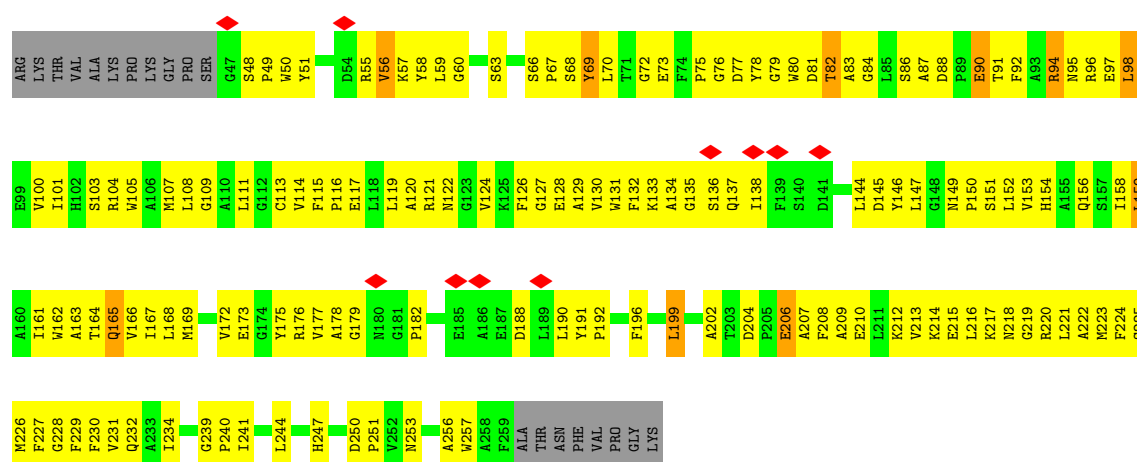
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic





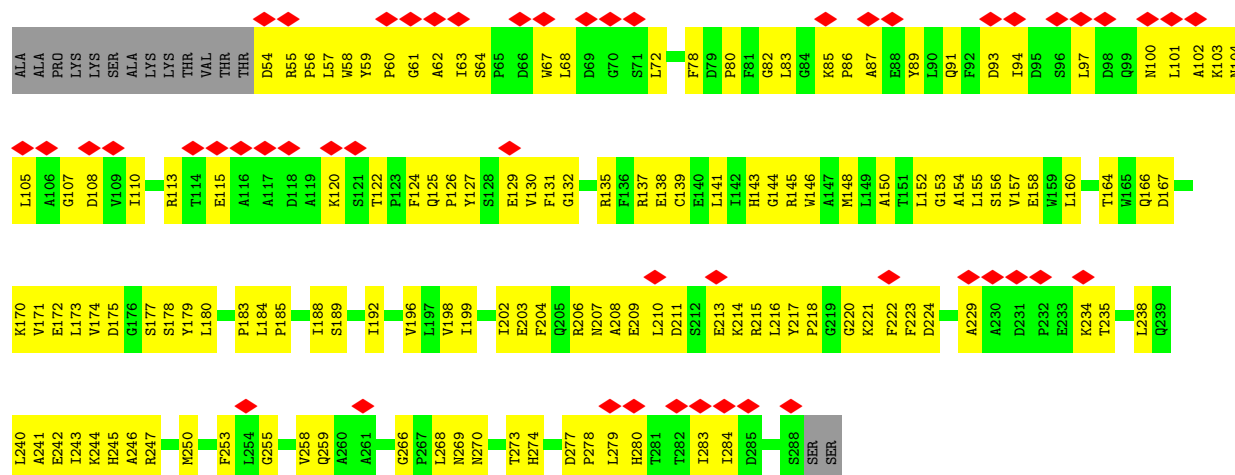
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 29% 59% 8%

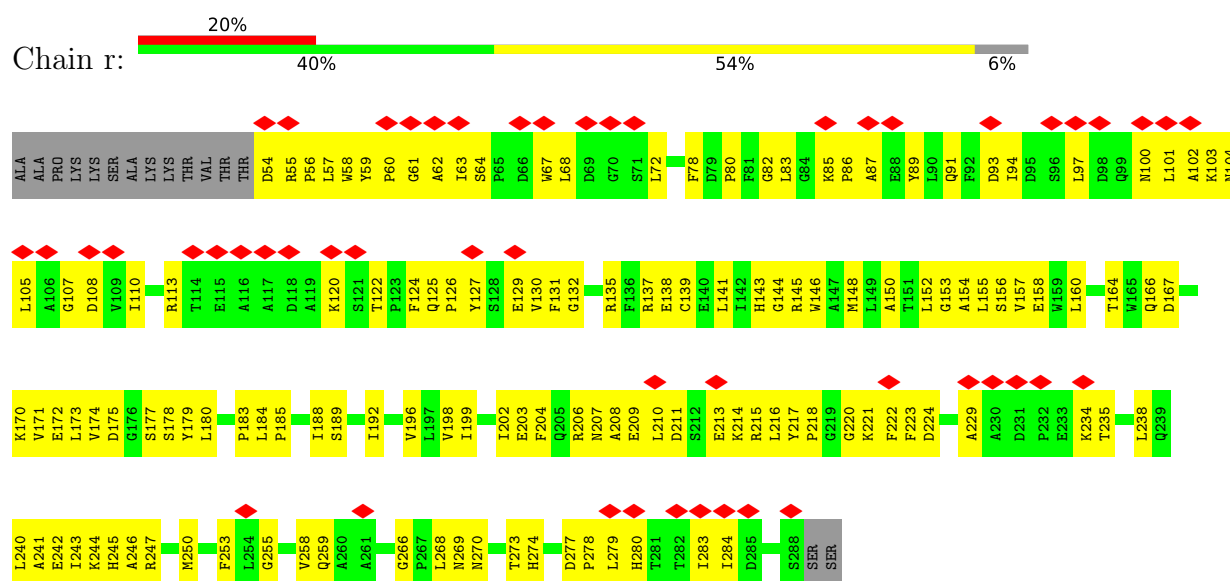


- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

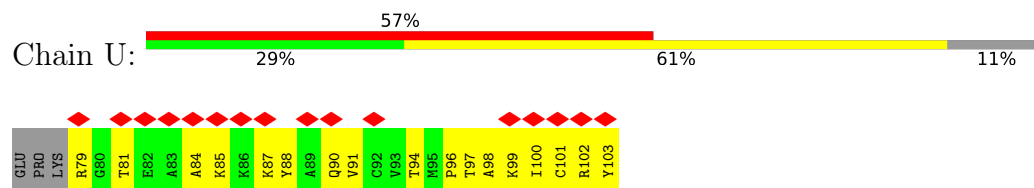
Chain R: 20% 39% 55% 6%



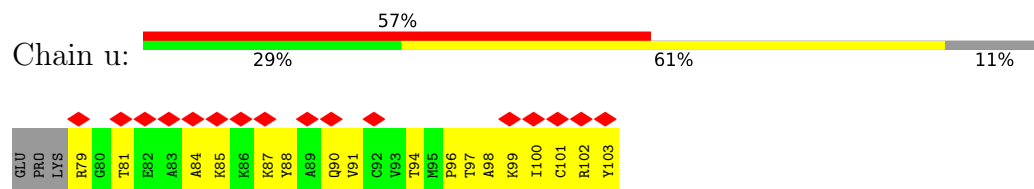
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.682	Depositor
Minimum map value	-19.496	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.976	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, CL, BCR, AJP, SQD, NEX, CA, LUT, DGD, HEM, CHL, PL9, BCT, XAT, LMG, PHO, FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.19	0/1582	0.45	0/2150
1	3	0.19	0/1582	0.45	0/2150
1	5	0.19	0/1582	0.45	0/2150
1	7	0.19	0/1582	0.45	0/2150
2	2	0.17	0/1640	0.42	0/2229
2	6	0.17	0/1640	0.42	0/2229
3	4	0.17	0/1652	0.43	0/2242
3	8	0.17	0/1652	0.43	0/2242
4	A	0.12	0/2626	0.34	0/3580
4	a	0.12	0/2626	0.34	0/3580
5	B	0.12	0/3940	0.29	0/5368
5	b	0.12	0/3940	0.29	0/5368
6	C	0.11	0/3487	0.26	0/4750
6	c	0.11	0/3487	0.26	0/4750
7	D	0.12	0/2815	0.28	0/3837
7	d	0.12	0/2815	0.28	0/3837
8	E	0.10	0/561	0.29	0/763
8	e	0.10	0/561	0.29	0/763
9	F	0.09	0/229	0.24	0/311
9	f	0.09	0/229	0.24	0/311
10	H	0.10	0/455	0.36	0/619
10	h	0.10	0/455	0.35	0/619
11	I	0.13	0/294	0.38	0/397
11	i	0.12	0/294	0.38	0/397
12	K	0.10	0/312	0.27	0/428
12	k	0.10	0/312	0.27	0/428
13	L	0.09	0/310	0.20	0/421
13	l	0.09	0/310	0.20	0/421
14	M	0.11	0/254	0.28	0/347
14	m	0.11	0/254	0.28	0/347
15	O	0.10	0/1548	0.31	0/2091

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.10	0/1548	0.31	0/2091
16	T	0.09	0/246	0.22	0/333
16	t	0.09	0/246	0.22	0/333
17	W	0.10	0/438	0.26	0/594
17	w	0.10	0/438	0.26	0/594
18	X	0.09	0/250	0.23	0/339
18	x	0.10	0/250	0.23	0/339
19	Z	0.15	0/474	0.30	0/649
19	z	0.15	0/474	0.30	0/649
20	S	0.12	0/1715	0.29	0/2328
20	s	0.12	0/1715	0.30	0/2328
21	G	0.19	0/1607	0.44	0/2184
21	N	0.19	0/1580	0.44	0/2146
21	Y	0.19	0/1669	0.44	0/2270
21	g	0.19	0/1607	0.44	0/2184
21	n	0.19	0/1580	0.44	0/2146
21	y	0.19	0/1669	0.44	0/2270
22	R	0.15	0/1878	0.34	0/2561
22	r	0.15	0/1878	0.34	0/2561
23	U	0.08	0/196	0.27	0/261
23	u	0.09	0/196	0.27	0/261
All	All	0.14	0/66680	0.35	0/90696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1537	0	1480	181	0
1	3	1537	0	1480	182	0
1	5	1537	0	1480	179	0
1	7	1537	0	1480	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1593	0	1543	287	0
2	6	1593	0	1543	292	0
3	4	1597	0	1534	197	0
3	8	1597	0	1534	200	0
4	A	2548	0	2460	229	0
4	a	2548	0	2460	233	0
5	B	3810	0	3688	326	0
5	b	3810	0	3688	327	0
6	C	3373	0	3302	277	0
6	c	3373	0	3302	284	0
7	D	2722	0	2615	251	0
7	d	2722	0	2615	255	0
8	E	543	0	519	38	0
8	e	543	0	519	37	0
9	F	224	0	233	14	0
9	f	224	0	233	14	0
10	H	446	0	471	58	0
10	h	446	0	471	60	0
11	I	286	0	295	32	0
11	i	286	0	295	32	0
12	K	301	0	313	28	0
12	k	301	0	313	28	0
13	L	302	0	291	29	0
13	l	302	0	291	30	0
14	M	250	0	279	41	0
14	m	250	0	279	41	0
15	O	1516	0	1494	133	0
15	o	1516	0	1494	131	0
16	T	239	0	255	19	0
16	t	239	0	255	20	0
17	W	427	0	405	33	0
17	w	427	0	405	34	0
18	X	248	0	266	43	0
18	x	248	0	266	43	0
19	Z	464	0	495	38	0
19	z	464	0	495	40	0
20	S	1670	0	1647	186	0
20	s	1670	0	1647	188	0
21	G	1562	0	1501	302	0
21	N	1536	0	1478	293	0
21	Y	1621	0	1546	306	0
21	g	1562	0	1501	300	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	n	1536	0	1478	295	0
21	y	1621	0	1546	307	0
22	R	1827	0	1777	212	0
22	r	1827	0	1777	211	0
23	U	194	0	206	36	0
23	u	194	0	206	35	0
24	1	92	0	62	18	0
24	2	110	0	91	29	0
24	5	92	0	62	17	0
24	6	110	0	91	30	0
24	G	335	0	296	78	0
24	N	348	0	321	117	0
24	R	195	0	146	23	0
24	S	184	0	124	28	0
24	Y	344	0	308	94	0
24	g	335	0	296	77	0
24	n	348	0	321	116	0
24	r	195	0	146	24	0
24	s	184	0	124	33	0
24	y	344	0	308	93	0
25	2	163	0	142	33	0
25	6	163	0	142	37	0
25	A	190	0	203	39	0
25	B	1040	0	1150	147	0
25	C	840	0	923	145	0
25	D	180	0	183	41	0
25	G	472	0	464	110	0
25	N	473	0	468	139	0
25	R	543	0	490	113	0
25	S	465	0	393	90	0
25	Y	470	0	465	123	0
25	a	190	0	203	39	0
25	b	1040	0	1150	149	0
25	c	840	0	923	157	0
25	d	180	0	183	42	0
25	g	472	0	464	115	0
25	n	473	0	468	136	0
25	r	543	0	490	121	0
25	s	465	0	393	92	0
25	y	470	0	465	120	0
26	2	47	0	67	14	0
26	6	47	0	67	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	142	0	206	18	0
26	C	147	74	222	10	0
26	D	49	0	74	10	0
26	L	49	0	74	5	0
26	N	49	0	74	11	0
26	R	42	0	56	14	0
26	S	98	0	148	13	0
26	Y	98	0	146	20	0
26	b	142	0	206	18	0
26	c	147	74	222	10	0
26	d	49	0	74	10	0
26	l	49	0	74	5	0
26	n	49	0	74	10	0
26	r	42	0	56	16	0
26	s	98	0	148	15	0
26	y	98	0	146	20	0
27	A	128	0	148	27	0
27	a	128	0	148	28	0
28	A	40	0	56	4	0
28	B	120	0	168	18	0
28	C	40	0	56	7	0
28	D	40	0	56	3	0
28	H	40	0	56	6	0
28	I	40	0	56	20	0
28	K	40	0	56	7	0
28	T	40	0	54	20	0
28	Z	40	0	56	5	0
28	a	40	0	56	5	0
28	b	120	0	168	19	0
28	c	40	0	56	7	0
28	d	40	0	56	3	0
28	h	40	0	56	8	0
28	i	40	0	56	20	0
28	k	40	0	56	9	0
28	t	40	0	54	21	0
28	z	40	0	56	5	0
29	A	104	0	145	13	0
29	L	96	0	126	25	0
29	a	104	0	145	12	0
29	l	96	0	126	25	0
30	A	88	0	116	6	0
30	B	106	0	158	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C	51	0	72	4	0
30	D	46	0	62	3	0
30	a	88	0	116	6	0
30	b	106	0	158	10	0
30	c	51	0	72	4	0
30	d	46	0	62	3	0
31	A	13	0	7	2	0
31	D	55	0	80	6	0
31	a	13	0	7	2	0
31	d	55	0	80	6	0
32	A	85	92	0	0	0
32	B	85	92	0	0	0
32	G	42	53	0	0	0
32	N	84	106	0	3	0
32	S	42	53	0	2	0
32	Y	210	265	0	7	0
32	a	85	92	0	0	0
32	b	85	92	0	0	0
32	g	42	53	0	0	0
32	n	84	106	0	3	0
32	s	42	53	0	2	0
32	y	210	265	0	7	0
33	A	4	0	1	2	0
33	a	4	0	1	1	0
34	A	1	0	0	0	0
34	a	1	0	0	0	0
35	A	59	0	76	3	0
35	B	62	0	82	5	0
35	C	117	0	150	18	0
35	a	59	0	76	3	0
35	b	62	0	82	6	0
35	c	117	0	150	17	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
37	D	1	0	0	1	0
37	d	1	0	0	1	0
38	F	43	0	30	7	0
38	f	43	0	30	8	0
39	G	84	0	112	30	0
39	N	84	0	112	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	R	42	0	56	6	0
39	S	84	0	112	27	0
39	Y	84	0	112	25	0
39	g	84	0	112	30	0
39	n	84	0	112	27	0
39	r	42	0	56	8	0
39	s	84	0	112	29	0
39	y	84	0	112	25	0
40	G	44	0	56	15	0
40	N	44	0	56	15	0
40	R	44	0	56	8	0
40	S	44	0	56	6	0
40	Y	44	0	56	7	0
40	g	44	0	56	15	0
40	n	44	0	56	13	0
40	r	44	0	56	10	0
40	s	44	0	56	5	0
40	y	44	0	56	10	0
41	R	44	0	56	20	0
41	r	44	0	56	22	0
42	A	23	0	0	0	0
42	B	10	0	0	3	0
42	C	14	0	0	1	0
42	D	14	0	0	0	0
42	H	1	0	0	0	0
42	I	1	0	0	0	0
42	L	3	0	0	2	0
42	M	1	0	0	0	0
42	T	1	0	0	0	0
42	W	1	0	0	0	0
42	a	23	0	0	1	0
42	b	10	0	0	3	0
42	c	14	0	0	1	0
42	d	14	0	0	0	0
42	h	1	0	0	0	0
42	i	1	0	0	0	0
42	l	3	0	0	2	0
42	m	2	0	0	0	0
42	t	1	0	0	0	0
42	w	1	0	0	0	0
All	All	84427	1470	83152	8481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 51.

All (8481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:196:TYR:HB2	15:O:212:LEU:HD21	1.21	1.19
10:h:56:ILE:HD13	18:x:84:LYS:HE3	1.25	1.17
21:n:138:ILE:HG21	24:n:606:CHL:HBC1	1.23	1.17
22:r:144:GLY:HA3	22:r:246:ALA:HB1	1.28	1.16
22:R:144:GLY:HA3	22:R:246:ALA:HB1	1.28	1.14
21:g:97:GLU:HG3	21:g:190:LEU:HD21	1.31	1.13
21:n:97:GLU:HG3	21:n:190:LEU:HD21	1.31	1.13
21:y:138:ILE:HG21	24:y:307:CHL:HBC1	1.26	1.12
21:G:97:GLU:HG3	21:G:190:LEU:HD21	1.31	1.12
2:2:175:GLY:HA3	2:2:181:LEU:HD11	1.32	1.12
1:5:178:ALA:HA	2:6:64:VAL:HG21	1.12	1.12
24:n:609:CHL:HAA2	21:y:82:THR:HG21	1.28	1.12
21:Y:97:GLU:HG3	21:Y:190:LEU:HD21	1.31	1.11
21:G:138:ILE:HG21	24:G:606:CHL:HBC1	1.17	1.11
1:1:97:GLU:HG3	1:1:190:LEU:HD21	1.31	1.11
1:5:97:GLU:HG3	1:5:190:LEU:HD21	1.31	1.11
1:7:97:GLU:HG3	1:7:190:LEU:HD21	1.31	1.11
21:n:97:GLU:HA	21:n:190:LEU:HD11	1.33	1.11
21:Y:138:ILE:HG21	24:Y:307:CHL:HBC1	1.26	1.11
2:6:97:ALA:HA	2:6:190:LEU:HD21	1.32	1.11
21:G:97:GLU:HA	21:G:190:LEU:HD11	1.33	1.10
24:N:609:CHL:HAA2	21:Y:82:THR:HG21	1.28	1.10
21:N:138:ILE:HG21	24:N:606:CHL:HBC1	1.23	1.09
21:Y:97:GLU:HA	21:Y:190:LEU:HD11	1.33	1.09
21:N:97:GLU:HG3	21:N:190:LEU:HD21	1.31	1.09
10:H:56:ILE:HD13	18:X:84:LYS:HE3	1.25	1.09
21:N:97:GLU:HA	21:N:190:LEU:HD11	1.33	1.09
15:o:196:TYR:HB2	15:o:212:LEU:HD21	1.21	1.09
21:G:76:GLY:HA3	21:G:216:LEU:HD23	1.35	1.08
21:N:76:GLY:HA3	21:N:216:LEU:HD23	1.35	1.08
21:y:76:GLY:HA3	21:y:216:LEU:HD23	1.35	1.08
1:1:178:ALA:HA	2:2:64:VAL:HG21	1.12	1.08
1:5:97:GLU:HA	1:5:190:LEU:HD11	1.33	1.08
1:1:76:GLY:HA3	1:1:216:LEU:HD23	1.35	1.08
1:3:97:GLU:HG3	1:3:190:LEU:HD21	1.31	1.08
21:y:98:LEU:HD22	25:y:304:CLA:HAA2	1.35	1.08
24:y:308:CHL:H8	24:y:308:CHL:H41	1.33	1.07
2:6:175:GLY:HA3	2:6:181:LEU:HD11	1.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:308:CHL:H8	24:Y:308:CHL:H41	1.33	1.07
1:7:76:GLY:HA3	1:7:216:LEU:HD23	1.35	1.07
21:g:138:ILE:HG21	24:g:606:CHL:HBC1	1.17	1.07
21:Y:76:GLY:HA3	21:Y:216:LEU:HD23	1.35	1.07
5:B:72:THR:HG23	5:B:80:ILE:HG22	1.36	1.06
1:7:97:GLU:HA	1:7:190:LEU:HD11	1.33	1.06
21:g:97:GLU:HA	21:g:190:LEU:HD11	1.33	1.06
21:y:97:GLU:HA	21:y:190:LEU:HD11	1.33	1.06
21:y:97:GLU:HG3	21:y:190:LEU:HD21	1.31	1.06
21:n:76:GLY:HA3	21:n:216:LEU:HD23	1.35	1.06
1:3:97:GLU:HA	1:3:190:LEU:HD11	1.33	1.06
24:n:607:CHL:H11	24:y:302:CHL:H191	1.37	1.06
2:2:97:ALA:HA	2:2:190:LEU:HD21	1.32	1.05
1:1:97:GLU:HA	1:1:190:LEU:HD11	1.33	1.05
1:3:76:GLY:HA3	1:3:216:LEU:HD23	1.35	1.05
23:u:85:LYS:HG2	23:u:101:CYS:HB3	1.36	1.05
5:b:72:THR:HG23	5:b:80:ILE:HG22	1.36	1.05
21:Y:98:LEU:HD22	25:Y:304:CLA:HAA2	1.35	1.04
21:Y:60:GLY:HA3	24:Y:302:CHL:HMC	1.39	1.04
21:g:76:GLY:HA3	21:g:216:LEU:HD23	1.35	1.03
1:3:55:ARG:HH12	1:3:72:GLY:HA3	1.23	1.03
1:5:76:GLY:HA3	1:5:216:LEU:HD23	1.35	1.03
1:7:55:ARG:HH12	1:7:72:GLY:HA3	1.23	1.03
2:6:178:ILE:HD11	1:7:62:PHE:HA	1.41	1.03
3:8:73:LEU:HG	3:8:82:GLY:HA2	1.41	1.02
3:8:133:GLN:HG2	3:8:134:PRO:HD3	1.41	1.02
21:g:55:ARG:HH12	21:g:72:GLY:HA3	1.23	1.02
21:y:60:GLY:HA3	24:y:302:CHL:HMC	1.39	1.02
25:y:311:CLA:H51	25:y:313:CLA:HMA1	1.37	1.02
23:U:85:LYS:HG2	23:U:101:CYS:HB3	1.36	1.02
25:B:607:CLA:H171	25:B:613:CLA:H161	1.38	1.02
3:4:133:GLN:HG2	3:4:134:PRO:HD3	1.42	1.02
21:Y:55:ARG:HH12	21:Y:72:GLY:HA3	1.23	1.02
1:1:55:ARG:HH12	1:1:72:GLY:HA3	1.23	1.01
25:Y:311:CLA:H51	25:Y:313:CLA:HMA1	1.37	1.01
3:8:78:PRO:HG3	3:8:225:LYS:HB3	1.38	1.01
24:N:607:CHL:H11	24:Y:302:CHL:H191	1.38	1.01
21:n:55:ARG:HH12	21:n:72:GLY:HA3	1.23	1.01
15:o:130:LYS:HE2	15:o:177:PRO:HB2	1.43	1.01
2:2:89:PRO:HA	2:2:92:PHE:HD2	1.22	1.01
1:5:55:ARG:HH12	1:5:72:GLY:HA3	1.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:55:ARG:HH12	21:G:72:GLY:HA3	1.23	1.00
2:2:179:ASN:HA	24:2:603:CHL:HMC	1.43	1.00
2:6:89:PRO:HA	2:6:92:PHE:HD2	1.22	1.00
25:b:607:CLA:H171	25:b:613:CLA:H161	1.38	1.00
21:N:55:ARG:HH12	21:N:72:GLY:HA3	1.23	1.00
3:4:78:PRO:HG3	3:4:225:LYS:HB3	1.38	1.00
2:6:120:GLN:HG3	2:6:125:VAL:HA	1.44	1.00
23:U:97:THR:HA	23:U:102:ARG:HH21	1.26	0.99
3:4:103:LEU:HD11	3:4:194:TYR:HD1	1.28	0.99
2:2:120:GLN:HG3	2:2:125:VAL:HA	1.44	0.99
22:R:58:TRP:HE1	25:R:601:CLA:HAA1	1.26	0.99
7:d:15:LEU:HD11	18:x:103:VAL:HG13	1.42	0.99
5:b:272:ARG:HH12	5:b:361:THR:HG21	1.26	0.99
7:d:173:SER:HB2	7:d:178:ALA:HB1	1.45	0.99
23:u:97:THR:HA	23:u:102:ARG:HH21	1.26	0.99
2:2:178:ILE:HD11	1:3:62:PHE:HA	1.41	0.99
7:D:15:LEU:HD11	18:X:103:VAL:HG13	1.42	0.99
15:O:130:LYS:HE2	15:O:177:PRO:HB2	1.43	0.99
3:8:222:GLU:HG2	3:8:225:LYS:HD3	1.45	0.99
7:D:173:SER:HB2	7:D:178:ALA:HB1	1.45	0.98
22:r:58:TRP:HE1	25:r:601:CLA:HAA1	1.26	0.98
3:4:73:LEU:HG	3:4:82:GLY:HA2	1.41	0.98
10:h:18:THR:HA	10:h:21:LYS:HD3	1.46	0.98
3:4:222:GLU:HG2	3:4:225:LYS:HD3	1.45	0.98
20:S:72:PRO:HG2	20:S:75:LEU:HD13	1.43	0.98
5:B:272:ARG:HH12	5:B:361:THR:HG21	1.26	0.98
11:i:33:GLY:O	11:i:34:ARG:HG3	1.64	0.98
5:B:243:ALA:HA	5:B:246:PHE:CE1	2.00	0.97
5:b:53:ASP:OD2	5:b:58:GLN:NE2	1.97	0.97
21:y:55:ARG:HH12	21:y:72:GLY:HA3	1.23	0.97
21:Y:251:PRO:HB2	25:Y:315:CLA:HMA1	1.46	0.97
40:Y:318:NEX:H28	40:Y:318:NEX:H361	1.45	0.97
2:6:179:ASN:HA	24:6:603:CHL:HMC	1.43	0.97
1:3:67:PRO:HG2	1:3:70:LEU:HD12	1.47	0.97
2:6:145:LEU:HD22	2:6:154:VAL:HG22	1.47	0.97
3:8:103:LEU:HD11	3:8:194:TYR:HD1	1.28	0.97
20:s:59:LEU:HD11	20:s:216:GLU:HG3	1.47	0.97
25:B:604:CLA:H142	25:B:615:CLA:HMA1	1.46	0.97
21:N:67:PRO:HG2	21:N:70:LEU:HD12	1.47	0.97
29:L:101:SQD:H132	29:L:101:SQD:H271	1.47	0.96
6:c:151:TRP:HB2	17:w:133:LEU:HD21	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:67:PRO:HG2	21:n:70:LEU:HD12	1.47	0.96
10:H:18:THR:HA	10:H:21:LYS:HD3	1.46	0.96
21:y:67:PRO:HG2	21:y:70:LEU:HD12	1.47	0.96
1:5:209:ALA:HA	1:5:212:LYS:HG3	1.48	0.96
20:S:236:MET:HE2	39:S:316:LUT:H12	1.48	0.96
21:G:67:PRO:HG2	21:G:70:LEU:HD12	1.47	0.96
21:Y:67:PRO:HG2	21:Y:70:LEU:HD12	1.47	0.96
5:b:243:ALA:HA	5:b:246:PHE:CE1	1.99	0.96
21:N:138:ILE:HG13	21:N:144:LEU:HB2	1.48	0.96
1:5:138:ILE:HG13	1:5:144:LEU:HB2	1.48	0.96
2:2:145:LEU:HD22	2:2:154:VAL:HG22	1.46	0.96
25:b:604:CLA:H142	25:b:615:CLA:HMA1	1.46	0.96
1:3:209:ALA:HA	1:3:212:LYS:HG3	1.48	0.95
5:B:53:ASP:OD2	5:B:58:GLN:NE2	1.97	0.95
21:g:209:ALA:HA	21:g:212:LYS:HG3	1.48	0.95
24:n:607:CHL:H203	25:y:303:CLA:H161	1.47	0.95
11:I:33:GLY:O	11:I:34:ARG:HG3	1.64	0.95
20:s:236:MET:HE2	39:s:316:LUT:H12	1.47	0.95
21:y:209:ALA:HA	21:y:212:LYS:HG3	1.48	0.95
7:D:183:ILE:HG23	25:D:402:CLA:HAC1	1.48	0.95
20:s:72:PRO:HG2	20:s:75:LEU:HD13	1.43	0.95
20:S:59:LEU:HD11	20:S:216:GLU:HG3	1.47	0.95
1:7:209:ALA:HA	1:7:212:LYS:HG3	1.48	0.95
21:g:98:LEU:HD22	25:g:603:CLA:HAA1	1.47	0.95
21:y:138:ILE:HG13	21:y:144:LEU:HB2	1.48	0.95
21:N:209:ALA:HA	21:N:212:LYS:HG3	1.48	0.95
21:Y:138:ILE:HG13	21:Y:144:LEU:HB2	1.48	0.95
21:Y:209:ALA:HA	21:Y:212:LYS:HG3	1.48	0.95
1:1:209:ALA:HA	1:1:212:LYS:HG3	1.48	0.94
21:g:138:ILE:HG13	21:g:144:LEU:HB2	1.48	0.94
24:r:607:CHL:HAB	24:r:607:CHL:H112	1.49	0.94
24:N:607:CHL:H203	25:Y:303:CLA:H161	1.47	0.94
21:Y:122:ASN:HB3	32:Y:320:AJP:C80	1.97	0.94
40:y:318:NEX:H28	40:y:318:NEX:H361	1.45	0.94
7:d:183:ILE:HG23	25:d:402:CLA:HAC1	1.48	0.94
1:7:67:PRO:HG2	1:7:70:LEU:HD12	1.47	0.94
21:y:251:PRO:HB2	25:y:315:CLA:HMA1	1.46	0.94
5:B:460:LEU:HD11	7:D:288:VAL:HG21	1.48	0.94
21:G:209:ALA:HA	21:G:212:LYS:HG3	1.48	0.94
4:a:235:GLU:HB3	7:d:264:ASN:HD21	1.32	0.94
21:G:91:THR:OG1	21:N:84:GLY:O	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:122:ASN:HB3	32:y:320:AJP:C80	1.97	0.94
21:G:98:LEU:HD22	25:G:603:CLA:HAA1	1.47	0.94
21:G:138:ILE:HG13	21:G:144:LEU:HB2	1.48	0.94
25:G:611:CLA:HHC	25:G:611:CLA:HBB1	1.49	0.94
21:n:138:ILE:HG13	21:n:144:LEU:HB2	1.48	0.94
21:g:91:THR:OG1	21:n:84:GLY:O	1.85	0.93
20:S:225:GLU:HB2	25:S:310:CLA:C1B	1.97	0.93
4:a:225:ARG:HD3	22:r:102:ALA:HB1	1.50	0.93
1:1:67:PRO:HG2	1:1:70:LEU:HD12	1.47	0.93
6:C:151:TRP:HB2	17:W:133:LEU:HD21	1.48	0.93
21:g:67:PRO:HG2	21:g:70:LEU:HD12	1.47	0.93
5:b:460:LEU:HD11	7:d:288:VAL:HG21	1.48	0.93
29:l:102:SQD:H132	29:l:102:SQD:H271	1.47	0.93
1:1:138:ILE:HG13	1:1:144:LEU:HB2	1.48	0.93
1:1:168:LEU:O	1:1:172:VAL:HG23	1.68	0.93
1:3:168:LEU:O	1:3:172:VAL:HG23	1.68	0.93
1:7:138:ILE:HG13	1:7:144:LEU:HB2	1.48	0.93
24:R:607:CHL:HAB	24:R:607:CHL:H112	1.49	0.93
20:s:225:GLU:HB2	25:s:310:CLA:C1B	1.97	0.93
21:g:168:LEU:O	21:g:172:VAL:HG23	1.68	0.93
21:n:168:LEU:O	21:n:172:VAL:HG23	1.69	0.93
21:n:209:ALA:HA	21:n:212:LYS:HG3	1.48	0.93
1:3:138:ILE:HG13	1:3:144:LEU:HB2	1.48	0.92
1:5:168:LEU:O	1:5:172:VAL:HG23	1.69	0.92
25:g:611:CLA:HHC	25:g:611:CLA:HBB1	1.49	0.92
21:y:168:LEU:O	21:y:172:VAL:HG23	1.69	0.92
1:5:67:PRO:HG2	1:5:70:LEU:HD12	1.47	0.92
1:7:168:LEU:O	1:7:172:VAL:HG23	1.69	0.92
3:4:103:LEU:HD13	3:4:193:GLY:HA3	1.52	0.92
2:2:174:GLU:CG	1:3:59:LEU:HD22	1.99	0.92
1:5:178:ALA:CA	2:6:64:VAL:HG21	1.99	0.92
21:N:168:LEU:O	21:N:172:VAL:HG23	1.68	0.92
3:8:103:LEU:HD13	3:8:193:GLY:HA3	1.52	0.92
15:o:298:GLU:OE1	15:o:328:TYR:OH	1.86	0.92
28:T:101:BCR:H362	28:T:101:BCR:H292	1.52	0.92
21:Y:168:LEU:O	21:Y:172:VAL:HG23	1.68	0.92
4:A:235:GLU:HB3	7:D:264:ASN:HD21	1.32	0.92
2:6:174:GLU:CG	1:7:59:LEU:HD22	1.99	0.92
2:6:178:ILE:CD1	1:7:62:PHE:HA	2.00	0.92
3:8:77:LEU:HG	3:8:78:PRO:HD2	1.51	0.92
15:o:113:GLN:HE21	17:w:80:LEU:HD11	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:70:GLY:HA2	5:B:178:VAL:HG11	1.50	0.92
21:y:104:ARG:HB3	25:y:311:CLA:HBC3	1.52	0.92
5:b:70:GLY:HA2	5:b:178:VAL:HG11	1.50	0.91
1:1:178:ALA:CA	2:2:64:VAL:HG21	1.99	0.91
2:2:178:ILE:CD1	1:3:62:PHE:HA	2.00	0.91
3:4:77:LEU:HG	3:4:78:PRO:HD2	1.51	0.91
4:A:225:ARG:HD3	22:R:102:ALA:HB1	1.50	0.91
21:G:168:LEU:O	21:G:172:VAL:HG23	1.68	0.91
15:O:298:GLU:OE1	15:O:328:TYR:OH	1.86	0.91
10:h:17:THR:HG23	10:h:20:GLY:H	1.34	0.91
25:6:605:CLA:HAA1	25:6:605:CLA:HBD	1.51	0.91
21:Y:104:ARG:HB3	25:Y:311:CLA:HBC3	1.52	0.91
3:4:194:TYR:HE2	3:4:221:LEU:HB2	1.35	0.91
1:1:55:ARG:NH1	1:1:72:GLY:HA3	1.86	0.91
20:s:115:LEU:HD12	20:s:200:LEU:HD13	1.53	0.91
10:H:17:THR:HG23	10:H:20:GLY:H	1.34	0.90
25:N:613:CLA:H143	25:N:613:CLA:H8	1.54	0.90
25:c:511:CLA:H162	19:z:20:LEU:HD12	1.53	0.90
21:G:55:ARG:NH1	21:G:72:GLY:HA3	1.86	0.90
1:7:55:ARG:NH1	1:7:72:GLY:HA3	1.86	0.90
4:a:192:ILE:HG21	25:a:402:CLA:HHD	1.53	0.90
5:b:141:ILE:HG21	25:b:615:CLA:HBB1	1.53	0.90
6:c:163:ILE:HG21	25:c:512:CLA:HAB	1.53	0.90
2:6:55:ARG:NH1	2:6:77:ASP:O	2.05	0.90
1:3:55:ARG:NH1	1:3:72:GLY:HA3	1.86	0.90
15:O:196:TYR:HB2	15:O:212:LEU:CD2	2.02	0.90
25:2:605:CLA:HBD	25:2:605:CLA:HAA1	1.51	0.90
7:d:187:GLN:HB2	25:d:402:CLA:HBC1	1.53	0.90
15:o:145:VAL:HG11	15:o:203:LEU:HD11	1.54	0.90
2:2:55:ARG:NH1	2:2:77:ASP:O	2.05	0.90
25:C:511:CLA:H162	19:Z:20:LEU:HD12	1.54	0.90
4:A:220:THR:O	7:D:140:ARG:NH2	2.04	0.89
6:C:163:ILE:HG21	25:C:512:CLA:HAB	1.53	0.89
21:N:55:ARG:NH1	21:N:72:GLY:HA3	1.86	0.89
7:D:187:GLN:HB2	25:D:402:CLA:HBC1	1.53	0.89
25:c:501:CLA:HHB	28:i:101:BCR:H271	1.54	0.89
25:n:613:CLA:H143	25:n:613:CLA:H8	1.53	0.89
2:2:145:LEU:HD23	2:2:154:VAL:HA	1.55	0.89
2:2:174:GLU:HB3	1:3:62:PHE:CB	2.03	0.89
1:5:55:ARG:NH1	1:5:72:GLY:HA3	1.86	0.89
3:8:194:TYR:HE2	3:8:221:LEU:HB2	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:t:101:BCR:H362	28:t:101:BCR:H292	1.52	0.89
2:6:179:ASN:HA	24:6:603:CHL:CMC	2.03	0.89
4:a:220:THR:O	7:d:140:ARG:NH2	2.04	0.89
11:I:34:ARG:HH11	11:I:35:GLU:HG2	1.38	0.89
1:7:114:VAL:HG13	1:7:241:LEU:HD11	1.55	0.89
25:C:501:CLA:HBB	28:I:101:BCR:H271	1.54	0.89
2:6:145:LEU:HD23	2:6:154:VAL:HA	1.55	0.89
2:6:174:GLU:HB3	1:7:62:PHE:CB	2.03	0.89
21:y:55:ARG:NH1	21:y:72:GLY:HA3	1.86	0.89
20:S:115:LEU:HD12	20:S:200:LEU:HD13	1.53	0.89
21:Y:55:ARG:NH1	21:Y:72:GLY:HA3	1.86	0.89
4:A:192:ILE:HG21	25:A:401:CLA:HHD	1.53	0.89
1:5:114:VAL:HG13	1:5:241:LEU:HD11	1.55	0.89
3:8:103:LEU:HD11	3:8:194:TYR:CD1	2.08	0.89
5:B:141:ILE:HG21	25:B:615:CLA:HBB1	1.53	0.89
15:o:196:TYR:HB2	15:o:212:LEU:CD2	2.02	0.89
21:n:55:ARG:NH1	21:n:72:GLY:HA3	1.86	0.89
25:G:611:CLA:HBC1	26:Y:301:LHG:H292	1.56	0.88
11:i:34:ARG:HH11	11:i:35:GLU:HG2	1.38	0.88
21:g:55:ARG:NH1	21:g:72:GLY:HA3	1.86	0.88
1:3:114:VAL:HG13	1:3:241:LEU:HD11	1.55	0.88
15:O:145:VAL:HG11	15:O:203:LEU:HD11	1.54	0.88
2:6:188:ASN:O	24:6:603:CHL:HBC1	1.73	0.88
25:y:304:CLA:HMC3	25:y:304:CLA:HBC3	1.55	0.88
6:c:221:GLU:O	6:c:226:SER:OG	1.91	0.88
2:2:179:ASN:HA	24:2:603:CHL:CMC	2.03	0.88
25:a:406:CLA:HMC1	11:i:11:VAL:HG11	1.56	0.88
25:r:610:CLA:HBC3	26:r:618:LHG:HC5	1.55	0.88
2:2:188:ASN:O	24:2:603:CHL:HBC1	1.73	0.88
15:O:113:GLN:HE21	17:W:80:LEU:HD11	1.35	0.88
25:g:611:CLA:HBC1	26:y:301:LHG:H292	1.56	0.88
25:R:614:CLA:HBC3	25:R:614:CLA:HHD	1.56	0.88
3:4:103:LEU:HD11	3:4:194:TYR:CD1	2.08	0.87
25:S:310:CLA:H51	25:S:312:CLA:HMA1	1.56	0.87
4:a:76:ASN:HB2	13:l:34:ASN:HD22	1.40	0.87
21:g:98:LEU:HD22	25:g:603:CLA:CAA	2.04	0.87
3:4:177:PRO:HG3	25:R:610:CLA:HBB2	1.57	0.87
21:G:94:ARG:HG3	21:N:82:THR:O	1.74	0.87
25:s:310:CLA:H51	25:s:312:CLA:HMA1	1.56	0.87
3:8:177:PRO:HG3	25:r:610:CLA:HBB2	1.57	0.87
4:a:74:GLY:HA3	7:d:305:ARG:NH1	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:610:CLA:H52	39:n:615:LUT:H28	1.57	0.87
5:B:472:ARG:HA	5:B:479:PHE:CE2	2.10	0.87
25:A:405:CLA:HMC1	11:I:11:VAL:HG11	1.56	0.87
21:G:231:VAL:HG11	25:G:613:CLA:HAC2	1.56	0.87
6:c:457:LYS:HE2	7:d:230:ALA:HB2	1.57	0.87
6:C:221:GLU:O	6:C:226:SER:OG	1.91	0.86
6:C:457:LYS:HE2	7:D:230:ALA:HB2	1.57	0.86
22:R:58:TRP:NE1	25:R:601:CLA:HAA1	1.90	0.86
1:1:114:VAL:HG13	1:1:241:LEU:HD11	1.55	0.86
8:E:27:ILE:HG23	8:E:28:PRO:HD3	1.57	0.86
21:n:231:VAL:HG21	25:n:613:CLA:HAC1	1.57	0.86
21:y:250:ASP:OD2	21:y:253:ASN:N	2.09	0.86
25:S:313:CLA:HBB	39:S:315:LUT:H3	1.56	0.86
8:e:27:ILE:HG23	8:e:28:PRO:HD3	1.58	0.86
24:G:601:CHL:H122	24:Y:308:CHL:HAB	1.58	0.86
24:Y:308:CHL:HHD	24:Y:308:CHL:HBC2	1.56	0.86
3:8:174:TRP:CE3	3:8:180:LYS:HD2	2.11	0.86
21:G:98:LEU:HD22	25:G:603:CLA:CAA	2.04	0.86
5:b:472:ARG:HA	5:b:479:PHE:CE2	2.10	0.86
4:A:76:ASN:HB2	13:L:34:ASN:HD22	1.40	0.86
21:G:243:ASN:ND2	25:G:613:CLA:O1D	2.09	0.86
21:G:232:GLN:HE21	25:G:613:CLA:C4D	1.85	0.86
12:k:40:MET:HA	12:k:43:ILE:HD12	1.57	0.86
25:s:313:CLA:HBB	39:s:315:LUT:H3	1.56	0.86
21:Y:109:GLY:HA2	39:Y:317:LUT:H181	1.58	0.86
7:d:183:ILE:CG2	25:d:402:CLA:HAC1	2.06	0.86
22:r:58:TRP:NE1	25:r:601:CLA:HAA1	1.90	0.86
25:R:610:CLA:HBC3	26:R:618:LHG:HC5	1.55	0.86
3:8:221:LEU:O	3:8:225:LYS:HG3	1.76	0.86
21:y:109:GLY:HA2	39:y:317:LUT:H181	1.58	0.86
7:D:55:PHE:O	8:E:49:SER:OG	1.94	0.86
20:S:246:THR:HG22	20:S:248:GLU:HG2	1.57	0.86
24:y:308:CHL:HHD	24:y:308:CHL:HBC2	1.56	0.86
3:4:221:LEU:O	3:4:225:LYS:HG3	1.76	0.85
24:N:607:CHL:H18	24:N:609:CHL:H71	1.57	0.85
25:Y:304:CLA:HMC3	25:Y:304:CLA:HBC3	1.55	0.85
21:g:94:ARG:HG3	21:n:82:THR:O	1.74	0.85
21:g:243:ASN:ND2	25:g:613:CLA:O1D	2.09	0.85
24:g:601:CHL:H122	24:y:308:CHL:HAB	1.58	0.85
25:n:602:CLA:H52	25:n:602:CLA:HMB3	1.58	0.85
21:n:104:ARG:HB3	25:n:610:CLA:HBC3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:614:CLA:HBC3	25:r:614:CLA:HHD	1.56	0.85
4:A:74:GLY:HA3	7:D:305:ARG:NH1	1.90	0.85
21:N:104:ARG:HB3	25:N:610:CLA:HBC3	1.59	0.85
1:1:220:ARG:HA	1:1:223:MET:HE3	1.59	0.85
20:s:89:VAL:HG11	20:s:111:GLN:NE2	1.91	0.85
25:N:602:CLA:HMB3	25:N:602:CLA:H52	1.58	0.85
21:Y:98:LEU:CD2	25:Y:304:CLA:HAA2	2.07	0.85
2:6:120:GLN:OE1	2:6:129:GLU:HG3	1.76	0.85
21:n:220:ARG:HA	21:n:223:MET:HE3	1.59	0.85
5:B:277:GLN:NE2	35:B:626:DGD:O5E	2.10	0.85
7:D:183:ILE:CG2	25:D:402:CLA:HAC1	2.06	0.85
21:N:159:LEU:HD11	21:Y:257:TRP:CG	2.11	0.85
12:K:40:MET:HA	12:K:43:ILE:HD12	1.57	0.85
20:s:246:THR:HG22	20:s:248:GLU:HG2	1.57	0.85
5:B:51:VAL:HG13	5:B:308:LYS:HG3	1.58	0.85
26:D:406:LHG:H321	16:T:21:ILE:HD11	1.58	0.85
18:X:84:LYS:O	18:X:87:LEU:HG	1.76	0.85
25:N:610:CLA:H52	39:N:615:LUT:H28	1.57	0.85
21:Y:250:ASP:OD2	21:Y:253:ASN:N	2.09	0.85
2:2:120:GLN:OE1	2:2:129:GLU:HG3	1.76	0.84
15:O:290:THR:HG22	15:O:291:LYS:H	1.41	0.84
21:G:220:ARG:HA	21:G:223:MET:HE3	1.59	0.84
2:6:117:GLU:HB2	2:6:241:PRO:HG2	1.58	0.84
24:n:607:CHL:H18	24:n:609:CHL:H71	1.57	0.84
2:2:146:ASP:O	2:2:152:ASN:ND2	2.11	0.84
21:N:231:VAL:HG21	25:N:613:CLA:HAC1	1.57	0.84
2:6:174:GLU:HG2	1:7:59:LEU:HD22	1.59	0.84
26:d:406:LHG:H321	16:t:21:ILE:HD11	1.58	0.84
18:x:84:LYS:O	18:x:87:LEU:HG	1.76	0.84
21:y:98:LEU:CD2	25:y:304:CLA:HAA2	2.07	0.84
1:3:220:ARG:HA	1:3:223:MET:HE3	1.59	0.84
21:Y:98:LEU:HD22	25:Y:304:CLA:CAA	2.07	0.84
5:b:460:LEU:CD1	7:d:288:VAL:HG21	2.07	0.84
7:d:56:VAL:HG21	7:d:111:LEU:CD1	2.08	0.84
3:4:175:ALA:HB2	22:R:59:TYR:HE2	1.41	0.84
5:b:51:VAL:HG13	5:b:308:LYS:HG3	1.58	0.84
15:o:202:GLN:HE21	15:o:206:GLY:HA2	1.43	0.84
5:B:460:LEU:CD1	7:D:288:VAL:HG21	2.07	0.84
13:L:5:ASN:ND2	13:L:8:GLU:OE1	2.10	0.84
21:Y:220:ARG:HA	21:Y:223:MET:HE3	1.59	0.84
7:d:55:PHE:O	8:e:49:SER:OG	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:220:ARG:HA	21:N:223:MET:HE3	1.59	0.84
3:4:174:TRP:CE3	3:4:180:LYS:HD2	2.11	0.84
1:5:220:ARG:HA	1:5:223:MET:HE3	1.59	0.84
25:c:502:CLA:HAA1	25:c:502:CLA:HBD	1.60	0.84
15:o:309:SER:N	15:o:319:LYS:O	2.10	0.84
21:g:220:ARG:HA	21:g:223:MET:HE3	1.59	0.84
23:u:84:ALA:HB1	23:u:100:ILE:HG23	1.57	0.84
25:B:615:CLA:H193	25:B:616:CLA:HBC3	1.59	0.84
7:D:56:VAL:HG21	7:D:111:LEU:CD1	2.08	0.84
20:S:89:VAL:HG11	20:S:111:GLN:NE2	1.91	0.84
25:B:604:CLA:H41	25:B:604:CLA:H92	1.59	0.84
26:C:518:LHG:H161	25:Y:312:CLA:HAB	1.58	0.84
15:O:228:THR:HG22	15:O:284:GLU:OE2	1.77	0.84
23:U:84:ALA:HB1	23:U:100:ILE:HG23	1.57	0.84
1:5:165:GLN:NE2	24:5:302:CHL:NB	2.26	0.84
2:6:89:PRO:HA	2:6:92:PHE:CD2	2.10	0.84
5:b:277:GLN:NE2	35:b:626:DGD:O5E	2.10	0.84
21:g:231:VAL:HG11	25:g:613:CLA:HAC2	1.56	0.84
21:n:232:GLN:HE21	25:n:613:CLA:C4D	1.82	0.84
15:O:309:SER:N	15:O:319:LYS:O	2.10	0.83
2:6:146:ASP:O	2:6:152:ASN:ND2	2.11	0.83
21:n:158:ILE:HD11	21:y:257:TRP:HE3	1.43	0.83
21:y:98:LEU:HD22	25:y:304:CLA:CAA	2.07	0.83
25:r:604:CLA:CHC	40:r:617:NEX:H222	2.08	0.83
2:2:117:GLU:HB2	2:2:241:PRO:HG2	1.58	0.83
25:R:604:CLA:CHC	40:R:617:NEX:H222	2.08	0.83
1:7:220:ARG:HA	1:7:223:MET:HE3	1.59	0.83
3:8:175:ALA:HB2	22:r:59:TYR:HE2	1.41	0.83
5:b:174:LEU:HD21	5:b:309:LEU:HD13	1.60	0.83
5:b:326:ARG:NH2	7:d:298:ASP:OD1	2.11	0.83
25:b:615:CLA:H193	25:b:616:CLA:HBC3	1.59	0.83
2:2:174:GLU:HG2	1:3:59:LEU:HD22	1.59	0.83
2:2:220:GLY:CA	25:2:602:CLA:HAC1	2.08	0.83
1:3:130:VAL:O	1:3:134:ALA:N	2.12	0.83
25:C:502:CLA:HAA1	25:C:502:CLA:HBD	1.60	0.83
26:c:518:LHG:H161	25:y:312:CLA:HAB	1.58	0.83
21:n:159:LEU:HD11	21:y:257:TRP:CG	2.11	0.83
21:y:165:GLN:OE1	21:y:165:GLN:HA	1.79	0.83
21:N:109:GLY:HA2	39:N:616:LUT:H181	1.60	0.83
6:c:310:SER:HB3	6:c:355:THR:HG22	1.60	0.83
1:1:165:GLN:OE1	1:1:165:GLN:HA	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:612:CLA:HHB	39:R:615:LUT:H42	1.61	0.83
25:b:604:CLA:H41	25:b:604:CLA:H92	1.59	0.83
13:l:5:ASN:ND2	13:l:8:GLU:OE1	2.10	0.83
25:S:312:CLA:HBA1	25:S:312:CLA:HMA2	1.61	0.83
7:d:226:ASP:HB2	7:d:235:ALA:HB1	1.58	0.83
22:r:120:LYS:N	22:r:126:PRO:O	2.11	0.83
5:B:326:ARG:NH2	7:D:298:ASP:OD1	2.11	0.83
6:C:331:ALA:O	15:O:196:TYR:OH	1.97	0.83
15:O:202:GLN:HE21	15:O:206:GLY:HA2	1.43	0.83
1:5:130:VAL:O	1:5:134:ALA:N	2.12	0.83
21:n:130:VAL:O	21:n:134:ALA:N	2.12	0.83
2:2:89:PRO:HA	2:2:92:PHE:CD2	2.10	0.83
22:R:120:LYS:N	22:R:126:PRO:O	2.11	0.83
5:B:233:ASN:O	5:B:236:THR:HG22	1.79	0.83
5:b:233:ASN:O	5:b:236:THR:HG22	1.79	0.83
1:1:213:VAL:O	1:1:217:LYS:HG3	1.79	0.83
1:3:213:VAL:O	1:3:217:LYS:HG3	1.79	0.83
7:D:226:ASP:HB2	7:D:235:ALA:HB1	1.58	0.83
15:o:290:THR:HG22	15:o:291:LYS:H	1.41	0.83
21:y:130:VAL:O	21:y:134:ALA:N	2.12	0.83
21:Y:213:VAL:O	21:Y:217:LYS:HG3	1.79	0.82
22:R:158:GLU:HB3	22:R:268:LEU:HD12	1.60	0.82
14:M:31:SER:HG	14:m:31:SER:HG	0.97	0.82
19:Z:19:LEU:HD21	19:Z:43:GLY:HA3	1.61	0.82
27:a:405:PHO:HBC3	7:d:280:LEU:HD12	1.61	0.82
21:g:165:GLN:OE1	21:g:165:GLN:HA	1.79	0.82
21:y:220:ARG:HA	21:y:223:MET:HE3	1.59	0.82
25:r:612:CLA:HHB	39:r:615:LUT:H42	1.61	0.82
5:B:159:THR:OG1	5:B:161:LEU:HD23	1.79	0.82
21:Y:130:VAL:O	21:Y:134:ALA:N	2.12	0.82
1:5:213:VAL:O	1:5:217:LYS:HG3	1.79	0.82
2:6:173:VAL:O	2:6:176:PHE:HB2	1.80	0.82
20:s:118:ALA:HB1	20:s:229:GLY:HA3	1.61	0.82
27:A:404:PHO:HBC3	7:D:280:LEU:HD12	1.61	0.82
21:N:158:ILE:HD11	21:Y:257:TRP:HE3	1.43	0.82
21:G:146:TYR:CE2	25:G:604:CLA:H2	2.15	0.82
21:G:213:VAL:O	21:G:217:LYS:HG3	1.79	0.82
21:N:130:VAL:O	21:N:134:ALA:N	2.12	0.82
22:R:137:ARG:HH21	25:R:602:CLA:HED3	1.44	0.82
15:o:228:THR:HG22	15:o:284:GLU:OE2	1.77	0.82
21:g:130:VAL:O	21:g:134:ALA:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:97:GLU:HG3	1:3:190:LEU:CD2	2.10	0.82
5:B:174:LEU:HD21	5:B:309:LEU:HD13	1.60	0.82
2:6:220:GLY:CA	25:6:602:CLA:HAC1	2.08	0.82
1:1:165:GLN:NE2	24:1:302:CHL:NB	2.26	0.82
5:B:157:HIS:CD2	5:B:164:PRO:HD2	2.15	0.82
21:N:213:VAL:O	21:N:217:LYS:HG3	1.79	0.82
21:Y:165:GLN:OE1	21:Y:165:GLN:HA	1.79	0.82
5:b:157:HIS:CD2	5:b:164:PRO:HD2	2.15	0.82
5:b:159:THR:OG1	5:b:161:LEU:HD23	1.79	0.82
8:e:27:ILE:CG2	8:e:28:PRO:HD3	2.09	0.82
22:r:158:GLU:HB3	22:r:268:LEU:HD12	1.60	0.82
1:1:130:VAL:O	1:1:134:ALA:N	2.12	0.82
25:N:603:CLA:H191	24:N:607:CHL:H111	1.61	0.82
22:R:269:ASN:O	22:R:273:THR:HG23	1.80	0.82
1:7:97:GLU:HG3	1:7:190:LEU:CD2	2.10	0.82
1:7:130:VAL:O	1:7:134:ALA:N	2.12	0.82
4:a:278:TRP:HB3	4:a:279:PRO:HD3	1.62	0.82
21:n:109:GLY:HA2	39:n:616:LUT:H181	1.60	0.82
21:n:165:GLN:OE1	21:n:165:GLN:HA	1.79	0.82
21:y:97:GLU:HG3	21:y:190:LEU:CD2	2.10	0.82
21:y:104:ARG:HB3	25:y:311:CLA:CBC	2.10	0.82
5:B:482:ILE:HG21	7:D:139:LEU:HD23	1.61	0.82
20:S:68:ARG:HH22	26:S:301:LHG:HC12	1.45	0.82
25:S:303:CLA:H71	25:S:304:CLA:HMA1	1.62	0.82
40:N:617:NEX:H12	40:N:617:NEX:H191	1.59	0.82
22:R:58:TRP:CE3	22:R:60:PRO:HG3	2.15	0.82
21:g:82:THR:HG22	24:y:310:CHL:HED3	1.61	0.82
21:n:213:VAL:O	21:n:217:LYS:HG3	1.79	0.82
40:n:617:NEX:H12	40:n:617:NEX:H191	1.60	0.82
21:y:213:VAL:O	21:y:217:LYS:HG3	1.79	0.82
22:r:58:TRP:CE3	22:r:60:PRO:HG3	2.15	0.82
1:1:97:GLU:HG3	1:1:190:LEU:CD2	2.09	0.82
21:G:130:VAL:O	21:G:134:ALA:N	2.12	0.82
21:N:165:GLN:OE1	21:N:165:GLN:HA	1.79	0.82
23:U:96:PRO:O	23:U:97:THR:OG1	1.97	0.82
25:s:312:CLA:HMA2	25:s:312:CLA:HBA1	1.61	0.82
8:E:27:ILE:CG2	8:E:28:PRO:HD3	2.09	0.81
21:Y:138:ILE:HG21	24:Y:307:CHL:CBC	2.10	0.81
2:2:175:GLY:HA3	2:2:181:LEU:CD1	2.10	0.81
4:A:278:TRP:HB3	4:A:279:PRO:HD3	1.62	0.81
1:7:213:VAL:O	1:7:217:LYS:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:19:LEU:HD21	19:z:43:GLY:HA3	1.61	0.81
21:g:146:TYR:CE2	25:g:604:CLA:H2	2.15	0.81
25:r:610:CLA:CMB	26:r:618:LHG:HC2	2.10	0.81
23:u:96:PRO:O	23:u:97:THR:OG1	1.97	0.81
2:2:204:ASP:O	2:2:208:THR:HG23	1.80	0.81
20:S:119:ARG:HD3	25:S:310:CLA:CHD	2.11	0.81
5:b:388:SER:HA	7:d:345:GLU:OE1	1.81	0.81
6:c:331:ALA:O	15:o:196:TYR:OH	1.97	0.81
21:g:213:VAL:O	21:g:217:LYS:HG3	1.79	0.81
20:S:118:ALA:HB1	20:S:229:GLY:HA3	1.61	0.81
21:G:107:MET:HG2	21:G:222:ALA:CB	2.11	0.81
25:R:610:CLA:CMB	26:R:618:LHG:HC2	2.10	0.81
2:6:184:VAL:HB	2:6:196:TYR:HE2	1.45	0.81
21:y:161:ILE:O	21:y:165:GLN:HB2	1.81	0.81
4:A:57:PRO:HD3	4:A:73:TYR:CE2	2.16	0.81
5:B:296:GLN:HE22	5:B:304:LYS:HD2	1.45	0.81
15:O:232:LEU:HD23	15:O:282:VAL:HG12	1.63	0.81
1:5:161:ILE:O	1:5:165:GLN:HB2	1.81	0.81
21:g:97:GLU:HG3	21:g:190:LEU:CD2	2.10	0.81
21:y:138:ILE:HG21	24:y:307:CHL:CBC	2.10	0.81
1:3:107:MET:HG2	1:3:222:ALA:CB	2.11	0.81
21:N:107:MET:HG2	21:N:222:ALA:CB	2.11	0.81
21:Y:104:ARG:HB3	25:Y:311:CLA:CBC	2.10	0.81
1:5:153:VAL:HG13	24:5:301:CHL:C1D	2.10	0.81
2:6:130:PRO:O	2:6:134:LYS:N	2.14	0.81
2:6:204:ASP:O	2:6:208:THR:HG23	1.80	0.81
1:1:161:ILE:O	1:1:165:GLN:HB2	1.81	0.81
21:G:165:GLN:OE1	21:G:165:GLN:HA	1.79	0.81
6:c:178:LYS:NZ	6:c:184:GLY:O	2.14	0.81
5:B:388:SER:HA	7:D:345:GLU:OE1	1.81	0.81
20:S:175:VAL:O	20:S:179:VAL:HG23	1.80	0.81
1:5:165:GLN:OE1	1:5:165:GLN:HA	1.79	0.81
1:7:165:GLN:HA	1:7:165:GLN:OE1	1.79	0.81
25:s:305:CLA:CHC	40:s:317:NEX:H222	2.11	0.81
22:r:269:ASN:O	22:r:273:THR:HG23	1.80	0.81
2:2:49:LEU:O	2:2:55:ARG:HA	1.80	0.81
2:2:184:VAL:HB	2:2:196:TYR:HE2	1.45	0.81
1:3:161:ILE:O	1:3:165:GLN:HB2	1.81	0.81
19:Z:26:VAL:HG21	19:Z:40:VAL:CG2	2.11	0.81
20:s:119:ARG:HD3	25:s:310:CLA:CHD	2.11	0.81
21:n:104:ARG:HB3	25:n:610:CLA:CBC	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:y:315:CLA:HBC1	39:y:316:LUT:H162	1.63	0.81
1:1:153:VAL:HG13	24:1:301:CHL:C1D	2.10	0.80
1:3:165:GLN:OE1	1:3:165:GLN:HA	1.79	0.80
6:C:310:SER:HB3	6:C:355:THR:HG22	1.60	0.80
21:N:104:ARG:HB3	25:N:610:CLA:CBC	2.11	0.80
21:Y:107:MET:HG2	21:Y:222:ALA:CB	2.11	0.80
2:6:49:LEU:O	2:6:55:ARG:HA	1.80	0.80
1:7:107:MET:HG2	1:7:222:ALA:CB	2.11	0.80
1:7:161:ILE:O	1:7:165:GLN:HB2	1.81	0.80
21:g:107:MET:HG2	21:g:222:ALA:CB	2.11	0.80
21:n:161:ILE:O	21:n:165:GLN:HB2	1.81	0.80
21:y:138:ILE:CG2	24:y:307:CHL:HBC1	2.11	0.80
22:r:72:LEU:HB3	22:r:137:ARG:HH12	1.46	0.80
3:4:229:ILE:HG13	3:4:230:LYS:H	1.45	0.80
6:C:265:VAL:HG22	17:W:131:LEU:HD12	1.63	0.80
21:Y:138:ILE:CG2	24:Y:307:CHL:HBC1	2.11	0.80
1:5:97:GLU:HG3	1:5:190:LEU:CD2	2.10	0.80
25:n:603:CLA:H191	24:n:607:CHL:H111	1.61	0.80
2:2:130:PRO:O	2:2:134:LYS:N	2.14	0.80
6:C:178:LYS:NZ	6:C:184:GLY:O	2.14	0.80
21:G:55:ARG:HH12	21:G:72:GLY:CA	1.95	0.80
21:n:107:MET:HG2	21:n:222:ALA:CB	2.11	0.80
21:Y:55:ARG:HH12	21:Y:72:GLY:CA	1.95	0.80
21:Y:161:ILE:O	21:Y:165:GLN:HB2	1.81	0.80
4:a:57:PRO:HD3	4:a:73:TYR:CE2	2.16	0.80
4:a:223:LEU:HB2	7:d:140:ARG:HH21	1.46	0.80
5:b:296:GLN:HE22	5:b:304:LYS:HD2	1.46	0.80
13:l:8:GLU:HB3	29:l:102:SQD:H62	1.63	0.80
1:1:107:MET:HG2	1:1:222:ALA:CB	2.11	0.80
2:2:173:VAL:O	2:2:176:PHE:HB2	1.80	0.80
21:G:82:THR:HG22	24:Y:310:CHL:HED3	1.61	0.80
21:N:161:ILE:O	21:N:165:GLN:HB2	1.81	0.80
1:3:135:GLY:O	1:3:138:ILE:HG22	1.82	0.80
21:G:161:ILE:O	21:G:165:GLN:HB2	1.81	0.80
21:N:231:VAL:HG11	25:N:613:CLA:HHD	1.63	0.80
21:n:55:ARG:HH12	21:n:72:GLY:CA	1.95	0.80
25:y:312:CLA:H122	25:y:313:CLA:H141	1.64	0.80
25:G:610:CLA:H52	39:G:615:LUT:H30	1.63	0.80
1:5:55:ARG:HH12	1:5:72:GLY:CA	1.95	0.80
1:5:107:MET:HG2	1:5:222:ALA:CB	2.11	0.80
5:b:482:ILE:HG21	7:d:139:LEU:HD23	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:132:GLU:HA	20:s:145:ALA:HB1	1.63	0.80
20:s:175:VAL:O	20:s:179:VAL:HG23	1.80	0.80
25:s:303:CLA:H71	25:s:304:CLA:HMA1	1.62	0.80
4:A:223:LEU:HB2	7:D:140:ARG:HH21	1.46	0.80
25:B:605:CLA:HMA1	25:B:606:CLA:H3A	1.64	0.80
21:Y:97:GLU:HG3	21:Y:190:LEU:CD2	2.10	0.80
1:5:135:GLY:O	1:5:138:ILE:HG22	1.82	0.80
19:z:26:VAL:HG21	19:z:40:VAL:CG2	2.11	0.80
21:n:97:GLU:HG3	21:n:190:LEU:CD2	2.09	0.80
21:n:231:VAL:HG11	25:n:613:CLA:HHD	1.63	0.80
22:r:137:ARG:HH21	25:r:602:CLA:HED3	1.44	0.80
21:G:97:GLU:HG3	21:G:190:LEU:CD2	2.10	0.80
21:N:135:GLY:O	21:N:138:ILE:HG22	1.82	0.80
25:d:403:CLA:H112	10:h:48:ALA:HB1	1.63	0.80
20:s:68:ARG:HH22	26:s:301:LHG:HC12	1.45	0.80
21:y:199:LEU:HG	39:y:316:LUT:H221	1.64	0.80
25:G:602:CLA:H121	25:G:602:CLA:H93	1.64	0.80
21:N:55:ARG:HH12	21:N:72:GLY:CA	1.95	0.80
21:Y:135:GLY:O	21:Y:138:ILE:HG22	1.82	0.80
5:b:467:ILE:HD12	7:d:127:MET:HE2	1.64	0.80
17:W:125:GLU:O	17:W:129:SER:OG	1.98	0.79
21:Y:226:MET:HG2	39:Y:317:LUT:H12	1.62	0.79
17:w:125:GLU:O	17:w:129:SER:OG	1.98	0.79
21:g:161:ILE:O	21:g:165:GLN:HB2	1.81	0.79
21:n:135:GLY:O	21:n:138:ILE:HG22	1.82	0.79
21:n:182:PRO:HB3	40:n:617:NEX:H171	1.63	0.79
21:y:55:ARG:HH12	21:y:72:GLY:CA	1.95	0.79
1:1:55:ARG:HH12	1:1:72:GLY:CA	1.95	0.79
1:1:135:GLY:O	1:1:138:ILE:HG22	1.82	0.79
21:G:135:GLY:O	21:G:138:ILE:HG22	1.82	0.79
3:8:229:ILE:HG13	3:8:230:LYS:H	1.45	0.79
21:y:135:GLY:O	21:y:138:ILE:HG22	1.82	0.79
25:S:305:CLA:CHC	40:S:317:NEX:H222	2.11	0.79
5:b:173:GLY:HA3	5:b:265:ILE:HD11	1.64	0.79
21:y:107:MET:HG2	21:y:222:ALA:CB	2.11	0.79
25:D:403:CLA:H112	10:H:48:ALA:HB1	1.63	0.79
20:S:132:GLU:HA	20:S:145:ALA:HB1	1.63	0.79
2:6:175:GLY:HA3	2:6:181:LEU:CD1	2.10	0.79
15:o:232:LEU:HD23	15:o:282:VAL:HG12	1.63	0.79
22:r:85:LYS:HG2	22:r:86:PRO:HD2	1.65	0.79
1:3:55:ARG:HH12	1:3:72:GLY:CA	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:315:CLA:HBC1	39:Y:316:LUT:H162	1.62	0.79
22:R:85:LYS:HG2	22:R:86:PRO:HD2	1.65	0.79
2:6:193:GLY:HA2	2:6:197:PHE:HD2	1.48	0.79
5:b:277:GLN:HB2	23:u:99:LYS:HG2	1.65	0.79
21:g:135:GLY:O	21:g:138:ILE:HG22	1.82	0.79
21:g:165:GLN:HE22	24:g:606:CHL:C1B	1.96	0.79
4:A:139:MET:HE3	7:D:222:THR:CG2	2.13	0.79
7:D:108:LEU:HD23	8:E:66:ILE:HD13	1.64	0.79
21:N:182:PRO:HB3	40:N:617:NEX:H171	1.63	0.79
21:G:165:GLN:HE22	24:G:606:CHL:C1B	1.96	0.79
1:5:153:VAL:HA	24:5:301:CHL:C4D	2.13	0.79
21:N:97:GLU:HG3	21:N:190:LEU:CD2	2.10	0.79
21:N:164:THR:HG21	24:N:606:CHL:HED3	1.64	0.79
1:5:138:ILE:HD12	1:5:144:LEU:HD13	1.65	0.79
5:b:73:ASN:ND2	5:b:79:ASN:OD1	2.16	0.79
7:D:20:ASP:OD2	7:D:24:ARG:NH1	2.15	0.79
21:N:138:ILE:HD12	21:N:144:LEU:HD13	1.65	0.79
1:7:55:ARG:HH12	1:7:72:GLY:CA	1.95	0.79
1:7:135:GLY:O	1:7:138:ILE:HG22	1.82	0.79
28:h:101:BCR:H403	28:h:101:BCR:H23C	1.65	0.79
15:o:207:GLU:OE1	15:o:209:VAL:HG23	1.83	0.79
25:g:610:CLA:H52	39:g:615:LUT:H30	1.63	0.79
21:y:226:MET:HG2	39:y:317:LUT:H12	1.62	0.79
22:r:214:LYS:NZ	22:r:218:PRO:O	2.13	0.79
2:2:205:ASP:O	2:2:208:THR:OG1	2.01	0.79
4:a:139:MET:HE3	7:d:222:THR:CG2	2.13	0.79
6:c:265:VAL:HG22	17:w:131:LEU:HD12	1.63	0.79
1:1:153:VAL:HA	24:1:301:CHL:C4D	2.13	0.78
8:E:77:ASP:O	8:E:81:ARG:HG3	1.83	0.78
21:Y:138:ILE:HD12	21:Y:144:LEU:HD13	1.65	0.78
21:Y:199:LEU:HG	39:Y:316:LUT:H221	1.64	0.78
4:a:288:LEU:O	4:a:292:THR:HG23	1.84	0.78
8:e:77:ASP:O	8:e:81:ARG:HG3	1.83	0.78
21:g:55:ARG:HH12	21:g:72:GLY:CA	1.95	0.78
5:B:73:ASN:ND2	5:B:79:ASN:OD1	2.16	0.78
5:B:277:GLN:HB2	23:U:99:LYS:HG2	1.65	0.78
13:L:8:GLU:HB3	29:L:101:SQD:H62	1.63	0.78
3:8:122:TRP:HA	3:8:127:TRP:HD1	1.48	0.78
3:8:175:ALA:HB2	22:r:59:TYR:CE2	2.19	0.78
25:b:605:CLA:HMA1	25:b:606:CLA:H3A	1.64	0.78
7:d:20:ASP:OD2	7:d:24:ARG:NH1	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:122:TRP:HA	3:4:127:TRP:HD1	1.48	0.78
15:O:207:GLU:OE1	15:O:209:VAL:HG23	1.83	0.78
4:a:60:ILE:HD12	4:a:84:PRO:HD2	1.64	0.78
21:g:138:ILE:HD12	21:g:144:LEU:HD13	1.65	0.78
21:g:215:GLU:HG3	25:g:610:CLA:NB	1.99	0.78
5:B:173:GLY:HA3	5:B:265:ILE:HD11	1.64	0.78
11:I:34:ARG:HD2	11:I:35:GLU:HG3	1.63	0.78
25:Y:312:CLA:H122	25:Y:313:CLA:H141	1.64	0.78
2:6:205:ASP:O	2:6:208:THR:OG1	2.01	0.78
2:2:70:LEU:HD13	2:2:79:GLY:HA2	1.65	0.78
25:2:602:CLA:HBD	25:2:602:CLA:HAA1	1.65	0.78
5:B:42:LEU:HD13	5:B:94:GLU:HG3	1.66	0.78
21:G:138:ILE:HD12	21:G:144:LEU:HD13	1.65	0.78
25:N:610:CLA:H51	25:N:612:CLA:HMA1	1.66	0.78
22:R:72:LEU:HB3	22:R:137:ARG:HH12	1.46	0.78
5:b:360:PRO:O	5:b:361:THR:HG22	1.84	0.78
10:h:56:ILE:HD13	18:x:84:LYS:CE	2.12	0.78
11:i:34:ARG:HD2	11:i:35:GLU:HG3	1.63	0.78
4:A:89:ILE:HD11	4:A:108:ASN:HB3	1.66	0.78
5:B:360:PRO:O	5:B:361:THR:HG22	1.84	0.78
24:N:609:CHL:CAA	21:Y:82:THR:HG21	2.13	0.78
21:y:138:ILE:HD12	21:y:144:LEU:HD13	1.65	0.78
3:4:170:GLN:HB2	3:4:183:GLU:HG2	1.63	0.78
28:H:101:BCR:H403	28:H:101:BCR:H23C	1.65	0.78
2:6:70:LEU:HD13	2:6:79:GLY:HA2	1.65	0.78
21:n:138:ILE:HD12	21:n:144:LEU:HD13	1.65	0.78
2:2:193:GLY:HA2	2:2:197:PHE:HD2	1.48	0.78
5:B:272:ARG:NH1	5:B:276:ASP:OD2	2.17	0.78
6:C:449:ARG:HH12	11:I:28:PRO:HG3	1.48	0.78
21:G:97:GLU:CA	21:G:190:LEU:HD11	2.14	0.78
1:7:57:LYS:HZ1	1:7:66:PRO:HG3	1.48	0.78
3:8:138:ALA:HB3	3:8:140:PHE:CE2	2.19	0.78
3:8:170:GLN:HB2	3:8:183:GLU:HG2	1.63	0.78
6:c:97:TRP:CH2	30:c:520:LMG:H172	2.19	0.78
20:s:132:GLU:HG2	20:s:251:VAL:HB	1.66	0.78
20:S:132:GLU:HG2	20:S:251:VAL:HB	1.66	0.78
22:R:214:LYS:NZ	22:R:218:PRO:O	2.13	0.78
2:6:152:ASN:O	2:6:154:VAL:HG23	1.84	0.78
5:b:478:VAL:O	7:d:140:ARG:HD3	1.84	0.78
6:c:449:ARG:HH12	11:i:28:PRO:HG3	1.48	0.78
7:d:108:LEU:HD23	8:e:66:ILE:HD13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:467:ILE:HD12	7:D:127:MET:HE2	1.64	0.77
6:C:322:GLN:HE22	6:C:384:ILE:HD12	1.49	0.77
7:D:292:LEU:HB2	7:D:294:LEU:HD13	1.66	0.77
5:b:51:VAL:HG13	5:b:308:LYS:CG	2.14	0.77
21:g:84:GLY:O	21:y:91:THR:OG1	2.02	0.77
21:g:97:GLU:CA	21:g:190:LEU:HD11	2.14	0.77
25:n:610:CLA:H51	25:n:612:CLA:HMA1	1.66	0.77
19:Z:26:VAL:HG21	19:Z:40:VAL:HG21	1.66	0.77
21:N:206:GLU:OE1	21:N:206:GLU:N	2.18	0.77
1:7:206:GLU:N	1:7:206:GLU:OE1	2.18	0.77
25:g:602:CLA:H121	25:g:602:CLA:H93	1.64	0.77
25:n:612:CLA:HHC	25:n:612:CLA:HBB1	1.65	0.77
1:1:138:ILE:HD12	1:1:144:LEU:HD13	1.65	0.77
2:2:239:LYS:HD2	2:2:242:LEU:CD1	2.14	0.77
4:A:60:ILE:HD12	4:A:84:PRO:HD2	1.64	0.77
5:B:280:PHE:CD2	5:B:312:TYR:HB3	2.19	0.77
6:C:97:TRP:CH2	30:C:520:LMG:H172	2.19	0.77
14:M:31:SER:O	14:M:32:GLN:HG2	1.85	0.77
2:6:239:LYS:HD2	2:6:242:LEU:CD1	2.14	0.77
5:b:42:LEU:HD13	5:b:94:GLU:HG3	1.66	0.77
1:1:206:GLU:OE1	1:1:206:GLU:N	2.18	0.77
5:B:51:VAL:HG13	5:B:308:LYS:CG	2.14	0.77
21:N:232:GLN:HE21	25:N:613:CLA:C4D	1.82	0.77
3:8:155:TRP:CD1	3:8:159:LYS:HZ1	2.03	0.77
21:y:206:GLU:OE1	21:y:206:GLU:N	2.18	0.77
1:3:206:GLU:OE1	1:3:206:GLU:N	2.18	0.77
4:A:292:THR:HG22	6:C:428:THR:HG23	1.66	0.77
24:N:607:CHL:H203	25:Y:303:CLA:C16	2.14	0.77
25:s:303:CLA:HAB	39:s:316:LUT:H30	1.66	0.77
1:1:97:GLU:CA	1:1:190:LEU:HD11	2.14	0.77
4:A:335:ASN:HA	7:D:351:ASN:HD22	1.50	0.77
25:B:603:CLA:H2	25:B:605:CLA:H91	1.65	0.77
4:a:335:ASN:HA	7:d:351:ASN:HD22	1.50	0.77
25:b:603:CLA:H2	25:b:605:CLA:H91	1.65	0.77
6:c:369:LEU:HD21	6:c:384:ILE:HG12	1.66	0.77
25:g:614:CLA:HBD	25:g:614:CLA:HAA1	1.67	0.77
3:4:175:ALA:HB2	22:R:59:TYR:CE2	2.19	0.77
15:O:169:TYR:OH	17:W:80:LEU:HA	1.84	0.77
25:N:612:CLA:HHC	25:N:612:CLA:HBB1	1.64	0.77
22:R:238:LEU:HB3	25:R:609:CLA:H3A	1.66	0.77
1:7:97:GLU:CA	1:7:190:LEU:HD11	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:322:GLN:HE22	6:c:384:ILE:HD12	1.49	0.77
21:g:232:GLN:HE21	25:g:613:CLA:C4D	1.85	0.77
3:4:138:ALA:HB3	3:4:140:PHE:CE2	2.19	0.77
4:A:288:LEU:O	4:A:292:THR:HG23	1.84	0.77
21:G:215:GLU:HG3	25:G:610:CLA:NB	1.99	0.77
40:G:617:NEX:H28	40:G:617:NEX:H361	1.67	0.77
21:Y:206:GLU:OE1	21:Y:206:GLU:N	2.18	0.77
21:g:64:GLY:HA3	21:y:178:ALA:HA	1.66	0.77
21:g:206:GLU:N	21:g:206:GLU:OE1	2.18	0.77
21:n:179:GLY:HA2	24:n:608:CHL:HAC1	1.67	0.77
25:r:603:CLA:C14	25:r:603:CLA:HMB2	2.14	0.77
5:B:451:PHE:HE2	25:B:604:CLA:HMA3	1.50	0.77
5:B:478:VAL:O	7:D:140:ARG:HD3	1.84	0.77
25:R:603:CLA:C14	25:R:603:CLA:HMB2	2.14	0.77
1:5:206:GLU:OE1	1:5:206:GLU:N	2.18	0.77
4:a:292:THR:HG22	6:c:428:THR:HG23	1.66	0.77
2:2:122:TRP:O	2:2:123:VAL:HG23	1.85	0.77
21:G:64:GLY:HA3	21:Y:178:ALA:HA	1.66	0.77
21:Y:231:VAL:HG21	25:Y:314:CLA:HAC2	1.66	0.77
2:6:122:TRP:O	2:6:123:VAL:HG23	1.85	0.77
2:6:127:PHE:HE2	2:6:145:LEU:HB2	1.50	0.77
1:7:138:ILE:HD12	1:7:144:LEU:HD13	1.65	0.77
1:1:57:LYS:HZ1	1:1:66:PRO:HG3	1.50	0.76
1:3:138:ILE:HD12	1:3:144:LEU:HD13	1.65	0.76
6:C:369:LEU:HD21	6:C:384:ILE:HG12	1.66	0.76
18:X:84:LYS:HA	18:X:87:LEU:CD2	2.15	0.76
21:G:196:PHE:HE2	24:G:608:CHL:HBC2	1.50	0.76
21:N:97:GLU:CA	21:N:190:LEU:HD11	2.14	0.76
7:d:292:LEU:HB2	7:d:294:LEU:HD13	1.66	0.76
18:x:84:LYS:HA	18:x:87:LEU:CD2	2.14	0.76
22:r:238:LEU:HB3	25:r:609:CLA:H3A	1.67	0.76
25:S:303:CLA:HAB	39:S:316:LUT:H30	1.66	0.76
26:d:406:LHG:H182	16:t:17:ILE:HD11	1.66	0.76
21:G:84:GLY:O	21:Y:91:THR:OG1	2.02	0.76
5:b:272:ARG:NH1	5:b:276:ASP:OD2	2.17	0.76
21:n:164:THR:HG21	24:n:606:CHL:HED3	1.65	0.76
6:C:86:LEU:HD13	6:C:89:LEU:HD12	1.68	0.76
19:Z:48:ILE:HG12	26:S:318:LHG:H222	1.67	0.76
22:R:68:LEU:HD11	25:R:602:CLA:CGD	2.16	0.76
4:a:89:ILE:HD11	4:a:108:ASN:HB3	1.66	0.76
5:b:280:PHE:CD2	5:b:312:TYR:HB3	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:m:31:SER:O	14:m:32:GLN:HG2	1.85	0.76
21:g:196:PHE:HE2	24:g:608:CHL:HBC2	1.50	0.76
21:n:97:GLU:CA	21:n:190:LEU:HD11	2.14	0.76
21:n:206:GLU:OE1	21:n:206:GLU:N	2.18	0.76
1:3:220:ARG:HA	1:3:223:MET:CE	2.15	0.76
25:g:610:CLA:H41	25:g:612:CLA:HMA2	1.68	0.76
21:n:220:ARG:HA	21:n:223:MET:CE	2.15	0.76
2:2:152:ASN:O	2:2:154:VAL:HG23	1.84	0.76
2:2:211:GLU:HA	2:2:214:VAL:HG12	1.68	0.76
3:4:219:GLU:CG	3:4:222:GLU:HB2	2.15	0.76
21:G:206:GLU:N	21:G:206:GLU:OE1	2.18	0.76
25:G:614:CLA:HBD	25:G:614:CLA:HAA1	1.67	0.76
21:N:220:ARG:HA	21:N:223:MET:CE	2.15	0.76
21:Y:220:ARG:HA	21:Y:223:MET:CE	2.15	0.76
2:6:211:GLU:HA	2:6:214:VAL:HG12	1.68	0.76
5:b:162:TYR:HA	26:b:621:LHG:HC2	1.68	0.76
25:c:502:CLA:HMC2	25:c:510:CLA:HBB1	1.67	0.76
19:z:48:ILE:HG12	26:s:318:LHG:H222	1.67	0.76
20:s:141:CYS:HB3	25:s:305:CLA:OBD	1.85	0.76
25:n:603:CLA:HMC3	25:n:603:CLA:HBC3	1.68	0.76
1:1:220:ARG:HA	1:1:223:MET:CE	2.15	0.76
4:A:328:MET:HG2	7:D:326:ILE:HG12	1.68	0.76
5:b:392:VAL:HG13	5:b:397:VAL:HG22	1.68	0.76
19:z:26:VAL:HG21	19:z:40:VAL:HG21	1.66	0.76
5:B:223:GLN:HA	10:H:33:VAL:HG11	1.67	0.76
26:D:406:LHG:H182	16:T:17:ILE:HD11	1.66	0.76
8:E:60:ARG:CZ	8:E:64:PRO:HG3	2.16	0.76
24:N:607:CHL:H192	25:Y:303:CLA:H151	1.68	0.76
2:6:69:TYR:CE1	2:6:70:LEU:HG	2.20	0.76
2:6:160:LEU:HD23	2:6:163:LEU:HD12	1.68	0.76
3:8:219:GLU:CG	3:8:222:GLU:HB2	2.15	0.76
5:B:162:TYR:HA	26:B:621:LHG:HC2	1.68	0.76
15:O:236:TYR:HB2	15:O:310:ASP:OD2	1.86	0.76
25:N:603:CLA:HMC3	25:N:603:CLA:HBC3	1.68	0.76
25:N:603:CLA:H101	24:N:609:CHL:H141	1.68	0.76
21:y:227:PHE:HD2	25:y:303:CLA:H202	1.51	0.76
1:3:97:GLU:CA	1:3:190:LEU:HD11	2.14	0.76
5:B:341:LEU:HD12	5:B:429:ILE:HG22	1.68	0.76
25:a:402:CLA:HMC3	25:a:402:CLA:HBC3	1.68	0.76
24:n:607:CHL:H203	25:y:303:CLA:C16	2.14	0.76
21:y:146:TYR:HB3	21:y:152:LEU:HD13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:TYR:CE1	2:2:70:LEU:HG	2.20	0.75
5:B:392:VAL:HG13	5:B:397:VAL:HG22	1.68	0.75
2:6:175:GLY:CA	2:6:181:LEU:HD11	2.15	0.75
5:b:272:ARG:NH1	5:b:361:THR:HG21	2.01	0.75
21:y:97:GLU:CA	21:y:190:LEU:HD11	2.14	0.75
23:u:88:TYR:HB2	23:u:100:ILE:HG21	1.68	0.75
3:8:225:LYS:HA	3:8:228:GLU:OE1	1.86	0.75
1:1:146:TYR:HB3	1:1:152:LEU:HD13	1.68	0.75
1:3:146:TYR:HB3	1:3:152:LEU:HD13	1.68	0.75
5:B:121:GLU:O	10:H:24:LYS:HE2	1.86	0.75
5:B:377:VAL:HG11	7:D:343:PRO:HG3	1.69	0.75
6:C:215:LYS:HG2	6:C:221:GLU:HB3	1.69	0.75
15:O:180:VAL:HA	15:O:186:VAL:HG12	1.68	0.75
21:G:220:ARG:HA	21:G:223:MET:CE	2.15	0.75
25:R:604:CLA:CHB	41:R:616:XAT:H42	2.17	0.75
1:5:57:LYS:HZ1	1:5:66:PRO:HG3	1.51	0.75
15:o:236:TYR:HB2	15:o:310:ASP:OD2	1.85	0.75
40:g:617:NEX:H28	40:g:617:NEX:H361	1.67	0.75
21:y:231:VAL:HG21	25:y:314:CLA:HAC2	1.66	0.75
25:r:610:CLA:HMB3	26:r:618:LHG:HC2	1.68	0.75
15:O:92:LEU:HB3	15:O:96:GLU:HG3	1.68	0.75
2:6:88:ASP:HB3	2:6:91:ALA:CB	2.17	0.75
2:6:239:LYS:HD2	2:6:242:LEU:HD12	1.68	0.75
15:o:169:TYR:OH	17:w:80:LEU:HA	1.84	0.75
21:g:220:ARG:HA	21:g:223:MET:CE	2.15	0.75
25:A:401:CLA:HMC3	25:A:401:CLA:HBC3	1.68	0.75
5:B:127:ARG:HG3	5:B:128:THR:HG23	1.69	0.75
20:S:141:CYS:HB3	25:S:305:CLA:OBD	1.85	0.75
25:6:602:CLA:HBD	25:6:602:CLA:HAA1	1.65	0.75
10:h:56:ILE:HA	18:x:84:LYS:HE2	1.69	0.75
21:n:132:PHE:HB2	24:n:607:CHL:H2A	1.68	0.75
22:r:68:LEU:HD11	25:r:602:CLA:CGD	2.16	0.75
2:2:175:GLY:CA	2:2:181:LEU:HD11	2.15	0.75
3:4:225:LYS:HA	3:4:228:GLU:OE1	1.86	0.75
3:4:226:LEU:HD12	3:4:229:ILE:HD11	1.67	0.75
3:8:226:LEU:HD12	3:8:229:ILE:HD11	1.67	0.75
5:b:377:VAL:HG11	7:d:343:PRO:HG3	1.69	0.75
6:c:215:LYS:HG2	6:c:221:GLU:HB3	1.68	0.75
8:e:60:ARG:CZ	8:e:64:PRO:HG3	2.16	0.75
21:N:132:PHE:HB2	24:N:607:CHL:H2A	1.68	0.75
21:N:146:TYR:HB3	21:N:152:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:220:ARG:HA	1:5:223:MET:CE	2.15	0.75
25:n:603:CLA:H101	24:n:609:CHL:H141	1.68	0.75
21:y:220:ARG:HA	21:y:223:MET:CE	2.15	0.75
2:2:127:PHE:HE2	2:2:145:LEU:HB2	1.50	0.75
27:A:403:PHO:HMB1	27:A:403:PHO:HBB1	1.68	0.75
26:B:625:LHG:O4	7:D:142:TYR:OH	2.04	0.75
22:R:72:LEU:HB3	22:R:137:ARG:NH1	2.01	0.75
6:c:86:LEU:HD13	6:c:89:LEU:HD12	1.68	0.75
21:g:146:TYR:HB3	21:g:152:LEU:HD13	1.68	0.75
21:y:105:TRP:HE1	24:y:309:CHL:HED2	1.52	0.75
2:2:127:PHE:HB3	2:2:140:PHE:CE2	2.22	0.75
3:4:133:GLN:HG2	3:4:134:PRO:CD	2.17	0.75
3:4:221:LEU:HD12	3:4:222:GLU:N	2.02	0.75
8:E:23:HIS:O	8:E:27:ILE:HG22	1.87	0.75
21:G:84:GLY:CA	21:Y:94:ARG:HG2	2.17	0.75
21:N:179:GLY:HA2	24:N:608:CHL:HAC1	1.67	0.75
21:Y:227:PHE:HD2	25:Y:303:CLA:H202	1.51	0.75
1:7:146:TYR:HB3	1:7:152:LEU:HD13	1.68	0.75
8:e:23:HIS:O	8:e:27:ILE:HG22	1.87	0.75
15:o:92:LEU:HB3	15:o:96:GLU:HG3	1.68	0.75
3:4:107:ARG:O	3:4:110:MET:HG3	1.87	0.74
25:C:502:CLA:HMC2	25:C:510:CLA:HBB1	1.67	0.74
21:G:169:MET:HG3	24:G:609:CHL:HMC	1.69	0.74
24:G:608:CHL:H12	24:G:608:CHL:H151	1.69	0.74
24:Y:308:CHL:HBC3	32:Y:322:AJP:O82	1.86	0.74
1:5:146:TYR:HB3	1:5:152:LEU:HD13	1.68	0.74
24:s:307:CHL:HBC2	32:s:319:AJP:O82	1.87	0.74
24:n:607:CHL:H192	25:y:303:CLA:H151	1.68	0.74
2:2:88:ASP:HB3	2:2:91:ALA:CB	2.17	0.74
2:2:130:PRO:HG2	2:2:133:PHE:HB2	1.70	0.74
2:2:130:PRO:HD3	2:2:239:LYS:HE2	1.69	0.74
21:Y:105:TRP:HE1	24:Y:309:CHL:HED2	1.52	0.74
2:6:130:PRO:HG2	2:6:133:PHE:HB2	1.70	0.74
1:7:220:ARG:HA	1:7:223:MET:CE	2.15	0.74
3:8:221:LEU:HD12	3:8:222:GLU:N	2.02	0.74
5:b:360:PRO:O	42:b:701:HOH:O	2.05	0.74
15:o:180:VAL:HA	15:o:186:VAL:HG12	1.68	0.74
21:y:117:GLU:OE2	21:y:239:GLY:HA3	1.88	0.74
2:2:239:LYS:HD2	2:2:242:LEU:HD12	1.68	0.74
4:A:230:ASN:OD1	22:R:100:ASN:HA	1.87	0.74
22:R:214:LYS:HG3	22:R:218:PRO:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:126:ASP:HA	2:6:148:LEU:HG	1.70	0.74
5:b:223:GLN:HA	10:h:33:VAL:HG11	1.67	0.74
25:b:604:CLA:HBD	25:b:604:CLA:HBA1	1.70	0.74
25:n:613:CLA:H141	25:n:614:CLA:HMD1	1.68	0.74
22:r:214:LYS:HG3	22:r:218:PRO:O	1.86	0.74
2:2:126:ASP:HA	2:2:148:LEU:HG	1.70	0.74
1:3:57:LYS:HZ1	1:3:66:PRO:HG3	1.51	0.74
25:A:405:CLA:CMC	11:I:11:VAL:HG11	2.17	0.74
21:N:117:GLU:OE2	21:N:239:GLY:HA3	1.87	0.74
21:N:227:PHE:HD2	25:N:602:CLA:H202	1.52	0.74
2:6:127:PHE:HB3	2:6:140:PHE:CE2	2.22	0.74
2:6:130:PRO:HD3	2:6:239:LYS:HE2	1.69	0.74
3:8:107:ARG:O	3:8:110:MET:HG3	1.87	0.74
5:b:214:LEU:HD11	25:r:608:CLA:H51	1.69	0.74
18:x:87:LEU:CD1	18:x:88:LEU:HD22	2.18	0.74
25:r:604:CLA:CHB	41:r:616:XAT:H42	2.17	0.74
1:1:57:LYS:NZ	1:1:66:PRO:HG3	2.02	0.74
18:X:87:LEU:CD1	18:X:88:LEU:HD22	2.18	0.74
25:G:610:CLA:H41	25:G:612:CLA:HMA2	1.68	0.74
25:R:610:CLA:HMB3	26:R:618:LHG:HC2	1.68	0.74
5:b:451:PHE:HE2	25:b:604:CLA:HMA3	1.50	0.74
24:n:609:CHL:H72	24:y:302:CHL:H111	1.69	0.74
24:y:308:CHL:HBC3	32:y:322:AJP:O82	1.86	0.74
22:r:72:LEU:HB3	22:r:137:ARG:NH1	2.01	0.74
1:3:117:GLU:OE2	1:3:239:GLY:HA3	1.88	0.74
5:B:282:GLN:CD	23:U:100:ILE:HD11	2.13	0.74
38:F:101:HEM:HBB2	38:F:101:HEM:HHC	1.70	0.74
25:N:613:CLA:H141	25:N:614:CLA:HMD1	1.68	0.74
4:a:328:MET:HG2	7:d:326:ILE:HG12	1.68	0.74
6:c:30:THR:HG23	6:c:31:THR:HG23	1.68	0.74
21:g:132:PHE:HB2	24:g:607:CHL:HMA3	1.68	0.74
21:n:227:PHE:HD2	25:n:602:CLA:H202	1.52	0.74
5:B:360:PRO:O	42:B:701:HOH:O	2.05	0.74
10:H:56:ILE:HA	18:X:84:LYS:HE2	1.68	0.74
24:N:609:CHL:H72	24:Y:302:CHL:H111	1.69	0.74
25:a:406:CLA:CMC	11:i:11:VAL:HG11	2.17	0.74
5:b:121:GLU:O	10:h:24:LYS:HE2	1.86	0.74
5:b:127:ARG:HG3	5:b:128:THR:HG23	1.69	0.74
1:1:117:GLU:OE2	1:1:239:GLY:HA3	1.88	0.74
2:2:246:LEU:O	2:2:249:LEU:HG	1.88	0.74
1:3:146:TYR:O	1:3:152:LEU:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:272:ARG:NH1	5:B:361:THR:HG21	2.01	0.74
10:H:56:ILE:HD13	18:X:84:LYS:CE	2.12	0.74
21:G:146:TYR:HB3	21:G:152:LEU:HD13	1.68	0.74
21:Y:146:TYR:O	21:Y:152:LEU:HD12	1.88	0.74
2:6:88:ASP:HB3	2:6:91:ALA:HB3	1.70	0.74
26:b:625:LHG:O4	7:d:142:TYR:OH	2.04	0.74
24:n:609:CHL:CAA	21:y:82:THR:HG21	2.13	0.74
5:B:214:LEU:HD11	25:R:608:CLA:H51	1.69	0.74
21:N:104:ARG:NH1	24:N:608:CHL:OBD	2.20	0.74
4:a:230:ASN:OD1	22:r:100:ASN:HA	1.87	0.74
24:S:307:CHL:HBC2	32:S:319:AJP:O82	1.87	0.74
2:6:246:LEU:O	2:6:249:LEU:HG	1.88	0.74
25:a:402:CLA:H52	25:a:403:CLA:HAB	1.70	0.74
21:n:159:LEU:HD11	21:y:257:TRP:CB	2.18	0.74
6:C:30:THR:HG23	6:C:31:THR:HG23	1.69	0.73
21:N:146:TYR:O	21:N:152:LEU:HD12	1.88	0.73
21:Y:59:LEU:HD23	24:Y:302:CHL:C2B	2.18	0.73
21:Y:97:GLU:CA	21:Y:190:LEU:HD11	2.14	0.73
25:c:504:CLA:C1C	35:c:516:DGD:HB51	2.18	0.73
21:y:59:LEU:HD23	24:y:302:CHL:C2B	2.18	0.73
21:Y:107:MET:HG2	21:Y:222:ALA:HB2	1.70	0.73
24:R:607:CHL:HBB2	40:R:617:NEX:H12	1.71	0.73
1:5:97:GLU:CA	1:5:190:LEU:HD11	2.14	0.73
2:6:155:HIS:NE2	2:6:161:ALA:HB2	2.03	0.73
5:b:341:LEU:HD12	5:b:429:ILE:HG22	1.68	0.73
25:N:603:CLA:HAB	39:N:616:LUT:C35	2.19	0.73
21:Y:146:TYR:HB3	21:Y:152:LEU:HD13	1.68	0.73
5:b:282:GLN:CD	23:u:100:ILE:HD11	2.13	0.73
1:1:107:MET:HG2	1:1:222:ALA:HB2	1.70	0.73
17:W:110:GLY:O	17:W:114:THR:HG23	1.89	0.73
21:G:103:SER:HB2	21:G:219:GLY:HA3	1.71	0.73
21:G:132:PHE:HB2	24:G:607:CHL:HMA3	1.68	0.73
21:N:159:LEU:HD11	21:Y:257:TRP:CB	2.18	0.73
23:U:88:TYR:HB2	23:U:100:ILE:HG21	1.68	0.73
1:5:70:LEU:HD13	1:5:79:GLY:HA2	1.71	0.73
7:d:56:VAL:HG21	7:d:111:LEU:HD12	1.69	0.73
20:s:192:ASN:OD1	20:s:195:ASP:HA	1.87	0.73
21:g:169:MET:HG3	24:g:609:CHL:HMC	1.69	0.73
1:3:57:LYS:NZ	1:3:66:PRO:HG3	2.02	0.73
5:B:14:ASN:ND2	22:R:97:LEU:O	2.18	0.73
25:B:604:CLA:HBD	25:B:604:CLA:HBA1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:56:VAL:HG21	7:D:111:LEU:HD12	1.69	0.73
21:G:107:MET:HG2	21:G:222:ALA:HB2	1.70	0.73
21:G:146:TYR:O	21:G:152:LEU:HD12	1.88	0.73
22:R:93:ASP:HB2	22:R:108:ASP:H	1.53	0.73
1:5:57:LYS:NZ	1:5:66:PRO:HG3	2.02	0.73
3:8:133:GLN:HG2	3:8:134:PRO:CD	2.16	0.73
25:d:401:CLA:HAB	25:d:402:CLA:H72	1.69	0.73
21:n:103:SER:HB2	21:n:219:GLY:HA3	1.71	0.73
21:y:107:MET:HG2	21:y:222:ALA:HB2	1.70	0.73
1:1:103:SER:HB2	1:1:219:GLY:HA3	1.71	0.73
3:4:219:GLU:HG3	3:4:222:GLU:HB2	1.69	0.73
10:H:62:ASN:OD1	10:H:63:SER:N	2.22	0.73
15:O:183:ASP:OD2	15:O:223:LYS:NZ	2.21	0.73
1:5:146:TYR:O	1:5:152:LEU:HD12	1.88	0.73
38:f:101:HEM:HBB2	38:f:101:HEM:HHC	1.70	0.73
21:g:70:LEU:HD13	21:g:79:GLY:HA2	1.71	0.73
21:g:117:GLU:OE2	21:g:239:GLY:HA3	1.88	0.73
21:n:146:TYR:HB3	21:n:152:LEU:HD13	1.69	0.73
21:n:146:TYR:O	21:n:152:LEU:HD12	1.88	0.73
21:y:146:TYR:O	21:y:152:LEU:HD12	1.88	0.73
2:2:160:LEU:HD23	2:2:163:LEU:HD12	1.68	0.73
25:R:612:CLA:H101	25:R:612:CLA:HAB	1.71	0.73
1:7:57:LYS:NZ	1:7:66:PRO:HG3	2.02	0.73
1:7:117:GLU:OE2	1:7:239:GLY:HA3	1.88	0.73
21:G:117:GLU:OE2	21:G:239:GLY:HA3	1.88	0.73
21:N:107:MET:HG2	21:N:222:ALA:HB2	1.70	0.73
21:Y:103:SER:HB2	21:Y:219:GLY:HA3	1.71	0.73
27:a:404:PHO:HBB1	27:a:404:PHO:HMB1	1.68	0.73
5:b:397:VAL:HG23	5:b:417:VAL:HG11	1.71	0.73
6:c:225:VAL:HG22	6:c:289:PHE:CE1	2.24	0.73
21:n:117:GLU:OE2	21:n:239:GLY:HA3	1.87	0.73
21:y:70:LEU:HD13	21:y:79:GLY:HA2	1.71	0.73
2:2:50:TRP:CD1	2:2:213:LYS:HD3	2.24	0.73
1:3:70:LEU:HD13	1:3:79:GLY:HA2	1.71	0.73
1:3:103:SER:HB2	1:3:219:GLY:HA3	1.71	0.73
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.71	0.73
25:C:504:CLA:C1C	35:C:516:DGD:HB51	2.18	0.73
1:5:103:SER:HB2	1:5:219:GLY:HA3	1.71	0.73
2:6:214:VAL:HA	2:6:217:ILE:HD11	1.69	0.73
3:8:142:PHE:CE1	3:8:146:LEU:HD11	2.24	0.73
3:8:221:LEU:HA	3:8:224:LEU:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:513:CLA:HBA1	25:c:513:CLA:HBD	1.71	0.73
17:w:110:GLY:O	17:w:114:THR:HG23	1.89	0.73
21:g:103:SER:HB2	21:g:219:GLY:HA3	1.71	0.73
24:g:606:CHL:HBA1	40:g:617:NEX:H403	1.71	0.73
24:r:607:CHL:HBB2	40:r:617:NEX:H12	1.71	0.73
2:2:220:GLY:HA3	25:2:602:CLA:HAC1	1.71	0.73
25:B:614:CLA:H8	28:B:617:BCR:H362	1.70	0.73
20:S:192:ASN:OD1	20:S:195:ASP:HA	1.87	0.73
21:G:215:GLU:HG3	25:G:610:CLA:C4B	2.19	0.73
21:N:103:SER:HB2	21:N:219:GLY:HA3	1.71	0.73
1:7:70:LEU:HD13	1:7:79:GLY:HA2	1.71	0.73
4:a:95:PRO:HG2	4:a:98:GLU:HG2	1.71	0.73
4:a:317:TRP:CZ3	7:d:181:ARG:HD3	2.24	0.73
5:b:172:TYR:CE2	5:b:283:GLU:HB2	2.24	0.73
15:o:310:ASP:OD1	15:o:311:THR:N	2.22	0.73
18:x:84:LYS:HA	18:x:87:LEU:HD23	1.71	0.73
21:g:84:GLY:CA	21:y:94:ARG:HG2	2.17	0.73
24:g:608:CHL:H12	24:g:608:CHL:H151	1.69	0.73
22:r:127:TYR:CD2	22:r:135:ARG:HD2	2.24	0.73
5:b:285:TYR:CE1	23:u:90:GLN:HG3	2.23	0.72
22:r:54:ASP:OD2	22:r:56:PRO:HD2	1.88	0.72
2:2:214:VAL:HA	2:2:217:ILE:HD11	1.69	0.72
5:B:285:TYR:CE1	23:U:90:GLN:HG3	2.23	0.72
21:G:197:ASP:OD1	25:G:610:CLA:HAA1	1.89	0.72
21:Y:70:LEU:HD13	21:Y:79:GLY:HA2	1.71	0.72
22:R:54:ASP:OD2	22:R:56:PRO:HD2	1.88	0.72
2:6:50:TRP:CD1	2:6:213:LYS:HD3	2.24	0.72
15:o:183:ASP:OD2	15:o:223:LYS:NZ	2.21	0.72
21:n:107:MET:HG2	21:n:222:ALA:HB2	1.70	0.72
22:r:93:ASP:HB2	22:r:108:ASP:H	1.53	0.72
1:1:146:TYR:O	1:1:152:LEU:HD12	1.88	0.72
5:B:172:TYR:CE2	5:B:283:GLU:HB2	2.24	0.72
5:B:382:PRO:HB3	7:D:345:GLU:OE2	1.90	0.72
18:X:84:LYS:HA	18:X:87:LEU:HD23	1.71	0.72
20:S:63:TYR:CE2	20:S:219:ALA:HB1	2.25	0.72
20:S:72:PRO:CG	20:S:75:LEU:HD13	2.19	0.72
2:6:213:LYS:O	2:6:217:ILE:HG12	1.89	0.72
1:7:103:SER:HB2	1:7:219:GLY:HA3	1.71	0.72
1:7:107:MET:HG2	1:7:222:ALA:HB2	1.70	0.72
21:g:107:MET:HG2	21:g:222:ALA:HB2	1.70	0.72
21:n:70:LEU:HD13	21:n:79:GLY:HA2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:104:ARG:NH1	24:n:608:CHL:OBD	2.20	0.72
6:C:57:ALA:O	6:C:61:VAL:HG23	1.89	0.72
21:N:70:LEU:HD13	21:N:79:GLY:HA2	1.71	0.72
2:6:130:PRO:HG2	2:6:133:PHE:CD2	2.25	0.72
25:b:614:CLA:H8	28:b:617:BCR:H362	1.70	0.72
21:g:146:TYR:O	21:g:152:LEU:HD12	1.88	0.72
3:4:221:LEU:HA	3:4:224:LEU:CD2	2.19	0.72
4:A:331:MET:CE	7:D:321:LEU:HB3	2.20	0.72
25:A:401:CLA:H52	25:A:402:CLA:HAB	1.70	0.72
5:B:128:THR:HG21	22:R:94:ILE:HD13	1.72	0.72
21:G:215:GLU:HG3	25:G:610:CLA:C1B	2.19	0.72
21:Y:117:GLU:OE2	21:Y:239:GLY:HA3	1.88	0.72
21:Y:169:MET:HG3	24:Y:310:CHL:CMC	2.19	0.72
1:5:107:MET:HG2	1:5:222:ALA:HB2	1.70	0.72
2:6:174:GLU:HB3	1:7:62:PHE:HB3	1.70	0.72
6:c:216:SER:OG	6:c:221:GLU:OE1	2.06	0.72
5:B:70:GLY:HA2	5:B:178:VAL:CG1	2.20	0.72
14:M:17:VAL:HB	14:M:18:PRO:HD3	1.72	0.72
21:N:127:GLY:O	21:N:128:GLU:HG2	1.90	0.72
1:5:117:GLU:OE2	1:5:239:GLY:HA3	1.88	0.72
25:c:508:CLA:H141	25:c:510:CLA:H18	1.72	0.72
4:A:283:ILE:HG13	27:A:403:PHO:HBC3	1.72	0.72
3:8:73:LEU:HG	3:8:82:GLY:CA	2.20	0.72
23:u:85:LYS:HG2	23:u:101:CYS:CB	2.19	0.72
2:2:88:ASP:HB3	2:2:91:ALA:HB3	1.70	0.72
4:A:317:TRP:CZ3	7:D:181:ARG:HD3	2.24	0.72
5:B:397:VAL:HG23	5:B:417:VAL:HG11	1.71	0.72
1:7:127:GLY:O	1:7:128:GLU:HG2	1.90	0.72
5:b:14:ASN:ND2	22:r:97:LEU:O	2.18	0.72
10:h:62:ASN:OD1	10:h:63:SER:N	2.22	0.72
21:g:215:GLU:HG3	25:g:610:CLA:C1B	2.19	0.72
2:2:174:GLU:HB3	1:3:62:PHE:HB3	1.70	0.72
1:3:107:MET:HG2	1:3:222:ALA:HB2	1.70	0.72
25:C:504:CLA:H42	35:C:516:DGD:HB32	1.72	0.72
24:G:606:CHL:HBA1	40:G:617:NEX:H403	1.71	0.72
21:Y:215:GLU:HG3	25:Y:311:CLA:NB	2.04	0.72
21:g:82:THR:CG2	24:y:310:CHL:HED3	2.20	0.72
21:y:169:MET:HG3	24:y:310:CHL:CMC	2.19	0.72
25:D:401:CLA:HAB	25:D:402:CLA:H72	1.69	0.72
4:a:283:ILE:HG13	27:a:404:PHO:HBC3	1.72	0.72
15:o:306:LEU:HD21	15:o:322:LYS:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:103:SER:HB2	21:y:219:GLY:HA3	1.71	0.72
21:y:127:GLY:O	21:y:128:GLU:HG2	1.90	0.72
2:2:130:PRO:HG2	2:2:133:PHE:CD2	2.25	0.71
5:B:141:ILE:CG2	25:B:615:CLA:HBB1	2.19	0.71
6:C:293:ASN:OD1	35:C:515:DGD:HE61	1.90	0.71
11:I:23:PHE:HB3	28:I:101:BCR:HC32	1.72	0.71
20:S:63:TYR:OH	20:S:90:ALA:HB2	1.90	0.71
4:a:329:GLU:HA	4:a:332:HIS:NE2	2.05	0.71
6:c:130:ILE:HG22	19:z:27:PHE:HD2	1.55	0.71
25:C:513:CLA:HBA1	25:C:513:CLA:HBD	1.71	0.71
21:G:231:VAL:HG11	25:G:613:CLA:HHD	1.73	0.71
4:a:308:ASP:OD1	8:e:55:TYR:HB2	1.90	0.71
4:A:329:GLU:HA	4:A:332:HIS:NE2	2.05	0.71
6:C:225:VAL:HG22	6:C:289:PHE:CE1	2.24	0.71
15:O:310:ASP:OD1	15:O:311:THR:N	2.22	0.71
2:6:104:ARG:NE	24:6:603:CHL:HBD	2.05	0.71
2:6:218:LYS:O	2:6:221:ARG:HG2	1.91	0.71
2:6:220:GLY:HA3	25:6:602:CLA:HAC1	1.71	0.71
1:7:146:TYR:O	1:7:152:LEU:HD12	1.88	0.71
20:s:63:TYR:OH	20:s:90:ALA:HB2	1.90	0.71
2:2:218:LYS:O	2:2:221:ARG:HG2	1.91	0.71
21:G:70:LEU:HD13	21:G:79:GLY:HA2	1.71	0.71
14:m:17:VAL:HB	14:m:18:PRO:HD3	1.72	0.71
21:y:215:GLU:HG3	25:y:311:CLA:NB	2.04	0.71
1:1:70:LEU:HD13	1:1:79:GLY:HA2	1.71	0.71
2:2:120:GLN:HA	2:2:124:ARG:O	1.90	0.71
2:2:155:HIS:NE2	2:2:161:ALA:HB2	2.03	0.71
3:4:142:PHE:CE1	3:4:146:LEU:HD11	2.24	0.71
4:A:229:GLU:O	4:A:232:SER:HB2	1.90	0.71
2:6:113:CYS:SG	2:6:131:VAL:HG21	2.30	0.71
25:c:504:CLA:H42	35:c:516:DGD:HB32	1.72	0.71
20:s:246:THR:CG2	20:s:248:GLU:HG2	2.21	0.71
25:n:613:CLA:H8	25:n:613:CLA:C14	2.21	0.71
15:O:306:LEU:HD21	15:O:322:LYS:HE2	1.70	0.71
22:R:127:TYR:CD2	22:R:135:ARG:HD2	2.24	0.71
3:8:219:GLU:HG3	3:8:222:GLU:HB2	1.69	0.71
5:b:460:LEU:HD11	7:d:288:VAL:CG2	2.21	0.71
6:c:131:TYR:OH	20:s:74:GLY:HA3	1.90	0.71
6:c:293:ASN:OD1	35:c:515:DGD:HE61	1.90	0.71
20:s:63:TYR:CE2	20:s:219:ALA:HB1	2.25	0.71
22:r:246:ALA:O	22:r:250:MET:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:127:GLY:O	1:1:128:GLU:HG2	1.90	0.71
20:S:141:CYS:SG	20:S:162:TYR:HA	2.31	0.71
25:N:610:CLA:HMC1	39:N:615:LUT:C31	2.21	0.71
1:5:128:GLU:HB2	1:5:137:GLN:HB2	1.73	0.71
11:i:23:PHE:HB3	28:i:101:BCR:HC32	1.72	0.71
25:n:603:CLA:HAB	39:n:616:LUT:C35	2.19	0.71
22:r:124:PHE:HD1	25:r:614:CLA:CHC	2.03	0.71
2:2:104:ARG:NE	24:2:603:CHL:HBD	2.04	0.71
1:3:127:GLY:O	1:3:128:GLU:HG2	1.90	0.71
3:4:94:PHE:HB3	3:4:98:TYR:HE2	1.56	0.71
25:A:405:CLA:HHD	28:A:406:BCR:H362	1.72	0.71
6:C:131:TYR:OH	20:S:74:GLY:HA3	1.90	0.71
1:7:138:ILE:HB	1:7:144:LEU:HD12	1.73	0.71
4:a:331:MET:CE	7:d:321:LEU:HB3	2.20	0.71
5:b:382:PRO:HB3	7:d:345:GLU:OE2	1.90	0.71
6:c:57:ALA:O	6:c:61:VAL:HG23	1.89	0.71
21:g:215:GLU:HG3	25:g:610:CLA:C4B	2.19	0.71
21:n:128:GLU:HB2	21:n:137:GLN:HB2	1.73	0.71
2:2:213:LYS:O	2:2:217:ILE:HG12	1.89	0.71
21:N:107:MET:HE1	25:N:610:CLA:HHC	1.73	0.71
25:N:613:CLA:H8	25:N:613:CLA:C14	2.21	0.71
5:b:70:GLY:HA2	5:b:178:VAL:CG1	2.20	0.71
7:d:57:THR:HG21	8:e:50:PRO:HD3	1.73	0.71
20:s:141:CYS:SG	20:s:162:TYR:HA	2.31	0.71
21:g:127:GLY:O	21:g:128:GLU:HG2	1.90	0.71
21:g:128:GLU:HB2	21:g:137:GLN:HB2	1.73	0.71
21:g:197:ASP:OD1	25:g:610:CLA:HAA1	1.89	0.71
25:r:612:CLA:H101	25:r:612:CLA:HAB	1.71	0.71
1:3:138:ILE:HB	1:3:144:LEU:HD12	1.73	0.71
3:4:168:ASP:HA	3:4:185:PHE:CZ	2.26	0.71
4:A:335:ASN:HA	7:D:351:ASN:ND2	2.05	0.71
2:6:97:ALA:CB	2:6:190:LEU:HD11	2.21	0.71
4:a:229:GLU:O	4:a:232:SER:HB2	1.90	0.71
25:a:406:CLA:HHD	28:a:407:BCR:H362	1.73	0.71
21:g:231:VAL:HG11	25:g:613:CLA:HHD	1.72	0.71
21:y:138:ILE:HB	21:y:144:LEU:HD12	1.73	0.71
21:N:231:VAL:HG11	25:N:613:CLA:HAC1	1.73	0.70
40:Y:318:NEX:H28	40:Y:318:NEX:C36	2.21	0.70
5:b:128:THR:HG21	22:r:94:ILE:HD13	1.72	0.70
5:b:272:ARG:HB2	5:b:319:PRO:HG2	1.73	0.70
19:z:14:ILE:O	19:z:18:ILE:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:73:GLU:HG2	21:g:73:GLU:O	1.91	0.70
21:n:107:MET:HE1	25:n:610:CLA:HHC	1.73	0.70
21:n:127:GLY:O	21:n:128:GLU:HG2	1.90	0.70
1:3:128:GLU:HB2	1:3:137:GLN:HB2	1.73	0.70
21:N:165:GLN:HE22	24:N:606:CHL:C1B	2.04	0.70
1:5:73:GLU:O	1:5:73:GLU:HG2	1.91	0.70
4:a:333:GLU:O	7:d:350:GLY:HA3	1.91	0.70
5:b:141:ILE:CG2	25:b:615:CLA:HBB1	2.20	0.70
25:g:610:CLA:HBB1	39:g:615:LUT:H32	1.73	0.70
40:y:318:NEX:H28	40:y:318:NEX:C36	2.21	0.70
2:2:217:ILE:HD12	25:2:604:CLA:CAD	2.21	0.70
5:B:460:LEU:HD11	7:D:288:VAL:CG2	2.21	0.70
15:O:163:LEU:O	15:O:164:MET:HE2	1.91	0.70
20:S:246:THR:CG2	20:S:248:GLU:HG2	2.21	0.70
21:N:138:ILE:HB	21:N:144:LEU:HD12	1.73	0.70
2:6:120:GLN:HA	2:6:124:ARG:O	1.90	0.70
3:8:113:VAL:HG13	3:8:114:LEU:HD12	1.72	0.70
4:a:74:GLY:HA3	7:d:305:ARG:HH12	1.54	0.70
4:a:183:MET:HB3	25:a:402:CLA:HBC2	1.73	0.70
3:4:219:GLU:OE1	3:4:219:GLU:N	2.25	0.70
4:A:183:MET:HB3	25:A:401:CLA:HBC2	1.73	0.70
21:G:82:THR:CG2	24:Y:310:CHL:HED3	2.20	0.70
21:N:128:GLU:HB2	21:N:137:GLN:HB2	1.73	0.70
3:8:219:GLU:OE1	3:8:219:GLU:N	2.24	0.70
6:c:163:ILE:HG21	25:c:512:CLA:CAB	2.21	0.70
26:d:406:LHG:HC62	13:l:16:THR:HG23	1.73	0.70
20:s:202:PRO:HG3	24:s:308:CHL:HBC2	1.74	0.70
25:n:610:CLA:HMC1	39:n:615:LUT:C31	2.21	0.70
2:2:97:ALA:CB	2:2:190:LEU:HD11	2.21	0.70
4:A:333:GLU:O	7:D:350:GLY:HA3	1.91	0.70
25:C:508:CLA:H141	25:C:510:CLA:H18	1.72	0.70
25:C:510:CLA:ND	25:C:510:CLA:H172	2.07	0.70
21:G:138:ILE:HB	21:G:144:LEU:HD12	1.73	0.70
21:N:215:GLU:HG3	25:N:610:CLA:C4B	2.22	0.70
22:R:246:ALA:O	22:R:250:MET:HG3	1.91	0.70
1:5:127:GLY:O	1:5:128:GLU:HG2	1.90	0.70
3:8:168:ASP:HA	3:8:185:PHE:CZ	2.26	0.70
6:c:151:TRP:CB	17:w:133:LEU:HD21	2.21	0.70
28:k:101:BCR:C33	19:z:12:LEU:HD23	2.22	0.70
16:t:14:LEU:HD12	28:t:101:BCR:H343	1.73	0.70
2:2:113:CYS:SG	2:2:131:VAL:HG21	2.30	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:241:SER:OG	25:B:612:CLA:OBD	2.06	0.70
6:C:369:LEU:HD22	6:C:380:LEU:HD23	1.74	0.70
16:T:1:MET:HG2	16:T:3:ALA:H	1.57	0.70
16:T:14:LEU:HD12	28:T:101:BCR:H343	1.73	0.70
22:R:184:LEU:HD23	24:y:306:CHL:HAA2	1.74	0.70
25:6:604:CLA:HAA1	25:6:604:CLA:HBD	1.74	0.70
3:8:94:PHE:HB3	3:8:98:TYR:HE2	1.56	0.70
4:a:335:ASN:HA	7:d:351:ASN:ND2	2.05	0.70
7:d:194:LEU:HD23	7:d:296:ALA:O	1.92	0.70
25:g:610:CLA:H2	39:g:615:LUT:H28	1.73	0.70
21:n:165:GLN:HE22	24:n:606:CHL:C1B	2.04	0.70
21:n:215:GLU:HG3	25:n:610:CLA:C4B	2.22	0.70
3:4:113:VAL:HG13	3:4:114:LEU:HD12	1.72	0.70
3:4:122:TRP:O	3:4:126:ALA:N	2.25	0.70
6:C:130:ILE:HG22	19:Z:27:PHE:HD2	1.55	0.70
7:D:15:LEU:HD11	18:X:103:VAL:CG1	2.21	0.70
22:R:124:PHE:HD1	25:R:614:CLA:CHC	2.03	0.70
3:8:225:LYS:HA	3:8:228:GLU:CD	2.17	0.70
15:o:163:LEU:O	15:o:164:MET:HE2	1.91	0.70
25:2:604:CLA:HBD	25:2:604:CLA:HAA1	1.74	0.70
3:4:225:LYS:HA	3:4:228:GLU:CD	2.17	0.70
25:B:615:CLA:H91	25:B:615:CLA:H172	1.73	0.70
21:G:127:GLY:O	21:G:128:GLU:HG2	1.90	0.70
21:N:73:GLU:O	21:N:73:GLU:HG2	1.91	0.70
21:Y:127:GLY:O	21:Y:128:GLU:HG2	1.90	0.70
22:R:93:ASP:HB2	22:R:108:ASP:N	2.06	0.70
4:a:235:GLU:OE1	7:d:266:ARG:HB2	1.92	0.70
5:b:332:ASN:ND2	30:b:620:LMG:O4	2.25	0.70
2:2:104:ARG:CZ	24:2:603:CHL:HBD	2.22	0.70
4:A:308:ASP:OD1	8:E:55:TYR:HB2	1.90	0.70
7:D:57:THR:HG21	8:E:50:PRO:HD3	1.73	0.70
21:G:98:LEU:CD2	25:G:603:CLA:HAA1	2.21	0.70
25:G:610:CLA:HBB1	39:G:615:LUT:H32	1.73	0.70
25:b:604:CLA:H142	25:b:615:CLA:CMA	2.21	0.70
21:y:202:ALA:HB1	21:y:208:PHE:HD1	1.57	0.70
4:A:232:SER:HB3	5:B:4:PRO:HD3	1.74	0.70
5:B:442:VAL:HG23	5:B:444:ARG:HH12	1.57	0.70
6:C:163:ILE:HG21	25:C:512:CLA:CAB	2.21	0.70
6:C:327:ASN:HD21	15:O:192:ASP:HB2	1.57	0.70
19:Z:14:ILE:O	19:Z:18:ILE:HD12	1.91	0.70
21:N:202:ALA:HB1	21:N:208:PHE:HD1	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:129:GLU:OE1	22:R:132:GLY:N	2.25	0.70
4:a:75:ASN:HB2	4:a:79:SER:OG	1.92	0.70
20:s:119:ARG:HD3	25:s:310:CLA:HHD	1.74	0.70
21:g:98:LEU:CD2	25:g:603:CLA:HAA1	2.21	0.70
21:y:73:GLU:O	21:y:73:GLU:HG2	1.91	0.70
4:A:74:GLY:HA3	7:D:305:ARG:HH12	1.54	0.69
5:B:272:ARG:HB2	5:B:319:PRO:HG2	1.73	0.69
6:C:255:LYS:NZ	17:W:127:GLU:OE2	2.22	0.69
7:D:78:ALA:HB2	7:D:175:GLY:HA3	1.74	0.69
29:L:101:SQD:H251	29:L:101:SQD:H111	1.74	0.69
14:M:28:LYS:HB2	14:m:27:VAL:CG1	2.22	0.69
2:6:104:ARG:CZ	24:6:603:CHL:HBD	2.22	0.69
1:7:128:GLU:HB2	1:7:137:GLN:HB2	1.73	0.69
4:a:232:SER:HB3	5:b:4:PRO:HD3	1.74	0.69
5:b:121:GLU:OE2	10:h:16:SER:OG	2.08	0.69
29:l:102:SQD:H251	29:l:102:SQD:H111	1.74	0.69
5:B:332:ASN:ND2	30:B:620:LMG:O4	2.25	0.69
21:G:215:GLU:HB2	25:G:610:CLA:C1B	2.22	0.69
21:N:215:GLU:HG3	25:N:610:CLA:NB	2.06	0.69
25:c:510:CLA:ND	25:c:510:CLA:H172	2.07	0.69
20:s:72:PRO:CG	20:s:75:LEU:HD13	2.19	0.69
20:s:109:LYS:O	20:s:113:PHE:HD2	1.75	0.69
21:g:138:ILE:HB	21:g:144:LEU:HD12	1.73	0.69
21:n:215:GLU:HG3	25:n:610:CLA:NB	2.06	0.69
1:3:138:ILE:CG1	1:3:144:LEU:HB2	2.23	0.69
7:D:298:ASP:HA	7:D:316:TYR:OH	1.92	0.69
28:K:101:BCR:C33	19:Z:12:LEU:HD23	2.22	0.69
25:G:610:CLA:H2	39:G:615:LUT:H28	1.73	0.69
21:Y:73:GLU:O	21:Y:73:GLU:HG2	1.91	0.69
7:d:78:ALA:HB2	7:d:175:GLY:HA3	1.74	0.69
21:y:128:GLU:HB2	21:y:137:GLN:HB2	1.73	0.69
21:y:131:TRP:HB2	39:y:317:LUT:H21	1.75	0.69
22:r:93:ASP:HB2	22:r:108:ASP:N	2.06	0.69
25:B:603:CLA:HAB	25:B:605:CLA:H152	1.74	0.69
20:S:109:LYS:O	20:S:113:PHE:HD2	1.75	0.69
2:6:178:ILE:HD12	1:7:62:PHE:HD1	1.58	0.69
4:a:133:LEU:HD23	7:d:257:ILE:HG12	1.74	0.69
7:d:298:ASP:HA	7:d:316:TYR:OH	1.92	0.69
15:o:230:LYS:HD3	15:o:284:GLU:OE1	1.93	0.69
21:n:202:ALA:HB1	21:n:208:PHE:HD1	1.57	0.69
1:1:138:ILE:HB	1:1:144:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:235:GLU:OE1	7:D:266:ARG:HB2	1.92	0.69
21:G:82:THR:HG21	24:Y:310:CHL:HAA1	1.74	0.69
24:Y:306:CHL:HAA2	22:r:184:LEU:HD23	1.74	0.69
25:b:613:CLA:HED2	25:b:613:CLA:H2	1.74	0.69
21:g:82:THR:HG21	24:y:310:CHL:HAA1	1.74	0.69
26:D:406:LHG:HC62	13:L:16:THR:HG23	1.73	0.69
21:N:138:ILE:CG1	21:N:144:LEU:HB2	2.22	0.69
21:Y:131:TRP:HB2	39:Y:317:LUT:H21	1.74	0.69
21:Y:138:ILE:HB	21:Y:144:LEU:HD12	1.73	0.69
1:5:202:ALA:HB1	1:5:208:PHE:HD1	1.57	0.69
2:6:210:ALA:HA	2:6:213:LYS:NZ	2.07	0.69
21:g:215:GLU:HB2	25:g:610:CLA:C1B	2.22	0.69
21:n:231:VAL:HG11	25:n:613:CLA:HAC1	1.73	0.69
1:1:128:GLU:HB2	1:1:137:GLN:HB2	1.73	0.69
2:2:104:ARG:NE	24:2:603:CHL:CBD	2.55	0.69
6:C:154:ARG:HG2	6:C:266:TRP:CE3	2.28	0.69
7:D:194:LEU:HD23	7:D:296:ALA:O	1.92	0.69
20:s:144:GLU:HB3	20:s:153:LEU:HD21	1.73	0.69
2:2:178:ILE:HD12	1:3:62:PHE:HD1	1.57	0.69
2:2:210:ALA:HA	2:2:213:LYS:NZ	2.07	0.69
3:4:155:TRP:CD1	3:4:159:LYS:HZ1	2.10	0.69
3:4:219:GLU:O	3:4:219:GLU:HG2	1.93	0.69
4:A:46:SER:O	4:A:50:ILE:HG12	1.93	0.69
26:L:102:LHG:H102	26:L:102:LHG:HC61	1.74	0.69
14:M:27:VAL:CG1	14:m:28:LYS:HB2	2.22	0.69
15:O:309:SER:OG	15:O:319:LYS:N	2.20	0.69
25:N:603:CLA:H191	24:N:607:CHL:C11	2.22	0.69
21:Y:128:GLU:HB2	21:Y:137:GLN:HB2	1.73	0.69
22:R:156:SER:HB3	25:R:604:CLA:HHD	1.75	0.69
1:5:138:ILE:HB	1:5:144:LEU:HD12	1.73	0.69
1:7:138:ILE:CG1	1:7:144:LEU:HB2	2.23	0.69
1:7:202:ALA:HB1	1:7:208:PHE:HD1	1.57	0.69
25:a:403:CLA:HBB	27:a:404:PHO:H203	1.74	0.69
25:b:606:CLA:CHC	26:b:622:LHG:H272	2.23	0.69
6:c:154:ARG:HG2	6:c:266:TRP:CE3	2.28	0.69
7:d:56:VAL:HG21	7:d:111:LEU:HD11	1.75	0.69
16:t:1:MET:HG2	16:t:3:ALA:H	1.57	0.69
17:w:116:PHE:O	17:w:120:THR:HG23	1.93	0.69
21:n:138:ILE:CG1	21:n:144:LEU:HB2	2.22	0.69
25:n:602:CLA:HMC3	25:n:602:CLA:HBC2	1.75	0.69
25:n:603:CLA:H191	24:n:607:CHL:C11	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:156:SER:HB3	25:r:604:CLA:HHD	1.75	0.69
2:2:150:ASN:O	2:2:154:VAL:HG21	1.92	0.69
3:4:157:GLU:O	3:4:161:TRP:HD1	1.76	0.69
3:4:176:THR:OG1	3:4:180:LYS:HA	1.93	0.69
3:4:219:GLU:HB2	3:4:222:GLU:HB2	1.75	0.69
7:D:162:PRO:HB3	7:D:171:ALA:HB2	1.75	0.69
21:Y:104:ARG:NH1	24:Y:309:CHL:OBD	2.20	0.69
6:c:369:LEU:HD22	6:c:380:LEU:HD23	1.74	0.69
21:g:202:ALA:HB1	21:g:208:PHE:HD1	1.57	0.69
4:A:75:ASN:HB2	4:A:79:SER:OG	1.92	0.69
17:W:116:PHE:O	17:W:120:THR:HG23	1.93	0.69
1:5:178:ALA:HA	2:6:64:VAL:CG2	2.07	0.69
2:6:150:ASN:O	2:6:154:VAL:HG21	1.93	0.69
3:8:176:THR:OG1	3:8:180:LYS:HA	1.93	0.69
3:8:224:LEU:O	3:8:228:GLU:OE1	2.10	0.69
21:g:87:ALA:HB1	21:y:90:GLU:CB	2.23	0.69
21:g:211:LEU:HB3	25:g:610:CLA:HMA1	1.74	0.69
21:n:138:ILE:CG2	24:n:606:CHL:HBC1	2.14	0.69
1:1:73:GLU:HG2	1:1:73:GLU:O	1.91	0.68
1:3:202:ALA:HB1	1:3:208:PHE:HD1	1.57	0.68
4:A:133:LEU:HD23	7:D:257:ILE:HG12	1.74	0.68
6:C:281:VAL:O	6:C:285:ILE:HG13	1.94	0.68
20:S:202:PRO:HG3	24:S:308:CHL:HBC2	1.74	0.68
21:G:128:GLU:HB2	21:G:137:GLN:HB2	1.73	0.68
22:R:202:ILE:HD12	24:R:607:CHL:HMA3	1.75	0.68
2:6:217:ILE:HD12	25:6:604:CLA:CAD	2.21	0.68
12:k:32:PHE:HZ	19:z:9:VAL:HG11	1.58	0.68
3:4:224:LEU:O	3:4:228:GLU:OE1	2.10	0.68
4:A:176:ILE:HD13	25:A:402:CLA:HED3	1.75	0.68
25:B:606:CLA:CHC	26:B:622:LHG:H272	2.23	0.68
25:B:613:CLA:HED2	25:B:613:CLA:H2	1.74	0.68
21:G:87:ALA:HB1	21:Y:90:GLU:CB	2.23	0.68
21:Y:244:LEU:HD22	39:Y:316:LUT:H163	1.75	0.68
2:6:174:GLU:OE1	1:7:62:PHE:HD2	1.76	0.68
3:8:219:GLU:HB2	3:8:222:GLU:HB2	1.75	0.68
6:c:26:ARG:NH2	6:c:41:ARG:O	2.26	0.68
6:c:281:VAL:O	6:c:285:ILE:HG13	1.94	0.68
6:C:26:ARG:NH2	6:C:41:ARG:O	2.26	0.68
20:S:236:MET:HE2	39:S:316:LUT:C12	2.23	0.68
21:G:138:ILE:CG1	21:G:144:LEU:HB2	2.23	0.68
21:G:211:LEU:HB3	25:G:610:CLA:HMA1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:609:CHL:HAA2	21:Y:82:THR:CG2	2.17	0.68
21:Y:256:ALA:HB2	25:Y:314:CLA:CAD	2.23	0.68
23:U:85:LYS:HG2	23:U:101:CYS:CB	2.19	0.68
3:8:122:TRP:O	3:8:126:ALA:N	2.25	0.68
20:s:225:GLU:HB2	25:s:310:CLA:CHB	2.22	0.68
21:n:73:GLU:O	21:n:73:GLU:HG2	1.91	0.68
22:r:198:VAL:O	22:r:202:ILE:HG23	1.94	0.68
2:2:131:VAL:O	2:2:134:LYS:HB2	1.94	0.68
2:2:251:ASN:HB3	25:2:605:CLA:HBB	1.75	0.68
21:G:73:GLU:HG2	21:G:73:GLU:O	1.91	0.68
21:N:234:ILE:HG21	32:N:620:AJP:C81	2.23	0.68
3:8:183:GLU:HB3	3:8:185:PHE:CD1	2.28	0.68
7:d:162:PRO:HB3	7:d:171:ALA:HB2	1.75	0.68
21:Y:56:VAL:HB	24:Y:302:CHL:HBC1	1.76	0.68
3:8:157:GLU:O	3:8:161:TRP:HD1	1.76	0.68
5:b:162:TYR:O	25:b:606:CLA:HHD	1.93	0.68
6:c:346:THR:OG1	6:c:348:GLU:OE1	2.09	0.68
25:c:504:CLA:CHC	35:c:516:DGD:HB51	2.24	0.68
26:l:103:LHG:H102	26:l:103:LHG:HC61	1.74	0.68
21:g:59:LEU:HD23	24:g:601:CHL:C2B	2.24	0.68
21:y:104:ARG:NH1	24:y:309:CHL:OBD	2.20	0.68
21:y:127:GLY:HA3	21:y:137:GLN:HG3	1.76	0.68
3:4:73:LEU:HG	3:4:82:GLY:CA	2.20	0.68
3:4:183:GLU:HB3	3:4:185:PHE:CD1	2.28	0.68
29:L:101:SQD:H122	14:m:23:LEU:HD13	1.74	0.68
20:S:59:LEU:CD1	20:S:216:GLU:HG3	2.24	0.68
20:S:262:PHE:HE2	25:S:314:CLA:H3A	1.59	0.68
21:Y:231:VAL:HG11	25:Y:314:CLA:HAC2	1.73	0.68
2:6:251:ASN:HB3	25:6:605:CLA:HBB	1.75	0.68
1:7:73:GLU:HG2	1:7:73:GLU:O	1.91	0.68
4:a:176:ILE:HD13	25:a:403:CLA:HED3	1.75	0.68
5:b:442:VAL:HG23	5:b:444:ARG:HH12	1.57	0.68
20:s:113:PHE:O	20:s:117:HIS:ND1	2.26	0.68
21:y:138:ILE:CG1	21:y:144:LEU:HB2	2.23	0.68
1:1:138:ILE:CG1	1:1:144:LEU:HB2	2.23	0.68
1:1:202:ALA:HB1	1:1:208:PHE:HD1	1.57	0.68
21:G:60:GLY:HA3	24:G:601:CHL:CMC	2.23	0.68
25:N:602:CLA:HMC3	25:N:602:CLA:HBC2	1.75	0.68
22:R:153:GLY:HA2	25:R:604:CLA:C4C	2.24	0.68
25:R:603:CLA:C1D	25:R:608:CLA:H92	1.95	0.68
24:6:601:CHL:H12	26:6:606:LHG:H181	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:46:SER:O	4:a:50:ILE:HG12	1.93	0.68
25:b:615:CLA:H91	25:b:615:CLA:H172	1.73	0.68
26:s:301:LHG:H272	25:s:311:CLA:HBB2	1.76	0.68
21:n:138:ILE:HB	21:n:144:LEU:HD12	1.73	0.68
21:y:231:VAL:HG11	25:y:314:CLA:HAC2	1.73	0.68
25:r:601:CLA:C4C	26:r:618:LHG:HC92	2.24	0.68
1:3:127:GLY:HA3	1:3:137:GLN:HG3	1.76	0.68
5:B:162:TYR:O	25:B:606:CLA:HHD	1.93	0.68
25:B:615:CLA:H51	25:B:616:CLA:H203	1.75	0.68
21:G:231:VAL:HG21	25:G:613:CLA:CAC	2.24	0.68
21:N:127:GLY:HA3	21:N:137:GLN:HG3	1.76	0.68
21:Y:151:SER:HB2	22:r:185:PRO:HD3	1.76	0.68
22:R:198:VAL:O	22:R:202:ILE:HG23	1.94	0.68
5:b:91:TRP:HE1	26:b:622:LHG:HC61	1.58	0.68
21:y:56:VAL:HB	24:y:302:CHL:HBC1	1.76	0.68
21:y:59:LEU:HD23	24:y:302:CHL:C1B	2.24	0.68
21:y:256:ALA:HB2	25:y:314:CLA:CAD	2.24	0.68
2:2:174:GLU:OE1	1:3:62:PHE:HD2	1.76	0.68
21:G:59:LEU:HD23	24:G:601:CHL:C2B	2.24	0.68
5:b:462:PHE:CZ	25:b:613:CLA:HMB3	2.29	0.68
25:b:603:CLA:HAB	25:b:605:CLA:H152	1.74	0.68
25:y:313:CLA:HBB1	39:y:316:LUT:C14	2.24	0.68
22:r:224:ASP:OD1	39:r:615:LUT:O23	2.12	0.68
1:3:73:GLU:O	1:3:73:GLU:HG2	1.91	0.68
15:O:230:LYS:HD3	15:O:284:GLU:OE1	1.93	0.68
20:S:144:GLU:HB3	20:S:153:LEU:HD21	1.73	0.68
20:S:225:GLU:HB2	25:S:310:CLA:CHB	2.22	0.68
26:S:301:LHG:H272	25:S:311:CLA:HBB2	1.76	0.68
2:6:128:LYS:HD3	2:6:133:PHE:HB3	1.76	0.68
2:6:131:VAL:O	2:6:134:LYS:HB2	1.94	0.68
2:6:168:ILE:O	2:6:172:LEU:HG	1.94	0.68
21:g:60:GLY:HA3	24:g:601:CHL:CMC	2.24	0.68
21:n:234:ILE:HG21	32:n:620:AJP:C81	2.23	0.68
21:y:176:ARG:NH2	24:y:310:CHL:O1D	2.27	0.68
2:2:168:ILE:O	2:2:172:LEU:HG	1.94	0.67
1:3:115:PHE:CZ	1:3:119:LEU:HD21	2.29	0.67
6:C:216:SER:OG	6:C:221:GLU:OE1	2.06	0.67
25:C:504:CLA:CHC	35:C:516:DGD:HB51	2.24	0.67
21:G:85:LEU:HD13	25:G:602:CLA:H42	1.75	0.67
21:G:202:ALA:HB1	21:G:208:PHE:HD1	1.57	0.67
21:Y:202:ALA:HB1	21:Y:208:PHE:HD1	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:309:CHL:H11	39:Y:316:LUT:H383	1.75	0.67
25:Y:313:CLA:HBB1	39:Y:316:LUT:C14	2.24	0.67
22:R:173:LEU:HD13	22:R:188:ILE:HG13	1.76	0.67
1:7:115:PHE:CZ	1:7:119:LEU:HD21	2.29	0.67
3:8:229:ILE:O	3:8:233:ARG:HD3	1.94	0.67
7:d:15:LEU:HD11	18:x:103:VAL:CG1	2.21	0.67
3:4:229:ILE:O	3:4:233:ARG:HD3	1.94	0.67
6:C:224:ILE:O	6:C:227:VAL:HG23	1.95	0.67
25:C:513:CLA:HMD1	20:S:75:LEU:HD11	1.77	0.67
14:M:23:LEU:HD13	29:l:102:SQD:H122	1.74	0.67
6:c:327:ASN:HD21	15:o:192:ASP:HB2	1.57	0.67
21:g:85:LEU:HD13	25:g:602:CLA:H42	1.75	0.67
22:r:202:ILE:HD12	24:r:607:CHL:HMA3	1.75	0.67
22:r:211:ASP:OD1	22:r:213:GLU:HG2	1.94	0.67
6:C:373:ASN:OD1	15:O:111:ALA:HA	1.95	0.67
20:S:119:ARG:HD3	25:S:310:CLA:HHD	1.74	0.67
21:N:138:ILE:CG2	24:N:606:CHL:HBC1	2.14	0.67
2:6:70:LEU:CD1	2:6:79:GLY:HA2	2.23	0.67
3:8:73:LEU:CG	3:8:82:GLY:HA2	2.22	0.67
6:c:224:ILE:O	6:c:227:VAL:HG23	1.95	0.67
6:c:255:LYS:NZ	17:w:127:GLU:OE2	2.22	0.67
6:c:335:THR:HG23	6:c:337:LEU:H	1.58	0.67
7:d:94:TRP:HE1	18:x:87:LEU:HD22	1.59	0.67
21:y:115:PHE:CZ	21:y:119:LEU:HD21	2.29	0.67
2:2:70:LEU:CD1	2:2:79:GLY:HA2	2.23	0.67
3:4:177:PRO:HG3	25:R:610:CLA:CBB	2.25	0.67
5:B:159:THR:HA	5:B:181:VAL:O	1.94	0.67
21:G:138:ILE:HG21	24:G:606:CHL:CBC	2.10	0.67
21:N:115:PHE:CZ	21:N:119:LEU:HD21	2.30	0.67
25:R:601:CLA:C4C	26:R:618:LHG:HC92	2.24	0.67
1:5:138:ILE:CG1	1:5:144:LEU:HB2	2.22	0.67
4:a:196:PRO:HG3	4:a:300:PHE:CE2	2.29	0.67
20:s:236:MET:HE2	39:s:316:LUT:C12	2.23	0.67
21:n:115:PHE:CZ	21:n:119:LEU:HD21	2.30	0.67
4:A:246:TYR:CE2	4:A:248:ILE:HG12	2.29	0.67
5:B:91:TRP:HE1	26:B:622:LHG:HC61	1.58	0.67
6:C:457:LYS:HE2	7:D:230:ALA:CB	2.24	0.67
25:C:501:CLA:CHC	25:C:503:CLA:H71	2.24	0.67
7:D:94:TRP:HE1	18:X:87:LEU:HD22	1.59	0.67
21:N:131:TRP:HB3	39:N:616:LUT:H41	1.76	0.67
21:Y:127:GLY:HA3	21:Y:137:GLN:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:115:PHE:CZ	1:5:119:LEU:HD21	2.30	0.67
13:l:13:LEU:HB2	14:m:25:ILE:HG22	1.77	0.67
15:o:309:SER:OG	15:o:319:LYS:N	2.20	0.67
24:y:309:CHL:H11	39:y:316:LUT:H383	1.75	0.67
22:r:153:GLY:HA2	25:r:604:CLA:C4C	2.24	0.67
23:u:97:THR:HA	23:u:102:ARG:NH2	2.06	0.67
25:C:505:CLA:HAA1	25:C:505:CLA:HBD	1.76	0.67
7:D:56:VAL:HG21	7:D:111:LEU:HD11	1.75	0.67
10:H:25:PRO:HG3	22:R:122:THR:HB	1.77	0.67
12:K:32:PHE:HZ	19:Z:9:VAL:HG11	1.58	0.67
21:N:153:VAL:HG13	24:N:605:CHL:CHD	2.25	0.67
21:Y:59:LEU:HD23	24:Y:302:CHL:C1B	2.24	0.67
21:Y:138:ILE:CG1	21:Y:144:LEU:HB2	2.23	0.67
3:8:219:GLU:HG2	3:8:219:GLU:O	1.93	0.67
3:8:226:LEU:HD12	3:8:229:ILE:CD1	2.24	0.67
6:c:373:ASN:OD1	15:o:111:ALA:HA	1.95	0.67
21:g:138:ILE:CG1	21:g:144:LEU:HB2	2.22	0.67
21:y:56:VAL:HB	24:y:302:CHL:CBC	2.25	0.67
5:B:462:PHE:CZ	25:B:613:CLA:HMB3	2.29	0.67
6:C:335:THR:HG23	6:C:337:LEU:H	1.58	0.67
24:S:302:CHL:HHC	24:S:302:CHL:HBB1	1.77	0.67
21:Y:176:ARG:NH2	24:Y:310:CHL:O1D	2.27	0.67
1:7:127:GLY:HA3	1:7:137:GLN:HG3	1.76	0.67
4:a:246:TYR:CE2	4:a:248:ILE:HG12	2.29	0.67
5:b:201:HIS:HE1	25:b:602:CLA:ND	1.93	0.67
21:n:75:PRO:HG3	21:n:212:LYS:HD3	1.77	0.67
25:n:613:CLA:H141	25:n:614:CLA:CMD	2.25	0.67
25:r:602:CLA:HMC1	41:r:616:XAT:C31	2.25	0.67
1:1:127:GLY:HA3	1:1:137:GLN:HG3	1.76	0.67
3:4:226:LEU:HD12	3:4:229:ILE:CD1	2.24	0.67
4:A:255:PHE:CE2	4:A:264:SER:HB3	2.30	0.67
20:S:146:VAL:HG11	20:S:149:LYS:HZ3	1.60	0.67
25:b:615:CLA:H51	25:b:616:CLA:H203	1.75	0.67
6:c:472:LEU:HD11	16:t:26:PRO:HB3	1.77	0.67
25:c:501:CLA:CHC	25:c:503:CLA:H71	2.24	0.67
22:r:170:LYS:O	22:r:174:VAL:HG22	1.95	0.67
25:r:604:CLA:HBB	41:r:616:XAT:H42	1.77	0.67
3:4:175:ALA:O	3:4:177:PRO:HD3	1.95	0.67
5:B:352:ARG:CZ	5:B:372:ASP:HB2	2.25	0.67
6:C:151:TRP:CB	17:W:133:LEU:HD21	2.21	0.67
21:N:107:MET:CE	25:N:610:CLA:HHC	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:170:LYS:O	22:R:174:VAL:HG22	1.95	0.67
22:R:185:PRO:HD3	21:y:151:SER:HB2	1.76	0.67
22:R:220:GLY:CA	22:R:224:ASP:HB3	2.25	0.67
25:6:604:CLA:C1C	26:6:606:LHG:HC5	2.25	0.67
3:8:175:ALA:O	3:8:177:PRO:HD3	1.95	0.67
4:a:255:PHE:CE2	4:a:264:SER:HB3	2.30	0.67
5:b:423:ARG:NH2	5:b:430:PHE:O	2.28	0.67
21:g:127:GLY:HA3	21:g:137:GLN:HG3	1.76	0.67
21:n:107:MET:CE	25:n:610:CLA:HHC	2.25	0.67
2:2:120:GLN:NE2	2:2:125:VAL:HG23	2.09	0.67
2:2:129:GLU:HB2	2:2:239:LYS:CE	2.24	0.67
25:B:604:CLA:H142	25:B:615:CLA:CMA	2.21	0.67
6:C:472:LEU:HD11	16:T:26:PRO:HB3	1.77	0.67
24:S:308:CHL:HHC	24:S:308:CHL:HBB1	1.77	0.67
2:6:117:GLU:HG2	2:6:239:LYS:HB3	1.76	0.67
2:6:129:GLU:HB2	2:6:239:LYS:CE	2.24	0.67
5:b:159:THR:HA	5:b:181:VAL:O	1.94	0.67
25:b:615:CLA:CMB	25:b:615:CLA:H201	2.25	0.67
21:g:100:VAL:CB	21:g:190:LEU:HD13	2.25	0.67
21:g:115:PHE:CZ	21:g:119:LEU:HD21	2.30	0.67
25:n:603:CLA:H171	24:n:607:CHL:H193	1.77	0.67
2:2:128:LYS:HD3	2:2:133:PHE:HB3	1.75	0.66
24:2:601:CHL:H12	26:2:606:LHG:H181	1.75	0.66
4:A:196:PRO:HG3	4:A:300:PHE:CE2	2.29	0.66
25:A:402:CLA:HHB	27:A:403:PHO:H203	1.74	0.66
21:G:75:PRO:HG3	21:G:212:LYS:HD3	1.77	0.66
21:Y:107:MET:HE1	25:Y:311:CLA:HHC	1.77	0.66
25:R:604:CLA:HHB	41:R:616:XAT:H42	1.77	0.66
1:5:100:VAL:CB	1:5:190:LEU:HD13	2.25	0.66
2:6:120:GLN:NE2	2:6:125:VAL:HG23	2.09	0.66
25:6:605:CLA:CBC	26:6:606:LHG:H362	2.25	0.66
4:a:225:ARG:HD3	22:r:102:ALA:CB	2.24	0.66
20:s:59:LEU:CD1	20:s:216:GLU:HG3	2.24	0.66
25:s:304:CLA:HMC2	39:s:316:LUT:C13	2.26	0.66
21:n:127:GLY:HA3	21:n:137:GLN:HG3	1.76	0.66
24:n:609:CHL:HAA2	21:y:82:THR:CG2	2.17	0.66
24:y:307:CHL:HHC	24:y:308:CHL:C2C	2.25	0.66
22:r:220:GLY:CA	22:r:224:ASP:HB3	2.25	0.66
1:1:115:PHE:CZ	1:1:119:LEU:HD21	2.29	0.66
2:2:128:LYS:HE3	2:2:140:PHE:CZ	2.31	0.66
4:A:231:GLU:HG2	5:B:1:MET:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:615:CLA:HMB1	25:B:615:CLA:H201	1.76	0.66
20:S:128:PHE:CE2	20:S:236:MET:HE1	2.31	0.66
25:G:603:CLA:HAB	39:G:616:LUT:C35	2.25	0.66
21:Y:75:PRO:HG3	21:Y:212:LYS:HD3	1.77	0.66
24:Y:307:CHL:HHC	24:Y:308:CHL:C2C	2.25	0.66
2:6:128:LYS:HE3	2:6:140:PHE:CZ	2.31	0.66
4:a:237:TYR:HB3	7:d:264:ASN:OD1	1.96	0.66
25:c:511:CLA:H3A	28:k:101:BCR:H271	1.78	0.66
15:o:139:GLU:OE1	17:w:80:LEU:N	2.28	0.66
21:n:100:VAL:CB	21:n:190:LEU:HD13	2.26	0.66
21:n:131:TRP:HB3	39:n:616:LUT:H41	1.77	0.66
25:n:613:CLA:H142	25:n:613:CLA:H2	1.76	0.66
25:2:604:CLA:C1C	26:2:606:LHG:HC5	2.25	0.66
1:3:75:PRO:HG3	1:3:212:LYS:HD3	1.77	0.66
25:C:501:CLA:HMB1	28:I:101:BCR:H23C	1.77	0.66
25:G:604:CLA:HBB1	39:G:616:LUT:H181	1.78	0.66
15:o:133:GLY:O	15:o:134:LYS:HE2	1.96	0.66
22:r:173:LEU:HD13	22:r:188:ILE:HG13	1.76	0.66
3:4:245:GLU:HB2	3:4:250:LYS:HB3	1.77	0.66
26:B:625:LHG:O9	26:L:102:LHG:HC81	1.96	0.66
15:O:146:LYS:HB2	15:O:158:PHE:CD1	2.31	0.66
21:N:75:PRO:HG3	21:N:212:LYS:HD3	1.77	0.66
21:Y:115:PHE:CZ	21:Y:119:LEU:HD21	2.30	0.66
15:o:140:PRO:HD2	15:o:169:TYR:CD2	2.30	0.66
20:s:246:THR:HG21	20:s:253:ASN:OD1	1.95	0.66
1:1:165:GLN:HE22	24:1:302:CHL:C1B	2.08	0.66
2:2:117:GLU:HG2	2:2:239:LYS:HB3	1.76	0.66
25:C:511:CLA:H3A	28:K:101:BCR:H271	1.78	0.66
20:S:113:PHE:CE1	25:S:304:CLA:HBD	2.31	0.66
25:S:304:CLA:HMC2	39:S:316:LUT:C13	2.26	0.66
21:G:127:GLY:HA3	21:G:137:GLN:HG3	1.76	0.66
24:G:606:CHL:HBC2	24:G:607:CHL:CHD	2.25	0.66
25:N:603:CLA:C17	24:N:607:CHL:H193	2.25	0.66
21:Y:107:MET:CE	25:Y:311:CLA:HHC	2.26	0.66
22:R:103:LYS:HE3	22:R:105:LEU:HD11	1.78	0.66
22:R:211:ASP:OD1	22:R:213:GLU:HG2	1.94	0.66
3:8:245:GLU:HB2	3:8:250:LYS:HB3	1.77	0.66
4:a:292:THR:CG2	6:c:428:THR:HG23	2.25	0.66
25:b:615:CLA:H201	25:b:615:CLA:HMB1	1.76	0.66
21:n:153:VAL:HG13	24:n:605:CHL:CHD	2.25	0.66
25:n:603:CLA:C17	24:n:607:CHL:H193	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:75:PRO:HG3	21:y:212:LYS:HD3	1.77	0.66
1:3:100:VAL:CB	1:3:190:LEU:HD13	2.25	0.66
5:B:44:VAL:HG23	5:B:60:MET:HE1	1.77	0.66
21:G:115:PHE:CZ	21:G:119:LEU:HD21	2.30	0.66
21:Y:231:VAL:HG11	25:Y:314:CLA:HHD	1.78	0.66
5:b:352:ARG:CZ	5:b:372:ASP:HB2	2.25	0.66
25:c:501:CLA:HMB1	28:i:101:BCR:H23C	1.77	0.66
20:s:128:PHE:CE2	20:s:236:MET:HE1	2.31	0.66
24:s:308:CHL:HHC	24:s:308:CHL:HBB1	1.77	0.66
21:y:244:LEU:HD22	39:y:316:LUT:H163	1.75	0.66
25:2:605:CLA:CBC	26:2:606:LHG:H362	2.25	0.66
3:4:73:LEU:CG	3:4:82:GLY:HA2	2.22	0.66
4:A:235:GLU:HB3	7:D:264:ASN:ND2	2.08	0.66
4:A:292:THR:CG2	6:C:428:THR:HG23	2.25	0.66
29:L:101:SQD:H92	29:L:101:SQD:C23	2.26	0.66
15:O:169:TYR:OH	17:W:80:LEU:HD23	1.95	0.66
20:S:246:THR:HG21	20:S:253:ASN:OD1	1.95	0.66
25:N:613:CLA:H142	25:N:613:CLA:H2	1.76	0.66
24:5:302:CHL:HHC	24:5:302:CHL:HBB1	1.78	0.66
5:b:44:VAL:HG23	5:b:60:MET:HE1	1.77	0.66
20:s:262:PHE:HE2	25:s:314:CLA:H3A	1.59	0.66
24:g:606:CHL:HBC2	24:g:607:CHL:CHD	2.25	0.66
2:2:116:PRO:HG3	2:2:134:LYS:HE3	1.76	0.66
5:B:45:PHE:CE2	5:B:47:PRO:HB3	2.31	0.66
5:B:121:GLU:OE2	10:H:16:SER:OG	2.08	0.66
5:B:475:PHE:HB2	5:B:479:PHE:CE2	2.31	0.66
25:B:615:CLA:H201	25:B:615:CLA:CMB	2.25	0.66
7:D:175:GLY:O	7:D:179:ILE:HG12	1.96	0.66
13:L:13:LEU:HB2	14:M:25:ILE:HG22	1.77	0.66
25:G:610:CLA:C4	25:G:612:CLA:HMA2	2.26	0.66
22:R:130:VAL:HG23	22:R:131:PHE:HD1	1.61	0.66
24:R:613:CHL:HHC	24:R:613:CHL:HBB1	1.78	0.66
3:8:194:TYR:CE2	3:8:221:LEU:HB2	2.24	0.66
15:o:146:LYS:HB2	15:o:158:PHE:CD1	2.31	0.66
21:g:231:VAL:HG21	25:g:613:CLA:CAC	2.24	0.66
2:2:130:PRO:CD	2:2:239:LYS:HE2	2.25	0.66
3:4:194:TYR:CE2	3:4:221:LEU:HB2	2.24	0.66
4:A:225:ARG:HD3	22:R:102:ALA:CB	2.24	0.66
5:B:478:VAL:HG13	7:D:140:ARG:HG2	1.78	0.66
1:5:127:GLY:HA3	1:5:137:GLN:HG3	1.76	0.66
20:s:113:PHE:CE1	25:s:304:CLA:HBD	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:107:MET:CE	25:y:311:CLA:HHC	2.26	0.66
4:A:139:MET:HE3	7:D:222:THR:HG22	1.78	0.66
15:O:133:GLY:O	15:O:134:LYS:HE2	1.96	0.66
15:O:139:GLU:OE1	17:W:80:LEU:N	2.28	0.66
20:S:113:PHE:O	20:S:117:HIS:ND1	2.26	0.66
25:R:604:CLA:HHB	41:R:616:XAT:H22	1.78	0.66
4:a:224:ILE:HD13	5:b:482:ILE:HG13	1.78	0.66
4:a:231:GLU:HG2	5:b:1:MET:HA	1.77	0.66
21:y:100:VAL:CB	21:y:190:LEU:HD13	2.26	0.66
1:1:100:VAL:CB	1:1:190:LEU:HD13	2.25	0.65
5:B:423:ARG:NH2	5:B:430:PHE:O	2.28	0.65
25:N:613:CLA:H141	25:N:614:CLA:CMD	2.25	0.65
21:Y:56:VAL:HB	24:Y:302:CHL:CBC	2.25	0.65
25:R:602:CLA:HMC1	41:R:616:XAT:C31	2.25	0.65
5:b:161:LEU:HD21	30:b:623:LMG:O3	1.96	0.65
6:c:162:GLY:HA2	6:c:248:GLY:HA2	1.79	0.65
25:c:512:CLA:C1B	28:c:514:BCR:H401	2.27	0.65
10:h:52:VAL:O	10:h:56:ILE:HG12	1.97	0.65
2:2:117:GLU:CB	2:2:241:PRO:HG2	2.26	0.65
5:B:128:THR:HG21	22:R:94:ILE:CD1	2.26	0.65
14:M:1:MET:HB2	14:M:3:VAL:HG13	1.78	0.65
20:S:135:ASN:ND2	20:S:141:CYS:H	1.95	0.65
21:G:104:ARG:NH1	24:G:608:CHL:OBD	2.28	0.65
21:N:100:VAL:CB	21:N:190:LEU:HD13	2.26	0.65
25:N:603:CLA:H101	24:N:609:CHL:C14	2.26	0.65
21:Y:100:VAL:CB	21:Y:190:LEU:HD13	2.26	0.65
2:6:117:GLU:CB	2:6:241:PRO:HG2	2.26	0.65
3:8:86:LEU:HB3	3:8:88:LEU:HD13	1.77	0.65
3:8:177:PRO:HG3	25:r:610:CLA:CBB	2.25	0.65
5:b:45:PHE:CE2	5:b:47:PRO:HB3	2.31	0.65
6:c:457:LYS:HE2	7:d:230:ALA:CB	2.24	0.65
25:g:603:CLA:HAB	39:g:616:LUT:C35	2.25	0.65
22:r:214:LYS:HA	22:r:217:TYR:O	1.97	0.65
25:r:604:CLA:HHB	41:r:616:XAT:H22	1.78	0.65
4:A:173:PRO:HB2	4:A:178:GLY:HA3	1.79	0.65
2:6:116:PRO:HG3	2:6:134:LYS:HE3	1.76	0.65
5:b:388:SER:HB2	5:b:391:SER:HB2	1.77	0.65
6:c:60:ILE:HA	25:c:510:CLA:HMC3	1.79	0.65
6:c:278:ALA:CB	25:c:507:CLA:HMA1	2.27	0.65
10:h:25:PRO:HG3	22:r:122:THR:HB	1.77	0.65
29:l:102:SQD:H251	29:l:102:SQD:C10	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:169:TYR:OH	17:w:80:LEU:HD23	1.95	0.65
21:n:209:ALA:O	21:n:212:LYS:HB2	1.96	0.65
25:y:304:CLA:H122	25:y:304:CLA:H203	1.78	0.65
24:1:302:CHL:HHC	24:1:302:CHL:HBB1	1.78	0.65
2:2:137:SER:HA	2:2:140:PHE:CD2	2.32	0.65
2:2:223:ALA:HB3	25:2:602:CLA:HMC2	1.78	0.65
1:3:209:ALA:O	1:3:212:LYS:HB2	1.96	0.65
3:4:86:LEU:HB3	3:4:88:LEU:HD13	1.77	0.65
3:4:136:ALA:HB1	3:4:140:PHE:HZ	1.61	0.65
21:G:224:PHE:CD2	26:Y:301:LHG:H281	2.31	0.65
22:R:138:GLU:HB2	22:R:216:LEU:HD11	1.79	0.65
2:6:125:VAL:HG13	2:6:148:LEU:CD1	2.26	0.65
6:c:305:THR:HG22	6:c:307:PRO:HD2	1.79	0.65
25:c:505:CLA:HBD	25:c:505:CLA:HAA1	1.77	0.65
7:d:194:LEU:HD22	7:d:316:TYR:HE1	1.61	0.65
15:o:117:ILE:CG2	15:o:298:GLU:HB3	2.27	0.65
21:n:227:PHE:O	21:n:231:VAL:HG23	1.97	0.65
21:y:209:ALA:O	21:y:212:LYS:HB2	1.96	0.65
22:r:130:VAL:HG23	22:r:131:PHE:HD1	1.61	0.65
10:H:52:VAL:HG22	18:X:88:LEU:HD12	1.78	0.65
15:O:140:PRO:HD2	15:O:169:TYR:CD2	2.30	0.65
21:G:227:PHE:O	21:G:231:VAL:HG23	1.97	0.65
21:N:209:ALA:O	21:N:212:LYS:HB2	1.97	0.65
1:5:75:PRO:HG3	1:5:212:LYS:HD3	1.77	0.65
1:5:227:PHE:O	1:5:231:VAL:HG23	1.97	0.65
25:a:406:CLA:HHD	28:a:407:BCR:C36	2.27	0.65
25:b:608:CLA:H152	25:b:609:CLA:H203	1.78	0.65
6:c:133:ALA:HB1	25:c:511:CLA:HMA2	1.78	0.65
25:d:403:CLA:H52	18:x:91:ALA:CB	2.27	0.65
25:r:612:CLA:CHB	39:r:615:LUT:H42	2.25	0.65
1:3:227:PHE:O	1:3:231:VAL:HG23	1.97	0.65
5:B:161:LEU:HD21	30:B:623:LMG:O3	1.96	0.65
25:B:608:CLA:H152	25:B:609:CLA:H203	1.78	0.65
6:C:162:GLY:HA2	6:C:248:GLY:HA2	1.78	0.65
29:L:101:SQD:H251	29:L:101:SQD:C11	2.27	0.65
1:7:100:VAL:CB	1:7:190:LEU:HD13	2.25	0.65
6:c:362:ARG:HG3	6:c:367:GLU:CD	2.22	0.65
25:c:511:CLA:H143	19:z:20:LEU:HD11	1.79	0.65
20:s:128:PHE:HE2	20:s:236:MET:HE1	1.62	0.65
21:g:138:ILE:HG21	24:g:606:CHL:CBC	2.10	0.65
21:g:227:PHE:O	21:g:231:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:603:CLA:H101	24:n:609:CHL:C14	2.26	0.65
2:2:125:VAL:HG13	2:2:148:LEU:CD1	2.26	0.65
6:C:87:ILE:HD13	25:C:504:CLA:CMB	2.27	0.65
6:C:346:THR:OG1	6:C:348:GLU:OE1	2.09	0.65
20:S:128:PHE:HE2	20:S:236:MET:HE1	1.61	0.65
25:R:612:CLA:CHB	39:R:615:LUT:H42	2.25	0.65
3:8:78:PRO:CG	3:8:225:LYS:HE2	2.27	0.65
26:b:625:LHG:O9	26:l:103:LHG:HC81	1.96	0.65
6:c:87:ILE:HD13	25:c:504:CLA:CMB	2.27	0.65
25:g:604:CLA:HBB1	39:g:616:LUT:H181	1.78	0.65
24:g:606:CHL:HBB1	24:g:606:CHL:HHC	1.78	0.65
24:r:613:CHL:HHC	24:r:613:CHL:HBB1	1.78	0.65
1:1:75:PRO:HG3	1:1:212:LYS:HD3	1.77	0.65
5:B:274:GLN:HG2	5:B:279:TYR:CD2	2.32	0.65
5:B:277:GLN:HA	23:U:98:ALA:HA	1.79	0.65
6:C:305:THR:HG22	6:C:307:PRO:HD2	1.79	0.65
6:C:362:ARG:HG3	6:C:367:GLU:CD	2.22	0.65
7:D:194:LEU:HD22	7:D:316:TYR:HE1	1.61	0.65
29:L:101:SQD:H251	29:L:101:SQD:C10	2.26	0.65
21:G:231:VAL:HG21	25:G:613:CLA:HAC2	1.79	0.65
21:N:227:PHE:O	21:N:231:VAL:HG23	1.97	0.65
1:5:153:VAL:HG13	24:5:301:CHL:CHD	2.27	0.65
2:6:130:PRO:CD	2:6:239:LYS:HE2	2.25	0.65
2:6:145:LEU:CD2	2:6:154:VAL:HA	2.27	0.65
24:n:606:CHL:HBC2	24:n:607:CHL:CHD	2.27	0.65
21:y:94:ARG:NE	21:y:94:ARG:HA	2.12	0.65
5:B:98:GLY:O	5:B:102:VAL:HG23	1.97	0.65
6:C:378:SER:O	6:C:382:LYS:HG2	1.97	0.65
8:E:73:LEU:HD23	8:E:77:ASP:OD2	1.97	0.65
10:H:52:VAL:O	10:H:56:ILE:HG12	1.97	0.65
25:N:603:CLA:H171	24:N:607:CHL:H193	1.77	0.65
25:Y:304:CLA:H122	25:Y:304:CLA:H203	1.78	0.65
22:R:214:LYS:HA	22:R:217:TYR:O	1.97	0.65
24:s:302:CHL:HHC	24:s:302:CHL:HBB1	1.77	0.65
21:g:209:ALA:O	21:g:212:LYS:HB2	1.97	0.65
24:y:302:CHL:HMB3	26:y:319:LHG:H161	1.79	0.65
22:r:139:CYS:O	22:r:143:HIS:ND1	2.29	0.65
3:4:77:LEU:CG	3:4:78:PRO:HD2	2.26	0.65
25:A:405:CLA:HHD	28:A:406:BCR:C36	2.27	0.65
5:B:201:HIS:HE1	25:B:602:CLA:ND	1.93	0.65
18:X:87:LEU:HD11	18:X:88:LEU:HD22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:100:VAL:CB	21:G:190:LEU:HD13	2.25	0.65
24:N:606:CHL:HBC2	24:N:607:CHL:CHD	2.27	0.65
22:R:224:ASP:OD1	39:R:615:LUT:O23	2.12	0.65
1:5:165:GLN:HE22	24:5:302:CHL:C1B	2.08	0.65
2:6:137:SER:HA	2:6:140:PHE:CD2	2.32	0.65
1:7:75:PRO:HG3	1:7:212:LYS:HD3	1.77	0.65
1:7:94:ARG:NE	1:7:94:ARG:HA	2.12	0.65
3:8:175:ALA:HB1	25:r:601:CLA:HHC	1.78	0.65
5:b:98:GLY:O	5:b:102:VAL:HG23	1.97	0.65
25:b:606:CLA:HMC1	26:b:622:LHG:H292	1.80	0.65
8:e:73:LEU:HD23	8:e:77:ASP:OD2	1.97	0.65
20:s:135:ASN:ND2	20:s:141:CYS:H	1.94	0.65
21:g:75:PRO:HG3	21:g:212:LYS:HD3	1.77	0.65
21:y:107:MET:HE1	25:y:311:CLA:HHC	1.78	0.65
21:y:227:PHE:O	21:y:231:VAL:HG23	1.97	0.65
21:y:231:VAL:HG11	25:y:314:CLA:HHD	1.78	0.65
1:1:227:PHE:O	1:1:231:VAL:HG23	1.97	0.64
3:4:78:PRO:CD	3:4:225:LYS:HE2	2.27	0.64
4:A:237:TYR:HB3	7:D:264:ASN:OD1	1.96	0.64
5:B:72:THR:HG23	5:B:80:ILE:CG2	2.22	0.64
5:B:336:ILE:HD12	5:B:436:THR:HG21	1.77	0.64
6:C:133:ALA:HB1	25:C:511:CLA:HMA2	1.78	0.64
6:C:272:LEU:HD21	25:C:508:CLA:CHB	2.27	0.64
25:C:512:CLA:C1B	28:C:514:BCR:H401	2.27	0.64
21:G:62:PHE:C	21:Y:178:ALA:HB2	2.22	0.64
24:N:607:CHL:H142	24:N:607:CHL:H93	1.79	0.64
22:R:209:GLU:CD	22:R:214:LYS:HD2	2.22	0.64
5:b:475:PHE:HB2	5:b:479:PHE:CE2	2.31	0.64
29:l:102:SQD:H92	29:l:102:SQD:C23	2.26	0.64
21:g:104:ARG:NH1	24:g:608:CHL:OBD	2.28	0.64
22:r:103:LYS:HE3	22:r:105:LEU:HD11	1.78	0.64
15:O:117:ILE:CG2	15:O:298:GLU:HB3	2.27	0.64
21:N:94:ARG:NE	21:N:94:ARG:HA	2.12	0.64
21:Y:94:ARG:NE	21:Y:94:ARG:HA	2.12	0.64
21:Y:209:ALA:O	21:Y:212:LYS:HB2	1.96	0.64
21:Y:215:GLU:HG3	25:Y:311:CLA:C4B	2.27	0.64
21:Y:227:PHE:O	21:Y:231:VAL:HG23	1.97	0.64
1:7:227:PHE:O	1:7:231:VAL:HG23	1.97	0.64
4:a:173:PRO:HB2	4:a:178:GLY:HA3	1.79	0.64
7:d:175:GLY:O	7:d:179:ILE:HG12	1.96	0.64
14:m:1:MET:HB2	14:m:3:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:164:THR:HG21	24:g:606:CHL:O1D	1.97	0.64
25:n:603:CLA:H192	24:n:607:CHL:H172	1.79	0.64
22:r:208:ALA:O	22:r:210:LEU:HD12	1.97	0.64
1:1:94:ARG:NE	1:1:94:ARG:HA	2.12	0.64
1:1:153:VAL:HG13	24:1:301:CHL:CHD	2.27	0.64
3:4:78:PRO:CG	3:4:225:LYS:HE2	2.27	0.64
5:B:388:SER:HB2	5:B:391:SER:HB2	1.78	0.64
6:C:278:ALA:CB	25:C:507:CLA:HMA1	2.27	0.64
7:D:189:PHE:O	7:D:295:ARG:NH1	2.31	0.64
28:K:101:BCR:H332	19:Z:12:LEU:HD23	1.79	0.64
28:T:101:BCR:H271	5:b:39:LEU:CD1	2.28	0.64
21:G:94:ARG:NE	21:G:94:ARG:HA	2.12	0.64
24:N:607:CHL:C1	24:Y:302:CHL:H191	2.23	0.64
24:Y:310:CHL:HHC	24:Y:310:CHL:HBB1	1.79	0.64
1:5:162:TRP:O	1:5:166:VAL:HG23	1.98	0.64
1:5:209:ALA:O	1:5:212:LYS:HB2	1.96	0.64
2:6:223:ALA:HB3	25:6:602:CLA:HMC2	1.79	0.64
1:7:209:ALA:O	1:7:212:LYS:HB2	1.96	0.64
5:b:128:THR:HG21	22:r:94:ILE:CD1	2.26	0.64
21:g:224:PHE:CD2	26:y:301:LHG:H281	2.31	0.64
24:g:601:CHL:HHB	24:y:310:CHL:HMB3	1.79	0.64
21:n:231:VAL:CG1	25:n:613:CLA:HHD	2.26	0.64
24:n:607:CHL:H93	24:n:607:CHL:H142	1.79	0.64
20:S:135:ASN:OD1	20:S:145:ALA:HB2	1.97	0.64
21:N:132:PHE:CE1	21:N:133:LYS:HG3	2.33	0.64
22:R:103:LYS:HE3	22:R:105:LEU:HD21	1.79	0.64
24:5:301:CHL:HHC	24:5:301:CHL:HBB1	1.80	0.64
5:b:335:GLY:HA3	5:b:432:LEU:HB3	1.80	0.64
6:c:272:LEU:HD21	25:c:508:CLA:CHB	2.27	0.64
6:c:428:THR:HG22	35:c:516:DGD:HBW1	1.78	0.64
15:o:158:PHE:CE2	15:o:322:LYS:HE3	2.33	0.64
20:s:135:ASN:OD1	20:s:145:ALA:HB2	1.97	0.64
22:r:68:LEU:HD11	25:r:602:CLA:O2D	1.97	0.64
22:r:209:GLU:CD	22:r:214:LYS:HD2	2.23	0.64
4:A:135:PHE:CE1	6:C:449:ARG:HG2	2.33	0.64
25:B:607:CLA:H171	25:B:613:CLA:C16	2.23	0.64
6:C:52:ALA:HB1	25:C:509:CLA:HBB1	1.80	0.64
21:N:158:ILE:CD1	21:Y:257:TRP:HE3	2.11	0.64
21:Y:57:LYS:HB2	21:Y:63:SER:OG	1.98	0.64
21:Y:179:GLY:HA2	24:Y:309:CHL:HAC1	1.79	0.64
3:8:136:ALA:HB1	3:8:140:PHE:HZ	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:336:ILE:HD12	5:b:436:THR:HG21	1.77	0.64
18:x:87:LEU:HD11	18:x:88:LEU:HD22	1.79	0.64
25:r:601:CLA:C4D	26:r:618:LHG:H102	2.03	0.64
1:1:51:TYR:CE2	1:1:209:ALA:HB1	2.33	0.64
2:2:145:LEU:CD2	2:2:154:VAL:HA	2.27	0.64
7:D:52:GLY:HA3	7:D:79:VAL:HG22	1.79	0.64
24:G:606:CHL:HBB1	24:G:606:CHL:HHC	1.78	0.64
25:G:610:CLA:HMC1	39:G:615:LUT:C31	2.27	0.64
3:8:77:LEU:CG	3:8:78:PRO:HD2	2.26	0.64
3:8:224:LEU:O	3:8:227:ALA:HB3	1.98	0.64
5:b:241:SER:OG	25:b:612:CLA:OBD	2.06	0.64
5:b:274:GLN:HG2	5:b:279:TYR:CD2	2.32	0.64
5:b:291:GLY:HA2	5:b:294:GLU:OE2	1.98	0.64
15:o:130:LYS:HD2	15:o:179:GLU:HB2	1.80	0.64
24:n:607:CHL:C1	24:y:302:CHL:H191	2.23	0.64
21:y:215:GLU:HG3	25:y:311:CLA:C4B	2.27	0.64
1:3:132:PHE:CE1	1:3:133:LYS:HG3	2.33	0.64
24:G:601:CHL:HBB	24:Y:310:CHL:HMB3	1.79	0.64
22:R:122:THR:OG1	22:R:125:GLN:O	2.16	0.64
22:R:220:GLY:HA2	22:R:224:ASP:N	2.13	0.64
1:5:94:ARG:HA	1:5:94:ARG:NE	2.12	0.64
5:b:478:VAL:HG13	7:d:140:ARG:HG2	1.78	0.64
25:g:610:CLA:C4	25:g:612:CLA:HMA2	2.26	0.64
25:g:610:CLA:HMC1	39:g:615:LUT:C31	2.27	0.64
21:n:57:LYS:HB2	21:n:63:SER:OG	1.98	0.64
21:y:86:SER:OG	25:y:303:CLA:O1A	2.16	0.64
1:1:209:ALA:O	1:1:212:LYS:HB2	1.96	0.64
1:3:202:ALA:HB1	1:3:208:PHE:CD1	2.33	0.64
3:4:175:ALA:HB1	25:R:601:CLA:HHC	1.78	0.64
4:A:224:ILE:HD13	5:B:482:ILE:HG13	1.78	0.64
5:B:335:GLY:HA3	5:B:432:LEU:HB3	1.80	0.64
25:B:606:CLA:HMC1	26:B:622:LHG:H292	1.80	0.64
6:C:138:GLU:HG3	6:C:139:THR:HG23	1.80	0.64
6:C:255:LYS:HG3	6:C:256:PRO:HD2	1.80	0.64
7:D:185:PHE:HA	7:D:330:MET:HE1	1.80	0.64
21:G:51:TYR:CE2	21:G:209:ALA:HB1	2.33	0.64
21:N:57:LYS:HB2	21:N:63:SER:OG	1.98	0.64
25:Y:314:CLA:HAA1	25:Y:314:CLA:HBD	1.79	0.64
22:R:208:ALA:O	22:R:210:LEU:HD12	1.97	0.64
2:6:220:GLY:HA2	25:6:602:CLA:HAC1	1.80	0.64
5:b:277:GLN:HA	23:u:98:ALA:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:513:CLA:OBD	20:s:72:PRO:HB2	1.97	0.64
7:d:185:PHE:HA	7:d:330:MET:HE1	1.80	0.64
29:l:102:SQD:H251	29:l:102:SQD:C11	2.27	0.64
21:g:62:PHE:C	21:y:178:ALA:HB2	2.22	0.64
21:n:202:ALA:HB1	21:n:208:PHE:CD1	2.33	0.64
22:r:138:GLU:HB2	22:r:216:LEU:HD11	1.79	0.64
22:r:220:GLY:HA2	22:r:224:ASP:N	2.13	0.64
1:3:57:LYS:HB2	1:3:63:SER:OG	1.98	0.64
4:A:332:HIS:HB3	7:D:322:LEU:HD21	1.80	0.64
5:B:39:LEU:CD1	28:t:101:BCR:H271	2.28	0.64
6:C:60:ILE:HA	25:C:510:CLA:HMC3	1.79	0.64
25:D:403:CLA:H52	18:X:91:ALA:CB	2.27	0.64
21:G:209:ALA:O	21:G:212:LYS:HB2	1.97	0.64
21:N:162:TRP:O	21:N:166:VAL:HG23	1.98	0.64
3:8:229:ILE:HG13	3:8:230:LYS:N	2.13	0.64
6:c:138:GLU:HG3	6:c:139:THR:HG23	1.80	0.64
6:c:199:ILE:O	6:c:200:THR:HG22	1.98	0.64
25:c:510:CLA:HMA2	25:c:510:CLA:H2	1.80	0.64
10:h:52:VAL:HG22	18:x:88:LEU:HD12	1.78	0.64
11:i:34:ARG:NH1	11:i:35:GLU:HG2	2.11	0.64
20:s:128:PHE:HE1	39:s:316:LUT:H173	1.63	0.64
25:s:304:CLA:HMA2	25:s:304:CLA:HBA1	1.80	0.64
21:n:132:PHE:CE1	21:n:133:LYS:HG3	2.33	0.64
21:n:224:PHE:CD1	25:n:602:CLA:H201	2.33	0.64
21:y:162:TRP:O	21:y:166:VAL:HG23	1.98	0.64
21:y:179:GLY:HA2	24:y:309:CHL:HAC1	1.79	0.64
1:1:132:PHE:CE1	1:1:133:LYS:HG3	2.33	0.64
5:B:291:GLY:HA2	5:B:294:GLU:OE2	1.98	0.64
25:C:513:CLA:OBD	20:S:72:PRO:HB2	1.97	0.64
25:S:313:CLA:HAA1	25:S:313:CLA:HBD	1.80	0.64
21:N:80:TRP:CE3	39:N:616:LUT:H383	2.33	0.64
4:a:139:MET:HE3	7:d:222:THR:HG22	1.78	0.64
6:c:185:VAL:HG23	6:c:230:LEU:HD13	1.80	0.64
6:c:348:GLU:OE2	15:o:106:LYS:HA	1.98	0.64
7:d:211:LEU:HA	7:d:214:ILE:HG22	1.80	0.64
13:l:11:VAL:HG11	14:m:25:ILE:HD12	1.80	0.64
21:g:51:TYR:CE2	21:g:209:ALA:HB1	2.33	0.64
21:g:231:VAL:HG21	25:g:613:CLA:HAC2	1.79	0.64
22:r:103:LYS:HE3	22:r:105:LEU:HD21	1.79	0.64
2:2:120:GLN:CG	2:2:125:VAL:HA	2.26	0.63
11:I:34:ARG:NH1	11:I:35:GLU:HG2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:32:PHE:CZ	19:Z:9:VAL:HG11	2.33	0.63
21:G:57:LYS:HB2	21:G:63:SER:OG	1.98	0.63
21:G:213:VAL:HG12	25:G:611:CLA:HED1	1.80	0.63
21:N:231:VAL:CG1	25:N:613:CLA:HHD	2.26	0.63
25:N:603:CLA:H192	24:N:607:CHL:H172	1.79	0.63
1:7:51:TYR:CE2	1:7:209:ALA:HB1	2.33	0.63
3:8:78:PRO:CD	3:8:225:LYS:HE2	2.27	0.63
6:c:73:ALA:HB2	12:k:26:LEU:HG	1.80	0.63
7:d:189:PHE:O	7:d:295:ARG:NH1	2.31	0.63
12:k:32:PHE:CZ	19:z:9:VAL:HG11	2.33	0.63
21:g:172:VAL:HG21	40:g:617:NEX:H34	1.80	0.63
24:n:607:CHL:H142	24:n:607:CHL:C9	2.28	0.63
6:C:308:GLU:HA	6:C:361:LEU:HD22	1.80	0.63
25:C:511:CLA:H143	19:Z:20:LEU:HD11	1.79	0.63
25:C:512:CLA:HBC3	25:C:512:CLA:HHD	1.80	0.63
15:O:130:LYS:HD2	15:O:179:GLU:HB2	1.80	0.63
16:T:2:GLU:O	16:T:5:VAL:HG22	1.98	0.63
21:G:132:PHE:CE1	21:G:133:LYS:HG3	2.33	0.63
21:G:164:THR:HG21	24:G:606:CHL:O1D	1.97	0.63
21:N:202:ALA:HB1	21:N:208:PHE:CD1	2.33	0.63
21:Y:164:THR:HG21	24:Y:307:CHL:O1D	1.98	0.63
1:5:132:PHE:CE1	1:5:133:LYS:HG3	2.33	0.63
2:6:51:TYR:HA	2:6:55:ARG:HD3	1.80	0.63
4:a:172:MET:HE1	25:a:403:CLA:HBC2	1.79	0.63
5:b:472:ARG:HA	5:b:479:PHE:CZ	2.33	0.63
7:d:13:LYS:HA	7:d:13:LYS:HE2	1.80	0.63
16:t:2:GLU:O	16:t:5:VAL:HG22	1.98	0.63
21:g:138:ILE:HD13	24:g:606:CHL:CBC	2.28	0.63
1:1:162:TRP:O	1:1:166:VAL:HG23	1.98	0.63
6:C:428:THR:HG22	35:C:516:DGD:HBW1	1.78	0.63
25:C:510:CLA:HMA2	25:C:510:CLA:H2	1.80	0.63
21:G:138:ILE:HD13	24:G:606:CHL:CBC	2.28	0.63
21:G:162:TRP:O	21:G:166:VAL:HG23	1.98	0.63
21:Y:202:ALA:HB1	21:Y:208:PHE:CD1	2.33	0.63
3:8:174:TRP:HE3	3:8:180:LYS:HD2	1.63	0.63
4:a:290:ILE:HG13	25:a:402:CLA:HED3	1.80	0.63
7:d:52:GLY:HA3	7:d:79:VAL:HG22	1.79	0.63
21:g:97:GLU:CG	21:g:190:LEU:HD21	2.20	0.63
25:g:603:CLA:HAB	39:g:616:LUT:C34	2.28	0.63
21:y:51:TYR:CE2	21:y:209:ALA:HB1	2.33	0.63
1:1:49:PRO:O	1:1:55:ARG:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:112:PHE:O	6:C:116:VAL:HG23	1.98	0.63
6:C:185:VAL:HG23	6:C:230:LEU:HD13	1.81	0.63
6:C:304:PRO:O	6:C:305:THR:HB	1.99	0.63
11:I:23:PHE:HB3	28:I:101:BCR:C3	2.29	0.63
20:S:128:PHE:HE1	39:S:316:LUT:H173	1.63	0.63
25:G:603:CLA:HAB	39:G:616:LUT:C34	2.29	0.63
25:N:603:CLA:H203	24:N:607:CHL:C19	2.29	0.63
23:U:97:THR:HA	23:U:102:ARG:NH2	2.06	0.63
1:7:132:PHE:CE1	1:7:133:LYS:HG3	2.33	0.63
3:8:78:PRO:HG3	3:8:225:LYS:HE2	1.79	0.63
6:c:308:GLU:HA	6:c:361:LEU:HD22	1.80	0.63
6:c:378:SER:O	6:c:382:LYS:HG2	1.98	0.63
21:g:213:VAL:HG12	25:g:611:CLA:HED1	1.81	0.63
21:g:218:ASN:OD1	25:g:611:CLA:HMD2	1.98	0.63
21:n:162:TRP:O	21:n:166:VAL:HG23	1.98	0.63
22:r:129:GLU:OE1	22:r:132:GLY:N	2.25	0.63
2:2:220:GLY:HA2	25:2:602:CLA:HAC1	1.80	0.63
1:3:94:ARG:NE	1:3:94:ARG:HA	2.12	0.63
4:A:172:MET:HE1	25:A:402:CLA:HBC2	1.79	0.63
25:B:601:CLA:HBB2	28:H:101:BCR:H351	1.81	0.63
6:C:38:GLY:HA3	25:C:511:CLA:HMD2	1.80	0.63
15:O:190:GLU:OE2	15:O:216:LYS:HA	1.99	0.63
25:S:304:CLA:HMA2	25:S:304:CLA:HBA1	1.80	0.63
24:G:605:CHL:HHC	24:G:605:CHL:HBB1	1.81	0.63
3:8:155:TRP:CE2	25:r:601:CLA:HMB1	2.34	0.63
4:a:132:GLU:O	4:a:136:ARG:HG2	1.99	0.63
15:o:158:PHE:CD2	15:o:322:LYS:HE3	2.33	0.63
21:y:57:LYS:HB2	21:y:63:SER:OG	1.98	0.63
24:y:310:CHL:HBB1	24:y:310:CHL:HHC	1.79	0.63
1:3:97:GLU:CG	1:3:190:LEU:HD21	2.20	0.63
4:A:147:TYR:O	4:A:150:PRO:HD2	1.98	0.63
6:C:199:ILE:O	6:C:200:THR:HG22	1.98	0.63
6:C:348:GLU:OE2	15:O:106:LYS:HA	1.98	0.63
21:N:51:TYR:CE2	21:N:209:ALA:HB1	2.33	0.63
21:Y:51:TYR:CE2	21:Y:209:ALA:HB1	2.33	0.63
24:Y:302:CHL:HMB3	26:Y:319:LHG:H161	1.79	0.63
1:5:57:LYS:HB2	1:5:63:SER:OG	1.98	0.63
1:7:114:VAL:CG1	1:7:241:LEU:HD11	2.27	0.63
3:8:159:LYS:HZ2	25:r:601:CLA:HMB2	1.62	0.63
4:a:135:PHE:CE1	6:c:449:ARG:HG2	2.33	0.63
5:b:60:MET:SD	5:b:63:ILE:HD12	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:122:ILE:CG2	10:h:20:GLY:HA2	2.29	0.63
21:g:162:TRP:O	21:g:166:VAL:HG23	1.98	0.63
22:r:67:TRP:HZ3	22:r:82:GLY:HA2	1.63	0.63
5:B:141:ILE:HG21	25:B:615:CLA:HHC	1.81	0.63
13:L:11:VAL:HG11	14:M:25:ILE:HD12	1.80	0.63
15:O:158:PHE:CD2	15:O:322:LYS:HE3	2.33	0.63
21:G:196:PHE:CE2	24:G:608:CHL:HBC2	2.33	0.63
21:G:202:ALA:HB1	21:G:208:PHE:CD1	2.33	0.63
21:N:49:PRO:O	21:N:55:ARG:HG2	1.99	0.63
2:6:120:GLN:CG	2:6:125:VAL:HA	2.26	0.63
6:c:112:PHE:O	6:c:116:VAL:HG23	1.98	0.63
26:c:518:LHG:O4	25:y:312:CLA:H3A	1.99	0.63
7:d:322:LEU:O	7:d:326:ILE:HG13	1.99	0.63
21:n:94:ARG:NE	21:n:94:ARG:HA	2.12	0.63
22:r:122:THR:OG1	22:r:125:GLN:O	2.16	0.63
2:2:51:TYR:HA	2:2:55:ARG:HD3	1.80	0.63
2:2:117:GLU:HB3	2:2:121:LYS:NZ	2.13	0.63
1:3:49:PRO:O	1:3:55:ARG:HG2	1.99	0.63
1:3:162:TRP:O	1:3:166:VAL:HG23	1.98	0.63
3:4:155:TRP:CE2	25:R:601:CLA:HMB1	2.34	0.63
3:4:229:ILE:HG13	3:4:230:LYS:N	2.13	0.63
6:C:73:ALA:HB2	12:K:26:LEU:HG	1.80	0.63
6:C:168:LEU:HD13	25:C:507:CLA:H43	1.81	0.63
21:G:94:ARG:HG2	21:N:84:GLY:N	2.14	0.63
21:G:204:ASP:HB3	21:G:207:ALA:HB3	1.81	0.63
40:G:617:NEX:H361	40:G:617:NEX:C28	2.29	0.63
21:N:224:PHE:CD1	25:N:602:CLA:H201	2.33	0.63
21:Y:132:PHE:CE1	21:Y:133:LYS:HG3	2.33	0.63
25:Y:304:CLA:O2A	25:Y:304:CLA:H2A	1.99	0.63
22:R:68:LEU:HD11	25:R:602:CLA:O2D	1.98	0.63
1:7:49:PRO:O	1:7:55:ARG:HG2	1.99	0.63
4:a:147:TYR:O	4:a:150:PRO:HD2	1.98	0.63
14:m:26:TYR:CZ	14:m:30:VAL:HG11	2.34	0.63
21:g:57:LYS:HB2	21:g:63:SER:OG	1.98	0.63
25:g:614:CLA:HMC1	25:g:614:CLA:HBC3	1.80	0.63
21:y:132:PHE:CE1	21:y:133:LYS:HG3	2.33	0.63
21:y:202:ALA:HB1	21:y:208:PHE:CD1	2.33	0.63
3:4:224:LEU:O	3:4:227:ALA:HB3	1.98	0.63
5:B:122:ILE:CG2	10:H:20:GLY:HA2	2.29	0.63
5:B:122:ILE:HG21	10:H:20:GLY:HA2	1.81	0.63
21:Y:162:TRP:O	21:Y:166:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:51:TYR:CE2	1:5:209:ALA:HB1	2.33	0.63
1:7:162:TRP:O	1:7:166:VAL:HG23	1.98	0.63
5:b:141:ILE:HG21	25:b:615:CLA:HHC	1.81	0.63
28:k:101:BCR:H332	19:z:12:LEU:HD23	1.78	0.63
20:s:144:GLU:CB	20:s:153:LEU:HD21	2.29	0.63
21:g:94:ARG:NE	21:g:94:ARG:HA	2.12	0.63
21:g:202:ALA:HB1	21:g:208:PHE:CD1	2.33	0.63
25:y:314:CLA:HAA1	25:y:314:CLA:HBD	1.79	0.63
1:3:51:TYR:CE2	1:3:209:ALA:HB1	2.33	0.62
3:4:78:PRO:HG3	3:4:225:LYS:HE2	1.79	0.62
6:C:289:PHE:CE2	25:C:501:CLA:H12	2.34	0.62
6:C:369:LEU:HD11	6:C:388:GLN:OE1	1.99	0.62
7:D:295:ARG:HG3	7:D:297:TYR:HB2	1.81	0.62
21:G:84:GLY:N	21:Y:94:ARG:HG2	2.14	0.62
21:Y:204:ASP:HB3	21:Y:207:ALA:HB3	1.81	0.62
24:Y:302:CHL:H8	24:Y:302:CHL:H143	1.81	0.62
2:6:117:GLU:HB3	2:6:121:LYS:NZ	2.13	0.62
5:b:157:HIS:HE1	25:b:606:CLA:C4A	2.09	0.62
25:b:605:CLA:HMB2	25:b:606:CLA:O2A	1.99	0.62
15:o:130:LYS:CE	15:o:177:PRO:HB2	2.25	0.62
20:s:232:ALA:O	20:s:236:MET:HG2	1.99	0.62
21:g:196:PHE:CE2	24:g:608:CHL:HBC2	2.33	0.62
25:n:603:CLA:H203	24:n:607:CHL:C19	2.29	0.62
21:y:164:THR:HG21	24:y:307:CHL:O1D	1.98	0.62
1:1:202:ALA:HB1	1:1:208:PHE:CD1	2.33	0.62
2:2:130:PRO:CG	2:2:133:PHE:HB2	2.29	0.62
5:B:472:ARG:HA	5:B:479:PHE:CZ	2.33	0.62
8:E:67:THR:O	23:U:102:ARG:HD3	1.99	0.62
21:G:218:ASN:OD1	25:G:611:CLA:HMD2	1.98	0.62
21:Y:49:PRO:O	21:Y:55:ARG:HG2	1.99	0.62
21:Y:231:VAL:HG21	25:Y:314:CLA:CAC	2.30	0.62
22:R:67:TRP:HZ3	22:R:82:GLY:HA2	1.63	0.62
2:6:69:TYR:CD1	2:6:70:LEU:HG	2.35	0.62
25:b:601:CLA:HBB2	28:h:101:BCR:H351	1.81	0.62
6:c:267:SER:HA	17:w:133:LEU:HD23	1.81	0.62
14:m:1:MET:CB	14:m:3:VAL:HG13	2.28	0.62
21:g:132:PHE:CE1	21:g:133:LYS:HG3	2.33	0.62
1:1:57:LYS:HB2	1:1:63:SER:OG	1.98	0.62
24:1:301:CHL:HHC	24:1:301:CHL:HBB1	1.80	0.62
1:3:114:VAL:CG1	1:3:241:LEU:HD11	2.27	0.62
4:A:132:GLU:O	4:A:136:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:94:ARG:NH2	21:G:97:GLU:OE1	2.33	0.62
21:G:172:VAL:HG21	40:G:617:NEX:H34	1.80	0.62
21:N:164:THR:CG2	24:N:606:CHL:HED3	2.28	0.62
24:N:607:CHL:H12	32:Y:321:AJP:C21	2.29	0.62
40:N:617:NEX:H191	40:N:617:NEX:C12	2.30	0.62
1:5:49:PRO:O	1:5:55:ARG:HG2	1.99	0.62
1:7:94:ARG:NH2	1:7:97:GLU:OE1	2.33	0.62
4:a:232:SER:OG	5:b:7:ARG:HD2	2.00	0.62
6:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.80	0.62
24:g:605:CHL:HBB1	24:g:605:CHL:HHC	1.81	0.62
21:n:80:TRP:CE3	39:n:616:LUT:H383	2.33	0.62
21:n:204:ASP:HB3	21:n:207:ALA:HB3	1.81	0.62
1:3:204:ASP:HB3	1:3:207:ALA:HB3	1.81	0.62
5:B:39:LEU:HB3	28:t:101:BCR:C38	2.28	0.62
5:B:157:HIS:HE1	25:B:606:CLA:C4A	2.09	0.62
25:C:511:CLA:HBD	25:C:511:CLA:HAA1	1.81	0.62
14:M:1:MET:CB	14:M:3:VAL:HG13	2.28	0.62
28:T:101:BCR:C38	5:b:39:LEU:HB3	2.28	0.62
20:S:232:ALA:O	20:S:236:MET:HG2	1.99	0.62
21:G:49:PRO:O	21:G:55:ARG:HG2	1.99	0.62
24:N:607:CHL:H142	24:N:607:CHL:C9	2.28	0.62
1:5:94:ARG:NH2	1:5:97:GLU:OE1	2.33	0.62
1:7:202:ALA:HB1	1:7:208:PHE:CD1	2.33	0.62
6:c:255:LYS:HG3	6:c:256:PRO:HD2	1.80	0.62
6:c:304:PRO:O	6:c:305:THR:HB	1.99	0.62
25:s:313:CLA:HAA1	25:s:313:CLA:HBD	1.80	0.62
21:g:94:ARG:NH2	21:g:97:GLU:OE1	2.33	0.62
21:g:94:ARG:HG2	21:n:84:GLY:N	2.14	0.62
21:g:131:TRP:HB3	39:g:616:LUT:H41	1.82	0.62
24:n:607:CHL:H12	32:y:321:AJP:C21	2.29	0.62
25:y:303:CLA:HAB	39:y:317:LUT:H32	1.81	0.62
6:C:279:LEU:HD12	25:C:509:CLA:HED3	1.81	0.62
7:D:13:LYS:HA	7:D:13:LYS:HE2	1.80	0.62
7:D:211:LEU:HA	7:D:214:ILE:HG22	1.80	0.62
18:X:84:LYS:O	18:X:88:LEU:HD23	1.99	0.62
1:5:114:VAL:CG1	1:5:241:LEU:HD11	2.28	0.62
1:5:202:ALA:HB1	1:5:208:PHE:CD1	2.33	0.62
2:6:232:VAL:HG13	2:6:243:GLU:OE1	2.00	0.62
6:c:52:ALA:HB1	25:c:509:CLA:HBB1	1.80	0.62
21:n:51:TYR:CE2	21:n:209:ALA:HB1	2.33	0.62
21:n:94:ARG:NH2	21:n:97:GLU:OE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:164:THR:CG2	24:n:606:CHL:HED3	2.29	0.62
21:n:232:GLN:NE2	25:n:613:CLA:C4D	2.40	0.62
5:B:60:MET:SD	5:B:63:ILE:HD12	2.39	0.62
25:B:605:CLA:HMB2	25:B:606:CLA:O2A	1.99	0.62
26:C:518:LHG:O4	25:Y:312:CLA:H3A	1.99	0.62
7:D:86:LEU:HD13	7:D:91:LEU:HD21	1.80	0.62
15:O:158:PHE:CE2	15:O:322:LYS:HE3	2.33	0.62
25:G:614:CLA:HMC1	25:G:614:CLA:HBC3	1.80	0.62
21:N:204:ASP:HB3	21:N:207:ALA:HB3	1.81	0.62
21:Y:86:SER:OG	25:Y:303:CLA:O1A	2.16	0.62
21:Y:94:ARG:NH2	21:Y:97:GLU:OE1	2.33	0.62
1:5:86:SER:HB3	1:5:92:PHE:HD1	1.65	0.62
4:a:332:HIS:HB3	7:d:322:LEU:HD21	1.80	0.62
6:c:168:LEU:HD13	25:c:507:CLA:H43	1.81	0.62
11:i:23:PHE:HB3	28:i:101:BCR:C3	2.29	0.62
21:g:49:PRO:O	21:g:55:ARG:HG2	1.99	0.62
21:g:131:TRP:HB2	39:g:616:LUT:H21	1.82	0.62
21:n:90:GLU:OE1	21:n:90:GLU:HA	2.00	0.62
21:y:49:PRO:O	21:y:55:ARG:HG2	1.99	0.62
4:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.35	0.62
6:C:267:SER:HA	17:W:133:LEU:HD23	1.81	0.62
6:C:350:ILE:HG21	6:C:359:TRP:HB2	1.82	0.62
21:G:90:GLU:OE1	21:G:90:GLU:HA	2.00	0.62
22:R:173:LEU:CD1	22:R:188:ILE:HG13	2.30	0.62
1:7:57:LYS:HB2	1:7:63:SER:OG	1.98	0.62
3:8:219:GLU:CB	3:8:222:GLU:HB2	2.30	0.62
6:c:289:PHE:CE2	25:c:501:CLA:H12	2.34	0.62
6:c:369:LEU:HD11	6:c:388:GLN:OE1	1.99	0.62
25:c:512:CLA:HBC3	25:c:512:CLA:HHD	1.80	0.62
18:x:84:LYS:O	18:x:88:LEU:HD23	1.99	0.62
25:r:601:CLA:HHB	26:r:618:LHG:H132	1.81	0.62
1:1:86:SER:HB3	1:1:92:PHE:HD1	1.65	0.62
2:2:120:GLN:HB3	2:2:129:GLU:OE2	2.00	0.62
1:3:94:ARG:NH2	1:3:97:GLU:OE1	2.33	0.62
4:A:232:SER:OG	5:B:7:ARG:HD2	2.00	0.62
12:K:53:VAL:CG2	28:Z:101:BCR:H21C	2.30	0.62
14:M:26:TYR:CZ	14:M:30:VAL:HG11	2.34	0.62
3:8:139:PRO:HB2	22:r:280:HIS:NE2	2.15	0.62
4:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.35	0.62
21:n:86:SER:HB3	21:n:92:PHE:HD1	1.65	0.62
22:r:173:LEU:CD1	22:r:188:ILE:HG13	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:ASP:HB3	1:1:207:ALA:HB3	1.81	0.62
2:2:69:TYR:CD1	2:2:70:LEU:HG	2.35	0.62
3:4:222:GLU:HA	3:4:225:LYS:CG	2.30	0.62
25:C:501:CLA:H171	25:C:507:CLA:H122	1.82	0.62
12:K:58:VAL:O	12:K:58:VAL:HG12	1.99	0.62
21:G:86:SER:HB3	21:G:92:PHE:HD1	1.65	0.62
2:6:130:PRO:CG	2:6:133:PHE:HB2	2.29	0.62
5:b:157:HIS:NE2	5:b:164:PRO:HD2	2.15	0.62
25:c:511:CLA:HAA1	25:c:511:CLA:HBD	1.81	0.62
8:e:67:THR:O	23:u:102:ARG:HD3	1.99	0.62
20:s:132:GLU:CG	20:s:251:VAL:HB	2.30	0.62
21:n:49:PRO:O	21:n:55:ARG:HG2	1.99	0.62
24:n:606:CHL:HBC2	24:n:607:CHL:HHD	1.82	0.62
21:y:231:VAL:HG21	25:y:314:CLA:CAC	2.29	0.62
24:y:302:CHL:H143	24:y:302:CHL:H8	1.81	0.62
5:B:141:ILE:HG13	5:B:217:LEU:HD21	1.82	0.62
6:C:163:ILE:O	6:C:167:LEU:HD23	2.00	0.62
6:C:288:CYS:SG	35:C:515:DGD:HB32	2.40	0.62
10:H:56:ILE:CD1	18:X:84:LYS:HE3	2.16	0.62
20:S:144:GLU:CB	20:S:153:LEU:HD21	2.29	0.62
20:S:218:GLY:O	20:S:222:LYS:HG3	2.00	0.62
21:Y:86:SER:HB3	21:Y:92:PHE:HD1	1.65	0.62
21:Y:90:GLU:OE1	21:Y:90:GLU:HA	2.00	0.62
21:Y:215:GLU:HG3	25:Y:311:CLA:C1B	2.30	0.62
2:6:100:VAL:HG22	2:6:216:GLU:OE2	2.00	0.62
3:8:205:LEU:HB3	3:8:220:LYS:NZ	2.15	0.62
4:a:81:ALA:HB2	4:a:175:GLY:HA3	1.82	0.62
25:b:609:CLA:HAA1	10:h:43:MET:SD	2.40	0.62
25:c:507:CLA:H142	28:i:101:BCR:H362	1.81	0.62
7:d:305:ARG:HD3	14:m:1:MET:HE1	1.82	0.62
15:o:285:ILE:HG12	15:o:287:LEU:HD11	1.82	0.62
40:g:617:NEX:H361	40:g:617:NEX:C28	2.29	0.62
22:r:283:ILE:HG13	25:r:612:CLA:HMD3	1.81	0.62
1:1:94:ARG:NH2	1:1:97:GLU:OE1	2.33	0.61
1:1:138:ILE:CD1	24:1:302:CHL:HMD3	2.30	0.61
2:2:117:GLU:HG3	2:2:239:LYS:HD3	1.82	0.61
2:2:232:VAL:HG13	2:2:243:GLU:OE1	2.00	0.61
3:4:139:PRO:HB2	22:R:280:HIS:NE2	2.15	0.61
6:C:199:ILE:HG23	6:C:231:GLU:HG3	1.82	0.61
7:D:305:ARG:HH11	14:M:1:MET:HE2	1.65	0.61
11:I:6:LEU:HD23	17:W:101:LEU:HD23	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:90:GLU:OE1	21:N:90:GLU:HA	2.00	0.61
22:R:172:GLU:OE1	22:R:177:SER:HA	2.00	0.61
22:R:283:ILE:HG13	25:R:612:CLA:HMD3	1.81	0.61
25:R:601:CLA:HHB	26:R:618:LHG:H132	1.81	0.61
1:5:138:ILE:CD1	24:5:302:CHL:HMD3	2.30	0.61
6:c:199:ILE:HG23	6:c:231:GLU:HG3	1.82	0.61
6:c:251:HIS:CE1	25:c:506:CLA:HMA3	2.35	0.61
6:c:288:CYS:SG	35:c:515:DGD:HB32	2.40	0.61
25:c:501:CLA:H171	25:c:507:CLA:H122	1.82	0.61
7:d:295:ARG:HG3	7:d:297:TYR:HB2	1.81	0.61
12:k:53:VAL:CG2	28:z:101:BCR:H21C	2.30	0.61
28:t:101:BCR:H292	28:t:101:BCR:C36	2.29	0.61
24:n:607:CHL:H202	24:n:609:CHL:C4	2.30	0.61
21:y:94:ARG:NH2	21:y:97:GLU:OE1	2.33	0.61
22:r:172:GLU:OE1	22:r:177:SER:HA	2.00	0.61
3:4:205:LEU:HB3	3:4:220:LYS:NZ	2.15	0.61
3:4:222:GLU:HG2	3:4:225:LYS:CD	2.27	0.61
14:M:15:ILE:O	14:M:19:THR:OG1	2.18	0.61
21:N:94:ARG:NH2	21:N:97:GLU:OE1	2.33	0.61
27:a:404:PHO:HBB1	27:a:404:PHO:CMB	2.30	0.61
11:i:6:LEU:HD23	17:w:101:LEU:HD23	1.80	0.61
21:y:204:ASP:HB3	21:y:207:ALA:HB3	1.81	0.61
1:1:90:GLU:OE1	1:1:90:GLU:HA	2.00	0.61
2:2:96:ARG:O	2:2:100:VAL:HG23	2.00	0.61
24:2:601:CHL:CGD	26:2:606:LHG:H142	2.30	0.61
5:B:153:PHE:O	5:B:158:VAL:HG23	2.00	0.61
7:D:133:LEU:O	7:D:137:VAL:HG22	2.01	0.61
21:G:215:GLU:CG	25:G:610:CLA:C1B	2.78	0.61
25:R:601:CLA:C4D	26:R:618:LHG:H102	2.03	0.61
2:6:181:LEU:HD13	24:6:603:CHL:CAB	2.30	0.61
24:6:601:CHL:CGD	26:6:606:LHG:H142	2.30	0.61
21:g:84:GLY:N	21:y:94:ARG:HG2	2.14	0.61
21:g:215:GLU:CG	25:g:610:CLA:C1B	2.78	0.61
25:n:613:CLA:HMC3	25:n:613:CLA:HBC2	1.81	0.61
21:y:224:PHE:HE2	25:y:314:CLA:HAB	1.65	0.61
2:2:100:VAL:HG22	2:2:216:GLU:OE2	2.00	0.61
3:4:219:GLU:CB	3:4:222:GLU:HB2	2.30	0.61
4:A:290:ILE:HG13	25:A:401:CLA:HED3	1.80	0.61
5:B:75:TRP:CD1	5:B:92:SER:HG	2.19	0.61
7:D:322:LEU:O	7:D:326:ILE:HG13	1.99	0.61
20:S:196:PHE:HD2	24:S:308:CHL:HBC3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:208:PHE:CE2	21:G:212:LYS:HE3	2.36	0.61
21:Y:231:VAL:CG1	25:Y:314:CLA:HHD	2.31	0.61
22:R:139:CYS:O	22:R:143:HIS:ND1	2.29	0.61
2:6:117:GLU:HG3	2:6:239:LYS:HD3	1.82	0.61
6:c:279:LEU:HD12	25:c:509:CLA:HED3	1.81	0.61
15:o:190:GLU:OE2	15:o:216:LYS:HA	1.99	0.61
1:1:208:PHE:CE2	1:1:212:LYS:HE3	2.36	0.61
1:3:78:TYR:OH	1:3:217:LYS:NZ	2.20	0.61
6:C:237:HIS:HE1	25:C:501:CLA:ND	1.98	0.61
21:G:215:GLU:HB2	25:G:610:CLA:C2B	2.30	0.61
24:Y:307:CHL:HMB2	24:Y:310:CHL:OMC	2.01	0.61
22:R:178:SER:OG	22:R:183:PRO:HA	2.00	0.61
22:R:274:HIS:O	22:R:278:PRO:HA	2.01	0.61
2:6:221:ARG:NH1	2:6:222:LEU:HD21	2.16	0.61
3:8:222:GLU:HA	3:8:225:LYS:CG	2.30	0.61
5:b:122:ILE:HG21	10:h:20:GLY:HA2	1.81	0.61
6:c:153:ASP:O	6:c:157:MET:HG2	2.00	0.61
6:c:350:ILE:HG21	6:c:359:TRP:HB2	1.82	0.61
10:h:18:THR:O	10:h:21:LYS:HB2	2.00	0.61
20:s:196:PHE:CD2	24:s:308:CHL:HBC3	2.36	0.61
21:y:215:GLU:HG3	25:y:311:CLA:C1B	2.30	0.61
3:4:142:PHE:CZ	3:4:146:LEU:HD11	2.36	0.61
5:B:282:GLN:NE2	23:U:100:ILE:HD11	2.15	0.61
15:O:227:PHE:CE2	15:O:287:LEU:HD13	2.36	0.61
20:S:182:LEU:HD23	24:S:306:CHL:HMA1	1.82	0.61
20:S:196:PHE:CD2	24:S:308:CHL:HBC3	2.36	0.61
20:S:267:LEU:HD13	25:S:314:CLA:HED1	1.81	0.61
21:G:199:LEU:HG	39:G:615:LUT:H221	1.83	0.61
24:G:601:CHL:HMD3	26:Y:301:LHG:HC61	1.83	0.61
25:Y:303:CLA:HBA1	39:Y:317:LUT:H382	1.83	0.61
1:5:97:GLU:CG	1:5:190:LEU:HD21	2.20	0.61
1:5:208:PHE:CE2	1:5:212:LYS:HE3	2.36	0.61
2:6:104:ARG:NE	24:6:603:CHL:CBD	2.55	0.61
1:7:191:TYR:CE2	1:7:212:LYS:HE2	2.36	0.61
4:a:235:GLU:HB3	7:d:264:ASN:ND2	2.08	0.61
6:c:227:VAL:HG21	28:i:101:BCR:H292	1.82	0.61
21:g:215:GLU:HB2	25:g:610:CLA:C2B	2.30	0.61
21:y:191:TYR:CE2	21:y:212:LYS:HE2	2.36	0.61
1:3:86:SER:HB3	1:3:92:PHE:HD1	1.65	0.61
5:B:161:LEU:HD21	30:B:623:LMG:C2	2.31	0.61
5:B:272:ARG:NH2	42:B:702:HOH:O	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:K:101:BCR:H343	19:Z:13:ILE:HD13	1.81	0.61
21:N:191:TYR:CE2	21:N:212:LYS:HE2	2.36	0.61
21:N:208:PHE:CE2	21:N:212:LYS:HE3	2.36	0.61
2:6:208:THR:O	2:6:212:LEU:HG	2.01	0.61
1:7:90:GLU:OE1	1:7:90:GLU:HA	2.00	0.61
5:b:141:ILE:HG13	5:b:217:LEU:HD21	1.82	0.61
7:d:86:LEU:HD13	7:d:91:LEU:HD21	1.80	0.61
21:g:204:ASP:HB3	21:g:207:ALA:HB3	1.81	0.61
21:g:208:PHE:CE2	21:g:212:LYS:HE3	2.36	0.61
24:g:601:CHL:HMD3	26:y:301:LHG:HC61	1.83	0.61
25:B:609:CLA:HAA1	10:H:43:MET:SD	2.40	0.61
26:C:518:LHG:H352	25:Y:315:CLA:HBB1	1.82	0.61
10:H:18:THR:O	10:H:21:LYS:HB2	2.00	0.61
20:S:113:PHE:HE1	25:S:304:CLA:HBD	1.66	0.61
21:G:131:TRP:HB2	39:G:616:LUT:H21	1.82	0.61
2:6:224:MET:HG2	25:6:602:CLA:HMC3	1.83	0.61
1:7:204:ASP:HB3	1:7:207:ALA:HB3	1.81	0.61
3:8:221:LEU:HA	3:8:224:LEU:HD21	1.82	0.61
4:a:172:MET:CE	25:a:403:CLA:HBC2	2.30	0.61
26:c:518:LHG:H352	25:y:315:CLA:HBB1	1.82	0.61
28:k:101:BCR:H343	19:z:13:ILE:HD13	1.81	0.61
15:o:143:PHE:CD2	17:w:81:VAL:HG11	2.36	0.61
20:s:196:PHE:HD2	24:s:308:CHL:HBC3	1.65	0.61
21:g:191:TYR:CE2	21:g:212:LYS:HE2	2.36	0.61
25:n:603:CLA:H203	24:n:607:CHL:H172	1.82	0.61
22:r:103:LYS:HG2	22:r:105:LEU:HD11	1.83	0.61
2:2:221:ARG:NH1	2:2:222:LEU:HD21	2.16	0.61
3:4:157:GLU:HG3	3:4:161:TRP:HE1	1.66	0.61
4:A:219:VAL:HG13	4:A:246:TYR:CD1	2.36	0.61
27:A:403:PHO:HBB1	27:A:403:PHO:CMB	2.30	0.61
25:A:405:CLA:HMC1	11:I:11:VAL:CG1	2.30	0.61
5:B:157:HIS:NE2	5:B:164:PRO:HD2	2.15	0.61
5:B:157:HIS:HB2	25:B:606:CLA:C4C	2.31	0.61
5:B:346:PHE:O	5:B:354:LEU:N	2.32	0.61
6:C:153:ASP:O	6:C:157:MET:HG2	2.00	0.61
7:D:30:PHE:O	7:D:129:ARG:NH1	2.33	0.61
7:D:127:MET:SD	7:D:151:ILE:HD12	2.41	0.61
11:I:24:LEU:HD13	28:I:101:BCR:HC41	1.83	0.61
15:O:285:ILE:HG12	15:O:287:LEU:HD11	1.82	0.61
20:S:132:GLU:CG	20:S:251:VAL:HB	2.30	0.61
21:G:131:TRP:HB3	39:G:616:LUT:H41	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:86:SER:HB3	21:N:92:PHE:HD1	1.65	0.61
21:N:199:LEU:HG	39:N:615:LUT:H221	1.83	0.61
24:N:607:CHL:H202	24:N:609:CHL:C4	2.30	0.61
25:Y:303:CLA:HAB	39:Y:317:LUT:H32	1.81	0.61
22:R:103:LYS:HG2	22:R:105:LEU:HD11	1.83	0.61
1:5:90:GLU:HA	1:5:90:GLU:OE1	2.00	0.61
1:5:138:ILE:HD11	24:5:302:CHL:HMD3	1.83	0.61
2:6:96:ARG:O	2:6:100:VAL:HG23	2.00	0.61
2:6:120:GLN:HB3	2:6:129:GLU:OE2	2.00	0.61
29:a:412:SQD:H131	16:t:21:ILE:HD12	1.82	0.61
6:c:237:HIS:HE1	25:c:501:CLA:ND	1.98	0.61
6:c:279:LEU:HD12	25:c:509:CLA:CED	2.31	0.61
20:s:267:LEU:HD13	25:s:314:CLA:HED1	1.81	0.61
21:g:86:SER:HB3	21:g:92:PHE:HD1	1.65	0.61
21:g:199:LEU:HG	39:g:615:LUT:H221	1.83	0.61
21:n:94:ARG:HG2	21:y:84:GLY:CA	2.31	0.61
21:y:86:SER:HB3	21:y:92:PHE:HD1	1.65	0.61
1:3:191:TYR:CE2	1:3:212:LYS:HE2	2.36	0.61
4:A:81:ALA:HB2	4:A:175:GLY:HA3	1.82	0.61
22:R:199:ILE:HA	22:R:202:ILE:HG12	1.83	0.61
1:5:191:TYR:CE2	1:5:212:LYS:HE2	2.36	0.61
3:8:157:GLU:HA	3:8:160:ARG:HG2	1.82	0.61
4:a:239:PHE:HB3	16:t:28:LYS:HG3	1.83	0.61
5:b:161:LEU:HD21	30:b:623:LMG:C2	2.31	0.61
5:b:392:VAL:HG13	5:b:397:VAL:CG2	2.31	0.61
12:k:58:VAL:O	12:k:58:VAL:HG12	1.99	0.61
15:o:227:PHE:CE2	15:o:287:LEU:HD13	2.36	0.61
21:n:199:LEU:HG	39:n:615:LUT:H221	1.83	0.61
1:1:114:VAL:CG1	1:1:241:LEU:HD11	2.28	0.60
1:1:191:TYR:CE2	1:1:212:LYS:HE2	2.36	0.60
6:C:269:GLU:HG2	6:C:448:ALA:HB2	1.83	0.60
11:I:34:ARG:O	11:I:35:GLU:HG3	2.01	0.60
25:Y:315:CLA:HAA1	25:Y:315:CLA:HED2	1.82	0.60
1:5:204:ASP:HB3	1:5:207:ALA:HB3	1.81	0.60
3:8:142:PHE:CZ	3:8:146:LEU:HD11	2.36	0.60
3:8:205:LEU:HB3	3:8:220:LYS:HZ3	1.64	0.60
27:a:404:PHO:H41	29:a:412:SQD:H192	1.83	0.60
5:b:272:ARG:NH2	42:b:702:HOH:O	2.11	0.60
7:d:133:LEU:O	7:d:137:VAL:HG22	2.01	0.60
21:g:112:GLY:HA3	25:g:604:CLA:CHC	2.31	0.60
21:y:138:ILE:HD13	24:y:307:CHL:HBC3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:58:TYR:OH	24:2:601:CHL:HAA2	2.01	0.60
5:B:71:ILE:HD13	25:B:606:CLA:HED3	1.84	0.60
5:B:272:ARG:HG3	5:B:320:ALA:HB2	1.83	0.60
6:C:279:LEU:HD12	25:C:509:CLA:CED	2.31	0.60
25:D:403:CLA:H162	18:X:92:SER:OG	2.01	0.60
21:N:94:ARG:HG2	21:Y:84:GLY:CA	2.31	0.60
21:Y:191:TYR:CE2	21:Y:212:LYS:HE2	2.36	0.60
21:Y:208:PHE:CE2	21:Y:212:LYS:HE3	2.36	0.60
22:R:85:LYS:CG	22:R:86:PRO:HD2	2.31	0.60
22:R:220:GLY:HA2	22:R:224:ASP:H	1.65	0.60
22:R:220:GLY:HA3	22:R:224:ASP:HB3	1.83	0.60
2:6:172:LEU:O	2:6:176:PHE:HD2	1.84	0.60
1:7:86:SER:HB3	1:7:92:PHE:HD1	1.65	0.60
3:8:84:ASP:OD2	3:8:87:GLY:HA2	2.02	0.60
5:b:327:ALA:HB1	30:b:620:LMG:HC8	1.83	0.60
20:s:237:LEU:O	20:s:241:ILE:HD12	2.01	0.60
24:n:609:CHL:HHC	24:n:609:CHL:HBB1	1.82	0.60
25:y:303:CLA:HBA1	39:y:317:LUT:H382	1.83	0.60
25:r:603:CLA:C1D	25:r:608:CLA:H92	1.95	0.60
2:2:208:THR:O	2:2:212:LEU:HG	2.01	0.60
4:A:172:MET:CE	25:A:402:CLA:HBC2	2.30	0.60
21:G:191:TYR:CE2	21:G:212:LYS:HE2	2.36	0.60
25:N:603:CLA:H203	24:N:607:CHL:H172	1.82	0.60
22:R:258:VAL:HB	25:R:612:CLA:HHD	1.83	0.60
2:6:58:TYR:OH	24:6:601:CHL:HAA2	2.01	0.60
1:7:208:PHE:CE2	1:7:212:LYS:HE3	2.36	0.60
4:a:328:MET:HG2	7:d:326:ILE:CG1	2.31	0.60
5:b:157:HIS:HB2	25:b:606:CLA:C4C	2.31	0.60
5:b:282:GLN:NE2	23:u:100:ILE:HD11	2.15	0.60
7:d:236:PHE:HD1	7:d:244:THR:HG21	1.66	0.60
24:g:606:CHL:CBA	40:g:617:NEX:H403	2.31	0.60
21:n:208:PHE:CE2	21:n:212:LYS:HE3	2.36	0.60
21:y:90:GLU:OE1	21:y:90:GLU:HA	2.00	0.60
22:r:247:ARG:HD3	25:r:602:CLA:CHD	2.31	0.60
2:2:107:MET:HG2	2:2:111:PHE:HE2	1.67	0.60
2:2:172:LEU:O	2:2:176:PHE:HD2	1.84	0.60
1:3:90:GLU:OE1	1:3:90:GLU:HA	2.00	0.60
6:C:251:HIS:CE1	25:C:506:CLA:HMA3	2.35	0.60
25:C:512:CLA:H192	26:S:301:LHG:H222	1.83	0.60
7:D:305:ARG:HD3	14:M:1:MET:HE1	1.82	0.60
15:O:232:LEU:O	15:O:234:PRO:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:603:CLA:H203	24:N:607:CHL:H193	1.84	0.60
22:R:100:ASN:OD1	22:R:101:LEU:N	2.34	0.60
22:R:103:LYS:HG2	22:R:105:LEU:CD1	2.32	0.60
22:R:185:PRO:HB3	21:y:151:SER:OG	2.01	0.60
3:8:222:GLU:HG2	3:8:225:LYS:CD	2.27	0.60
4:a:129:ARG:NH2	7:d:257:ILE:O	2.34	0.60
6:c:163:ILE:O	6:c:167:LEU:HD23	2.00	0.60
6:c:269:GLU:HG2	6:c:448:ALA:HB2	1.83	0.60
7:d:127:MET:SD	7:d:151:ILE:HD12	2.41	0.60
7:d:280:LEU:HD21	25:d:402:CLA:HBA2	1.83	0.60
7:d:305:ARG:HH11	14:m:1:MET:HE2	1.65	0.60
4:A:239:PHE:HB3	16:T:28:LYS:HG3	1.83	0.60
4:A:259:ILE:HG23	4:A:259:ILE:O	2.02	0.60
27:A:403:PHO:H41	29:A:411:SQD:H192	1.83	0.60
21:Y:97:GLU:CG	21:Y:190:LEU:HD21	2.20	0.60
2:6:139:ILE:O	2:6:139:ILE:HG22	2.01	0.60
5:b:153:PHE:O	5:b:158:VAL:HG23	2.00	0.60
21:n:158:ILE:CD1	21:y:257:TRP:HE3	2.11	0.60
21:y:208:PHE:CE2	21:y:212:LYS:HE3	2.36	0.60
25:y:315:CLA:HED2	25:y:315:CLA:HAA1	1.82	0.60
22:r:100:ASN:OD1	22:r:101:LEU:N	2.34	0.60
22:r:258:VAL:HB	25:r:612:CLA:HHD	1.83	0.60
2:2:139:ILE:O	2:2:139:ILE:HG22	2.01	0.60
2:2:224:MET:HG2	25:2:602:CLA:HMC3	1.82	0.60
1:3:208:PHE:CE2	1:3:212:LYS:HE3	2.36	0.60
3:4:157:GLU:HA	3:4:160:ARG:HG2	1.82	0.60
5:B:392:VAL:HG13	5:B:397:VAL:CG2	2.31	0.60
16:T:7:THR:HG21	28:T:101:BCR:H363	1.84	0.60
21:G:215:GLU:HB2	25:G:610:CLA:CHB	2.31	0.60
21:Y:224:PHE:HE2	25:Y:314:CLA:HAB	1.65	0.60
22:R:247:ARG:HD3	25:R:602:CLA:CHD	2.31	0.60
1:7:97:GLU:CG	1:7:190:LEU:HD21	2.20	0.60
11:i:24:LEU:HD13	28:i:101:BCR:HC41	1.83	0.60
15:o:232:LEU:O	15:o:234:PRO:HD3	2.02	0.60
20:s:182:LEU:HD23	24:s:306:CHL:HMA1	1.83	0.60
21:g:90:GLU:OE1	21:g:90:GLU:HA	2.00	0.60
21:n:191:TYR:CE2	21:n:212:LYS:HE2	2.36	0.60
22:r:103:LYS:HG2	22:r:105:LEU:CD1	2.32	0.60
2:2:145:LEU:CD2	2:2:154:VAL:HG22	2.26	0.60
5:B:47:PRO:HG3	5:B:78:TRP:CE2	2.36	0.60
5:B:327:ALA:HB1	30:B:620:LMG:HC8	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:507:CLA:H142	28:I:101:BCR:H362	1.81	0.60
9:F:21:ALA:HB1	38:F:101:HEM:HAC	1.84	0.60
21:Y:172:VAL:HG21	40:Y:318:NEX:H34	1.84	0.60
4:a:259:ILE:HG23	4:a:259:ILE:O	2.02	0.60
7:d:157:VAL:HG12	7:d:172:PRO:HG2	1.84	0.60
20:s:113:PHE:HE1	25:s:304:CLA:HBD	1.66	0.60
21:y:231:VAL:CG1	25:y:314:CLA:HHD	2.31	0.60
22:r:220:GLY:HA2	22:r:224:ASP:H	1.65	0.60
2:2:179:ASN:ND2	2:2:188:ASN:O	2.35	0.60
2:2:193:GLY:HA2	2:2:197:PHE:CD2	2.34	0.60
3:4:84:ASP:OD2	3:4:87:GLY:HA2	2.02	0.60
3:4:174:TRP:HE3	3:4:180:LYS:HD2	1.63	0.60
29:A:411:SQD:H131	16:T:21:ILE:HD12	1.82	0.60
6:C:215:LYS:CG	6:C:221:GLU:HB3	2.31	0.60
6:C:225:VAL:HG22	6:C:289:PHE:CD1	2.37	0.60
6:C:285:ILE:HG22	6:C:289:PHE:CZ	2.37	0.60
15:O:143:PHE:CD2	17:W:81:VAL:HG11	2.36	0.60
20:S:237:LEU:O	20:S:241:ILE:HD12	2.01	0.60
24:G:606:CHL:CBA	40:G:617:NEX:H403	2.31	0.60
22:R:144:GLY:O	22:R:148:MET:HG3	2.02	0.60
22:R:253:PHE:CZ	41:R:616:XAT:H10	2.37	0.60
2:6:179:ASN:ND2	2:6:188:ASN:O	2.35	0.60
4:a:77:ILE:HD13	13:l:30:VAL:HG13	1.84	0.60
4:a:219:VAL:HG13	4:a:246:TYR:CD1	2.36	0.60
5:b:47:PRO:HG3	5:b:78:TRP:CE2	2.36	0.60
5:b:388:SER:HA	7:d:345:GLU:CD	2.26	0.60
21:g:100:VAL:HG21	21:g:190:LEU:HD13	1.84	0.60
21:g:215:GLU:HB2	25:g:610:CLA:CHB	2.31	0.60
21:n:169:MET:HG3	24:n:609:CHL:CMC	2.32	0.60
22:r:178:SER:OG	22:r:183:PRO:HA	2.00	0.60
1:1:138:ILE:HD11	24:1:302:CHL:HMD3	1.83	0.60
1:3:100:VAL:HG21	1:3:190:LEU:HD13	1.84	0.60
4:A:222:SER:OG	4:A:246:TYR:HB2	2.02	0.60
4:A:248:ILE:HD13	4:A:268:SER:OG	2.02	0.60
4:A:328:MET:HG2	7:D:326:ILE:CG1	2.31	0.60
6:C:175:LEU:HD22	25:C:501:CLA:C3D	2.32	0.60
19:Z:3:ILE:O	19:Z:7:LEU:HD23	2.02	0.60
21:Y:151:SER:OG	22:r:185:PRO:HB3	2.01	0.60
4:a:248:ILE:HD13	4:a:268:SER:OG	2.02	0.60
6:c:87:ILE:HD13	25:c:504:CLA:HMB2	1.84	0.60
6:c:91:HIS:O	6:c:95:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:t:7:THR:HG21	28:t:101:BCR:H363	1.84	0.60
2:2:111:PHE:O	2:2:115:THR:HG23	2.02	0.60
4:A:235:GLU:OE1	7:D:264:ASN:ND2	2.35	0.60
30:A:408:LMG:HC61	6:C:221:GLU:OE2	2.02	0.60
5:B:333:GLY:O	5:B:441:GLY:N	2.34	0.60
21:G:112:GLY:HA3	25:G:604:CLA:CHC	2.31	0.60
21:N:67:PRO:CG	21:N:70:LEU:HD12	2.29	0.60
24:N:606:CHL:HBC2	24:N:607:CHL:HHD	1.82	0.60
25:N:613:CLA:HMC1	25:N:613:CLA:HBC3	1.83	0.60
2:6:107:MET:HG2	2:6:111:PHE:HE2	1.67	0.60
3:8:138:ALA:HB3	3:8:140:PHE:CD2	2.37	0.60
6:c:215:LYS:CG	6:c:221:GLU:HB3	2.31	0.60
22:r:144:GLY:O	22:r:148:MET:HG3	2.02	0.60
23:u:84:ALA:HB1	23:u:100:ILE:CG2	2.31	0.60
4:A:179:THR:HG21	25:A:402:CLA:CHD	2.32	0.59
5:B:336:ILE:HG22	5:B:336:ILE:O	2.02	0.59
6:C:327:ASN:HD22	6:C:330:SER:HB2	1.67	0.59
24:N:609:CHL:HHC	24:N:609:CHL:HBB1	1.82	0.59
25:N:610:CLA:CBB	25:N:612:CLA:H3A	2.32	0.59
22:R:93:ASP:O	22:R:107:GLY:HA3	2.02	0.59
22:R:150:ALA:HA	41:R:616:XAT:C18	2.32	0.59
2:6:184:VAL:HB	2:6:196:TYR:CE2	2.33	0.59
4:a:235:GLU:OE1	7:d:264:ASN:ND2	2.35	0.59
30:a:409:LMG:HC61	6:c:221:GLU:OE2	2.02	0.59
29:l:102:SQD:H312	14:m:17:VAL:HG13	1.84	0.59
21:n:138:ILE:HD12	21:n:144:LEU:CD1	2.33	0.59
25:n:610:CLA:CBB	25:n:612:CLA:H3A	2.32	0.59
24:y:307:CHL:HMB2	24:y:310:CHL:OMC	2.01	0.59
22:r:274:HIS:O	22:r:278:PRO:HA	2.01	0.59
6:C:87:ILE:HD13	25:C:504:CLA:HMB2	1.84	0.59
15:O:100:LYS:HE3	15:O:105:VAL:HG22	1.84	0.59
25:N:602:CLA:HMC1	39:N:616:LUT:C31	2.32	0.59
21:Y:111:LEU:HD23	25:Y:305:CLA:HMC2	1.84	0.59
21:Y:138:ILE:HD13	24:Y:307:CHL:HBC3	1.83	0.59
1:5:100:VAL:HG21	1:5:190:LEU:HD13	1.84	0.59
2:6:214:VAL:HA	2:6:217:ILE:CD1	2.32	0.59
4:a:45:THR:HG23	25:a:403:CLA:H201	1.84	0.59
5:b:467:ILE:HG21	7:d:127:MET:CE	2.32	0.59
25:b:607:CLA:H171	25:b:613:CLA:C16	2.23	0.59
6:c:285:ILE:HG22	6:c:289:PHE:CZ	2.37	0.59
6:c:327:ASN:HD22	6:c:330:SER:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:511:CLA:H142	12:k:47:PHE:CE2	2.37	0.59
25:c:512:CLA:H192	26:s:301:LHG:H222	1.84	0.59
25:d:403:CLA:H162	18:x:92:SER:OG	2.01	0.59
2:2:214:VAL:HA	2:2:217:ILE:CD1	2.32	0.59
4:A:328:MET:CG	7:D:326:ILE:HG12	2.33	0.59
6:C:91:HIS:O	6:C:95:LEU:HD13	2.02	0.59
6:C:131:TYR:CE1	6:C:135:LEU:HD22	2.38	0.59
7:D:157:VAL:HG12	7:D:172:PRO:HG2	1.84	0.59
7:D:236:PHE:HD1	7:D:244:THR:HG21	1.66	0.59
21:N:169:MET:HG3	24:N:609:CHL:CMC	2.32	0.59
3:8:78:PRO:HB2	3:8:229:ILE:CG2	2.32	0.59
7:d:56:VAL:O	7:d:67:SER:HB3	2.02	0.59
11:i:34:ARG:O	11:i:35:GLU:HG3	2.01	0.59
20:s:119:ARG:HH11	25:s:310:CLA:CHD	2.15	0.59
20:s:218:GLY:O	20:s:222:LYS:HG3	2.00	0.59
21:g:244:LEU:HD22	39:g:615:LUT:H163	1.84	0.59
21:n:100:VAL:HG21	21:n:190:LEU:HD13	1.84	0.59
25:n:603:CLA:H191	24:n:607:CHL:H122	1.84	0.59
2:2:181:LEU:HD13	24:2:603:CHL:CAB	2.30	0.59
1:3:229:PHE:CD2	1:3:240:PRO:HB3	2.38	0.59
25:C:510:CLA:HHD	25:C:510:CLA:HBC3	1.84	0.59
20:S:119:ARG:HH11	25:S:310:CLA:CHD	2.15	0.59
21:G:244:LEU:HD22	39:G:615:LUT:H163	1.84	0.59
2:6:127:PHE:O	2:6:128:LYS:HG3	2.03	0.59
2:6:155:HIS:HE1	2:6:158:SER:HA	1.67	0.59
5:b:241:SER:O	5:b:245:VAL:HG23	2.02	0.59
5:b:272:ARG:HG3	5:b:320:ALA:HB2	1.83	0.59
21:y:97:GLU:CG	21:y:190:LEU:HD21	2.20	0.59
21:y:153:VAL:HG13	24:y:306:CHL:CHD	2.32	0.59
22:r:150:ALA:HA	41:r:616:XAT:C18	2.32	0.59
22:r:199:ILE:HA	22:r:202:ILE:HG12	1.83	0.59
20:S:169:ILE:HG13	24:S:306:CHL:OBD	2.03	0.59
20:S:223:VAL:O	20:S:226:ILE:HG22	2.03	0.59
21:Y:67:PRO:CG	21:Y:70:LEU:HD12	2.29	0.59
4:a:19:ASN:O	4:a:23:SER:HB2	2.03	0.59
5:b:71:ILE:HD13	25:b:606:CLA:HED3	1.84	0.59
25:n:603:CLA:H203	24:n:607:CHL:H193	1.84	0.59
21:y:111:LEU:HD23	25:y:305:CLA:HMC2	1.84	0.59
22:r:93:ASP:O	22:r:107:GLY:HA3	2.02	0.59
22:r:253:PHE:CZ	41:r:616:XAT:H10	2.37	0.59
1:1:229:PHE:CD2	1:1:240:PRO:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:121:LYS:NZ	2:2:241:PRO:HB2	2.17	0.59
3:4:78:PRO:HB2	3:4:229:ILE:CG2	2.32	0.59
3:4:138:ALA:HB3	3:4:140:PHE:CD2	2.37	0.59
4:A:331:MET:HE2	7:D:321:LEU:HB3	1.83	0.59
5:B:241:SER:O	5:B:245:VAL:HG23	2.02	0.59
5:B:388:SER:HA	7:D:345:GLU:CD	2.26	0.59
6:C:227:VAL:HG21	28:I:101:BCR:H292	1.82	0.59
6:C:449:ARG:HH12	11:I:28:PRO:CG	2.16	0.59
25:C:511:CLA:H102	19:Z:24:PRO:HB3	1.83	0.59
20:S:83:GLU:OE2	20:S:96:ASP:HB3	2.03	0.59
25:N:603:CLA:H191	24:N:607:CHL:H122	1.84	0.59
21:Y:100:VAL:HG21	21:Y:190:LEU:HD13	1.84	0.59
4:a:222:SER:OG	4:a:246:TYR:HB2	2.02	0.59
6:c:225:VAL:HG22	6:c:289:PHE:CD1	2.37	0.59
15:o:158:PHE:CE2	15:o:322:LYS:HB2	2.36	0.59
18:x:97:LEU:O	18:x:101:ILE:HG12	2.01	0.59
25:y:304:CLA:H2A	25:y:304:CLA:O2A	1.99	0.59
22:r:220:GLY:HA3	22:r:224:ASP:HB3	1.83	0.59
2:2:121:LYS:HZ2	2:2:241:PRO:HB2	1.68	0.59
2:2:127:PHE:O	2:2:128:LYS:HG3	2.03	0.59
3:4:146:LEU:O	3:4:150:LEU:HG	2.03	0.59
4:A:129:ARG:NH2	7:D:257:ILE:O	2.34	0.59
4:A:158:PHE:O	4:A:162:PRO:HG2	2.03	0.59
4:A:192:ILE:HD13	25:A:401:CLA:C1D	2.32	0.59
25:C:511:CLA:H142	12:K:47:PHE:CE2	2.37	0.59
15:O:158:PHE:CE2	15:O:322:LYS:HB2	2.36	0.59
18:X:97:LEU:O	18:X:101:ILE:HG12	2.01	0.59
20:S:141:CYS:C	20:S:143:PRO:HA	2.28	0.59
21:G:67:PRO:CG	21:G:70:LEU:HD12	2.29	0.59
21:Y:153:VAL:HG13	24:Y:306:CHL:CHD	2.32	0.59
2:6:112:GLY:O	2:6:116:PRO:HD3	2.03	0.59
1:7:229:PHE:CD2	1:7:240:PRO:HB3	2.38	0.59
4:a:192:ILE:HD13	25:a:402:CLA:C1D	2.33	0.59
6:c:175:LEU:HD22	25:c:501:CLA:C3D	2.32	0.59
25:c:511:CLA:H102	19:z:24:PRO:HB3	1.83	0.59
20:s:141:CYS:C	20:s:143:PRO:HA	2.28	0.59
20:s:169:ILE:HG13	24:s:306:CHL:OBD	2.03	0.59
20:s:223:VAL:O	20:s:226:ILE:HG22	2.03	0.59
22:r:240:LEU:O	22:r:243:ILE:HG22	2.03	0.59
3:4:221:LEU:HA	3:4:224:LEU:HD21	1.82	0.59
4:A:127:MET:HG3	4:A:144:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:28:GLN:OE1	7:D:231:ASN:ND2	2.35	0.59
6:C:66:ALA:N	6:C:119:LEU:HD21	2.18	0.59
6:C:154:ARG:HB3	6:C:256:PRO:HG2	1.85	0.59
6:C:369:LEU:CD2	6:C:380:LEU:HD23	2.33	0.59
28:T:101:BCR:H292	28:T:101:BCR:C36	2.29	0.59
21:Y:104:ARG:HD3	25:Y:311:CLA:CHD	2.33	0.59
22:R:240:LEU:O	22:R:243:ILE:HG22	2.03	0.59
3:8:146:LEU:O	3:8:150:LEU:HG	2.03	0.59
5:b:41:GLU:OE1	5:b:63:ILE:HG13	2.03	0.59
6:c:154:ARG:HB3	6:c:256:PRO:HG2	1.85	0.59
25:c:511:CLA:C16	19:z:20:LEU:HD12	2.31	0.59
20:s:83:GLU:OE2	20:s:96:ASP:HB3	2.03	0.59
24:s:307:CHL:HBC3	24:s:307:CHL:HMC	1.85	0.59
25:y:311:CLA:HMC1	39:y:316:LUT:C31	2.33	0.59
2:2:184:VAL:HB	2:2:196:TYR:CE2	2.33	0.59
7:D:153:VAL:HG21	7:D:280:LEU:HD22	1.85	0.59
25:N:613:CLA:HMC1	25:N:613:CLA:CBC	2.32	0.59
25:Y:303:CLA:HBB1	25:Y:303:CLA:HMB3	1.83	0.59
25:Y:311:CLA:HMC1	39:Y:316:LUT:C31	2.33	0.59
2:6:121:LYS:NZ	2:6:241:PRO:HB2	2.17	0.59
2:6:127:PHE:HB3	2:6:140:PHE:CD2	2.38	0.59
2:6:145:LEU:CD2	2:6:154:VAL:HG22	2.26	0.59
2:6:193:GLY:HA2	2:6:197:PHE:CD2	2.34	0.59
6:c:28:GLN:OE1	7:d:231:ASN:ND2	2.35	0.59
6:c:272:LEU:CD2	25:c:508:CLA:HHB	2.33	0.59
8:e:27:ILE:HG23	8:e:28:PRO:CD	2.32	0.59
9:f:21:ALA:HB1	38:f:101:HEM:HAC	1.84	0.59
21:g:146:TYR:HE2	25:g:604:CLA:H2	1.65	0.59
21:n:229:PHE:CD2	21:n:240:PRO:HB3	2.38	0.59
4:A:19:ASN:O	4:A:23:SER:HB2	2.03	0.59
25:B:601:CLA:C1B	25:B:602:CLA:HBB2	2.32	0.59
7:D:56:VAL:O	7:D:67:SER:HB3	2.02	0.59
20:S:146:VAL:HG11	20:S:149:LYS:NZ	2.17	0.59
21:N:98:LEU:HD22	25:N:603:CLA:HAA2	1.85	0.59
21:N:111:LEU:HD23	25:N:604:CLA:HMC2	1.85	0.59
3:8:125:VAL:HB	3:8:127:TRP:CD1	2.38	0.59
4:a:133:LEU:CD2	7:d:257:ILE:HG12	2.33	0.59
4:a:202:VAL:HG22	25:a:402:CLA:CHB	2.32	0.59
5:b:357:ARG:CZ	23:u:96:PRO:HD2	2.33	0.59
21:n:67:PRO:CG	21:n:70:LEU:HD12	2.29	0.59
21:n:221:LEU:HD12	26:n:618:LHG:H272	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:178:ALA:HA	2:2:64:VAL:CG2	2.07	0.58
4:A:149:ALA:HB3	4:A:150:PRO:HD3	1.85	0.58
26:B:625:LHG:HC5	7:D:270:PHE:HZ	1.68	0.58
7:D:280:LEU:HD21	25:D:402:CLA:HBA2	1.83	0.58
8:E:27:ILE:HG23	8:E:28:PRO:CD	2.32	0.58
15:O:92:LEU:HA	15:O:96:GLU:OE2	2.04	0.58
21:G:226:MET:HG2	39:G:616:LUT:H12	1.85	0.58
22:R:91:GLN:NE2	22:R:113:ARG:HD2	2.18	0.58
24:R:605:CHL:HBB1	41:R:616:XAT:H162	1.85	0.58
4:a:224:ILE:HD13	5:b:482:ILE:CG1	2.32	0.58
5:b:191:ASP:OD1	10:h:70:ILE:HD13	2.03	0.58
25:b:601:CLA:C1B	25:b:602:CLA:HBB2	2.32	0.58
25:c:510:CLA:HBC3	25:c:510:CLA:HHD	1.85	0.58
25:n:613:CLA:HMC3	25:n:613:CLA:CBC	2.33	0.58
4:A:133:LEU:CD2	7:D:257:ILE:HG12	2.33	0.58
4:A:329:GLU:HA	4:A:332:HIS:CD2	2.38	0.58
5:B:357:ARG:CZ	23:U:96:PRO:HD2	2.33	0.58
5:B:451:PHE:CE2	25:B:604:CLA:HMA3	2.36	0.58
5:B:467:ILE:HG21	7:D:127:MET:CE	2.32	0.58
6:C:67:MET:HE3	6:C:71:GLU:HG3	1.84	0.58
11:I:24:LEU:CD1	28:I:101:BCR:HC41	2.33	0.58
25:G:614:CLA:HAA1	25:G:614:CLA:CBD	2.33	0.58
21:Y:138:ILE:HD12	21:Y:144:LEU:CD1	2.32	0.58
3:8:157:GLU:HG3	3:8:161:TRP:HE1	1.66	0.58
3:8:177:PRO:HD2	3:8:178:TRP:CZ3	2.38	0.58
4:a:131:TRP:HZ2	6:c:449:ARG:HD2	1.67	0.58
4:a:179:THR:HG21	25:a:403:CLA:CHD	2.32	0.58
6:c:66:ALA:N	6:c:119:LEU:HD21	2.18	0.58
6:c:308:GLU:HA	6:c:361:LEU:CD2	2.34	0.58
20:s:146:VAL:HG11	20:s:149:LYS:NZ	2.17	0.58
21:g:62:PHE:CZ	21:y:175:TYR:HE1	2.21	0.58
21:n:97:GLU:CG	21:n:190:LEU:HD21	2.20	0.58
21:n:138:ILE:HD13	24:n:606:CHL:CBC	2.33	0.58
21:y:104:ARG:HD3	25:y:311:CLA:CHD	2.33	0.58
25:y:303:CLA:HBB1	25:y:303:CLA:HMB3	1.83	0.58
1:1:100:VAL:HG21	1:1:190:LEU:HD13	1.84	0.58
3:4:147:GLY:O	3:4:151:LEU:HD23	2.03	0.58
4:A:77:ILE:HD13	13:L:30:VAL:HG13	1.84	0.58
5:B:191:ASP:OD1	10:H:70:ILE:HD13	2.03	0.58
6:C:289:PHE:CD2	25:C:501:CLA:H12	2.39	0.58
15:O:306:LEU:HD21	15:O:322:LYS:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:190:ILE:HG13	20:S:191:THR:N	2.19	0.58
21:G:62:PHE:CZ	21:Y:175:TYR:HE1	2.21	0.58
21:G:78:TYR:OH	21:G:217:LYS:NZ	2.20	0.58
21:G:229:PHE:CD2	21:G:240:PRO:HB3	2.38	0.58
25:G:610:CLA:HMC1	39:G:615:LUT:C32	2.33	0.58
21:N:221:LEU:HD12	26:N:618:LHG:H272	1.85	0.58
21:N:232:GLN:NE2	25:N:613:CLA:C4D	2.40	0.58
22:R:274:HIS:ND1	25:R:612:CLA:HAA2	2.18	0.58
4:a:158:PHE:O	4:a:162:PRO:HG2	2.03	0.58
25:a:403:CLA:C1B	27:a:404:PHO:H192	2.34	0.58
5:b:244:ALA:CB	25:b:610:CLA:HMA1	2.33	0.58
21:n:231:VAL:HG21	25:n:613:CLA:CAC	2.30	0.58
22:r:85:LYS:CG	22:r:86:PRO:HD2	2.31	0.58
2:2:112:GLY:O	2:2:116:PRO:HD3	2.03	0.58
5:B:41:GLU:OE1	5:B:63:ILE:HG13	2.03	0.58
6:C:272:LEU:CD2	25:C:508:CLA:HHB	2.33	0.58
6:C:308:GLU:HA	6:C:361:LEU:CD2	2.34	0.58
7:D:190:HIS:HA	7:D:295:ARG:HD3	1.86	0.58
21:N:97:GLU:CG	21:N:190:LEU:HD21	2.20	0.58
2:6:111:PHE:O	2:6:115:THR:HG23	2.02	0.58
1:7:138:ILE:HD12	1:7:144:LEU:CD1	2.33	0.58
26:b:625:LHG:HC5	7:d:270:PHE:HZ	1.68	0.58
6:c:272:LEU:HD21	25:c:508:CLA:C1B	2.34	0.58
25:c:506:CLA:H52	26:c:517:LHG:H261	1.86	0.58
25:c:512:CLA:HMA2	25:c:513:CLA:H203	1.85	0.58
19:z:3:ILE:O	19:z:7:LEU:HD23	2.02	0.58
25:g:610:CLA:HMC1	39:g:615:LUT:C32	2.33	0.58
21:n:98:LEU:HD22	25:n:603:CLA:HAA2	1.85	0.58
21:y:172:VAL:HG21	40:y:318:NEX:H34	1.84	0.58
21:y:229:PHE:CD2	21:y:240:PRO:HB3	2.38	0.58
1:3:138:ILE:HD12	1:3:144:LEU:CD1	2.33	0.58
3:4:78:PRO:HB2	3:4:229:ILE:HG21	1.86	0.58
4:A:224:ILE:HD13	5:B:482:ILE:CG1	2.32	0.58
4:A:283:ILE:O	4:A:286:THR:HG22	2.03	0.58
6:C:457:LYS:HE2	7:D:230:ALA:CA	2.34	0.58
25:C:511:CLA:C16	19:Z:20:LEU:HD12	2.31	0.58
29:L:101:SQD:H312	14:M:17:VAL:HG13	1.84	0.58
15:O:190:GLU:OE1	15:O:215:VAL:HG13	2.04	0.58
20:S:266:LEU:HD13	25:S:313:CLA:CMD	2.34	0.58
21:G:100:VAL:HG21	21:G:190:LEU:HD13	1.84	0.58
21:Y:122:ASN:CB	32:Y:320:AJP:C80	2.79	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:89:GLY:HA3	3:8:95:LEU:HD21	1.85	0.58
3:8:147:GLY:O	3:8:151:LEU:HD23	2.03	0.58
13:l:3:GLN:HG3	13:l:4:SER:H	1.68	0.58
21:y:100:VAL:HG21	21:y:190:LEU:HD13	1.84	0.58
25:y:304:CLA:HAB	39:y:317:LUT:C35	2.33	0.58
22:r:91:GLN:NE2	22:r:113:ARG:HD2	2.18	0.58
3:4:125:VAL:HB	3:4:127:TRP:CD1	2.38	0.58
6:C:272:LEU:HD21	25:C:508:CLA:C1B	2.34	0.58
25:C:512:CLA:HMA2	25:C:513:CLA:H203	1.85	0.58
10:H:59:GLU:OE1	18:X:84:LYS:HD2	2.04	0.58
2:6:105:TRP:CD1	24:6:603:CHL:HED1	2.39	0.58
5:b:346:PHE:O	5:b:354:LEU:N	2.32	0.58
7:d:30:PHE:O	7:d:129:ARG:NH1	2.33	0.58
15:o:100:LYS:HE3	15:o:105:VAL:HG22	1.84	0.58
15:o:190:GLU:OE1	15:o:215:VAL:HG13	2.04	0.58
21:g:107:MET:HE3	25:g:610:CLA:HMC2	1.86	0.58
21:g:115:PHE:CD2	25:g:604:CLA:HHD	2.38	0.58
25:n:602:CLA:HMC1	39:n:616:LUT:C31	2.32	0.58
21:y:138:ILE:HD12	21:y:144:LEU:CD1	2.33	0.58
2:2:145:LEU:HD13	2:2:150:ASN:N	2.19	0.58
4:A:131:TRP:HZ2	6:C:449:ARG:HD2	1.67	0.58
25:A:402:CLA:C1B	27:A:403:PHO:H192	2.34	0.58
5:B:464:PHE:HB2	7:D:281:TRP:CZ2	2.38	0.58
25:D:403:CLA:H52	18:X:91:ALA:HB3	1.84	0.58
21:N:100:VAL:HG21	21:N:190:LEU:HD13	1.84	0.58
25:N:603:CLA:H191	24:N:607:CHL:C12	2.34	0.58
2:6:104:ARG:NH2	24:6:603:CHL:HBD	2.19	0.58
2:6:129:GLU:HB2	2:6:239:LYS:HE2	1.86	0.58
1:7:100:VAL:HG21	1:7:190:LEU:HD13	1.84	0.58
5:b:464:PHE:HB2	7:d:281:TRP:CZ2	2.38	0.58
25:b:607:CLA:H151	26:b:625:LHG:C19	2.33	0.58
25:b:608:CLA:HAB	7:d:124:ILE:HG12	1.85	0.58
6:c:67:MET:HE3	6:c:71:GLU:HG3	1.84	0.58
7:d:153:VAL:HG21	7:d:280:LEU:HD22	1.85	0.58
7:d:173:SER:HB2	7:d:178:ALA:CB	2.28	0.58
10:h:22:LEU:HG	22:r:124:PHE:HE2	1.69	0.58
20:s:130:ILE:HD12	25:s:305:CLA:HAC1	1.86	0.58
21:g:229:PHE:CD2	21:g:240:PRO:HB3	2.38	0.58
25:n:610:CLA:H52	39:n:615:LUT:C28	2.32	0.58
21:y:103:SER:HB2	21:y:219:GLY:CA	2.34	0.58
22:r:274:HIS:ND1	25:r:612:CLA:HAA2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:155:HIS:HE1	2:2:158:SER:HA	1.67	0.58
1:3:67:PRO:CG	1:3:70:LEU:HD12	2.29	0.58
5:B:477:ASP:HA	22:R:104:ASN:O	2.04	0.58
29:L:101:SQD:H282	29:L:101:SQD:H121	1.86	0.58
21:N:165:GLN:HE21	24:N:607:CHL:HMC	1.69	0.58
25:Y:304:CLA:HAB	39:Y:317:LUT:C35	2.33	0.58
4:a:232:SER:HG	5:b:7:ARG:HD2	1.69	0.58
4:a:331:MET:HE2	7:d:321:LEU:HB3	1.83	0.58
6:c:131:TYR:CE1	6:c:135:LEU:HD22	2.38	0.58
25:d:403:CLA:H52	18:x:91:ALA:HB3	1.84	0.58
21:g:138:ILE:HD12	21:g:144:LEU:CD1	2.33	0.58
22:r:158:GLU:CB	22:r:268:LEU:HD12	2.31	0.58
4:A:45:THR:HG23	25:A:402:CLA:H201	1.84	0.58
4:A:202:VAL:HG22	25:A:401:CLA:CHB	2.32	0.58
29:A:407:SQD:H151	26:C:519:LHG:H342	1.86	0.58
5:B:155:ALA:O	5:B:159:THR:OG1	2.19	0.58
25:B:607:CLA:H151	26:B:625:LHG:C19	2.33	0.58
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.86	0.58
35:B:626:DGD:O5D	35:B:626:DGD:O4D	2.18	0.58
7:D:181:ARG:HD2	7:D:334:ASP:OD1	2.04	0.58
14:M:24:ILE:HG23	14:m:27:VAL:HG21	1.86	0.58
15:O:130:LYS:CE	15:O:177:PRO:HB2	2.25	0.58
21:G:115:PHE:CD2	25:G:604:CLA:HHD	2.38	0.58
22:R:158:GLU:CB	22:R:268:LEU:HD12	2.31	0.58
2:6:145:LEU:HD13	2:6:150:ASN:N	2.19	0.58
4:a:140:ARG:NH1	26:c:519:LHG:O5	2.33	0.58
5:b:75:TRP:CD1	5:b:92:SER:HG	2.21	0.58
7:d:190:HIS:HA	7:d:295:ARG:HD3	1.86	0.58
9:f:13:ARG:O	9:f:17:VAL:HG22	2.03	0.58
21:g:139:PHE:HD2	24:g:607:CHL:OBD	1.87	0.58
3:4:177:PRO:HD2	3:4:178:TRP:CZ3	2.38	0.58
4:A:139:MET:HE3	7:D:222:THR:HG23	1.86	0.58
21:Y:103:SER:HB2	21:Y:219:GLY:CA	2.34	0.58
21:Y:229:PHE:CD2	21:Y:240:PRO:HB3	2.38	0.58
1:5:229:PHE:CD2	1:5:240:PRO:HB3	2.38	0.58
2:6:107:MET:HG2	2:6:111:PHE:CE2	2.39	0.58
3:8:156:VAL:HG22	3:8:160:ARG:HE	1.69	0.58
4:a:329:GLU:HA	4:a:332:HIS:CD2	2.38	0.58
25:b:615:CLA:C19	25:b:616:CLA:HBC3	2.33	0.58
6:c:369:LEU:CD2	6:c:380:LEU:HD23	2.33	0.58
7:d:350:GLY:O	7:d:353:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:i:24:LEU:CD1	28:i:101:BCR:HC41	2.33	0.58
15:o:117:ILE:HG12	15:o:300:ILE:HG21	1.85	0.58
20:s:63:TYR:HE2	20:s:219:ALA:HB1	1.66	0.58
20:s:266:LEU:HD13	25:s:313:CLA:CMD	2.34	0.58
21:n:78:TYR:OH	21:n:217:LYS:NZ	2.20	0.58
25:r:603:CLA:HMD1	25:r:608:CLA:C1	2.34	0.58
1:3:81:ASP:OD2	1:3:84:GLY:HA2	2.04	0.57
1:3:133:LYS:O	1:3:136:SER:OG	2.20	0.57
25:B:608:CLA:HAB	7:D:124:ILE:HG12	1.85	0.57
25:D:403:CLA:H18	18:X:92:SER:HB3	1.86	0.57
15:O:117:ILE:HG12	15:O:300:ILE:HG21	1.85	0.57
25:S:304:CLA:HMC2	39:S:316:LUT:C12	2.34	0.57
21:G:97:GLU:CG	21:G:190:LEU:HD21	2.20	0.57
21:N:229:PHE:CD2	21:N:240:PRO:HB3	2.38	0.57
1:7:164:THR:CG2	1:7:168:LEU:HD12	2.34	0.57
25:a:406:CLA:HMC1	11:i:11:VAL:CG1	2.30	0.57
6:c:291:TRP:O	6:c:305:THR:HG23	2.04	0.57
25:c:508:CLA:HAB	25:c:510:CLA:H3A	1.86	0.57
29:l:102:SQD:H282	29:l:102:SQD:H121	1.86	0.57
20:s:111:GLN:HA	25:s:303:CLA:HMA1	1.86	0.57
20:s:190:ILE:HG13	20:s:191:THR:N	2.19	0.57
24:s:306:CHL:HHC	24:s:306:CHL:HBB1	1.86	0.57
21:g:82:THR:O	21:y:94:ARG:HG3	2.04	0.57
21:g:98:LEU:CD2	25:g:603:CLA:CAA	2.78	0.57
1:1:81:ASP:OD2	1:1:84:GLY:HA2	2.05	0.57
1:1:97:GLU:CG	1:1:190:LEU:HD21	2.20	0.57
1:1:152:LEU:HD23	24:1:301:CHL:HED3	1.86	0.57
2:2:127:PHE:CD2	2:2:148:LEU:HD23	2.39	0.57
1:3:164:THR:CG2	1:3:168:LEU:HD12	2.34	0.57
3:4:156:VAL:HG22	3:4:160:ARG:HE	1.69	0.57
5:B:222:PRO:HB3	10:H:38:GLY:H	1.69	0.57
25:C:506:CLA:H52	26:C:517:LHG:H261	1.86	0.57
25:C:508:CLA:HAB	25:C:510:CLA:H3A	1.86	0.57
7:D:237:ASN:OD1	7:D:238:PRO:HD2	2.05	0.57
9:F:13:ARG:O	9:F:17:VAL:HG22	2.03	0.57
24:S:307:CHL:HBC3	24:S:307:CHL:HMC	1.85	0.57
21:G:62:PHE:O	21:Y:178:ALA:HB2	2.04	0.57
21:N:182:PRO:HG3	40:N:617:NEX:H161	1.86	0.57
21:Y:164:THR:CG2	21:Y:168:LEU:HD12	2.34	0.57
22:R:207:ASN:OD1	22:R:215:ARG:NH2	2.37	0.57
25:6:604:CLA:HBC3	26:6:606:LHG:C38	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:127:MET:HG3	4:a:144:ALA:HB1	1.85	0.57
5:b:281:GLN:OE1	23:u:91:VAL:HG13	2.04	0.57
6:c:319:VAL:O	6:c:322:GLN:HG2	2.04	0.57
25:d:403:CLA:H18	18:x:92:SER:HB3	1.86	0.57
1:1:133:LYS:O	1:1:136:SER:OG	2.20	0.57
2:2:121:LYS:HD3	2:2:245:LEU:HD12	1.87	0.57
3:4:131:GLY:O	3:4:134:PRO:HD2	2.04	0.57
4:A:283:ILE:HA	4:A:286:THR:HG22	1.86	0.57
30:A:410:LMG:H301	35:A:415:DGD:HB22	1.87	0.57
6:C:237:HIS:HD2	28:I:101:BCR:H272	1.69	0.57
6:C:319:VAL:O	6:C:322:GLN:HG2	2.04	0.57
16:T:11:VAL:HG13	28:T:101:BCR:H331	1.86	0.57
21:G:164:THR:CG2	21:G:168:LEU:HD12	2.34	0.57
21:N:228:GLY:O	21:N:232:GLN:OE1	2.23	0.57
21:Y:228:GLY:O	21:Y:232:GLN:OE1	2.23	0.57
22:R:283:ILE:HA	25:R:612:CLA:CAD	2.34	0.57
1:7:103:SER:HB2	1:7:219:GLY:CA	2.34	0.57
5:b:336:ILE:HG22	5:b:336:ILE:O	2.02	0.57
6:c:289:PHE:CD2	25:c:501:CLA:H12	2.39	0.57
13:l:26:PHE:O	13:l:30:VAL:HG23	2.05	0.57
21:g:62:PHE:O	21:y:178:ALA:HB2	2.04	0.57
25:n:603:CLA:H191	24:n:607:CHL:C12	2.34	0.57
22:r:207:ASN:OD1	22:r:215:ARG:NH2	2.37	0.57
24:r:605:CHL:HBB1	41:r:616:XAT:H162	1.85	0.57
1:1:164:THR:CG2	1:1:168:LEU:HD12	2.34	0.57
1:1:228:GLY:O	1:1:232:GLN:OE1	2.23	0.57
2:2:129:GLU:HB2	2:2:239:LYS:HE2	1.86	0.57
5:B:281:GLN:OE1	23:U:91:VAL:HG13	2.04	0.57
6:C:363:ALA:O	6:C:367:GLU:HG2	2.04	0.57
7:D:236:PHE:CD1	7:D:244:THR:HG21	2.38	0.57
9:F:13:ARG:NE	38:F:101:HEM:O2D	2.32	0.57
14:M:28:LYS:HB2	14:m:27:VAL:HG11	1.87	0.57
21:N:81:ASP:OD2	21:N:84:GLY:HA2	2.04	0.57
21:N:138:ILE:HD12	21:N:144:LEU:CD1	2.33	0.57
40:Y:318:NEX:H361	40:Y:318:NEX:C28	2.25	0.57
25:R:610:CLA:C2B	26:R:618:LHG:HC2	2.34	0.57
23:U:81:THR:OG1	23:U:103:TYR:O	2.23	0.57
1:5:103:SER:HB2	1:5:219:GLY:CA	2.34	0.57
1:7:81:ASP:OD2	1:7:84:GLY:HA2	2.05	0.57
4:a:149:ALA:HB3	4:a:150:PRO:HD3	1.85	0.57
4:a:328:MET:CG	7:d:326:ILE:HG12	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:222:PRO:HB3	10:h:38:GLY:H	1.70	0.57
5:b:477:ASP:HA	22:r:104:ASN:O	2.04	0.57
25:b:612:CLA:H171	25:b:613:CLA:HBB2	1.86	0.57
7:d:247:MET:HE3	31:d:405:PL9:H522	1.85	0.57
10:h:29:GLU:HA	22:r:113:ARG:HH12	1.69	0.57
10:h:59:GLU:OE1	18:x:84:LYS:HD2	2.04	0.57
21:n:94:ARG:HG2	21:y:84:GLY:HA3	1.86	0.57
21:y:81:ASP:OD2	21:y:84:GLY:HA2	2.05	0.57
21:y:228:GLY:O	21:y:232:GLN:OE1	2.23	0.57
2:2:127:PHE:HB3	2:2:140:PHE:CD2	2.38	0.57
25:2:604:CLA:HBC3	26:2:606:LHG:C38	2.35	0.57
6:C:199:ILE:CG2	6:C:231:GLU:HG3	2.35	0.57
10:H:29:GLU:HA	22:R:113:ARG:HH12	1.69	0.57
12:K:58:VAL:O	12:K:61:ARG:HG3	2.04	0.57
18:X:96:VAL:O	18:X:100:ILE:HG12	2.05	0.57
21:G:228:GLY:O	21:G:232:GLN:OE1	2.23	0.57
21:N:164:THR:CG2	21:N:168:LEU:HD12	2.34	0.57
21:Y:132:PHE:CB	24:Y:308:CHL:HMA3	2.34	0.57
22:R:93:ASP:OD1	22:R:110:ILE:HD11	2.05	0.57
1:5:164:THR:CG2	1:5:168:LEU:HD12	2.34	0.57
2:6:121:LYS:HD3	2:6:245:LEU:HD12	1.87	0.57
4:a:84:PRO:HA	4:a:112:TYR:CG	2.39	0.57
4:a:283:ILE:HA	4:a:286:THR:HG22	1.86	0.57
5:b:451:PHE:CE2	25:b:604:CLA:HMA3	2.36	0.57
7:d:236:PHE:CD1	7:d:244:THR:HG21	2.38	0.57
20:s:153:LEU:HB3	20:s:159:THR:HG22	1.87	0.57
21:n:215:GLU:HG3	25:n:610:CLA:C1B	2.35	0.57
26:n:618:LHG:H291	26:n:618:LHG:H121	1.86	0.57
5:B:388:SER:HB3	7:D:345:GLU:OE2	2.04	0.57
21:N:103:SER:HB2	21:N:219:GLY:CA	2.34	0.57
21:N:138:ILE:HD13	24:N:606:CHL:CBC	2.33	0.57
25:N:610:CLA:H52	39:N:615:LUT:H30	1.87	0.57
26:N:618:LHG:H291	26:N:618:LHG:H121	1.86	0.57
3:8:221:LEU:O	3:8:224:LEU:HD23	2.05	0.57
25:b:604:CLA:H171	26:b:622:LHG:H311	1.85	0.57
6:c:154:ARG:HH22	17:w:128:GLU:HA	1.70	0.57
15:o:307:GLN:O	15:o:321:VAL:HG12	2.05	0.57
21:y:164:THR:CG2	21:y:168:LEU:HD12	2.34	0.57
22:r:220:GLY:HA2	22:r:224:ASP:HB3	1.87	0.57
24:r:607:CHL:H93	24:r:607:CHL:HMB3	1.85	0.57
1:1:138:ILE:HD12	1:1:144:LEU:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:129:GLU:HB2	2:2:239:LYS:NZ	2.19	0.57
4:A:46:SER:OG	35:A:415:DGD:HBH2	2.05	0.57
5:B:244:ALA:CB	25:B:610:CLA:HMA1	2.33	0.57
6:C:304:PRO:O	6:C:305:THR:CB	2.53	0.57
7:D:350:GLY:O	7:D:353:LEU:HD23	2.04	0.57
13:L:26:PHE:O	13:L:30:VAL:HG23	2.05	0.57
20:S:173:LEU:HA	20:S:176:VAL:HG22	1.87	0.57
21:G:82:THR:O	21:Y:94:ARG:HG3	2.04	0.57
21:G:107:MET:HE3	25:G:610:CLA:HMC2	1.85	0.57
22:R:206:ARG:NH2	25:R:608:CLA:HMA3	2.20	0.57
24:R:607:CHL:H93	24:R:607:CHL:HMB3	1.85	0.57
1:5:133:LYS:O	1:5:136:SER:OG	2.20	0.57
2:6:50:TRP:CG	2:6:213:LYS:HD3	2.40	0.57
1:7:228:GLY:O	1:7:232:GLN:OE1	2.23	0.57
3:8:136:ALA:HB1	3:8:140:PHE:CZ	2.40	0.57
4:a:255:PHE:CD2	4:a:264:SER:HB3	2.40	0.57
4:a:283:ILE:O	4:a:286:THR:HG22	2.03	0.57
29:a:408:SQD:H151	26:c:519:LHG:H342	1.86	0.57
6:c:50:LEU:O	6:c:54:VAL:HG23	2.05	0.57
7:d:94:TRP:NE1	18:x:87:LEU:HD22	2.20	0.57
15:o:218:LEU:HA	15:o:231:PHE:HB3	1.87	0.57
15:o:306:LEU:HD21	15:o:322:LYS:CE	2.33	0.57
18:x:96:VAL:O	18:x:100:ILE:HG12	2.05	0.57
21:g:228:GLY:O	21:g:232:GLN:OE1	2.23	0.57
21:n:111:LEU:HD23	25:n:604:CLA:HMC2	1.85	0.57
21:n:165:GLN:HE21	24:n:607:CHL:HMC	1.69	0.57
23:u:81:THR:OG1	23:u:103:TYR:O	2.23	0.57
1:1:117:GLU:O	1:1:121:ARG:HG3	2.05	0.57
2:2:104:ARG:NH2	24:2:603:CHL:HBD	2.19	0.57
2:2:105:TRP:CD1	24:2:603:CHL:HED1	2.39	0.57
3:4:205:LEU:HB3	3:4:220:LYS:HZ3	1.70	0.57
4:A:255:PHE:CD2	4:A:264:SER:HB3	2.40	0.57
4:A:256:GLY:O	4:A:261:GLN:HA	2.05	0.57
10:H:22:LEU:HG	22:R:124:PHE:HE2	1.69	0.57
21:N:76:GLY:HA3	21:N:216:LEU:CD2	2.24	0.57
21:N:215:GLU:HG3	25:N:610:CLA:C1B	2.35	0.57
25:R:603:CLA:HMD1	25:R:608:CLA:C1	2.34	0.57
1:5:117:GLU:O	1:5:121:ARG:HG3	2.05	0.57
1:5:138:ILE:HD12	1:5:144:LEU:CD1	2.33	0.57
1:7:78:TYR:OH	1:7:217:LYS:NZ	2.20	0.57
5:b:144:PHE:CE1	5:b:210:ILE:HG23	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:87:ILE:HD13	25:c:504:CLA:C2B	2.35	0.57
6:c:457:LYS:HE2	7:d:230:ALA:CA	2.34	0.57
7:d:67:SER:OG	7:d:70:GLU:HG3	2.04	0.57
7:d:181:ARG:HD2	7:d:334:ASP:OD1	2.04	0.57
9:f:13:ARG:NE	38:f:101:HEM:O2D	2.32	0.57
12:k:58:VAL:O	12:k:61:ARG:HG3	2.04	0.57
15:o:92:LEU:HA	15:o:96:GLU:OE2	2.04	0.57
21:g:218:ASN:OD1	25:g:611:CLA:CMD	2.52	0.57
1:1:67:PRO:CG	1:1:70:LEU:HD12	2.29	0.57
2:2:172:LEU:HD22	24:2:603:CHL:HMB3	1.87	0.57
2:2:210:ALA:HA	2:2:213:LYS:HZ2	1.69	0.57
3:4:89:GLY:HA3	3:4:95:LEU:HD21	1.85	0.57
3:4:221:LEU:O	3:4:224:LEU:HD23	2.05	0.57
5:B:329:SER:O	5:B:444:ARG:HD3	2.05	0.57
6:C:237:HIS:CD2	28:I:101:BCR:H272	2.39	0.57
25:C:501:CLA:HMB3	28:I:101:BCR:C26	2.34	0.57
7:D:67:SER:OG	7:D:70:GLU:HG3	2.04	0.57
14:M:27:VAL:HG21	14:m:24:ILE:HG23	1.86	0.57
15:O:227:PHE:CZ	15:O:287:LEU:HB2	2.40	0.57
15:O:307:GLN:O	15:O:321:VAL:HG12	2.05	0.57
21:G:146:TYR:HE2	25:G:604:CLA:H2	1.65	0.57
21:G:218:ASN:OD1	25:G:611:CLA:CMD	2.52	0.57
21:Y:117:GLU:O	21:Y:121:ARG:HG3	2.05	0.57
1:5:78:TYR:OH	1:5:217:LYS:NZ	2.20	0.57
1:5:228:GLY:O	1:5:232:GLN:OE1	2.23	0.57
4:a:139:MET:HE3	7:d:222:THR:HG23	1.86	0.57
4:a:274:PHE:HD1	29:a:408:SQD:H132	1.70	0.57
5:b:341:LEU:HD21	5:b:431:GLU:HB2	1.87	0.57
5:b:388:SER:HB3	7:d:345:GLU:OE2	2.04	0.57
6:c:363:ALA:O	6:c:367:GLU:HG2	2.04	0.57
6:c:449:ARG:HH12	11:i:28:PRO:CG	2.16	0.57
21:g:81:ASP:OD2	21:g:84:GLY:HA2	2.05	0.57
21:g:226:MET:HG2	39:g:616:LUT:H12	1.85	0.57
21:n:164:THR:CG2	21:n:168:LEU:HD12	2.34	0.57
4:A:84:PRO:HA	4:A:112:TYR:CG	2.39	0.57
13:L:3:GLN:HG3	13:L:4:SER:H	1.68	0.57
20:S:130:ILE:HD12	25:S:305:CLA:HAC1	1.86	0.57
21:G:98:LEU:CD2	25:G:603:CLA:CAA	2.78	0.57
21:G:139:PHE:HD2	24:G:607:CHL:OBD	1.87	0.57
24:G:601:CHL:CMB	26:Y:301:LHG:H161	2.35	0.57
22:R:158:GLU:OE2	22:R:164:THR:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:129:GLU:OE1	2:6:239:LYS:NZ	2.27	0.57
1:7:117:GLU:O	1:7:121:ARG:HG3	2.05	0.57
3:8:181:THR:O	3:8:182:ALA:HB2	2.05	0.57
4:a:64:ARG:HG2	6:c:337:LEU:HD21	1.87	0.57
5:b:333:GLY:O	5:b:441:GLY:N	2.34	0.57
25:c:513:CLA:HMD3	20:s:75:LEU:HD11	1.85	0.57
7:d:237:ASN:OD1	7:d:238:PRO:HD2	2.05	0.57
8:e:19:TYR:N	8:e:22:ILE:HG22	2.20	0.57
21:g:103:SER:HB2	21:g:219:GLY:CA	2.34	0.57
21:n:182:PRO:HG3	40:n:617:NEX:H161	1.86	0.57
21:y:78:TYR:OH	21:y:217:LYS:NZ	2.20	0.57
21:y:132:PHE:CB	24:y:308:CHL:HMA3	2.34	0.57
2:2:50:TRP:CG	2:2:213:LYS:HD3	2.40	0.56
6:C:291:TRP:O	6:C:305:THR:HG23	2.04	0.56
21:G:84:GLY:HA3	21:Y:94:ARG:HG2	1.87	0.56
21:N:188:ASP:OD2	21:N:191:TYR:HB2	2.05	0.56
1:5:188:ASP:OD2	1:5:191:TYR:HB2	2.05	0.56
3:8:142:PHE:O	3:8:146:LEU:HD13	2.05	0.56
35:a:401:DGD:HB22	30:a:411:LMG:H301	1.87	0.56
6:c:237:HIS:HD2	28:i:101:BCR:H272	1.69	0.56
16:t:11:VAL:HG13	28:t:101:BCR:H331	1.86	0.56
20:s:146:VAL:HG21	20:s:149:LYS:HZ1	1.70	0.56
21:g:117:GLU:O	21:g:121:ARG:HG3	2.05	0.56
21:g:215:GLU:HB2	25:g:610:CLA:HHB	1.87	0.56
24:g:601:CHL:CMB	26:y:301:LHG:H161	2.35	0.56
21:y:188:ASP:OD2	21:y:191:TYR:HB2	2.05	0.56
21:y:251:PRO:HB2	25:y:315:CLA:CMA	2.30	0.56
1:1:138:ILE:HG21	24:1:302:CHL:HBC1	1.87	0.56
2:2:175:GLY:O	2:2:179:ASN:N	2.38	0.56
3:4:218:PHE:HB3	3:4:219:GLU:OE1	2.05	0.56
25:B:604:CLA:H171	26:B:622:LHG:H311	1.86	0.56
6:C:163:ILE:CG2	25:C:512:CLA:HAB	2.32	0.56
7:D:247:MET:HE3	31:D:405:PL9:H522	1.85	0.56
13:L:21:GLY:O	13:L:25:ILE:HG12	2.04	0.56
20:S:202:PRO:CG	24:S:308:CHL:HBC2	2.35	0.56
21:G:81:ASP:OD2	21:G:84:GLY:HA2	2.04	0.56
21:G:103:SER:HB2	21:G:219:GLY:CA	2.34	0.56
21:G:215:GLU:HB2	25:G:610:CLA:HHB	1.87	0.56
21:N:131:TRP:HB2	39:N:616:LUT:H21	1.87	0.56
25:c:501:CLA:HMB3	28:i:101:BCR:C26	2.34	0.56
15:o:220:ALA:HA	15:o:229:GLY:HA3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:81:ASP:OD2	21:n:84:GLY:HA2	2.04	0.56
25:y:315:CLA:HBC3	25:y:315:CLA:HHD	1.87	0.56
22:r:158:GLU:OE2	22:r:164:THR:HA	2.05	0.56
25:r:610:CLA:C2B	26:r:618:LHG:HC2	2.34	0.56
1:3:103:SER:HB2	1:3:219:GLY:CA	2.34	0.56
3:4:89:GLY:O	3:4:95:LEU:HD11	2.05	0.56
3:4:123:SER:HA	3:4:133:GLN:OE1	2.06	0.56
5:B:341:LEU:HD21	5:B:431:GLU:HB2	1.87	0.56
5:B:347:ARG:O	5:B:397:VAL:HA	2.05	0.56
6:C:50:LEU:O	6:C:54:VAL:HG23	2.05	0.56
6:C:87:ILE:HD13	25:C:504:CLA:C2B	2.35	0.56
25:D:403:CLA:H101	18:X:92:SER:OG	2.06	0.56
8:E:19:TYR:N	8:E:22:ILE:HG22	2.20	0.56
15:O:117:ILE:HG12	15:O:300:ILE:CG2	2.36	0.56
19:Z:14:ILE:HG23	19:Z:18:ILE:CD1	2.36	0.56
21:G:69:TYR:CE2	21:G:87:ALA:HA	2.41	0.56
21:G:126:PHE:CE1	21:G:147:LEU:HA	2.41	0.56
21:G:227:PHE:CD2	25:G:602:CLA:H161	2.40	0.56
21:N:94:ARG:HG2	21:Y:84:GLY:HA3	1.86	0.56
24:N:606:CHL:HHC	24:N:606:CHL:HBB1	1.87	0.56
22:R:58:TRP:CH2	22:R:80:PRO:HG3	2.41	0.56
22:R:253:PHE:CD2	41:R:616:XAT:H12	2.41	0.56
1:5:138:ILE:HG21	24:5:302:CHL:HBC1	1.87	0.56
2:6:55:ARG:NH1	2:6:77:ASP:OD1	2.38	0.56
2:6:97:ALA:HB2	2:6:190:LEU:HD11	1.87	0.56
2:6:127:PHE:CD2	2:6:148:LEU:HD23	2.39	0.56
2:6:128:LYS:HD2	2:6:133:PHE:O	2.05	0.56
2:6:130:PRO:O	2:6:134:LYS:HG3	2.05	0.56
2:6:179:ASN:CA	24:6:603:CHL:HMC	2.28	0.56
2:6:211:GLU:HA	2:6:214:VAL:CG1	2.33	0.56
3:8:131:GLY:O	3:8:134:PRO:HD2	2.04	0.56
4:a:256:GLY:O	4:a:261:GLN:HA	2.05	0.56
5:b:3:LEU:HD11	13:l:9:GLN:HB3	1.88	0.56
5:b:347:ARG:O	5:b:397:VAL:HA	2.05	0.56
6:c:199:ILE:CG2	6:c:231:GLU:HG3	2.35	0.56
6:c:237:HIS:CD2	28:i:101:BCR:H272	2.39	0.56
13:l:21:GLY:O	13:l:25:ILE:HG12	2.04	0.56
15:o:312:ASP:OD1	15:o:313:LEU:N	2.38	0.56
25:s:304:CLA:HMC2	39:s:316:LUT:C12	2.34	0.56
21:g:164:THR:CG2	21:g:168:LEU:HD12	2.34	0.56
22:r:58:TRP:CH2	22:r:80:PRO:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:206:ARG:NH2	25:r:608:CLA:HMA3	2.20	0.56
22:r:283:ILE:HA	25:r:612:CLA:CAD	2.35	0.56
1:l:103:SER:HB2	1:l:219:GLY:CA	2.34	0.56
5:B:3:LEU:CD1	13:L:9:GLN:HB3	2.35	0.56
5:B:3:LEU:HD11	13:L:9:GLN:HB3	1.88	0.56
6:C:60:ILE:HG23	25:C:510:CLA:HMC1	1.87	0.56
7:D:94:TRP:NE1	18:X:87:LEU:HD22	2.20	0.56
14:M:27:VAL:HG11	14:m:28:LYS:HB2	1.87	0.56
20:S:153:LEU:HB3	20:S:159:THR:HG22	1.87	0.56
25:R:601:CLA:CHA	26:R:618:LHG:H121	2.35	0.56
4:a:218:LEU:HD12	31:a:410:PL9:O1	2.05	0.56
4:a:223:LEU:HB2	7:d:140:ARG:NH2	2.18	0.56
5:b:471:ALA:HB2	7:d:131:PHE:HE1	1.71	0.56
6:c:161:LEU:HD11	25:c:506:CLA:HBB1	1.88	0.56
6:c:304:PRO:O	6:c:305:THR:CB	2.53	0.56
25:c:501:CLA:CHB	28:i:101:BCR:H271	2.33	0.56
13:l:13:LEU:O	14:m:29:THR:HG21	2.05	0.56
21:n:228:GLY:O	21:n:232:GLN:OE1	2.23	0.56
22:r:144:GLY:HA3	22:r:246:ALA:CB	2.20	0.56
25:r:601:CLA:CHB	26:r:618:LHG:H112	2.35	0.56
1:l:146:TYR:HB3	1:l:152:LEU:CD1	2.36	0.56
2:2:130:PRO:O	2:2:134:LYS:HG3	2.05	0.56
1:3:228:GLY:O	1:3:232:GLN:OE1	2.23	0.56
4:A:14:TRP:HB3	17:W:119:TYR:HB2	1.88	0.56
5:B:454:GLY:HA2	30:B:620:LMG:H211	1.87	0.56
15:O:220:ALA:HA	15:O:229:GLY:HA3	1.86	0.56
20:S:111:GLN:HA	25:S:303:CLA:HMA1	1.86	0.56
24:S:306:CHL:HHC	24:S:306:CHL:HBB1	1.86	0.56
25:G:614:CLA:HBC3	25:G:614:CLA:CMC	2.35	0.56
24:N:607:CHL:H161	24:Y:302:CHL:H142	1.88	0.56
22:R:220:GLY:HA2	22:R:224:ASP:HB3	1.87	0.56
1:5:146:TYR:HB3	1:5:152:LEU:CD1	2.36	0.56
1:5:152:LEU:HD23	24:5:301:CHL:HED3	1.86	0.56
2:6:129:GLU:HB2	2:6:239:LYS:NZ	2.19	0.56
3:8:78:PRO:HB2	3:8:229:ILE:HG21	1.86	0.56
25:y:315:CLA:HBD	25:y:315:CLA:HBA2	1.88	0.56
22:r:124:PHE:HD1	25:r:614:CLA:HHC	1.70	0.56
22:r:146:TRP:CH2	25:r:608:CLA:HBC3	2.40	0.56
2:2:246:LEU:HA	2:2:249:LEU:CD2	2.36	0.56
5:B:482:ILE:HG21	7:D:139:LEU:CD2	2.33	0.56
21:G:146:TYR:HB3	21:G:152:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:69:TYR:CE2	21:N:87:ALA:HA	2.41	0.56
25:Y:315:CLA:HBA2	25:Y:315:CLA:HBD	1.88	0.56
22:R:152:LEU:HD13	25:R:611:CLA:HBB2	1.88	0.56
23:U:84:ALA:HB1	23:U:100:ILE:CG2	2.31	0.56
2:6:172:LEU:HD22	24:6:603:CHL:HMB3	1.87	0.56
3:8:184:ASN:O	3:8:195:PRO:HA	2.05	0.56
5:b:3:LEU:CD1	13:l:9:GLN:HB3	2.35	0.56
25:b:601:CLA:H101	25:b:601:CLA:CGA	2.35	0.56
22:r:67:TRP:CZ2	22:r:85:LYS:HG3	2.41	0.56
22:r:152:LEU:HD13	25:r:611:CLA:HBB2	1.87	0.56
22:r:253:PHE:CD2	41:r:616:XAT:H12	2.41	0.56
25:r:601:CLA:CHA	26:r:618:LHG:H121	2.35	0.56
1:3:188:ASP:OD2	1:3:191:TYR:HB2	2.06	0.56
3:4:142:PHE:O	3:4:146:LEU:HD13	2.05	0.56
5:B:26:HIS:O	5:B:30:VAL:HG23	2.05	0.56
5:B:41:GLU:HB3	5:B:60:MET:SD	2.46	0.56
25:B:601:CLA:H101	25:B:601:CLA:CGA	2.35	0.56
6:C:161:LEU:HD11	25:C:506:CLA:HBB1	1.88	0.56
6:C:272:LEU:HD21	25:C:508:CLA:HHB	1.87	0.56
13:L:13:LEU:O	14:M:29:THR:HG21	2.05	0.56
21:G:188:ASP:OD2	21:G:191:TYR:HB2	2.05	0.56
21:G:224:PHE:HE2	25:G:613:CLA:HAB	1.71	0.56
21:N:133:LYS:O	21:N:136:SER:OG	2.20	0.56
21:Y:227:PHE:HE2	25:Y:303:CLA:H162	1.71	0.56
1:5:126:PHE:CE1	1:5:147:LEU:HA	2.41	0.56
3:8:123:SER:HA	3:8:133:GLN:OE1	2.06	0.56
4:a:46:SER:OG	35:a:401:DGD:HBH2	2.05	0.56
6:c:272:LEU:HD21	25:c:508:CLA:HHB	1.87	0.56
6:c:393:ALA:O	6:c:396:MET:HG2	2.06	0.56
38:f:101:HEM:O1D	38:f:101:HEM:HHA	2.06	0.56
21:n:117:GLU:O	21:n:121:ARG:HG3	2.05	0.56
25:n:610:CLA:H52	39:n:615:LUT:H30	1.87	0.56
21:y:69:TYR:CE2	21:y:87:ALA:HA	2.41	0.56
21:y:126:PHE:CE1	21:y:147:LEU:HA	2.41	0.56
2:2:107:MET:HG2	2:2:111:PHE:CE2	2.39	0.56
2:2:128:LYS:HD2	2:2:133:PHE:O	2.05	0.56
3:4:184:ASN:O	3:4:195:PRO:HA	2.05	0.56
4:A:224:ILE:HD11	4:A:247:ASN:OD1	2.05	0.56
20:S:63:TYR:HE2	20:S:219:ALA:HB1	1.66	0.56
20:S:170:ASN:OD1	20:S:171:LEU:N	2.36	0.56
21:N:117:GLU:O	21:N:121:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:132:PHE:CB	24:N:607:CHL:HMA3	2.36	0.56
21:Y:81:ASP:OD2	21:Y:84:GLY:HA2	2.04	0.56
21:Y:126:PHE:CE1	21:Y:147:LEU:HA	2.41	0.56
1:5:138:ILE:HG13	1:5:144:LEU:CB	2.31	0.56
2:6:90:GLU:O	2:6:94:LYS:HG2	2.06	0.56
5:b:72:THR:HG23	5:b:80:ILE:CG2	2.23	0.56
5:b:155:ALA:O	5:b:159:THR:OG1	2.19	0.56
18:x:87:LEU:HD12	18:x:88:LEU:HD22	1.88	0.56
20:s:146:VAL:HG11	20:s:149:LYS:HZ3	1.71	0.56
20:s:262:PHE:HD2	25:s:314:CLA:HMA1	1.71	0.56
21:n:133:LYS:O	21:n:136:SER:OG	2.20	0.56
2:2:55:ARG:NH1	2:2:77:ASP:OD1	2.38	0.56
2:2:217:ILE:CD1	25:2:604:CLA:CAD	2.84	0.56
1:3:117:GLU:O	1:3:121:ARG:HG3	2.05	0.56
3:4:155:TRP:CD1	3:4:159:LYS:NZ	2.74	0.56
3:4:181:THR:O	3:4:182:ALA:HB2	2.05	0.56
4:A:64:ARG:HG2	6:C:337:LEU:HD21	1.87	0.56
4:A:218:LEU:HD12	31:A:409:PL9:O1	2.05	0.56
5:B:237:VAL:CG2	25:B:610:CLA:HBC2	2.36	0.56
6:C:160:ILE:HG12	25:C:512:CLA:HMC3	1.88	0.56
6:C:393:ALA:O	6:C:396:MET:HG2	2.06	0.56
25:C:511:CLA:H102	19:Z:24:PRO:CB	2.35	0.56
15:O:136:PHE:HB2	15:O:174:ILE:O	2.05	0.56
21:G:117:GLU:O	21:G:121:ARG:HG3	2.05	0.56
21:N:96:ARG:O	21:N:100:VAL:HG23	2.06	0.56
25:N:602:CLA:HBC1	26:N:618:LHG:H251	1.88	0.56
22:R:67:TRP:CZ2	22:R:85:LYS:HG3	2.41	0.56
22:R:146:TRP:CH2	25:R:608:CLA:HBC3	2.40	0.56
25:R:601:CLA:CHB	26:R:618:LHG:H112	2.35	0.56
1:5:67:PRO:CG	1:5:70:LEU:HD12	2.29	0.56
2:6:100:VAL:CB	2:6:190:LEU:HD23	2.36	0.56
1:7:76:GLY:HA3	1:7:216:LEU:CD2	2.24	0.56
6:c:26:ARG:NH2	6:c:41:ARG:HB3	2.20	0.56
25:c:511:CLA:H162	19:z:20:LEU:CD1	2.32	0.56
7:d:22:TRP:CD1	7:d:25:ARG:HH12	2.24	0.56
25:d:403:CLA:H101	18:x:92:SER:OG	2.06	0.56
28:d:404:BCR:H382	28:d:404:BCR:H23C	1.87	0.56
14:m:26:TYR:O	14:m:29:THR:HG22	2.06	0.56
20:s:173:LEU:HA	20:s:176:VAL:HG22	1.87	0.56
21:g:146:TYR:HB3	21:g:152:LEU:CD1	2.36	0.56
21:g:224:PHE:HE2	25:g:613:CLA:HAB	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:50:TRP:C	21:n:55:ARG:HD2	2.31	0.56
21:n:103:SER:HB2	21:n:219:GLY:CA	2.34	0.56
21:n:126:PHE:CE1	21:n:147:LEU:HA	2.41	0.56
25:n:610:CLA:H71	25:n:612:CLA:H102	1.88	0.56
2:2:211:GLU:HA	2:2:214:VAL:CG1	2.33	0.56
5:B:37:MET:HE2	5:B:37:MET:HA	1.88	0.56
6:C:26:ARG:NH2	6:C:41:ARG:HB3	2.20	0.56
6:C:154:ARG:HH22	17:W:128:GLU:HA	1.70	0.56
25:S:305:CLA:HBB1	39:S:316:LUT:H181	1.87	0.56
25:S:312:CLA:HBB1	39:S:315:LUT:H14	1.87	0.56
21:G:95:ASN:C	25:G:602:CLA:HMA1	2.31	0.56
25:Y:303:CLA:H72	25:Y:303:CLA:H122	1.88	0.56
2:6:217:ILE:CD1	25:6:604:CLA:CAD	2.84	0.56
2:6:246:LEU:HA	2:6:249:LEU:CD2	2.36	0.56
3:8:162:VAL:O	3:8:166:ASN:N	2.33	0.56
4:a:224:ILE:HD11	4:a:247:ASN:OD1	2.05	0.56
5:b:41:GLU:HB3	5:b:60:MET:SD	2.46	0.56
5:b:355:PHE:HB3	23:u:94:THR:HG22	1.88	0.56
10:h:56:ILE:CD1	18:x:84:LYS:HE3	2.16	0.56
20:s:202:PRO:CG	24:s:308:CHL:HBC2	2.35	0.56
25:s:312:CLA:HBB1	39:s:315:LUT:H14	1.87	0.56
21:g:69:TYR:CE2	21:g:87:ALA:HA	2.41	0.56
21:n:132:PHE:HB3	24:n:607:CHL:HMA3	1.88	0.56
21:y:50:TRP:C	21:y:55:ARG:HD2	2.31	0.56
21:y:146:TYR:HB3	21:y:152:LEU:CD1	2.36	0.56
3:4:166:ASN:ND2	22:R:61:GLY:O	2.39	0.55
5:B:144:PHE:CE1	5:B:210:ILE:HG23	2.40	0.55
25:B:606:CLA:CAD	26:B:622:LHG:HC62	2.36	0.55
6:C:175:LEU:HD23	6:C:237:HIS:ND1	2.22	0.55
25:C:511:CLA:H162	19:Z:20:LEU:CD1	2.33	0.55
38:F:101:HEM:O1D	38:F:101:HEM:HHA	2.06	0.55
13:L:13:LEU:HB2	14:M:25:ILE:CG2	2.36	0.55
15:O:218:LEU:HA	15:O:231:PHE:HB3	1.86	0.55
17:W:108:VAL:O	17:W:112:ILE:HD12	2.06	0.55
21:N:231:VAL:HG21	25:N:613:CLA:CAC	2.30	0.55
24:N:607:CHL:H201	24:N:609:CHL:H62	1.88	0.55
21:Y:128:GLU:OE1	21:Y:133:LYS:HB3	2.06	0.55
2:6:121:LYS:HZ2	2:6:241:PRO:HB2	1.71	0.55
3:8:89:GLY:O	3:8:95:LEU:HD11	2.05	0.55
21:n:69:TYR:CE2	21:n:87:ALA:HA	2.41	0.55
21:n:138:ILE:HG13	21:n:144:LEU:CB	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:606:CHL:HHC	24:n:606:CHL:HBB1	1.87	0.55
25:y:303:CLA:HBB1	25:y:303:CLA:CMB	2.36	0.55
25:y:303:CLA:H72	25:y:303:CLA:H122	1.88	0.55
1:1:126:PHE:CE1	1:1:147:LEU:HA	2.41	0.55
1:3:126:PHE:CE1	1:3:147:LEU:HA	2.41	0.55
1:3:146:TYR:HB3	1:3:152:LEU:CD1	2.36	0.55
3:4:183:GLU:CD	3:4:185:PHE:HE1	2.15	0.55
4:A:274:PHE:HD1	29:A:407:SQD:H132	1.70	0.55
6:C:369:LEU:CD2	6:C:384:ILE:HG12	2.36	0.55
16:T:20:ALA:O	16:T:24:ARG:HB3	2.06	0.55
20:S:178:GLU:OE1	24:S:307:CHL:HMC	2.06	0.55
21:G:138:ILE:HD12	21:G:144:LEU:CD1	2.32	0.55
21:N:138:ILE:HD13	24:N:606:CHL:HBC3	1.87	0.55
21:N:224:PHE:HZ	25:N:613:CLA:H93	1.71	0.55
25:N:604:CLA:HBA2	40:N:617:NEX:H241	1.88	0.55
21:Y:116:PRO:HB2	21:Y:129:ALA:O	2.07	0.55
21:Y:133:LYS:O	21:Y:136:SER:OG	2.20	0.55
1:7:126:PHE:CE1	1:7:147:LEU:HA	2.41	0.55
1:7:146:TYR:HB3	1:7:152:LEU:CD1	2.36	0.55
3:8:218:PHE:HB3	3:8:219:GLU:OE1	2.05	0.55
5:b:329:SER:O	5:b:444:ARG:HD3	2.05	0.55
6:c:437:LEU:HD22	25:c:502:CLA:CBC	2.37	0.55
7:d:147:PHE:O	7:d:150:PRO:HD2	2.06	0.55
15:o:227:PHE:CZ	15:o:287:LEU:HB2	2.40	0.55
20:s:135:ASN:HD21	20:s:141:CYS:HB2	1.72	0.55
21:g:126:PHE:CE1	21:g:147:LEU:HA	2.41	0.55
21:g:188:ASP:OD2	21:g:191:TYR:HB2	2.05	0.55
21:g:218:ASN:ND2	25:g:612:CLA:C4A	2.62	0.55
21:g:227:PHE:CD2	25:g:602:CLA:H161	2.40	0.55
21:n:116:PRO:HB2	21:n:129:ALA:O	2.07	0.55
21:n:127:GLY:CA	21:n:137:GLN:HG3	2.37	0.55
21:n:188:ASP:OD2	21:n:191:TYR:HB2	2.05	0.55
21:n:224:PHE:HZ	25:n:613:CLA:H93	1.71	0.55
21:y:117:GLU:O	21:y:121:ARG:HG3	2.05	0.55
21:y:227:PHE:HE2	25:y:303:CLA:H162	1.71	0.55
23:u:97:THR:CA	23:u:102:ARG:HH21	2.09	0.55
2:2:97:ALA:HB2	2:2:190:LEU:HD11	1.87	0.55
1:3:58:TYR:CD1	1:3:80:TRP:HB2	2.42	0.55
3:4:159:LYS:HZ2	25:R:601:CLA:HMB2	1.69	0.55
3:4:164:PHE:HB2	3:4:192:GLN:OE1	2.06	0.55
28:D:404:BCR:H382	28:D:404:BCR:H23C	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:69:ILE:HG13	20:S:71:LEU:O	2.07	0.55
21:G:50:TRP:C	21:G:55:ARG:HD2	2.31	0.55
25:G:613:CLA:C3B	39:G:615:LUT:H183	2.37	0.55
21:N:128:GLU:OE1	21:N:133:LYS:HB3	2.06	0.55
21:Y:50:TRP:C	21:Y:55:ARG:HD2	2.31	0.55
21:Y:188:ASP:OD2	21:Y:191:TYR:HB2	2.05	0.55
1:5:69:TYR:CE2	1:5:87:ALA:HA	2.41	0.55
1:5:72:GLY:HA2	1:5:77:ASP:OD2	2.07	0.55
4:a:14:TRP:HB3	17:w:119:TYR:HB2	1.88	0.55
5:b:170:ASP:HB2	5:b:171:PRO:HD2	1.87	0.55
5:b:454:GLY:HA2	30:b:620:LMG:H211	1.87	0.55
25:s:312:CLA:HHC	39:s:315:LUT:C13	2.36	0.55
25:g:613:CLA:C3B	39:g:615:LUT:H183	2.37	0.55
22:r:93:ASP:OD1	22:r:110:ILE:HD11	2.05	0.55
2:2:158:SER:O	2:2:161:ALA:HB3	2.07	0.55
2:2:242:LEU:O	2:2:246:LEU:HG	2.06	0.55
1:3:69:TYR:CE2	1:3:87:ALA:HA	2.41	0.55
1:3:76:GLY:HA3	1:3:216:LEU:CD2	2.24	0.55
8:E:57:THR:HG23	8:E:60:ARG:H	1.72	0.55
25:S:305:CLA:C2B	39:S:316:LUT:H183	2.37	0.55
21:G:127:GLY:CA	21:G:137:GLN:HG3	2.37	0.55
21:N:56:VAL:HG21	26:N:618:LHG:O2	2.07	0.55
21:N:58:TYR:CD1	21:N:80:TRP:HB2	2.42	0.55
21:Y:69:TYR:CE2	21:Y:87:ALA:HA	2.41	0.55
21:Y:96:ARG:O	21:Y:100:VAL:HG23	2.06	0.55
1:5:50:TRP:C	1:5:55:ARG:HD2	2.31	0.55
1:5:81:ASP:OD2	1:5:84:GLY:HA2	2.05	0.55
1:7:127:GLY:CA	1:7:137:GLN:HG3	2.37	0.55
3:8:94:PHE:O	3:8:98:TYR:CD2	2.60	0.55
4:a:140:ARG:NH2	7:d:220:GLU:HG2	2.22	0.55
4:a:238:ARG:NH2	4:a:241:GLN:HB2	2.22	0.55
25:c:511:CLA:H102	19:z:24:PRO:CB	2.35	0.55
17:w:108:VAL:O	17:w:112:ILE:HD12	2.06	0.55
21:g:67:PRO:CG	21:g:70:LEU:HD12	2.29	0.55
21:g:127:GLY:CA	21:g:137:GLN:HG3	2.37	0.55
21:n:132:PHE:CB	24:n:607:CHL:HMA3	2.36	0.55
21:y:67:PRO:CG	21:y:70:LEU:HD12	2.29	0.55
21:y:72:GLY:HA2	21:y:77:ASP:OD2	2.07	0.55
21:y:128:GLU:OE1	21:y:133:LYS:HB3	2.06	0.55
25:y:313:CLA:HAC2	25:y:314:CLA:H191	1.87	0.55
25:r:612:CLA:C1B	39:r:615:LUT:H183	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:90:GLU:O	2:2:94:LYS:HG2	2.06	0.55
2:2:100:VAL:CB	2:2:190:LEU:HD23	2.36	0.55
1:3:50:TRP:C	1:3:55:ARG:HD2	2.31	0.55
7:D:147:PHE:O	7:D:150:PRO:HD2	2.06	0.55
20:S:85:LEU:HD23	20:S:94:GLY:HA2	1.88	0.55
20:S:110:TYR:CD2	25:S:303:CLA:H12	2.42	0.55
20:S:122:MET:HB3	39:S:315:LUT:C34	2.37	0.55
21:N:98:LEU:HD11	21:Y:83:ALA:HA	1.88	0.55
21:N:226:MET:HG2	39:N:616:LUT:H12	1.89	0.55
25:N:611:CLA:HBC2	25:N:612:CLA:HAC1	1.87	0.55
22:R:130:VAL:HG23	22:R:131:PHE:CD1	2.42	0.55
1:5:116:PRO:HB2	1:5:129:ALA:O	2.07	0.55
1:7:58:TYR:CD1	1:7:80:TRP:HB2	2.42	0.55
1:7:69:TYR:CE2	1:7:87:ALA:HA	2.41	0.55
5:b:26:HIS:O	5:b:30:VAL:HG23	2.05	0.55
5:b:237:VAL:HG22	25:b:610:CLA:HBC2	1.89	0.55
5:b:272:ARG:O	5:b:272:ARG:HD3	2.06	0.55
6:c:60:ILE:HG23	25:c:510:CLA:HMC1	1.87	0.55
25:c:511:CLA:HBA2	12:k:54:TRP:CH2	2.42	0.55
19:z:13:ILE:HD12	28:z:101:BCR:HC31	1.89	0.55
20:s:69:ILE:HG13	20:s:71:LEU:O	2.07	0.55
20:s:122:MET:HB3	39:s:315:LUT:C34	2.37	0.55
21:g:116:PRO:HB2	21:g:129:ALA:O	2.07	0.55
21:g:128:GLU:OE1	21:g:133:LYS:HB3	2.06	0.55
21:y:96:ARG:O	21:y:100:VAL:HG23	2.06	0.55
26:y:319:LHG:H271	26:y:319:LHG:HC82	1.89	0.55
1:3:127:GLY:CA	1:3:137:GLN:HG3	2.37	0.55
5:B:237:VAL:HG22	25:B:610:CLA:HBC2	1.89	0.55
6:C:187:ASP:OD2	6:C:197:ARG:NH2	2.40	0.55
20:S:262:PHE:HD2	25:S:314:CLA:HMA1	1.71	0.55
21:G:58:TYR:CD1	21:G:80:TRP:HB2	2.42	0.55
24:G:609:CHL:O2D	24:G:609:CHL:H2A	2.07	0.55
21:N:60:GLY:HA3	24:N:601:CHL:HMC	1.89	0.55
21:N:132:PHE:HB3	24:N:607:CHL:HMA3	1.88	0.55
25:N:610:CLA:H51	25:N:612:CLA:CMA	2.37	0.55
21:Y:165:GLN:OE1	24:Y:307:CHL:CHB	2.55	0.55
25:Y:313:CLA:HAC2	25:Y:314:CLA:H191	1.87	0.55
25:Y:315:CLA:HBC3	25:Y:315:CLA:HHD	1.87	0.55
24:R:607:CHL:H112	24:R:607:CHL:CAB	2.31	0.55
25:R:612:CLA:C1B	39:R:615:LUT:H183	2.37	0.55
2:6:69:TYR:HE1	2:6:70:LEU:HG	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:188:ASP:OD2	1:7:191:TYR:HB2	2.06	0.55
3:8:166:ASN:ND2	22:r:61:GLY:O	2.39	0.55
6:c:79:LYS:HG2	6:c:80:PRO:HD2	1.89	0.55
16:t:20:ALA:O	16:t:24:ARG:HB3	2.06	0.55
19:z:14:ILE:HG23	19:z:18:ILE:CD1	2.36	0.55
25:s:305:CLA:HBB1	39:s:316:LUT:H181	1.87	0.55
25:g:614:CLA:HBC3	25:g:614:CLA:CMC	2.35	0.55
21:n:138:ILE:HD13	24:n:606:CHL:HBC3	1.87	0.55
23:u:85:LYS:HE2	23:u:101:CYS:HB2	1.88	0.55
1:1:50:TRP:C	1:1:55:ARG:HD2	2.31	0.55
1:1:69:TYR:CE2	1:1:87:ALA:HA	2.41	0.55
1:1:90:GLU:OE1	1:1:90:GLU:CA	2.55	0.55
1:3:96:ARG:O	1:3:100:VAL:HG23	2.06	0.55
3:4:110:MET:SD	3:4:111:ALA:N	2.80	0.55
3:4:169:SER:O	3:4:183:GLU:HG2	2.07	0.55
6:C:79:LYS:HG2	6:C:80:PRO:HD2	1.89	0.55
18:X:87:LEU:HD12	18:X:88:LEU:HD22	1.88	0.55
21:G:128:GLU:OE1	21:G:133:LYS:HB3	2.06	0.55
21:N:230:PHE:O	21:N:234:ILE:HG13	2.07	0.55
21:Y:60:GLY:CA	24:Y:302:CHL:HMC	2.27	0.55
26:Y:319:LHG:HC82	26:Y:319:LHG:H271	1.89	0.55
2:6:174:GLU:HB3	1:7:62:PHE:HB2	1.88	0.55
2:6:210:ALA:HA	2:6:213:LYS:HZ3	1.69	0.55
1:7:138:ILE:HG13	1:7:144:LEU:CB	2.31	0.55
5:b:237:VAL:CG2	25:b:610:CLA:HBC2	2.36	0.55
25:b:606:CLA:CAD	26:b:622:LHG:HC62	2.36	0.55
6:c:369:LEU:CD2	6:c:384:ILE:HG12	2.36	0.55
21:g:50:TRP:C	21:g:55:ARG:HD2	2.31	0.55
21:g:58:TYR:CD1	21:g:80:TRP:HB2	2.42	0.55
21:n:72:GLY:HA2	21:n:77:ASP:OD2	2.07	0.55
21:n:95:ASN:C	25:n:602:CLA:HMA1	2.32	0.55
24:n:601:CHL:HBC3	24:n:601:CHL:CMC	2.37	0.55
1:1:116:PRO:HB2	1:1:129:ALA:O	2.07	0.55
1:1:128:GLU:OE1	1:1:133:LYS:HB3	2.06	0.55
2:2:145:LEU:HB3	2:2:149:GLY:O	2.07	0.55
1:3:128:GLU:OE1	1:3:133:LYS:HB3	2.07	0.55
3:4:221:LEU:CD1	3:4:222:GLU:HG3	2.37	0.55
5:B:224:ARG:HG2	10:H:37:TRP:CH2	2.42	0.55
5:B:272:ARG:O	5:B:272:ARG:HD3	2.06	0.55
25:B:607:CLA:H152	25:B:613:CLA:H152	1.89	0.55
25:B:615:CLA:C19	25:B:616:CLA:HBC3	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:437:LEU:HD22	25:C:502:CLA:CBC	2.37	0.55
21:G:90:GLU:OE1	21:G:90:GLU:CA	2.55	0.55
21:N:162:TRP:CE3	21:Y:257:TRP:CH2	2.95	0.55
25:N:603:CLA:O1A	21:Y:83:ALA:HB1	2.07	0.55
25:N:610:CLA:H52	39:N:615:LUT:C28	2.32	0.55
25:Y:315:CLA:HBA2	25:Y:315:CLA:CHA	2.37	0.55
22:R:124:PHE:HD1	25:R:614:CLA:HHC	1.70	0.55
1:7:116:PRO:HB2	1:7:129:ALA:O	2.07	0.55
6:c:81:MET:HE2	6:c:89:LEU:HB3	1.89	0.55
6:c:160:ILE:HG12	25:c:512:CLA:HMC3	1.88	0.55
15:o:136:PHE:HB2	15:o:174:ILE:O	2.05	0.55
21:y:86:SER:OG	25:y:303:CLA:HAA2	2.06	0.55
21:y:116:PRO:HB2	21:y:129:ALA:O	2.07	0.55
22:r:130:VAL:HG23	22:r:131:PHE:CD1	2.42	0.55
27:A:404:PHO:H42	27:A:404:PHO:O1A	2.07	0.55
5:B:355:PHE:HB3	23:U:94:THR:HG22	1.88	0.55
7:D:81:THR:HG22	7:D:112:TRP:CE2	2.42	0.55
7:D:96:PRO:HG2	10:H:63:SER:OG	2.07	0.55
15:O:296:THR:HB	15:O:298:GLU:HG2	1.89	0.55
20:S:153:LEU:CB	20:S:159:THR:HG22	2.37	0.55
20:S:266:LEU:HA	25:S:313:CLA:OBD	2.07	0.55
21:G:72:GLY:HA2	21:G:77:ASP:OD2	2.07	0.55
21:G:107:MET:HE3	25:G:610:CLA:CMC	2.37	0.55
21:G:138:ILE:HD12	24:G:606:CHL:HAC1	1.89	0.55
21:N:104:ARG:HD3	25:N:610:CLA:CHD	2.36	0.55
21:N:126:PHE:CE1	21:N:147:LEU:HA	2.41	0.55
21:N:146:TYR:HB3	21:N:152:LEU:CD1	2.36	0.55
21:Y:86:SER:OG	25:Y:303:CLA:HAA2	2.06	0.55
21:Y:90:GLU:OE1	21:Y:90:GLU:CA	2.55	0.55
21:Y:213:VAL:HG12	25:Y:312:CLA:HED2	1.89	0.55
22:R:59:TYR:N	22:R:60:PRO:HD3	2.22	0.55
2:6:158:SER:O	2:6:161:ALA:HB3	2.07	0.55
2:6:242:LEU:O	2:6:246:LEU:HG	2.06	0.55
1:7:50:TRP:C	1:7:55:ARG:HD2	2.31	0.55
1:7:72:GLY:HA2	1:7:77:ASP:OD2	2.07	0.55
1:7:90:GLU:OE1	1:7:90:GLU:CA	2.55	0.55
1:7:133:LYS:O	1:7:136:SER:OG	2.20	0.55
4:a:140:ARG:HH21	7:d:220:GLU:HG2	1.72	0.55
29:l:101:SQD:H251	42:l:203:HOH:O	2.07	0.55
20:s:153:LEU:CB	20:s:159:THR:HG22	2.37	0.55
21:n:60:GLY:HA3	24:n:601:CHL:HMC	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:104:ARG:HD3	25:n:610:CLA:CHD	2.36	0.55
21:n:131:TRP:HB2	39:n:616:LUT:H21	1.87	0.55
21:y:230:PHE:O	21:y:234:ILE:HG13	2.07	0.55
25:y:315:CLA:HBA2	25:y:315:CLA:CHA	2.37	0.55
22:r:59:TYR:N	22:r:60:PRO:HD3	2.22	0.55
1:1:188:ASP:OD2	1:1:191:TYR:HB2	2.05	0.55
4:A:140:ARG:NH2	7:D:220:GLU:HG2	2.22	0.55
4:A:140:ARG:NH1	26:C:519:LHG:O5	2.33	0.55
15:O:134:LYS:HE2	15:O:175:GLU:HB2	1.89	0.55
21:G:116:PRO:HB2	21:G:129:ALA:O	2.07	0.55
1:5:128:GLU:OE1	1:5:133:LYS:HB3	2.06	0.55
20:s:110:TYR:CD2	25:s:303:CLA:H12	2.42	0.55
25:s:304:CLA:CHC	39:s:316:LUT:H15	2.36	0.55
25:s:305:CLA:C2B	39:s:316:LUT:H183	2.37	0.55
21:g:133:LYS:O	21:g:136:SER:OG	2.20	0.55
25:g:604:CLA:NC	40:g:617:NEX:O23	2.41	0.55
21:y:132:PHE:HB2	24:y:308:CHL:HMA3	1.89	0.55
21:y:165:GLN:OE1	24:y:307:CHL:CHB	2.55	0.55
1:1:72:GLY:HA2	1:1:77:ASP:OD2	2.07	0.54
2:2:202:LEU:H	2:2:202:LEU:HD23	1.73	0.54
1:3:72:GLY:HA2	1:3:77:ASP:OD2	2.07	0.54
4:A:140:ARG:HH21	7:D:220:GLU:HG2	1.72	0.54
7:D:22:TRP:CD1	7:D:25:ARG:HH12	2.24	0.54
15:O:285:ILE:HG12	15:O:287:LEU:CD1	2.37	0.54
15:O:290:THR:HG22	15:O:291:LYS:N	2.19	0.54
25:S:304:CLA:CHC	39:S:316:LUT:H15	2.36	0.54
21:Y:176:ARG:HG3	24:Y:309:CHL:CHD	2.37	0.54
1:5:230:PHE:O	1:5:234:ILE:HG13	2.07	0.54
5:b:224:ARG:HG2	10:h:37:TRP:CH2	2.42	0.54
6:c:60:ILE:HG12	25:c:510:CLA:CMC	2.37	0.54
6:c:175:LEU:HD23	6:c:237:HIS:ND1	2.21	0.54
25:c:505:CLA:C19	35:c:515:DGD:HA81	2.37	0.54
28:h:101:BCR:C23	28:h:101:BCR:H392	2.36	0.54
15:o:117:ILE:HG12	15:o:300:ILE:CG2	2.36	0.54
15:o:296:THR:HB	15:o:298:GLU:HG2	1.89	0.54
20:s:85:LEU:HD23	20:s:94:GLY:HA2	1.88	0.54
20:s:130:ILE:HD12	25:s:305:CLA:CAC	2.38	0.54
20:s:142:GLY:N	20:s:143:PRO:HA	2.22	0.54
21:g:90:GLU:OE1	21:g:90:GLU:CA	2.55	0.54
21:n:230:PHE:O	21:n:234:ILE:HG13	2.07	0.54
25:n:611:CLA:HBC2	25:n:612:CLA:HAC1	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:59:LEU:O	21:y:63:SER:OG	2.22	0.54
1:1:59:LEU:O	1:1:63:SER:OG	2.22	0.54
1:1:96:ARG:O	1:1:100:VAL:HG23	2.07	0.54
2:2:174:GLU:HB3	1:3:62:PHE:CG	2.42	0.54
3:4:220:LYS:O	3:4:224:LEU:HD23	2.07	0.54
4:A:269:ARG:HH11	7:D:232:THR:HB	1.72	0.54
29:A:407:SQD:H302	12:K:52:PHE:CZ	2.42	0.54
5:B:170:ASP:HB2	5:B:171:PRO:HD2	1.87	0.54
5:B:471:ALA:HB2	7:D:131:PHE:HE1	1.71	0.54
6:C:60:ILE:HG12	25:C:510:CLA:HMC1	1.89	0.54
7:D:305:ARG:HD3	14:M:1:MET:CE	2.37	0.54
12:K:58:VAL:CG1	12:K:61:ARG:HD2	2.37	0.54
14:M:26:TYR:O	14:M:29:THR:HG22	2.06	0.54
15:O:174:ILE:HG21	15:O:190:GLU:OE1	2.08	0.54
16:T:14:LEU:CD1	28:T:101:BCR:H343	2.37	0.54
21:N:72:GLY:HA2	21:N:77:ASP:OD2	2.07	0.54
21:N:116:PRO:HB2	21:N:129:ALA:O	2.07	0.54
21:N:127:GLY:CA	21:N:137:GLN:HG3	2.37	0.54
2:6:88:ASP:HB3	2:6:91:ALA:HB2	1.89	0.54
2:6:122:TRP:O	2:6:123:VAL:CG2	2.54	0.54
2:6:211:GLU:CA	2:6:214:VAL:HG12	2.37	0.54
1:7:88:ASP:OD2	1:7:90:GLU:HB2	2.08	0.54
1:7:96:ARG:O	1:7:100:VAL:HG23	2.06	0.54
3:8:164:PHE:HB2	3:8:192:GLN:OE1	2.06	0.54
4:a:269:ARG:HH11	7:d:232:THR:HB	1.72	0.54
29:a:408:SQD:H302	12:k:52:PHE:CZ	2.42	0.54
5:b:144:PHE:O	5:b:148:VAL:HG23	2.07	0.54
5:b:223:GLN:HA	10:h:33:VAL:CG1	2.38	0.54
7:d:81:THR:HG22	7:d:112:TRP:CE2	2.42	0.54
7:d:88:HIS:CD2	7:d:167:GLY:HA2	2.43	0.54
14:m:2:GLU:O	14:m:3:VAL:HG22	2.07	0.54
21:n:128:GLU:OE1	21:n:133:LYS:HB3	2.06	0.54
21:n:219:GLY:C	21:n:223:MET:HE2	2.33	0.54
2:2:155:HIS:CE1	2:2:158:SER:HA	2.42	0.54
2:2:179:ASN:CA	24:2:603:CHL:HMC	2.28	0.54
3:4:136:ALA:HB1	3:4:140:PHE:CZ	2.40	0.54
6:C:293:ASN:ND2	6:C:296:ALA:H	2.05	0.54
6:C:338:GLY:HA2	15:O:196:TYR:OH	2.07	0.54
6:C:452:ALA:HB1	17:W:131:LEU:HB3	1.90	0.54
6:C:462:ASP:OD1	6:C:463:PHE:N	2.41	0.54
25:C:505:CLA:C19	35:C:515:DGD:HA81	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:101:BCR:C23	28:H:101:BCR:H392	2.36	0.54
20:S:142:GLY:N	20:S:143:PRO:HA	2.22	0.54
21:G:182:PRO:HG2	24:G:608:CHL:HBB2	1.89	0.54
24:G:609:CHL:HBB1	24:G:609:CHL:HHC	1.90	0.54
21:N:219:GLY:O	21:N:223:MET:HE2	2.08	0.54
24:N:605:CHL:HHC	24:N:605:CHL:HBB1	1.88	0.54
21:Y:58:TYR:CD1	21:Y:80:TRP:HB2	2.42	0.54
1:5:88:ASP:OD2	1:5:90:GLU:HB2	2.08	0.54
1:5:127:GLY:CA	1:5:137:GLN:HG3	2.37	0.54
2:6:145:LEU:HB3	2:6:149:GLY:O	2.07	0.54
1:7:128:GLU:OE1	1:7:133:LYS:HB3	2.06	0.54
3:8:221:LEU:CD1	3:8:222:GLU:HG3	2.37	0.54
27:a:405:PHO:O1A	27:a:405:PHO:H42	2.07	0.54
6:c:293:ASN:ND2	6:c:296:ALA:H	2.05	0.54
25:c:510:CLA:HMA2	25:c:510:CLA:C2	2.37	0.54
21:g:219:GLY:C	21:g:223:MET:HE2	2.33	0.54
21:g:230:PHE:O	21:g:234:ILE:HG13	2.07	0.54
21:n:58:TYR:CD1	21:n:80:TRP:HB2	2.42	0.54
21:n:162:TRP:CE3	21:y:257:TRP:CH2	2.95	0.54
21:n:219:GLY:O	21:n:223:MET:HE2	2.08	0.54
25:n:603:CLA:O1A	21:y:83:ALA:HB1	2.07	0.54
25:r:601:CLA:HMA2	25:r:601:CLA:O2A	2.08	0.54
1:1:58:TYR:CD1	1:1:80:TRP:HB2	2.42	0.54
1:1:127:GLY:CA	1:1:137:GLN:HG3	2.37	0.54
1:1:219:GLY:O	1:1:223:MET:HE2	2.08	0.54
1:1:230:PHE:O	1:1:234:ILE:HG13	2.07	0.54
20:S:128:PHE:CE1	39:S:316:LUT:H173	2.42	0.54
20:S:134:LEU:HD23	24:N:605:CHL:HAA2	1.90	0.54
25:S:312:CLA:HHC	39:S:315:LUT:C13	2.36	0.54
21:G:219:GLY:C	21:G:223:MET:HE2	2.33	0.54
21:G:229:PHE:CE2	21:G:240:PRO:HB3	2.43	0.54
21:G:230:PHE:O	21:G:234:ILE:HG13	2.07	0.54
21:N:50:TRP:C	21:N:55:ARG:HD2	2.31	0.54
21:N:131:TRP:CE3	21:N:132:PHE:HB3	2.43	0.54
21:N:233:ALA:HB1	32:N:619:AJP:C18	2.38	0.54
24:N:601:CHL:CMC	24:N:601:CHL:HBC3	2.37	0.54
21:Y:219:GLY:C	21:Y:223:MET:HE2	2.33	0.54
22:R:189:SER:O	22:R:192:ILE:HG22	2.08	0.54
22:R:258:VAL:HG21	25:R:612:CLA:HAC2	1.89	0.54
1:5:59:LEU:O	1:5:63:SER:OG	2.22	0.54
1:5:229:PHE:CE2	1:5:240:PRO:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:55:ARG:NE	2:6:72:GLY:HA3	2.23	0.54
1:7:229:PHE:CE2	1:7:240:PRO:HB3	2.43	0.54
3:8:110:MET:SD	3:8:111:ALA:N	2.80	0.54
3:8:169:SER:O	3:8:183:GLU:HG2	2.07	0.54
25:c:504:CLA:HBC1	12:k:42:VAL:HA	1.89	0.54
7:d:96:PRO:HG2	10:h:63:SER:OG	2.07	0.54
13:l:13:LEU:HB2	14:m:25:ILE:CG2	2.36	0.54
21:g:88:ASP:OD2	21:g:90:GLU:HB2	2.08	0.54
21:g:96:ARG:O	21:g:100:VAL:HG23	2.07	0.54
21:n:59:LEU:O	21:n:63:SER:OG	2.22	0.54
25:n:602:CLA:HBC1	26:n:618:LHG:H251	1.88	0.54
2:2:211:GLU:CA	2:2:214:VAL:HG12	2.37	0.54
3:4:94:PHE:O	3:4:98:TYR:CD2	2.60	0.54
6:C:81:MET:HE2	6:C:89:LEU:HB3	1.89	0.54
25:C:510:CLA:H192	25:C:510:CLA:CHD	2.38	0.54
7:D:57:THR:CB	7:D:70:GLU:OE1	2.55	0.54
19:Z:13:ILE:HD12	28:Z:101:BCR:HC31	1.89	0.54
20:S:135:ASN:HD21	20:S:141:CYS:HB2	1.72	0.54
21:G:96:ARG:O	21:G:100:VAL:HG23	2.07	0.54
21:N:95:ASN:C	25:N:602:CLA:HMA1	2.32	0.54
25:N:610:CLA:H71	25:N:612:CLA:H102	1.88	0.54
21:Y:72:GLY:HA2	21:Y:77:ASP:OD2	2.07	0.54
21:Y:127:GLY:CA	21:Y:137:GLN:HG3	2.37	0.54
23:U:85:LYS:HE2	23:U:101:CYS:HB2	1.88	0.54
1:5:131:TRP:CE3	1:5:132:PHE:HB3	2.43	0.54
2:6:50:TRP:HB2	2:6:213:LYS:CE	2.38	0.54
2:6:202:LEU:HD23	2:6:202:LEU:H	1.73	0.54
3:8:181:THR:HG21	3:8:198:ARG:HH21	1.72	0.54
30:a:409:LMG:H292	6:c:216:SER:HA	1.89	0.54
6:c:187:ASP:OD2	6:c:197:ARG:NH2	2.40	0.54
7:d:57:THR:OG1	7:d:70:GLU:OE1	2.25	0.54
7:d:89:SER:O	7:d:91:LEU:HD12	2.08	0.54
29:l:102:SQD:H292	29:l:102:SQD:H152	1.90	0.54
20:s:178:GLU:OE1	24:s:307:CHL:HMC	2.06	0.54
20:s:186:GLU:HG3	25:s:309:CLA:C4B	2.38	0.54
21:g:78:TYR:OH	21:g:217:LYS:NZ	2.20	0.54
21:g:95:ASN:C	25:g:602:CLA:HMA1	2.31	0.54
21:g:218:ASN:HD22	25:g:612:CLA:C4A	2.21	0.54
21:g:229:PHE:CE2	21:g:240:PRO:HB3	2.43	0.54
21:n:105:TRP:CZ3	24:n:609:CHL:HAC2	2.43	0.54
21:n:130:VAL:HB	21:n:133:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:607:CHL:H201	24:n:609:CHL:H62	1.88	0.54
24:n:607:CHL:H161	24:y:302:CHL:H142	1.88	0.54
25:n:610:CLA:H8	39:n:615:LUT:C30	2.38	0.54
25:n:613:CLA:HAA1	25:n:613:CLA:HBD	1.90	0.54
21:y:58:TYR:CD1	21:y:80:TRP:HB2	2.42	0.54
21:y:88:ASP:OD2	21:y:90:GLU:HB2	2.08	0.54
25:r:608:CLA:HBC2	25:r:608:CLA:CMC	2.38	0.54
1:1:88:ASP:OD2	1:1:90:GLU:HB2	2.08	0.54
3:4:181:THR:HG21	3:4:198:ARG:HH21	1.72	0.54
4:A:131:TRP:HZ2	6:C:449:ARG:CD	2.21	0.54
25:C:511:CLA:HBA2	12:K:54:TRP:CH2	2.42	0.54
21:N:105:TRP:CZ3	24:N:609:CHL:HAC2	2.43	0.54
21:Y:229:PHE:CE2	21:Y:240:PRO:HB3	2.43	0.54
25:Y:303:CLA:HBB1	25:Y:303:CLA:CMB	2.36	0.54
1:5:58:TYR:CD1	1:5:80:TRP:HB2	2.42	0.54
1:5:219:GLY:C	1:5:223:MET:HE2	2.33	0.54
2:6:50:TRP:HB2	2:6:213:LYS:HE2	1.90	0.54
1:7:67:PRO:CG	1:7:70:LEU:HD12	2.29	0.54
4:a:254:TYR:CE1	7:d:133:LEU:HB3	2.42	0.54
7:d:57:THR:CB	7:d:70:GLU:OE1	2.55	0.54
8:e:57:THR:HG23	8:e:60:ARG:H	1.72	0.54
15:o:291:LYS:O	15:o:300:ILE:HG12	2.07	0.54
21:n:96:ARG:O	21:n:100:VAL:HG23	2.07	0.54
21:n:98:LEU:HD11	21:y:83:ALA:HA	1.88	0.54
21:n:229:PHE:CE2	21:n:240:PRO:HB3	2.43	0.54
1:1:105:TRP:HZ3	24:1:302:CHL:CMB	2.20	0.54
24:2:601:CHL:O1D	26:2:606:LHG:H142	2.08	0.54
1:3:116:PRO:HB2	1:3:129:ALA:O	2.07	0.54
4:A:324:ALA:O	4:A:328:MET:HG3	2.08	0.54
25:C:502:CLA:CMC	25:C:510:CLA:HBB1	2.38	0.54
15:O:291:LYS:O	15:O:300:ILE:HG12	2.07	0.54
20:S:186:GLU:HG3	25:S:309:CLA:C4B	2.38	0.54
24:G:608:CHL:H152	40:G:617:NEX:H402	1.90	0.54
21:Y:131:TRP:CE3	21:Y:132:PHE:HB3	2.43	0.54
25:R:608:CLA:CMC	25:R:608:CLA:HBC2	2.38	0.54
2:6:155:HIS:CE1	2:6:158:SER:HA	2.42	0.54
1:7:59:LEU:O	1:7:63:SER:OG	2.22	0.54
7:d:147:PHE:C	7:d:150:PRO:HD2	2.33	0.54
15:o:117:ILE:HG21	15:o:298:GLU:HB3	1.89	0.54
21:g:72:GLY:HA2	21:g:77:ASP:OD2	2.07	0.54
21:y:213:VAL:HG12	25:y:312:CLA:HED2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:221:LYS:HD2	22:r:222:PHE:CD2	2.43	0.54
25:2:602:CLA:HBC1	26:2:606:LHG:H251	1.89	0.54
1:3:90:GLU:OE1	1:3:90:GLU:CA	2.55	0.54
4:A:254:TYR:CE1	7:D:133:LEU:HB3	2.42	0.54
5:B:36:SER:OG	28:B:618:BCR:H362	2.08	0.54
25:C:504:CLA:HBC1	12:K:42:VAL:HA	1.89	0.54
7:D:89:SER:O	7:D:91:LEU:HD12	2.08	0.54
25:S:304:CLA:HBD	25:S:304:CLA:HAA2	1.89	0.54
21:G:219:GLY:O	21:G:223:MET:HE2	2.08	0.54
21:N:225:SER:OG	39:N:615:LUT:H192	2.08	0.54
25:N:603:CLA:HMC1	39:N:616:LUT:C13	2.38	0.54
21:Y:104:ARG:HD3	25:Y:311:CLA:C4C	2.38	0.54
1:5:90:GLU:OE1	1:5:90:GLU:CA	2.55	0.54
1:7:230:PHE:O	1:7:234:ILE:HG13	2.07	0.54
3:8:173:GLU:HB3	22:r:59:TYR:CZ	2.43	0.54
4:a:27:ARG:NH2	7:d:259:GLY:O	2.36	0.54
15:o:172:ASP:OD1	15:o:173:GLU:N	2.41	0.54
15:o:233:VAL:HB	15:o:281:SER:O	2.08	0.54
20:s:119:ARG:HD2	24:s:308:CHL:OBD	2.07	0.54
20:s:170:ASN:H	20:s:173:LEU:HB2	1.73	0.54
21:g:219:GLY:O	21:g:223:MET:HE2	2.08	0.54
21:n:56:VAL:HG11	24:n:601:CHL:HBC1	1.90	0.54
21:n:172:VAL:HG13	24:n:608:CHL:C1B	2.38	0.54
21:n:233:ALA:HB1	32:n:619:AJP:C18	2.37	0.54
24:n:608:CHL:H42	39:n:615:LUT:H362	1.90	0.54
22:r:255:GLY:O	22:r:259:GLN:HG3	2.07	0.54
3:4:173:GLU:HB3	22:R:59:TYR:CZ	2.43	0.54
4:A:238:ARG:NH2	4:A:241:GLN:HB2	2.22	0.54
6:C:60:ILE:HG12	25:C:510:CLA:CMC	2.37	0.54
25:C:501:CLA:CHB	28:I:101:BCR:H271	2.33	0.54
25:C:510:CLA:HMA2	25:C:510:CLA:C2	2.37	0.54
8:E:19:TYR:HB3	8:E:20:TRP:CE3	2.43	0.54
29:L:103:SQD:H251	42:L:203:HOH:O	2.07	0.54
15:O:172:ASP:OD1	15:O:173:GLU:N	2.41	0.54
20:S:122:MET:HE3	20:S:229:GLY:CA	2.38	0.54
21:G:131:TRP:CE3	21:G:132:PHE:HB3	2.43	0.54
25:G:603:CLA:HAC1	24:G:607:CHL:HBB2	1.90	0.54
21:N:172:VAL:HG13	24:N:608:CHL:C1B	2.38	0.54
21:Y:230:PHE:O	21:Y:234:ILE:HG13	2.07	0.54
22:R:184:LEU:HD13	24:R:605:CHL:OBD	2.08	0.54
25:R:601:CLA:HMA2	25:R:601:CLA:O2A	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:608:CLA:HBC2	25:R:608:CLA:HMC3	1.90	0.54
2:6:175:GLY:O	2:6:179:ASN:N	2.38	0.54
1:7:219:GLY:C	1:7:223:MET:HE2	2.33	0.54
25:b:607:CLA:H152	25:b:613:CLA:H152	1.89	0.54
35:b:626:DGD:O5D	35:b:626:DGD:O4D	2.18	0.54
15:o:117:ILE:HG22	15:o:298:GLU:HB3	1.89	0.54
15:o:174:ILE:HG21	15:o:190:GLU:OE1	2.08	0.54
20:s:266:LEU:HA	25:s:313:CLA:OBD	2.07	0.54
25:g:614:CLA:HAA1	25:g:614:CLA:CBD	2.33	0.54
21:n:56:VAL:HG21	26:n:618:LHG:O2	2.07	0.54
21:n:226:MET:HG2	39:n:616:LUT:H12	1.89	0.54
25:n:603:CLA:HMC1	39:n:616:LUT:C13	2.38	0.54
21:y:127:GLY:CA	21:y:137:GLN:HG3	2.37	0.54
1:1:78:TYR:OH	1:1:217:LYS:NZ	2.20	0.54
1:1:165:GLN:O	1:1:169:MET:HB2	2.08	0.54
1:3:130:VAL:HB	1:3:133:LYS:HB2	1.90	0.54
4:A:27:ARG:NH2	7:D:259:GLY:O	2.36	0.54
4:A:184:ILE:HG23	4:A:328:MET:SD	2.48	0.54
7:D:88:HIS:CD2	7:D:167:GLY:HA2	2.43	0.54
7:D:222:THR:HG21	7:D:250:ALA:HB2	1.90	0.54
21:N:90:GLU:OE1	21:N:90:GLU:CA	2.55	0.54
1:5:96:ARG:O	1:5:100:VAL:HG23	2.06	0.54
2:6:174:GLU:HB3	1:7:62:PHE:CG	2.42	0.54
1:7:165:GLN:O	1:7:169:MET:HB2	2.08	0.54
5:b:37:MET:HA	5:b:37:MET:HE2	1.88	0.54
6:c:365:TRP:O	6:c:368:PRO:HD2	2.08	0.54
6:c:452:ALA:HB1	17:w:131:LEU:HB3	1.90	0.54
15:o:285:ILE:HG12	15:o:287:LEU:CD1	2.37	0.54
21:n:90:GLU:OE1	21:n:90:GLU:CA	2.55	0.54
2:2:55:ARG:NE	2:2:72:GLY:HA3	2.23	0.53
25:B:607:CLA:HBB1	25:B:607:CLA:HMB1	1.91	0.53
14:M:2:GLU:O	14:M:3:VAL:HG22	2.07	0.53
15:O:158:PHE:CD2	15:O:322:LYS:HB2	2.43	0.53
25:S:311:CLA:HAA1	25:S:311:CLA:HBD	1.90	0.53
21:N:165:GLN:O	21:N:169:MET:HB2	2.08	0.53
21:Y:219:GLY:O	21:Y:223:MET:HE2	2.08	0.53
24:Y:302:CHL:CMB	26:Y:319:LHG:H161	2.38	0.53
24:6:601:CHL:O1D	26:6:606:LHG:H142	2.08	0.53
25:6:602:CLA:HBC1	26:6:606:LHG:H251	1.89	0.53
5:b:314:TYR:CE2	5:b:316:GLY:HA3	2.43	0.53
6:c:338:GLY:HA2	15:o:196:TYR:OH	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:462:ASP:OD1	6:c:463:PHE:N	2.41	0.53
12:k:58:VAL:CG1	12:k:61:ARG:HD2	2.37	0.53
15:o:158:PHE:CD2	15:o:322:LYS:HB2	2.43	0.53
25:s:304:CLA:HAB	39:s:316:LUT:C15	2.39	0.53
21:g:59:LEU:O	21:g:63:SER:OG	2.22	0.53
21:g:87:ALA:HB1	21:y:90:GLU:HB3	1.90	0.53
21:g:182:PRO:HG2	24:g:608:CHL:HBB2	1.89	0.53
21:n:165:GLN:O	21:n:169:MET:HB2	2.08	0.53
21:n:210:GLU:OE1	21:n:214:LYS:NZ	2.38	0.53
21:n:231:VAL:CG2	25:n:613:CLA:HAC1	2.35	0.53
25:n:604:CLA:HBA2	40:n:617:NEX:H241	1.89	0.53
21:y:90:GLU:OE1	21:y:90:GLU:CA	2.55	0.53
21:y:122:ASN:CB	32:y:320:AJP:C80	2.79	0.53
21:y:131:TRP:CE3	21:y:132:PHE:HB3	2.43	0.53
24:y:302:CHL:CMB	26:y:319:LHG:H161	2.38	0.53
1:1:219:GLY:C	1:1:223:MET:HE2	2.33	0.53
1:3:165:GLN:O	1:3:169:MET:HB2	2.08	0.53
1:3:230:PHE:O	1:3:234:ILE:HG13	2.07	0.53
3:4:69:ASP:N	3:4:70:PRO:HD2	2.23	0.53
4:A:51:ALA:HB3	4:A:82:ILE:HD12	1.90	0.53
5:B:16:PRO:HB3	5:B:133:LEU:HD11	1.91	0.53
5:B:144:PHE:O	5:B:148:VAL:HG23	2.07	0.53
5:B:368:VAL:HB	5:B:381:VAL:HB	1.90	0.53
25:S:304:CLA:HAB	39:S:316:LUT:C15	2.39	0.53
21:G:88:ASP:OD2	21:G:90:GLU:HB2	2.08	0.53
21:Y:132:PHE:HB2	24:Y:308:CHL:HMA3	1.90	0.53
22:R:255:GLY:O	22:R:259:GLN:HG3	2.07	0.53
3:8:69:ASP:N	3:8:70:PRO:HD2	2.23	0.53
3:8:220:LYS:O	3:8:224:LEU:HD23	2.07	0.53
4:a:131:TRP:HZ2	6:c:449:ARG:CD	2.21	0.53
4:a:286:THR:OG1	25:a:402:CLA:O1D	2.25	0.53
6:c:60:ILE:HG12	25:c:510:CLA:HMC1	1.89	0.53
15:o:134:LYS:HE2	15:o:175:GLU:HB2	1.89	0.53
20:s:170:ASN:OD1	20:s:171:LEU:N	2.36	0.53
25:s:304:CLA:HBD	25:s:304:CLA:HAA2	1.89	0.53
21:g:84:GLY:HA3	21:y:94:ARG:HG2	1.88	0.53
21:g:131:TRP:CE3	21:g:132:PHE:HB3	2.43	0.53
24:g:609:CHL:O2D	24:g:609:CHL:H2A	2.07	0.53
24:n:605:CHL:HHC	24:n:605:CHL:HBB1	1.88	0.53
25:n:610:CLA:H71	25:n:612:CLA:C10	2.38	0.53
21:y:176:ARG:HG3	24:y:309:CHL:CHD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:219:GLY:C	21:y:223:MET:HE2	2.33	0.53
22:r:258:VAL:HG21	25:r:612:CLA:HAC2	1.89	0.53
1:1:69:TYR:OH	1:1:81:ASP:OD2	2.20	0.53
2:2:174:GLU:HB3	1:3:62:PHE:HB2	1.88	0.53
27:A:404:PHO:HBB1	27:A:404:PHO:CMB	2.38	0.53
5:B:331:ASP:HA	5:B:335:GLY:O	2.08	0.53
7:D:147:PHE:C	7:D:150:PRO:HD2	2.33	0.53
20:S:119:ARG:HD2	24:S:308:CHL:OBD	2.07	0.53
21:G:130:VAL:HB	21:G:133:LYS:HB2	1.90	0.53
21:N:130:VAL:HB	21:N:133:LYS:HB2	1.90	0.53
21:N:229:PHE:CE2	21:N:240:PRO:HB3	2.43	0.53
2:6:126:ASP:HA	2:6:148:LEU:CG	2.37	0.53
3:8:221:LEU:HD12	3:8:222:GLU:HG3	1.91	0.53
5:b:368:VAL:HB	5:b:381:VAL:HB	1.90	0.53
7:d:299:PHE:O	7:d:303:GLU:HG2	2.09	0.53
7:d:305:ARG:HD3	14:m:1:MET:CE	2.37	0.53
20:s:122:MET:HE3	20:s:229:GLY:CA	2.38	0.53
20:s:266:LEU:O	20:s:270:ILE:HG23	2.09	0.53
21:n:76:GLY:HA3	21:n:216:LEU:CD2	2.24	0.53
21:n:159:LEU:HD11	21:y:257:TRP:HB3	1.88	0.53
1:1:130:VAL:HB	1:1:133:LYS:HB2	1.90	0.53
1:1:131:TRP:CE3	1:1:132:PHE:HB3	2.43	0.53
2:2:126:ASP:HA	2:2:148:LEU:CG	2.37	0.53
1:3:219:GLY:C	1:3:223:MET:HE2	2.33	0.53
1:3:219:GLY:O	1:3:223:MET:HE2	2.08	0.53
3:4:118:VAL:HG23	3:4:122:TRP:CE2	2.44	0.53
3:4:173:GLU:OE1	22:R:59:TYR:HA	2.08	0.53
5:B:274:GLN:HB3	5:B:279:TYR:HB3	1.90	0.53
6:C:365:TRP:O	6:C:368:PRO:HD2	2.07	0.53
6:C:461:ARG:NH1	7:D:242:GLU:HG3	2.23	0.53
8:E:19:TYR:CA	8:E:22:ILE:HG22	2.39	0.53
10:H:65:VAL:HG22	18:X:80:SER:OG	2.09	0.53
21:G:138:ILE:HG13	21:G:144:LEU:CB	2.31	0.53
21:G:172:VAL:CG1	24:G:608:CHL:C1B	2.86	0.53
21:N:78:TYR:OH	21:N:217:LYS:NZ	2.20	0.53
21:N:88:ASP:OD2	21:N:90:GLU:HB2	2.08	0.53
25:N:603:CLA:HBC1	24:N:609:CHL:HBC2	1.91	0.53
1:5:105:TRP:HZ3	24:5:302:CHL:CMB	2.20	0.53
3:8:94:PHE:O	3:8:98:TYR:HD2	1.92	0.53
25:c:510:CLA:H192	25:c:510:CLA:CHD	2.38	0.53
15:o:144:THR:OG1	15:o:322:LYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:177:ALA:CB	24:s:306:CHL:HED2	2.38	0.53
20:s:266:LEU:HD13	25:s:313:CLA:HMD2	1.91	0.53
21:g:172:VAL:CG1	24:g:608:CHL:C1B	2.86	0.53
24:g:609:CHL:HHC	24:g:609:CHL:HBB1	1.90	0.53
21:n:88:ASP:OD2	21:n:90:GLU:HB2	2.08	0.53
25:n:611:CLA:HMC2	26:n:618:LHG:H341	1.91	0.53
21:y:219:GLY:O	21:y:223:MET:HE2	2.08	0.53
1:1:229:PHE:CE2	1:1:240:PRO:HB3	2.43	0.53
2:2:104:ARG:HG3	24:2:603:CHL:CED	2.39	0.53
2:2:122:TRP:O	2:2:123:VAL:CG2	2.54	0.53
1:3:88:ASP:OD2	1:3:90:GLU:HB2	2.08	0.53
3:4:221:LEU:HD12	3:4:222:GLU:HG3	1.90	0.53
4:A:133:LEU:HD21	7:D:256:GLN:HB2	1.90	0.53
5:B:161:LEU:HD21	30:B:623:LMG:O2	2.08	0.53
6:C:209:ILE:HG13	6:C:239:TRP:NE1	2.23	0.53
7:D:57:THR:OG1	7:D:70:GLU:OE1	2.25	0.53
7:D:173:SER:HB2	7:D:178:ALA:CB	2.28	0.53
10:H:56:ILE:HA	18:X:84:LYS:CE	2.37	0.53
29:L:101:SQD:H152	29:L:101:SQD:H292	1.90	0.53
15:O:140:PRO:HD2	15:O:169:TYR:HD2	1.71	0.53
21:N:115:PHE:CD2	25:N:604:CLA:HHD	2.44	0.53
21:N:219:GLY:C	21:N:223:MET:HE2	2.33	0.53
25:N:610:CLA:H8	39:N:615:LUT:C30	2.38	0.53
21:Y:59:LEU:O	21:Y:63:SER:OG	2.22	0.53
2:6:97:ALA:HB1	2:6:190:LEU:HD11	1.91	0.53
2:6:104:ARG:HH21	24:6:603:CHL:HBA2	1.73	0.53
1:7:131:TRP:CE3	1:7:132:PHE:HB3	2.43	0.53
3:8:118:VAL:HG23	3:8:122:TRP:CE2	2.44	0.53
3:8:183:GLU:CD	3:8:185:PHE:HE1	2.15	0.53
4:a:133:LEU:HD21	7:d:256:GLN:HB2	1.90	0.53
7:d:350:GLY:HA2	7:d:353:LEU:CD2	2.39	0.53
20:s:223:VAL:HG12	25:s:311:CLA:HED1	1.91	0.53
21:g:231:VAL:CG1	25:g:613:CLA:HHD	2.39	0.53
24:g:608:CHL:H152	40:g:617:NEX:H402	1.89	0.53
26:n:618:LHG:H321	26:n:618:LHG:H122	1.90	0.53
21:y:138:ILE:HG13	21:y:144:LEU:CB	2.31	0.53
21:y:165:GLN:O	21:y:169:MET:HB2	2.08	0.53
2:2:50:TRP:HB2	2:2:213:LYS:HE2	1.90	0.53
2:2:104:ARG:HH21	24:2:603:CHL:HBA2	1.73	0.53
1:3:59:LEU:O	1:3:63:SER:OG	2.22	0.53
4:A:56:PRO:HB2	15:O:208:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:408:LMG:HB2	6:C:216:SER:HA	1.89	0.53
25:B:608:CLA:C15	25:B:609:CLA:H203	2.39	0.53
7:D:220:GLU:HA	7:D:223:LEU:HG	1.91	0.53
7:D:299:PHE:O	7:D:303:GLU:HG2	2.09	0.53
15:O:117:ILE:HG21	15:O:298:GLU:HB3	1.89	0.53
20:S:196:PHE:HB2	24:S:308:CHL:CB	2.39	0.53
21:N:159:LEU:HD11	21:Y:257:TRP:HB3	1.88	0.53
25:N:613:CLA:HBD	25:N:613:CLA:HAA1	1.90	0.53
21:Y:130:VAL:HB	21:Y:133:LYS:HB2	1.90	0.53
1:5:219:GLY:O	1:5:223:MET:HE2	2.08	0.53
2:6:130:PRO:HG2	2:6:133:PHE:CB	2.37	0.53
2:6:178:ILE:HG12	1:7:64:GLY:CA	2.39	0.53
4:a:184:ILE:HG23	4:a:328:MET:SD	2.48	0.53
27:a:405:PHO:CMB	27:a:405:PHO:HBB1	2.38	0.53
5:b:36:SER:OG	28:b:618:BCR:H362	2.08	0.53
5:b:110:ALA:HB1	25:b:616:CLA:HBB	1.91	0.53
6:c:209:ILE:HG13	6:c:239:TRP:NE1	2.23	0.53
6:c:461:ARG:NH1	7:d:242:GLU:HG3	2.23	0.53
8:e:19:TYR:HB3	8:e:20:TRP:CE3	2.43	0.53
15:o:177:PRO:CG	15:o:189:LYS:HE3	2.39	0.53
21:g:138:ILE:HD12	24:g:606:CHL:HAC1	1.89	0.53
21:g:165:GLN:O	21:g:169:MET:HB2	2.08	0.53
21:n:225:SER:OG	39:n:615:LUT:H192	2.08	0.53
21:y:130:VAL:HB	21:y:133:LYS:HB2	1.90	0.53
22:r:85:LYS:HG2	22:r:86:PRO:CD	2.38	0.53
22:r:184:LEU:HD13	24:r:605:CHL:OBD	2.08	0.53
25:2:604:CLA:HHC	26:2:606:LHG:HC41	1.90	0.53
3:4:110:MET:O	3:4:113:VAL:HG12	2.09	0.53
5:B:320:ALA:HB1	7:D:293:ASN:HD22	1.73	0.53
20:S:177:ALA:CB	24:S:306:CHL:HED2	2.38	0.53
21:G:115:PHE:HB3	21:G:116:PRO:HD3	1.91	0.53
21:N:56:VAL:HG11	24:N:601:CHL:HBC1	1.90	0.53
21:N:144:LEU:HD22	24:N:606:CHL:HMD2	1.91	0.53
21:N:227:PHE:CD2	25:N:602:CLA:H171	2.44	0.53
21:Y:88:ASP:OD2	21:Y:90:GLU:HB2	2.08	0.53
21:Y:108:LEU:HD11	25:Y:311:CLA:CB	2.39	0.53
21:Y:131:TRP:CZ3	21:Y:132:PHE:HB3	2.44	0.53
1:7:130:VAL:HB	1:7:133:LYS:HB2	1.90	0.53
1:7:219:GLY:O	1:7:223:MET:HE2	2.08	0.53
4:a:51:ALA:HB3	4:a:82:ILE:HD12	1.90	0.53
7:d:287:VAL:HG21	25:d:402:CLA:HED2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:188:TYR:OH	40:s:317:NEX:H162	2.08	0.53
25:g:603:CLA:HAC1	24:g:607:CHL:HBB2	1.90	0.53
21:n:131:TRP:CZ3	21:n:132:PHE:HB3	2.44	0.53
21:y:229:PHE:CE2	21:y:240:PRO:HB3	2.43	0.53
22:r:238:LEU:HD22	25:r:609:CLA:O1A	2.09	0.53
2:2:50:TRP:HB2	2:2:213:LYS:CE	2.38	0.53
4:A:49:ILE:HA	31:D:405:PL9:H503	1.91	0.53
4:A:335:ASN:HB3	6:C:334:PRO:HB3	1.91	0.53
5:B:110:ALA:HB1	25:B:616:CLA:HBB	1.91	0.53
6:C:451:ALA:HB2	6:C:456:GLU:OE1	2.08	0.53
25:C:501:CLA:C1C	25:C:503:CLA:H71	2.39	0.53
25:C:505:CLA:H191	35:C:515:DGD:HA81	1.91	0.53
7:D:237:ASN:HB3	7:D:240:GLN:HB2	1.90	0.53
13:L:5:ASN:HD22	13:L:8:GLU:HB2	1.74	0.53
15:O:188:PHE:HD2	15:O:218:LEU:HD11	1.74	0.53
15:O:233:VAL:HB	15:O:281:SER:O	2.08	0.53
15:O:312:ASP:OD1	15:O:313:LEU:N	2.38	0.53
20:S:188:TYR:OH	40:S:317:NEX:H162	2.08	0.53
20:S:223:VAL:HG12	25:S:311:CLA:HED1	1.91	0.53
21:G:179:GLY:HA2	24:G:608:CHL:HAC1	1.91	0.53
24:G:606:CHL:CBB	39:G:616:LUT:H161	2.39	0.53
24:N:607:CHL:HBA2	24:Y:302:CHL:H201	1.90	0.53
1:5:115:PHE:HB3	1:5:116:PRO:HD3	1.91	0.53
2:6:191:TYR:CZ	2:6:212:LEU:HD22	2.44	0.53
1:7:100:VAL:CG2	1:7:190:LEU:HD13	2.39	0.53
1:7:131:TRP:CZ3	1:7:132:PHE:HB3	2.44	0.53
7:d:220:GLU:HA	7:d:223:LEU:HG	1.91	0.53
22:r:67:TRP:CZ3	22:r:82:GLY:HA2	2.44	0.53
22:r:189:SER:O	22:r:192:ILE:HG22	2.08	0.53
2:2:191:TYR:CZ	2:2:212:LEU:HD22	2.44	0.53
3:4:162:VAL:O	3:4:166:ASN:N	2.33	0.53
4:A:56:PRO:HD2	4:A:106:LEU:HB3	1.91	0.53
4:A:76:ASN:ND2	13:L:34:ASN:HB3	2.24	0.53
4:A:255:PHE:HE2	4:A:264:SER:HB3	1.74	0.53
5:B:218:SER:O	22:R:130:VAL:HG21	2.09	0.53
15:O:177:PRO:CG	15:O:189:LYS:HE3	2.39	0.53
25:G:604:CLA:NC	40:G:617:NEX:O23	2.41	0.53
25:N:610:CLA:H71	25:N:612:CLA:C10	2.38	0.53
25:N:611:CLA:HMC2	26:N:618:LHG:H341	1.91	0.53
21:Y:78:TYR:OH	21:Y:217:LYS:NZ	2.20	0.53
25:Y:303:CLA:HMB1	25:Y:303:CLA:C2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:97:THR:CA	23:U:102:ARG:HH21	2.09	0.53
1:5:131:TRP:CZ3	1:5:132:PHE:HB3	2.44	0.53
1:5:165:GLN:O	1:5:169:MET:HB2	2.08	0.53
4:a:324:ALA:O	4:a:328:MET:HG3	2.08	0.53
5:b:19:LEU:O	5:b:22:VAL:HG22	2.08	0.53
5:b:274:GLN:HB3	5:b:279:TYR:HB3	1.90	0.53
6:c:225:VAL:HG22	6:c:289:PHE:HE1	1.73	0.53
6:c:451:ALA:HB2	6:c:456:GLU:OE1	2.08	0.53
7:d:194:LEU:HD22	7:d:316:TYR:CE1	2.42	0.53
7:d:237:ASN:HB3	7:d:240:GLN:HB2	1.90	0.53
14:m:5:ILE:HG13	14:m:6:LEU:HD12	1.91	0.53
15:o:145:VAL:HG11	15:o:203:LEU:CD1	2.35	0.53
21:g:69:TYR:OH	21:g:81:ASP:OD2	2.20	0.53
21:g:107:MET:HE3	25:g:610:CLA:CMC	2.38	0.53
21:g:198:PRO:HD2	39:g:615:LUT:H23	1.91	0.53
24:g:606:CHL:CBB	39:g:616:LUT:H161	2.39	0.53
21:y:131:TRP:CZ3	21:y:132:PHE:HB3	2.44	0.53
24:r:607:CHL:H93	24:r:607:CHL:CMB	2.39	0.53
25:r:608:CLA:HBC2	25:r:608:CLA:HMC3	1.90	0.53
1:1:131:TRP:CZ3	1:1:132:PHE:HB3	2.44	0.53
2:2:161:ALA:HB1	2:2:165:PHE:CE2	2.44	0.53
1:3:100:VAL:HG11	1:3:190:LEU:HD13	1.91	0.53
1:3:131:TRP:CE3	1:3:132:PHE:HB3	2.43	0.53
5:B:19:LEU:O	5:B:22:VAL:HG22	2.08	0.53
6:C:189:TRP:CH2	6:C:362:ARG:HG2	2.44	0.53
7:D:350:GLY:HA2	7:D:353:LEU:CD2	2.39	0.53
10:H:29:GLU:HA	22:R:113:ARG:HH22	1.74	0.53
14:M:5:ILE:HG13	14:M:6:LEU:HD12	1.91	0.53
15:O:117:ILE:HG22	15:O:298:GLU:HB3	1.89	0.53
20:S:266:LEU:O	20:S:270:ILE:HG23	2.09	0.53
21:G:131:TRP:CZ3	21:G:132:PHE:HB3	2.44	0.53
25:G:613:CLA:C1B	39:G:615:LUT:H42	2.39	0.53
21:N:131:TRP:CZ3	21:N:132:PHE:HB3	2.44	0.53
21:N:176:ARG:HG3	24:N:608:CHL:CHD	2.39	0.53
22:R:144:GLY:HA3	22:R:246:ALA:CB	2.20	0.53
22:R:150:ALA:CB	41:R:616:XAT:H181	2.39	0.53
2:6:161:ALA:HB1	2:6:165:PHE:CE2	2.44	0.53
3:8:103:LEU:HD22	3:8:193:GLY:CA	2.39	0.53
4:a:56:PRO:HB2	15:o:208:ARG:NH2	2.24	0.53
5:b:331:ASP:HA	5:b:335:GLY:O	2.08	0.53
5:b:482:ILE:HG21	7:d:139:LEU:CD2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:513:CLA:CMB	25:c:513:CLA:HBB1	2.39	0.53
13:l:5:ASN:HD22	13:l:8:GLU:HB2	1.74	0.53
21:g:94:ARG:HG2	21:n:84:GLY:CA	2.38	0.53
21:g:100:VAL:CG2	21:g:190:LEU:HD13	2.39	0.53
24:g:606:CHL:HBC2	24:g:607:CHL:HHD	1.90	0.53
21:y:100:VAL:CG2	21:y:190:LEU:HD13	2.39	0.53
21:y:104:ARG:HD3	25:y:311:CLA:C4C	2.38	0.53
22:r:94:ILE:H	22:r:94:ILE:HD12	1.74	0.53
2:2:69:TYR:HE1	2:2:70:LEU:HG	1.70	0.52
1:3:229:PHE:CE2	1:3:240:PRO:HB3	2.43	0.52
3:4:114:LEU:O	3:4:118:VAL:HG12	2.09	0.52
21:G:133:LYS:O	21:G:136:SER:OG	2.20	0.52
21:N:164:THR:HG23	21:N:168:LEU:HD12	1.92	0.52
21:Y:165:GLN:O	21:Y:169:MET:HB2	2.08	0.52
22:R:238:LEU:HD22	25:R:609:CLA:O1A	2.09	0.52
2:6:104:ARG:HG3	24:6:603:CHL:CED	2.39	0.52
3:8:155:TRP:CD1	3:8:159:LYS:NZ	2.74	0.52
3:8:173:GLU:OE1	22:r:59:TYR:HA	2.08	0.52
5:b:320:ALA:HB1	7:d:293:ASN:HD22	1.73	0.52
5:b:380:ASP:OD2	7:d:343:PRO:HG2	2.09	0.52
11:i:14:PHE:CZ	11:i:18:LEU:HD11	2.44	0.52
24:s:307:CHL:HBC3	24:s:307:CHL:CMC	2.39	0.52
25:s:311:CLA:HAA1	25:s:311:CLA:HBD	1.90	0.52
21:n:56:VAL:HB	24:n:601:CHL:HBC2	1.91	0.52
40:n:617:NEX:H42	40:n:617:NEX:H172	1.91	0.52
21:y:108:LEU:HD11	25:y:311:CLA:CBC	2.39	0.52
22:r:245:HIS:CD2	25:r:610:CLA:HMD1	2.45	0.52
25:r:604:CLA:HHC	40:r:617:NEX:H222	1.91	0.52
1:1:164:THR:HG23	1:1:168:LEU:HD12	1.92	0.52
2:2:117:GLU:HB3	2:2:121:LYS:CE	2.40	0.52
1:3:131:TRP:CZ3	1:3:132:PHE:HB3	2.44	0.52
20:S:170:ASN:H	20:S:173:LEU:HB2	1.73	0.52
21:G:94:ARG:HG2	21:N:84:GLY:CA	2.38	0.52
21:G:165:GLN:O	21:G:169:MET:HB2	2.08	0.52
21:G:218:ASN:HD22	25:G:612:CLA:C4A	2.21	0.52
24:N:608:CHL:H42	39:N:615:LUT:H362	1.90	0.52
24:Y:308:CHL:H2	32:Y:322:AJP:O79	2.09	0.52
22:R:143:HIS:HB3	22:R:250:MET:HE3	1.91	0.52
24:R:607:CHL:H93	24:R:607:CHL:CMB	2.38	0.52
1:5:100:VAL:CG2	1:5:190:LEU:HD13	2.39	0.52
25:6:604:CLA:HHC	26:6:606:LHG:HC41	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:114:LEU:O	3:8:118:VAL:HG12	2.09	0.52
25:c:505:CLA:H191	35:c:515:DGD:HA81	1.91	0.52
8:e:19:TYR:CA	8:e:22:ILE:HG22	2.39	0.52
8:e:55:TYR:O	8:e:60:ARG:NH1	2.35	0.52
10:h:29:GLU:HA	22:r:113:ARG:HH22	1.75	0.52
10:h:67:LEU:O	10:h:68:ASP:HB2	2.08	0.52
21:n:131:TRP:CE3	21:n:132:PHE:HB3	2.43	0.52
21:n:176:ARG:HG3	24:n:608:CHL:CHD	2.39	0.52
21:n:227:PHE:CD2	25:n:602:CLA:H171	2.44	0.52
25:n:610:CLA:H51	25:n:612:CLA:CMA	2.37	0.52
21:y:164:THR:HG23	21:y:168:LEU:HD12	1.92	0.52
22:r:143:HIS:HB3	22:r:250:MET:HE3	1.91	0.52
1:1:100:VAL:HG11	1:1:190:LEU:HD13	1.92	0.52
1:1:115:PHE:HB3	1:1:116:PRO:HD3	1.91	0.52
2:2:116:PRO:HG3	2:2:134:LYS:CE	2.40	0.52
3:4:78:PRO:C	3:4:229:ILE:HG21	2.35	0.52
4:A:57:PRO:HB2	4:A:66:PRO:HB2	1.91	0.52
4:A:223:LEU:HB2	7:D:140:ARG:NH2	2.18	0.52
25:A:401:CLA:HMC1	25:D:402:CLA:CAC	2.40	0.52
5:B:314:TYR:CE2	5:B:316:GLY:HA3	2.43	0.52
25:B:615:CLA:HMA2	25:B:615:CLA:HBA1	1.91	0.52
28:B:617:BCR:H322	30:B:620:LMG:H111	1.92	0.52
6:C:316:THR:HA	6:C:319:VAL:HG12	1.91	0.52
7:D:287:VAL:HG21	25:D:402:CLA:HED2	1.91	0.52
20:S:81:ILE:O	20:S:81:ILE:HG22	2.09	0.52
21:G:100:VAL:HG11	21:G:190:LEU:HD13	1.92	0.52
21:G:164:THR:HG23	21:G:168:LEU:HD12	1.92	0.52
21:G:232:GLN:NE2	25:G:613:CLA:C4D	2.44	0.52
25:N:603:CLA:C19	24:N:607:CHL:H172	2.39	0.52
21:Y:100:VAL:CG2	21:Y:190:LEU:HD13	2.39	0.52
21:Y:215:GLU:HB2	25:Y:311:CLA:CHB	2.40	0.52
1:7:115:PHE:HB3	1:7:116:PRO:HD3	1.91	0.52
1:7:164:THR:HG23	1:7:168:LEU:HD12	1.92	0.52
3:8:110:MET:O	3:8:113:VAL:HG12	2.08	0.52
4:a:76:ASN:ND2	13:l:34:ASN:HB3	2.24	0.52
25:a:402:CLA:HMC1	25:d:402:CLA:CAC	2.40	0.52
25:a:402:CLA:H191	26:d:406:LHG:H161	1.92	0.52
5:b:188:GLU:O	5:b:194:VAL:HG21	2.10	0.52
25:b:608:CLA:C15	25:b:609:CLA:H203	2.39	0.52
7:d:222:THR:HG21	7:d:250:ALA:HB2	1.90	0.52
11:i:24:LEU:HD12	28:i:101:BCR:HC31	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:t:14:LEU:CD1	28:t:101:BCR:H343	2.37	0.52
20:s:134:LEU:HD23	24:n:605:CHL:HAA2	1.90	0.52
25:g:613:CLA:C1B	39:g:615:LUT:H42	2.39	0.52
21:n:86:SER:OG	25:n:602:CLA:HAA2	2.10	0.52
21:y:76:GLY:HA3	21:y:216:LEU:CD2	2.25	0.52
25:y:303:CLA:C2	25:y:303:CLA:HMB1	2.39	0.52
22:r:57:LEU:HB2	22:r:59:TYR:CD1	2.45	0.52
22:r:150:ALA:CB	41:r:616:XAT:H181	2.39	0.52
1:1:138:ILE:HG13	1:1:144:LEU:CB	2.31	0.52
2:2:88:ASP:HB3	2:2:91:ALA:HB2	1.89	0.52
2:2:178:ILE:HG12	1:3:64:GLY:CA	2.39	0.52
1:3:115:PHE:HB3	1:3:116:PRO:HD3	1.91	0.52
3:4:94:PHE:O	3:4:98:TYR:HD2	1.92	0.52
4:A:161:TYR:HA	4:A:294:ALA:CB	2.39	0.52
19:Z:14:ILE:HG23	19:Z:18:ILE:HD11	1.92	0.52
20:S:115:LEU:O	20:S:119:ARG:HG3	2.09	0.52
20:S:130:ILE:HD12	25:S:305:CLA:CAC	2.38	0.52
20:S:135:ASN:ND2	20:S:141:CYS:HB2	2.25	0.52
25:N:613:CLA:H142	25:N:613:CLA:C2	2.40	0.52
21:Y:164:THR:HG23	21:Y:168:LEU:HD12	1.92	0.52
22:R:56:PRO:C	22:R:57:LEU:HD22	2.35	0.52
22:R:57:LEU:HB2	22:R:59:TYR:CD1	2.44	0.52
22:R:221:LYS:HD2	22:R:222:PHE:CD2	2.43	0.52
22:R:270:ASN:HB3	25:R:612:CLA:HED3	1.92	0.52
2:6:116:PRO:HG3	2:6:134:LYS:CE	2.40	0.52
2:6:117:GLU:HB3	2:6:121:LYS:CE	2.40	0.52
2:6:184:VAL:HG12	2:6:185:GLY:O	2.09	0.52
1:7:100:VAL:HG11	1:7:190:LEU:HD13	1.91	0.52
5:b:161:LEU:HD21	30:b:623:LMG:O2	2.08	0.52
6:c:51:GLY:HA2	6:c:132:HIS:HB2	1.91	0.52
6:c:459:ILE:HG21	6:c:464:GLU:HG3	1.92	0.52
20:s:196:PHE:HB2	24:s:308:CHL:CB	2.39	0.52
25:s:305:CLA:O1A	25:s:305:CLA:H3A	2.09	0.52
25:n:603:CLA:HBC1	24:n:609:CHL:HBC2	1.91	0.52
25:r:610:CLA:CB	26:r:618:LHG:HC5	2.33	0.52
25:S:305:CLA:O1A	25:S:305:CLA:H3A	2.09	0.52
21:N:60:GLY:H	24:N:601:CHL:CHC	2.23	0.52
40:N:617:NEX:H42	40:N:617:NEX:H172	1.91	0.52
25:Y:304:CLA:HMD3	24:Y:310:CHL:C4D	2.40	0.52
22:R:229:ALA:O	22:R:235:THR:OG1	2.26	0.52
27:a:405:PHO:H193	25:d:401:CLA:HHB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:277:GLN:OE1	23:u:99:LYS:NZ	2.33	0.52
6:c:87:ILE:CD1	25:c:504:CLA:HMB2	2.40	0.52
7:d:57:THR:HB	7:d:70:GLU:OE1	2.09	0.52
13:l:13:LEU:CB	14:m:25:ILE:HG22	2.40	0.52
24:n:607:CHL:HBA2	24:y:302:CHL:H201	1.91	0.52
3:4:110:MET:O	3:4:114:LEU:HD13	2.10	0.52
7:D:194:LEU:HD22	7:D:316:TYR:CE1	2.42	0.52
10:H:67:LEU:O	10:H:68:ASP:HB2	2.08	0.52
11:I:14:PHE:CZ	11:I:18:LEU:HD11	2.44	0.52
25:S:305:CLA:C1C	40:S:317:NEX:H222	2.39	0.52
21:G:100:VAL:CG2	21:G:190:LEU:HD13	2.39	0.52
21:G:224:PHE:CE2	25:G:613:CLA:HAB	2.45	0.52
24:G:606:CHL:HBC2	24:G:607:CHL:HHD	1.90	0.52
21:N:86:SER:OG	25:N:602:CLA:HAA2	2.10	0.52
21:N:115:PHE:HB3	21:N:116:PRO:HD3	1.91	0.52
21:Y:115:PHE:HB3	21:Y:116:PRO:HD3	1.91	0.52
1:5:100:VAL:HG11	1:5:190:LEU:HD13	1.92	0.52
2:6:127:PHE:N	2:6:148:LEU:HD21	2.25	0.52
5:b:16:PRO:HB3	5:b:133:LEU:HD11	1.90	0.52
5:b:45:PHE:O	5:b:58:GLN:OE1	2.27	0.52
9:f:17:VAL:HG23	9:f:18:HIS:CD2	2.45	0.52
9:f:20:LEU:O	9:f:24:THR:OG1	2.15	0.52
15:o:188:PHE:HD2	15:o:218:LEU:HD11	1.74	0.52
18:x:99:VAL:O	18:x:103:VAL:HG23	2.10	0.52
21:g:225:SER:O	21:g:229:PHE:CD1	2.63	0.52
25:g:602:CLA:H121	25:g:602:CLA:C9	2.38	0.52
21:n:100:VAL:CG2	21:n:190:LEU:HD13	2.39	0.52
21:n:115:PHE:HB3	21:n:116:PRO:HD3	1.91	0.52
21:y:215:GLU:HB2	25:y:311:CLA:CHB	2.40	0.52
22:r:138:GLU:OE2	25:r:608:CLA:HED3	2.09	0.52
22:r:202:ILE:HG13	22:r:203:GLU:N	2.25	0.52
2:2:100:VAL:HG11	2:2:190:LEU:HD23	1.91	0.52
4:A:297:LEU:HD11	6:C:425:TRP:CZ3	2.45	0.52
30:A:408:LMG:O5	17:W:87:THR:O	2.27	0.52
5:B:380:ASP:OD2	7:D:343:PRO:HG2	2.09	0.52
25:B:604:CLA:H92	25:B:604:CLA:C4	2.34	0.52
9:F:17:VAL:HG23	9:F:18:HIS:CD2	2.45	0.52
21:N:56:VAL:HB	24:N:601:CHL:HBC2	1.91	0.52
21:N:86:SER:HB3	21:N:92:PHE:CD1	2.45	0.52
21:Y:100:VAL:HB	21:Y:190:LEU:HD13	1.92	0.52
22:R:138:GLU:OE2	25:R:608:CLA:HED3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:602:CLA:O2D	25:R:602:CLA:H2A	2.10	0.52
24:6:603:CHL:CMC	24:6:603:CHL:HBC3	2.40	0.52
4:a:161:TYR:HA	4:a:294:ALA:CB	2.39	0.52
6:c:79:LYS:HD3	6:c:83:GLU:HB3	1.92	0.52
20:s:128:PHE:CE1	39:s:316:LUT:H173	2.42	0.52
21:g:69:TYR:CE1	21:y:90:GLU:HG3	2.44	0.52
21:g:115:PHE:HB3	21:g:116:PRO:HD3	1.91	0.52
21:g:131:TRP:CZ3	21:g:132:PHE:HB3	2.44	0.52
21:n:115:PHE:CD2	25:n:604:CLA:HHD	2.44	0.52
24:n:609:CHL:HBC3	24:y:302:CHL:C9	2.40	0.52
1:1:225:SER:O	1:1:229:PHE:CD1	2.63	0.52
3:4:183:GLU:HB3	3:4:185:PHE:CE1	2.45	0.52
3:4:253:LEU:HD12	3:4:254:GLY:N	2.25	0.52
5:B:122:ILE:HA	10:H:24:LYS:CD	2.40	0.52
5:B:341:LEU:HD12	5:B:429:ILE:CG2	2.38	0.52
25:B:601:CLA:HMC1	28:H:101:BCR:C19	2.40	0.52
6:C:79:LYS:HD3	6:C:83:GLU:HB3	1.92	0.52
6:C:447:ARG:HD3	25:C:508:CLA:HED1	1.92	0.52
7:D:12:GLU:OE1	7:D:12:GLU:N	2.43	0.52
7:D:12:GLU:HG2	7:D:13:LYS:N	2.25	0.52
15:O:144:THR:OG1	15:O:322:LYS:HB3	2.09	0.52
28:T:101:BCR:H271	5:b:39:LEU:CB	2.39	0.52
21:Y:138:ILE:HD13	24:Y:307:CHL:CBC	2.39	0.52
1:5:94:ARG:HA	1:5:94:ARG:HE	1.75	0.52
1:7:225:SER:O	1:7:229:PHE:CD1	2.63	0.52
4:a:40:THR:HG23	25:a:406:CLA:HBB1	1.92	0.52
4:a:49:ILE:HA	31:d:405:PL9:H503	1.91	0.52
4:a:56:PRO:HD2	4:a:106:LEU:HB3	1.91	0.52
25:b:615:CLA:HMA2	25:b:615:CLA:HBA1	1.91	0.52
6:c:320:ARG:O	6:c:323:ARG:HB2	2.10	0.52
7:d:12:GLU:OE1	7:d:12:GLU:N	2.43	0.52
15:o:290:THR:HG22	15:o:291:LYS:N	2.19	0.52
21:g:100:VAL:HG11	21:g:190:LEU:HD13	1.92	0.52
21:g:224:PHE:CE2	25:g:613:CLA:HAB	2.45	0.52
21:n:144:LEU:HD22	24:n:606:CHL:HMD2	1.91	0.52
21:y:69:TYR:OH	21:y:81:ASP:OD2	2.20	0.52
21:y:86:SER:HB3	21:y:92:PHE:CD1	2.45	0.52
25:y:304:CLA:HMD3	24:y:310:CHL:C4D	2.40	0.52
1:1:100:VAL:CG2	1:1:190:LEU:HD13	2.39	0.52
2:2:127:PHE:N	2:2:148:LEU:HD21	2.25	0.52
2:2:173:VAL:HA	2:2:176:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:103:LEU:HD22	3:4:193:GLY:CA	2.39	0.52
4:A:170:ASP:OD2	6:C:357:ARG:NH1	2.43	0.52
5:B:154:GLY:HA3	5:B:202:HIS:CB	2.40	0.52
5:B:340:TRP:O	5:B:405:GLU:HG3	2.10	0.52
9:F:31:ILE:O	9:F:35:GLN:HG2	2.10	0.52
13:L:13:LEU:CB	14:M:25:ILE:HG22	2.40	0.52
15:O:130:LYS:CD	15:O:179:GLU:HB2	2.40	0.52
20:S:58:GLU:OE1	20:S:61:LYS:NZ	2.35	0.52
21:G:69:TYR:CE1	21:Y:90:GLU:HG3	2.44	0.52
21:G:107:MET:HE1	25:G:610:CLA:CHC	2.40	0.52
24:G:606:CHL:CBA	40:G:617:NEX:H30	2.40	0.52
26:N:618:LHG:H122	26:N:618:LHG:H321	1.90	0.52
21:Y:51:TYR:HE2	21:Y:209:ALA:HB1	1.75	0.52
21:Y:146:TYR:HB3	21:Y:152:LEU:CD1	2.36	0.52
22:R:94:ILE:H	22:R:94:ILE:HD12	1.74	0.52
1:5:130:VAL:HB	1:5:133:LYS:HB2	1.90	0.52
4:a:57:PRO:HB2	4:a:66:PRO:HB2	1.90	0.52
4:a:223:LEU:HD12	7:d:140:ARG:HH22	1.74	0.52
4:a:297:LEU:HD11	6:c:425:TRP:CZ3	2.45	0.52
5:b:154:GLY:HA3	5:b:202:HIS:HB2	1.92	0.52
25:b:607:CLA:HBB1	25:b:607:CLA:HMB1	1.91	0.52
6:c:30:THR:HG23	6:c:31:THR:CG2	2.37	0.52
6:c:189:TRP:CH2	6:c:362:ARG:HG2	2.44	0.52
25:c:501:CLA:C1C	25:c:503:CLA:H71	2.39	0.52
7:d:12:GLU:HG2	7:d:13:LYS:N	2.25	0.52
10:h:65:VAL:HG22	18:x:80:SER:OG	2.09	0.52
25:s:305:CLA:C1C	40:s:317:NEX:H222	2.39	0.52
21:g:107:MET:HE1	25:g:610:CLA:CHC	2.40	0.52
25:g:602:CLA:H92	25:g:603:CLA:H122	1.91	0.52
24:g:606:CHL:CBA	40:g:617:NEX:H30	2.40	0.52
21:n:60:GLY:H	24:n:601:CHL:CHC	2.23	0.52
21:n:100:VAL:HG11	21:n:190:LEU:HD13	1.92	0.52
21:n:164:THR:HG23	21:n:168:LEU:HD12	1.92	0.52
1:1:100:VAL:HB	1:1:190:LEU:HD13	1.92	0.52
2:2:130:PRO:HG2	2:2:133:PHE:CB	2.37	0.52
2:2:211:GLU:O	2:2:214:VAL:HG12	2.09	0.52
24:2:603:CHL:CMC	24:2:603:CHL:HBC3	2.40	0.52
1:3:94:ARG:HA	1:3:94:ARG:HE	1.75	0.52
1:3:100:VAL:CG2	1:3:190:LEU:HD13	2.39	0.52
4:A:331:MET:HE1	7:D:321:LEU:HD22	1.92	0.52
25:A:401:CLA:H191	26:D:406:LHG:H161	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:404:PHO:H202	25:D:401:CLA:C1B	2.40	0.52
5:B:39:LEU:CB	28:t:101:BCR:H271	2.39	0.52
11:I:24:LEU:HD12	28:I:101:BCR:HC31	1.92	0.52
18:X:99:VAL:O	18:X:103:VAL:HG23	2.10	0.52
25:S:311:CLA:CHB	26:S:318:LHG:HC31	2.40	0.52
21:G:131:TRP:O	21:G:134:ALA:HB3	2.10	0.52
21:G:231:VAL:CG1	25:G:613:CLA:HHD	2.39	0.52
21:N:100:VAL:HB	21:N:190:LEU:HD13	1.92	0.52
21:N:225:SER:O	21:N:229:PHE:CD1	2.63	0.52
21:Y:131:TRP:O	21:Y:134:ALA:HB3	2.10	0.52
24:Y:306:CHL:HHC	24:Y:306:CHL:HBB1	1.92	0.52
25:R:603:CLA:HMC1	41:R:616:XAT:C13	2.40	0.52
2:6:100:VAL:HG11	2:6:190:LEU:HD23	1.91	0.52
3:8:183:GLU:HB3	3:8:185:PHE:CE1	2.45	0.52
4:a:335:ASN:HB3	6:c:334:PRO:HB3	1.91	0.52
5:b:478:VAL:O	5:b:478:VAL:HG22	2.10	0.52
6:c:316:THR:HA	6:c:319:VAL:HG12	1.91	0.52
7:d:150:PRO:HB3	25:d:402:CLA:H41	1.92	0.52
21:g:164:THR:HG23	21:g:168:LEU:HD12	1.92	0.52
21:y:115:PHE:HB3	21:y:116:PRO:HD3	1.91	0.52
21:y:133:LYS:O	21:y:136:SER:OG	2.20	0.52
25:r:602:CLA:O2D	25:r:602:CLA:H2A	2.10	0.52
2:2:181:LEU:HD12	24:2:603:CHL:CHC	2.40	0.51
1:3:86:SER:HB3	1:3:92:PHE:CD1	2.45	0.51
5:B:154:GLY:HA3	5:B:202:HIS:HB2	1.91	0.51
5:B:188:GLU:O	5:B:194:VAL:HG21	2.10	0.51
26:B:625:LHG:HC5	7:D:270:PHE:CZ	2.46	0.51
6:C:267:SER:CB	17:W:133:LEU:HD23	2.40	0.51
25:C:513:CLA:CMB	25:C:513:CLA:HBB1	2.39	0.51
20:S:266:LEU:HD13	25:S:313:CLA:HMD2	1.90	0.51
25:G:602:CLA:H121	25:G:602:CLA:C9	2.38	0.51
21:Y:98:LEU:HD22	25:Y:304:CLA:CBA	2.40	0.51
2:6:228:PHE:O	2:6:232:VAL:HG23	2.10	0.51
1:7:69:TYR:OH	1:7:81:ASP:OD2	2.20	0.51
28:b:617:BCR:H322	30:b:620:LMG:H111	1.92	0.51
6:c:433:LEU:HD13	25:c:502:CLA:CHC	2.41	0.51
15:o:140:PRO:HD2	15:o:169:TYR:HD2	1.71	0.51
20:s:135:ASN:ND2	20:s:141:CYS:HB2	2.25	0.51
25:s:303:CLA:HAB	39:s:316:LUT:H32	1.91	0.51
21:g:130:VAL:HB	21:g:133:LYS:HB2	1.90	0.51
21:n:146:TYR:HB3	21:n:152:LEU:CD1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:603:CLA:HMC1	41:r:616:XAT:C13	2.40	0.51
2:2:101:ILE:O	2:2:104:ARG:HB3	2.11	0.51
1:3:51:TYR:HE2	1:3:209:ALA:HB1	1.75	0.51
6:C:30:THR:HG23	6:C:31:THR:CG2	2.37	0.51
21:G:51:TYR:HE2	21:G:209:ALA:HB1	1.75	0.51
21:G:59:LEU:O	21:G:63:SER:OG	2.22	0.51
21:G:198:PRO:HD2	39:G:615:LUT:H23	1.91	0.51
25:G:602:CLA:H92	25:G:603:CLA:H122	1.91	0.51
21:N:59:LEU:O	21:N:63:SER:OG	2.22	0.51
21:N:100:VAL:CG2	21:N:190:LEU:HD13	2.39	0.51
21:N:172:VAL:CG1	24:N:608:CHL:C1B	2.88	0.51
3:8:94:PHE:HB3	3:8:98:TYR:CE2	2.42	0.51
27:a:405:PHO:H202	25:d:401:CLA:C1B	2.40	0.51
7:d:94:TRP:O	18:x:83:LEU:HD23	2.10	0.51
21:g:100:VAL:HB	21:g:190:LEU:HD13	1.92	0.51
21:y:100:VAL:HG11	21:y:190:LEU:HD13	1.92	0.51
1:3:225:SER:O	1:3:229:PHE:CD1	2.63	0.51
4:A:223:LEU:HD12	7:D:140:ARG:HH22	1.74	0.51
5:B:39:LEU:HB3	28:t:101:BCR:H381	1.93	0.51
5:B:223:GLN:HA	10:H:33:VAL:CG1	2.38	0.51
25:C:505:CLA:HAA1	25:C:505:CLA:CBD	2.39	0.51
26:C:519:LHG:HC5	7:D:220:GLU:OE2	2.11	0.51
7:D:57:THR:HB	7:D:70:GLU:OE1	2.09	0.51
7:D:94:TRP:O	18:X:83:LEU:HD23	2.10	0.51
20:S:262:PHE:CE2	25:S:314:CLA:H3A	2.43	0.51
21:G:100:VAL:HB	21:G:190:LEU:HD13	1.92	0.51
25:N:602:CLA:HBC2	25:N:602:CLA:CMC	2.40	0.51
2:6:210:ALA:O	2:6:213:LYS:HG2	2.10	0.51
3:8:78:PRO:C	3:8:229:ILE:HG21	2.35	0.51
5:b:218:SER:O	22:r:130:VAL:HG21	2.09	0.51
25:c:513:CLA:HMD3	20:s:75:LEU:CD1	2.41	0.51
15:o:296:THR:HG22	15:o:296:THR:O	2.09	0.51
20:s:115:LEU:O	20:s:119:ARG:HG3	2.09	0.51
20:s:115:LEU:HB3	20:s:119:ARG:HH21	1.75	0.51
21:n:69:TYR:OH	21:n:81:ASP:OD2	2.20	0.51
21:n:225:SER:O	21:n:229:PHE:CD1	2.63	0.51
24:y:308:CHL:H2	32:y:322:AJP:O79	2.09	0.51
22:r:270:ASN:HB3	25:r:612:CLA:HED3	1.92	0.51
2:2:210:ALA:O	2:2:213:LYS:HG2	2.10	0.51
3:4:156:VAL:O	3:4:159:LYS:HB2	2.11	0.51
4:A:58:VAL:HB	4:A:83:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:45:PHE:O	5:B:58:GLN:OE1	2.27	0.51
24:S:307:CHL:HBC3	24:S:307:CHL:CMC	2.39	0.51
21:Y:100:VAL:HG11	21:Y:190:LEU:HD13	1.92	0.51
1:5:131:TRP:O	1:5:134:ALA:HB3	2.10	0.51
1:5:146:TYR:CD1	1:5:147:LEU:HG	2.46	0.51
2:6:173:VAL:HA	2:6:176:PHE:CD2	2.44	0.51
2:6:181:LEU:HD12	24:6:603:CHL:CHC	2.40	0.51
1:7:100:VAL:HB	1:7:190:LEU:HD13	1.92	0.51
1:7:128:GLU:CB	1:7:137:GLN:HB2	2.41	0.51
5:b:340:TRP:O	5:b:405:GLU:HG3	2.10	0.51
6:c:80:PRO:HD2	6:c:83:GLU:OE1	2.10	0.51
12:k:58:VAL:HG12	12:k:61:ARG:HD2	1.92	0.51
25:s:311:CLA:CHB	26:s:318:LHG:HC31	2.40	0.51
21:g:131:TRP:O	21:g:134:ALA:HB3	2.11	0.51
21:y:225:SER:O	21:y:229:PHE:CD1	2.63	0.51
24:y:306:CHL:HHC	24:y:306:CHL:HBB1	1.92	0.51
1:1:210:GLU:OE1	1:1:214:LYS:NZ	2.38	0.51
2:2:104:ARG:HE	24:2:603:CHL:CBD	2.13	0.51
2:2:129:GLU:OE1	2:2:239:LYS:NZ	2.27	0.51
2:2:210:ALA:HA	2:2:213:LYS:HZ3	1.76	0.51
27:A:404:PHO:HAB	25:D:402:CLA:C1	2.41	0.51
6:C:320:ARG:O	6:C:323:ARG:HB2	2.10	0.51
6:C:459:ILE:HG21	6:C:464:GLU:HG3	1.92	0.51
25:C:513:CLA:HMD1	20:S:75:LEU:CD1	2.39	0.51
21:G:128:GLU:CB	21:G:137:GLN:HB2	2.41	0.51
21:G:225:SER:O	21:G:229:PHE:CD1	2.63	0.51
21:N:104:ARG:HD3	25:N:610:CLA:C4C	2.41	0.51
25:N:610:CLA:H18	40:N:617:NEX:H372	1.92	0.51
21:Y:227:PHE:CD2	25:Y:303:CLA:H202	2.40	0.51
1:5:164:THR:HG23	1:5:168:LEU:HD12	1.92	0.51
1:5:225:SER:O	1:5:229:PHE:CD1	2.63	0.51
3:8:110:MET:O	3:8:114:LEU:HD13	2.10	0.51
3:8:253:LEU:HD12	3:8:254:GLY:N	2.25	0.51
4:a:58:VAL:HB	4:a:83:ILE:HB	1.93	0.51
5:b:203:ILE:O	5:b:207:THR:HG23	2.10	0.51
11:i:6:LEU:HD23	17:w:101:LEU:CD2	2.41	0.51
20:s:81:ILE:O	20:s:81:ILE:HG22	2.09	0.51
20:s:182:LEU:HD23	24:s:306:CHL:CMA	2.41	0.51
20:s:230:ARG:HD3	25:s:303:CLA:CHD	2.40	0.51
21:g:146:TYR:CD1	21:g:147:LEU:HG	2.46	0.51
21:g:179:GLY:HA2	24:g:608:CHL:HAC1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:172:VAL:CG1	24:n:608:CHL:C1B	2.89	0.51
25:n:603:CLA:C19	24:n:607:CHL:H172	2.39	0.51
21:y:100:VAL:HB	21:y:190:LEU:HD13	1.92	0.51
21:y:107:MET:HE1	25:y:311:CLA:CHC	2.40	0.51
1:1:131:TRP:O	1:1:134:ALA:HB3	2.10	0.51
2:2:239:LYS:HB2	2:2:242:LEU:HB2	1.92	0.51
1:3:146:TYR:CD1	1:3:147:LEU:HG	2.46	0.51
4:A:43:THR:O	4:A:47:VAL:HG23	2.11	0.51
4:A:50:ILE:HG22	28:A:406:BCR:H271	1.92	0.51
25:B:602:CLA:HBC3	25:B:602:CLA:HHD	1.93	0.51
25:B:614:CLA:HBD	25:B:614:CLA:HAA1	1.93	0.51
6:C:51:GLY:HA2	6:C:132:HIS:HB2	1.91	0.51
6:C:80:PRO:HD2	6:C:83:GLU:OE1	2.10	0.51
6:C:318:LEU:HD12	6:C:340:TYR:HB3	1.93	0.51
8:E:73:LEU:O	8:E:77:ASP:OD2	2.29	0.51
14:M:32:GLN:HG3	14:m:32:GLN:HG3	1.92	0.51
20:S:115:LEU:HB3	20:S:119:ARG:HH21	1.75	0.51
21:G:87:ALA:HB1	21:Y:90:GLU:HB3	1.90	0.51
21:N:108:LEU:HD11	25:N:610:CLA:CBC	2.41	0.51
24:N:609:CHL:HBC3	24:Y:302:CHL:C9	2.40	0.51
21:Y:196:PHE:HZ	24:Y:309:CHL:C1C	2.24	0.51
21:Y:225:SER:O	21:Y:229:PHE:CD1	2.63	0.51
22:R:245:HIS:CD2	25:R:610:CLA:HMD1	2.45	0.51
1:5:100:VAL:HB	1:5:190:LEU:HD13	1.92	0.51
2:6:211:GLU:O	2:6:214:VAL:HG12	2.09	0.51
2:6:236:VAL:O	2:6:237:THR:OG1	2.24	0.51
2:6:239:LYS:HB2	2:6:242:LEU:HB2	1.92	0.51
2:6:244:ASN:O	2:6:248:HIS:ND1	2.44	0.51
5:b:41:GLU:HB3	5:b:63:ILE:CD1	2.41	0.51
5:b:154:GLY:HA3	5:b:202:HIS:CB	2.40	0.51
5:b:187:VAL:HG13	25:b:601:CLA:HMD2	1.93	0.51
25:b:601:CLA:HMC1	28:h:101:BCR:C19	2.39	0.51
6:c:267:SER:CB	17:w:133:LEU:HD23	2.40	0.51
7:d:262:PHE:O	31:d:405:PL9:H522	2.11	0.51
8:e:73:LEU:O	8:e:77:ASP:OD2	2.29	0.51
15:o:215:VAL:HG22	15:o:218:LEU:HB3	1.93	0.51
20:s:262:PHE:CD2	25:s:314:CLA:HMA1	2.46	0.51
21:n:100:VAL:HB	21:n:190:LEU:HD13	1.92	0.51
21:n:108:LEU:HD11	25:n:610:CLA:CBC	2.41	0.51
21:n:131:TRP:O	21:n:134:ALA:HB3	2.10	0.51
21:n:132:PHE:CD2	24:n:607:CHL:HED1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:128:GLU:CB	21:y:137:GLN:HB2	2.41	0.51
21:y:138:ILE:HD13	24:y:307:CHL:CBC	2.39	0.51
23:u:96:PRO:C	23:u:97:THR:HG1	2.07	0.51
2:2:184:VAL:HG12	2:2:185:GLY:O	2.09	0.51
3:4:225:LYS:HA	3:4:228:GLU:OE2	2.11	0.51
27:A:404:PHO:HBB1	27:A:404:PHO:HMB3	1.93	0.51
5:B:382:PRO:HB3	7:D:345:GLU:CD	2.35	0.51
15:O:146:LYS:HB2	15:O:158:PHE:CE1	2.46	0.51
20:S:105:GLU:O	20:S:109:LYS:HG3	2.11	0.51
20:S:182:LEU:HD23	24:S:306:CHL:CMA	2.41	0.51
21:G:104:ARG:HD3	25:G:610:CLA:CHD	2.40	0.51
21:N:104:ARG:HB3	25:N:610:CLA:HBC2	1.92	0.51
21:N:146:TYR:CD1	21:N:147:LEU:HG	2.46	0.51
21:Y:156:GLN:HB2	24:Y:306:CHL:CBB	2.41	0.51
25:R:603:CLA:CHD	25:R:608:CLA:H92	2.29	0.51
2:6:125:VAL:HG13	2:6:148:LEU:HD11	1.92	0.51
1:7:146:TYR:CD1	1:7:147:LEU:HG	2.46	0.51
3:8:156:VAL:O	3:8:159:LYS:HB2	2.11	0.51
4:a:202:VAL:HG22	25:a:402:CLA:HHB	1.92	0.51
25:b:615:CLA:H51	25:b:616:CLA:C20	2.41	0.51
25:c:511:CLA:HBA1	28:k:101:BCR:H271	1.93	0.51
26:c:519:LHG:HC5	7:d:220:GLU:OE2	2.11	0.51
15:o:130:LYS:CD	15:o:179:GLU:HB2	2.40	0.51
19:z:14:ILE:HG23	19:z:18:ILE:HD11	1.92	0.51
21:n:94:ARG:HA	21:n:94:ARG:HE	1.75	0.51
1:1:86:SER:HB3	1:1:92:PHE:CD1	2.45	0.51
2:2:244:ASN:O	2:2:248:HIS:ND1	2.44	0.51
5:B:462:PHE:CE2	25:B:613:CLA:HMB3	2.46	0.51
6:C:87:ILE:CD1	25:C:504:CLA:HMB2	2.40	0.51
21:G:95:ASN:HA	21:G:98:LEU:HB2	1.93	0.51
21:G:131:TRP:HA	39:G:616:LUT:O3	2.11	0.51
21:N:131:TRP:O	21:N:134:ALA:HB3	2.10	0.51
21:N:231:VAL:CG2	25:N:613:CLA:HAC1	2.35	0.51
21:Y:146:TYR:CD1	21:Y:147:LEU:HG	2.46	0.51
1:7:131:TRP:O	1:7:134:ALA:HB3	2.10	0.51
4:a:43:THR:O	4:a:47:VAL:HG23	2.11	0.51
5:b:110:ALA:CB	25:b:616:CLA:HHB	2.40	0.51
5:b:360:PRO:O	5:b:361:THR:CG2	2.58	0.51
6:c:447:ARG:HD3	25:c:508:CLA:HED1	1.92	0.51
11:i:27:ASP:HB3	11:i:28:PRO:HD3	1.93	0.51
15:o:187:ASN:OD1	15:o:187:ASN:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:83:GLU:HG3	20:s:83:GLU:O	2.10	0.51
20:s:187:TYR:HA	20:s:190:ILE:HG12	1.93	0.51
21:g:94:ARG:HA	21:g:94:ARG:HE	1.75	0.51
21:n:128:GLU:CB	21:n:137:GLN:HB2	2.41	0.51
21:y:60:GLY:HA3	24:y:302:CHL:CMC	2.28	0.51
40:y:318:NEX:H361	40:y:318:NEX:C28	2.25	0.51
22:r:204:PHE:CE1	25:r:614:CLA:HAC2	2.46	0.51
1:1:146:TYR:CD1	1:1:147:LEU:HG	2.46	0.51
2:2:228:PHE:O	2:2:232:VAL:HG23	2.10	0.51
5:B:203:ILE:O	5:B:207:THR:HG23	2.10	0.51
6:C:433:LEU:HD13	25:C:502:CLA:CHC	2.41	0.51
20:S:230:ARG:HD3	25:S:303:CLA:CHD	2.40	0.51
25:R:604:CLA:HHC	40:R:617:NEX:H222	1.91	0.51
3:8:215:GLU:HB3	3:8:216:PRO:HD3	1.93	0.51
5:b:7:ARG:HD3	25:b:611:CLA:HED1	1.93	0.51
5:b:122:ILE:HA	10:h:24:LYS:CD	2.40	0.51
6:c:163:ILE:CG2	25:c:512:CLA:HAB	2.32	0.51
7:d:85:SER:OG	23:u:102:ARG:NH1	2.44	0.51
15:o:140:PRO:HD2	15:o:169:TYR:CE2	2.46	0.51
21:g:87:ALA:HB1	21:y:90:GLU:HB2	1.93	0.51
21:g:104:ARG:HD3	25:g:610:CLA:CHD	2.40	0.51
21:y:95:ASN:HA	21:y:98:LEU:HB2	1.93	0.51
21:y:196:PHE:HZ	24:y:309:CHL:C1C	2.24	0.51
22:r:56:PRO:C	22:r:57:LEU:HD22	2.35	0.51
3:4:75:GLY:HA2	3:4:80:ASP:HB3	1.93	0.51
6:C:76:VAL:O	6:C:76:VAL:HG13	2.11	0.51
15:O:296:THR:HG22	15:O:296:THR:O	2.09	0.51
19:Z:3:ILE:HD12	19:Z:3:ILE:H	1.76	0.51
20:S:83:GLU:HG3	20:S:83:GLU:O	2.10	0.51
21:G:210:GLU:OE1	21:G:214:LYS:NZ	2.38	0.51
21:N:100:VAL:HG11	21:N:190:LEU:HD13	1.92	0.51
21:N:132:PHE:CD2	24:N:607:CHL:HED1	2.45	0.51
21:Y:107:MET:HE1	25:Y:311:CLA:CHC	2.40	0.51
25:R:602:CLA:HAB	41:R:616:XAT:H30	1.93	0.51
2:6:57:LYS:HD3	2:6:63:SER:CB	2.41	0.51
2:6:130:PRO:HG3	2:6:239:LYS:HE2	1.93	0.51
3:8:183:GLU:HB3	3:8:185:PHE:HD1	1.75	0.51
3:8:225:LYS:HA	3:8:228:GLU:OE2	2.11	0.51
4:a:170:ASP:OD2	6:c:357:ARG:NH1	2.43	0.51
4:a:205:VAL:HG12	7:d:205:VAL:HG12	1.93	0.51
6:c:203:THR:HG21	6:c:208:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:240:GLN:HE22	7:d:242:GLU:CG	2.24	0.51
20:s:221:LEU:HB3	25:s:310:CLA:H3A	1.93	0.51
21:n:85:LEU:HD13	25:n:602:CLA:H42	1.92	0.51
24:n:609:CHL:H91	24:n:609:CHL:H142	1.93	0.51
21:y:51:TYR:HE2	21:y:209:ALA:HB1	1.75	0.51
2:2:57:LYS:HD3	2:2:63:SER:CB	2.41	0.50
2:2:97:ALA:HB1	2:2:190:LEU:HD11	1.91	0.50
1:3:100:VAL:HB	1:3:190:LEU:HD13	1.92	0.50
1:3:164:THR:HG23	1:3:168:LEU:HD12	1.92	0.50
4:A:40:THR:HG23	25:A:405:CLA:HBB1	1.92	0.50
4:A:205:VAL:HG12	7:D:205:VAL:HG12	1.93	0.50
5:B:110:ALA:CB	25:B:616:CLA:HHB	2.40	0.50
26:B:625:LHG:H122	26:B:625:LHG:H331	1.92	0.50
6:C:471:PRO:O	6:C:472:LEU:HB2	2.11	0.50
12:K:58:VAL:HG12	12:K:61:ARG:HD2	1.92	0.50
15:O:187:ASN:OD1	15:O:187:ASN:O	2.28	0.50
18:X:93:GLY:O	18:X:96:VAL:HG22	2.11	0.50
20:S:169:ILE:HD12	24:S:306:CHL:HED1	1.92	0.50
20:S:209:LEU:O	21:N:195:SER:HA	2.11	0.50
21:Y:95:ASN:HA	21:Y:98:LEU:HB2	1.93	0.50
22:R:144:GLY:CA	22:R:246:ALA:HB1	2.19	0.50
22:R:154:ALA:O	22:R:157:VAL:HG12	2.11	0.50
22:R:202:ILE:HG13	22:R:203:GLU:N	2.25	0.50
22:R:277:ASP:HB2	22:R:280:HIS:HD1	1.75	0.50
24:R:607:CHL:CBB	40:R:617:NEX:H12	2.40	0.50
5:b:382:PRO:HB3	7:d:345:GLU:CD	2.35	0.50
5:b:458:PHE:HB3	25:b:604:CLA:HBC2	1.93	0.50
21:n:146:TYR:CD1	21:n:147:LEU:HG	2.46	0.50
21:y:131:TRP:O	21:y:134:ALA:HB3	2.10	0.50
24:y:302:CHL:C9	24:y:302:CHL:H51	2.41	0.50
25:y:312:CLA:H52	25:y:312:CLA:H92	1.92	0.50
22:r:240:LEU:HG	22:r:244:LYS:HD2	1.93	0.50
25:r:602:CLA:HAB	41:r:616:XAT:H30	1.93	0.50
1:1:117:GLU:HB2	1:1:241:LEU:HD12	1.93	0.50
2:2:127:PHE:HB3	2:2:140:PHE:HE2	1.75	0.50
4:A:202:VAL:HG22	25:A:401:CLA:HHB	1.92	0.50
27:A:404:PHO:H193	25:D:401:CLA:HHB	1.92	0.50
25:B:616:CLA:CMC	25:B:616:CLA:HBC2	2.42	0.50
25:C:503:CLA:HAA1	25:C:503:CLA:HBD	1.94	0.50
25:C:513:CLA:HBB1	25:C:513:CLA:HMB3	1.93	0.50
7:D:78:ALA:CB	7:D:175:GLY:HA3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:28:PRO:O	8:E:32:ILE:HG12	2.12	0.50
15:O:140:PRO:HD2	15:O:169:TYR:CE2	2.46	0.50
25:S:305:CLA:H43	40:S:317:NEX:H23	1.93	0.50
21:G:59:LEU:HD23	24:G:601:CHL:C1B	2.41	0.50
21:N:98:LEU:HD22	25:N:603:CLA:CAA	2.40	0.50
21:N:136:SER:HB3	24:N:607:CHL:O1D	2.11	0.50
2:6:210:ALA:HA	2:6:213:LYS:HZ2	1.76	0.50
4:a:85:THR:CG2	4:a:89:ILE:HD12	2.41	0.50
4:a:89:ILE:HD13	4:a:94:TYR:CD2	2.46	0.50
4:a:331:MET:HE1	7:d:321:LEU:HD22	1.92	0.50
5:b:271:THR:O	5:b:272:ARG:HB3	2.12	0.50
25:b:616:CLA:CMC	25:b:616:CLA:HBC2	2.42	0.50
6:c:61:VAL:HG12	6:c:118:HIS:O	2.12	0.50
6:c:318:LEU:HD12	6:c:340:TYR:HB3	1.93	0.50
25:c:505:CLA:HAA1	25:c:505:CLA:CBD	2.39	0.50
7:d:108:LEU:HD21	8:e:72:SER:HB2	1.93	0.50
20:s:72:PRO:HG3	24:s:302:CHL:CBB	2.41	0.50
20:s:105:GLU:O	20:s:109:LYS:HG3	2.11	0.50
20:s:209:LEU:O	21:n:195:SER:HA	2.11	0.50
21:g:86:SER:HB3	21:g:92:PHE:CD1	2.45	0.50
21:n:98:LEU:HD22	25:n:603:CLA:CAA	2.40	0.50
21:n:104:ARG:HD3	25:n:610:CLA:C4C	2.41	0.50
21:y:146:TYR:CD1	21:y:147:LEU:HG	2.46	0.50
24:y:308:CHL:HHD	24:y:308:CHL:CBC	2.36	0.50
22:r:277:ASP:HB2	22:r:280:HIS:HD1	1.75	0.50
1:1:158:ILE:O	1:1:161:ILE:HB	2.12	0.50
4:A:290:ILE:HG13	25:A:401:CLA:CED	2.41	0.50
5:B:59:GLY:O	25:B:607:CLA:HED2	2.12	0.50
5:B:360:PRO:O	5:B:361:THR:CG2	2.58	0.50
5:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.93	0.50
5:B:478:VAL:O	5:B:478:VAL:HG22	2.10	0.50
6:C:199:ILE:HG13	6:C:234:ILE:HG13	1.93	0.50
8:E:38:VAL:HG21	9:F:30:SER:O	2.11	0.50
20:S:188:TYR:CD1	20:S:193:GLY:HA3	2.46	0.50
21:G:154:HIS:O	21:G:154:HIS:ND1	2.43	0.50
21:N:85:LEU:HD13	25:N:602:CLA:H42	1.92	0.50
24:N:609:CHL:H91	24:N:609:CHL:H142	1.93	0.50
22:R:85:LYS:HG2	22:R:86:PRO:CD	2.38	0.50
22:R:124:PHE:CD1	25:R:614:CLA:HHC	2.46	0.50
1:7:86:SER:HB3	1:7:92:PHE:CD1	2.45	0.50
3:8:123:SER:OG	3:8:133:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:232:SER:OG	5:b:7:ARG:NH1	2.44	0.50
5:b:462:PHE:CE2	25:b:613:CLA:HMB3	2.46	0.50
15:o:296:THR:HG22	15:o:298:GLU:OE2	2.12	0.50
25:s:303:CLA:CAB	39:s:316:LUT:H32	2.42	0.50
22:r:150:ALA:HA	41:r:616:XAT:H181	1.94	0.50
2:2:120:GLN:HB3	2:2:129:GLU:CG	2.41	0.50
6:C:28:GLN:O	6:C:32:GLY:N	2.42	0.50
6:C:175:LEU:HB2	25:C:501:CLA:CMD	2.41	0.50
6:C:236:GLY:HA2	6:C:239:TRP:HD1	1.77	0.50
26:D:406:LHG:HC42	13:L:16:THR:HG21	1.94	0.50
18:X:79:ILE:H	18:X:79:ILE:HD12	1.77	0.50
24:Y:302:CHL:C9	24:Y:302:CHL:H51	2.42	0.50
25:Y:311:CLA:HAB	39:Y:316:LUT:H32	1.94	0.50
22:R:72:LEU:HB3	22:R:137:ARG:CZ	2.41	0.50
25:R:610:CLA:CBC	26:R:618:LHG:HC5	2.33	0.50
5:b:377:VAL:HG11	7:d:343:PRO:CG	2.41	0.50
25:b:607:CLA:H193	25:b:613:CLA:H141	1.94	0.50
6:c:76:VAL:O	6:c:76:VAL:HG13	2.11	0.50
6:c:290:VAL:HG21	25:c:502:CLA:CED	2.41	0.50
25:c:502:CLA:CMC	25:c:510:CLA:HBB1	2.38	0.50
7:d:135:ARG:NH2	7:d:138:GLN:OE1	2.42	0.50
15:o:114:CYS:SG	15:o:139:GLU:HB2	2.52	0.50
15:o:146:LYS:HB2	15:o:158:PHE:CE1	2.46	0.50
20:s:144:GLU:HB3	20:s:153:LEU:CD2	2.41	0.50
20:s:171:LEU:O	20:s:175:VAL:HG23	2.11	0.50
25:s:305:CLA:H43	40:s:317:NEX:H23	1.93	0.50
21:n:95:ASN:HA	21:n:98:LEU:HB2	1.93	0.50
2:2:130:PRO:HG3	2:2:239:LYS:CE	2.42	0.50
2:2:179:ASN:CA	24:2:603:CHL:CMC	2.85	0.50
1:3:131:TRP:O	1:3:134:ALA:HB3	2.10	0.50
4:A:286:THR:OG1	25:A:401:CLA:O1D	2.25	0.50
5:B:41:GLU:HB3	5:B:63:ILE:CD1	2.41	0.50
7:D:240:GLN:HE22	7:D:242:GLU:CG	2.24	0.50
15:O:296:THR:HG22	15:O:298:GLU:OE2	2.11	0.50
20:S:119:ARG:HD3	25:S:310:CLA:C4C	2.41	0.50
20:S:124:GLY:HA2	39:S:316:LUT:H181	1.92	0.50
21:G:158:ILE:O	21:G:161:ILE:HB	2.12	0.50
21:G:215:GLU:HG3	25:G:610:CLA:C2B	2.41	0.50
24:G:606:CHL:HBB1	39:G:616:LUT:H161	1.94	0.50
21:N:128:GLU:CB	21:N:137:GLN:HB2	2.41	0.50
21:N:204:ASP:O	21:N:208:PHE:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:611:CLA:CMC	26:N:618:LHG:H341	2.42	0.50
21:Y:86:SER:HB3	21:Y:92:PHE:CD1	2.45	0.50
2:6:131:VAL:HA	2:6:134:LYS:HD2	1.94	0.50
3:8:177:PRO:HD2	3:8:178:TRP:CE3	2.47	0.50
20:s:58:GLU:OE1	20:s:61:LYS:NZ	2.35	0.50
20:s:119:ARG:HD3	25:s:310:CLA:C4C	2.41	0.50
20:s:131:PRO:HG3	25:s:305:CLA:C1D	2.42	0.50
21:g:131:TRP:HA	39:g:616:LUT:O3	2.11	0.50
21:n:214:LYS:HG2	25:n:611:CLA:O2D	2.11	0.50
21:y:214:LYS:HG2	25:y:312:CLA:O2D	2.12	0.50
22:r:68:LEU:HD11	25:r:602:CLA:CED	2.42	0.50
22:r:154:ALA:O	22:r:157:VAL:HG12	2.11	0.50
2:2:103:GLY:HA3	2:2:219:ASN:HB3	1.93	0.50
1:3:95:ASN:HA	1:3:98:LEU:HB2	1.93	0.50
3:4:157:GLU:HG3	3:4:161:TRP:NE1	2.26	0.50
4:A:57:PRO:HB2	4:A:66:PRO:CB	2.42	0.50
4:A:220:THR:O	4:A:223:LEU:HG	2.12	0.50
7:D:108:LEU:HD21	8:E:72:SER:HB2	1.93	0.50
11:I:6:LEU:HD23	17:W:101:LEU:CD2	2.41	0.50
20:S:146:VAL:HG21	20:S:149:LYS:HZ1	1.77	0.50
25:S:310:CLA:H51	25:S:312:CLA:CMA	2.33	0.50
21:G:138:ILE:CD1	24:G:606:CHL:HAC1	2.42	0.50
21:G:146:TYR:CD1	21:G:147:LEU:HG	2.46	0.50
21:G:215:GLU:CB	25:G:610:CLA:C2B	2.90	0.50
24:N:607:CHL:H203	25:Y:303:CLA:C15	2.42	0.50
21:Y:158:ILE:O	21:Y:161:ILE:HB	2.12	0.50
2:6:127:PHE:HB3	2:6:140:PHE:HE2	1.75	0.50
2:6:179:ASN:CA	24:6:603:CHL:CMC	2.85	0.50
2:6:183:GLY:O	2:6:184:VAL:HG23	2.12	0.50
4:a:50:ILE:HG22	28:a:407:BCR:H271	1.92	0.50
27:a:405:PHO:HBB1	27:a:405:PHO:HMB3	1.93	0.50
27:a:405:PHO:HAB	25:d:402:CLA:C1	2.41	0.50
5:b:59:GLY:O	25:b:607:CLA:HED2	2.12	0.50
25:b:614:CLA:HBA1	28:b:617:BCR:H403	1.94	0.50
26:b:625:LHG:H331	26:b:625:LHG:H122	1.92	0.50
6:c:175:LEU:HB2	25:c:501:CLA:CMD	2.41	0.50
6:c:457:LYS:CD	7:d:230:ALA:HA	2.42	0.50
9:f:31:ILE:O	9:f:35:GLN:HG2	2.10	0.50
10:h:22:LEU:CG	22:r:124:PHE:HE2	2.25	0.50
19:z:3:ILE:HD12	19:z:3:ILE:H	1.76	0.50
21:g:138:ILE:HG13	21:g:144:LEU:CB	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:215:GLU:HG3	25:g:610:CLA:C2B	2.41	0.50
21:y:156:GLN:HB2	24:y:306:CHL:CBB	2.41	0.50
21:y:227:PHE:CD2	25:y:303:CLA:H171	2.47	0.50
25:y:311:CLA:HAB	39:y:316:LUT:H32	1.94	0.50
2:2:125:VAL:HG13	2:2:148:LEU:HD11	1.92	0.50
4:A:64:ARG:CG	6:C:337:LEU:HD21	2.42	0.50
4:A:85:THR:CG2	4:A:89:ILE:HD12	2.41	0.50
5:B:214:LEU:HD13	25:R:603:CLA:HED1	1.94	0.50
6:C:447:ARG:CD	25:C:508:CLA:HED1	2.42	0.50
7:D:19:MET:SD	18:X:103:VAL:HG22	2.52	0.50
11:I:27:ASP:HB3	11:I:28:PRO:HD3	1.93	0.50
14:M:6:LEU:O	14:M:9:ILE:HG22	2.12	0.50
20:S:72:PRO:HG3	24:S:302:CHL:CBB	2.41	0.50
25:S:303:CLA:CAB	39:S:316:LUT:H32	2.42	0.50
21:G:94:ARG:HA	21:G:94:ARG:HE	1.75	0.50
21:N:158:ILE:O	21:N:161:ILE:HB	2.12	0.50
21:N:210:GLU:OE1	21:N:214:LYS:NZ	2.38	0.50
25:R:603:CLA:C1B	25:R:608:CLA:H111	2.42	0.50
1:5:103:SER:O	1:5:107:MET:HG3	2.12	0.50
1:5:158:ILE:O	1:5:161:ILE:HB	2.12	0.50
2:6:69:TYR:HH	2:6:81:ASP:CG	2.19	0.50
4:a:77:ILE:HB	13:l:34:ASN:HD21	1.77	0.50
4:a:290:ILE:HG13	25:a:402:CLA:CED	2.41	0.50
25:b:614:CLA:HBD	25:b:614:CLA:HAA1	1.93	0.50
6:c:87:ILE:HD13	25:c:504:CLA:C1B	2.42	0.50
10:h:56:ILE:HA	18:x:84:LYS:CE	2.37	0.50
12:k:40:MET:N	12:k:41:PRO:HD2	2.27	0.50
18:x:79:ILE:H	18:x:79:ILE:HD12	1.77	0.50
25:n:610:CLA:H18	40:n:617:NEX:H372	1.92	0.50
21:y:94:ARG:HA	21:y:94:ARG:HE	1.75	0.50
2:2:121:LYS:HD3	2:2:242:LEU:HD23	1.93	0.50
2:2:130:PRO:HG3	2:2:239:LYS:HE2	1.93	0.50
4:A:77:ILE:HB	13:L:34:ASN:HD21	1.77	0.50
4:A:89:ILE:HD13	4:A:94:TYR:CD2	2.46	0.50
4:A:224:ILE:O	7:D:266:ARG:NH2	2.43	0.50
5:B:121:GLU:HG2	10:H:15:ARG:O	2.12	0.50
25:B:607:CLA:H193	25:B:613:CLA:H141	1.94	0.50
6:C:87:ILE:HD13	25:C:504:CLA:C1B	2.41	0.50
6:C:203:THR:HG21	6:C:208:VAL:HG11	1.93	0.50
6:C:379:ARG:HG2	6:C:383:ASP:OD2	2.11	0.50
7:D:85:SER:OG	23:U:102:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:12:LEU:HD13	19:Z:50:LEU:HB3	1.94	0.50
25:S:303:CLA:C7	25:S:304:CLA:HMA1	2.39	0.50
21:G:76:GLY:HA3	21:G:216:LEU:CD2	2.24	0.50
21:G:215:GLU:HG3	25:G:610:CLA:C3B	2.42	0.50
21:N:103:SER:O	21:N:107:MET:HG3	2.12	0.50
25:N:604:CLA:HBB	39:N:616:LUT:H3	1.94	0.50
21:Y:127:GLY:HA3	21:Y:137:GLN:CG	2.42	0.50
22:R:204:PHE:CE1	25:R:614:CLA:HAC2	2.46	0.50
22:R:220:GLY:HA2	22:R:224:ASP:CB	2.42	0.50
2:6:101:ILE:O	2:6:104:ARG:HB3	2.11	0.50
2:6:120:GLN:HB3	2:6:129:GLU:CG	2.41	0.50
1:7:94:ARG:HA	1:7:94:ARG:HE	1.75	0.50
1:7:154:HIS:O	1:7:154:HIS:ND1	2.44	0.50
25:a:402:CLA:H51	27:a:404:PHO:C3B	2.42	0.50
5:b:280:PHE:O	5:b:281:GLN:HB2	2.12	0.50
30:b:623:LMG:H371	25:r:608:CLA:C13	2.42	0.50
6:c:447:ARG:CD	25:c:508:CLA:HED1	2.42	0.50
7:d:320:ILE:O	7:d:324:GLU:HG3	2.12	0.50
20:s:124:GLY:HA2	39:s:316:LUT:H181	1.93	0.50
20:s:169:ILE:HD12	24:s:306:CHL:HED1	1.92	0.50
21:g:158:ILE:O	21:g:161:ILE:HB	2.12	0.50
21:g:209:ALA:CA	21:g:212:LYS:HG3	2.34	0.50
25:n:602:CLA:HBC2	25:n:602:CLA:CMC	2.40	0.50
25:n:604:CLA:HBB	39:n:616:LUT:H3	1.94	0.50
21:y:103:SER:O	21:y:107:MET:HG3	2.12	0.50
21:y:127:GLY:HA3	21:y:137:GLN:CG	2.42	0.50
21:y:158:ILE:O	21:y:161:ILE:HB	2.12	0.50
22:r:124:PHE:CD1	25:r:614:CLA:HHC	2.46	0.50
3:4:215:GLU:HB3	3:4:216:PRO:HD3	1.93	0.50
6:C:435:PHE:O	6:C:439:VAL:HG23	2.12	0.50
6:C:457:LYS:CD	7:D:230:ALA:HA	2.42	0.50
7:D:150:PRO:HB3	25:D:402:CLA:H41	1.92	0.50
28:T:101:BCR:H381	5:b:39:LEU:HB3	1.93	0.50
20:S:171:LEU:O	20:S:175:VAL:HG23	2.11	0.50
20:S:221:LEU:HB3	25:S:310:CLA:H3A	1.93	0.50
25:S:303:CLA:HAB	39:S:316:LUT:H32	1.91	0.50
21:G:69:TYR:OH	21:G:81:ASP:OD2	2.20	0.50
25:N:603:CLA:C20	24:N:607:CHL:H172	2.42	0.50
25:Y:312:CLA:H52	25:Y:312:CLA:H92	1.92	0.50
22:R:67:TRP:CZ3	22:R:82:GLY:HA2	2.44	0.50
2:6:103:GLY:HA3	2:6:219:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:72:THR:CG2	5:b:80:ILE:HG22	2.26	0.50
5:b:341:LEU:HD12	5:b:429:ILE:CG2	2.39	0.50
6:c:97:TRP:HH2	30:c:520:LMG:H172	1.75	0.50
25:c:510:CLA:H2	25:c:510:CLA:CMA	2.41	0.50
7:d:179:ILE:HG21	25:d:401:CLA:C4C	2.42	0.50
14:m:6:LEU:O	14:m:9:ILE:HG22	2.12	0.50
21:g:215:GLU:CB	25:g:610:CLA:C2B	2.90	0.50
21:n:136:SER:HB3	24:n:607:CHL:O1D	2.11	0.50
21:y:98:LEU:HD22	25:y:304:CLA:CBA	2.40	0.50
25:r:603:CLA:C1B	25:r:608:CLA:H111	2.42	0.50
40:r:617:NEX:H12	40:r:617:NEX:H191	1.93	0.50
2:2:246:LEU:HA	2:2:249:LEU:HD23	1.94	0.49
3:4:177:PRO:HD2	3:4:178:TRP:CE3	2.47	0.49
25:A:401:CLA:H51	27:A:403:PHO:C3B	2.42	0.49
5:B:7:ARG:HD3	25:B:611:CLA:HED1	1.93	0.49
25:B:601:CLA:CHB	25:B:602:CLA:HBB2	2.42	0.49
25:B:614:CLA:HBA1	28:B:617:BCR:H403	1.94	0.49
25:B:615:CLA:H51	25:B:616:CLA:C20	2.41	0.49
6:C:257:PHE:O	6:C:261:ARG:HG3	2.12	0.49
6:C:378:SER:OG	6:C:382:LYS:HE3	2.12	0.49
12:K:40:MET:N	12:K:41:PRO:HD2	2.27	0.49
25:N:603:CLA:H192	24:N:607:CHL:C17	2.42	0.49
21:Y:227:PHE:CD2	25:Y:303:CLA:H171	2.47	0.49
22:R:68:LEU:HD11	25:R:602:CLA:CED	2.42	0.49
40:R:617:NEX:H12	40:R:617:NEX:H191	1.93	0.49
1:5:57:LYS:HD2	1:5:63:SER:CB	2.42	0.49
1:5:117:GLU:HB2	1:5:241:LEU:HD12	1.93	0.49
1:5:154:HIS:O	1:5:154:HIS:ND1	2.43	0.49
2:6:64:VAL:HG12	2:6:65:GLN:N	2.27	0.49
2:6:130:PRO:HG3	2:6:239:LYS:CE	2.42	0.49
3:8:158:SER:O	3:8:162:VAL:HG12	2.12	0.49
4:a:40:THR:HA	4:a:118:HIS:HD1	1.77	0.49
4:a:64:ARG:CG	6:c:337:LEU:HD21	2.42	0.49
4:a:255:PHE:HE2	4:a:264:SER:HB3	1.74	0.49
5:b:460:LEU:HD21	7:d:160:ILE:CD1	2.42	0.49
25:b:601:CLA:CHB	25:b:602:CLA:HBB2	2.42	0.49
26:b:625:LHG:HC5	7:d:270:PHE:CZ	2.46	0.49
7:d:78:ALA:CB	7:d:175:GLY:HA3	2.42	0.49
21:g:59:LEU:HD23	24:g:601:CHL:C1B	2.41	0.49
21:n:104:ARG:HB3	25:n:610:CLA:HBC2	1.92	0.49
22:r:144:GLY:CA	22:r:246:ALA:HB1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:603:CLA:CHD	25:r:608:CLA:H92	2.29	0.49
3:4:213:VAL:O	3:4:213:VAL:HG12	2.12	0.49
30:B:623:LMG:H371	25:R:608:CLA:C13	2.42	0.49
25:C:510:CLA:H2	25:C:510:CLA:CMA	2.41	0.49
25:C:511:CLA:HAA1	25:C:511:CLA:CBD	2.42	0.49
10:H:22:LEU:CG	22:R:124:PHE:HE2	2.25	0.49
20:S:187:TYR:HA	20:S:190:ILE:HG12	1.93	0.49
21:N:214:LYS:HG2	25:N:611:CLA:O2D	2.11	0.49
21:Y:196:PHE:CE2	24:Y:309:CHL:HBC2	2.48	0.49
4:a:214:MET:HE1	27:a:405:PHO:CAD	2.43	0.49
25:b:602:CLA:H191	35:b:626:DGD:HBT1	1.95	0.49
25:b:602:CLA:HBC3	25:b:602:CLA:HHD	1.93	0.49
25:b:604:CLA:H92	25:b:604:CLA:C4	2.34	0.49
6:c:379:ARG:HG2	6:c:383:ASP:OD2	2.11	0.49
25:c:503:CLA:HAA1	25:c:503:CLA:HBD	1.94	0.49
25:c:513:CLA:HBB1	25:c:513:CLA:HMB3	1.93	0.49
26:d:406:LHG:HC42	13:l:16:THR:HG21	1.94	0.49
19:z:12:LEU:HD13	19:z:50:LEU:HB3	1.94	0.49
20:s:188:TYR:CD1	20:s:193:GLY:HA3	2.46	0.49
21:g:103:SER:O	21:g:107:MET:HG3	2.12	0.49
25:n:603:CLA:H142	25:y:304:CLA:C14	2.42	0.49
24:y:307:CHL:CMC	24:y:308:CHL:C4C	2.90	0.49
2:2:116:PRO:CG	2:2:134:LYS:HE3	2.42	0.49
2:2:183:GLY:O	2:2:184:VAL:HG23	2.12	0.49
2:2:249:LEU:HD12	2:2:250:ASP:N	2.28	0.49
3:4:77:LEU:HD23	3:4:78:PRO:O	2.11	0.49
3:4:123:SER:OG	3:4:133:GLN:HB2	2.11	0.49
27:A:404:PHO:H152	25:D:401:CLA:HMB2	1.95	0.49
5:B:187:VAL:HG13	25:B:601:CLA:HMD2	1.93	0.49
5:B:277:GLN:OE1	23:U:99:LYS:NZ	2.33	0.49
6:C:25:GLY:O	6:C:26:ARG:HG3	2.12	0.49
6:C:61:VAL:HG12	6:C:118:HIS:O	2.12	0.49
15:O:145:VAL:HG11	15:O:203:LEU:CD1	2.35	0.49
20:S:262:PHE:CD2	25:S:314:CLA:HMA1	2.46	0.49
21:G:57:LYS:HD2	21:G:63:SER:CB	2.42	0.49
21:G:90:GLU:CB	21:N:87:ALA:HB1	2.42	0.49
21:Y:57:LYS:HD2	21:Y:63:SER:CB	2.42	0.49
22:R:150:ALA:HB1	41:R:616:XAT:H181	1.95	0.49
1:5:107:MET:HG2	1:5:222:ALA:HB3	1.94	0.49
2:6:55:ARG:HE	2:6:72:GLY:HA3	1.77	0.49
2:6:211:GLU:O	2:6:215:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:95:ASN:HA	1:7:98:LEU:HB2	1.93	0.49
3:8:77:LEU:HD23	3:8:78:PRO:O	2.11	0.49
3:8:157:GLU:HG3	3:8:161:TRP:NE1	2.26	0.49
4:a:85:THR:O	4:a:169:SER:HB3	2.12	0.49
5:b:121:GLU:HG2	10:h:15:ARG:O	2.12	0.49
25:b:614:CLA:H71	29:l:102:SQD:C15	2.43	0.49
6:c:257:PHE:O	6:c:261:ARG:HG3	2.12	0.49
6:c:327:ASN:ND2	15:o:192:ASP:HB2	2.26	0.49
21:g:57:LYS:HD2	21:g:63:SER:CB	2.42	0.49
21:g:138:ILE:CD1	24:g:606:CHL:HAC1	2.42	0.49
24:g:606:CHL:HBB1	39:g:616:LUT:H161	1.94	0.49
21:n:51:TYR:HE2	21:n:209:ALA:HB1	1.75	0.49
21:n:57:LYS:HD2	21:n:63:SER:CB	2.42	0.49
21:n:172:VAL:HG22	40:n:617:NEX:H201	1.94	0.49
25:n:603:CLA:CAC	24:y:302:CHL:H102	2.42	0.49
21:y:56:VAL:CB	24:y:302:CHL:HBC1	2.43	0.49
21:y:196:PHE:CE2	24:y:309:CHL:HBC2	2.47	0.49
25:y:315:CLA:HBA2	25:y:315:CLA:CBD	2.42	0.49
22:r:63:ILE:HG13	22:r:63:ILE:O	2.12	0.49
22:r:158:GLU:OE2	22:r:266:GLY:HA3	2.12	0.49
2:2:130:PRO:HG2	2:2:133:PHE:CG	2.47	0.49
2:2:131:VAL:HA	2:2:134:LYS:HD2	1.94	0.49
1:3:117:GLU:HB2	1:3:241:LEU:HD12	1.95	0.49
1:3:158:ILE:O	1:3:161:ILE:HB	2.12	0.49
3:4:219:GLU:HG3	3:4:222:GLU:CB	2.41	0.49
4:A:85:THR:O	4:A:169:SER:HB3	2.12	0.49
6:C:277:ALA:HB2	6:C:441:HIS:CG	2.47	0.49
6:C:290:VAL:HG21	25:C:502:CLA:CED	2.41	0.49
20:S:131:PRO:HG3	25:S:305:CLA:C1D	2.42	0.49
21:N:95:ASN:HA	21:N:98:LEU:HB2	1.93	0.49
24:Y:307:CHL:CMC	24:Y:308:CHL:C4C	2.90	0.49
22:R:67:TRP:CE2	22:R:85:LYS:HA	2.48	0.49
22:R:279:LEU:H	22:R:279:LEU:HD12	1.76	0.49
25:R:603:CLA:HMB2	25:R:603:CLA:H143	1.94	0.49
23:U:79:ARG:O	23:U:84:ALA:HB2	2.13	0.49
2:6:121:LYS:HD3	2:6:242:LEU:HD23	1.93	0.49
8:e:28:PRO:O	8:e:32:ILE:HG12	2.12	0.49
20:s:262:PHE:CE2	25:s:314:CLA:H3A	2.43	0.49
21:y:57:LYS:HD2	21:y:63:SER:CB	2.42	0.49
24:y:310:CHL:NA	24:y:310:CHL:HBA1	2.27	0.49
22:r:220:GLY:HA2	22:r:224:ASP:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:94:ARG:HA	1:1:94:ARG:HE	1.75	0.49
2:2:117:GLU:O	2:2:121:LYS:HB2	2.13	0.49
2:2:145:LEU:HB3	2:2:149:GLY:C	2.37	0.49
25:C:511:CLA:HBA1	28:K:101:BCR:H271	1.93	0.49
7:D:135:ARG:NH2	7:D:138:GLN:OE1	2.42	0.49
15:O:177:PRO:CD	15:O:189:LYS:HE3	2.43	0.49
21:G:86:SER:HB3	21:G:92:PHE:CD1	2.45	0.49
21:N:57:LYS:HD2	21:N:63:SER:CB	2.42	0.49
21:N:154:HIS:O	21:N:154:HIS:ND1	2.44	0.49
25:N:603:CLA:CAC	24:Y:302:CHL:H102	2.42	0.49
25:Y:315:CLA:HBA2	25:Y:315:CLA:CBD	2.42	0.49
22:R:150:ALA:HA	41:R:616:XAT:H181	1.94	0.49
1:7:57:LYS:HD2	1:7:63:SER:CB	2.42	0.49
27:a:405:PHO:H152	25:d:401:CLA:HMB2	1.95	0.49
25:b:607:CLA:HMC2	28:b:618:BCR:H323	1.95	0.49
6:c:95:LEU:HD23	25:c:502:CLA:H143	1.95	0.49
18:x:93:GLY:O	18:x:96:VAL:HG22	2.12	0.49
20:s:225:GLU:HB2	25:s:310:CLA:C2B	2.42	0.49
21:g:144:LEU:HD11	25:g:604:CLA:HAA2	1.95	0.49
21:n:176:ARG:NH2	24:n:609:CHL:O1D	2.44	0.49
25:n:603:CLA:H192	24:n:607:CHL:C17	2.42	0.49
24:n:607:CHL:H203	25:y:303:CLA:C15	2.42	0.49
2:2:64:VAL:HG12	2:2:65:GLN:N	2.27	0.49
4:A:232:SER:OG	5:B:7:ARG:NH1	2.44	0.49
5:B:280:PHE:O	5:B:281:GLN:HB2	2.12	0.49
5:B:453:PHE:HB2	7:D:292:LEU:HD12	1.93	0.49
25:B:613:CLA:H172	28:B:618:BCR:H312	1.94	0.49
10:H:32:LYS:HB2	22:R:113:ARG:NH1	2.28	0.49
15:O:215:VAL:HG22	15:O:218:LEU:HB3	1.93	0.49
21:G:215:GLU:CB	25:G:610:CLA:C1B	2.89	0.49
22:R:158:GLU:OE2	22:R:266:GLY:HA3	2.12	0.49
22:R:164:THR:HG23	22:R:167:ASP:H	1.78	0.49
1:5:86:SER:HB3	1:5:92:PHE:CD1	2.45	0.49
1:7:51:TYR:HE2	1:7:209:ALA:HB1	1.75	0.49
1:7:103:SER:O	1:7:107:MET:HG3	2.12	0.49
30:a:409:LMG:O5	17:w:87:THR:O	2.27	0.49
7:d:44:PHE:HB3	7:d:114:PHE:CE2	2.48	0.49
7:d:240:GLN:OE1	7:d:242:GLU:HG2	2.13	0.49
21:n:132:PHE:HD2	24:n:607:CHL:HED1	1.77	0.49
21:y:227:PHE:CD2	25:y:303:CLA:H202	2.40	0.49
22:r:72:LEU:HB3	22:r:137:ARG:CZ	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:279:LEU:H	22:r:279:LEU:HD12	1.76	0.49
1:1:57:LYS:HD2	1:1:63:SER:CB	2.42	0.49
1:1:116:PRO:HA	1:1:126:PHE:HE2	1.78	0.49
2:2:204:ASP:C	2:2:208:THR:HG23	2.38	0.49
2:2:236:VAL:O	2:2:237:THR:OG1	2.24	0.49
3:4:158:SER:O	3:4:162:VAL:HG12	2.12	0.49
5:B:377:VAL:HG11	7:D:343:PRO:CG	2.41	0.49
25:B:609:CLA:HMA2	25:B:610:CLA:HMC2	1.94	0.49
25:B:614:CLA:H71	29:L:101:SQD:C15	2.43	0.49
6:C:227:VAL:HG21	28:I:101:BCR:C29	2.43	0.49
7:D:262:PHE:O	31:D:405:PL9:H522	2.11	0.49
7:D:320:ILE:O	7:D:324:GLU:HG3	2.12	0.49
15:O:179:GLU:HB3	15:O:187:ASN:OD1	2.12	0.49
20:S:135:ASN:HA	20:S:138:GLY:O	2.12	0.49
21:G:103:SER:O	21:G:107:MET:HG3	2.12	0.49
21:G:144:LEU:HD11	25:G:604:CLA:HAA2	1.95	0.49
24:N:609:CHL:H72	24:Y:302:CHL:C11	2.40	0.49
21:Y:214:LYS:HG2	25:Y:312:CLA:O2D	2.12	0.49
4:a:57:PRO:HB2	4:a:66:PRO:CB	2.42	0.49
4:a:131:TRP:CZ2	6:c:449:ARG:HD2	2.48	0.49
4:a:162:PRO:HB3	4:a:168:PHE:HA	1.94	0.49
5:b:453:PHE:HB2	7:d:292:LEU:HD12	1.93	0.49
5:b:471:ALA:HB2	7:d:131:PHE:CE1	2.48	0.49
6:c:135:LEU:O	6:c:135:LEU:HD23	2.13	0.49
6:c:435:PHE:O	6:c:439:VAL:HG23	2.12	0.49
7:d:19:MET:SD	18:x:103:VAL:HG22	2.52	0.49
20:s:119:ARG:HB3	25:s:310:CLA:HAC1	1.95	0.49
20:s:135:ASN:HA	20:s:138:GLY:O	2.12	0.49
20:s:188:TYR:HD1	20:s:193:GLY:HA3	1.77	0.49
21:g:95:ASN:HA	21:g:98:LEU:HB2	1.93	0.49
25:n:611:CLA:CMC	26:n:618:LHG:H341	2.42	0.49
21:y:204:ASP:O	21:y:208:PHE:N	2.40	0.49
1:3:116:PRO:HA	1:3:126:PHE:HE2	1.78	0.49
1:3:127:GLY:HA3	1:3:137:GLN:CG	2.42	0.49
3:4:221:LEU:HA	3:4:224:LEU:HD23	1.95	0.49
4:A:254:TYR:HE1	7:D:134:ALA:N	2.11	0.49
5:B:164:PRO:HG3	25:B:606:CLA:O1D	2.12	0.49
5:B:360:PRO:C	5:B:361:THR:HG22	2.38	0.49
6:C:213:LEU:HD11	28:I:101:BCR:H373	1.95	0.49
6:C:361:LEU:HD12	35:C:515:DGD:O3E	2.13	0.49
21:G:127:GLY:HA3	21:G:137:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:51:TYR:HE2	21:N:209:ALA:HB1	1.75	0.49
21:N:227:PHE:CD2	25:N:602:CLA:H202	2.41	0.49
21:Y:154:HIS:O	21:Y:154:HIS:ND1	2.44	0.49
1:5:95:ASN:HA	1:5:98:LEU:HB2	1.93	0.49
1:5:209:ALA:CA	1:5:212:LYS:HG3	2.34	0.49
2:6:116:PRO:HG2	2:6:117:GLU:OE1	2.13	0.49
2:6:249:LEU:HD12	2:6:250:ASP:N	2.28	0.49
1:7:127:GLY:HA3	1:7:137:GLN:CG	2.42	0.49
3:8:75:GLY:HA2	3:8:80:ASP:HB3	1.93	0.49
5:b:245:VAL:HG21	25:b:612:CLA:CED	2.43	0.49
6:c:97:TRP:HE1	6:c:178:LYS:CE	2.25	0.49
6:c:321:ASP:OD2	6:c:340:TYR:OH	2.27	0.49
6:c:378:SER:OG	6:c:382:LYS:HE3	2.12	0.49
6:c:457:LYS:HD3	7:d:230:ALA:HA	1.94	0.49
7:d:341:ILE:HG23	7:d:341:ILE:O	2.13	0.49
8:e:38:VAL:HG21	9:f:30:SER:O	2.11	0.49
15:o:177:PRO:CD	15:o:189:LYS:HE3	2.43	0.49
21:g:90:GLU:CB	21:n:87:ALA:HB1	2.42	0.49
21:n:107:MET:HE1	25:n:610:CLA:CHC	2.42	0.49
22:r:218:PRO:HB2	22:r:223:PHE:CD2	2.48	0.49
2:2:137:SER:HA	2:2:140:PHE:CE2	2.48	0.49
1:3:138:ILE:HG13	1:3:144:LEU:CB	2.31	0.49
5:B:245:VAL:HG21	25:B:612:CLA:CED	2.43	0.49
5:B:271:THR:O	5:B:272:ARG:HB3	2.12	0.49
7:D:44:PHE:HB3	7:D:114:PHE:CE2	2.48	0.49
7:D:179:ILE:HG21	25:D:401:CLA:C4C	2.42	0.49
7:D:192:TRP:CE3	7:D:290:LEU:HD11	2.48	0.49
7:D:198:HIS:HE1	25:D:402:CLA:C1C	2.26	0.49
7:D:240:GLN:OE1	7:D:242:GLU:HG2	2.13	0.49
10:H:25:PRO:CG	22:R:122:THR:HB	2.42	0.49
15:O:113:GLN:NE2	17:W:80:LEU:HD11	2.16	0.49
21:G:97:GLU:HA	21:G:190:LEU:CD1	2.24	0.49
25:G:612:CLA:HBD	25:G:612:CLA:HAA2	1.95	0.49
21:N:107:MET:HE1	25:N:610:CLA:CHC	2.42	0.49
25:N:603:CLA:H142	25:Y:304:CLA:C14	2.42	0.49
21:Y:103:SER:O	21:Y:107:MET:HG3	2.12	0.49
24:R:605:CHL:HAB	25:R:608:CLA:CBC	2.43	0.49
23:U:97:THR:HG22	23:U:102:ARG:NH2	2.28	0.49
2:6:130:PRO:HG2	2:6:133:PHE:CG	2.47	0.49
1:7:117:GLU:HB2	1:7:241:LEU:HD12	1.95	0.49
3:8:73:LEU:HB3	3:8:80:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:220:THR:O	4:a:223:LEU:HG	2.12	0.49
29:a:408:SQD:H441	7:d:233:PHE:CE2	2.48	0.49
25:b:608:CLA:H18	25:d:403:CLA:HBA1	1.95	0.49
10:h:22:LEU:HB3	22:r:124:PHE:CE2	2.48	0.49
14:m:26:TYR:O	14:m:30:VAL:HG13	2.13	0.49
21:g:76:GLY:HA3	21:g:216:LEU:CD2	2.24	0.49
25:2:604:CLA:HBD	25:2:604:CLA:CAA	2.41	0.49
3:4:187:ASN:O	3:4:188:TYR:HB2	2.12	0.49
4:A:40:THR:HA	4:A:118:HIS:HD1	1.77	0.49
25:C:504:CLA:H101	35:C:516:DGD:HBH2	1.94	0.49
19:Z:58:ASN:O	19:Z:61:ILE:HG12	2.13	0.49
21:G:209:ALA:CA	21:G:212:LYS:HG3	2.34	0.49
21:N:60:GLY:HA3	24:N:601:CHL:CMC	2.43	0.49
21:N:116:PRO:HA	21:N:126:PHE:HE2	1.78	0.49
21:N:127:GLY:HA3	21:N:137:GLN:CG	2.42	0.49
21:N:138:ILE:HG13	21:N:144:LEU:CB	2.31	0.49
24:N:607:CHL:H202	24:N:609:CHL:C3	2.43	0.49
21:Y:251:PRO:HB2	25:Y:315:CLA:CMA	2.30	0.49
24:5:301:CHL:HHD	24:5:301:CHL:HBC2	1.95	0.49
3:8:213:VAL:O	3:8:213:VAL:HG12	2.12	0.49
27:a:404:PHO:H42	26:d:406:LHG:H342	1.95	0.49
5:b:296:GLN:NE2	5:b:304:LYS:HD2	2.22	0.49
25:b:613:CLA:H172	28:b:618:BCR:H312	1.94	0.49
6:c:25:GLY:O	6:c:26:ARG:HG3	2.12	0.49
7:d:141:PRO:O	7:d:145:ILE:HD12	2.13	0.49
7:d:194:LEU:O	13:l:35:TYR:OH	2.14	0.49
14:m:15:ILE:O	14:m:19:THR:OG1	2.18	0.49
15:o:113:GLN:NE2	17:w:80:LEU:HD11	2.16	0.49
15:o:145:VAL:CG1	15:o:203:LEU:HD11	2.37	0.49
21:g:107:MET:HG2	21:g:222:ALA:HB3	1.93	0.49
21:g:116:PRO:HA	21:g:126:PHE:HE2	1.78	0.49
21:g:139:PHE:CD2	24:g:607:CHL:OBD	2.66	0.49
21:g:215:GLU:CB	25:g:610:CLA:C1B	2.89	0.49
21:n:158:ILE:O	21:n:161:ILE:HB	2.12	0.49
22:r:67:TRP:CE2	22:r:85:LYS:HA	2.48	0.49
22:r:160:LEU:HD13	22:r:180:LEU:HD21	1.95	0.49
2:2:55:ARG:HE	2:2:72:GLY:HA3	1.77	0.48
4:A:202:VAL:HG13	25:A:401:CLA:HMB2	1.95	0.48
5:B:460:LEU:HD21	7:D:160:ILE:CD1	2.42	0.48
7:D:343:PRO:HD2	7:D:346:VAL:HG21	1.95	0.48
20:S:132:GLU:HA	20:S:145:ALA:CB	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:86:SER:OG	25:G:602:CLA:O1A	2.23	0.48
21:N:132:PHE:HD2	24:N:607:CHL:HED1	1.77	0.48
25:N:604:CLA:C1C	40:N:617:NEX:H222	2.42	0.48
21:Y:69:TYR:OH	21:Y:81:ASP:OD2	2.20	0.48
22:R:63:ILE:O	22:R:63:ILE:HG13	2.12	0.48
22:R:160:LEU:HD13	22:R:180:LEU:HD21	1.95	0.48
1:5:204:ASP:O	1:5:208:PHE:N	2.40	0.48
2:6:116:PRO:CG	2:6:134:LYS:HE3	2.42	0.48
2:6:117:GLU:O	2:6:121:LYS:HB2	2.13	0.48
2:6:127:PHE:HE2	2:6:145:LEU:CB	2.24	0.48
25:6:604:CLA:CHC	26:6:606:LHG:HC5	2.43	0.48
4:a:202:VAL:HG13	25:a:402:CLA:HMB2	1.95	0.48
5:b:164:PRO:HG3	25:b:606:CLA:O1D	2.12	0.48
6:c:223:TRP:CG	6:c:224:ILE:H	2.31	0.48
25:c:504:CLA:H101	35:c:516:DGD:HBH2	1.94	0.48
25:c:511:CLA:H142	12:k:47:PHE:HE2	1.77	0.48
7:d:343:PRO:HD2	7:d:346:VAL:HG21	1.95	0.48
10:h:32:LYS:HB2	22:r:113:ARG:NH1	2.28	0.48
21:g:215:GLU:HG3	25:g:610:CLA:C3B	2.42	0.48
25:n:603:CLA:C20	24:n:607:CHL:H172	2.42	0.48
25:n:613:CLA:H142	25:n:613:CLA:C2	2.40	0.48
22:r:72:LEU:CB	22:r:137:ARG:HH22	2.26	0.48
22:r:164:THR:HG23	22:r:167:ASP:H	1.78	0.48
22:r:192:ILE:O	22:r:196:VAL:HG23	2.13	0.48
2:2:127:PHE:HE2	2:2:145:LEU:CB	2.24	0.48
1:3:57:LYS:HD2	1:3:63:SER:CB	2.42	0.48
1:3:103:SER:O	1:3:107:MET:HG3	2.12	0.48
25:B:608:CLA:H18	25:D:403:CLA:HBA1	1.95	0.48
6:C:97:TRP:HE1	6:C:178:LYS:CE	2.25	0.48
6:C:135:LEU:O	6:C:135:LEU:HD23	2.13	0.48
6:C:175:LEU:HD23	6:C:237:HIS:CE1	2.48	0.48
6:C:211:GLY:O	6:C:215:LYS:HB2	2.13	0.48
25:C:506:CLA:H141	25:C:506:CLA:H162	1.63	0.48
7:D:162:PRO:CB	7:D:171:ALA:HB2	2.42	0.48
12:K:34:ASN:N	12:K:35:PRO:HD2	2.28	0.48
15:O:114:CYS:SG	15:O:139:GLU:HB2	2.52	0.48
21:G:224:PHE:CG	26:Y:301:LHG:H281	2.49	0.48
24:G:605:CHL:H3A	24:G:605:CHL:HBA2	1.36	0.48
21:N:172:VAL:HG22	40:N:617:NEX:H201	1.94	0.48
21:N:176:ARG:NH2	24:N:609:CHL:O1D	2.44	0.48
2:6:145:LEU:HB3	2:6:149:GLY:C	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:209:PHE:C	2:6:213:LYS:HZ2	2.22	0.48
1:7:204:ASP:O	1:7:208:PHE:N	2.40	0.48
3:8:187:ASN:O	3:8:188:TYR:HB2	2.12	0.48
3:8:222:GLU:HA	3:8:225:LYS:HB2	1.95	0.48
5:b:236:THR:HB	5:b:473:THR:HG21	1.95	0.48
6:c:175:LEU:HD23	6:c:237:HIS:CE1	2.48	0.48
6:c:199:ILE:HG13	6:c:234:ILE:HG13	1.93	0.48
6:c:279:LEU:O	25:c:502:CLA:HBC1	2.13	0.48
6:c:332:GLN:HG2	15:o:238:GLY:O	2.14	0.48
7:d:192:TRP:CE3	7:d:290:LEU:HD11	2.48	0.48
15:o:171:LEU:HD22	15:o:194:ILE:O	2.13	0.48
15:o:179:GLU:HB3	15:o:187:ASN:OD1	2.12	0.48
24:n:601:CHL:HBC3	24:n:601:CHL:HMC	1.94	0.48
1:1:95:ASN:HA	1:1:98:LEU:HB2	1.93	0.48
3:4:175:ALA:CB	25:R:601:CLA:HHC	2.43	0.48
4:A:60:ILE:HB	4:A:83:ILE:CG2	2.44	0.48
5:B:285:TYR:CZ	23:U:90:GLN:HG3	2.49	0.48
5:B:368:VAL:HG21	5:B:422:ARG:HG2	1.95	0.48
25:B:602:CLA:H191	35:B:626:DGD:HBT1	1.95	0.48
25:B:607:CLA:HMC2	28:B:618:BCR:H323	1.95	0.48
6:C:332:GLN:HG2	15:O:238:GLY:O	2.14	0.48
6:C:457:LYS:HD3	7:D:230:ALA:HA	1.94	0.48
20:S:119:ARG:HB3	25:S:310:CLA:HAC1	1.95	0.48
21:G:60:GLY:H	24:G:601:CHL:CHC	2.26	0.48
22:R:240:LEU:HG	22:R:244:LYS:HD2	1.93	0.48
2:6:246:LEU:HA	2:6:249:LEU:HD23	1.94	0.48
1:7:158:ILE:O	1:7:161:ILE:HB	2.12	0.48
4:a:60:ILE:HB	4:a:83:ILE:HG22	1.96	0.48
4:a:140:ARG:NH2	7:d:220:GLU:O	2.40	0.48
25:a:402:CLA:H102	27:a:404:PHO:HAA1	1.95	0.48
25:b:609:CLA:HMA2	25:b:610:CLA:HMC2	1.94	0.48
6:c:140:LEU:HD22	25:c:513:CLA:CMA	2.44	0.48
6:c:471:PRO:O	6:c:472:LEU:HB2	2.11	0.48
25:c:501:CLA:HHC	25:c:501:CLA:HBB1	1.96	0.48
11:i:34:ARG:C	11:i:35:GLU:HG3	2.39	0.48
25:s:310:CLA:H51	25:s:312:CLA:CMA	2.34	0.48
21:g:127:GLY:HA3	21:g:137:GLN:CG	2.42	0.48
21:g:128:GLU:CB	21:g:137:GLN:HB2	2.41	0.48
24:g:606:CHL:HAA1	40:g:617:NEX:H381	1.96	0.48
21:n:103:SER:O	21:n:107:MET:HG3	2.12	0.48
25:n:602:CLA:HMB1	25:n:602:CLA:C2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:164:THR:CG2	22:r:167:ASP:HB2	2.43	0.48
23:u:97:THR:HG22	23:u:102:ARG:NH2	2.28	0.48
1:1:58:TYR:CE1	1:1:80:TRP:HA	2.49	0.48
1:1:103:SER:O	1:1:107:MET:HG3	2.12	0.48
2:2:114:ILE:O	2:2:118:VAL:HG23	2.13	0.48
4:A:272:HIS:CD2	7:D:219:VAL:HG21	2.48	0.48
25:A:401:CLA:H102	27:A:403:PHO:HAA1	1.95	0.48
5:B:236:THR:HB	5:B:473:THR:HG21	1.95	0.48
7:D:141:PRO:O	7:D:145:ILE:HD12	2.13	0.48
15:O:171:LEU:HD22	15:O:194:ILE:O	2.13	0.48
25:G:603:CLA:ND	24:G:609:CHL:H8	2.28	0.48
21:N:94:ARG:HA	21:N:94:ARG:HE	1.75	0.48
25:N:602:CLA:HMB1	25:N:602:CLA:C2	2.44	0.48
21:Y:210:GLU:OE1	21:Y:214:LYS:NZ	2.38	0.48
22:R:185:PRO:CD	21:y:151:SER:HB2	2.43	0.48
6:c:277:ALA:HB2	6:c:441:HIS:CG	2.47	0.48
25:s:305:CLA:HBB1	25:s:305:CLA:HMB1	1.95	0.48
25:g:610:CLA:H41	25:g:612:CLA:CMA	2.41	0.48
25:n:604:CLA:C1C	40:n:617:NEX:H222	2.43	0.48
22:r:58:TRP:CD2	22:r:78:PHE:HD1	2.31	0.48
24:r:607:CHL:H112	24:r:607:CHL:CAB	2.31	0.48
25:r:614:CLA:HHD	25:r:614:CLA:CBC	2.37	0.48
1:1:107:MET:HG2	1:1:222:ALA:HB3	1.94	0.48
2:2:69:TYR:HH	2:2:81:ASP:CG	2.21	0.48
2:2:175:GLY:HA3	2:2:181:LEU:CG	2.44	0.48
25:2:604:CLA:H41	25:2:604:CLA:H61	1.61	0.48
3:4:222:GLU:HA	3:4:225:LYS:HB2	1.95	0.48
3:4:225:LYS:CA	3:4:228:GLU:OE1	2.61	0.48
6:C:279:LEU:O	25:C:502:CLA:HBC1	2.13	0.48
10:H:22:LEU:HB3	22:R:124:PHE:CE2	2.48	0.48
11:I:34:ARG:C	11:I:35:GLU:HG3	2.38	0.48
20:S:67:ARG:HH11	20:S:87:GLY:HA2	1.78	0.48
25:S:305:CLA:HBB1	25:S:305:CLA:HMB1	1.95	0.48
21:Y:94:ARG:HA	21:Y:94:ARG:HE	1.75	0.48
21:Y:116:PRO:HA	21:Y:126:PHE:HE2	1.78	0.48
21:Y:151:SER:HB2	22:r:185:PRO:CD	2.43	0.48
21:Y:209:ALA:CA	21:Y:212:LYS:HG3	2.34	0.48
22:R:164:THR:CG2	22:R:167:ASP:HB2	2.44	0.48
1:5:128:GLU:CB	1:5:137:GLN:HB2	2.41	0.48
2:6:104:ARG:HE	24:6:603:CHL:CBD	2.13	0.48
2:6:131:VAL:HA	2:6:134:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:175:ALA:CB	25:r:601:CLA:HHC	2.43	0.48
4:a:51:ALA:HA	4:a:55:ALA:HB2	1.95	0.48
4:a:131:TRP:CZ2	25:c:505:CLA:HAA2	2.49	0.48
4:a:139:MET:SD	7:d:253:PHE:HB2	2.54	0.48
19:z:56:ILE:HG23	20:s:270:ILE:CD1	2.44	0.48
24:g:609:CHL:CAA	21:n:82:THR:HG21	2.43	0.48
25:n:602:CLA:H142	25:n:602:CLA:H112	1.63	0.48
24:y:307:CHL:HHC	24:y:308:CHL:CMC	2.44	0.48
1:1:154:HIS:O	1:1:154:HIS:ND1	2.43	0.48
2:2:131:VAL:HA	2:2:134:LYS:HB2	1.96	0.48
1:3:107:MET:HG2	1:3:222:ALA:HB3	1.94	0.48
4:A:214:MET:HE1	27:A:404:PHO:CAD	2.43	0.48
29:A:407:SQD:H441	7:D:233:PHE:CE2	2.48	0.48
5:B:115:TRP:CH2	25:B:614:CLA:HMA2	2.49	0.48
5:B:223:GLN:HG2	10:H:36:GLY:N	2.28	0.48
6:C:223:TRP:CG	6:C:224:ILE:H	2.31	0.48
7:D:58:SER:OG	7:D:80:SER:OG	2.25	0.48
20:S:188:TYR:HD1	20:S:193:GLY:HA3	1.77	0.48
20:S:225:GLU:HB2	25:S:310:CLA:C2B	2.42	0.48
21:G:58:TYR:CE1	21:G:80:TRP:HA	2.49	0.48
21:G:107:MET:HG2	21:G:222:ALA:HB3	1.93	0.48
21:Y:56:VAL:CB	24:Y:302:CHL:HBC1	2.43	0.48
23:U:96:PRO:C	23:U:97:THR:HG1	2.09	0.48
1:5:116:PRO:HA	1:5:126:PHE:HE2	1.78	0.48
4:a:95:PRO:HD2	4:a:98:GLU:HG3	1.96	0.48
5:b:200:SER:O	5:b:201:HIS:C	2.56	0.48
5:b:280:PHE:O	5:b:281:GLN:CB	2.61	0.48
5:b:422:ARG:O	5:b:425:GLN:HG2	2.13	0.48
26:b:622:LHG:H201	26:b:622:LHG:H352	1.96	0.48
6:c:227:VAL:HG21	28:i:101:BCR:C29	2.43	0.48
25:c:504:CLA:H92	25:c:504:CLA:H62	1.52	0.48
25:c:513:CLA:HMC1	28:c:514:BCR:H372	1.96	0.48
7:d:198:HIS:HE1	25:d:402:CLA:C1C	2.26	0.48
11:i:33:GLY:C	11:i:34:ARG:HG3	2.36	0.48
25:g:602:CLA:H111	25:g:602:CLA:H72	1.45	0.48
24:g:606:CHL:HBA2	40:g:617:NEX:H30	1.96	0.48
21:n:86:SER:HB3	21:n:92:PHE:CD1	2.45	0.48
2:2:116:PRO:HG2	2:2:117:GLU:OE1	2.13	0.48
4:A:51:ALA:HA	4:A:55:ALA:HB2	1.95	0.48
5:B:57:ARG:HG3	5:B:57:ARG:O	2.14	0.48
5:B:296:GLN:NE2	5:B:304:LYS:HD2	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:379:ALA:HB2	5:B:395:VAL:HG11	1.95	0.48
25:C:513:CLA:HMC1	28:C:514:BCR:H372	1.96	0.48
8:E:27:ILE:HG22	8:E:28:PRO:HD3	1.92	0.48
13:L:20:TRP:CE3	26:L:102:LHG:H132	2.49	0.48
15:O:100:LYS:HE3	15:O:105:VAL:CG2	2.43	0.48
15:O:143:PHE:HD1	15:O:323:ILE:HG13	1.78	0.48
20:S:239:PHE:CE1	39:S:315:LUT:H41	2.49	0.48
24:N:601:CHL:HMC	24:N:601:CHL:HBC3	1.95	0.48
21:Y:58:TYR:CE1	21:Y:80:TRP:HA	2.49	0.48
24:Y:310:CHL:NA	24:Y:310:CHL:HBA1	2.27	0.48
4:a:60:ILE:HB	4:a:83:ILE:CG2	2.44	0.48
5:b:191:ASP:HB3	5:b:194:VAL:HG13	1.95	0.48
5:b:214:LEU:HD13	25:r:603:CLA:HED1	1.94	0.48
5:b:360:PRO:C	5:b:361:THR:HG22	2.38	0.48
5:b:368:VAL:HG21	5:b:422:ARG:HG2	1.95	0.48
6:c:211:GLY:O	6:c:215:LYS:HB2	2.13	0.48
6:c:224:ILE:CD1	6:c:289:PHE:HZ	2.27	0.48
9:f:21:ALA:O	9:f:25:VAL:HG23	2.14	0.48
15:o:100:LYS:HE3	15:o:105:VAL:CG2	2.43	0.48
19:z:58:ASN:O	19:z:61:ILE:HG12	2.13	0.48
20:s:67:ARG:HH11	20:s:87:GLY:HA2	1.78	0.48
20:s:127:GLY:O	20:s:131:PRO:HD2	2.13	0.48
21:g:231:VAL:CG1	25:g:613:CLA:HAC2	2.36	0.48
21:n:127:GLY:HA3	21:n:137:GLN:CG	2.42	0.48
24:n:607:CHL:H202	24:n:609:CHL:C3	2.43	0.48
24:n:609:CHL:H72	24:y:302:CHL:C11	2.40	0.48
24:y:309:CHL:H11	39:y:316:LUT:C38	2.43	0.48
24:r:605:CHL:HAB	25:r:608:CLA:CBC	2.43	0.48
24:r:607:CHL:CBB	40:r:617:NEX:H12	2.40	0.48
25:2:604:CLA:HBA2	25:2:604:CLA:CHA	2.44	0.48
25:2:605:CLA:HBD	25:2:605:CLA:CAA	2.35	0.48
1:3:128:GLU:CB	1:3:137:GLN:HB2	2.41	0.48
3:4:94:PHE:HB3	3:4:98:TYR:CE2	2.42	0.48
3:4:222:GLU:HA	3:4:225:LYS:CD	2.44	0.48
4:A:95:PRO:HD2	4:A:98:GLU:HG3	1.96	0.48
4:A:139:MET:SD	7:D:253:PHE:HB2	2.54	0.48
4:A:162:PRO:HB3	4:A:168:PHE:HA	1.94	0.48
5:B:121:GLU:HB3	10:H:14:PRO:HB2	1.95	0.48
25:D:403:CLA:H122	18:X:92:SER:OG	2.14	0.48
25:S:311:CLA:CHD	26:S:318:LHG:HC62	2.43	0.48
24:G:609:CHL:CAA	21:N:82:THR:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:72:LEU:CB	22:R:137:ARG:HH22	2.26	0.48
22:R:166:GLN:HG2	22:R:167:ASP:N	2.28	0.48
2:6:137:SER:HA	2:6:140:PHE:CE2	2.48	0.48
3:8:222:GLU:HA	3:8:225:LYS:CD	2.44	0.48
4:a:135:PHE:CZ	11:i:31:ASN:HB3	2.49	0.48
5:b:240:SER:HB3	25:b:610:CLA:NB	2.28	0.48
25:b:607:CLA:H91	25:b:607:CLA:H111	1.62	0.48
6:c:361:LEU:HD12	35:c:515:DGD:O3E	2.13	0.48
7:d:350:GLY:HA2	7:d:353:LEU:HD23	1.96	0.48
16:t:11:VAL:HG13	28:t:101:BCR:C33	2.43	0.48
16:t:14:LEU:HD12	28:t:101:BCR:C34	2.42	0.48
25:s:303:CLA:C7	25:s:304:CLA:HMA1	2.39	0.48
21:g:60:GLY:H	24:g:601:CHL:CHC	2.26	0.48
25:g:612:CLA:HAA2	25:g:612:CLA:HBD	1.95	0.48
23:u:79:ARG:O	23:u:84:ALA:HB2	2.13	0.48
2:2:204:ASP:O	2:2:208:THR:N	2.45	0.48
2:2:211:GLU:O	2:2:215:LYS:HG3	2.13	0.48
6:C:376:ASP:OD2	6:C:379:ARG:NE	2.47	0.48
14:M:26:TYR:O	14:M:30:VAL:HG13	2.13	0.48
16:T:14:LEU:HD12	28:T:101:BCR:C34	2.42	0.48
20:S:127:GLY:O	20:S:131:PRO:HD2	2.13	0.48
24:G:606:CHL:HAA1	40:G:617:NEX:H381	1.96	0.48
25:G:613:CLA:HHB	39:G:615:LUT:H3	1.96	0.48
21:N:50:TRP:O	21:N:55:ARG:HD2	2.14	0.48
21:N:58:TYR:CE1	21:N:80:TRP:HA	2.49	0.48
21:N:139:PHE:HD2	24:N:607:CHL:OBD	1.97	0.48
21:N:196:PHE:HZ	24:N:608:CHL:C1C	2.27	0.48
22:R:57:LEU:HB2	22:R:59:TYR:CE1	2.49	0.48
22:R:242:GLU:HB2	25:R:609:CLA:CHB	2.44	0.48
2:6:117:GLU:HG3	2:6:129:GLU:HB3	1.96	0.48
2:6:175:GLY:HA3	2:6:181:LEU:CG	2.44	0.48
24:6:601:CHL:H62	24:6:601:CHL:H102	1.58	0.48
3:8:169:SER:OG	3:8:173:GLU:OE2	2.31	0.48
4:a:272:HIS:CD2	7:d:219:VAL:HG21	2.48	0.48
5:b:121:GLU:HB3	10:h:14:PRO:HB2	1.95	0.48
5:b:139:PHE:HB2	25:b:610:CLA:CMD	2.44	0.48
5:b:249:ALA:HA	5:b:252:VAL:HG22	1.96	0.48
5:b:290:ALA:O	5:b:293:ALA:HB3	2.14	0.48
6:c:106:ILE:HG13	6:c:107:ASP:N	2.28	0.48
6:c:466:VAL:HG21	7:d:249:THR:HG23	1.96	0.48
13:l:29:ALA:CB	14:m:15:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:s:311:CLA:CHD	26:s:318:LHG:HC62	2.43	0.48
21:g:51:TYR:HE2	21:g:209:ALA:HB1	1.75	0.48
25:g:603:CLA:ND	24:g:609:CHL:H8	2.28	0.48
21:n:134:ALA:HB1	25:n:604:CLA:HED2	1.96	0.48
21:y:116:PRO:HA	21:y:126:PHE:HE2	1.78	0.48
21:y:154:HIS:O	21:y:154:HIS:ND1	2.44	0.48
25:y:305:CLA:HBC2	25:y:305:CLA:CMC	2.44	0.48
22:r:166:GLN:HG2	22:r:167:ASP:N	2.28	0.48
1:1:127:GLY:HA3	1:1:137:GLN:CG	2.42	0.48
1:3:58:TYR:CE1	1:3:80:TRP:HA	2.49	0.48
3:4:169:SER:HA	3:4:172:VAL:HG12	1.96	0.48
3:4:231:HIS:O	3:4:234:LEU:HG	2.14	0.48
4:A:131:TRP:HZ2	6:C:449:ARG:NE	2.12	0.48
5:B:139:PHE:HB2	25:B:610:CLA:CMD	2.44	0.48
5:B:240:SER:HB3	25:B:610:CLA:NB	2.28	0.48
5:B:290:ALA:O	5:B:293:ALA:HB3	2.14	0.48
25:B:614:CLA:CBA	28:B:617:BCR:H403	2.44	0.48
6:C:140:LEU:HD22	25:C:513:CLA:CMA	2.44	0.48
6:C:213:LEU:O	6:C:223:TRP:NE1	2.40	0.48
6:C:224:ILE:CD1	6:C:289:PHE:HZ	2.27	0.48
25:C:509:CLA:HBA2	42:C:607:HOH:O	2.14	0.48
25:C:511:CLA:H142	12:K:47:PHE:HE2	1.77	0.48
7:D:341:ILE:HG23	7:D:341:ILE:O	2.13	0.48
13:L:29:ALA:CB	14:M:15:ILE:HD11	2.43	0.48
29:L:103:SQD:H262	42:L:202:HOH:O	2.14	0.48
25:S:310:CLA:H41	25:S:310:CLA:H62	1.68	0.48
25:S:311:CLA:NC	26:S:318:LHG:HC41	2.29	0.48
25:Y:304:CLA:H142	25:Y:304:CLA:H112	1.74	0.48
22:R:127:TYR:CD2	22:R:135:ARG:CD	2.97	0.48
22:R:192:ILE:O	22:R:196:VAL:HG23	2.13	0.48
25:6:604:CLA:H61	25:6:604:CLA:H41	1.60	0.48
1:7:116:PRO:HA	1:7:126:PHE:HE2	1.78	0.48
4:a:104:GLU:OE2	15:o:166:ARG:CG	2.62	0.48
6:c:235:GLY:O	6:c:239:TRP:CD1	2.67	0.48
25:c:501:CLA:CGA	25:c:501:CLA:H3A	2.44	0.48
7:d:99:GLN:OE1	8:e:73:LEU:HD13	2.14	0.48
7:d:237:ASN:OD1	7:d:238:PRO:CD	2.62	0.48
12:k:34:ASN:N	12:k:35:PRO:HD2	2.28	0.48
20:s:186:GLU:OE1	20:s:189:ARG:NH2	2.46	0.48
21:n:58:TYR:CE1	21:n:80:TRP:HA	2.49	0.48
21:n:116:PRO:HA	21:n:126:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:139:PHE:HD2	24:n:607:CHL:OBD	1.97	0.48
25:n:614:CLA:HAA1	25:n:614:CLA:HBD	1.96	0.48
21:y:58:TYR:CE1	21:y:80:TRP:HA	2.49	0.48
1:l:50:TRP:CB	1:l:213:VAL:HG21	2.44	0.47
2:2:52:GLY:O	2:2:55:ARG:HG3	2.14	0.47
25:2:604:CLA:CHC	26:2:606:LHG:HC5	2.43	0.47
27:A:403:PHO:H42	26:D:406:LHG:H342	1.95	0.47
25:B:604:CLA:H143	25:B:610:CLA:H93	1.96	0.47
16:T:11:VAL:HG13	28:T:101:BCR:C33	2.43	0.47
20:S:176:VAL:O	20:S:180:VAL:HG23	2.14	0.47
20:S:262:PHE:HD2	25:S:314:CLA:CMA	2.27	0.47
21:Y:173:GLU:OE2	24:Y:310:CHL:NA	2.47	0.47
22:R:218:PRO:HB2	22:R:223:PHE:CD2	2.48	0.47
1:5:50:TRP:CB	1:5:213:VAL:HG21	2.44	0.47
5:b:223:GLN:HG2	10:h:36:GLY:N	2.28	0.47
25:b:614:CLA:CBA	28:b:617:BCR:H403	2.44	0.47
6:c:316:THR:O	6:c:319:VAL:HG12	2.14	0.47
25:c:502:CLA:HAA1	25:c:502:CLA:CBD	2.40	0.47
7:d:12:GLU:O	7:d:13:LYS:HB2	2.13	0.47
13:l:20:TRP:CE3	26:l:103:LHG:H132	2.49	0.47
20:s:132:GLU:OE1	20:s:145:ALA:HB3	2.14	0.47
20:s:196:PHE:HB2	24:s:308:CHL:HBC3	1.96	0.47
20:s:262:PHE:HD2	25:s:314:CLA:CMA	2.27	0.47
25:s:304:CLA:HHC	39:s:316:LUT:H15	1.95	0.47
25:s:311:CLA:NC	26:s:318:LHG:HC41	2.29	0.47
21:g:86:SER:OG	25:g:602:CLA:O1A	2.23	0.47
21:g:224:PHE:CG	26:y:301:LHG:H281	2.48	0.47
21:n:50:TRP:O	21:n:55:ARG:HD2	2.14	0.47
22:r:87:ALA:HB1	22:r:89:TYR:CE2	2.49	0.47
22:r:120:LYS:HB2	22:r:126:PRO:O	2.14	0.47
1:3:154:HIS:O	1:3:154:HIS:ND1	2.44	0.47
4:A:77:ILE:H	13:L:34:ASN:ND2	2.12	0.47
5:B:67:THR:HA	5:B:71:ILE:O	2.14	0.47
6:C:316:THR:O	6:C:319:VAL:HG12	2.14	0.47
25:C:501:CLA:H3A	25:C:501:CLA:CGA	2.44	0.47
21:Y:164:THR:HG21	24:Y:307:CHL:HED3	1.96	0.47
21:Y:224:PHE:CE2	25:Y:314:CLA:HAB	2.48	0.47
24:Y:307:CHL:HHC	24:Y:308:CHL:CMC	2.44	0.47
3:8:250:LYS:NZ	3:8:255:ALA:HA	2.29	0.47
4:a:254:TYR:HE1	7:d:134:ALA:N	2.11	0.47
5:b:283:GLU:HG3	5:b:287:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:519:LHG:H381	26:c:519:LHG:H222	1.95	0.47
25:g:603:CLA:HMD3	24:g:609:CHL:C4D	2.45	0.47
25:g:610:CLA:CBB	39:g:615:LUT:H32	2.43	0.47
21:n:204:ASP:O	21:n:208:PHE:N	2.40	0.47
24:n:607:CHL:C18	24:n:609:CHL:H71	2.38	0.47
21:y:107:MET:HG2	21:y:222:ALA:HB3	1.94	0.47
1:1:97:GLU:HA	1:1:190:LEU:CD1	2.24	0.47
2:2:188:ASN:HB2	2:2:192:PRO:HA	1.96	0.47
4:A:100:ALA:HB2	17:W:84:ARG:CZ	2.45	0.47
4:A:131:TRP:CZ2	25:C:505:CLA:HAA2	2.49	0.47
4:A:202:VAL:HG22	25:A:401:CLA:C1B	2.44	0.47
4:A:321:ILE:HD11	7:D:180:PHE:HB2	1.96	0.47
27:A:403:PHO:H141	27:A:403:PHO:H161	1.52	0.47
25:B:608:CLA:H18	25:D:403:CLA:HMA2	1.96	0.47
6:C:322:GLN:HE22	6:C:384:ILE:CD1	2.24	0.47
25:C:504:CLA:H92	25:C:504:CLA:H62	1.52	0.47
7:D:12:GLU:O	7:D:13:LYS:HB2	2.13	0.47
7:D:107:GLN:HE21	8:E:48:GLY:HA3	1.79	0.47
7:D:237:ASN:OD1	7:D:238:PRO:CD	2.62	0.47
8:E:55:TYR:O	8:E:60:ARG:NH1	2.34	0.47
20:S:179:VAL:HG22	32:S:319:AJP:C01	2.45	0.47
20:S:237:LEU:HG	39:S:316:LUT:C40	2.45	0.47
20:S:257:HIS:ND1	20:S:261:PRO:HA	2.29	0.47
21:G:116:PRO:HA	21:G:126:PHE:HE2	1.78	0.47
21:G:131:TRP:CB	39:G:616:LUT:H41	2.44	0.47
21:G:139:PHE:CD2	24:G:607:CHL:OBD	2.66	0.47
21:G:139:PHE:CE2	24:G:607:CHL:CMD	2.97	0.47
25:G:603:CLA:HMD3	24:G:609:CHL:C4D	2.45	0.47
22:R:120:LYS:HB2	22:R:126:PRO:O	2.14	0.47
1:5:51:TYR:HE2	1:5:209:ALA:HB1	1.75	0.47
2:6:66:THR:HG23	2:6:67:PRO:HD2	1.96	0.47
25:6:605:CLA:HBC1	26:6:606:LHG:H362	1.95	0.47
1:7:145:ASP:HB3	1:7:149:ASN:O	2.15	0.47
5:b:67:THR:HA	5:b:71:ILE:O	2.14	0.47
5:b:154:GLY:O	5:b:159:THR:HG23	2.15	0.47
6:c:213:LEU:HD11	28:i:101:BCR:H373	1.95	0.47
25:c:511:CLA:HAA1	25:c:511:CLA:CBP	2.42	0.47
12:k:33:LEU:HD13	28:k:101:BCR:H312	1.96	0.47
29:l:101:SQD:H262	42:l:202:HOH:O	2.14	0.47
14:m:1:MET:HB2	14:m:3:VAL:CG1	2.43	0.47
20:s:113:PHE:HD1	20:s:117:HIS:HE1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:131:TRP:CB	39:g:616:LUT:H41	2.44	0.47
24:g:601:CHL:H72	24:g:601:CHL:H111	1.62	0.47
21:y:164:THR:HG21	24:y:307:CHL:HED3	1.96	0.47
22:r:242:GLU:HB2	25:r:609:CLA:CHB	2.44	0.47
1:3:50:TRP:O	1:3:55:ARG:HD2	2.14	0.47
4:A:135:PHE:CZ	11:I:31:ASN:HB3	2.49	0.47
5:B:268:PHE:HB2	5:B:448:ARG:NH2	2.30	0.47
6:C:95:LEU:HD23	25:C:502:CLA:H143	1.95	0.47
25:S:304:CLA:HHC	39:S:316:LUT:H15	1.95	0.47
21:Y:131:TRP:HB3	39:Y:317:LUT:H41	1.97	0.47
21:Y:209:ALA:HA	21:Y:212:LYS:CG	2.34	0.47
26:Y:301:LHG:H301	26:Y:301:LHG:H271	1.62	0.47
24:Y:309:CHL:H11	39:Y:316:LUT:C38	2.43	0.47
22:R:58:TRP:CD2	22:R:78:PHE:HD1	2.31	0.47
1:5:145:ASP:HB3	1:5:149:ASN:O	2.15	0.47
2:6:172:LEU:O	2:6:176:PHE:CD2	2.67	0.47
25:b:608:CLA:H18	25:d:403:CLA:HMA2	1.96	0.47
15:o:143:PHE:HD1	15:o:323:ILE:HG13	1.78	0.47
15:o:146:LYS:HG3	15:o:156:PRO:HB2	1.97	0.47
17:w:104:ILE:O	17:w:108:VAL:HG23	2.14	0.47
20:s:239:PHE:CE1	39:s:315:LUT:H41	2.49	0.47
20:s:257:HIS:ND1	20:s:261:PRO:HA	2.29	0.47
21:g:50:TRP:CB	21:g:213:VAL:HG21	2.45	0.47
21:g:139:PHE:CE2	24:g:607:CHL:CMD	2.97	0.47
21:g:209:ALA:HA	21:g:212:LYS:CG	2.34	0.47
21:n:56:VAL:HB	24:n:601:CHL:CBC	2.45	0.47
21:n:171:ALA:HB2	26:y:319:LHG:H211	1.96	0.47
25:n:611:CLA:H3A	25:n:611:CLA:HBA2	1.40	0.47
21:y:50:TRP:O	21:y:55:ARG:HD2	2.14	0.47
25:r:610:CLA:H3A	25:r:610:CLA:C1	2.45	0.47
1:1:76:GLY:HA3	1:1:216:LEU:CD2	2.25	0.47
2:2:172:LEU:O	2:2:176:PHE:CD2	2.67	0.47
3:4:58:ILE:O	3:4:58:ILE:HG22	2.15	0.47
3:4:169:SER:OG	3:4:173:GLU:OE2	2.31	0.47
3:4:250:LYS:NZ	3:4:255:ALA:HA	2.29	0.47
4:A:17:PHE:O	4:A:18:CYS:SG	2.73	0.47
4:A:157:VAL:CG1	4:A:172:MET:HE3	2.45	0.47
25:A:402:CLA:H151	25:A:402:CLA:H111	1.59	0.47
5:B:280:PHE:O	5:B:281:GLN:CB	2.61	0.47
5:B:354:LEU:HD22	5:B:378:ARG:HG3	1.96	0.47
5:B:422:ARG:O	5:B:425:GLN:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:466:VAL:HG21	7:D:249:THR:HG23	1.96	0.47
25:C:501:CLA:HHC	25:C:501:CLA:HBB1	1.96	0.47
35:C:516:DGD:HAN2	35:C:516:DGD:HAW2	1.43	0.47
7:D:350:GLY:HA2	7:D:353:LEU:HD23	1.96	0.47
25:S:314:CLA:C4A	25:S:314:CLA:HBA2	2.44	0.47
21:N:171:ALA:HB2	26:Y:319:LHG:H211	1.96	0.47
21:Y:50:TRP:CB	21:Y:213:VAL:HG21	2.45	0.47
22:R:72:LEU:HB3	22:R:137:ARG:NH2	2.29	0.47
1:5:76:GLY:HA3	1:5:216:LEU:CD2	2.24	0.47
2:6:114:ILE:O	2:6:118:VAL:HG23	2.13	0.47
1:7:50:TRP:O	1:7:55:ARG:HD2	2.14	0.47
4:a:157:VAL:CG1	4:a:172:MET:HE3	2.45	0.47
5:b:28:ALA:HB2	5:b:107:CYS:HB3	1.96	0.47
5:b:330:MET:HE1	5:b:446:SER:HB3	1.96	0.47
26:b:621:LHG:H321	22:r:192:ILE:HD11	1.96	0.47
21:g:132:PHE:HB2	24:g:607:CHL:CMA	2.43	0.47
21:g:211:LEU:CB	25:g:610:CLA:HMA1	2.44	0.47
21:n:60:GLY:HA3	24:n:601:CHL:CMC	2.43	0.47
21:y:60:GLY:CA	24:y:302:CHL:HMC	2.27	0.47
22:r:137:ARG:HH21	25:r:602:CLA:CED	2.22	0.47
2:2:71:THR:HG22	2:2:71:THR:O	2.13	0.47
4:A:60:ILE:HB	4:A:83:ILE:HG22	1.95	0.47
4:A:291:SER:O	4:A:294:ALA:HB3	2.14	0.47
5:B:154:GLY:O	5:B:159:THR:HG23	2.15	0.47
7:D:273:LEU:C	7:D:273:LEU:HD23	2.40	0.47
7:D:280:LEU:CD2	25:D:402:CLA:HBA2	2.45	0.47
11:I:34:ARG:HD2	11:I:35:GLU:CG	2.41	0.47
12:K:33:LEU:HD13	28:K:101:BCR:H312	1.96	0.47
15:O:223:LYS:HE2	15:O:223:LYS:HA	1.97	0.47
21:G:145:ASP:HB3	21:G:149:ASN:O	2.15	0.47
21:G:172:VAL:CG1	24:G:608:CHL:NB	2.78	0.47
25:Y:305:CLA:HBC2	25:Y:305:CLA:CMC	2.44	0.47
22:R:87:ALA:HB1	22:R:89:TYR:CE2	2.49	0.47
22:R:164:THR:OG1	22:R:166:GLN:OE1	2.31	0.47
25:R:609:CLA:H61	25:R:609:CLA:H92	1.67	0.47
2:6:120:GLN:HA	2:6:124:ARG:C	2.40	0.47
2:6:211:GLU:C	2:6:214:VAL:HG12	2.40	0.47
25:6:602:CLA:H71	25:6:602:CLA:H111	1.68	0.47
25:6:605:CLA:HAA1	25:6:605:CLA:CBD	2.28	0.47
3:8:231:HIS:O	3:8:234:LEU:HG	2.14	0.47
4:a:202:VAL:HG22	25:a:402:CLA:C1B	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:268:PHE:HB2	5:b:448:ARG:NH2	2.29	0.47
5:b:357:ARG:NH2	7:d:338:GLU:OE1	2.47	0.47
6:c:157:MET:HE2	6:c:271:TYR:CE2	2.50	0.47
6:c:311:GLN:HG3	6:c:361:LEU:HD23	1.97	0.47
6:c:343:ARG:NH1	6:c:347:GLY:O	2.48	0.47
6:c:376:ASP:OD2	6:c:379:ARG:NE	2.47	0.47
7:d:162:PRO:CB	7:d:171:ALA:HB2	2.42	0.47
20:s:176:VAL:O	20:s:180:VAL:HG23	2.14	0.47
24:s:302:CHL:C1D	26:s:318:LHG:HC82	2.44	0.47
21:g:154:HIS:O	21:g:154:HIS:ND1	2.43	0.47
21:y:131:TRP:HB3	39:y:317:LUT:H41	1.97	0.47
22:r:164:THR:OG1	22:r:166:GLN:OE1	2.31	0.47
1:1:145:ASP:HB3	1:1:149:ASN:O	2.15	0.47
24:1:301:CHL:HBC2	24:1:301:CHL:HHD	1.95	0.47
2:2:117:GLU:HG3	2:2:129:GLU:HB3	1.95	0.47
2:2:205:ASP:HA	2:2:208:THR:OG1	2.15	0.47
2:2:223:ALA:O	2:2:226:SER:OG	2.32	0.47
1:3:206:GLU:OE1	1:3:206:GLU:CA	2.63	0.47
1:3:216:LEU:O	1:3:220:ARG:HG3	2.15	0.47
3:4:75:GLY:H	3:4:80:ASP:CG	2.22	0.47
4:A:43:THR:HG21	4:A:118:HIS:CE1	2.50	0.47
4:A:220:THR:HA	4:A:223:LEU:HG	1.96	0.47
5:B:20:LEU:O	5:B:24:ILE:HG13	2.15	0.47
5:B:191:ASP:HB3	5:B:194:VAL:HG13	1.95	0.47
5:B:200:SER:O	5:B:201:HIS:C	2.56	0.47
5:B:382:PRO:CB	7:D:345:GLU:OE2	2.62	0.47
25:B:604:CLA:H93	25:B:604:CLA:H61	1.59	0.47
6:C:49:LEU:HD11	25:C:509:CLA:C1C	2.45	0.47
6:C:235:GLY:O	6:C:239:TRP:CD1	2.67	0.47
6:C:327:ASN:ND2	15:O:192:ASP:HB2	2.26	0.47
6:C:429:SER:HB3	35:C:516:DGD:HB92	1.96	0.47
25:C:507:CLA:HAA2	25:C:507:CLA:CGD	2.44	0.47
26:C:519:LHG:H381	26:C:519:LHG:H222	1.95	0.47
7:D:41:CYS:SG	25:D:403:CLA:CMB	3.03	0.47
7:D:343:PRO:HD2	7:D:346:VAL:CG2	2.45	0.47
9:F:20:LEU:O	9:F:24:THR:OG1	2.15	0.47
9:F:21:ALA:O	9:F:25:VAL:HG23	2.14	0.47
12:K:53:VAL:HG23	28:Z:101:BCR:H21C	1.95	0.47
29:L:103:SQD:H312	29:L:103:SQD:H352	1.97	0.47
15:O:145:VAL:CG1	15:O:203:LEU:HD11	2.37	0.47
19:Z:56:ILE:HG23	20:S:270:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:196:PHE:HB2	24:S:308:CHL:HBC3	1.96	0.47
20:S:230:ARG:HD3	25:S:303:CLA:HHD	1.97	0.47
21:N:227:PHE:HB2	39:N:616:LUT:H401	1.97	0.47
24:N:609:CHL:HBC3	24:Y:302:CHL:H91	1.97	0.47
25:N:614:CLA:HAA1	25:N:614:CLA:HBD	1.96	0.47
21:Y:138:ILE:HG13	21:Y:144:LEU:CB	2.31	0.47
21:Y:145:ASP:HB3	21:Y:149:ASN:O	2.15	0.47
26:Y:319:LHG:H252	26:Y:319:LHG:H282	1.66	0.47
22:R:247:ARG:HD3	25:R:602:CLA:HHD	1.97	0.47
22:R:283:ILE:HG22	24:R:613:CHL:HED1	1.96	0.47
1:5:216:LEU:O	1:5:220:ARG:HG3	2.15	0.47
2:6:134:LYS:O	2:6:137:SER:OG	2.22	0.47
2:6:174:GLU:HG3	1:7:59:LEU:HD22	1.93	0.47
2:6:197:PHE:HB3	2:6:202:LEU:HD22	1.97	0.47
25:6:604:CLA:HBD	25:6:604:CLA:CAA	2.41	0.47
1:7:58:TYR:CE1	1:7:80:TRP:HA	2.49	0.47
3:8:219:GLU:HG3	3:8:222:GLU:CB	2.41	0.47
4:a:17:PHE:O	4:a:18:CYS:SG	2.73	0.47
4:a:103:ASP:HB3	15:o:202:GLN:OE1	2.15	0.47
4:a:291:SER:O	4:a:294:ALA:HB3	2.15	0.47
25:a:403:CLA:H111	25:a:403:CLA:H151	1.59	0.47
25:b:610:CLA:H13	25:b:612:CLA:H2	1.97	0.47
6:c:236:GLY:HA2	6:c:239:TRP:HD1	1.77	0.47
6:c:437:LEU:HD22	25:c:502:CLA:HBC1	1.97	0.47
7:d:328:ALA:CB	7:d:348:PRO:HD2	2.45	0.47
15:o:115:PRO:HB2	15:o:328:TYR:CE2	2.50	0.47
17:w:125:GLU:O	17:w:126:ASP:HB3	2.15	0.47
20:s:202:PRO:CB	24:s:308:CHL:HBC2	2.45	0.47
20:s:237:LEU:HG	39:s:316:LUT:C40	2.45	0.47
21:g:50:TRP:O	21:g:55:ARG:HD2	2.14	0.47
21:g:145:ASP:HB3	21:g:149:ASN:O	2.15	0.47
24:g:601:CHL:H52	24:g:601:CHL:H8	1.70	0.47
21:n:108:LEU:HD11	25:n:610:CLA:HBC1	1.96	0.47
21:n:206:GLU:OE1	21:n:206:GLU:CA	2.63	0.47
21:y:145:ASP:HB3	21:y:149:ASN:O	2.15	0.47
25:y:314:CLA:HBA2	25:y:314:CLA:H3A	1.57	0.47
22:r:56:PRO:O	22:r:57:LEU:HD22	2.15	0.47
22:r:141:LEU:HD21	22:r:145:ARG:NH2	2.30	0.47
22:r:229:ALA:O	22:r:235:THR:OG1	2.26	0.47
22:r:283:ILE:HG22	24:r:613:CHL:HED1	1.96	0.47
25:r:601:CLA:H3A	25:r:601:CLA:HBA1	1.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:ASP:O	1:1:208:PHE:N	2.40	0.47
1:3:50:TRP:CB	1:3:213:VAL:HG21	2.45	0.47
1:3:204:ASP:O	1:3:208:PHE:N	2.40	0.47
3:4:73:LEU:HB3	3:4:80:ASP:OD1	2.13	0.47
5:B:257:TRP:CE2	7:D:292:LEU:HD22	2.49	0.47
5:B:471:ALA:HB2	7:D:131:PHE:CE1	2.48	0.47
25:B:610:CLA:H13	25:B:612:CLA:H2	1.97	0.47
7:D:22:TRP:NE1	18:X:105:VAL:HG12	2.30	0.47
28:T:101:BCR:C18	28:T:101:BCR:H272	2.44	0.47
17:W:104:ILE:O	17:W:108:VAL:HG23	2.14	0.47
17:W:125:GLU:O	17:W:126:ASP:HB3	2.15	0.47
20:S:128:PHE:HE2	20:S:236:MET:CE	2.27	0.47
20:S:186:GLU:OE1	20:S:189:ARG:NH2	2.47	0.47
20:S:202:PRO:CB	24:S:308:CHL:HBC2	2.45	0.47
25:G:613:CLA:H101	26:Y:301:LHG:H341	1.96	0.47
21:N:50:TRP:CB	21:N:213:VAL:HG21	2.45	0.47
21:N:56:VAL:HB	24:N:601:CHL:CBC	2.45	0.47
40:N:617:NEX:H201	40:N:617:NEX:H15	1.55	0.47
26:Y:319:LHG:HC92	26:Y:319:LHG:H121	1.60	0.47
22:R:56:PRO:O	22:R:57:LEU:HD22	2.15	0.47
24:R:605:CHL:HAB	25:R:608:CLA:HBC2	1.97	0.47
1:5:55:ARG:HE	1:5:55:ARG:HB2	1.37	0.47
1:5:58:TYR:CE1	1:5:80:TRP:HA	2.49	0.47
1:5:97:GLU:HA	1:5:190:LEU:CD1	2.24	0.47
4:a:84:PRO:HB2	4:a:169:SER:HA	1.97	0.47
4:a:231:GLU:HA	5:b:1:MET:H2	1.78	0.47
5:b:57:ARG:HG3	5:b:57:ARG:O	2.14	0.47
5:b:224:ARG:HG2	10:h:37:TRP:CZ2	2.50	0.47
5:b:257:TRP:CE2	7:d:292:LEU:HD22	2.49	0.47
5:b:265:ILE:O	5:b:269:GLY:N	2.47	0.47
5:b:354:LEU:HD22	5:b:378:ARG:HG3	1.96	0.47
6:c:97:TRP:NE1	6:c:178:LYS:HE3	2.30	0.47
25:c:507:CLA:HAA2	25:c:507:CLA:CGD	2.44	0.47
8:e:27:ILE:HG22	8:e:28:PRO:HD3	1.92	0.47
25:g:613:CLA:HBB	39:g:615:LUT:H3	1.96	0.47
21:n:97:GLU:HA	21:n:190:LEU:CD1	2.24	0.47
21:n:227:PHE:HB2	39:n:616:LUT:H401	1.97	0.47
24:y:307:CHL:HAA1	40:y:318:NEX:H27	1.96	0.47
1:1:216:LEU:O	1:1:220:ARG:HG3	2.15	0.47
2:2:130:PRO:CG	2:2:239:LYS:HE2	2.45	0.47
2:2:150:ASN:N	2:2:151:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:604:CLA:CHC	26:2:606:LHG:HC41	2.45	0.47
3:4:173:GLU:HB3	22:R:59:TYR:CE1	2.50	0.47
5:B:249:ALA:HA	5:B:252:VAL:HG22	1.96	0.47
25:B:601:CLA:HBD	25:B:601:CLA:HAA1	1.97	0.47
25:B:607:CLA:H161	25:B:607:CLA:H141	1.54	0.47
26:B:622:LHG:H201	26:B:622:LHG:H352	1.96	0.47
6:C:97:TRP:NE1	6:C:178:LYS:HE3	2.30	0.47
6:C:106:ILE:HG13	6:C:107:ASP:N	2.28	0.47
6:C:157:MET:HE2	6:C:271:TYR:CE2	2.50	0.47
6:C:343:ARG:NH1	6:C:347:GLY:O	2.48	0.47
7:D:328:ALA:CB	7:D:348:PRO:HD2	2.45	0.47
8:E:26:THR:HB	38:F:101:HEM:CAB	2.44	0.47
20:S:68:ARG:NH2	26:S:301:LHG:HC12	2.23	0.47
21:G:50:TRP:CB	21:G:213:VAL:HG21	2.45	0.47
21:G:197:ASP:OD1	25:G:610:CLA:CAA	2.62	0.47
24:G:606:CHL:HBA2	40:G:617:NEX:H30	1.96	0.47
25:N:610:CLA:H92	25:N:610:CLA:H61	1.71	0.47
25:Y:315:CLA:CBC	39:Y:316:LUT:H162	2.39	0.47
22:R:240:LEU:O	22:R:244:LYS:HG3	2.15	0.47
2:6:52:GLY:O	2:6:55:ARG:HG3	2.14	0.47
3:8:222:GLU:HA	3:8:225:LYS:HG3	1.97	0.47
4:a:43:THR:HG21	4:a:118:HIS:CE1	2.50	0.47
4:a:329:GLU:HA	4:a:332:HIS:HE2	1.79	0.47
29:a:408:SQD:O8	29:a:408:SQD:H4	2.15	0.47
5:b:115:TRP:CH2	25:b:614:CLA:HMA2	2.49	0.47
5:b:258:TYR:HB3	35:b:626:DGD:HD62	1.97	0.47
5:b:379:ALA:HB2	5:b:395:VAL:HG11	1.96	0.47
6:c:304:PRO:O	6:c:308:GLU:OE1	2.33	0.47
25:c:513:CLA:CMD	20:s:75:LEU:HD11	2.45	0.47
7:d:107:GLN:HE21	8:e:48:GLY:HA3	1.79	0.47
8:e:26:THR:HB	38:f:101:HEM:CAB	2.44	0.47
9:f:18:HIS:CE1	38:f:101:HEM:NB	2.83	0.47
10:h:25:PRO:CG	22:r:122:THR:HB	2.42	0.47
11:i:34:ARG:HD2	11:i:35:GLU:CG	2.41	0.47
21:g:216:LEU:O	21:g:220:ARG:HG3	2.15	0.47
25:g:610:CLA:H111	25:g:610:CLA:H142	1.60	0.47
21:n:196:PHE:HZ	24:n:608:CHL:C1C	2.27	0.47
21:y:173:GLU:OE2	24:y:310:CHL:NA	2.47	0.47
21:y:224:PHE:CE2	25:y:314:CLA:HAB	2.48	0.47
22:r:57:LEU:HB2	22:r:59:TYR:CE1	2.49	0.47
24:r:605:CHL:CBB	41:r:616:XAT:H162	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:611:CLA:H3A	25:r:611:CLA:HBA1	1.43	0.47
2:2:66:THR:HG23	2:2:67:PRO:HD2	1.96	0.47
2:2:127:PHE:HZ	2:2:145:LEU:HD12	1.80	0.47
2:2:211:GLU:C	2:2:214:VAL:HG12	2.40	0.47
3:4:144:SER:CB	22:R:279:LEU:O	2.63	0.47
4:A:104:GLU:OE2	15:O:166:ARG:CG	2.62	0.47
4:A:215:HIS:NE2	33:A:413:BCT:O2	2.48	0.47
5:B:223:GLN:CD	10:H:36:GLY:H	2.23	0.47
5:B:357:ARG:NH2	7:D:338:GLU:OE1	2.47	0.47
5:B:475:PHE:O	5:B:478:VAL:HG12	2.15	0.47
26:B:621:LHG:H321	22:R:192:ILE:HD11	1.96	0.47
15:O:146:LYS:HG3	15:O:156:PRO:HB2	1.97	0.47
20:S:113:PHE:HD1	20:S:117:HIS:HE1	1.63	0.47
20:S:132:GLU:CA	20:S:145:ALA:HB1	2.40	0.47
20:S:242:GLN:HE22	25:S:313:CLA:CHB	2.28	0.47
21:G:100:VAL:CG1	21:G:190:LEU:HD13	2.45	0.47
21:G:216:LEU:O	21:G:220:ARG:HG3	2.15	0.47
24:Y:308:CHL:HHD	24:Y:308:CHL:CBC	2.36	0.47
1:5:100:VAL:CG1	1:5:190:LEU:HD13	2.45	0.47
1:5:127:GLY:HA3	1:5:137:GLN:CG	2.42	0.47
25:6:604:CLA:HBA2	25:6:604:CLA:CHA	2.44	0.47
3:8:225:LYS:CA	3:8:228:GLU:OE1	2.61	0.47
4:a:77:ILE:H	13:l:34:ASN:ND2	2.12	0.47
4:a:321:ILE:HD11	7:d:180:PHE:HB2	1.96	0.47
5:b:5:TRP:O	25:b:611:CLA:H42	2.15	0.47
5:b:37:MET:HE2	5:b:37:MET:CA	2.45	0.47
5:b:214:LEU:HB3	25:r:603:CLA:HED1	1.97	0.47
6:c:49:LEU:HD11	25:c:509:CLA:C1C	2.45	0.47
7:d:217:ALA:O	7:d:221:ASN:ND2	2.47	0.47
25:d:403:CLA:H122	18:x:92:SER:OG	2.14	0.47
15:o:130:LYS:HD2	15:o:179:GLU:CB	2.45	0.47
28:t:101:BCR:C18	28:t:101:BCR:H272	2.44	0.47
25:s:314:CLA:C4A	25:s:314:CLA:HBA2	2.44	0.47
21:g:206:GLU:OE1	21:g:206:GLU:CA	2.63	0.47
21:n:50:TRP:CB	21:n:213:VAL:HG21	2.45	0.47
22:r:150:ALA:HB1	41:r:616:XAT:H181	1.95	0.47
1:1:50:TRP:O	1:1:55:ARG:HD2	2.14	0.46
1:1:206:GLU:OE1	1:1:206:GLU:CA	2.63	0.46
2:2:161:ALA:O	2:2:162:VAL:C	2.59	0.46
3:4:69:ASP:N	3:4:70:PRO:CD	2.79	0.46
3:4:226:LEU:CD1	3:4:229:ILE:HD11	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:161:TYR:HB3	4:A:162:PRO:HD3	1.96	0.46
6:C:36:TRP:O	25:C:508:CLA:H11	2.15	0.46
6:C:311:GLN:HG3	6:C:361:LEU:HD23	1.97	0.46
25:C:509:CLA:HMC1	25:C:509:CLA:HBC2	1.97	0.46
7:D:318:LYS:HE3	37:D:408:CL:CL	2.53	0.46
20:S:241:ILE:HG22	25:S:313:CLA:HMD3	1.97	0.46
21:G:50:TRP:O	21:G:55:ARG:HD2	2.14	0.46
21:N:131:TRP:HA	39:N:616:LUT:O3	2.15	0.46
21:N:134:ALA:HB1	25:N:604:CLA:HED2	1.96	0.46
21:Y:76:GLY:HA3	21:Y:216:LEU:CD2	2.24	0.46
21:Y:100:VAL:CG1	21:Y:190:LEU:HD13	2.45	0.46
2:6:127:PHE:HZ	2:6:145:LEU:HD12	1.80	0.46
2:6:150:ASN:N	2:6:151:PRO:CD	2.78	0.46
5:b:139:PHE:HB2	25:b:610:CLA:HMD3	1.97	0.46
6:c:428:THR:HG22	35:c:516:DGD:CCB	2.44	0.46
7:d:41:CYS:SG	25:d:403:CLA:CMB	3.03	0.46
12:k:53:VAL:HG23	28:z:101:BCR:H21C	1.96	0.46
20:s:230:ARG:HD3	25:s:303:CLA:HHD	1.97	0.46
21:g:172:VAL:CG1	24:g:608:CHL:NB	2.78	0.46
25:g:611:CLA:H112	25:g:611:CLA:H142	1.59	0.46
25:g:613:CLA:H101	26:y:301:LHG:H341	1.96	0.46
21:y:216:LEU:O	21:y:220:ARG:HG3	2.15	0.46
2:2:120:GLN:HA	2:2:124:ARG:C	2.39	0.46
1:3:97:GLU:HA	1:3:190:LEU:CD1	2.24	0.46
4:A:103:ASP:HB3	15:O:202:GLN:OE1	2.15	0.46
5:B:37:MET:HE2	5:B:37:MET:CA	2.45	0.46
5:B:224:ARG:HG2	10:H:37:TRP:CZ2	2.50	0.46
9:F:18:HIS:CE1	38:F:101:HEM:NB	2.83	0.46
10:H:18:THR:O	10:H:22:LEU:HD13	2.16	0.46
14:M:1:MET:HB2	14:M:3:VAL:CG1	2.43	0.46
20:S:132:GLU:OE1	20:S:145:ALA:HB3	2.14	0.46
20:S:144:GLU:HB3	20:S:153:LEU:CD2	2.41	0.46
24:S:302:CHL:C1D	26:S:318:LHG:HC82	2.44	0.46
21:G:87:ALA:HB1	21:Y:90:GLU:HB2	1.93	0.46
21:N:107:MET:HG2	21:N:222:ALA:HB3	1.94	0.46
21:N:224:PHE:HE2	25:N:613:CLA:HAB	1.81	0.46
24:R:607:CHL:HMB2	40:R:617:NEX:H14	1.97	0.46
25:R:610:CLA:H3A	25:R:610:CLA:C1	2.45	0.46
1:5:50:TRP:O	1:5:55:ARG:HD2	2.14	0.46
2:6:204:ASP:C	2:6:208:THR:HG23	2.38	0.46
25:6:604:CLA:CHC	26:6:606:LHG:HC41	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:69:ASP:N	3:8:70:PRO:CD	2.79	0.46
4:a:100:ALA:HB2	17:w:84:ARG:CZ	2.45	0.46
4:a:131:TRP:HZ2	6:c:449:ARG:NE	2.12	0.46
5:b:51:VAL:HG13	5:b:308:LYS:HG2	1.95	0.46
5:b:285:TYR:CZ	23:u:90:GLN:HG3	2.49	0.46
25:b:604:CLA:H143	25:b:610:CLA:H93	1.96	0.46
7:d:22:TRP:NE1	18:x:105:VAL:HG12	2.30	0.46
7:d:273:LEU:C	7:d:273:LEU:HD23	2.40	0.46
15:o:146:LYS:HD3	15:o:158:PHE:HE1	1.80	0.46
15:o:223:LYS:HE2	15:o:223:LYS:HA	1.97	0.46
25:s:305:CLA:O1A	40:s:317:NEX:H382	2.15	0.46
21:g:58:TYR:CE1	21:g:80:TRP:HA	2.49	0.46
21:g:82:THR:N	39:g:616:LUT:O23	2.42	0.46
25:g:610:CLA:H62	25:g:612:CLA:HMA1	1.97	0.46
21:y:50:TRP:CB	21:y:213:VAL:HG21	2.45	0.46
22:r:72:LEU:HB3	22:r:137:ARG:NH2	2.29	0.46
25:r:610:CLA:HBC3	26:r:618:LHG:C5	2.37	0.46
1:1:154:HIS:CE1	1:1:156:GLN:OE1	2.69	0.46
2:2:197:PHE:HB3	2:2:202:LEU:HD22	1.97	0.46
5:B:28:ALA:HB2	5:B:107:CYS:HB3	1.96	0.46
5:B:58:GLN:HG2	5:B:331:ASP:OD2	2.16	0.46
6:C:304:PRO:O	6:C:308:GLU:OE1	2.33	0.46
25:S:305:CLA:O1A	40:S:317:NEX:H382	2.15	0.46
21:N:56:VAL:CG1	24:N:601:CHL:HBC1	2.46	0.46
21:N:216:LEU:O	21:N:220:ARG:HG3	2.15	0.46
21:Y:128:GLU:CB	21:Y:137:GLN:HB2	2.41	0.46
21:Y:164:THR:HG23	21:Y:168:LEU:CD1	2.46	0.46
1:5:154:HIS:CE1	1:5:156:GLN:OE1	2.69	0.46
1:5:164:THR:HG23	1:5:168:LEU:CD1	2.46	0.46
2:6:71:THR:O	2:6:71:THR:HG22	2.14	0.46
3:8:169:SER:HA	3:8:172:VAL:HG12	1.96	0.46
3:8:173:GLU:HB3	22:r:59:TYR:CE1	2.50	0.46
4:a:161:TYR:HB3	4:a:162:PRO:HD3	1.96	0.46
4:a:214:MET:HE1	27:a:405:PHO:C3D	2.45	0.46
5:b:256:MET:HG3	5:b:448:ARG:HG3	1.97	0.46
6:c:429:SER:HB3	35:c:516:DGD:HB92	1.96	0.46
25:c:510:CLA:H2	25:c:510:CLA:H61	1.67	0.46
10:h:26:LEU:HD23	25:r:614:CLA:HMA1	1.97	0.46
21:g:154:HIS:CE1	21:g:156:GLN:OE1	2.69	0.46
21:g:210:GLU:OE1	21:g:214:LYS:NZ	2.38	0.46
1:1:100:VAL:CG1	1:1:190:LEU:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:209:PHE:C	2:2:213:LYS:HZ2	2.23	0.46
2:2:217:ILE:HD13	25:2:604:CLA:O2D	2.15	0.46
1:3:69:TYR:OH	1:3:81:ASP:OD2	2.20	0.46
4:A:221:SER:HB2	7:D:140:ARG:O	2.16	0.46
5:B:5:TRP:O	25:B:611:CLA:H42	2.15	0.46
21:G:55:ARG:HE	21:G:55:ARG:HB2	1.36	0.46
25:G:610:CLA:H62	25:G:612:CLA:HMA1	1.97	0.46
21:N:98:LEU:CD2	25:N:603:CLA:HAA2	2.46	0.46
21:N:226:MET:O	21:N:230:PHE:CD2	2.69	0.46
25:N:602:CLA:CBC	26:N:618:LHG:H251	2.45	0.46
21:Y:108:LEU:HD11	25:Y:311:CLA:HBC1	1.97	0.46
24:Y:307:CHL:HAA1	40:Y:318:NEX:H27	1.96	0.46
22:R:170:LYS:HB2	24:R:606:CHL:O1D	2.15	0.46
2:6:205:ASP:HA	2:6:208:THR:OG1	2.15	0.46
2:6:217:ILE:HD13	25:6:604:CLA:O2D	2.15	0.46
27:a:404:PHO:NB	7:d:210:LEU:HD12	2.31	0.46
5:b:325:PHE:CG	13:l:35:TYR:HB3	2.51	0.46
7:d:318:LYS:HE3	37:d:408:CL:CL	2.53	0.46
8:e:24:SER:O	8:e:28:PRO:HG2	2.16	0.46
20:s:179:VAL:HG22	32:s:319:AJP:C01	2.45	0.46
21:g:87:ALA:CB	21:y:90:GLU:HB3	2.46	0.46
21:g:100:VAL:CG1	21:g:190:LEU:HD13	2.45	0.46
25:g:603:CLA:H3A	25:g:603:CLA:HBA1	1.58	0.46
21:n:100:VAL:CG1	21:n:190:LEU:HD13	2.45	0.46
21:n:216:LEU:O	21:n:220:ARG:HG3	2.15	0.46
21:y:107:MET:HA	21:y:222:ALA:HB1	1.98	0.46
21:y:154:HIS:CE1	21:y:156:GLN:OE1	2.69	0.46
24:y:302:CHL:H51	24:y:302:CHL:H92	1.97	0.46
22:r:203:GLU:OE2	25:r:608:CLA:C4A	2.63	0.46
1:1:209:ALA:CA	1:1:212:LYS:HG3	2.34	0.46
1:1:226:MET:O	1:1:230:PHE:CD2	2.69	0.46
2:2:122:TRP:O	2:2:123:VAL:CB	2.64	0.46
2:2:223:ALA:HB3	25:2:602:CLA:CMC	2.45	0.46
1:3:51:TYR:C	1:3:55:ARG:HD3	2.41	0.46
4:A:84:PRO:HB2	4:A:169:SER:HA	1.97	0.46
4:A:231:GLU:HA	5:B:1:MET:H2	1.81	0.46
29:A:407:SQD:O8	29:A:407:SQD:H4	2.15	0.46
6:C:459:ILE:CG2	6:C:464:GLU:HG3	2.45	0.46
8:E:71:ASP:HB3	23:U:103:TYR:CE1	2.50	0.46
15:O:115:PRO:HB2	15:O:328:TYR:CE2	2.50	0.46
15:O:146:LYS:HD3	15:O:158:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:87:ALA:CB	21:Y:90:GLU:HB3	2.46	0.46
21:G:164:THR:HG23	21:G:168:LEU:CD1	2.46	0.46
21:N:100:VAL:CG1	21:N:190:LEU:HD13	2.45	0.46
21:N:164:THR:HG23	21:N:168:LEU:CD1	2.46	0.46
24:Y:302:CHL:H51	24:Y:302:CHL:H92	1.97	0.46
22:R:124:PHE:CD1	25:R:614:CLA:CHC	2.93	0.46
22:R:179:TYR:HD1	22:R:180:LEU:N	2.14	0.46
22:R:203:GLU:OE2	25:R:608:CLA:C4A	2.63	0.46
22:R:241:ALA:O	22:R:245:HIS:HD2	1.98	0.46
25:R:603:CLA:HMD1	25:R:608:CLA:H12	1.97	0.46
25:R:612:CLA:HBA2	25:R:612:CLA:H3A	1.57	0.46
2:6:61:PRO:HD2	24:6:601:CHL:HBB1	1.97	0.46
2:6:117:GLU:HB3	2:6:121:LYS:HZ2	1.77	0.46
1:7:50:TRP:CB	1:7:213:VAL:HG21	2.45	0.46
1:7:107:MET:HG2	1:7:222:ALA:HB3	1.94	0.46
3:8:152:LEU:O	3:8:155:TRP:HB3	2.16	0.46
4:a:221:SER:HB2	7:d:140:ARG:O	2.16	0.46
4:a:224:ILE:O	7:d:266:ARG:NH2	2.43	0.46
5:b:413:ASP:O	5:b:417:VAL:HG23	2.16	0.46
13:l:21:GLY:HA2	26:l:103:LHG:H261	1.96	0.46
20:s:242:GLN:HE22	25:s:313:CLA:CHB	2.28	0.46
20:s:265:ASN:OD1	20:s:268:THR:HG23	2.16	0.46
26:s:301:LHG:H341	26:s:301:LHG:H312	1.76	0.46
21:g:164:THR:HG23	21:g:168:LEU:CD1	2.46	0.46
21:g:197:ASP:OD1	25:g:610:CLA:CAA	2.62	0.46
21:n:224:PHE:HE2	25:n:613:CLA:HAB	1.81	0.46
25:n:610:CLA:H62	25:n:610:CLA:H41	1.67	0.46
21:y:51:TYR:C	21:y:55:ARG:HD3	2.41	0.46
22:r:274:HIS:HD1	25:r:612:CLA:HAA2	1.79	0.46
1:1:58:TYR:HE1	1:1:79:GLY:O	1.99	0.46
1:3:208:PHE:CZ	1:3:212:LYS:HE3	2.51	0.46
27:A:403:PHO:NB	7:D:210:LEU:HD12	2.31	0.46
6:C:256:PRO:HA	25:C:506:CLA:HED2	1.98	0.46
7:D:99:GLN:OE1	8:E:73:LEU:HD13	2.14	0.46
7:D:278:THR:O	7:D:282:MET:HG2	2.16	0.46
14:M:14:PHE:O	14:M:18:PRO:HD2	2.16	0.46
21:N:51:TYR:C	21:N:55:ARG:HD3	2.41	0.46
21:Y:51:TYR:C	21:Y:55:ARG:HD3	2.41	0.46
21:Y:172:VAL:CG1	24:Y:309:CHL:C1B	2.94	0.46
21:Y:226:MET:O	21:Y:230:PHE:CD2	2.69	0.46
22:R:57:LEU:HD11	22:R:64:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:258:VAL:HG12	25:R:612:CLA:CMD	2.45	0.46
24:R:605:CHL:CBB	41:R:616:XAT:H162	2.45	0.46
2:6:50:TRP:C	2:6:55:ARG:HG2	2.41	0.46
1:7:154:HIS:CE1	1:7:156:GLN:OE1	2.69	0.46
1:7:208:PHE:CZ	1:7:212:LYS:HE3	2.51	0.46
5:b:18:ARG:O	5:b:22:VAL:HG13	2.15	0.46
5:b:20:LEU:O	5:b:24:ILE:HG13	2.15	0.46
5:b:475:PHE:O	5:b:478:VAL:HG12	2.16	0.46
6:c:79:LYS:CG	6:c:80:PRO:HD2	2.45	0.46
6:c:316:THR:HG21	6:c:396:MET:SD	2.56	0.46
7:d:89:SER:HB3	8:e:69:ARG:HH11	1.80	0.46
21:n:51:TYR:C	21:n:55:ARG:HD3	2.41	0.46
21:n:58:TYR:HE1	21:n:79:GLY:O	1.99	0.46
21:n:153:VAL:HG13	24:n:605:CHL:C1D	2.45	0.46
21:y:208:PHE:CZ	21:y:212:LYS:HE3	2.51	0.46
22:r:241:ALA:O	22:r:245:HIS:HD2	1.98	0.46
25:r:612:CLA:H3A	25:r:612:CLA:HBA2	1.57	0.46
1:1:51:TYR:HE2	1:1:209:ALA:HB1	1.75	0.46
2:2:122:TRP:C	2:2:123:VAL:HG23	2.40	0.46
1:3:100:VAL:CG1	1:3:190:LEU:HD13	2.45	0.46
1:3:145:ASP:HB3	1:3:149:ASN:O	2.15	0.46
1:3:154:HIS:CE1	1:3:156:GLN:OE1	2.69	0.46
1:3:209:ALA:CA	1:3:212:LYS:HG3	2.34	0.46
1:3:226:MET:O	1:3:230:PHE:CD2	2.69	0.46
3:4:221:LEU:C	3:4:224:LEU:HD23	2.41	0.46
4:A:331:MET:CE	7:D:321:LEU:HD22	2.46	0.46
5:B:258:TYR:HB3	35:B:626:DGD:HD62	1.97	0.46
5:B:330:MET:HE1	5:B:446:SER:HB3	1.96	0.46
25:B:611:CLA:H112	25:B:611:CLA:H72	1.67	0.46
6:C:79:LYS:CG	6:C:80:PRO:HD2	2.45	0.46
28:T:101:BCR:C16	28:T:101:BCR:H351	2.45	0.46
18:X:87:LEU:HD12	18:X:88:LEU:N	2.31	0.46
20:S:67:ARG:HH22	20:S:85:LEU:HB3	1.81	0.46
20:S:99:GLY:O	20:S:100:LEU:HB2	2.16	0.46
20:S:113:PHE:C	20:S:117:HIS:HD1	2.22	0.46
20:S:265:ASN:OD1	20:S:268:THR:HG23	2.16	0.46
21:G:51:TYR:C	21:G:55:ARG:HD3	2.41	0.46
25:G:610:CLA:H41	25:G:612:CLA:CMA	2.41	0.46
21:Y:216:LEU:O	21:Y:220:ARG:HG3	2.15	0.46
25:Y:303:CLA:H93	25:Y:303:CLA:C12	2.46	0.46
22:R:283:ILE:HG23	22:R:284:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:226:MET:O	1:5:230:PHE:CD2	2.69	0.46
2:6:188:ASN:HB2	2:6:192:PRO:HA	1.96	0.46
24:6:601:CHL:HBA1	24:6:601:CHL:H3A	1.83	0.46
1:7:51:TYR:C	1:7:55:ARG:HD3	2.41	0.46
1:7:206:GLU:OE1	1:7:206:GLU:CA	2.63	0.46
1:7:226:MET:O	1:7:230:PHE:CD2	2.69	0.46
3:8:144:SER:CB	22:r:279:LEU:O	2.63	0.46
6:c:189:TRP:HH2	6:c:362:ARG:HG2	1.81	0.46
6:c:233:ILE:HA	28:i:101:BCR:H282	1.97	0.46
6:c:459:ILE:CG2	6:c:464:GLU:HG3	2.45	0.46
7:d:85:SER:CB	23:u:102:ARG:HD2	2.46	0.46
7:d:247:MET:HE3	31:d:405:PL9:C52	2.46	0.46
7:d:343:PRO:HD2	7:d:346:VAL:CG2	2.45	0.46
12:k:35:PRO:O	12:k:38:ASP:HB2	2.16	0.46
18:x:87:LEU:HD12	18:x:88:LEU:N	2.31	0.46
25:s:310:CLA:H61	25:s:310:CLA:H92	1.51	0.46
25:s:312:CLA:HBA1	25:s:312:CLA:CMA	2.38	0.46
21:g:58:TYR:HE1	21:g:79:GLY:O	1.99	0.46
21:g:204:ASP:O	21:g:208:PHE:N	2.40	0.46
21:g:226:MET:O	21:g:230:PHE:CD2	2.69	0.46
24:g:605:CHL:H3A	24:g:605:CHL:HBA2	1.37	0.46
21:n:145:ASP:HB3	21:n:149:ASN:O	2.15	0.46
21:y:105:TRP:NE1	24:y:309:CHL:HED2	2.26	0.46
21:y:132:PHE:HB3	24:y:308:CHL:HMA3	1.97	0.46
22:r:57:LEU:HD11	22:r:64:SER:HB2	1.98	0.46
24:r:607:CHL:H3A	24:r:607:CHL:HBA2	1.60	0.46
1:1:75:PRO:HG3	1:1:212:LYS:HB3	1.98	0.46
4:A:54:ALA:HA	4:A:70:SER:OG	2.16	0.46
25:A:402:CLA:C2B	27:A:403:PHO:H192	2.46	0.46
5:B:139:PHE:HB2	25:B:610:CLA:HMD3	1.98	0.46
5:B:221:PRO:HA	25:B:609:CLA:HED3	1.98	0.46
25:B:605:CLA:HBD	25:B:605:CLA:HAA1	1.98	0.46
25:C:502:CLA:HBA1	25:C:502:CLA:H3A	1.78	0.46
28:H:101:BCR:C8	28:H:101:BCR:H331	2.46	0.46
20:S:143:PRO:HD2	20:S:153:LEU:HD11	1.98	0.46
21:G:58:TYR:HE1	21:G:79:GLY:O	1.99	0.46
21:G:75:PRO:HG3	21:G:212:LYS:HB3	1.98	0.46
21:G:154:HIS:CE1	21:G:156:GLN:OE1	2.69	0.46
21:G:164:THR:HG21	24:G:606:CHL:CED	2.46	0.46
21:G:206:GLU:OE1	21:G:206:GLU:CA	2.63	0.46
21:N:107:MET:HA	21:N:222:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:145:ASP:HB3	21:N:149:ASN:O	2.15	0.46
21:N:208:PHE:CZ	21:N:212:LYS:HE3	2.51	0.46
21:Y:50:TRP:O	21:Y:55:ARG:HD2	2.14	0.46
40:Y:318:NEX:H31	40:Y:318:NEX:H391	1.49	0.46
22:R:103:LYS:CE	22:R:105:LEU:HD11	2.45	0.46
25:R:612:CLA:H71	25:R:612:CLA:HHC	1.98	0.46
1:5:208:PHE:CZ	1:5:212:LYS:HE3	2.51	0.46
2:6:89:PRO:O	2:6:92:PHE:HB2	2.16	0.46
24:6:601:CHL:H62	24:6:601:CHL:H41	1.56	0.46
25:6:605:CLA:HBD	25:6:605:CLA:CAA	2.35	0.46
4:a:149:ALA:HB1	4:a:283:ILE:HB	1.97	0.46
4:a:220:THR:HA	4:a:223:LEU:HG	1.96	0.46
5:b:58:GLN:HG2	5:b:331:ASP:OD2	2.16	0.46
5:b:108:PHE:CZ	5:b:112:ILE:HD11	2.51	0.46
5:b:194:VAL:HG23	5:b:194:VAL:O	2.15	0.46
6:c:133:ALA:HB1	25:c:511:CLA:CMA	2.45	0.46
25:c:509:CLA:HBC2	25:c:509:CLA:HMC1	1.98	0.46
7:d:194:LEU:O	7:d:194:LEU:HG	2.16	0.46
20:s:95:TYR:OH	24:s:302:CHL:O1A	2.30	0.46
20:s:241:ILE:HG22	25:s:313:CLA:HMD3	1.97	0.46
21:n:164:THR:HG23	21:n:168:LEU:CD1	2.46	0.46
25:n:613:CLA:H2	25:n:613:CLA:H122	1.98	0.46
25:y:304:CLA:H91	25:y:304:CLA:C12	2.46	0.46
40:y:318:NEX:C36	40:y:318:NEX:C28	2.90	0.46
1:3:107:MET:HA	1:3:222:ALA:HB1	1.98	0.46
4:A:149:ALA:HB1	4:A:283:ILE:HB	1.97	0.46
5:B:283:GLU:HG3	5:B:287:ARG:HD2	1.96	0.46
5:B:413:ASP:O	5:B:417:VAL:HG23	2.16	0.46
28:B:617:BCR:H15C	28:B:617:BCR:H351	1.81	0.46
6:C:316:THR:HG21	6:C:396:MET:SD	2.56	0.46
6:C:437:LEU:HD22	25:C:502:CLA:HBC1	1.97	0.46
15:O:130:LYS:HD2	15:O:179:GLU:CB	2.45	0.46
15:O:228:THR:CG2	15:O:284:GLU:OE2	2.57	0.46
25:N:602:CLA:H61	25:N:602:CLA:H93	1.49	0.46
1:5:75:PRO:HG3	1:5:212:LYS:HB3	1.98	0.46
1:5:206:GLU:OE1	1:5:206:GLU:CA	2.63	0.46
1:7:75:PRO:HG3	1:7:212:LYS:HB3	1.98	0.46
1:7:100:VAL:CG1	1:7:190:LEU:HD13	2.45	0.46
3:8:221:LEU:C	3:8:224:LEU:HD23	2.41	0.46
25:b:609:CLA:HMB1	25:b:610:CLA:C1B	2.46	0.46
6:c:251:HIS:HE1	25:c:506:CLA:HMA3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:505:CLA:H92	25:c:505:CLA:H61	1.74	0.46
29:l:101:SQD:H312	29:l:101:SQD:H352	1.97	0.46
28:t:101:BCR:H351	28:t:101:BCR:C16	2.45	0.46
17:w:81:VAL:HG23	17:w:82:ASP:OD2	2.16	0.46
20:s:113:PHE:C	20:s:117:HIS:HD1	2.22	0.46
20:s:267:LEU:HD13	25:s:314:CLA:CED	2.44	0.46
21:g:208:PHE:CZ	21:g:212:LYS:HE3	2.51	0.46
21:n:56:VAL:CG1	24:n:601:CHL:HBC1	2.46	0.46
21:n:107:MET:HA	21:n:222:ALA:HB1	1.98	0.46
21:n:215:GLU:OE1	25:n:610:CLA:C4A	2.64	0.46
25:n:602:CLA:H51	25:n:603:CLA:HBA1	1.97	0.46
26:y:301:LHG:H301	26:y:301:LHG:H271	1.62	0.46
22:r:170:LYS:HB2	24:r:606:CHL:O1D	2.15	0.46
22:r:240:LEU:O	22:r:244:LYS:HG3	2.15	0.46
2:2:61:PRO:HD2	24:2:601:CHL:HBB1	1.97	0.46
1:3:58:TYR:HE1	1:3:79:GLY:C	2.24	0.46
3:4:152:LEU:O	3:4:155:TRP:HB3	2.16	0.46
3:4:171:SER:N	3:4:183:GLU:OE2	2.48	0.46
4:A:30:ILE:HD11	29:A:411:SQD:H442	1.98	0.46
4:A:57:PRO:O	15:O:208:ARG:NH1	2.49	0.46
4:A:131:TRP:CZ2	6:C:449:ARG:HD2	2.48	0.46
4:A:214:MET:HE1	27:A:404:PHO:C3D	2.45	0.46
25:A:402:CLA:O1A	25:A:402:CLA:H43	2.16	0.46
5:B:18:ARG:O	5:B:22:VAL:HG13	2.15	0.46
5:B:108:PHE:CZ	5:B:112:ILE:HD11	2.51	0.46
5:B:194:VAL:O	5:B:194:VAL:HG23	2.15	0.46
5:B:248:ALA:HB2	25:B:603:CLA:H52	1.97	0.46
6:C:133:ALA:HB1	25:C:511:CLA:CMA	2.45	0.46
6:C:225:VAL:HG22	6:C:289:PHE:HE1	1.73	0.46
6:C:233:ILE:HA	28:I:101:BCR:H282	1.97	0.46
25:C:510:CLA:HHD	25:C:510:CLA:H192	1.98	0.46
7:D:97:GLU:HG3	8:E:69:ARG:HG3	1.98	0.46
25:D:403:CLA:H52	18:X:91:ALA:HB1	1.98	0.46
11:I:33:GLY:C	11:I:34:ARG:HG3	2.36	0.46
13:L:21:GLY:HA2	26:L:102:LHG:H261	1.96	0.46
20:S:67:ARG:NH2	20:S:85:LEU:O	2.49	0.46
25:S:310:CLA:CBB	25:S:312:CLA:H3A	2.46	0.46
21:N:154:HIS:CE1	21:N:156:GLN:OE1	2.69	0.46
25:N:611:CLA:HMD2	25:N:612:CLA:HHD	1.98	0.46
22:R:83:LEU:HD12	41:R:616:XAT:H23	1.98	0.46
22:R:141:LEU:HD21	22:R:145:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:58:TYR:HE1	1:5:79:GLY:O	1.99	0.46
2:6:130:PRO:CG	2:6:239:LYS:HE2	2.45	0.46
25:6:605:CLA:HBA2	25:6:605:CLA:H3A	1.26	0.46
3:8:97:TRP:HD1	3:8:164:PHE:CE2	2.34	0.46
3:8:221:LEU:HA	3:8:224:LEU:HD23	1.95	0.46
4:a:30:ILE:HD11	29:a:412:SQD:H442	1.98	0.46
4:a:215:HIS:NE2	33:a:414:BCT:O2	2.48	0.46
4:a:331:MET:CE	7:d:321:LEU:HD22	2.46	0.46
5:b:148:VAL:HG11	26:b:622:LHG:H212	1.98	0.46
5:b:330:MET:CE	5:b:446:SER:HB3	2.46	0.46
28:b:618:BCR:C8	28:b:618:BCR:H331	2.46	0.46
6:c:36:TRP:O	25:c:508:CLA:H11	2.15	0.46
6:c:113:VAL:HG13	28:c:514:BCR:H313	1.98	0.46
25:c:504:CLA:HAA1	35:c:516:DGD:HD61	1.97	0.46
25:c:511:CLA:C14	19:z:20:LEU:HD11	2.45	0.46
20:s:99:GLY:O	20:s:100:LEU:HB2	2.16	0.46
20:s:132:GLU:HA	20:s:145:ALA:CB	2.39	0.46
25:s:310:CLA:CBB	25:s:312:CLA:H3A	2.46	0.46
21:n:227:PHE:CD2	25:n:602:CLA:H202	2.41	0.46
21:y:131:TRP:HA	39:y:317:LUT:O3	2.16	0.46
22:r:127:TYR:CD2	22:r:135:ARG:CD	2.97	0.46
40:r:617:NEX:H201	40:r:617:NEX:H15	1.41	0.46
1:1:55:ARG:HE	1:1:55:ARG:HB2	1.36	0.45
1:1:128:GLU:CB	1:1:137:GLN:HB2	2.41	0.45
1:1:153:VAL:HA	24:1:301:CHL:ND	2.30	0.45
1:1:164:THR:HG23	1:1:168:LEU:CD1	2.46	0.45
2:2:69:TYR:CD1	2:2:70:LEU:N	2.85	0.45
24:2:601:CHL:H62	24:2:601:CHL:H41	1.56	0.45
1:3:58:TYR:HE1	1:3:79:GLY:O	1.99	0.45
1:3:75:PRO:HG3	1:3:212:LYS:HB3	1.98	0.45
4:A:157:VAL:HG11	4:A:172:MET:HE3	1.98	0.45
4:A:231:GLU:HG2	5:B:1:MET:CA	2.45	0.45
5:B:285:TYR:HE2	23:U:87:LYS:O	1.99	0.45
25:B:609:CLA:H3A	25:B:609:CLA:HBA1	1.47	0.45
10:H:26:LEU:HD23	25:R:614:CLA:HMA1	1.97	0.45
20:S:146:VAL:HG11	20:S:148:PHE:CZ	2.52	0.45
21:G:183:LEU:HG	24:G:608:CHL:CBB	2.46	0.45
25:G:610:CLA:CBB	39:G:615:LUT:H32	2.43	0.45
21:N:50:TRP:HB3	21:N:213:VAL:HG21	1.98	0.45
21:N:58:TYR:HE1	21:N:79:GLY:O	1.99	0.45
21:Y:97:GLU:HA	21:Y:190:LEU:CD1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:105:TRP:NE1	24:Y:309:CHL:HED2	2.26	0.45
21:Y:107:MET:HA	21:Y:222:ALA:HB1	1.98	0.45
2:6:122:TRP:C	2:6:123:VAL:HG23	2.40	0.45
1:7:120:ALA:HA	1:7:124:VAL:O	2.16	0.45
3:8:171:SER:N	3:8:183:GLU:OE2	2.49	0.45
4:a:54:ALA:HA	4:a:70:SER:OG	2.16	0.45
4:a:136:ARG:NH2	11:i:27:ASP:OD2	2.48	0.45
25:b:601:CLA:HBD	25:b:601:CLA:HAA1	1.97	0.45
6:c:51:GLY:CA	6:c:132:HIS:HB2	2.46	0.45
6:c:457:LYS:HZ3	7:d:228:ASP:C	2.22	0.45
25:c:509:CLA:HBA2	42:c:607:HOH:O	2.14	0.45
10:h:18:THR:O	10:h:22:LEU:HD13	2.16	0.45
14:m:14:PHE:O	14:m:18:PRO:HD2	2.16	0.45
15:o:228:THR:CG2	15:o:284:GLU:OE2	2.57	0.45
15:o:311:THR:HG21	15:o:316:LYS:O	2.16	0.45
20:s:146:VAL:HG11	20:s:148:PHE:CZ	2.51	0.45
24:s:306:CHL:CBB	39:s:316:LUT:H161	2.46	0.45
21:g:75:PRO:HG3	21:g:212:LYS:HB3	1.98	0.45
25:g:602:CLA:C2	25:g:602:CLA:HMB1	2.47	0.45
21:y:100:VAL:CG1	21:y:190:LEU:HD13	2.45	0.45
21:y:161:ILE:HG21	24:y:308:CHL:HBC1	1.99	0.45
21:y:206:GLU:OE1	21:y:206:GLU:CA	2.63	0.45
24:y:306:CHL:HBC3	24:y:306:CHL:HMC	1.98	0.45
40:y:318:NEX:H31	40:y:318:NEX:H391	1.49	0.45
22:r:247:ARG:HD3	25:r:602:CLA:HHD	1.97	0.45
22:r:258:VAL:HG12	25:r:612:CLA:CMD	2.45	0.45
2:2:100:VAL:HB	2:2:190:LEU:HD23	1.98	0.45
4:A:329:GLU:HA	4:A:332:HIS:HE2	1.79	0.45
5:B:214:LEU:HB3	25:R:603:CLA:HED1	1.97	0.45
5:B:256:MET:HG3	5:B:448:ARG:HG3	1.98	0.45
5:B:257:TRP:CD2	7:D:292:LEU:HD22	2.52	0.45
25:B:604:CLA:H152	25:B:604:CLA:H112	1.57	0.45
6:C:51:GLY:CA	6:C:132:HIS:HB2	2.46	0.45
25:C:504:CLA:HAA1	35:C:516:DGD:HD61	1.97	0.45
7:D:85:SER:CB	23:U:102:ARG:HD2	2.46	0.45
7:D:247:MET:HE3	31:D:405:PL9:C52	2.46	0.45
18:X:92:SER:O	18:X:96:VAL:HG13	2.17	0.45
21:G:226:MET:O	21:G:230:PHE:CD2	2.69	0.45
24:G:606:CHL:HBB1	39:G:616:LUT:C16	2.47	0.45
21:N:108:LEU:HD11	25:N:610:CLA:HBC1	1.96	0.45
21:N:153:VAL:HG13	24:N:605:CHL:C1D	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:602:CLA:H51	25:N:603:CLA:HBA1	1.98	0.45
21:Y:58:TYR:HE1	21:Y:79:GLY:O	1.99	0.45
25:Y:315:CLA:HED2	25:Y:315:CLA:HBD	1.82	0.45
22:R:137:ARG:HH21	25:R:602:CLA:CED	2.22	0.45
1:5:120:ALA:HA	1:5:124:VAL:O	2.16	0.45
2:6:69:TYR:CD1	2:6:70:LEU:N	2.84	0.45
2:6:122:TRP:O	2:6:123:VAL:CB	2.64	0.45
2:6:161:ALA:HB1	2:6:165:PHE:HE2	1.81	0.45
1:7:216:LEU:O	1:7:220:ARG:HG3	2.15	0.45
30:a:411:LMG:H291	11:i:4:LEU:CD2	2.46	0.45
5:b:281:GLN:CD	23:u:91:VAL:HG13	2.42	0.45
5:b:285:TYR:HE2	23:u:87:LYS:O	1.99	0.45
25:b:601:CLA:H192	25:b:601:CLA:H162	1.69	0.45
25:b:616:CLA:H91	25:b:616:CLA:H111	1.72	0.45
6:c:146:PHE:CE2	26:s:301:LHG:HC62	2.51	0.45
7:d:278:THR:O	7:d:282:MET:HG2	2.16	0.45
21:n:50:TRP:HB3	21:n:213:VAL:HG21	1.98	0.45
21:n:107:MET:HG2	21:n:222:ALA:HB3	1.94	0.45
25:n:602:CLA:CBC	26:n:618:LHG:H251	2.45	0.45
40:n:617:NEX:H191	40:n:617:NEX:C12	2.30	0.45
21:y:58:TYR:HE1	21:y:79:GLY:O	1.99	0.45
21:y:164:THR:HG23	21:y:168:LEU:CD1	2.46	0.45
22:r:274:HIS:CD2	24:r:613:CHL:NC	2.84	0.45
24:r:605:CHL:HAB	25:r:608:CLA:HBC2	1.97	0.45
24:r:607:CHL:HMB2	40:r:617:NEX:H14	1.97	0.45
1:1:120:ALA:HA	1:1:124:VAL:O	2.16	0.45
2:2:89:PRO:O	2:2:92:PHE:HB2	2.16	0.45
3:4:97:TRP:HD1	3:4:164:PHE:CE2	2.34	0.45
4:A:105:TRP:CZ3	4:A:111:PRO:HG3	2.51	0.45
4:A:174:LEU:HD22	27:A:403:PHO:H143	1.98	0.45
5:B:41:GLU:CD	5:B:62:VAL:HG22	2.41	0.45
6:C:189:TRP:HH2	6:C:362:ARG:HG2	1.81	0.45
6:C:311:GLN:HG3	6:C:361:LEU:CD2	2.47	0.45
6:C:311:GLN:HE21	6:C:358:PHE:HB2	1.81	0.45
6:C:428:THR:HG22	35:C:516:DGD:CCB	2.44	0.45
25:C:511:CLA:C14	19:Z:20:LEU:HD11	2.45	0.45
7:D:89:SER:HB3	8:E:69:ARG:HH11	1.80	0.45
21:G:107:MET:HA	21:G:222:ALA:HB1	1.98	0.45
21:G:218:ASN:ND2	25:G:612:CLA:C4A	2.62	0.45
24:G:608:CHL:H18	40:G:617:NEX:H361	1.98	0.45
25:N:603:CLA:HBC1	24:N:609:CHL:CBC	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:75:PRO:HG3	21:Y:212:LYS:HB3	1.98	0.45
21:Y:132:PHE:HB3	24:Y:308:CHL:HMA3	1.97	0.45
21:Y:206:GLU:OE1	21:Y:206:GLU:CA	2.63	0.45
22:R:234:LYS:HA	22:R:234:LYS:HE2	1.99	0.45
1:5:51:TYR:C	1:5:55:ARG:HD3	2.41	0.45
3:8:120:GLN:OE1	3:8:253:LEU:HD23	2.16	0.45
5:b:460:LEU:HD12	7:d:288:VAL:HG21	1.94	0.45
25:c:511:CLA:C3B	28:k:101:BCR:H393	2.46	0.45
7:d:97:GLU:HG3	8:e:69:ARG:HG3	1.98	0.45
29:l:102:SQD:H462	14:m:28:LYS:HD2	1.98	0.45
25:s:305:CLA:H3A	25:s:305:CLA:CGA	2.46	0.45
21:g:164:THR:HG21	24:g:606:CHL:CED	2.46	0.45
21:y:120:ALA:HA	21:y:124:VAL:O	2.16	0.45
21:y:226:MET:O	21:y:230:PHE:CD2	2.69	0.45
25:y:303:CLA:C12	25:y:303:CLA:H93	2.46	0.45
25:r:603:CLA:HMD1	25:r:608:CLA:H12	1.98	0.45
2:2:121:LYS:HD3	2:2:245:LEU:CD1	2.46	0.45
2:2:174:GLU:HG3	1:3:59:LEU:HD22	1.93	0.45
2:2:218:LYS:HA	2:2:221:ARG:HE	1.81	0.45
1:3:164:THR:HG23	1:3:168:LEU:CD1	2.46	0.45
3:4:120:GLN:OE1	3:4:253:LEU:HD23	2.16	0.45
30:A:410:LMG:H351	30:A:410:LMG:H382	1.83	0.45
30:A:410:LMG:H291	11:I:4:LEU:CD2	2.46	0.45
5:B:245:VAL:HG21	25:B:612:CLA:HED3	1.99	0.45
25:B:608:CLA:HBC3	25:B:608:CLA:HHD	1.98	0.45
25:B:609:CLA:HMB1	25:B:610:CLA:C1B	2.46	0.45
25:B:611:CLA:HAB	25:B:613:CLA:H3A	1.98	0.45
6:C:146:PHE:CE2	26:S:301:LHG:HC62	2.51	0.45
7:D:81:THR:HG22	7:D:112:TRP:NE1	2.32	0.45
12:K:35:PRO:O	12:K:38:ASP:HB2	2.16	0.45
15:O:290:THR:HB	15:O:300:ILE:HG13	1.98	0.45
15:O:290:THR:O	15:O:291:LYS:C	2.59	0.45
15:O:311:THR:HG21	15:O:316:LYS:O	2.16	0.45
28:T:101:BCR:H271	5:b:39:LEU:HD13	1.98	0.45
25:S:312:CLA:HBB1	39:S:315:LUT:C14	2.47	0.45
21:G:82:THR:N	39:G:616:LUT:O23	2.42	0.45
25:G:603:CLA:H3A	25:G:603:CLA:HBA1	1.58	0.45
21:N:59:LEU:HD23	24:N:601:CHL:C1B	2.46	0.45
25:N:613:CLA:H2	25:N:613:CLA:H122	1.98	0.45
21:Y:154:HIS:CE1	21:Y:156:GLN:OE1	2.69	0.45
25:Y:304:CLA:H91	25:Y:304:CLA:C12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:304:CLA:H161	25:Y:304:CLA:H192	1.74	0.45
24:Y:309:CHL:H91	24:Y:309:CHL:H112	1.60	0.45
1:5:153:VAL:HA	24:5:301:CHL:ND	2.30	0.45
2:6:161:ALA:O	2:6:162:VAL:C	2.58	0.45
4:a:210:LEU:HD12	27:a:405:PHO:NB	2.31	0.45
5:b:223:GLN:CD	10:h:36:GLY:H	2.23	0.45
5:b:355:PHE:O	5:b:371:VAL:HG22	2.16	0.45
6:c:185:VAL:HG23	6:c:230:LEU:CD1	2.47	0.45
6:c:372:PRO:O	6:c:373:ASN:HB2	2.16	0.45
8:e:71:ASP:HB3	23:u:103:TYR:CE1	2.50	0.45
20:s:67:ARG:NH2	20:s:85:LEU:O	2.49	0.45
21:g:107:MET:HA	21:g:222:ALA:HB1	1.98	0.45
25:g:612:CLA:H111	25:g:612:CLA:H142	1.51	0.45
21:n:58:TYR:HE1	21:n:79:GLY:C	2.24	0.45
21:n:131:TRP:HA	39:n:616:LUT:O3	2.15	0.45
21:n:226:MET:O	21:n:230:PHE:CD2	2.69	0.45
24:n:609:CHL:HBC3	24:y:302:CHL:H91	1.97	0.45
21:y:172:VAL:CG1	24:y:309:CHL:C1B	2.94	0.45
24:y:309:CHL:H141	24:y:309:CHL:H162	1.86	0.45
22:r:83:LEU:HD12	41:r:616:XAT:H23	1.98	0.45
2:2:192:PRO:HB3	24:2:603:CHL:HBC2	1.99	0.45
2:2:197:PHE:HB3	2:2:202:LEU:CD2	2.47	0.45
25:2:605:CLA:HBC1	26:2:606:LHG:H362	1.95	0.45
5:B:39:LEU:HD13	28:t:101:BCR:H271	1.98	0.45
25:B:613:CLA:H111	25:B:613:CLA:H142	1.67	0.45
6:C:376:ASP:OD1	6:C:379:ARG:HB2	2.17	0.45
25:C:511:CLA:C3B	28:K:101:BCR:H393	2.46	0.45
29:L:101:SQD:H92	29:L:101:SQD:O10	2.16	0.45
20:S:267:LEU:HD13	25:S:314:CLA:CED	2.44	0.45
24:S:306:CHL:CBB	39:S:316:LUT:H161	2.46	0.45
24:S:306:CHL:HBC2	24:S:307:CHL:CHD	2.46	0.45
21:G:132:PHE:CB	24:G:607:CHL:HMA3	2.41	0.45
21:N:206:GLU:OE1	21:N:206:GLU:CA	2.63	0.45
25:N:612:CLA:H62	25:N:612:CLA:H2	1.71	0.45
25:Y:312:CLA:H142	25:Y:312:CLA:H111	1.54	0.45
1:5:58:TYR:HE1	1:5:79:GLY:C	2.24	0.45
1:5:107:MET:HA	1:5:222:ALA:HB1	1.98	0.45
2:6:69:TYR:CG	2:6:92:PHE:CZ	3.05	0.45
2:6:197:PHE:HB3	2:6:202:LEU:CD2	2.47	0.45
1:7:164:THR:HG23	1:7:168:LEU:CD1	2.46	0.45
4:a:205:VAL:CG1	7:d:205:VAL:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:28:ALA:HB2	5:b:107:CYS:CB	2.47	0.45
28:d:404:BCR:H403	30:d:407:LMG:H141	1.99	0.45
20:s:143:PRO:HD2	20:s:153:LEU:HD11	1.98	0.45
21:g:83:ALA:HA	21:y:98:LEU:HD11	1.98	0.45
21:n:75:PRO:HG3	21:n:212:LYS:HB3	1.98	0.45
21:n:98:LEU:CD2	25:n:603:CLA:HAA2	2.46	0.45
21:n:120:ALA:HA	21:n:124:VAL:O	2.16	0.45
1:1:51:TYR:C	1:1:55:ARG:HD3	2.41	0.45
25:2:604:CLA:H52	25:2:604:CLA:H12	1.77	0.45
3:4:222:GLU:HA	3:4:225:LYS:HG3	1.97	0.45
4:A:205:VAL:CG1	7:D:205:VAL:HG12	2.47	0.45
5:B:220:ARG:HG3	10:H:32:LYS:HE3	1.99	0.45
5:B:325:PHE:CG	13:L:35:TYR:HB3	2.51	0.45
25:B:602:CLA:H62	25:B:602:CLA:H41	1.79	0.45
15:O:196:TYR:CB	15:O:212:LEU:HD21	2.16	0.45
19:Z:57:LEU:HD23	19:Z:60:LEU:HD12	1.98	0.45
20:S:190:ILE:HG13	20:S:191:THR:H	1.81	0.45
21:N:58:TYR:HE1	21:N:79:GLY:C	2.24	0.45
21:N:128:GLU:CB	21:N:133:LYS:O	2.65	0.45
21:N:215:GLU:OE1	25:N:610:CLA:C4A	2.64	0.45
21:N:224:PHE:HD1	25:N:602:CLA:H201	1.81	0.45
24:N:607:CHL:C18	24:N:609:CHL:H71	2.38	0.45
21:Y:114:VAL:HG13	21:Y:241:ILE:HD11	1.98	0.45
21:Y:208:PHE:CZ	21:Y:212:LYS:HE3	2.51	0.45
2:6:218:LYS:HA	2:6:221:ARG:HE	1.81	0.45
2:6:232:VAL:CG1	2:6:243:GLU:OE1	2.65	0.45
25:6:604:CLA:HBC3	26:6:606:LHG:H372	1.98	0.45
1:7:50:TRP:HB3	1:7:213:VAL:HG21	1.99	0.45
1:7:107:MET:HA	1:7:222:ALA:HB1	1.98	0.45
3:8:170:GLN:HB2	3:8:183:GLU:CG	2.42	0.45
4:a:51:ALA:CB	4:a:82:ILE:HD12	2.47	0.45
4:a:105:TRP:CZ3	4:a:111:PRO:HG3	2.51	0.45
27:a:405:PHO:HAB	25:d:402:CLA:H11	1.98	0.45
5:b:41:GLU:CD	5:b:62:VAL:HG22	2.41	0.45
25:b:605:CLA:HBD	25:b:605:CLA:HAA1	1.98	0.45
25:c:504:CLA:C4	35:c:516:DGD:HB32	2.45	0.45
25:c:510:CLA:HHD	25:c:510:CLA:H192	1.98	0.45
28:h:101:BCR:H331	28:h:101:BCR:C8	2.46	0.45
15:o:290:THR:HB	15:o:300:ILE:HG13	1.98	0.45
15:o:290:THR:O	15:o:291:LYS:C	2.59	0.45
20:s:67:ARG:HH22	20:s:85:LEU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:s:306:CHL:HBC2	24:s:307:CHL:CHD	2.46	0.45
21:g:51:TYR:C	21:g:55:ARG:HD3	2.41	0.45
21:g:183:LEU:HG	24:g:608:CHL:CBB	2.46	0.45
21:n:208:PHE:CZ	21:n:212:LYS:HE3	2.51	0.45
25:y:315:CLA:CBC	39:y:316:LUT:H162	2.39	0.45
22:r:234:LYS:HE2	22:r:234:LYS:HA	1.99	0.45
2:2:50:TRP:C	2:2:55:ARG:HG2	2.41	0.45
2:2:69:TYR:CG	2:2:92:PHE:CZ	3.05	0.45
2:2:232:VAL:CG1	2:2:243:GLU:OE1	2.65	0.45
3:4:183:GLU:HB3	3:4:185:PHE:HD1	1.75	0.45
5:B:355:PHE:O	5:B:371:VAL:HG22	2.16	0.45
6:C:236:GLY:HA2	6:C:239:TRP:CD1	2.52	0.45
6:C:372:PRO:O	6:C:373:ASN:HB2	2.16	0.45
7:D:172:PRO:HG3	7:D:182:PHE:CE2	2.52	0.45
7:D:309:ASP:OD1	7:D:311:GLU:HG3	2.17	0.45
8:E:24:SER:O	8:E:28:PRO:HG2	2.16	0.45
15:O:130:LYS:HE2	15:O:177:PRO:CB	2.30	0.45
25:S:305:CLA:H3A	25:S:305:CLA:CGA	2.46	0.45
21:G:80:TRP:CE3	39:G:616:LUT:H383	2.52	0.45
21:G:120:ALA:HA	21:G:124:VAL:O	2.16	0.45
21:G:204:ASP:O	21:G:208:PHE:N	2.40	0.45
25:G:613:CLA:H3A	25:G:613:CLA:HBA2	1.59	0.45
25:G:613:CLA:H91	26:Y:301:LHG:H322	1.99	0.45
21:N:227:PHE:HB2	39:N:616:LUT:C40	2.47	0.45
25:N:602:CLA:H93	25:N:602:CLA:H111	1.52	0.45
25:Y:304:CLA:HMD1	24:Y:310:CHL:C1D	2.47	0.45
25:Y:313:CLA:H142	25:Y:313:CLA:H111	1.50	0.45
26:Y:319:LHG:H171	26:Y:319:LHG:H202	1.70	0.45
22:R:155:LEU:HD22	22:R:268:LEU:HD21	1.99	0.45
1:5:50:TRP:HB3	1:5:213:VAL:HG21	1.98	0.45
1:5:128:GLU:CB	1:5:133:LYS:O	2.65	0.45
2:6:174:GLU:CD	1:7:59:LEU:HD22	2.42	0.45
1:7:163:ALA:O	1:7:167:ILE:HG13	2.17	0.45
3:8:58:ILE:O	3:8:58:ILE:HG22	2.15	0.45
27:a:404:PHO:H141	27:a:404:PHO:H161	1.52	0.45
29:a:412:SQD:H132	29:a:412:SQD:H162	1.70	0.45
5:b:248:ALA:HB2	25:b:603:CLA:H52	1.97	0.45
5:b:377:VAL:O	5:b:378:ARG:HB2	2.17	0.45
25:b:607:CLA:H161	25:b:607:CLA:H141	1.55	0.45
26:b:625:LHG:H351	26:b:625:LHG:H101	1.99	0.45
6:c:225:VAL:HG13	6:c:289:PHE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:256:PRO:HA	25:c:506:CLA:HED2	1.98	0.45
7:d:172:PRO:HG3	7:d:182:PHE:CE2	2.52	0.45
7:d:280:LEU:CD2	25:d:402:CLA:HBA2	2.45	0.45
25:s:310:CLA:H62	25:s:310:CLA:H41	1.68	0.45
21:g:58:TYR:HE1	21:g:79:GLY:C	2.24	0.45
24:g:608:CHL:H18	40:g:617:NEX:H361	1.98	0.45
21:n:163:ALA:O	21:n:167:ILE:HG13	2.17	0.45
21:n:227:PHE:HB2	39:n:616:LUT:C40	2.47	0.45
24:n:601:CHL:H3A	24:n:601:CHL:HBA1	1.63	0.45
21:y:104:ARG:HB3	25:y:311:CLA:HBC2	1.96	0.45
22:r:103:LYS:CD	22:r:105:LEU:HD11	2.47	0.45
22:r:179:TYR:HD1	22:r:180:LEU:N	2.14	0.45
25:r:611:CLA:HAA2	25:r:611:CLA:H12	1.98	0.45
3:4:122:TRP:HA	3:4:127:TRP:CD1	2.40	0.45
3:4:169:SER:O	3:4:170:GLN:HB2	2.17	0.45
3:4:236:MET:HA	3:4:239:MET:HE3	1.98	0.45
5:B:296:GLN:HE21	5:B:300:GLU:HB3	1.82	0.45
5:B:330:MET:CE	5:B:446:SER:HB3	2.46	0.45
5:B:372:ASP:OD1	5:B:376:ILE:N	2.49	0.45
25:B:616:CLA:HMD3	10:H:17:THR:HG21	1.98	0.45
6:C:113:VAL:HG13	28:C:514:BCR:H313	1.98	0.45
7:D:161:TYR:HA	7:D:291:ALA:HB2	1.99	0.45
15:O:146:LYS:HD3	15:O:158:PHE:CE1	2.52	0.45
25:S:311:CLA:HBA1	25:S:311:CLA:H3A	1.69	0.45
21:N:164:THR:HG21	24:N:606:CHL:O1D	2.16	0.45
25:Y:303:CLA:H111	25:Y:303:CLA:H143	1.61	0.45
22:R:141:LEU:CD2	22:R:216:LEU:HB3	2.47	0.45
25:R:601:CLA:H3A	25:R:601:CLA:HBA1	1.45	0.45
1:5:163:ALA:O	1:5:167:ILE:HG13	2.17	0.45
1:7:97:GLU:HA	1:7:190:LEU:CD1	2.24	0.45
3:8:144:SER:HB3	22:r:279:LEU:O	2.17	0.45
3:8:169:SER:O	3:8:170:GLN:HB2	2.17	0.45
4:a:30:ILE:HD11	29:a:412:SQD:C44	2.47	0.45
5:b:110:ALA:HB1	25:b:616:CLA:CHB	2.47	0.45
25:b:602:CLA:H62	25:b:602:CLA:H41	1.79	0.45
6:c:364:PRO:O	6:c:368:PRO:HD3	2.17	0.45
21:g:50:TRP:HB3	21:g:213:VAL:HG21	1.98	0.45
21:n:154:HIS:CE1	21:n:156:GLN:OE1	2.69	0.45
21:n:158:ILE:HD11	21:y:257:TRP:CE3	2.35	0.45
21:y:56:VAL:HB	24:y:302:CHL:HBC2	1.98	0.45
21:y:75:PRO:HG3	21:y:212:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:128:GLU:CB	21:y:133:LYS:O	2.65	0.45
25:y:304:CLA:H101	25:y:304:CLA:H62	1.40	0.45
25:y:314:CLA:H141	25:y:314:CLA:H162	1.53	0.45
22:r:141:LEU:CD2	22:r:216:LEU:HB3	2.47	0.45
22:r:283:ILE:HG23	22:r:284:ILE:N	2.31	0.45
25:r:602:CLA:H43	25:r:603:CLA:HBA1	1.99	0.45
1:1:58:TYR:HE1	1:1:79:GLY:C	2.24	0.45
1:1:107:MET:HA	1:1:222:ALA:HB1	1.98	0.45
4:A:30:ILE:HD11	29:A:411:SQD:C44	2.47	0.45
4:A:37:MET:HB2	4:A:125:CYS:CB	2.47	0.45
4:A:238:ARG:O	4:A:241:GLN:HB3	2.17	0.45
6:C:227:VAL:CG2	28:I:101:BCR:H292	2.47	0.45
25:C:513:CLA:CMD	20:S:75:LEU:HD11	2.45	0.45
7:D:157:VAL:HG12	7:D:172:PRO:CG	2.47	0.45
7:D:194:LEU:HG	7:D:194:LEU:O	2.16	0.45
17:W:81:VAL:HG23	17:W:82:ASP:OD2	2.16	0.45
21:G:83:ALA:HA	21:Y:98:LEU:HD11	1.98	0.45
21:N:120:ALA:HA	21:N:124:VAL:O	2.16	0.45
24:N:607:CHL:HHC	24:N:607:CHL:HBB1	1.98	0.45
24:N:608:CHL:H13	40:N:617:NEX:C40	2.46	0.45
25:N:613:CLA:H143	25:N:613:CLA:C8	2.38	0.45
25:N:613:CLA:HBA1	25:N:614:CLA:C3D	2.47	0.45
21:Y:115:PHE:HZ	32:Y:320:AJP:C83	2.30	0.45
21:Y:131:TRP:HA	39:Y:317:LUT:O3	2.16	0.45
24:Y:302:CHL:HBB1	24:Y:302:CHL:HHC	1.98	0.45
22:R:67:TRP:CH2	22:R:85:LYS:HB2	2.51	0.45
22:R:177:SER:HB2	24:R:605:CHL:CMD	2.47	0.45
2:6:100:VAL:HB	2:6:190:LEU:HD23	1.98	0.45
5:b:372:ASP:OD1	5:b:376:ILE:N	2.49	0.45
25:b:613:CLA:H111	25:b:613:CLA:H142	1.67	0.45
8:e:18:ARG:HB3	8:e:21:VAL:HB	1.98	0.45
28:i:101:BCR:H15C	28:i:101:BCR:H351	1.84	0.45
12:k:58:VAL:O	12:k:58:VAL:CG1	2.65	0.45
20:s:128:PHE:HE2	20:s:236:MET:CE	2.27	0.45
20:s:190:ILE:HG13	20:s:191:THR:HG23	1.99	0.45
20:s:224:LYS:HG2	25:s:311:CLA:CED	2.47	0.45
20:s:238:GLY:O	20:s:242:GLN:HG3	2.17	0.45
20:s:260:ASP:OD2	20:s:263:GLY:HA3	2.17	0.45
21:g:128:GLU:CB	21:g:133:LYS:O	2.65	0.45
21:n:128:GLU:CB	21:n:133:LYS:O	2.65	0.45
25:n:603:CLA:H142	25:y:304:CLA:H143	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:608:CHL:H13	40:n:617:NEX:C40	2.46	0.45
25:n:612:CLA:H62	25:n:612:CLA:H2	1.71	0.45
21:y:50:TRP:HB3	21:y:213:VAL:HG21	1.99	0.45
21:y:114:VAL:HG13	21:y:241:ILE:HD11	1.98	0.45
21:y:115:PHE:CD2	25:y:305:CLA:HHD	2.52	0.45
25:y:311:CLA:C2B	25:y:311:CLA:H2	2.46	0.45
41:r:616:XAT:H35	41:r:616:XAT:H401	1.60	0.45
2:2:86:SER:HB2	2:2:92:PHE:CD1	2.52	0.45
24:2:601:CHL:H62	24:2:601:CHL:H102	1.58	0.45
3:4:231:HIS:HA	3:4:234:LEU:HG	1.99	0.45
4:A:94:TYR:OH	4:A:105:TRP:HA	2.17	0.45
5:B:141:ILE:CG1	5:B:217:LEU:HD21	2.46	0.45
6:C:281:VAL:CG1	6:C:285:ILE:HD11	2.47	0.45
25:C:503:CLA:H193	25:C:503:CLA:H161	1.60	0.45
30:C:520:LMG:H141	20:S:262:PHE:CD1	2.52	0.45
20:S:144:GLU:OE2	20:S:149:LYS:HE2	2.17	0.45
21:G:208:PHE:CZ	21:G:212:LYS:HE3	2.51	0.45
21:N:78:TYR:CE1	24:N:601:CHL:HMD1	2.52	0.45
21:Y:128:GLU:CB	21:Y:133:LYS:O	2.65	0.45
21:Y:163:ALA:O	21:Y:167:ILE:HG13	2.17	0.45
25:R:611:CLA:HAA2	25:R:611:CLA:H12	1.98	0.45
3:8:103:LEU:HD13	3:8:193:GLY:CA	2.36	0.45
3:8:118:VAL:HG23	3:8:122:TRP:CZ2	2.52	0.45
3:8:181:THR:HG21	3:8:198:ARG:NH2	2.32	0.45
3:8:236:MET:HA	3:8:239:MET:HE3	1.98	0.45
25:a:403:CLA:O1A	25:a:403:CLA:H43	2.16	0.45
5:b:41:GLU:HB3	5:b:63:ILE:HD11	1.99	0.45
5:b:69:LEU:HD13	25:b:606:CLA:HHB	1.99	0.45
5:b:388:SER:CB	5:b:391:SER:HB2	2.45	0.45
25:b:611:CLA:HAB	25:b:613:CLA:H3A	1.98	0.45
25:b:616:CLA:HMD3	10:h:17:THR:HG21	1.98	0.45
6:c:311:GLN:HE21	6:c:358:PHE:HB2	1.81	0.45
25:c:504:CLA:H111	25:c:504:CLA:H91	1.70	0.45
15:o:143:PHE:CE2	17:w:81:VAL:HG11	2.52	0.45
20:s:144:GLU:OE2	20:s:149:LYS:HE2	2.17	0.45
21:g:120:ALA:HA	21:g:124:VAL:O	2.16	0.45
1:1:128:GLU:CB	1:1:133:LYS:O	2.65	0.44
1:3:50:TRP:HB3	1:3:213:VAL:HG21	1.99	0.44
3:4:219:GLU:O	3:4:223:ARG:N	2.49	0.44
4:A:157:VAL:CG1	4:A:172:MET:HB2	2.47	0.44
4:A:233:ALA:O	4:A:235:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2:GLY:H	13:L:12:GLU:CD	2.25	0.44
5:B:91:TRP:NE1	26:B:622:LHG:HC61	2.29	0.44
5:B:122:ILE:HA	10:H:24:LYS:HD3	1.99	0.44
25:B:609:CLA:H13	25:B:609:CLA:H171	1.79	0.44
26:B:625:LHG:H351	26:B:625:LHG:H101	1.99	0.44
6:C:89:LEU:HD22	6:C:111:TYR:CD2	2.52	0.44
6:C:267:SER:CA	17:W:133:LEU:HD23	2.47	0.44
30:C:520:LMG:H362	25:S:314:CLA:OBD	2.17	0.44
25:D:403:CLA:H61	25:D:403:CLA:H102	1.80	0.44
19:Z:40:VAL:O	19:Z:41:PHE:C	2.61	0.44
20:S:142:GLY:N	20:S:160:LEU:O	2.50	0.44
21:G:58:TYR:HE1	21:G:79:GLY:C	2.24	0.44
21:G:84:GLY:N	21:Y:94:ARG:CG	2.80	0.44
21:G:163:ALA:O	21:G:167:ILE:HG13	2.17	0.44
25:G:611:CLA:H3A	25:G:611:CLA:HBA2	1.28	0.44
21:N:163:ALA:O	21:N:167:ILE:HG13	2.17	0.44
25:N:603:CLA:H142	25:Y:304:CLA:H143	1.99	0.44
21:Y:120:ALA:HA	21:Y:124:VAL:O	2.16	0.44
25:Y:311:CLA:C2B	25:Y:311:CLA:H2	2.46	0.44
25:Y:314:CLA:H92	25:Y:314:CLA:H61	1.56	0.44
2:6:66:THR:CG2	2:6:67:PRO:HD2	2.48	0.44
4:a:37:MET:HB2	4:a:125:CYS:CB	2.47	0.44
4:a:155:THR:HG21	35:c:515:DGD:HBW1	1.99	0.44
25:a:403:CLA:C2B	27:a:404:PHO:H192	2.46	0.44
5:b:220:ARG:HG3	10:h:32:LYS:HE3	1.99	0.44
25:b:609:CLA:H3A	25:b:609:CLA:HBA1	1.47	0.44
28:b:618:BCR:H20C	28:b:618:BCR:H361	1.85	0.44
6:c:28:GLN:O	6:c:32:GLY:N	2.42	0.44
30:c:520:LMG:H141	20:s:262:PHE:CD1	2.52	0.44
30:c:520:LMG:H362	25:s:314:CLA:OBD	2.17	0.44
7:d:58:SER:OG	7:d:80:SER:OG	2.25	0.44
7:d:81:THR:HG22	7:d:112:TRP:NE1	2.32	0.44
7:d:309:ASP:OD1	7:d:311:GLU:HG3	2.17	0.44
25:d:403:CLA:H3A	25:d:403:CLA:HBA2	1.55	0.44
12:k:58:VAL:HG12	12:k:61:ARG:CD	2.47	0.44
29:l:102:SQD:H92	29:l:102:SQD:O10	2.16	0.44
14:m:1:MET:HB3	14:m:3:VAL:HG13	1.99	0.44
15:o:227:PHE:CZ	15:o:287:LEU:HD22	2.52	0.44
28:t:101:BCR:H20C	28:t:101:BCR:H361	1.83	0.44
20:s:190:ILE:HG13	20:s:191:THR:H	1.81	0.44
25:g:610:CLA:H13	25:g:610:CLA:H172	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:g:617:NEX:C28	40:g:617:NEX:C36	2.95	0.44
21:n:154:HIS:O	21:n:154:HIS:ND1	2.44	0.44
21:n:164:THR:HG21	24:n:606:CHL:O1D	2.16	0.44
21:n:215:GLU:HB2	25:n:610:CLA:CHB	2.48	0.44
24:n:607:CHL:H112	24:n:607:CHL:H91	1.71	0.44
21:y:58:TYR:HE1	21:y:79:GLY:C	2.24	0.44
22:r:177:SER:HB2	24:r:605:CHL:CMD	2.47	0.44
25:r:612:CLA:H71	25:r:612:CLA:HHC	1.98	0.44
2:2:129:GLU:N	2:2:130:PRO:CD	2.80	0.44
2:2:193:GLY:CA	2:2:197:PHE:HD2	2.25	0.44
1:3:163:ALA:O	1:3:167:ILE:HG13	2.17	0.44
3:4:203:LEU:HB3	3:4:205:LEU:HD13	1.99	0.44
4:A:210:LEU:HD12	27:A:404:PHO:NB	2.31	0.44
25:B:610:CLA:CBD	25:B:610:CLA:HAA2	2.47	0.44
6:C:225:VAL:HG13	6:C:289:PHE:HA	1.99	0.44
6:C:364:PRO:O	6:C:368:PRO:HD3	2.17	0.44
25:C:511:CLA:H91	25:C:511:CLA:H111	1.79	0.44
25:C:512:CLA:CMA	25:C:513:CLA:H203	2.47	0.44
7:D:135:ARG:HH21	7:D:138:GLN:CD	2.25	0.44
10:H:52:VAL:HG22	18:X:88:LEU:CD1	2.45	0.44
11:I:24:LEU:HD12	28:I:101:BCR:C3	2.47	0.44
12:K:58:VAL:O	12:K:58:VAL:CG1	2.65	0.44
15:O:189:LYS:HD2	15:O:189:LYS:O	2.18	0.44
20:S:260:ASP:OD2	20:S:263:GLY:HA3	2.16	0.44
25:N:602:CLA:H142	25:N:602:CLA:H112	1.63	0.44
21:Y:50:TRP:HB3	21:Y:213:VAL:HG21	1.98	0.44
21:Y:107:MET:HG2	21:Y:222:ALA:HB3	1.93	0.44
21:Y:204:ASP:O	21:Y:208:PHE:N	2.40	0.44
39:Y:317:LUT:H11	39:Y:317:LUT:H191	1.85	0.44
25:R:602:CLA:HBC1	26:R:618:LHG:H282	2.00	0.44
25:R:612:CLA:H112	25:R:612:CLA:H91	1.58	0.44
2:6:126:ASP:OD1	2:6:129:GLU:HA	2.17	0.44
2:6:192:PRO:HB3	24:6:603:CHL:HBC2	1.99	0.44
2:6:221:ARG:HG3	2:6:222:LEU:N	2.32	0.44
1:7:58:TYR:HE1	1:7:79:GLY:O	1.99	0.44
3:8:75:GLY:H	3:8:80:ASP:CG	2.22	0.44
3:8:231:HIS:HA	3:8:234:LEU:HG	1.99	0.44
4:a:135:PHE:CE2	6:c:449:ARG:HD3	2.52	0.44
4:a:174:LEU:HD22	27:a:404:PHO:H143	1.98	0.44
5:b:157:HIS:CE1	25:b:606:CLA:C4A	2.96	0.44
5:b:296:GLN:HE21	5:b:300:GLU:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:608:CLA:HBC3	25:b:608:CLA:HHD	1.98	0.44
6:c:281:VAL:CG1	6:c:285:ILE:HD11	2.47	0.44
6:c:294:ASN:OD1	35:c:515:DGD:HE4	2.17	0.44
6:c:376:ASP:OD1	6:c:379:ARG:HB2	2.17	0.44
28:d:404:BCR:H20C	28:d:404:BCR:H361	1.84	0.44
26:d:406:LHG:H302	16:t:21:ILE:HD11	1.99	0.44
10:h:25:PRO:HG3	22:r:122:THR:CB	2.47	0.44
10:h:52:VAL:HG22	18:x:88:LEU:CD1	2.45	0.44
29:l:101:SQD:H102	29:l:101:SQD:H131	1.47	0.44
15:o:146:LYS:HD3	15:o:158:PHE:CE1	2.52	0.44
18:x:92:SER:O	18:x:96:VAL:HG13	2.17	0.44
20:s:119:ARG:HH11	25:s:310:CLA:C1D	2.30	0.44
20:s:254:LEU:HD22	39:s:315:LUT:H163	1.99	0.44
24:n:609:CHL:H121	32:n:619:AJP:C01	2.48	0.44
22:r:141:LEU:HD23	22:r:216:LEU:HB3	1.98	0.44
40:r:617:NEX:H11	40:r:617:NEX:H203	1.65	0.44
1:l:208:PHE:CZ	1:l:212:LYS:HE3	2.51	0.44
2:2:123:VAL:HG12	2:2:124:ARG:HH21	1.83	0.44
3:4:181:THR:HG21	3:4:198:ARG:NH2	2.32	0.44
4:A:40:THR:CG2	25:A:405:CLA:HBB1	2.48	0.44
4:A:120:LEU:O	4:A:123:VAL:HG22	2.18	0.44
4:A:155:THR:HG21	35:C:515:DGD:HBW1	1.99	0.44
27:A:404:PHO:HAB	25:D:402:CLA:H11	1.98	0.44
5:B:69:LEU:HD13	25:B:606:CLA:HBB	1.99	0.44
5:B:330:MET:HE3	5:B:446:SER:N	2.32	0.44
28:B:618:BCR:C8	28:B:618:BCR:H331	2.46	0.44
7:D:201:GLY:O	7:D:205:VAL:HG23	2.18	0.44
20:S:114:GLU:HB2	25:S:303:CLA:CHB	2.47	0.44
20:S:254:LEU:HD22	39:S:315:LUT:H163	1.99	0.44
21:G:128:GLU:CB	21:G:133:LYS:O	2.65	0.44
21:G:181:GLY:HA3	24:G:608:CHL:HMC	2.00	0.44
24:G:609:CHL:HBA1	24:N:601:CHL:HBA2	2.00	0.44
25:N:603:CLA:HBC2	24:N:609:CHL:HMD2	2.00	0.44
21:Y:80:TRP:HE3	25:Y:303:CLA:CMD	2.30	0.44
21:Y:115:PHE:CD2	25:Y:305:CLA:HHD	2.52	0.44
2:6:123:VAL:HG12	2:6:124:ARG:HH21	1.83	0.44
3:8:159:LYS:HZ2	25:r:601:CLA:CMB	2.29	0.44
4:a:157:VAL:HG11	4:a:172:MET:HE3	1.98	0.44
5:b:330:MET:HE3	5:b:446:SER:N	2.32	0.44
25:b:604:CLA:H112	25:b:604:CLA:H152	1.57	0.44
25:b:610:CLA:CBD	25:b:610:CLA:HAA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:275:SER:OG	25:c:509:CLA:OBD	2.30	0.44
25:c:501:CLA:H193	25:c:506:CLA:C1B	2.48	0.44
25:c:510:CLA:H112	25:c:510:CLA:H151	1.60	0.44
7:d:161:TYR:HA	7:d:291:ALA:HB2	1.99	0.44
12:k:39:VAL:O	12:k:42:VAL:HG22	2.17	0.44
28:t:101:BCR:H272	28:t:101:BCR:C17	2.48	0.44
25:s:312:CLA:HBB1	39:s:315:LUT:C14	2.47	0.44
21:g:181:GLY:HA3	24:g:608:CHL:CMC	2.47	0.44
25:g:604:CLA:HBB1	39:g:616:LUT:C18	2.47	0.44
25:g:610:CLA:H92	25:g:610:CLA:H61	1.69	0.44
21:n:59:LEU:HD23	24:n:601:CHL:C1B	2.46	0.44
21:n:206:GLU:N	21:n:206:GLU:CD	2.76	0.44
25:n:602:CLA:H93	25:n:602:CLA:H61	1.49	0.44
24:n:607:CHL:HHC	24:n:607:CHL:HBB1	1.98	0.44
25:n:611:CLA:HMD2	25:n:612:CLA:HHD	1.98	0.44
21:y:108:LEU:HD11	25:y:311:CLA:HBC1	1.97	0.44
21:y:163:ALA:O	21:y:167:ILE:HG13	2.17	0.44
2:2:221:ARG:HG3	2:2:222:LEU:N	2.32	0.44
1:3:120:ALA:HA	1:3:124:VAL:O	2.16	0.44
1:3:128:GLU:CB	1:3:133:LYS:O	2.65	0.44
3:4:231:HIS:HA	3:4:234:LEU:HD21	2.00	0.44
4:A:258:LEU:HA	7:D:133:LEU:CD1	2.47	0.44
5:B:281:GLN:CD	23:U:91:VAL:HG13	2.42	0.44
25:B:611:CLA:HMA1	25:B:612:CLA:CMC	2.48	0.44
8:E:18:ARG:HB3	8:E:21:VAL:HB	1.98	0.44
15:O:227:PHE:CZ	15:O:287:LEU:HD22	2.52	0.44
28:T:101:BCR:H272	28:T:101:BCR:C17	2.47	0.44
20:S:238:GLY:O	20:S:242:GLN:HG3	2.17	0.44
21:G:176:ARG:HG3	24:G:608:CHL:CHD	2.48	0.44
21:G:181:GLY:HA3	24:G:608:CHL:CMC	2.47	0.44
21:G:209:ALA:HA	21:G:212:LYS:CG	2.34	0.44
25:N:603:CLA:H71	25:N:603:CLA:H112	1.74	0.44
21:Y:58:TYR:HE1	21:Y:79:GLY:C	2.24	0.44
25:Y:304:CLA:H2	25:Y:304:CLA:H61	1.86	0.44
24:Y:306:CHL:HBC3	24:Y:306:CHL:HMC	1.98	0.44
25:Y:311:CLA:C5	25:Y:313:CLA:HMA1	2.28	0.44
22:R:67:TRP:CD2	22:R:85:LYS:HA	2.52	0.44
22:R:274:HIS:CD2	24:R:613:CHL:NC	2.84	0.44
25:R:610:CLA:H3A	25:R:610:CLA:HBA2	1.38	0.44
1:7:58:TYR:HE1	1:7:79:GLY:C	2.24	0.44
1:7:128:GLU:CB	1:7:133:LYS:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:225:SER:O	1:7:229:PHE:HD1	2.01	0.44
4:a:258:LEU:HA	7:d:133:LEU:CD1	2.47	0.44
5:b:217:LEU:HB3	25:r:614:CLA:HBA1	2.00	0.44
5:b:257:TRP:CD2	7:d:292:LEU:HD22	2.52	0.44
5:b:357:ARG:NH2	23:u:96:PRO:HG2	2.33	0.44
25:b:603:CLA:H193	25:b:603:CLA:H162	1.54	0.44
25:b:608:CLA:H122	7:d:121:PHE:CZ	2.53	0.44
6:c:297:TYR:HB3	6:c:302:TYR:CD2	2.53	0.44
7:d:343:PRO:O	7:d:346:VAL:HG22	2.17	0.44
15:o:189:LYS:HD2	15:o:189:LYS:O	2.18	0.44
20:s:130:ILE:HB	20:s:131:PRO:HD3	2.00	0.44
21:g:115:PHE:HB2	25:g:604:CLA:HBC3	2.00	0.44
21:g:176:ARG:HG3	24:g:608:CHL:CHD	2.48	0.44
21:g:206:GLU:N	21:g:206:GLU:CD	2.76	0.44
21:n:231:VAL:CG1	25:n:613:CLA:HAC1	2.46	0.44
25:n:602:CLA:H172	25:n:602:CLA:H13	1.80	0.44
25:n:603:CLA:HBC1	24:n:609:CHL:CBC	2.47	0.44
21:y:115:PHE:HZ	32:y:320:AJP:C83	2.30	0.44
25:y:312:CLA:HBA2	25:y:312:CLA:H12	1.90	0.44
2:2:197:PHE:C	2:2:199:PRO:HD2	2.43	0.44
3:4:118:VAL:HG23	3:4:122:TRP:CZ2	2.52	0.44
3:4:144:SER:HB3	22:R:279:LEU:O	2.17	0.44
4:A:140:ARG:NH2	7:D:220:GLU:O	2.40	0.44
5:B:110:ALA:HB1	25:B:616:CLA:CHB	2.47	0.44
6:C:240:LEU:HD22	25:C:501:CLA:CAB	2.47	0.44
29:L:101:SQD:H121	29:L:101:SQD:C28	2.47	0.44
14:M:27:VAL:HA	14:M:30:VAL:HG22	2.00	0.44
15:O:143:PHE:CE2	17:W:81:VAL:HG11	2.52	0.44
20:S:237:LEU:O	20:S:241:ILE:CD1	2.65	0.44
21:G:115:PHE:HD2	25:G:604:CLA:HHD	1.83	0.44
25:G:602:CLA:C2	25:G:602:CLA:HMB1	2.47	0.44
25:G:610:CLA:H142	25:G:610:CLA:H111	1.61	0.44
21:N:97:GLU:HA	21:N:190:LEU:CD1	2.24	0.44
21:N:208:PHE:O	21:N:212:LYS:HG3	2.18	0.44
21:N:209:ALA:CA	21:N:212:LYS:HG3	2.34	0.44
21:Y:225:SER:O	21:Y:229:PHE:HD1	2.01	0.44
25:Y:304:CLA:H122	25:Y:304:CLA:H91	1.99	0.44
22:R:150:ALA:CA	41:R:616:XAT:H181	2.48	0.44
25:R:602:CLA:H43	25:R:603:CLA:HBA1	1.99	0.44
40:R:617:NEX:H401	40:R:617:NEX:H35	1.52	0.44
2:6:100:VAL:CG1	2:6:190:LEU:HD23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:159:LEU:HD13	1:7:159:LEU:N	2.33	0.44
3:8:222:GLU:HA	3:8:225:LYS:HD3	1.99	0.44
5:b:242:ILE:HG22	5:b:466:HIS:HB2	2.00	0.44
25:b:609:CLA:H171	25:b:609:CLA:H13	1.79	0.44
6:c:311:GLN:HG3	6:c:361:LEU:CD2	2.47	0.44
7:d:229:GLY:O	7:d:230:ALA:HB3	2.18	0.44
20:s:114:GLU:HB2	25:s:303:CLA:CHB	2.47	0.44
24:g:601:CHL:HBC1	26:y:301:LHG:O3	2.18	0.44
21:y:177:VAL:HG21	24:y:310:CHL:CMA	2.48	0.44
21:y:208:PHE:O	21:y:212:LYS:HG3	2.18	0.44
22:r:67:TRP:CH2	22:r:85:LYS:HB2	2.51	0.44
22:r:177:SER:O	22:r:184:LEU:N	2.35	0.44
2:2:161:ALA:HB1	2:2:165:PHE:HE2	1.81	0.44
2:2:174:GLU:CD	1:3:59:LEU:HD22	2.42	0.44
2:2:217:ILE:HD13	25:2:604:CLA:CGD	2.48	0.44
3:4:155:TRP:CZ2	25:R:601:CLA:HBB1	2.53	0.44
4:A:49:ILE:HG23	31:D:405:PL9:H501	2.00	0.44
4:A:51:ALA:CB	4:A:82:ILE:HD12	2.47	0.44
5:B:28:ALA:HB2	5:B:107:CYS:CB	2.47	0.44
5:B:148:VAL:HG11	26:B:622:LHG:H212	1.98	0.44
5:B:346:PHE:O	5:B:353:GLU:HA	2.18	0.44
5:B:361:THR:HG22	42:B:701:HOH:O	2.17	0.44
6:C:297:TYR:HB3	6:C:302:TYR:CD2	2.53	0.44
7:D:30:PHE:O	7:D:129:ARG:NH2	2.51	0.44
21:N:158:ILE:CD1	21:Y:257:TRP:CE3	2.98	0.44
25:N:610:CLA:H141	25:N:610:CLA:H162	1.63	0.44
21:Y:161:ILE:HG21	24:Y:308:CHL:HBC1	1.98	0.44
21:Y:206:GLU:N	21:Y:206:GLU:CD	2.76	0.44
22:R:177:SER:HB2	24:R:605:CHL:HMD3	1.99	0.44
1:5:225:SER:O	1:5:229:PHE:HD1	2.01	0.44
24:5:301:CHL:CHD	24:5:301:CHL:HBC2	2.48	0.44
2:6:86:SER:HB2	2:6:92:PHE:CD1	2.52	0.44
2:6:126:ASP:C	2:6:148:LEU:HD21	2.42	0.44
2:6:129:GLU:N	2:6:130:PRO:CD	2.80	0.44
2:6:193:GLY:CA	2:6:197:PHE:HD2	2.25	0.44
4:a:23:SER:OG	4:a:25:GLU:OE1	2.35	0.44
4:a:49:ILE:HG23	31:d:405:PL9:H501	2.00	0.44
4:a:64:ARG:NH1	15:o:165:THR:HG21	2.33	0.44
4:a:94:TYR:OH	4:a:105:TRP:HA	2.17	0.44
35:a:401:DGD:HA71	35:a:401:DGD:HAT1	1.64	0.44
25:a:403:CLA:H91	31:d:405:PL9:H402	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:410:PL9:O1	31:a:410:PL9:HC8	2.17	0.44
5:b:2:GLY:H	13:l:12:GLU:CD	2.25	0.44
5:b:221:PRO:HA	25:b:609:CLA:HED3	1.98	0.44
25:b:607:CLA:HMB1	25:b:607:CLA:CBB	2.47	0.44
25:b:610:CLA:HMA2	25:b:610:CLA:HBA1	1.99	0.44
25:b:616:CLA:H92	25:b:616:CLA:H62	1.76	0.44
28:b:617:BCR:H382	28:b:617:BCR:H23C	2.00	0.44
6:c:89:LEU:HD22	6:c:111:TYR:CD2	2.52	0.44
25:c:512:CLA:CMA	25:c:513:CLA:H203	2.47	0.44
15:o:209:VAL:CG2	15:o:319:LYS:HD2	2.48	0.44
19:z:57:LEU:HD23	19:z:60:LEU:HD12	1.98	0.44
21:n:78:TYR:CE1	24:n:601:CHL:HMD1	2.52	0.44
25:n:610:CLA:H141	25:n:610:CLA:H162	1.63	0.44
25:n:613:CLA:HBA1	25:n:614:CLA:C3D	2.47	0.44
24:y:310:CHL:H92	24:y:310:CHL:H62	1.86	0.44
22:r:67:TRP:CD2	22:r:85:LYS:HA	2.52	0.44
25:2:604:CLA:HBC3	26:2:606:LHG:H372	1.98	0.44
1:3:208:PHE:O	1:3:212:LYS:HG3	2.18	0.44
3:4:219:GLU:O	3:4:223:ARG:HB2	2.18	0.44
4:A:64:ARG:NH1	15:O:165:THR:HG21	2.33	0.44
5:B:204:ALA:CB	25:B:602:CLA:HAB	2.48	0.44
5:B:462:PHE:HZ	25:B:613:CLA:HMB3	1.80	0.44
25:C:501:CLA:H193	25:C:506:CLA:C1B	2.48	0.44
7:D:68:TYR:O	30:D:407:LMG:HC61	2.18	0.44
8:E:67:THR:C	23:U:102:ARG:HH11	2.26	0.44
15:O:218:LEU:HD23	15:O:218:LEU:H	1.83	0.44
20:S:130:ILE:HB	20:S:131:PRO:HD3	2.00	0.44
20:S:132:GLU:O	20:S:136:LYS:HG2	2.18	0.44
25:S:303:CLA:H93	25:S:303:CLA:H111	1.53	0.44
25:G:610:CLA:C5	39:G:615:LUT:H30	2.41	0.44
21:N:75:PRO:HG3	21:N:212:LYS:HB3	1.98	0.44
21:Y:60:GLY:HA3	24:Y:302:CHL:CMC	2.28	0.44
26:6:606:LHG:H152	26:6:606:LHG:H301	1.99	0.44
4:a:157:VAL:CG1	4:a:172:MET:HB2	2.47	0.44
13:l:18:LEU:HD11	14:m:23:LEU:HD23	1.99	0.44
15:o:145:VAL:HG11	15:o:203:LEU:HD21	2.00	0.44
20:s:236:MET:CE	39:s:316:LUT:H12	2.33	0.44
20:s:237:LEU:O	20:s:241:ILE:CD1	2.65	0.44
21:g:80:TRP:CE3	39:g:616:LUT:H383	2.52	0.44
24:g:606:CHL:HBB1	39:g:616:LUT:C16	2.47	0.44
21:n:209:ALA:HA	21:n:212:LYS:CG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:n:612:CLA:HHC	25:n:612:CLA:CBB	2.44	0.44
25:y:304:CLA:H122	25:y:304:CLA:H91	1.99	0.44
25:y:311:CLA:C5	25:y:313:CLA:HMA1	2.28	0.44
1:1:225:SER:O	1:1:229:PHE:HD1	2.01	0.44
2:2:251:ASN:N	2:2:252:PRO:CD	2.81	0.44
1:3:159:LEU:HD13	1:3:159:LEU:N	2.33	0.44
3:4:73:LEU:HD12	3:4:80:ASP:OD1	2.18	0.44
3:4:171:SER:HB3	3:4:183:GLU:OE2	2.18	0.44
3:4:184:ASN:OD1	3:4:197:GLY:HA3	2.18	0.44
5:B:41:GLU:HB3	5:B:63:ILE:HD11	1.99	0.44
5:B:377:VAL:O	5:B:378:ARG:HB2	2.17	0.44
25:B:610:CLA:HMA2	25:B:610:CLA:HBA1	1.99	0.44
25:C:504:CLA:H91	25:C:504:CLA:H111	1.70	0.44
7:D:181:ARG:NH1	7:D:334:ASP:OD1	2.51	0.44
25:D:401:CLA:HMA2	30:D:407:LMG:H212	1.99	0.44
26:D:406:LHG:H302	16:T:21:ILE:HD11	1.99	0.44
12:K:39:VAL:O	12:K:42:VAL:HG22	2.17	0.44
21:G:50:TRP:HB3	21:G:213:VAL:HG21	1.98	0.44
21:G:226:MET:O	21:G:230:PHE:HD2	2.01	0.44
21:N:113:CYS:HB3	21:N:131:TRP:CD1	2.53	0.44
21:N:226:MET:O	21:N:230:PHE:HD2	2.01	0.44
24:N:601:CHL:HBA1	24:N:601:CHL:H3A	1.62	0.44
25:N:613:CLA:CBC	25:N:613:CLA:CMC	2.95	0.44
21:Y:215:GLU:CG	25:Y:311:CLA:C1B	2.95	0.44
21:Y:226:MET:O	21:Y:230:PHE:HD2	2.01	0.44
22:R:103:LYS:CD	22:R:105:LEU:HD11	2.47	0.44
1:5:113:CYS:HB3	1:5:131:TRP:CD1	2.53	0.44
1:5:226:MET:O	1:5:230:PHE:HD2	2.01	0.44
4:a:57:PRO:O	15:o:208:ARG:NH1	2.49	0.44
25:c:506:CLA:H193	25:c:506:CLA:H161	1.70	0.44
7:d:201:GLY:O	7:d:205:VAL:HG23	2.18	0.44
11:i:24:LEU:HD12	28:i:101:BCR:C3	2.47	0.44
21:y:196:PHE:HE2	24:y:309:CHL:HBC2	1.83	0.44
25:y:304:CLA:HMD1	24:y:310:CHL:C1D	2.47	0.44
25:y:313:CLA:HAA2	25:y:313:CLA:HBD	2.00	0.44
40:y:318:NEX:H27	40:y:318:NEX:H381	1.91	0.44
22:r:177:SER:HB2	24:r:605:CHL:HMD3	1.99	0.44
29:A:407:SQD:H45	29:A:407:SQD:H81	1.64	0.44
5:B:168:VAL:HG21	5:B:181:VAL:HG12	2.00	0.44
5:B:357:ARG:NH2	23:U:96:PRO:HG2	2.33	0.44
25:B:607:CLA:HMB1	25:B:607:CLA:CBB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:608:CLA:H122	7:D:121:PHE:CZ	2.53	0.44
28:B:619:BCR:H24C	28:B:619:BCR:H371	1.79	0.44
25:C:505:CLA:H3A	25:C:505:CLA:HBA2	1.74	0.44
25:C:510:CLA:HMA2	25:C:510:CLA:C1	2.48	0.44
7:D:229:GLY:O	7:D:230:ALA:HB3	2.18	0.44
28:D:404:BCR:H403	30:D:407:LMG:H141	1.99	0.44
12:K:58:VAL:HG12	12:K:61:ARG:CD	2.47	0.44
15:O:114:CYS:SG	15:O:139:GLU:N	2.91	0.44
20:S:95:TYR:CE1	24:S:302:CHL:HAA2	2.53	0.44
40:S:317:NEX:H35	40:S:317:NEX:H401	1.77	0.44
25:G:611:CLA:H142	25:G:611:CLA:H112	1.59	0.44
21:N:57:LYS:HD2	21:N:63:SER:HB2	2.00	0.44
21:N:69:TYR:OH	21:N:81:ASP:OD2	2.20	0.44
21:N:215:GLU:HB2	25:N:610:CLA:CHB	2.48	0.44
25:Y:303:CLA:HBB	25:Y:303:CLA:H12	1.99	0.44
22:R:135:ARG:NE	25:R:614:CLA:OBD	2.51	0.44
2:6:217:ILE:HD13	25:6:604:CLA:CGD	2.48	0.44
2:6:223:ALA:O	2:6:226:SER:OG	2.32	0.44
2:6:227:MET:HG3	2:6:231:PHE:CE2	2.53	0.44
1:7:208:PHE:O	1:7:212:LYS:HG3	2.18	0.44
1:7:226:MET:O	1:7:230:PHE:HD2	2.01	0.44
4:a:11:GLU:OE2	4:a:15:GLY:HA3	2.17	0.44
4:a:161:TYR:HA	4:a:294:ALA:HB2	1.99	0.44
5:b:359:MET:HA	5:b:360:PRO:HD3	1.86	0.44
25:c:505:CLA:H3A	25:c:505:CLA:HBA2	1.74	0.44
25:c:510:CLA:H141	25:c:510:CLA:H161	1.67	0.44
7:d:193:THR:HG23	25:d:402:CLA:HBC2	1.99	0.44
25:d:403:CLA:H52	18:x:91:ALA:HB1	1.98	0.44
10:h:54:LEU:O	10:h:57:ILE:HG12	2.18	0.44
20:s:266:LEU:HD22	25:s:313:CLA:H43	2.00	0.44
21:g:86:SER:OG	25:g:602:CLA:HAA2	2.18	0.44
21:g:163:ALA:O	21:g:167:ILE:HG13	2.17	0.44
21:n:244:LEU:HD11	25:n:614:CLA:HAC1	2.00	0.44
24:n:601:CHL:CMD	26:n:618:LHG:HC41	2.48	0.44
21:y:50:TRP:NE1	25:y:312:CLA:HED3	2.33	0.44
21:y:226:MET:O	21:y:230:PHE:HD2	2.01	0.44
21:y:244:LEU:CD1	25:y:315:CLA:HBC2	2.48	0.44
25:y:314:CLA:H122	25:y:315:CLA:HMD2	2.00	0.44
1:1:50:TRP:HB3	1:1:213:VAL:HG21	1.98	0.43
1:1:126:PHE:HE1	1:1:147:LEU:HA	1.83	0.43
2:2:100:VAL:CG1	2:2:190:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:217:ILE:CD1	25:2:604:CLA:CGD	2.97	0.43
3:4:222:GLU:HA	3:4:225:LYS:HD3	1.99	0.43
4:A:40:THR:O	4:A:43:THR:HG22	2.18	0.43
25:A:402:CLA:H91	31:D:405:PL9:H402	2.00	0.43
25:B:615:CLA:HMA2	25:B:615:CLA:CBA	2.48	0.43
28:C:514:BCR:H15C	28:C:514:BCR:H351	1.87	0.43
10:H:22:LEU:HD23	22:R:124:PHE:CZ	2.53	0.43
13:L:18:LEU:HD11	14:M:23:LEU:HD23	1.99	0.43
29:L:101:SQD:H261	14:M:21:PHE:HD1	1.83	0.43
15:O:184:GLY:O	15:O:224:PRO:HD3	2.18	0.43
15:O:224:PRO:O	15:O:289:VAL:HB	2.18	0.43
20:S:119:ARG:HH11	25:S:310:CLA:C1D	2.30	0.43
21:G:113:CYS:HB3	21:G:131:TRP:CD1	2.53	0.43
21:G:225:SER:O	21:G:229:PHE:HD1	2.01	0.43
21:N:232:GLN:HE21	25:N:613:CLA:CHA	2.17	0.43
21:Y:208:PHE:O	21:Y:212:LYS:HG3	2.18	0.43
21:Y:244:LEU:CD1	25:Y:315:CLA:HBC2	2.48	0.43
25:R:602:CLA:HBC1	26:R:618:LHG:C28	2.47	0.43
24:R:607:CHL:H3A	24:R:607:CHL:HBA2	1.60	0.43
2:6:87:ALA:HA	2:6:92:PHE:CZ	2.53	0.43
2:6:121:LYS:HD3	2:6:245:LEU:CD1	2.46	0.43
2:6:173:VAL:HA	2:6:176:PHE:CG	2.53	0.43
3:8:155:TRP:CZ2	25:r:601:CLA:HBB1	2.53	0.43
3:8:189:THR:O	3:8:189:THR:HG23	2.18	0.43
5:b:141:ILE:CG1	5:b:217:LEU:HD21	2.46	0.43
25:b:604:CLA:H141	25:b:604:CLA:H161	1.83	0.43
6:c:240:LEU:HD22	25:c:501:CLA:CAB	2.47	0.43
25:c:510:CLA:HMA2	25:c:510:CLA:C1	2.48	0.43
7:d:22:TRP:CZ2	18:x:105:VAL:HG11	2.53	0.43
25:d:401:CLA:HMA2	30:d:407:LMG:H212	1.99	0.43
10:h:43:MET:HE2	10:h:43:MET:HB3	1.91	0.43
11:i:31:ASN:HB2	11:i:32:PRO:HD2	2.00	0.43
29:l:102:SQD:H261	14:m:21:PHE:HD1	1.83	0.43
15:o:128:PRO:HA	15:o:180:VAL:HG13	1.99	0.43
15:o:224:PRO:O	15:o:289:VAL:HB	2.18	0.43
16:t:11:VAL:HG22	28:t:101:BCR:H342	2.00	0.43
20:s:132:GLU:O	20:s:136:LYS:HG2	2.18	0.43
21:g:56:VAL:HG11	26:y:301:LHG:HC2	1.99	0.43
25:n:603:CLA:HAB	39:n:616:LUT:C15	2.48	0.43
21:y:206:GLU:N	21:y:206:GLU:CD	2.76	0.43
22:r:103:LYS:CE	22:r:105:LEU:HD11	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:155:LEU:HD22	22:r:268:LEU:HD21	1.99	0.43
1:1:163:ALA:O	1:1:167:ILE:HG13	2.17	0.43
2:2:104:ARG:CZ	24:2:603:CHL:HED3	2.49	0.43
27:A:404:PHO:HAB	25:D:402:CLA:H12	2.01	0.43
31:A:409:PL9:O1	31:A:409:PL9:HC8	2.17	0.43
5:B:193:PHE:HE2	35:B:626:DGD:HE2	1.83	0.43
5:B:242:ILE:HG22	5:B:466:HIS:HB2	2.00	0.43
25:B:609:CLA:H2	25:B:609:CLA:H61	1.72	0.43
8:E:67:THR:HA	23:U:102:ARG:NH1	2.33	0.43
11:I:19:PHE:CE2	11:I:23:PHE:HE2	2.36	0.43
15:O:158:PHE:HE2	15:O:306:LEU:HD22	1.83	0.43
28:T:101:BCR:H271	5:b:39:LEU:HD12	1.99	0.43
21:G:126:PHE:HE1	21:G:147:LEU:HA	1.83	0.43
24:G:601:CHL:HBC1	26:Y:301:LHG:O3	2.18	0.43
21:N:97:GLU:CB	21:N:190:LEU:HD11	2.48	0.43
21:N:182:PRO:CB	40:N:617:NEX:H171	2.43	0.43
21:Y:196:PHE:HE2	24:Y:309:CHL:HBC2	1.83	0.43
21:Y:215:GLU:OE1	25:Y:311:CLA:C4A	2.66	0.43
22:R:127:TYR:CE2	22:R:135:ARG:HD2	2.54	0.43
22:R:274:HIS:HD1	25:R:612:CLA:HAA2	1.79	0.43
25:R:612:CLA:H61	25:R:612:CLA:H92	1.56	0.43
2:6:86:SER:O	2:6:88:ASP:N	2.51	0.43
2:6:197:PHE:C	2:6:199:PRO:HD2	2.43	0.43
2:6:216:GLU:O	2:6:219:ASN:HB2	2.18	0.43
1:7:57:LYS:HD2	1:7:63:SER:HB2	2.00	0.43
1:7:206:GLU:N	1:7:206:GLU:CD	2.76	0.43
1:7:209:ALA:CA	1:7:212:LYS:HG3	2.34	0.43
3:8:219:GLU:O	3:8:223:ARG:HB2	2.18	0.43
4:a:106:LEU:HD11	28:a:407:BCR:H402	2.00	0.43
4:a:276:ALA:O	4:a:280:VAL:HG23	2.18	0.43
5:b:361:THR:HG22	42:b:701:HOH:O	2.17	0.43
25:b:611:CLA:H112	25:b:611:CLA:H72	1.67	0.43
25:b:611:CLA:HMA1	25:b:612:CLA:CMC	2.48	0.43
6:c:236:GLY:HA2	6:c:239:TRP:CD1	2.52	0.43
7:d:140:ARG:NH1	7:d:142:TYR:CE2	2.86	0.43
26:d:406:LHG:H221	16:t:10:LEU:HD22	2.00	0.43
8:e:67:THR:HA	23:u:102:ARG:NH1	2.33	0.43
20:s:70:PHE:CG	20:s:95:TYR:HB2	2.53	0.43
25:g:611:CLA:HHC	25:g:611:CLA:CBB	2.36	0.43
25:g:613:CLA:H91	26:y:301:LHG:H322	1.99	0.43
21:n:101:ILE:O	21:n:105:TRP:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:y:225:SER:O	21:y:229:PHE:HD1	2.01	0.43
25:y:303:CLA:HBB	25:y:303:CLA:H12	2.00	0.43
2:2:57:LYS:CD	2:2:63:SER:OG	2.66	0.43
2:2:66:THR:CG2	2:2:67:PRO:HD2	2.48	0.43
25:2:604:CLA:H3A	3:4:178:TRP:CB	2.48	0.43
6:C:112:PHE:HE2	28:C:514:BCR:HC31	1.84	0.43
6:C:294:ASN:OD1	35:C:515:DGD:HE4	2.17	0.43
25:C:510:CLA:H91	25:C:510:CLA:H111	1.69	0.43
7:D:343:PRO:O	7:D:346:VAL:HG22	2.17	0.43
29:L:101:SQD:H462	14:M:28:LYS:HD2	1.98	0.43
15:O:209:VAL:CG2	15:O:319:LYS:HD2	2.48	0.43
20:S:224:LYS:HG2	25:S:311:CLA:CED	2.47	0.43
21:N:162:TRP:CE3	21:Y:257:TRP:HH2	2.37	0.43
21:N:244:LEU:HD11	25:N:614:CLA:HAC1	2.00	0.43
21:Y:56:VAL:HB	24:Y:302:CHL:HBC2	1.98	0.43
22:R:141:LEU:HD23	22:R:216:LEU:HB3	1.98	0.43
1:5:57:LYS:HD2	1:5:63:SER:HB2	2.00	0.43
2:6:217:ILE:CD1	25:6:604:CLA:CGD	2.97	0.43
3:8:73:LEU:HD12	3:8:80:ASP:OD1	2.18	0.43
3:8:79:GLY:N	3:8:229:ILE:HD13	2.33	0.43
3:8:104:ILE:H	3:8:104:ILE:HD12	1.84	0.43
3:8:140:PHE:HA	22:r:280:HIS:CD2	2.54	0.43
4:a:231:GLU:HG2	5:b:1:MET:CA	2.45	0.43
4:a:238:ARG:O	4:a:241:GLN:HB3	2.17	0.43
5:b:122:ILE:HA	10:h:24:LYS:HD3	1.99	0.43
25:b:603:CLA:C4B	25:b:605:CLA:H93	2.48	0.43
25:b:609:CLA:H61	25:b:609:CLA:H2	1.72	0.43
28:b:617:BCR:H15C	28:b:617:BCR:H351	1.81	0.43
7:d:157:VAL:HG12	7:d:172:PRO:CG	2.47	0.43
11:i:19:PHE:CE2	11:i:23:PHE:HE2	2.36	0.43
21:n:57:LYS:HD2	21:n:63:SER:HB2	2.00	0.43
21:n:221:LEU:CD1	26:n:618:LHG:H272	2.48	0.43
21:n:226:MET:O	21:n:230:PHE:HD2	2.01	0.43
24:n:607:CHL:H18	24:n:609:CHL:C7	2.39	0.43
25:n:613:CLA:CBC	25:n:613:CLA:CMC	2.95	0.43
24:y:302:CHL:HHC	24:y:302:CHL:HBB1	1.98	0.43
25:r:601:CLA:C1B	26:r:618:LHG:H112	2.49	0.43
25:r:602:CLA:HBC1	26:r:618:LHG:H282	2.00	0.43
1:1:101:ILE:O	1:1:105:TRP:HD1	2.02	0.43
1:1:226:MET:O	1:1:230:PHE:HD2	2.01	0.43
3:4:221:LEU:CA	3:4:224:LEU:HD23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:135:PHE:CE2	6:C:449:ARG:HD3	2.52	0.43
5:B:217:LEU:HB3	25:R:614:CLA:HBA1	2.00	0.43
7:D:119:GLY:O	7:D:123:LEU:HG	2.18	0.43
21:N:209:ALA:HA	21:N:212:LYS:CG	2.34	0.43
21:Y:59:LEU:CD2	24:Y:302:CHL:C2B	2.94	0.43
21:Y:97:GLU:CB	21:Y:190:LEU:HD11	2.48	0.43
25:Y:304:CLA:H101	25:Y:304:CLA:H62	1.40	0.43
24:Y:308:CHL:HBC2	24:Y:308:CHL:CHD	2.37	0.43
25:R:603:CLA:CMC	41:R:616:XAT:H203	2.49	0.43
41:R:616:XAT:H35	41:R:616:XAT:H401	1.60	0.43
1:5:101:ILE:O	1:5:105:TRP:HD1	2.02	0.43
1:5:159:LEU:HD13	1:5:159:LEU:N	2.33	0.43
1:5:208:PHE:O	1:5:212:LYS:HG3	2.18	0.43
2:6:57:LYS:CD	2:6:63:SER:OG	2.66	0.43
2:6:174:GLU:OE2	1:7:59:LEU:HD22	2.19	0.43
2:6:202:LEU:O	2:6:208:THR:HG22	2.19	0.43
2:6:204:ASP:O	2:6:208:THR:N	2.45	0.43
3:8:130:ALA:O	3:8:134:PRO:HD3	2.18	0.43
3:8:231:HIS:HA	3:8:234:LEU:HD21	2.00	0.43
4:a:74:GLY:CA	14:m:1:MET:HE2	2.49	0.43
5:b:245:VAL:HG21	25:b:612:CLA:HED3	1.99	0.43
5:b:346:PHE:O	5:b:353:GLU:HA	2.18	0.43
5:b:387:GLU:O	7:d:345:GLU:CD	2.62	0.43
25:b:607:CLA:H62	25:b:607:CLA:H93	1.51	0.43
25:b:613:CLA:HMD2	28:b:618:BCR:H341	2.00	0.43
25:b:615:CLA:HMA2	25:b:615:CLA:CBA	2.48	0.43
6:c:204:LEU:C	6:c:239:TRP:HZ2	2.26	0.43
7:d:90:LEU:O	7:d:92:LEU:N	2.49	0.43
7:d:119:GLY:O	7:d:123:LEU:HG	2.18	0.43
7:d:181:ARG:NH1	7:d:334:ASP:OD1	2.51	0.43
15:o:114:CYS:SG	15:o:139:GLU:N	2.91	0.43
21:g:159:LEU:HD13	21:g:159:LEU:N	2.33	0.43
24:n:607:CHL:CBB	24:y:302:CHL:H91	2.48	0.43
21:y:244:LEU:CD2	39:y:316:LUT:H163	2.47	0.43
25:y:314:CLA:C4B	39:y:316:LUT:H183	2.49	0.43
25:r:603:CLA:CMC	41:r:616:XAT:H203	2.49	0.43
1:1:113:CYS:HB3	1:1:131:TRP:CD1	2.53	0.43
1:1:137:GLN:HE22	1:1:144:LEU:HA	1.84	0.43
2:2:88:ASP:O	2:2:92:PHE:N	2.50	0.43
2:2:173:VAL:HA	2:2:176:PHE:CG	2.54	0.43
1:3:97:GLU:CB	1:3:190:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:141:PRO:HG3	6:C:446:GLY:C	2.43	0.43
25:A:405:CLA:H11	11:I:9:TYR:CZ	2.54	0.43
6:C:274:TYR:HE1	25:C:505:CLA:O2D	2.01	0.43
25:C:510:CLA:H193	25:C:510:CLA:H162	1.88	0.43
7:D:65:ALA:CB	7:D:70:GLU:OE2	2.67	0.43
7:D:217:ALA:O	7:D:221:ASN:ND2	2.47	0.43
11:I:9:TYR:O	11:I:13:ILE:HG22	2.18	0.43
14:M:1:MET:HB3	14:M:3:VAL:HG13	1.99	0.43
15:O:174:ILE:HG12	15:O:195:ASP:OD1	2.19	0.43
19:Z:16:SER:HB3	28:Z:101:BCR:H312	2.00	0.43
25:S:313:CLA:H3A	25:S:313:CLA:HBA2	1.60	0.43
21:G:56:VAL:HG11	26:Y:301:LHG:HC2	1.99	0.43
21:G:57:LYS:HD2	21:G:63:SER:HB2	2.00	0.43
21:G:208:PHE:O	21:G:212:LYS:HG3	2.18	0.43
21:G:211:LEU:CB	25:G:610:CLA:HMA1	2.44	0.43
40:G:617:NEX:C28	40:G:617:NEX:C36	2.95	0.43
25:N:603:CLA:HAB	39:N:616:LUT:C15	2.48	0.43
24:N:605:CHL:HHD	24:N:606:CHL:OBD	2.18	0.43
21:Y:101:ILE:O	21:Y:105:TRP:HD1	2.01	0.43
21:Y:126:PHE:HE1	21:Y:147:LEU:HA	1.83	0.43
21:Y:177:VAL:HG21	24:Y:310:CHL:CMA	2.48	0.43
22:R:72:LEU:HB3	22:R:137:ARG:HH22	1.83	0.43
25:R:610:CLA:HBC3	26:R:618:LHG:C5	2.37	0.43
2:6:178:ILE:HG22	2:6:180:GLY:H	1.84	0.43
1:7:126:PHE:HE1	1:7:147:LEU:HA	1.84	0.43
3:8:216:PRO:O	3:8:220:LYS:N	2.52	0.43
4:a:141:PRO:HG3	6:c:446:GLY:C	2.43	0.43
27:a:405:PHO:H193	25:d:401:CLA:CHB	2.49	0.43
5:b:157:HIS:HE1	25:b:606:CLA:CHB	2.26	0.43
5:b:276:ASP:OD1	5:b:361:THR:HG21	2.19	0.43
5:b:382:PRO:CB	7:d:345:GLU:OE2	2.62	0.43
25:b:614:CLA:H91	26:l:103:LHG:H372	2.00	0.43
6:c:112:PHE:HE2	28:c:514:BCR:HC31	1.84	0.43
6:c:227:VAL:CG2	28:i:101:BCR:H292	2.47	0.43
9:f:18:HIS:HE1	38:f:101:HEM:C4A	2.37	0.43
10:h:22:LEU:HD23	22:r:124:PHE:CZ	2.53	0.43
15:o:158:PHE:HE2	15:o:306:LEU:HD22	1.83	0.43
15:o:218:LEU:HD23	15:o:218:LEU:H	1.83	0.43
21:g:208:PHE:O	21:g:212:LYS:HG3	2.18	0.43
21:g:213:VAL:CG1	25:g:611:CLA:HED1	2.48	0.43
25:g:613:CLA:H3A	25:g:613:CLA:HBA2	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:113:CYS:HB3	21:n:131:TRP:CD1	2.53	0.43
24:n:605:CHL:HHD	24:n:606:CHL:OBD	2.18	0.43
24:n:609:CHL:NC	24:y:302:CHL:H52	2.34	0.43
21:y:80:TRP:O	39:y:317:LUT:H24	2.19	0.43
21:y:101:ILE:O	21:y:105:TRP:HD1	2.01	0.43
21:y:159:LEU:HD13	21:y:159:LEU:N	2.33	0.43
21:y:215:GLU:OE1	25:y:311:CLA:C4A	2.66	0.43
24:y:308:CHL:HBC2	24:y:308:CHL:CHD	2.36	0.43
22:r:72:LEU:HB3	22:r:137:ARG:HH22	1.83	0.43
26:2:606:LHG:H301	26:2:606:LHG:H152	1.99	0.43
1:3:113:CYS:HB3	1:3:131:TRP:CD1	2.53	0.43
1:3:206:GLU:N	1:3:206:GLU:CD	2.76	0.43
3:4:79:GLY:N	3:4:229:ILE:HD13	2.33	0.43
4:A:74:GLY:CA	14:M:1:MET:HE2	2.49	0.43
4:A:192:ILE:HD13	25:A:401:CLA:C2D	2.49	0.43
4:A:276:ALA:O	4:A:280:VAL:HG23	2.18	0.43
25:B:613:CLA:HMD2	28:B:618:BCR:H341	2.00	0.43
25:B:614:CLA:HMD2	29:L:101:SQD:H242	2.01	0.43
25:B:616:CLA:H11	25:B:616:CLA:H51	1.75	0.43
28:B:617:BCR:H382	28:B:617:BCR:H23C	2.00	0.43
25:C:502:CLA:H203	25:C:502:CLA:H161	1.84	0.43
7:D:22:TRP:CZ2	18:X:105:VAL:HG11	2.53	0.43
7:D:140:ARG:NH1	7:D:142:TYR:CE2	2.86	0.43
25:D:402:CLA:HBC3	25:D:402:CLA:HHD	2.01	0.43
8:E:56:PHE:HA	8:E:60:ARG:NH1	2.34	0.43
10:H:43:MET:HE2	10:H:43:MET:HB3	1.91	0.43
28:I:101:BCR:C8	28:I:101:BCR:H331	2.48	0.43
15:O:92:LEU:HB3	15:O:96:GLU:CG	2.43	0.43
20:S:189:ARG:NH2	25:S:309:CLA:HMA3	2.33	0.43
20:S:236:MET:CE	39:S:316:LUT:H12	2.33	0.43
20:S:266:LEU:HD22	25:S:313:CLA:H43	2.00	0.43
21:G:115:PHE:HB2	25:G:604:CLA:HBC3	2.00	0.43
21:G:213:VAL:CG1	25:G:611:CLA:HED1	2.48	0.43
21:N:86:SER:OG	25:N:602:CLA:O1A	2.33	0.43
1:5:97:GLU:CB	1:5:190:LEU:HD11	2.48	0.43
2:6:118:VAL:O	2:6:122:TRP:HB2	2.19	0.43
2:6:217:ILE:HG13	2:6:218:LYS:N	2.32	0.43
2:6:251:ASN:N	2:6:252:PRO:CD	2.81	0.43
1:7:113:CYS:HB3	1:7:131:TRP:CD1	2.53	0.43
4:a:192:ILE:HD13	25:a:402:CLA:C2D	2.49	0.43
5:b:168:VAL:HG21	5:b:181:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:356:VAL:O	5:b:356:VAL:HG13	2.19	0.43
25:b:608:CLA:H61	25:b:608:CLA:H92	1.86	0.43
25:c:502:CLA:HBA1	25:c:502:CLA:H3A	1.78	0.43
8:e:67:THR:C	23:u:102:ARG:HH11	2.26	0.43
20:s:95:TYR:CE1	24:s:302:CHL:HAA2	2.53	0.43
21:g:57:LYS:HD2	21:g:63:SER:HB2	2.00	0.43
21:g:126:PHE:HE1	21:g:147:LEU:HA	1.83	0.43
21:g:231:VAL:HG21	25:g:613:CLA:HAC1	2.00	0.43
21:n:132:PHE:HB2	24:n:607:CHL:HMA3	2.01	0.43
21:n:165:GLN:NE2	24:n:606:CHL:NB	2.63	0.43
21:y:209:ALA:CA	21:y:212:LYS:HG3	2.34	0.43
21:y:215:GLU:HB2	25:y:311:CLA:C1B	2.49	0.43
25:y:311:CLA:H122	39:y:316:LUT:H403	2.01	0.43
22:r:135:ARG:NE	25:r:614:CLA:OBD	2.51	0.43
2:2:87:ALA:HA	2:2:92:PHE:CZ	2.53	0.43
2:2:202:LEU:O	2:2:208:THR:HG22	2.19	0.43
2:2:227:MET:HG3	2:2:231:PHE:CE2	2.53	0.43
1:3:101:ILE:O	1:3:105:TRP:HD1	2.02	0.43
1:3:126:PHE:HE1	1:3:147:LEU:HA	1.84	0.43
3:4:78:PRO:HB2	3:4:229:ILE:HG23	2.01	0.43
4:A:136:ARG:NH2	11:I:27:ASP:OD2	2.48	0.43
5:B:476:ARG:HG2	5:B:476:ARG:HH11	1.83	0.43
6:C:75:PHE:O	12:K:25:LYS:HD3	2.18	0.43
6:C:185:VAL:HG23	6:C:230:LEU:CD1	2.47	0.43
25:C:512:CLA:C19	26:S:301:LHG:H222	2.48	0.43
8:E:25:ILE:O	8:E:29:SER:OG	2.28	0.43
28:I:101:BCR:H15C	28:I:101:BCR:H351	1.84	0.43
15:O:163:LEU:C	15:O:164:MET:HE2	2.44	0.43
20:S:190:ILE:HG13	20:S:191:THR:HG23	1.99	0.43
21:G:101:ILE:O	21:G:105:TRP:HD1	2.02	0.43
21:G:206:GLU:N	21:G:206:GLU:CD	2.76	0.43
24:N:609:CHL:H121	32:N:619:AJP:C01	2.48	0.43
25:N:613:CLA:HBA1	25:N:614:CLA:CAD	2.49	0.43
21:Y:113:CYS:HB3	21:Y:131:TRP:CD1	2.53	0.43
25:Y:312:CLA:H92	25:Y:312:CLA:C5	2.49	0.43
25:Y:313:CLA:HAA2	25:Y:313:CLA:HBD	2.00	0.43
25:Y:314:CLA:H122	25:Y:315:CLA:HMD2	2.00	0.43
25:Y:315:CLA:HED2	25:Y:315:CLA:CAA	2.48	0.43
22:R:85:LYS:CG	22:R:86:PRO:CD	2.96	0.43
25:6:604:CLA:H3A	3:8:178:TRP:CB	2.48	0.43
3:8:203:LEU:HB3	3:8:205:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:606:CLA:H203	28:b:619:BCR:H363	2.00	0.43
25:b:606:CLA:H172	25:b:616:CLA:H93	2.00	0.43
25:c:512:CLA:C19	26:s:301:LHG:H222	2.48	0.43
7:d:162:PRO:HG3	7:d:171:ALA:HB2	2.00	0.43
11:i:9:TYR:O	11:i:13:ILE:HG22	2.18	0.43
19:z:40:VAL:O	19:z:41:PHE:C	2.61	0.43
20:s:91:GLY:O	20:s:230:ARG:NH1	2.37	0.43
25:s:303:CLA:HAB	39:s:316:LUT:C30	2.44	0.43
25:s:303:CLA:H52	25:s:303:CLA:H8	1.74	0.43
21:g:97:GLU:HA	21:g:190:LEU:CD1	2.24	0.43
21:g:97:GLU:CB	21:g:190:LEU:HD11	2.48	0.43
21:g:215:GLU:HB2	25:g:610:CLA:CMB	2.49	0.43
21:g:225:SER:O	21:g:229:PHE:HD1	2.01	0.43
25:g:610:CLA:H72	25:g:610:CLA:H112	1.89	0.43
21:n:208:PHE:O	21:n:212:LYS:HG3	2.18	0.43
25:n:613:CLA:C14	25:n:613:CLA:H2	2.45	0.43
21:y:80:TRP:HE3	25:y:303:CLA:CMD	2.30	0.43
25:y:304:CLA:CMD	24:y:310:CHL:C4D	2.96	0.43
22:r:150:ALA:CA	41:r:616:XAT:H181	2.48	0.43
1:1:208:PHE:O	1:1:212:LYS:HG3	2.18	0.43
3:4:130:ALA:O	3:4:134:PRO:HD3	2.18	0.43
3:4:173:GLU:HG2	22:R:62:ALA:HB2	2.01	0.43
4:A:11:GLU:OE2	4:A:15:GLY:HA3	2.17	0.43
4:A:161:TYR:HA	4:A:294:ALA:HB2	1.99	0.43
4:A:331:MET:HE3	7:D:321:LEU:HB3	1.99	0.43
27:A:404:PHO:H193	25:D:401:CLA:CHB	2.49	0.43
5:B:291:GLY:HA2	5:B:294:GLU:CD	2.44	0.43
7:D:162:PRO:HG3	7:D:171:ALA:HB2	2.00	0.43
7:D:193:THR:HG23	25:D:402:CLA:HBC2	1.99	0.43
29:L:103:SQD:H281	29:L:103:SQD:C32	2.49	0.43
20:S:135:ASN:HD21	20:S:141:CYS:CA	2.32	0.43
21:G:137:GLN:HE22	21:G:144:LEU:HA	1.84	0.43
21:G:215:GLU:HB2	25:G:610:CLA:HMB3	2.01	0.43
21:G:215:GLU:HB2	25:G:610:CLA:CMB	2.49	0.43
24:N:601:CHL:CMD	26:N:618:LHG:HC41	2.48	0.43
21:Y:104:ARG:HB3	25:Y:311:CLA:HBC2	1.96	0.43
24:Y:302:CHL:CMC	24:Y:302:CHL:HBC3	2.49	0.43
25:Y:304:CLA:HMC3	25:Y:304:CLA:CBC	2.39	0.43
25:Y:304:CLA:CMD	24:Y:310:CHL:C4D	2.96	0.43
25:Y:304:CLA:H93	24:Y:310:CHL:H91	2.01	0.43
24:Y:310:CHL:H92	24:Y:310:CHL:H62	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:101:ILE:O	1:7:105:TRP:HD1	2.02	0.43
3:8:221:LEU:CA	3:8:224:LEU:HD23	2.48	0.43
4:a:47:VAL:HG21	4:a:114:LEU:HD22	2.00	0.43
4:a:142:TRP:CZ2	6:c:447:ARG:HG3	2.54	0.43
5:b:204:ALA:CB	25:b:602:CLA:HAB	2.48	0.43
28:b:618:BCR:H15C	28:b:618:BCR:H351	1.83	0.43
6:c:75:PHE:O	12:k:25:LYS:HD3	2.18	0.43
6:c:319:VAL:HG23	6:c:322:GLN:HE21	1.84	0.43
7:d:202:VAL:HG13	25:d:402:CLA:HBB1	2.01	0.43
7:d:287:VAL:CG2	25:d:402:CLA:HED2	2.49	0.43
8:e:56:PHE:HA	8:e:60:ARG:NH1	2.34	0.43
29:l:101:SQD:H281	29:l:101:SQD:C32	2.49	0.43
14:m:23:LEU:O	14:m:27:VAL:HG23	2.19	0.43
25:s:303:CLA:H93	25:s:303:CLA:H111	1.53	0.43
21:g:152:LEU:HD23	24:g:605:CHL:HED3	2.01	0.43
24:n:606:CHL:HMB1	24:n:609:CHL:HAC1	2.01	0.43
25:y:304:CLA:H93	24:y:310:CHL:H91	2.00	0.43
25:r:603:CLA:H92	25:r:603:CLA:H61	1.72	0.43
2:2:105:TRP:HD1	24:2:603:CHL:HED1	1.83	0.43
2:2:126:ASP:C	2:2:148:LEU:HD21	2.42	0.43
2:2:174:GLU:OE2	1:3:59:LEU:HD22	2.19	0.43
2:2:216:GLU:O	2:2:219:ASN:HB2	2.19	0.43
2:2:217:ILE:HG13	2:2:218:LYS:N	2.32	0.43
1:3:226:MET:O	1:3:230:PHE:HD2	2.01	0.43
4:A:106:LEU:HD11	28:A:406:BCR:H402	2.00	0.43
5:B:51:VAL:HG13	5:B:308:LYS:HG2	1.95	0.43
25:B:606:CLA:H203	28:B:619:BCR:H363	2.00	0.43
25:B:608:CLA:CAB	7:D:124:ILE:HG12	2.49	0.43
25:B:614:CLA:H61	25:B:614:CLA:H92	1.52	0.43
28:B:618:BCR:H15C	28:B:618:BCR:H351	1.83	0.43
6:C:162:GLY:CA	6:C:248:GLY:HA2	2.48	0.43
6:C:182:PHE:HE1	20:S:258:LEU:O	2.02	0.43
6:C:298:PRO:O	6:C:299:SER:HB3	2.19	0.43
6:C:399:ALA:HB1	6:C:400:PRO:HD2	2.01	0.43
15:O:128:PRO:HA	15:O:180:VAL:HG13	1.99	0.43
24:S:306:CHL:HBB1	39:S:316:LUT:C16	2.49	0.43
24:G:601:CHL:HBA1	24:G:601:CHL:H3A	1.89	0.43
21:N:159:LEU:HD13	21:N:159:LEU:N	2.33	0.43
21:N:215:GLU:HB2	25:N:610:CLA:C1B	2.48	0.43
25:N:613:CLA:CHB	39:N:615:LUT:H42	2.49	0.43
21:Y:159:LEU:HD13	21:Y:159:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:314:CLA:H141	25:Y:314:CLA:H162	1.53	0.43
1:5:126:PHE:HE1	1:5:147:LEU:HA	1.84	0.43
2:6:178:ILE:HD12	1:7:62:PHE:HA	1.97	0.43
3:8:184:ASN:OD1	3:8:197:GLY:HA3	2.18	0.43
3:8:228:GLU:O	3:8:229:ILE:C	2.61	0.43
4:a:161:TYR:HA	4:a:294:ALA:HB1	2.00	0.43
4:a:233:ALA:O	4:a:235:GLU:HG2	2.17	0.43
25:a:406:CLA:H11	11:i:9:TYR:CZ	2.54	0.43
25:b:607:CLA:C17	25:b:613:CLA:H161	2.28	0.43
6:c:97:TRP:HE1	6:c:178:LYS:HE3	1.83	0.43
6:c:273:SER:HB2	6:c:445:ALA:HB2	2.01	0.43
25:c:510:CLA:H91	25:c:510:CLA:H111	1.69	0.43
7:d:65:ALA:CB	7:d:70:GLU:OE2	2.67	0.43
7:d:197:PHE:HA	7:d:200:MET:HE3	2.01	0.43
7:d:268:LEU:HD23	7:d:268:LEU:C	2.44	0.43
25:d:402:CLA:HBC3	25:d:402:CLA:HHD	2.01	0.43
10:h:31:GLY:O	10:h:33:VAL:HG23	2.19	0.43
21:g:101:ILE:O	21:g:105:TRP:HD1	2.02	0.43
21:g:113:CYS:HB3	21:g:131:TRP:CD1	2.53	0.43
21:g:127:GLY:C	21:g:137:GLN:HG3	2.44	0.43
21:g:181:GLY:HA3	24:g:608:CHL:HMC	2.00	0.43
24:g:609:CHL:HBA1	24:n:601:CHL:HBA2	2.00	0.43
21:n:159:LEU:HD13	21:n:159:LEU:N	2.33	0.43
25:n:610:CLA:H52	39:n:615:LUT:C30	2.49	0.43
21:y:97:GLU:CB	21:y:190:LEU:HD11	2.48	0.43
21:y:113:CYS:HB3	21:y:131:TRP:CD1	2.53	0.43
21:y:121:ARG:HD2	21:y:241:ILE:HG22	2.01	0.43
21:y:244:LEU:HD13	25:y:315:CLA:HBC2	2.00	0.43
1:1:209:ALA:HA	1:1:212:LYS:CG	2.34	0.43
2:2:86:SER:O	2:2:88:ASP:N	2.51	0.43
4:A:279:PRO:O	4:A:283:ILE:HG12	2.19	0.43
5:B:135:LEU:HD12	5:B:231:MET:O	2.19	0.43
5:B:265:ILE:O	5:B:269:GLY:N	2.47	0.43
25:B:603:CLA:C4B	25:B:605:CLA:H93	2.48	0.43
6:C:204:LEU:C	6:C:239:TRP:HZ2	2.26	0.43
6:C:319:VAL:HG23	6:C:322:GLN:HE21	1.84	0.43
26:C:517:LHG:H332	26:C:517:LHG:H362	1.68	0.43
9:F:18:HIS:HE1	38:F:101:HEM:C4A	2.37	0.43
12:K:30:TYR:CZ	19:Z:5:PHE:HZ	2.36	0.43
18:X:96:VAL:O	18:X:100:ILE:HG23	2.19	0.43
25:S:303:CLA:H112	25:S:304:CLA:CMB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:172:VAL:HG13	24:G:608:CHL:C1B	2.49	0.43
24:G:601:CHL:H72	24:G:601:CHL:H111	1.62	0.43
25:G:602:CLA:H72	25:G:602:CLA:H111	1.45	0.43
24:G:609:CHL:H2	24:G:609:CHL:H61	1.73	0.43
25:G:610:CLA:H62	25:G:612:CLA:CMA	2.49	0.43
21:N:101:ILE:O	21:N:105:TRP:HD1	2.02	0.43
21:N:215:GLU:CG	25:N:610:CLA:C1B	2.97	0.43
21:Y:137:GLN:HE22	21:Y:144:LEU:HA	1.84	0.43
21:Y:182:PRO:HB3	40:Y:318:NEX:C18	2.49	0.43
22:R:258:VAL:HG12	25:R:612:CLA:HMD2	2.01	0.43
25:R:601:CLA:C1B	26:R:618:LHG:H112	2.49	0.43
25:R:611:CLA:HAB	39:R:615:LUT:C15	2.49	0.43
2:6:219:ASN:O	2:6:220:GLY:C	2.61	0.43
4:a:40:THR:CG2	25:a:406:CLA:HBB1	2.48	0.43
29:a:408:SQD:H441	7:d:233:PHE:CD2	2.54	0.43
5:b:336:ILE:O	5:b:336:ILE:CG2	2.67	0.43
6:c:179:ALA:HA	6:c:185:VAL:HG13	2.01	0.43
6:c:227:VAL:HG11	6:c:233:ILE:CG1	2.49	0.43
28:i:101:BCR:C8	28:i:101:BCR:H331	2.48	0.43
14:m:27:VAL:HA	14:m:30:VAL:HG22	2.00	0.43
15:o:307:GLN:HG3	15:o:321:VAL:CG1	2.49	0.43
19:z:16:SER:HB3	28:z:101:BCR:H312	2.00	0.43
20:s:83:GLU:HG3	20:s:85:LEU:HD13	2.01	0.43
20:s:248:GLU:CD	20:s:252:GLU:HG3	2.44	0.43
21:g:132:PHE:CB	24:g:607:CHL:HMA3	2.41	0.43
25:n:603:CLA:HBC2	24:n:609:CHL:HMD2	2.00	0.43
21:y:126:PHE:HE1	21:y:147:LEU:HA	1.83	0.43
21:y:182:PRO:HB3	40:y:318:NEX:C18	2.49	0.43
22:r:103:LYS:CG	22:r:105:LEU:HD11	2.49	0.43
22:r:253:PHE:CE2	41:r:616:XAT:H10	2.54	0.43
25:r:602:CLA:HBC1	26:r:618:LHG:C28	2.48	0.43
1:1:97:GLU:CB	1:1:190:LEU:HD11	2.48	0.42
1:3:225:SER:O	1:3:229:PHE:HD1	2.01	0.42
4:A:199:MET:SD	25:D:401:CLA:HED2	2.59	0.42
5:B:242:ILE:O	5:B:246:PHE:CD1	2.72	0.42
5:B:276:ASP:OD1	5:B:361:THR:HG21	2.19	0.42
5:B:387:GLU:O	7:D:345:GLU:CD	2.62	0.42
25:B:611:CLA:H61	25:B:611:CLA:H2	1.78	0.42
6:C:221:GLU:CD	17:W:91:GLY:HA2	2.44	0.42
6:C:321:ASP:OD2	6:C:340:TYR:OH	2.27	0.42
20:S:83:GLU:HG3	20:S:85:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:159:LEU:HD13	21:G:159:LEU:N	2.33	0.42
24:G:601:CHL:H8	24:G:601:CHL:H52	1.69	0.42
40:G:617:NEX:H381	40:G:617:NEX:H27	1.63	0.42
24:N:607:CHL:CBB	24:Y:302:CHL:H91	2.48	0.42
24:N:608:CHL:H203	24:N:608:CHL:H161	1.84	0.42
21:Y:244:LEU:HD13	25:Y:315:CLA:HBC2	2.00	0.42
1:5:151:SER:O	24:5:301:CHL:HMA3	2.19	0.42
3:8:173:GLU:HG2	22:r:62:ALA:HB2	2.01	0.42
3:8:241:ILE:O	3:8:245:GLU:HG2	2.19	0.42
4:a:199:MET:SD	25:d:401:CLA:HED2	2.59	0.42
4:a:329:GLU:OE1	4:a:332:HIS:NE2	2.52	0.42
27:a:405:PHO:HAB	25:d:402:CLA:H12	2.01	0.42
5:b:188:GLU:OE1	10:h:68:ASP:HB3	2.19	0.42
28:b:619:BCR:H20C	28:b:619:BCR:H361	1.80	0.42
6:c:267:SER:CA	17:w:133:LEU:HD23	2.47	0.42
6:c:274:TYR:HE1	25:c:505:CLA:O2D	2.01	0.42
6:c:298:PRO:O	6:c:299:SER:HB3	2.19	0.42
25:c:504:CLA:H61	25:c:504:CLA:H41	1.49	0.42
15:o:100:LYS:CE	15:o:105:VAL:HG22	2.48	0.42
19:z:61:ILE:HG13	19:z:62:SER:N	2.34	0.42
24:s:307:CHL:HBA1	24:s:307:CHL:H3A	1.26	0.42
26:s:318:LHG:H372	26:s:318:LHG:H342	1.86	0.42
21:n:215:GLU:HB2	25:n:610:CLA:C1B	2.48	0.42
25:n:610:CLA:C5	39:n:615:LUT:H30	2.48	0.42
25:y:311:CLA:H61	25:y:311:CLA:H92	1.82	0.42
25:r:603:CLA:HMB2	25:r:603:CLA:H143	1.94	0.42
25:r:611:CLA:HAB	39:r:615:LUT:C15	2.49	0.42
1:1:145:ASP:OD2	1:1:150:PRO:HA	2.19	0.42
2:2:178:ILE:HG22	2:2:180:GLY:H	1.84	0.42
2:2:249:LEU:HD12	2:2:250:ASP:HB2	2.00	0.42
1:3:57:LYS:HD2	1:3:63:SER:HB2	2.00	0.42
1:3:210:GLU:OE1	1:3:214:LYS:NZ	2.38	0.42
4:A:47:VAL:HG21	4:A:114:LEU:HD22	1.99	0.42
4:A:161:TYR:HA	4:A:294:ALA:HB1	2.00	0.42
29:A:407:SQD:H441	7:D:233:PHE:CD2	2.54	0.42
25:B:607:CLA:H62	25:B:607:CLA:H93	1.51	0.42
25:B:610:CLA:HHC	25:B:610:CLA:HBB1	2.01	0.42
25:B:614:CLA:H91	26:L:102:LHG:H372	2.00	0.42
6:C:251:HIS:HE1	25:C:506:CLA:HMA3	1.80	0.42
7:D:268:LEU:HD23	7:D:268:LEU:C	2.44	0.42
7:D:287:VAL:CG2	25:D:402:CLA:HED2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:54:LEU:O	10:H:57:ILE:HG12	2.18	0.42
11:I:31:ASN:HB2	11:I:32:PRO:HD2	2.00	0.42
29:L:103:SQD:H131	29:L:103:SQD:H102	1.47	0.42
15:O:286:THR:O	15:O:286:THR:HG23	2.19	0.42
15:O:307:GLN:HG3	15:O:321:VAL:CG1	2.49	0.42
20:S:70:PHE:CG	20:S:95:TYR:HB2	2.54	0.42
24:N:607:CHL:H61	24:N:607:CHL:H41	1.93	0.42
21:Y:228:GLY:O	21:Y:231:VAL:N	2.53	0.42
1:5:137:GLN:HE22	1:5:144:LEU:HA	1.84	0.42
2:6:223:ALA:HB3	25:6:602:CLA:CMC	2.45	0.42
3:8:171:SER:HB3	3:8:183:GLU:OE2	2.18	0.42
4:a:327:GLY:O	4:a:330:VAL:HG22	2.19	0.42
5:b:378:ARG:HA	5:b:378:ARG:NE	2.33	0.42
6:c:146:PHE:CD2	26:s:301:LHG:HC5	2.54	0.42
6:c:213:LEU:O	6:c:223:TRP:NE1	2.40	0.42
6:c:267:SER:HA	17:w:133:LEU:CD2	2.49	0.42
7:d:20:ASP:CG	7:d:24:ARG:HH11	2.25	0.42
7:d:218:THR:CG2	7:d:250:ALA:HB1	2.49	0.42
29:l:102:SQD:H121	29:l:102:SQD:C28	2.47	0.42
15:o:158:PHE:HE2	15:o:322:LYS:HB2	1.82	0.42
15:o:184:GLY:O	15:o:224:PRO:HD3	2.18	0.42
20:s:135:ASN:HD21	20:s:141:CYS:CA	2.32	0.42
20:s:189:ARG:NH2	25:s:309:CLA:HMA3	2.33	0.42
21:g:114:VAL:HG13	21:g:241:ILE:HD11	2.01	0.42
21:g:215:GLU:HB2	25:g:610:CLA:HMB3	2.01	0.42
21:n:232:GLN:HE21	25:n:613:CLA:CHA	2.17	0.42
40:n:617:NEX:C28	40:n:617:NEX:H381	2.48	0.42
24:y:302:CHL:H18	32:y:321:AJP:C13	2.49	0.42
41:r:616:XAT:H11	41:r:616:XAT:H191	1.79	0.42
1:1:164:THR:HG21	24:1:302:CHL:O1D	2.20	0.42
24:1:301:CHL:CHD	24:1:301:CHL:HBC2	2.48	0.42
2:2:126:ASP:OD1	2:2:129:GLU:HA	2.17	0.42
2:2:127:PHE:CZ	2:2:145:LEU:HD12	2.55	0.42
2:2:202:LEU:O	2:2:202:LEU:HG	2.19	0.42
25:2:604:CLA:HBC3	26:2:606:LHG:H382	2.00	0.42
3:4:104:ILE:H	3:4:104:ILE:HD12	1.84	0.42
4:A:327:GLY:O	4:A:330:VAL:HG22	2.19	0.42
5:B:188:GLU:OE1	10:H:68:ASP:HB3	2.19	0.42
5:B:371:VAL:HA	5:B:376:ILE:O	2.19	0.42
5:B:378:ARG:HA	5:B:378:ARG:NE	2.33	0.42
5:B:378:ARG:O	5:B:390:TYR:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:436:THR:HG23	5:B:437:LEU:N	2.34	0.42
25:B:602:CLA:H143	25:B:602:CLA:H162	1.72	0.42
6:C:146:PHE:CD2	26:S:301:LHG:HC5	2.54	0.42
6:C:201:ASN:O	6:C:231:GLU:CG	2.68	0.42
7:D:218:THR:CG2	7:D:250:ALA:HB1	2.49	0.42
25:S:313:CLA:HAA1	25:S:313:CLA:CBD	2.48	0.42
21:G:86:SER:OG	25:G:602:CLA:HAA2	2.18	0.42
21:G:231:VAL:HG21	25:G:613:CLA:HAC1	2.00	0.42
21:G:231:VAL:CG1	25:G:613:CLA:HAC2	2.36	0.42
24:G:601:CHL:H61	24:G:601:CHL:H41	1.55	0.42
25:N:604:CLA:HBC2	25:N:604:CLA:CMC	2.50	0.42
24:N:609:CHL:HBA1	24:N:609:CHL:H3A	1.82	0.42
21:Y:50:TRP:NE1	25:Y:312:CLA:HED3	2.33	0.42
24:Y:306:CHL:HBA2	24:Y:306:CHL:H3A	1.66	0.42
25:Y:314:CLA:C4B	39:Y:316:LUT:H183	2.49	0.42
1:5:206:GLU:N	1:5:206:GLU:CD	2.76	0.42
2:6:107:MET:HG3	2:6:222:LEU:HD12	2.01	0.42
2:6:175:GLY:HA3	2:6:181:LEU:HD21	2.02	0.42
2:6:239:LYS:HD2	2:6:242:LEU:HD11	1.99	0.42
1:7:127:GLY:C	1:7:137:GLN:HG3	2.44	0.42
4:a:279:PRO:O	4:a:283:ILE:HG12	2.19	0.42
5:b:242:ILE:O	5:b:246:PHE:CD1	2.72	0.42
5:b:243:ALA:HA	5:b:246:PHE:HE1	1.71	0.42
5:b:476:ARG:HG2	5:b:476:ARG:HH11	1.83	0.42
28:b:619:BCR:H24C	28:b:619:BCR:H371	1.79	0.42
25:c:506:CLA:H92	25:c:506:CLA:H61	1.62	0.42
26:c:517:LHG:H332	26:c:517:LHG:H362	1.68	0.42
7:d:160:ILE:HG21	7:d:288:VAL:HG22	2.02	0.42
12:k:30:TYR:CZ	19:z:5:PHE:HZ	2.36	0.42
12:k:58:VAL:O	12:k:59:SER:HB2	2.19	0.42
18:x:96:VAL:O	18:x:100:ILE:HG23	2.19	0.42
19:z:19:LEU:HD21	19:z:43:GLY:CA	2.41	0.42
20:s:142:GLY:N	20:s:160:LEU:O	2.50	0.42
21:g:50:TRP:NE1	25:g:611:CLA:HED2	2.34	0.42
21:g:84:GLY:N	21:y:94:ARG:CG	2.80	0.42
21:g:137:GLN:HE22	21:g:144:LEU:HA	1.84	0.42
21:n:127:GLY:C	21:n:137:GLN:HG3	2.44	0.42
25:n:613:CLA:HBA1	25:n:614:CLA:CAD	2.49	0.42
21:y:57:LYS:HD2	21:y:63:SER:HB2	2.00	0.42
25:y:312:CLA:H92	25:y:312:CLA:C5	2.49	0.42
22:r:258:VAL:HG12	25:r:612:CLA:HMD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:609:CLA:H52	39:r:615:LUT:C30	2.49	0.42
1:1:206:GLU:N	1:1:206:GLU:CD	2.76	0.42
2:2:107:MET:HG3	2:2:222:LEU:HD12	2.01	0.42
1:3:127:GLY:C	1:3:137:GLN:HG3	2.44	0.42
4:A:47:VAL:HG21	4:A:114:LEU:CD2	2.49	0.42
5:B:37:MET:HE1	25:B:607:CLA:HHD	2.01	0.42
5:B:367:PRO:HB3	7:D:346:VAL:HB	2.02	0.42
5:B:388:SER:CB	5:B:391:SER:HB2	2.45	0.42
25:B:614:CLA:HMD2	29:L:101:SQD:C24	2.49	0.42
6:C:109:PHE:O	6:C:113:VAL:HG23	2.19	0.42
6:C:287:CYS:SG	6:C:427:SER:HB3	2.60	0.42
7:D:258:PHE:CZ	26:D:406:LHG:H312	2.55	0.42
28:H:101:BCR:H351	28:H:101:BCR:H15C	1.90	0.42
21:G:132:PHE:HB2	24:G:607:CHL:CMA	2.43	0.42
21:G:228:GLY:O	21:G:231:VAL:N	2.53	0.42
21:N:127:GLY:C	21:N:137:GLN:HG3	2.44	0.42
21:N:221:LEU:CD1	26:N:618:LHG:H272	2.48	0.42
25:N:610:CLA:C5	39:N:615:LUT:H30	2.48	0.42
21:Y:132:PHE:CD1	21:Y:133:LYS:N	2.88	0.42
21:Y:191:TYR:N	21:Y:192:PRO:CD	2.82	0.42
21:Y:218:ASN:OD1	25:Y:312:CLA:CMD	2.67	0.42
25:Y:303:CLA:H41	25:Y:304:CLA:O1A	2.20	0.42
22:R:177:SER:O	22:R:184:LEU:N	2.35	0.42
1:7:131:TRP:CD1	1:7:131:TRP:H	2.38	0.42
3:8:89:GLY:CA	3:8:95:LEU:HD21	2.49	0.42
3:8:251:THR:HG23	3:8:254:GLY:H	1.83	0.42
4:a:335:ASN:HB3	6:c:334:PRO:CB	2.49	0.42
5:b:52:LEU:C	5:b:54:PRO:HD3	2.44	0.42
5:b:91:TRP:NE1	26:b:622:LHG:HC61	2.29	0.42
5:b:160:GLY:HA3	5:b:180:PRO:HB3	2.01	0.42
25:b:614:CLA:HMD2	29:l:102:SQD:H242	2.01	0.42
25:c:506:CLA:H13	25:c:506:CLA:H91	2.01	0.42
25:c:511:CLA:H3A	25:c:511:CLA:HBA1	1.68	0.42
12:k:27:PRO:HB2	12:k:30:TYR:HD1	1.85	0.42
15:o:92:LEU:HB3	15:o:96:GLU:CG	2.43	0.42
24:g:607:CHL:CMB	24:g:607:CHL:HBB1	2.50	0.42
25:g:610:CLA:C5	39:g:615:LUT:H30	2.41	0.42
21:n:97:GLU:CB	21:n:190:LEU:HD11	2.48	0.42
25:n:602:CLA:H52	25:n:602:CLA:CMB	2.41	0.42
21:y:210:GLU:O	21:y:214:LYS:HG3	2.20	0.42
1:1:57:LYS:HD2	1:1:63:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:210:GLU:O	1:1:214:LYS:HG3	2.20	0.42
2:2:192:PRO:HB2	2:2:196:TYR:CD2	2.55	0.42
3:4:189:THR:O	3:4:189:THR:HG23	2.18	0.42
3:4:193:GLY:O	3:4:195:PRO:HD3	2.20	0.42
3:4:216:PRO:O	3:4:220:LYS:N	2.52	0.42
5:B:52:LEU:C	5:B:54:PRO:HD3	2.44	0.42
6:C:147:PHE:CD1	25:C:513:CLA:HMB1	2.55	0.42
25:C:504:CLA:C4	35:C:516:DGD:HB32	2.45	0.42
26:C:517:LHG:HC82	17:W:113:TRP:HE1	1.84	0.42
7:D:197:PHE:HA	7:D:200:MET:HE3	2.01	0.42
7:D:243:GLU:HG2	7:D:245:TYR:H	1.83	0.42
7:D:297:TYR:O	7:D:316:TYR:OH	2.30	0.42
8:E:67:THR:CA	23:U:102:ARG:HH11	2.33	0.42
14:M:23:LEU:O	14:M:27:VAL:HG23	2.19	0.42
18:X:86:PHE:O	18:X:90:ILE:HG13	2.20	0.42
20:S:135:ASN:ND2	20:S:141:CYS:N	2.66	0.42
20:S:248:GLU:CD	20:S:252:GLU:HG3	2.44	0.42
21:G:127:GLY:C	21:G:137:GLN:HG3	2.44	0.42
21:N:228:GLY:O	21:N:231:VAL:N	2.53	0.42
24:N:609:CHL:NC	24:Y:302:CHL:H52	2.34	0.42
21:Y:176:ARG:HG3	24:Y:309:CHL:C1D	2.49	0.42
21:Y:221:LEU:HD21	25:Y:313:CLA:HAC1	2.01	0.42
25:R:603:CLA:H43	25:R:603:CLA:HED3	2.01	0.42
25:R:603:CLA:H93	25:R:603:CLA:H111	1.62	0.42
2:6:104:ARG:CZ	24:6:603:CHL:HED3	2.49	0.42
1:7:145:ASP:OD2	1:7:150:PRO:HA	2.20	0.42
1:7:191:TYR:N	1:7:192:PRO:CD	2.82	0.42
4:a:40:THR:O	4:a:43:THR:HG22	2.18	0.42
4:a:120:LEU:O	4:a:123:VAL:HG22	2.18	0.42
5:b:193:PHE:HE2	35:b:626:DGD:HE2	1.83	0.42
5:b:436:THR:HG23	5:b:437:LEU:N	2.34	0.42
25:b:605:CLA:H162	25:b:609:CLA:HBB2	2.01	0.42
25:b:614:CLA:HMD2	29:l:102:SQD:C24	2.49	0.42
6:c:185:VAL:CG2	6:c:230:LEU:HD13	2.49	0.42
6:c:221:GLU:CD	17:w:91:GLY:HA2	2.44	0.42
7:d:68:TYR:O	30:d:407:LMG:HC61	2.18	0.42
7:d:135:ARG:HH21	7:d:138:GLN:CD	2.25	0.42
17:w:131:LEU:HD23	17:w:131:LEU:HA	1.82	0.42
25:s:305:CLA:HMB1	25:s:305:CLA:CBB	2.49	0.42
21:g:145:ASP:OD2	21:g:150:PRO:HA	2.20	0.42
21:g:172:VAL:HG13	24:g:608:CHL:C4B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:226:MET:O	21:g:230:PHE:HD2	2.01	0.42
21:n:215:GLU:CG	25:n:610:CLA:C1B	2.97	0.42
25:n:604:CLA:HMA2	24:n:606:CHL:CAC	2.50	0.42
22:r:85:LYS:CG	22:r:86:PRO:CD	2.96	0.42
25:r:603:CLA:H43	25:r:603:CLA:HED3	2.01	0.42
25:r:614:CLA:HBD	25:r:614:CLA:HAA1	2.02	0.42
1:1:132:PHE:CD1	1:1:133:LYS:N	2.88	0.42
1:1:159:LEU:N	1:1:159:LEU:HD13	2.33	0.42
2:2:174:GLU:HB3	1:3:62:PHE:CD2	2.55	0.42
3:4:140:PHE:HA	22:R:280:HIS:CD2	2.54	0.42
3:4:245:GLU:O	3:4:249:GLY:N	2.53	0.42
28:B:617:BCR:H312	30:B:620:LMG:H341	2.02	0.42
6:C:135:LEU:HD23	6:C:135:LEU:C	2.45	0.42
6:C:227:VAL:HG11	6:C:233:ILE:CG1	2.49	0.42
6:C:235:GLY:O	6:C:239:TRP:HD1	2.02	0.42
6:C:267:SER:HA	17:W:133:LEU:CD2	2.49	0.42
6:C:304:PRO:O	6:C:308:GLU:HB3	2.19	0.42
25:C:512:CLA:H162	25:C:513:CLA:H152	2.02	0.42
7:D:160:ILE:HG21	7:D:288:VAL:HG22	2.02	0.42
15:O:145:VAL:HG11	15:O:203:LEU:HD21	2.00	0.42
15:O:225:ASP:O	15:O:288:LYS:HA	2.20	0.42
16:T:11:VAL:HG22	28:T:101:BCR:H342	2.00	0.42
25:S:303:CLA:H61	25:S:303:CLA:H41	1.90	0.42
21:G:145:ASP:OD2	21:G:150:PRO:HA	2.19	0.42
21:G:172:VAL:HG13	24:G:608:CHL:C4B	2.49	0.42
25:G:604:CLA:HBB1	39:G:616:LUT:C18	2.47	0.42
21:N:137:GLN:HE22	21:N:144:LEU:HA	1.84	0.42
21:N:210:GLU:O	21:N:214:LYS:HG3	2.20	0.42
21:N:247:HIS:HD1	21:N:247:HIS:C	2.28	0.42
25:N:604:CLA:HMA2	24:N:606:CHL:CAC	2.50	0.42
21:Y:57:LYS:HD2	21:Y:63:SER:HB2	2.00	0.42
21:Y:80:TRP:O	39:Y:317:LUT:H24	2.19	0.42
21:Y:145:ASP:OD2	21:Y:150:PRO:HA	2.20	0.42
21:Y:215:GLU:HB2	25:Y:311:CLA:C1B	2.49	0.42
21:Y:247:HIS:HD1	21:Y:247:HIS:C	2.28	0.42
24:Y:302:CHL:H18	32:Y:321:AJP:C13	2.49	0.42
22:R:137:ARG:NH2	25:R:602:CLA:HED3	2.24	0.42
2:6:174:GLU:HB3	1:7:62:PHE:CD2	2.55	0.42
2:6:202:LEU:O	2:6:202:LEU:HG	2.19	0.42
4:a:184:ILE:CG2	7:d:322:LEU:HD13	2.50	0.42
5:b:135:LEU:HD12	5:b:231:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:608:CLA:CAB	7:d:124:ILE:HG12	2.49	0.42
25:b:609:CLA:HAA1	25:b:609:CLA:HBD	2.01	0.42
6:c:182:PHE:HE1	20:s:258:LEU:O	2.02	0.42
8:e:25:ILE:O	8:e:29:SER:OG	2.28	0.42
15:o:180:VAL:CA	15:o:186:VAL:HG12	2.45	0.42
18:x:86:PHE:O	18:x:90:ILE:HG13	2.20	0.42
19:z:42:SER:O	19:z:43:GLY:C	2.63	0.42
21:g:172:VAL:HG13	24:g:608:CHL:C1B	2.48	0.42
21:g:191:TYR:N	21:g:192:PRO:CD	2.82	0.42
21:g:228:GLY:O	21:g:231:VAL:N	2.53	0.42
40:g:617:NEX:H391	40:g:617:NEX:H31	1.57	0.42
21:n:137:GLN:HE22	21:n:144:LEU:HA	1.84	0.42
25:n:603:CLA:H61	25:n:603:CLA:H92	1.50	0.42
21:y:127:GLY:C	21:y:137:GLN:HG3	2.44	0.42
21:y:215:GLU:CG	25:y:311:CLA:C1B	2.95	0.42
24:y:302:CHL:CMC	24:y:302:CHL:HBC3	2.49	0.42
25:y:303:CLA:H41	25:y:304:CLA:O1A	2.20	0.42
25:y:304:CLA:H161	25:y:304:CLA:H192	1.74	0.42
22:r:103:LYS:HE3	22:r:105:LEU:CD1	2.47	0.42
22:r:171:VAL:O	22:r:175:ASP:HB2	2.19	0.42
25:r:612:CLA:HBD	25:r:612:CLA:HAA1	2.02	0.42
1:1:127:GLY:C	1:1:137:GLN:HG3	2.44	0.42
2:2:118:VAL:O	2:2:122:TRP:HB2	2.19	0.42
1:3:191:TYR:N	1:3:192:PRO:CD	2.82	0.42
3:4:89:GLY:CA	3:4:95:LEU:HD21	2.49	0.42
4:A:184:ILE:CG2	7:D:322:LEU:HD13	2.50	0.42
4:A:223:LEU:O	5:B:482:ILE:HG12	2.19	0.42
4:A:292:THR:CB	6:C:428:THR:HG23	2.50	0.42
4:A:328:MET:O	4:A:332:HIS:CD2	2.73	0.42
5:B:187:VAL:HG23	5:B:188:GLU:OE1	2.20	0.42
6:C:97:TRP:HE1	6:C:178:LYS:HE3	1.83	0.42
6:C:281:VAL:HG12	6:C:285:ILE:HD11	2.01	0.42
7:D:172:PRO:HG3	7:D:182:PHE:CZ	2.55	0.42
7:D:316:TYR:O	7:D:320:ILE:HG12	2.19	0.42
10:H:31:GLY:O	10:H:33:VAL:HG23	2.19	0.42
14:M:29:THR:HG23	14:M:30:VAL:N	2.35	0.42
21:G:49:PRO:O	21:G:55:ARG:HA	2.20	0.42
21:G:172:VAL:HG13	24:G:608:CHL:NB	2.35	0.42
21:G:191:TYR:CE2	21:G:212:LYS:CE	3.03	0.42
24:G:607:CHL:CMB	24:G:607:CHL:HBB1	2.50	0.42
21:Y:49:PRO:O	21:Y:55:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:171:VAL:O	22:R:175:ASP:HB2	2.19	0.42
22:R:253:PHE:CE2	41:R:616:XAT:H10	2.54	0.42
1:5:228:GLY:O	1:5:231:VAL:N	2.53	0.42
2:6:137:SER:CA	2:6:140:PHE:CD2	3.02	0.42
2:6:149:GLY:O	2:6:152:ASN:HB2	2.20	0.42
2:6:192:PRO:HB2	2:6:196:TYR:CD2	2.55	0.42
3:8:118:VAL:HG13	3:8:119:GLY:N	2.35	0.42
3:8:164:PHE:HB2	3:8:192:GLN:CD	2.45	0.42
30:a:411:LMG:H351	30:a:411:LMG:H382	1.83	0.42
5:b:256:MET:O	5:b:448:ARG:HD3	2.20	0.42
25:b:604:CLA:H93	25:b:604:CLA:H61	1.59	0.42
6:c:147:PHE:CD1	25:c:513:CLA:HMB1	2.55	0.42
6:c:299:SER:HA	6:c:423:ARG:HH21	1.85	0.42
6:c:304:PRO:O	6:c:308:GLU:HB3	2.19	0.42
8:e:30:LEU:HD13	9:f:22:VAL:HG13	2.02	0.42
20:s:68:ARG:NH2	26:s:301:LHG:HC12	2.23	0.42
21:g:173:GLU:OE2	24:g:609:CHL:NA	2.53	0.42
21:n:80:TRP:HE3	25:n:602:CLA:CMD	2.32	0.42
25:n:604:CLA:HBC2	25:n:604:CLA:CMC	2.50	0.42
21:y:95:ASN:C	25:y:303:CLA:HMA1	2.45	0.42
21:y:137:GLN:HE22	21:y:144:LEU:HA	1.84	0.42
21:y:152:LEU:O	21:y:153:VAL:C	2.63	0.42
22:r:103:LYS:HE3	22:r:105:LEU:CD2	2.47	0.42
22:r:124:PHE:CD1	25:r:614:CLA:CHC	2.93	0.42
25:r:610:CLA:HMB3	26:r:618:LHG:C2	2.45	0.42
24:r:613:CHL:HBC3	24:r:613:CHL:OMC	2.20	0.42
25:r:614:CLA:HBC3	25:r:614:CLA:CHD	2.37	0.42
2:2:128:LYS:HB3	2:2:130:PRO:HD2	2.01	0.42
1:3:132:PHE:CD1	1:3:133:LYS:N	2.88	0.42
1:3:152:LEU:O	1:3:153:VAL:C	2.63	0.42
25:B:601:CLA:H161	25:B:601:CLA:H141	1.84	0.42
25:B:607:CLA:H192	25:B:607:CLA:H162	1.87	0.42
6:C:79:LYS:HG2	6:C:80:PRO:CD	2.49	0.42
12:K:30:TYR:CE2	19:Z:5:PHE:HZ	2.38	0.42
20:S:186:GLU:HG3	25:S:309:CLA:NB	2.34	0.42
20:S:252:GLU:O	20:S:256:LYS:HG2	2.20	0.42
21:G:152:LEU:HD23	24:G:605:CHL:HED3	2.01	0.42
21:N:80:TRP:HE3	25:N:602:CLA:CMD	2.32	0.42
21:N:191:TYR:N	21:N:192:PRO:CD	2.82	0.42
24:N:606:CHL:HMB1	24:N:609:CHL:HAC1	2.01	0.42
25:R:609:CLA:H52	39:R:615:LUT:C30	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:613:CHL:HBC3	24:R:613:CHL:OMC	2.20	0.42
25:6:604:CLA:HBC3	26:6:606:LHG:H382	2.00	0.42
3:8:226:LEU:CD1	3:8:229:ILE:HD11	2.43	0.42
4:a:47:VAL:HG21	4:a:114:LEU:CD2	2.50	0.42
5:b:51:VAL:HG22	5:b:308:LYS:HD2	2.01	0.42
6:c:209:ILE:HG13	6:c:239:TRP:CD1	2.55	0.42
25:c:501:CLA:H151	25:c:507:CLA:H102	2.02	0.42
7:d:280:LEU:HD23	7:d:280:LEU:HA	1.85	0.42
28:h:101:BCR:H20C	28:h:101:BCR:H361	1.79	0.42
29:l:102:SQD:H251	29:l:102:SQD:H102	2.01	0.42
14:m:29:THR:HG23	14:m:30:VAL:N	2.35	0.42
15:o:236:TYR:CB	15:o:310:ASP:OD2	2.63	0.42
20:s:132:GLU:CA	20:s:145:ALA:HB1	2.40	0.42
20:s:252:GLU:O	20:s:256:LYS:HG2	2.20	0.42
24:s:306:CHL:HBB1	39:s:316:LUT:C16	2.49	0.42
24:g:601:CHL:H142	24:g:601:CHL:H112	1.84	0.42
24:g:607:CHL:CMB	24:g:607:CHL:CBB	2.97	0.42
24:n:601:CHL:H62	24:n:601:CHL:H41	1.58	0.42
24:n:606:CHL:HAA1	40:n:617:NEX:H28	2.02	0.42
25:n:613:CLA:CHB	39:n:615:LUT:H42	2.49	0.42
21:y:131:TRP:CD1	21:y:131:TRP:H	2.38	0.42
21:y:165:GLN:OE1	24:y:307:CHL:C4A	2.68	0.42
21:y:221:LEU:HD21	25:y:313:CLA:HAC1	2.01	0.42
25:y:313:CLA:H142	25:y:313:CLA:H111	1.50	0.42
25:y:315:CLA:HBD	25:y:315:CLA:CBA	2.49	0.42
26:y:319:LHG:H292	26:y:319:LHG:H322	1.79	0.42
24:r:606:CHL:O2A	24:r:606:CHL:H2A	2.20	0.42
1:1:151:SER:O	24:1:301:CHL:HMA3	2.19	0.42
2:2:104:ARG:NH1	2:2:108:LEU:HD11	2.34	0.42
2:2:175:GLY:HA3	2:2:181:LEU:HD21	2.02	0.42
1:3:228:GLY:O	1:3:231:VAL:N	2.53	0.42
3:4:122:TRP:HB3	3:4:127:TRP:HB2	2.02	0.42
5:B:65:PHE:CE2	25:B:604:CLA:HMA2	2.55	0.42
5:B:127:ARG:HH22	10:H:31:GLY:HA3	1.85	0.42
25:B:601:CLA:H111	25:B:601:CLA:H93	1.71	0.42
25:B:606:CLA:H172	25:B:616:CLA:H93	2.00	0.42
25:B:613:CLA:H2A	25:B:613:CLA:O1D	2.20	0.42
6:C:179:ALA:HA	6:C:185:VAL:HG13	2.01	0.42
7:D:151:ILE:O	7:D:155:VAL:HG23	2.20	0.42
8:E:40:THR:OG1	8:E:42:LEU:HD13	2.20	0.42
12:K:58:VAL:O	12:K:59:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:3:GLN:HG3	13:L:4:SER:N	2.34	0.42
19:Z:61:ILE:HG13	19:Z:62:SER:N	2.34	0.42
25:S:303:CLA:H52	25:S:303:CLA:H8	1.74	0.42
21:G:160:ALA:HB3	24:G:605:CHL:OMC	2.20	0.42
24:N:607:CHL:H171	25:Y:303:CLA:H162	2.02	0.42
40:N:617:NEX:C28	40:N:617:NEX:H381	2.48	0.42
1:5:127:GLY:C	1:5:137:GLN:HG3	2.44	0.42
1:5:145:ASP:OD2	1:5:150:PRO:HA	2.19	0.42
2:6:128:LYS:HB3	2:6:130:PRO:HD2	2.01	0.42
2:6:249:LEU:HD12	2:6:250:ASP:HB2	2.00	0.42
4:a:98:GLU:HA	4:a:98:GLU:OE2	2.20	0.42
4:a:328:MET:O	4:a:332:HIS:CD2	2.73	0.42
5:b:291:GLY:HA2	5:b:294:GLU:CD	2.44	0.42
6:c:79:LYS:HG2	6:c:80:PRO:CD	2.49	0.42
6:c:287:CYS:SG	6:c:427:SER:HB3	2.60	0.42
7:d:243:GLU:HG2	7:d:245:TYR:H	1.83	0.42
7:d:305:ARG:NH1	14:m:1:MET:HE2	2.34	0.42
15:o:174:ILE:HG12	15:o:195:ASP:OD1	2.19	0.42
15:o:214:THR:HG21	15:o:233:VAL:HA	2.01	0.42
15:o:225:ASP:O	15:o:288:LYS:HA	2.20	0.42
18:x:87:LEU:HD12	18:x:87:LEU:C	2.45	0.42
20:s:186:GLU:HG3	25:s:309:CLA:NB	2.34	0.42
21:n:114:VAL:HG13	21:n:241:ILE:HD11	2.01	0.42
21:n:228:GLY:O	21:n:231:VAL:N	2.53	0.42
22:r:255:GLY:HA2	25:r:612:CLA:C4C	2.50	0.42
25:r:603:CLA:NB	25:r:608:CLA:H111	2.35	0.42
25:r:609:CLA:H61	25:r:609:CLA:H92	1.67	0.42
1:1:152:LEU:O	1:1:153:VAL:C	2.63	0.42
2:2:218:LYS:HA	2:2:221:ARG:NE	2.35	0.42
3:4:118:VAL:HG13	3:4:119:GLY:N	2.35	0.42
3:4:194:TYR:OH	3:4:225:LYS:CG	2.68	0.42
3:4:245:GLU:HB2	3:4:250:LYS:O	2.20	0.42
4:A:79:SER:CB	7:D:302:GLN:HE22	2.33	0.42
5:B:294:GLU:O	5:B:295:ASN:HB2	2.20	0.42
5:B:336:ILE:O	5:B:336:ILE:CG2	2.67	0.42
5:B:342:GLY:HA3	5:B:403:GLY:O	2.20	0.42
25:B:610:CLA:HAA2	25:B:610:CLA:HBD	2.02	0.42
6:C:273:SER:HB2	6:C:445:ALA:HB2	2.01	0.42
10:H:24:LYS:HB3	10:H:25:PRO:HD3	2.02	0.42
25:S:305:CLA:HMB1	25:S:305:CLA:CBB	2.50	0.42
21:G:131:TRP:CD1	21:G:131:TRP:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:137:GLN:O	21:N:140:SER:OG	2.30	0.42
25:N:613:CLA:H8	25:N:613:CLA:C13	2.47	0.42
25:R:604:CLA:HMA2	24:R:605:CHL:HAC2	2.02	0.42
25:R:612:CLA:HBD	25:R:612:CLA:HAA1	2.02	0.42
1:5:152:LEU:O	1:5:153:VAL:C	2.63	0.42
24:6:603:CHL:HBC3	24:6:603:CHL:OMC	2.20	0.42
1:7:97:GLU:CB	1:7:190:LEU:HD11	2.48	0.42
1:7:137:GLN:HE22	1:7:144:LEU:HA	1.84	0.42
1:7:152:LEU:O	1:7:153:VAL:C	2.63	0.42
1:7:228:GLY:O	1:7:231:VAL:N	2.53	0.42
3:8:148:THR:HG23	3:8:149:GLN:N	2.35	0.42
5:b:130:LYS:HB3	5:b:131:PRO:HD2	2.02	0.42
5:b:371:VAL:HA	5:b:376:ILE:O	2.20	0.42
5:b:378:ARG:O	5:b:390:TYR:HB3	2.20	0.42
6:c:281:VAL:HG12	6:c:285:ILE:HD11	2.01	0.42
6:c:322:GLN:HE22	6:c:384:ILE:CD1	2.24	0.42
25:c:502:CLA:H161	25:c:502:CLA:H203	1.84	0.42
7:d:258:PHE:CZ	26:d:406:LHG:H312	2.55	0.42
25:d:403:CLA:H102	25:d:403:CLA:H61	1.79	0.42
21:g:172:VAL:HG13	24:g:608:CHL:NB	2.35	0.42
21:g:210:GLU:O	21:g:214:LYS:HG3	2.20	0.42
25:g:610:CLA:HBA2	39:g:615:LUT:O23	2.20	0.42
25:n:602:CLA:H93	25:n:602:CLA:H111	1.52	0.42
24:n:607:CHL:H142	24:n:607:CHL:H91	2.01	0.42
21:y:191:TYR:N	21:y:192:PRO:CD	2.82	0.42
25:y:305:CLA:HMA1	39:y:317:LUT:H3	2.01	0.42
25:y:312:CLA:H62	25:y:312:CLA:H2	1.70	0.42
26:y:319:LHG:HC92	26:y:319:LHG:H121	1.60	0.42
41:r:616:XAT:H31	41:r:616:XAT:H391	1.76	0.42
1:1:228:GLY:O	1:1:231:VAL:N	2.53	0.41
2:2:149:GLY:O	2:2:152:ASN:HB2	2.20	0.41
1:3:145:ASP:OD2	1:3:150:PRO:HA	2.19	0.41
4:A:72:LEU:HG	4:A:72:LEU:O	2.20	0.41
4:A:142:TRP:CZ2	6:C:447:ARG:HG3	2.54	0.41
35:A:415:DGD:HAT1	35:A:415:DGD:HA71	1.64	0.41
5:B:115:TRP:HH2	25:B:614:CLA:HMA2	1.84	0.41
5:B:130:LYS:HB3	5:B:131:PRO:HD2	2.02	0.41
5:B:168:VAL:HG13	5:B:195:PRO:HG2	2.02	0.41
5:B:475:PHE:CD1	7:D:141:PRO:HG3	2.55	0.41
25:B:606:CLA:H192	25:B:616:CLA:H52	2.02	0.41
25:B:607:CLA:C17	25:B:613:CLA:H161	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:619:BCR:H361	28:B:619:BCR:H20C	1.80	0.41
6:C:209:ILE:HG13	6:C:239:TRP:CD1	2.55	0.41
6:C:239:TRP:CZ3	25:Y:315:CLA:CMB	3.03	0.41
25:C:509:CLA:H3A	25:C:509:CLA:HBA1	1.90	0.41
7:D:90:LEU:O	7:D:92:LEU:HG	2.20	0.41
7:D:202:VAL:HG13	25:D:402:CLA:HBB1	2.01	0.41
26:D:406:LHG:H221	16:T:10:LEU:HD22	2.00	0.41
8:E:30:LEU:HD13	9:F:22:VAL:HG13	2.02	0.41
13:L:15:ARG:HG2	13:L:19:TYR:CE1	2.55	0.41
18:X:87:LEU:HD12	18:X:87:LEU:C	2.45	0.41
19:Z:19:LEU:HD21	19:Z:43:GLY:CA	2.41	0.41
25:S:312:CLA:HBA1	25:S:312:CLA:CMA	2.38	0.41
25:S:313:CLA:H61	25:S:313:CLA:H2	1.83	0.41
21:G:114:VAL:HG13	21:G:241:ILE:HD11	2.01	0.41
21:G:152:LEU:O	21:G:153:VAL:C	2.63	0.41
21:N:152:LEU:O	21:N:153:VAL:C	2.63	0.41
21:N:225:SER:O	21:N:229:PHE:HD1	2.01	0.41
25:N:603:CLA:H202	25:N:603:CLA:H162	1.72	0.41
22:R:55:ARG:O	22:R:57:LEU:HD23	2.20	0.41
22:R:103:LYS:CG	22:R:105:LEU:HD11	2.49	0.41
41:R:616:XAT:H391	41:R:616:XAT:H31	1.76	0.41
1:5:191:TYR:N	1:5:192:PRO:CD	2.82	0.41
2:6:127:PHE:CZ	2:6:145:LEU:HD12	2.55	0.41
2:6:178:ILE:HD12	1:7:62:PHE:CD1	2.45	0.41
3:8:245:GLU:HB2	3:8:250:LYS:O	2.20	0.41
4:a:331:MET:HE3	7:d:321:LEU:HB3	1.99	0.41
5:b:37:MET:HE1	25:b:607:CLA:HHD	2.01	0.41
25:b:606:CLA:H192	25:b:616:CLA:H52	2.02	0.41
25:c:512:CLA:H203	25:c:513:CLA:H111	2.02	0.41
25:c:512:CLA:H162	25:c:513:CLA:H152	2.02	0.41
7:d:90:LEU:O	7:d:92:LEU:HG	2.20	0.41
9:f:11:THR:O	9:f:11:THR:HG22	2.20	0.41
13:l:15:ARG:HG2	13:l:19:TYR:CE1	2.55	0.41
15:o:163:LEU:C	15:o:164:MET:HE2	2.44	0.41
15:o:196:TYR:CB	15:o:212:LEU:HD21	2.16	0.41
25:s:303:CLA:H112	25:s:304:CLA:CMB	2.49	0.41
21:g:132:PHE:CD1	21:g:133:LYS:N	2.88	0.41
21:n:159:LEU:CD1	21:y:257:TRP:CG	2.95	0.41
21:n:162:TRP:CE3	21:y:257:TRP:HH2	2.37	0.41
21:y:145:ASP:OD2	21:y:150:PRO:HA	2.20	0.41
21:y:231:VAL:CG1	25:y:314:CLA:HAC2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:189:SER:HA	22:r:192:ILE:HG22	2.02	0.41
1:1:191:TYR:N	1:1:192:PRO:CD	2.82	0.41
2:2:219:ASN:O	2:2:220:GLY:C	2.61	0.41
24:2:603:CHL:HBC3	24:2:603:CHL:OMC	2.20	0.41
1:3:137:GLN:HE22	1:3:144:LEU:HA	1.84	0.41
4:A:56:PRO:CD	4:A:106:LEU:HD13	2.49	0.41
4:A:273:PHE:HB2	7:D:220:GLU:OE1	2.20	0.41
4:A:335:ASN:HB3	6:C:334:PRO:CB	2.49	0.41
5:B:160:GLY:HA3	5:B:180:PRO:HB3	2.01	0.41
5:B:226:TYR:CD2	5:B:231:MET:HB2	2.55	0.41
5:B:347:ARG:HA	5:B:352:ARG:O	2.20	0.41
25:B:613:CLA:H162	25:B:613:CLA:H143	1.55	0.41
6:C:449:ARG:NH1	11:I:28:PRO:HG3	2.27	0.41
25:C:505:CLA:H92	25:C:505:CLA:H61	1.74	0.41
25:C:510:CLA:H141	25:C:510:CLA:H161	1.67	0.41
7:D:205:VAL:HG21	25:D:402:CLA:H3A	2.02	0.41
12:K:27:PRO:HB2	12:K:30:TYR:HD1	1.85	0.41
29:L:103:SQD:H312	29:L:103:SQD:C35	2.51	0.41
15:O:100:LYS:CE	15:O:105:VAL:HG22	2.48	0.41
15:O:158:PHE:HE2	15:O:322:LYS:HB2	1.82	0.41
20:S:81:ILE:CG2	20:S:85:LEU:HD22	2.50	0.41
21:G:50:TRP:NE1	25:G:611:CLA:HED2	2.34	0.41
21:G:112:GLY:HA3	25:G:604:CLA:C1C	2.50	0.41
21:G:176:ARG:HG3	24:G:608:CHL:C1D	2.50	0.41
21:G:191:TYR:N	21:G:192:PRO:CD	2.82	0.41
25:N:603:CLA:C16	24:N:607:CHL:H193	2.50	0.41
21:Y:121:ARG:HD2	21:Y:241:ILE:HG22	2.01	0.41
21:Y:127:GLY:C	21:Y:137:GLN:HG3	2.44	0.41
21:Y:210:GLU:O	21:Y:214:LYS:HG3	2.20	0.41
21:Y:231:VAL:CG1	25:Y:314:CLA:HAC2	2.48	0.41
25:Y:315:CLA:HBD	25:Y:315:CLA:CBA	2.49	0.41
1:5:210:GLU:O	1:5:214:LYS:HG3	2.20	0.41
3:8:103:LEU:CD1	3:8:194:TYR:HD1	2.16	0.41
3:8:131:GLY:C	3:8:134:PRO:HD2	2.46	0.41
3:8:219:GLU:O	3:8:223:ARG:N	2.49	0.41
4:a:223:LEU:O	5:b:482:ILE:HG12	2.19	0.41
4:a:292:THR:CB	6:c:428:THR:HG23	2.50	0.41
28:b:619:BCR:H11C	28:b:619:BCR:H341	1.94	0.41
6:c:399:ALA:HB1	6:c:400:PRO:HD2	2.01	0.41
7:d:172:PRO:HG3	7:d:182:PHE:CZ	2.55	0.41
8:e:40:THR:OG1	8:e:42:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:188:TYR:O	20:s:192:ASN:N	2.54	0.41
25:g:610:CLA:H62	25:g:612:CLA:CMA	2.49	0.41
21:n:49:PRO:O	21:n:55:ARG:HA	2.20	0.41
21:y:132:PHE:CD1	21:y:133:LYS:N	2.88	0.41
25:r:603:CLA:C4C	25:r:608:CLA:H92	2.49	0.41
25:r:604:CLA:HMA2	24:r:605:CHL:HAC2	2.02	0.41
1:l:165:GLN:NE2	24:l:302:CHL:C1B	2.79	0.41
2:2:227:MET:HE3	2:2:231:PHE:CE2	2.55	0.41
1:3:191:TYR:CE2	1:3:212:LYS:CE	3.03	0.41
5:B:51:VAL:HG22	5:B:308:LYS:HD2	2.01	0.41
5:B:125:ASP:OD2	5:B:127:ARG:HG2	2.20	0.41
5:B:157:HIS:HE1	25:B:606:CLA:CHB	2.26	0.41
5:B:325:PHE:CD2	13:L:35:TYR:HB3	2.56	0.41
25:B:607:CLA:H91	25:B:607:CLA:H111	1.62	0.41
25:B:614:CLA:H91	25:B:614:CLA:H112	1.90	0.41
25:B:616:CLA:HBC2	25:B:616:CLA:HMC3	2.03	0.41
6:C:60:ILE:HG23	25:C:510:CLA:CMC	2.50	0.41
7:D:41:CYS:SG	25:D:403:CLA:HMB1	2.60	0.41
28:D:404:BCR:H11C	28:D:404:BCR:H341	1.96	0.41
15:O:290:THR:OG1	15:O:301:GLY:HA2	2.21	0.41
19:Z:23:VAL:HG22	19:Z:40:VAL:HG13	2.02	0.41
21:G:132:PHE:CD1	21:G:133:LYS:N	2.88	0.41
21:N:176:ARG:HG3	24:N:608:CHL:C1D	2.50	0.41
21:Y:91:THR:HA	21:Y:94:ARG:HB2	2.02	0.41
21:Y:191:TYR:CE2	21:Y:212:LYS:CE	3.03	0.41
25:Y:303:CLA:H13	25:Y:303:CLA:H172	1.80	0.41
25:Y:304:CLA:H93	24:Y:310:CHL:C9	2.50	0.41
25:Y:305:CLA:HMA1	39:Y:317:LUT:H3	2.01	0.41
2:6:227:MET:HE3	2:6:231:PHE:CE2	2.55	0.41
24:6:601:CHL:H112	24:6:601:CHL:H152	1.79	0.41
1:7:132:PHE:CD1	1:7:133:LYS:N	2.88	0.41
3:8:245:GLU:O	3:8:249:GLY:N	2.53	0.41
4:a:43:THR:HG21	4:a:118:HIS:ND1	2.36	0.41
5:b:69:LEU:HD21	25:b:603:CLA:OBD	2.20	0.41
5:b:475:PHE:CD1	7:d:141:PRO:HG3	2.55	0.41
6:c:109:PHE:O	6:c:113:VAL:HG23	2.19	0.41
6:c:135:LEU:HD23	6:c:135:LEU:C	2.45	0.41
7:d:316:TYR:O	7:d:320:ILE:HG12	2.20	0.41
10:h:24:LYS:HB3	10:h:25:PRO:HD3	2.02	0.41
21:g:160:ALA:HB3	24:g:605:CHL:OMC	2.20	0.41
21:n:57:LYS:NZ	21:n:66:SER:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:145:ASP:OD2	21:n:150:PRO:HA	2.19	0.41
24:n:607:CHL:HBA2	24:n:607:CHL:H3A	1.81	0.41
40:n:617:NEX:H201	40:n:617:NEX:H15	1.55	0.41
21:y:97:GLU:HA	21:y:190:LEU:CD1	2.24	0.41
21:y:218:ASN:OD1	25:y:312:CLA:CMD	2.67	0.41
22:r:55:ARG:O	22:r:57:LEU:HD23	2.20	0.41
1:1:49:PRO:O	1:1:55:ARG:HA	2.20	0.41
3:4:164:PHE:HB2	3:4:192:GLN:CD	2.45	0.41
3:4:251:THR:HG23	3:4:254:GLY:H	1.83	0.41
29:A:411:SQD:H132	29:A:411:SQD:H162	1.70	0.41
5:B:460:LEU:HD12	7:D:288:VAL:HG21	1.94	0.41
26:B:621:LHG:H311	26:B:621:LHG:H352	2.02	0.41
6:C:299:SER:HA	6:C:423:ARG:HH21	1.85	0.41
25:C:501:CLA:H151	25:C:507:CLA:H102	2.02	0.41
28:C:514:BCR:H20C	28:C:514:BCR:H361	1.84	0.41
7:D:92:LEU:HD22	25:D:403:CLA:HAA2	2.02	0.41
15:O:190:GLU:CD	15:O:215:VAL:HG13	2.45	0.41
28:T:101:BCR:HC31	28:b:618:BCR:H382	2.01	0.41
20:S:146:VAL:O	20:S:150:THR:OG1	2.38	0.41
21:G:62:PHE:CZ	21:Y:175:TYR:CE1	3.06	0.41
24:G:601:CHL:H122	24:Y:308:CHL:CAB	2.41	0.41
25:G:611:CLA:H41	25:G:611:CLA:H62	1.60	0.41
21:N:132:PHE:HB2	24:N:607:CHL:HMA3	2.01	0.41
25:N:613:CLA:C2C	25:N:613:CLA:H62	2.50	0.41
21:Y:165:GLN:OE1	24:Y:307:CHL:C4A	2.68	0.41
22:R:154:ALA:HA	22:R:157:VAL:HG12	2.03	0.41
22:R:255:GLY:HA2	25:R:612:CLA:C4C	2.50	0.41
2:6:92:PHE:HB3	2:6:96:ARG:CZ	2.50	0.41
25:6:602:CLA:HBA1	25:6:602:CLA:H3A	1.45	0.41
3:8:78:PRO:HB2	3:8:229:ILE:HG23	2.01	0.41
3:8:113:VAL:HG13	3:8:114:LEU:N	2.35	0.41
3:8:122:TRP:HB3	3:8:127:TRP:HB2	2.02	0.41
3:8:125:VAL:O	3:8:125:VAL:HG12	2.20	0.41
4:a:317:TRP:CE3	7:d:181:ARG:HD3	2.55	0.41
5:b:191:ASP:HB2	10:h:69:GLY:O	2.20	0.41
5:b:226:TYR:CD2	5:b:231:MET:HB2	2.55	0.41
6:c:47:GLY:HA3	6:c:137:PRO:O	2.21	0.41
6:c:201:ASN:O	6:c:231:GLU:CG	2.68	0.41
6:c:230:LEU:HD23	6:c:233:ILE:HD12	2.03	0.41
6:c:369:LEU:HD22	6:c:380:LEU:CD2	2.47	0.41
21:g:112:GLY:HA3	25:g:604:CLA:C1C	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:176:ARG:HG3	24:g:608:CHL:C1D	2.50	0.41
21:n:132:PHE:CD1	21:n:133:LYS:N	2.88	0.41
21:n:247:HIS:HD1	21:n:247:HIS:C	2.28	0.41
25:n:611:CLA:HBD	25:n:611:CLA:HAA1	2.02	0.41
40:y:318:NEX:H201	40:y:318:NEX:H15	1.71	0.41
25:r:612:CLA:HHB	39:r:615:LUT:C4	2.42	0.41
2:2:125:VAL:O	2:2:148:LEU:HD12	2.21	0.41
1:3:49:PRO:O	1:3:55:ARG:HA	2.20	0.41
4:A:194:MET:HE1	4:A:302:PHE:HD2	1.86	0.41
4:A:329:GLU:OE1	4:A:332:HIS:NE2	2.52	0.41
25:A:401:CLA:H142	25:A:401:CLA:H112	1.90	0.41
5:B:191:ASP:CG	10:H:70:ILE:HD13	2.46	0.41
5:B:356:VAL:O	5:B:356:VAL:HG13	2.19	0.41
25:B:601:CLA:H192	25:B:601:CLA:H162	1.69	0.41
25:B:609:CLA:HAA1	25:B:609:CLA:HBD	2.01	0.41
6:C:47:GLY:HA3	6:C:137:PRO:O	2.21	0.41
6:C:225:VAL:HG13	6:C:289:PHE:HD1	1.86	0.41
35:C:515:DGD:HE4	35:C:515:DGD:HO5E	1.68	0.41
20:S:173:LEU:O	20:S:176:VAL:HG22	2.21	0.41
21:G:244:LEU:HD22	39:G:615:LUT:H172	2.03	0.41
24:G:601:CHL:HMB1	26:Y:301:LHG:H161	2.02	0.41
40:G:617:NEX:H31	40:G:617:NEX:H391	1.57	0.41
21:N:114:VAL:HG13	21:N:241:ILE:HD11	2.02	0.41
21:N:132:PHE:CD1	21:N:133:LYS:N	2.88	0.41
25:N:610:CLA:C5	39:N:615:LUT:H28	2.41	0.41
22:R:103:LYS:HE3	22:R:105:LEU:CG	2.50	0.41
22:R:241:ALA:O	22:R:245:HIS:CD2	2.73	0.41
1:5:58:TYR:HD2	1:5:59:LEU:HG	1.86	0.41
24:6:601:CHL:HBB1	24:6:601:CHL:HHC	2.02	0.41
1:7:145:ASP:OD1	1:7:154:HIS:HA	2.21	0.41
1:7:210:GLU:O	1:7:214:LYS:HG3	2.20	0.41
4:a:56:PRO:CD	4:a:106:LEU:HD13	2.50	0.41
4:a:194:MET:HE1	4:a:302:PHE:HD2	1.86	0.41
5:b:7:ARG:HD3	25:b:611:CLA:CED	2.50	0.41
5:b:45:PHE:O	5:b:46:ASP:HB3	2.20	0.41
5:b:181:VAL:O	5:b:181:VAL:HG23	2.19	0.41
5:b:242:ILE:O	5:b:246:PHE:HD1	2.03	0.41
6:c:230:LEU:HD23	6:c:230:LEU:HA	1.85	0.41
25:c:503:CLA:H61	25:c:503:CLA:H101	1.81	0.41
8:e:67:THR:CA	23:u:102:ARG:HH11	2.33	0.41
12:k:30:TYR:CE2	19:z:5:PHE:HZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:k:43:ILE:O	12:k:46:PHE:HB2	2.21	0.41
28:k:101:BCR:H15C	28:k:101:BCR:H351	1.84	0.41
19:z:14:ILE:O	19:z:18:ILE:CD1	2.65	0.41
25:s:311:CLA:HBA1	25:s:311:CLA:H3A	1.69	0.41
21:g:152:LEU:O	21:g:153:VAL:C	2.63	0.41
25:g:611:CLA:HBA2	25:g:611:CLA:H3A	1.28	0.41
21:y:49:PRO:O	21:y:55:ARG:HA	2.20	0.41
25:y:304:CLA:H93	24:y:310:CHL:C9	2.50	0.41
22:r:103:LYS:HE3	22:r:105:LEU:CG	2.50	0.41
22:r:154:ALA:HA	22:r:157:VAL:HG12	2.02	0.41
22:r:241:ALA:O	22:r:245:HIS:CD2	2.73	0.41
25:r:612:CLA:H91	25:r:612:CLA:H112	1.58	0.41
40:r:617:NEX:H35	40:r:617:NEX:H401	1.52	0.41
2:2:118:VAL:O	2:2:122:TRP:CB	2.69	0.41
3:4:113:VAL:HG13	3:4:114:LEU:N	2.35	0.41
3:4:125:VAL:O	3:4:125:VAL:HG12	2.20	0.41
5:B:53:ASP:N	5:B:54:PRO:HD3	2.36	0.41
5:B:72:THR:CG2	5:B:80:ILE:HG22	2.26	0.41
5:B:191:ASP:HB2	10:H:69:GLY:O	2.20	0.41
6:C:30:THR:CG2	6:C:31:THR:HG23	2.46	0.41
6:C:130:ILE:HD11	25:C:511:CLA:H13	2.03	0.41
6:C:175:LEU:HD13	25:C:501:CLA:HMD1	2.03	0.41
7:D:240:GLN:NE2	7:D:242:GLU:HG2	2.36	0.41
25:D:403:CLA:H162	25:D:403:CLA:H122	1.57	0.41
15:O:220:ALA:CA	15:O:229:GLY:HA3	2.50	0.41
20:S:66:ASP:HA	20:S:78:ARG:NH2	2.36	0.41
21:G:97:GLU:CB	21:G:190:LEU:HD11	2.48	0.41
24:G:607:CHL:CMB	24:G:607:CHL:CBB	2.97	0.41
25:G:610:CLA:H92	25:G:610:CLA:H61	1.69	0.41
21:N:59:LEU:HD23	24:N:601:CHL:C2B	2.51	0.41
21:N:131:TRP:CD1	21:N:131:TRP:H	2.38	0.41
21:N:145:ASP:OD1	21:N:154:HIS:HA	2.21	0.41
21:N:191:TYR:CE2	21:N:212:LYS:CE	3.03	0.41
25:N:611:CLA:HBA2	25:N:611:CLA:H3A	1.40	0.41
21:Y:145:ASP:OD1	21:Y:154:HIS:HA	2.21	0.41
25:Y:303:CLA:HMC2	39:Y:317:LUT:C31	2.51	0.41
24:R:606:CHL:O2A	24:R:606:CHL:H2A	2.20	0.41
1:5:49:PRO:O	1:5:55:ARG:HA	2.20	0.41
1:5:164:THR:HG21	24:5:302:CHL:O1D	2.20	0.41
2:6:116:PRO:HG3	2:6:134:LYS:NZ	2.36	0.41
25:6:604:CLA:H52	25:6:604:CLA:H12	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:122:TRP:HA	3:8:127:TRP:CD1	2.40	0.41
3:8:194:TYR:OH	3:8:225:LYS:CG	2.68	0.41
4:a:72:LEU:O	4:a:72:LEU:HG	2.20	0.41
5:b:30:VAL:HG12	25:b:605:CLA:HMD3	2.02	0.41
5:b:65:PHE:CE2	25:b:604:CLA:HMA2	2.55	0.41
5:b:115:TRP:HH2	25:b:614:CLA:HMA2	1.84	0.41
5:b:125:ASP:OD2	5:b:127:ARG:HG2	2.20	0.41
5:b:367:PRO:HB3	7:d:346:VAL:HB	2.02	0.41
25:b:610:CLA:HAA2	25:b:610:CLA:HBD	2.02	0.41
25:b:610:CLA:HBB1	25:b:610:CLA:HHC	2.01	0.41
25:b:615:CLA:H61	25:b:615:CLA:H2	1.87	0.41
6:c:162:GLY:CA	6:c:248:GLY:HA2	2.48	0.41
15:o:146:LYS:CG	15:o:156:PRO:HB2	2.51	0.41
16:t:7:THR:CG2	28:t:101:BCR:H363	2.50	0.41
18:x:104:VAL:O	18:x:107:VAL:HG22	2.20	0.41
19:z:23:VAL:HG22	19:z:40:VAL:HG13	2.03	0.41
20:s:135:ASN:HD21	20:s:141:CYS:N	2.18	0.41
21:n:145:ASP:OD1	21:n:154:HIS:HA	2.21	0.41
21:n:210:GLU:O	21:n:214:LYS:HG3	2.20	0.41
25:y:303:CLA:HMC2	39:y:317:LUT:C31	2.51	0.41
25:y:314:CLA:H92	25:y:314:CLA:H61	1.56	0.41
2:2:100:VAL:HG21	2:2:190:LEU:HD23	2.02	0.41
1:3:145:ASP:OD1	1:3:154:HIS:HA	2.21	0.41
3:4:219:GLU:CG	3:4:219:GLU:O	2.66	0.41
3:4:231:HIS:HA	3:4:234:LEU:CD2	2.51	0.41
4:A:120:LEU:HA	4:A:123:VAL:HG22	2.03	0.41
5:B:45:PHE:O	5:B:46:ASP:HB3	2.20	0.41
5:B:217:LEU:HB3	25:R:614:CLA:CBA	2.50	0.41
5:B:290:ALA:O	5:B:294:GLU:OE1	2.39	0.41
6:C:75:PHE:CD1	6:C:86:LEU:HD11	2.56	0.41
9:F:11:THR:O	9:F:11:THR:HG22	2.20	0.41
10:H:59:GLU:HA	10:H:62:ASN:OD1	2.20	0.41
29:L:101:SQD:H251	29:L:101:SQD:H92	2.03	0.41
20:S:175:VAL:HG22	24:S:307:CHL:HBC1	2.02	0.41
21:G:109:GLY:HA2	39:G:616:LUT:H181	2.03	0.41
21:G:210:GLU:O	21:G:214:LYS:HG3	2.20	0.41
25:G:603:CLA:HED3	39:N:616:LUT:H372	2.02	0.41
25:G:610:CLA:HBA2	39:G:615:LUT:O23	2.20	0.41
25:G:614:CLA:HBA2	25:G:614:CLA:H3A	1.15	0.41
21:N:57:LYS:NZ	21:N:66:SER:HB2	2.35	0.41
21:N:139:PHE:CD2	24:N:607:CHL:OBD	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:145:ASP:OD2	21:N:150:PRO:HA	2.19	0.41
21:N:165:GLN:NE2	24:N:606:CHL:NB	2.63	0.41
25:N:612:CLA:HHC	25:N:612:CLA:CBB	2.44	0.41
21:Y:58:TYR:HD2	21:Y:59:LEU:HG	1.86	0.41
21:Y:95:ASN:C	25:Y:303:CLA:HMA1	2.45	0.41
25:R:602:CLA:H41	25:R:602:CLA:H62	1.89	0.41
25:R:614:CLA:HAA1	25:R:614:CLA:HBD	2.02	0.41
1:5:145:ASP:OD1	1:5:154:HIS:HA	2.21	0.41
2:6:205:ASP:O	2:6:209:PHE:CD1	2.74	0.41
2:6:218:LYS:HA	2:6:221:ARG:NE	2.35	0.41
1:7:58:TYR:CE2	1:7:59:LEU:HD12	2.56	0.41
4:a:79:SER:CB	7:d:302:GLN:HE22	2.33	0.41
5:b:127:ARG:HH22	10:h:31:GLY:HA3	1.85	0.41
5:b:187:VAL:HG23	5:b:188:GLU:OE1	2.20	0.41
5:b:342:GLY:HA3	5:b:403:GLY:O	2.20	0.41
25:b:613:CLA:O1D	25:b:613:CLA:H2A	2.20	0.41
6:c:75:PHE:CD1	6:c:86:LEU:HD11	2.56	0.41
6:c:215:LYS:CD	6:c:221:GLU:HB3	2.51	0.41
6:c:239:TRP:CZ3	25:y:315:CLA:CMB	3.03	0.41
25:c:510:CLA:H172	25:c:510:CLA:C1D	2.51	0.41
7:d:151:ILE:O	7:d:155:VAL:HG23	2.20	0.41
7:d:297:TYR:O	7:d:316:TYR:OH	2.30	0.41
15:o:286:THR:HG23	15:o:286:THR:O	2.19	0.41
20:s:135:ASN:ND2	20:s:141:CYS:N	2.66	0.41
25:s:305:CLA:HBB1	39:s:316:LUT:C18	2.51	0.41
21:g:49:PRO:O	21:g:55:ARG:HA	2.20	0.41
21:g:58:TYR:HD2	21:g:59:LEU:HG	1.86	0.41
21:g:215:GLU:CG	25:g:610:CLA:NB	2.78	0.41
24:g:601:CHL:HHC	24:g:601:CHL:HBB1	2.03	0.41
25:g:602:CLA:HAB	39:g:616:LUT:H32	2.03	0.41
24:g:609:CHL:H2	24:g:609:CHL:H61	1.73	0.41
40:g:617:NEX:H30	40:g:617:NEX:C40	2.51	0.41
21:n:131:TRP:CD1	21:n:131:TRP:H	2.38	0.41
21:n:244:LEU:HD12	21:n:244:LEU:HA	1.90	0.41
24:n:607:CHL:H171	25:y:303:CLA:H162	2.01	0.41
24:n:609:CHL:H143	24:n:609:CHL:H111	1.91	0.41
2:2:120:GLN:HB3	2:2:129:GLU:HG2	2.03	0.41
1:3:229:PHE:CE2	1:3:240:PRO:CB	3.04	0.41
3:4:103:LEU:HD22	3:4:193:GLY:HA2	2.02	0.41
3:4:131:GLY:C	3:4:134:PRO:HD2	2.46	0.41
4:A:43:THR:HG21	4:A:118:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:PHE:HE2	29:A:407:SQD:H92	1.86	0.41
5:B:7:ARG:HD3	25:B:611:CLA:CED	2.50	0.41
5:B:256:MET:O	5:B:448:ARG:HD3	2.20	0.41
28:B:618:BCR:H382	28:t:101:BCR:HC31	2.01	0.41
28:B:619:BCR:H15C	28:B:619:BCR:H351	1.87	0.41
11:I:28:PRO:HB3	17:W:131:LEU:CD1	2.51	0.41
15:O:214:THR:HG21	15:O:233:VAL:HA	2.01	0.41
19:Z:58:ASN:C	19:Z:58:ASN:HD22	2.27	0.41
25:S:312:CLA:HAA2	25:S:312:CLA:HBD	2.03	0.41
21:G:58:TYR:CE2	21:G:59:LEU:HD12	2.56	0.41
21:G:229:PHE:CE2	21:G:240:PRO:CB	3.04	0.41
21:N:49:PRO:O	21:N:55:ARG:HA	2.20	0.41
21:N:91:THR:HA	21:N:94:ARG:HB2	2.02	0.41
21:N:206:GLU:N	21:N:206:GLU:CD	2.76	0.41
25:N:613:CLA:C14	25:N:613:CLA:H2	2.45	0.41
21:Y:58:TYR:CE2	21:Y:59:LEU:HD12	2.56	0.41
21:Y:107:MET:CE	25:Y:311:CLA:CHC	2.97	0.41
25:Y:311:CLA:H122	39:Y:316:LUT:H403	2.01	0.41
22:R:155:LEU:HD23	22:R:155:LEU:HA	1.90	0.41
1:5:131:TRP:CD1	1:5:131:TRP:H	2.38	0.41
2:6:104:ARG:NH1	2:6:108:LEU:HD11	2.34	0.41
2:6:125:VAL:O	2:6:148:LEU:HD12	2.21	0.41
2:6:139:ILE:O	2:6:139:ILE:CG2	2.68	0.41
3:8:103:LEU:HD22	3:8:193:GLY:HA2	2.02	0.41
4:a:273:PHE:HB2	7:d:220:GLU:OE1	2.20	0.41
29:a:412:SQD:H131	16:t:21:ILE:CD1	2.51	0.41
5:b:157:HIS:HE2	5:b:164:PRO:HD2	1.85	0.41
5:b:207:THR:HG21	30:b:623:LMG:H332	2.02	0.41
5:b:223:GLN:HG2	10:h:36:GLY:H	1.86	0.41
6:c:130:ILE:HD11	25:c:511:CLA:H13	2.03	0.41
6:c:166:ILE:O	6:c:170:VAL:HG23	2.21	0.41
6:c:322:GLN:NE2	6:c:384:ILE:HD12	2.27	0.41
10:h:59:GLU:HA	10:h:62:ASN:OD1	2.20	0.41
20:s:175:VAL:HG22	24:s:307:CHL:HBC1	2.02	0.41
20:s:220:LEU:O	20:s:224:LYS:HG3	2.20	0.41
20:s:242:GLN:HG2	25:s:313:CLA:ND	2.36	0.41
24:s:306:CHL:HBB1	39:s:316:LUT:H161	2.03	0.41
21:g:191:TYR:CE2	21:g:212:LYS:CE	3.03	0.41
25:g:604:CLA:CHC	40:g:617:NEX:H222	2.51	0.41
24:g:608:CHL:H93	24:g:608:CHL:H62	1.82	0.41
21:n:55:ARG:HE	21:n:55:ARG:HB2	1.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:86:SER:OG	25:n:602:CLA:O1A	2.33	0.41
21:n:176:ARG:HG3	24:n:608:CHL:C1D	2.50	0.41
25:n:610:CLA:HMC1	39:n:615:LUT:H31	2.00	0.41
25:n:613:CLA:C2C	25:n:613:CLA:H62	2.51	0.41
21:y:58:TYR:HD2	21:y:59:LEU:HG	1.86	0.41
21:y:176:ARG:HG3	24:y:309:CHL:C1D	2.50	0.41
21:y:228:GLY:O	21:y:231:VAL:N	2.53	0.41
21:y:231:VAL:CG2	25:y:314:CLA:HAC2	2.43	0.41
21:y:247:HIS:HD1	21:y:247:HIS:C	2.28	0.41
26:y:319:LHG:H181	26:y:319:LHG:H152	1.91	0.41
22:r:127:TYR:CE2	22:r:135:ARG:HD2	2.54	0.41
25:r:602:CLA:H62	25:r:602:CLA:H41	1.89	0.41
1:1:58:TYR:CE2	1:1:59:LEU:HD12	2.56	0.41
2:2:116:PRO:HG3	2:2:134:LYS:NZ	2.36	0.41
1:3:58:TYR:HD2	1:3:59:LEU:HG	1.86	0.41
1:3:209:ALA:HA	1:3:212:LYS:CG	2.34	0.41
3:4:148:THR:O	3:4:152:LEU:HD13	2.21	0.41
3:4:157:GLU:O	3:4:161:TRP:CD1	2.65	0.41
3:4:241:ILE:O	3:4:245:GLU:HG2	2.19	0.41
4:A:21:ILE:O	4:A:30:ILE:O	2.39	0.41
5:B:39:LEU:HD12	28:t:101:BCR:H271	1.99	0.41
5:B:84:THR:HG21	15:o:204:PRO:CG	2.51	0.41
5:B:181:VAL:O	5:B:181:VAL:HG23	2.19	0.41
5:B:242:ILE:O	5:B:246:PHE:HD1	2.03	0.41
5:B:285:TYR:HD2	23:U:88:TYR:CD2	2.39	0.41
25:B:605:CLA:H162	25:B:609:CLA:HBB2	2.01	0.41
6:C:261:ARG:HA	6:C:266:TRP:HE1	1.86	0.41
6:C:322:GLN:NE2	6:C:384:ILE:HD12	2.27	0.41
25:C:506:CLA:H13	25:C:506:CLA:H91	2.01	0.41
25:C:512:CLA:H203	25:C:513:CLA:H111	2.02	0.41
26:D:406:LHG:H302	16:T:17:ILE:HG23	2.03	0.41
15:O:204:PRO:CG	5:b:84:THR:HG21	2.51	0.41
18:X:78:GLY:O	18:X:81:PRO:HG2	2.21	0.41
19:Z:18:ILE:HD12	19:Z:18:ILE:H	1.86	0.41
20:S:67:ARG:NH1	20:S:87:GLY:HA2	2.35	0.41
20:S:129:ILE:HD11	20:S:239:PHE:CE1	2.56	0.41
20:S:135:ASN:HD21	20:S:141:CYS:N	2.18	0.41
20:S:242:GLN:HG2	25:S:313:CLA:ND	2.36	0.41
24:S:306:CHL:HBB1	39:S:316:LUT:H161	2.03	0.41
21:G:58:TYR:HD2	21:G:59:LEU:HG	1.85	0.41
21:G:78:TYR:CE1	24:G:601:CHL:HMD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:145:ASP:OD1	21:G:154:HIS:HA	2.21	0.41
21:G:173:GLU:OE2	24:G:609:CHL:NA	2.53	0.41
25:G:604:CLA:CHC	40:G:617:NEX:H222	2.51	0.41
21:N:121:ARG:HD2	21:N:241:ILE:HG22	2.03	0.41
24:N:601:CHL:HMD2	26:N:618:LHG:HC41	2.03	0.41
25:N:604:CLA:HBA1	25:N:604:CLA:H3A	1.79	0.41
24:N:607:CHL:H112	24:N:607:CHL:H91	1.71	0.41
25:N:611:CLA:HAA1	25:N:611:CLA:HBD	2.03	0.41
21:Y:57:LYS:NZ	21:Y:66:SER:HB3	2.36	0.41
21:Y:152:LEU:O	21:Y:153:VAL:C	2.63	0.41
21:Y:229:PHE:CD2	21:Y:240:PRO:CB	3.04	0.41
21:Y:229:PHE:CE2	21:Y:240:PRO:CB	3.04	0.41
21:Y:252:VAL:O	21:Y:255:ASN:ND2	2.54	0.41
24:Y:302:CHL:H202	24:Y:302:CHL:H161	1.75	0.41
25:Y:303:CLA:H101	39:Y:317:LUT:H371	2.02	0.41
22:R:103:LYS:HE3	22:R:105:LEU:CD2	2.47	0.41
22:R:167:ASP:O	22:R:171:VAL:HG23	2.21	0.41
25:R:603:CLA:NB	25:R:608:CLA:H111	2.35	0.41
25:R:603:CLA:C4C	25:R:608:CLA:H92	2.49	0.41
1:5:132:PHE:CD1	1:5:133:LYS:N	2.88	0.41
1:7:91:THR:HA	1:7:94:ARG:HB2	2.02	0.41
1:7:229:PHE:CD2	1:7:240:PRO:CB	3.04	0.41
3:8:193:GLY:O	3:8:195:PRO:HD3	2.20	0.41
4:a:201:GLY:HA3	4:a:286:THR:HB	2.03	0.41
4:a:214:MET:HE2	4:a:214:MET:HB2	1.91	0.41
28:a:407:BCR:H371	28:a:407:BCR:H24C	1.77	0.41
5:b:200:SER:OG	25:b:602:CLA:HMB1	2.21	0.41
5:b:324:LEU:HD11	5:b:453:PHE:CZ	2.56	0.41
5:b:391:SER:HB3	5:b:394:GLN:CD	2.46	0.41
25:b:602:CLA:H93	25:b:602:CLA:H61	1.67	0.41
6:c:235:GLY:O	6:c:239:TRP:HD1	2.02	0.41
6:c:327:ASN:ND2	6:c:330:SER:HB2	2.34	0.41
25:c:503:CLA:H193	25:c:503:CLA:H161	1.60	0.41
25:c:506:CLA:H141	25:c:506:CLA:H162	1.63	0.41
35:c:516:DGD:HAN2	35:c:516:DGD:HAW2	1.43	0.41
7:d:240:GLN:NE2	7:d:242:GLU:HG2	2.36	0.41
29:l:102:SQD:H271	29:l:102:SQD:C13	2.35	0.41
19:z:16:SER:HB3	28:z:101:BCR:C31	2.51	0.41
20:s:81:ILE:CG2	20:s:85:LEU:HD22	2.50	0.41
20:s:177:ALA:HB1	24:s:306:CHL:HED2	2.02	0.41
25:s:312:CLA:HAA2	25:s:312:CLA:HBD	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:115:PHE:HD2	25:g:604:CLA:HHD	1.83	0.41
21:g:131:TRP:CD1	21:g:131:TRP:H	2.38	0.41
21:g:145:ASP:OD1	21:g:154:HIS:HA	2.21	0.41
21:g:244:LEU:HD22	39:g:615:LUT:H172	2.03	0.41
24:g:608:CHL:CMC	24:g:608:CHL:HBC3	2.51	0.41
25:g:611:CLA:H62	25:g:611:CLA:H41	1.60	0.41
25:g:611:CLA:HBC2	25:g:611:CLA:CMC	2.51	0.41
21:n:58:TYR:HD2	21:n:59:LEU:HG	1.86	0.41
21:n:152:LEU:O	21:n:153:VAL:C	2.63	0.41
21:n:191:TYR:N	21:n:192:PRO:CD	2.82	0.41
21:n:225:SER:O	21:n:229:PHE:HD1	2.01	0.41
21:n:227:PHE:HD2	25:n:602:CLA:C20	2.29	0.41
25:n:603:CLA:C16	24:n:607:CHL:H193	2.50	0.41
21:y:55:ARG:HE	21:y:55:ARG:HB2	1.36	0.41
21:y:59:LEU:CD2	24:y:302:CHL:C2B	2.94	0.41
21:y:145:ASP:OD1	21:y:154:HIS:HA	2.21	0.41
24:y:307:CHL:H12	24:y:307:CHL:HED1	2.03	0.41
24:y:309:CHL:H91	24:y:309:CHL:H112	1.60	0.41
25:y:315:CLA:HED2	25:y:315:CLA:HBD	1.82	0.41
26:y:319:LHG:H361	26:y:319:LHG:H331	1.71	0.41
25:r:603:CLA:H111	25:r:603:CLA:H93	1.62	0.41
25:r:604:CLA:HMA2	24:r:605:CHL:C3C	2.51	0.41
1:1:91:THR:HA	1:1:94:ARG:HB2	2.03	0.41
2:2:92:PHE:HB3	2:2:96:ARG:CZ	2.50	0.41
2:2:134:LYS:O	2:2:137:SER:OG	2.22	0.41
2:2:205:ASP:O	2:2:209:PHE:CD1	2.74	0.41
25:2:605:CLA:HAA1	25:2:605:CLA:CBF	2.28	0.41
1:3:131:TRP:CD1	1:3:131:TRP:H	2.38	0.41
4:A:98:GLU:HA	4:A:98:GLU:OE2	2.20	0.41
25:A:405:CLA:H112	25:A:405:CLA:H93	1.81	0.41
25:B:604:CLA:H161	25:B:604:CLA:H141	1.83	0.41
6:C:56:HIS:O	6:C:60:ILE:HG13	2.21	0.41
6:C:67:MET:HB3	6:C:88:LEU:CD1	2.51	0.41
25:C:508:CLA:O2A	25:C:510:CLA:H43	2.20	0.41
25:C:513:CLA:H11	28:C:514:BCR:H381	2.02	0.41
7:D:347:LEU:HD23	7:D:347:LEU:HA	1.92	0.41
21:G:91:THR:HA	21:G:94:ARG:HB2	2.03	0.41
25:G:611:CLA:HBC3	26:Y:301:LHG:H252	2.03	0.41
22:R:113:ARG:HG2	22:R:115:GLU:OE2	2.21	0.41
2:6:57:LYS:HD3	2:6:63:SER:OG	2.21	0.41
2:6:118:VAL:O	2:6:122:TRP:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:49:PRO:O	1:7:55:ARG:HA	2.20	0.41
3:8:231:HIS:HA	3:8:234:LEU:CD2	2.51	0.41
3:8:240:LEU:HG	3:8:244:PHE:CE2	2.56	0.41
4:a:96:ILE:HG22	25:a:406:CLA:OBD	2.21	0.41
4:a:104:GLU:OE2	15:o:166:ARG:HD2	2.21	0.41
4:a:141:PRO:HB3	42:a:513:HOH:O	2.21	0.41
4:a:147:TYR:C	4:a:150:PRO:HD2	2.46	0.41
25:a:402:CLA:HBD	25:a:403:CLA:HAC2	2.03	0.41
5:b:168:VAL:HG13	5:b:195:PRO:HG2	2.03	0.41
5:b:217:LEU:HB3	25:r:614:CLA:CBA	2.50	0.41
5:b:290:ALA:O	5:b:294:GLU:OE1	2.39	0.41
25:b:601:CLA:H92	28:h:101:BCR:H402	2.03	0.41
25:b:611:CLA:H122	25:b:611:CLA:H162	1.73	0.41
28:b:617:BCR:H312	30:b:620:LMG:H341	2.02	0.41
26:b:621:LHG:H311	26:b:621:LHG:H352	2.02	0.41
6:c:175:LEU:HD13	25:c:501:CLA:HMD1	2.03	0.41
25:c:513:CLA:H11	28:c:514:BCR:H381	2.02	0.41
25:c:513:CLA:H93	28:c:514:BCR:H393	2.03	0.41
25:c:513:CLA:H43	24:s:302:CHL:CBB	2.51	0.41
10:h:47:MET:HE2	10:h:47:MET:HB3	1.91	0.41
29:l:102:SQD:H251	29:l:102:SQD:H92	2.03	0.41
20:s:67:ARG:HH12	20:s:92:ASP:CG	2.29	0.41
26:s:301:LHG:HC91	24:s:302:CHL:OMC	2.21	0.41
21:n:59:LEU:HD23	24:n:601:CHL:C2B	2.51	0.41
21:n:91:THR:HA	21:n:94:ARG:HB2	2.03	0.41
24:n:607:CHL:H51	24:n:607:CHL:H8	1.66	0.41
21:y:58:TYR:CE2	21:y:59:LEU:HD12	2.56	0.41
25:y:303:CLA:H101	39:y:317:LUT:H371	2.02	0.41
40:r:617:NEX:H191	40:r:617:NEX:C12	2.51	0.41
2:2:86:SER:HG	2:2:92:PHE:HE1	1.65	0.40
1:3:58:TYR:CE2	1:3:59:LEU:HD12	2.56	0.40
1:3:91:THR:HA	1:3:94:ARG:HB2	2.02	0.40
1:3:210:GLU:O	1:3:214:LYS:HG3	2.20	0.40
25:A:401:CLA:HBD	25:A:402:CLA:HAC2	2.03	0.40
5:B:73:ASN:O	5:B:92:SER:HB2	2.21	0.40
5:B:207:THR:HG21	30:B:623:LMG:H332	2.02	0.40
6:C:185:VAL:CG2	6:C:230:LEU:HD13	2.49	0.40
25:C:510:CLA:H2	25:C:510:CLA:H61	1.67	0.40
7:D:20:ASP:CG	7:D:24:ARG:HH11	2.25	0.40
7:D:65:ALA:HB1	7:D:70:GLU:OE2	2.21	0.40
7:D:201:GLY:C	25:D:402:CLA:HMA1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:67:THR:HA	23:U:102:ARG:HH11	1.86	0.40
9:F:38:GLN:O	9:F:39:ARG:HB2	2.21	0.40
12:K:43:ILE:O	12:K:46:PHE:HB2	2.21	0.40
20:S:68:ARG:NH2	26:S:301:LHG:O3	2.53	0.40
20:S:220:LEU:O	20:S:224:LYS:HG3	2.20	0.40
21:G:121:ARG:HD2	21:G:241:ILE:HG22	2.02	0.40
21:N:58:TYR:CE2	21:N:59:LEU:HD12	2.56	0.40
24:N:606:CHL:HMB2	40:N:617:NEX:C39	2.51	0.40
24:N:606:CHL:HAA1	40:N:617:NEX:H28	2.02	0.40
25:N:610:CLA:H52	39:N:615:LUT:C30	2.49	0.40
24:Y:309:CHL:C1	39:Y:316:LUT:H383	2.47	0.40
1:7:191:TYR:CE2	1:7:212:LYS:CE	3.03	0.40
5:b:42:LEU:HD11	5:b:93:TYR:HB3	2.04	0.40
5:b:73:ASN:O	5:b:92:SER:HB2	2.21	0.40
6:c:225:VAL:HG13	6:c:289:PHE:HD1	1.86	0.40
26:c:517:LHG:HC82	17:w:113:TRP:HE1	1.84	0.40
7:d:341:ILE:O	7:d:341:ILE:CG2	2.69	0.40
11:i:28:PRO:HB3	17:w:131:LEU:CD1	2.51	0.40
20:s:129:ILE:HD11	20:s:239:PHE:CE1	2.56	0.40
21:g:62:PHE:CZ	21:y:175:TYR:CE1	3.06	0.40
21:g:214:LYS:HG2	25:g:611:CLA:O2D	2.21	0.40
25:g:603:CLA:HED3	39:n:616:LUT:H372	2.02	0.40
21:n:139:PHE:CD2	24:n:607:CHL:OBD	2.74	0.40
21:n:152:LEU:HD23	21:n:152:LEU:HA	1.92	0.40
21:n:158:ILE:CD1	21:y:257:TRP:CE3	2.98	0.40
21:n:229:PHE:CE2	21:n:240:PRO:CB	3.04	0.40
25:y:315:CLA:HED2	25:y:315:CLA:CAA	2.48	0.40
1:1:131:TRP:CD1	1:1:131:TRP:H	2.38	0.40
4:A:196:PRO:HG3	4:A:300:PHE:CZ	2.57	0.40
4:A:215:HIS:CE1	33:A:413:BCT:O2	2.75	0.40
5:B:13:LEU:HD23	5:B:13:LEU:C	2.47	0.40
5:B:42:LEU:HD11	5:B:93:TYR:HB3	2.04	0.40
5:B:391:SER:HB3	5:B:394:GLN:OE1	2.21	0.40
5:B:467:ILE:HG21	7:D:127:MET:HE2	2.03	0.40
25:B:615:CLA:H121	25:B:616:CLA:HMA3	2.02	0.40
6:C:369:LEU:HD21	6:C:384:ILE:CG1	2.46	0.40
25:C:502:CLA:HAA1	25:C:502:CLA:CBD	2.40	0.40
19:Z:42:SER:O	19:Z:43:GLY:C	2.63	0.40
24:G:608:CHL:CMC	24:G:608:CHL:HBC3	2.51	0.40
25:G:611:CLA:CMC	25:G:611:CLA:HBC2	2.51	0.40
21:N:196:PHE:CE2	24:N:608:CHL:HBC2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:229:PHE:CE2	21:N:240:PRO:CB	3.04	0.40
21:N:231:VAL:CG1	25:N:613:CLA:HAC1	2.46	0.40
25:N:610:CLA:H62	25:N:610:CLA:H41	1.67	0.40
21:Y:161:ILE:CG2	24:Y:308:CHL:HBC1	2.52	0.40
22:R:189:SER:HA	22:R:192:ILE:HG22	2.02	0.40
1:5:229:PHE:CE2	1:5:240:PRO:CB	3.04	0.40
1:7:209:ALA:HA	1:7:212:LYS:CG	2.34	0.40
4:a:223:LEU:HD12	7:d:140:ARG:NH2	2.36	0.40
5:b:53:ASP:N	5:b:54:PRO:HD3	2.36	0.40
5:b:347:ARG:HA	5:b:352:ARG:O	2.20	0.40
25:b:605:CLA:H141	25:b:605:CLA:H161	1.73	0.40
35:b:626:DGD:HA81	35:b:626:DGD:HA52	1.83	0.40
6:c:56:HIS:O	6:c:60:ILE:HG13	2.21	0.40
6:c:319:VAL:HG13	6:c:320:ARG:N	2.36	0.40
25:c:501:CLA:H162	25:c:501:CLA:H143	1.81	0.40
25:c:505:CLA:H142	25:c:505:CLA:H111	1.90	0.40
25:c:508:CLA:CBB	25:c:509:CLA:HMA3	2.51	0.40
25:c:508:CLA:O2A	25:c:510:CLA:H43	2.20	0.40
25:c:508:CLA:CAB	25:c:510:CLA:H3A	2.50	0.40
7:d:41:CYS:SG	25:d:403:CLA:HMB1	2.60	0.40
7:d:179:ILE:HG21	25:d:401:CLA:CHD	2.52	0.40
26:d:406:LHG:H302	16:t:17:ILE:HG23	2.03	0.40
9:f:38:GLN:O	9:f:39:ARG:HB2	2.20	0.40
28:h:101:BCR:H403	28:h:101:BCR:C23	2.42	0.40
11:i:21:PHE:O	11:i:25:SER:OG	2.37	0.40
19:z:18:ILE:HD12	19:z:18:ILE:H	1.86	0.40
25:s:311:CLA:HHC	25:s:311:CLA:HBB1	2.03	0.40
21:g:82:THR:HG21	24:y:310:CHL:CAA	2.49	0.40
21:g:229:PHE:CE2	21:g:240:PRO:CB	3.04	0.40
21:y:57:LYS:NZ	21:y:66:SER:HB3	2.36	0.40
21:y:191:TYR:CE2	21:y:212:LYS:CE	3.03	0.40
22:r:167:ASP:O	22:r:171:VAL:HG23	2.21	0.40
22:r:174:VAL:HG23	22:r:175:ASP:N	2.36	0.40
25:r:609:CLA:HAB	39:r:615:LUT:H32	2.03	0.40
25:r:609:CLA:O1D	25:r:609:CLA:H2A	2.21	0.40
4:A:81:ALA:CB	4:A:175:GLY:HA3	2.49	0.40
4:A:110:GLY:N	4:A:111:PRO:CD	2.85	0.40
5:B:198:ILE:O	5:B:201:HIS:HB3	2.21	0.40
5:B:223:GLN:HG2	10:H:36:GLY:H	1.86	0.40
5:B:288:VAL:O	5:B:292:LEU:HG	2.22	0.40
5:B:324:LEU:HD11	5:B:453:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:603:CLA:H193	25:B:603:CLA:H162	1.54	0.40
6:C:118:HIS:CE1	30:C:520:LMG:H212	2.57	0.40
7:D:341:ILE:O	7:D:341:ILE:CG2	2.69	0.40
15:O:131:TYR:O	15:O:177:PRO:HA	2.21	0.40
15:O:217:GLN:OE1	15:O:232:LEU:HD12	2.21	0.40
16:T:7:THR:CG2	28:T:101:BCR:H363	2.50	0.40
17:W:101:LEU:O	17:W:105:LEU:HD13	2.22	0.40
18:X:104:VAL:O	18:X:107:VAL:HG22	2.20	0.40
20:S:188:TYR:O	20:S:192:ASN:N	2.54	0.40
20:S:213:LYS:HE3	20:S:213:LYS:HB3	1.91	0.40
24:G:601:CHL:HMB3	26:Y:301:LHG:H161	2.03	0.40
25:G:602:CLA:H51	25:G:602:CLA:HMB3	2.04	0.40
21:Y:107:MET:HE3	25:Y:311:CLA:HHC	2.03	0.40
24:Y:308:CHL:CBC	24:Y:308:CHL:CHD	2.98	0.40
22:R:174:VAL:HG23	22:R:175:ASP:N	2.36	0.40
2:6:100:VAL:HG21	2:6:190:LEU:HD23	2.02	0.40
2:6:120:GLN:HB3	2:6:129:GLU:HG2	2.03	0.40
25:6:604:CLA:HAA2	3:8:178:TRP:O	2.22	0.40
1:7:229:PHE:CE2	1:7:240:PRO:CB	3.04	0.40
4:a:95:PRO:HB2	4:a:97:TRP:CE2	2.56	0.40
5:b:191:ASP:CG	10:h:70:ILE:HD13	2.46	0.40
5:b:294:GLU:O	5:b:295:ASN:HB2	2.20	0.40
5:b:324:LEU:O	5:b:450:TRP:HH2	2.04	0.40
25:b:616:CLA:HBC2	25:b:616:CLA:HMC3	2.03	0.40
6:c:30:THR:CG2	6:c:31:THR:HG23	2.46	0.40
6:c:67:MET:HB3	6:c:88:LEU:CD1	2.51	0.40
25:c:509:CLA:H161	25:c:509:CLA:H141	1.75	0.40
7:d:92:LEU:HD22	25:d:403:CLA:HAA2	2.02	0.40
28:k:101:BCR:H24C	28:k:101:BCR:H371	1.83	0.40
13:l:3:GLN:HG3	13:l:4:SER:N	2.34	0.40
15:o:190:GLU:CD	15:o:215:VAL:HG13	2.45	0.40
15:o:290:THR:OG1	15:o:301:GLY:HA2	2.21	0.40
19:z:58:ASN:HD22	19:z:58:ASN:C	2.27	0.40
25:s:312:CLA:HAA2	25:s:312:CLA:CBD	2.52	0.40
24:g:601:CHL:HMB1	26:y:301:LHG:H161	2.02	0.40
25:g:611:CLA:HBC2	26:y:301:LHG:H312	2.03	0.40
21:n:80:TRP:CZ3	39:n:616:LUT:H383	2.57	0.40
21:y:56:VAL:CG1	24:y:302:CHL:HBC1	2.51	0.40
21:y:60:GLY:H	24:y:302:CHL:CHC	2.35	0.40
21:y:229:PHE:CE2	21:y:240:PRO:CB	3.04	0.40
25:y:313:CLA:HBB1	39:y:316:LUT:H14	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:153:GLY:HA2	25:r:604:CLA:C3C	2.51	0.40
1:1:145:ASP:OD1	1:1:154:HIS:HA	2.21	0.40
1:3:229:PHE:HD2	1:3:240:PRO:CG	2.35	0.40
4:A:74:GLY:HA3	14:M:1:MET:HE2	2.04	0.40
5:B:223:GLN:CA	10:H:33:VAL:HG11	2.45	0.40
5:B:391:SER:HB3	5:B:394:GLN:CD	2.46	0.40
25:C:510:CLA:CHB	25:C:510:CLA:H13	2.52	0.40
7:D:54:THR:HG22	9:F:34:MET:HE1	2.04	0.40
29:L:101:SQD:H292	29:L:101:SQD:C15	2.52	0.40
15:O:146:LYS:CG	15:O:156:PRO:HB2	2.51	0.40
19:Z:16:SER:HB3	28:Z:101:BCR:C31	2.51	0.40
24:G:609:CHL:H43	24:N:601:CHL:H12	2.03	0.40
21:N:58:TYR:HD2	21:N:59:LEU:HG	1.86	0.40
25:N:602:CLA:HAB	39:N:616:LUT:H30	2.02	0.40
25:Y:313:CLA:HBA1	25:Y:313:CLA:HMA2	2.04	0.40
22:R:103:LYS:HE3	22:R:105:LEU:CD1	2.47	0.40
22:R:127:TYR:OH	22:R:138:GLU:OE2	2.38	0.40
25:R:603:CLA:C1D	25:R:608:CLA:H61	2.52	0.40
1:5:91:THR:HA	1:5:94:ARG:HB2	2.02	0.40
2:6:251:ASN:HB3	25:6:605:CLA:CHB	2.50	0.40
1:7:58:TYR:HD2	1:7:59:LEU:HG	1.86	0.40
3:8:155:TRP:O	3:8:159:LYS:HG3	2.21	0.40
4:a:275:LEU:O	4:a:279:PRO:HD2	2.21	0.40
25:a:402:CLA:H112	25:a:402:CLA:H142	1.90	0.40
5:b:325:PHE:CD2	13:l:35:TYR:HB3	2.56	0.40
25:b:615:CLA:H121	25:b:616:CLA:HMA3	2.02	0.40
6:c:60:ILE:HG23	25:c:510:CLA:CMC	2.50	0.40
6:c:75:PHE:CZ	6:c:77:PRO:HA	2.56	0.40
25:c:507:CLA:H62	25:c:507:CLA:H41	1.80	0.40
9:f:16:ALA:O	9:f:20:LEU:HD13	2.22	0.40
38:f:101:HEM:HHC	38:f:101:HEM:CBB	2.46	0.40
10:h:54:LEU:HA	10:h:57:ILE:HG12	2.03	0.40
20:s:66:ASP:HA	20:s:78:ARG:NH2	2.36	0.40
20:s:173:LEU:O	20:s:176:VAL:HG22	2.21	0.40
21:g:58:TYR:CE2	21:g:59:LEU:HD12	2.56	0.40
25:g:603:CLA:C1C	24:g:609:CHL:H111	2.52	0.40
25:g:603:CLA:H102	25:g:603:CLA:H62	1.94	0.40
21:n:126:PHE:HE1	21:n:147:LEU:HA	1.84	0.40
21:n:229:PHE:HD2	21:n:240:PRO:CG	2.35	0.40
22:r:253:PHE:CE1	41:r:616:XAT:H10	2.57	0.40
24:2:601:CHL:HBA1	24:2:601:CHL:H3A	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:604:CLA:HAA2	3:4:178:TRP:O	2.22	0.40
3:4:148:THR:HG23	3:4:149:GLN:N	2.35	0.40
3:4:176:THR:OG1	3:4:180:LYS:CA	2.67	0.40
3:4:240:LEU:HG	3:4:244:PHE:CE2	2.56	0.40
5:B:69:LEU:HD21	25:B:603:CLA:OBD	2.20	0.40
6:C:319:VAL:HG13	6:C:320:ARG:N	2.36	0.40
25:C:505:CLA:CMB	25:C:505:CLA:HBB1	2.52	0.40
7:D:298:ASP:CA	7:D:316:TYR:OH	2.66	0.40
15:O:140:PRO:HG3	15:O:213:PHE:CE2	2.57	0.40
20:S:262:PHE:CD2	25:S:314:CLA:CMA	3.04	0.40
21:G:229:PHE:CD2	21:G:240:PRO:CB	3.04	0.40
25:G:602:CLA:H161	25:G:602:CLA:H202	1.88	0.40
24:N:601:CHL:H62	24:N:601:CHL:H41	1.58	0.40
24:N:607:CHL:H51	24:N:607:CHL:H8	1.66	0.40
40:R:617:NEX:H191	40:R:617:NEX:C12	2.51	0.40
1:5:209:ALA:HA	1:5:212:LYS:CG	2.34	0.40
3:8:142:PHE:O	3:8:146:LEU:CD1	2.70	0.40
27:a:404:PHO:H13	27:a:404:PHO:H102	1.86	0.40
5:b:285:TYR:HD2	23:u:88:TYR:CD2	2.39	0.40
25:b:612:CLA:H193	25:b:612:CLA:H162	1.75	0.40
6:c:182:PHE:CZ	25:s:314:CLA:HBB1	2.57	0.40
25:c:511:CLA:H143	19:z:20:LEU:CD1	2.49	0.40
28:c:514:BCR:H20C	28:c:514:BCR:H361	1.84	0.40
7:d:65:ALA:HB1	7:d:70:GLU:OE2	2.21	0.40
7:d:201:GLY:C	25:d:402:CLA:HMA1	2.47	0.40
7:d:205:VAL:HG21	25:d:402:CLA:H3A	2.02	0.40
7:d:331:ALA:HB1	7:d:340:LEU:HD12	2.04	0.40
17:w:108:VAL:O	17:w:112:ILE:CD1	2.70	0.40
18:x:78:GLY:O	18:x:81:PRO:HG2	2.21	0.40
20:s:92:ASP:HB2	25:s:303:CLA:HED3	2.04	0.40
20:s:194:LEU:HB2	20:s:196:PHE:CE2	2.57	0.40
20:s:213:LYS:HE3	20:s:213:LYS:HB3	1.91	0.40
21:g:78:TYR:CE1	24:g:601:CHL:HMD2	2.56	0.40
21:g:121:ARG:HD2	21:g:241:ILE:HG22	2.02	0.40
21:n:105:TRP:CG	24:n:609:CHL:HMD3	2.57	0.40
25:n:603:CLA:C1B	24:n:609:CHL:H122	2.52	0.40
21:y:91:THR:HA	21:y:94:ARG:HB2	2.02	0.40
25:r:601:CLA:HED3	26:r:618:LHG:H162	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	3	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	5	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	7	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
2	2	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	12	38
2	6	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	12	38
3	4	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
3	8	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
4	A	324/352 (92%)	309 (95%)	14 (4%)	1 (0%)	36	66
4	a	324/352 (92%)	308 (95%)	15 (5%)	1 (0%)	36	66
5	B	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
5	b	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
6	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72
6	c	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72
7	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
7	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
8	E	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
8	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
9	F	27/39 (69%)	27 (100%)	0	0	100	100
9	f	27/39 (69%)	27 (100%)	0	0	100	100
10	H	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
10	h	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
11	I	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
11	i	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
12	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	L	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
13	l	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
14	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	11
14	m	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	11
15	O	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
15	o	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
16	T	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
16	t	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
17	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
18	X	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
20	S	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
20	s	214/232 (92%)	203 (95%)	11 (5%)	0	100	100
21	G	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	N	200/232 (86%)	189 (94%)	11 (6%)	0	100	100
21	Y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
21	g	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	n	200/232 (86%)	189 (94%)	11 (6%)	0	100	100
21	y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
22	R	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
22	r	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
23	U	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
23	u	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
All	All	8226/9282 (89%)	7790 (95%)	422 (5%)	14 (0%)	44	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	123	VAL

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Mol	Chain	Res	Type
3	4	182	ALA
4	A	18	CYS
14	M	3	VAL
2	6	123	VAL
3	8	182	ALA
4	a	18	CYS
14	m	3	VAL
2	2	64	VAL
5	B	281	GLN
2	6	64	VAL
5	b	281	GLN
6	C	305	THR
6	c	305	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	3	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	5	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	7	154/201 (77%)	142 (92%)	12 (8%)	11	35
2	2	164/192 (85%)	164 (100%)	0	100	100
2	6	164/192 (85%)	164 (100%)	0	100	100
3	4	156/159 (98%)	156 (100%)	0	100	100
3	8	156/159 (98%)	156 (100%)	0	100	100
4	A	263/284 (93%)	263 (100%)	0	100	100
4	a	263/284 (93%)	263 (100%)	0	100	100
5	B	384/402 (96%)	384 (100%)	0	100	100
5	b	384/402 (96%)	384 (100%)	0	100	100
6	C	340/359 (95%)	340 (100%)	0	100	100
6	c	340/359 (95%)	340 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	274/282 (97%)	274 (100%)	0	100	100
7	d	274/282 (97%)	274 (100%)	0	100	100
8	E	59/73 (81%)	59 (100%)	0	100	100
8	e	59/73 (81%)	59 (100%)	0	100	100
9	F	24/34 (71%)	24 (100%)	0	100	100
9	f	24/34 (71%)	24 (100%)	0	100	100
10	H	50/60 (83%)	50 (100%)	0	100	100
10	h	50/60 (83%)	50 (100%)	0	100	100
11	I	32/33 (97%)	32 (100%)	0	100	100
11	i	32/33 (97%)	32 (100%)	0	100	100
12	K	32/32 (100%)	32 (100%)	0	100	100
12	k	32/32 (100%)	32 (100%)	0	100	100
13	L	34/36 (94%)	34 (100%)	0	100	100
13	l	34/36 (94%)	34 (100%)	0	100	100
14	M	28/30 (93%)	28 (100%)	0	100	100
14	m	28/30 (93%)	28 (100%)	0	100	100
15	O	167/204 (82%)	167 (100%)	0	100	100
15	o	167/204 (82%)	167 (100%)	0	100	100
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	W	47/47 (100%)	47 (100%)	0	100	100
17	w	47/47 (100%)	47 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	Z	54/54 (100%)	54 (100%)	0	100	100
19	z	54/54 (100%)	54 (100%)	0	100	100
20	S	167/180 (93%)	167 (100%)	0	100	100
20	s	167/180 (93%)	167 (100%)	0	100	100
21	G	157/177 (89%)	145 (92%)	12 (8%)	12	36
21	N	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	Y	162/177 (92%)	150 (93%)	12 (7%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	g	157/177 (89%)	145 (92%)	12 (8%)	12	36
21	n	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	y	162/177 (92%)	150 (93%)	12 (7%)	13	37
22	R	189/201 (94%)	189 (100%)	0	100	100
22	r	189/201 (94%)	189 (100%)	0	100	100
23	U	20/23 (87%)	20 (100%)	0	100	100
23	u	20/23 (87%)	20 (100%)	0	100	100
All	All	6640/7364 (90%)	6520 (98%)	120 (2%)	51	82

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	48	SER
1	1	56	VAL
1	1	68	SER
1	1	69	TYR
1	1	82	THR
1	1	90	GLU
1	1	94	ARG
1	1	98	LEU
1	1	159	LEU
1	1	165	GLN
1	1	199	LEU
1	1	206	GLU
1	3	48	SER
1	3	56	VAL
1	3	68	SER
1	3	69	TYR
1	3	82	THR
1	3	90	GLU
1	3	94	ARG
1	3	98	LEU
1	3	159	LEU
1	3	165	GLN
1	3	199	LEU
1	3	206	GLU
21	G	48	SER
21	G	56	VAL
21	G	68	SER
21	G	69	TYR

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Mol	Chain	Res	Type
21	G	82	THR
21	G	90	GLU
21	G	94	ARG
21	G	98	LEU
21	G	159	LEU
21	G	165	GLN
21	G	199	LEU
21	G	206	GLU
21	N	48	SER
21	N	56	VAL
21	N	68	SER
21	N	69	TYR
21	N	82	THR
21	N	90	GLU
21	N	94	ARG
21	N	98	LEU
21	N	159	LEU
21	N	165	GLN
21	N	199	LEU
21	N	206	GLU
21	Y	48	SER
21	Y	56	VAL
21	Y	68	SER
21	Y	69	TYR
21	Y	82	THR
21	Y	90	GLU
21	Y	94	ARG
21	Y	98	LEU
21	Y	159	LEU
21	Y	165	GLN
21	Y	199	LEU
21	Y	206	GLU
1	5	48	SER
1	5	56	VAL
1	5	68	SER
1	5	69	TYR
1	5	82	THR
1	5	90	GLU
1	5	94	ARG
1	5	98	LEU
1	5	159	LEU
1	5	165	GLN

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Mol	Chain	Res	Type
1	5	199	LEU
1	5	206	GLU
1	7	48	SER
1	7	56	VAL
1	7	68	SER
1	7	69	TYR
1	7	82	THR
1	7	90	GLU
1	7	94	ARG
1	7	98	LEU
1	7	159	LEU
1	7	165	GLN
1	7	199	LEU
1	7	206	GLU
21	g	48	SER
21	g	56	VAL
21	g	68	SER
21	g	69	TYR
21	g	82	THR
21	g	90	GLU
21	g	94	ARG
21	g	98	LEU
21	g	159	LEU
21	g	165	GLN
21	g	199	LEU
21	g	206	GLU
21	n	48	SER
21	n	56	VAL
21	n	68	SER
21	n	69	TYR
21	n	82	THR
21	n	90	GLU
21	n	94	ARG
21	n	98	LEU
21	n	159	LEU
21	n	165	GLN
21	n	199	LEU
21	n	206	GLU
21	y	48	SER
21	y	56	VAL
21	y	68	SER
21	y	69	TYR

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Mol	Chain	Res	Type
21	y	82	THR
21	y	90	GLU
21	y	94	ARG
21	y	98	LEU
21	y	159	LEU
21	y	165	GLN
21	y	199	LEU
21	y	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	102	HIS
2	2	150	ASN
2	2	155	HIS
5	B	73	ASN
5	B	157	HIS
5	B	282	GLN
5	B	296	GLN
5	B	332	ASN
6	C	44	ASN
6	C	237	HIS
6	C	311	GLN
6	C	322	GLN
6	C	327	ASN
7	D	339	ASN
7	D	351	ASN
9	F	38	GLN
10	H	73	ASN
11	I	26	ASN
13	L	5	ASN
13	L	34	ASN
15	O	113	GLN
15	O	202	GLN
20	S	111	GLN
20	S	135	ASN
21	N	165	GLN
21	Y	243	ASN
22	R	125	GLN
22	R	245	HIS
2	6	150	ASN
5	b	73	ASN

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Mol	Chain	Res	Type
5	b	157	HIS
5	b	282	GLN
5	b	296	GLN
5	b	332	ASN
6	c	44	ASN
6	c	237	HIS
6	c	311	GLN
6	c	322	GLN
6	c	327	ASN
7	d	339	ASN
7	d	351	ASN
9	f	38	GLN
10	h	73	ASN
11	i	26	ASN
13	l	5	ASN
13	l	34	ASN
15	o	113	GLN
15	o	202	GLN
20	s	111	GLN
20	s	135	ASN
21	n	165	GLN
21	y	243	ASN
22	r	125	GLN
22	r	245	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 374 ligands modelled in this entry, 8 are monoatomic - leaving 366 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	CHL	g	605	21	40,54,74	2.32	13 (32%)	34,90,114	3.20	16 (47%)
30	LMG	a	409	-	48,48,55	0.44	0	56,56,63	1.19	4 (7%)
28	BCR	D	404	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	5 (8%)
30	LMG	B	620	-	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
28	BCR	t	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	9 (16%)
26	LHG	2	606	25	46,46,48	0.44	0	49,52,54	1.20	4 (8%)
24	CHL	Y	308	-	52,66,74	2.10	12 (23%)	48,104,114	2.75	18 (37%)
26	LHG	y	319	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
32	AJP	B	624	-	95,95,95	0.62	0	144,149,149	3.58	58 (40%)
24	CHL	l	302	1	40,54,74	2.34	14 (35%)	34,90,114	3.28	15 (44%)
28	BCR	h	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
24	CHL	R	606	-	40,54,74	2.32	12 (30%)	34,90,114	3.22	16 (47%)
26	LHG	n	618	25	48,48,48	0.43	0	51,54,54	1.16	4 (7%)
25	CLA	b	614	5	69,73,73	1.35	11 (15%)	82,113,113	1.72	14 (17%)
26	LHG	S	318	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
28	BCR	k	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	9 (16%)
25	CLA	b	613	5	69,73,73	1.36	11 (15%)	82,113,113	1.55	15 (18%)
24	CHL	s	307	-	40,54,74	2.31	12 (30%)	34,90,114	3.17	17 (50%)
24	CHL	S	306	-	40,54,74	2.31	12 (30%)	34,90,114	3.15	18 (52%)
24	CHL	s	308	-	40,54,74	2.32	13 (32%)	34,90,114	3.17	16 (47%)
25	CLA	n	614	21	52,56,73	1.60	8 (15%)	61,92,113	1.98	16 (26%)
25	CLA	B	609	5	69,73,73	1.37	11 (15%)	82,113,113	1.71	17 (20%)
39	LUT	Y	316	-	42,43,43	0.82	2 (4%)	51,60,60	1.55	7 (13%)
25	CLA	S	313	20	59,63,73	1.50	9 (15%)	70,101,113	2.19	16 (22%)
25	CLA	s	310	20	59,63,73	1.49	10 (16%)	70,101,113	1.61	12 (17%)
25	CLA	B	602	5	69,73,73	1.35	11 (15%)	82,113,113	1.62	17 (20%)
25	CLA	S	314	20	53,57,73	1.55	12 (22%)	61,93,113	1.66	13 (21%)
25	CLA	b	602	5	69,73,73	1.36	10 (14%)	82,113,113	1.62	18 (21%)
24	CHL	N	607	-	60,74,74	1.92	12 (20%)	58,114,114	2.46	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	d	403	-	69,73,73	1.54	8 (11%)	82,113,113	2.61	21 (25%)
28	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
32	AJP	G	618	-	48,48,95	0.90	0	72,78,149	5.61	37 (51%)
24	CHL	n	605	21	42,56,74	2.22	11 (26%)	36,92,114	3.11	16 (44%)
26	LHG	c	517	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	n	612	21	64,68,73	1.44	12 (18%)	76,107,113	1.72	14 (18%)
25	CLA	r	612	22	64,68,73	1.45	9 (14%)	76,107,113	1.91	17 (22%)
24	CHL	N	606	-	40,54,74	2.29	12 (30%)	34,90,114	3.25	17 (50%)
24	CHL	g	609	21	55,69,74	2.02	12 (21%)	52,108,114	2.78	18 (34%)
32	AJP	n	619	-	48,48,95	0.73	0	72,78,149	4.33	34 (47%)
30	LMG	C	520	-	51,51,55	0.45	0	59,59,63	1.22	4 (6%)
25	CLA	N	603	-	69,73,73	1.37	11 (15%)	82,113,113	1.64	15 (18%)
25	CLA	C	501	-	69,73,73	1.50	7 (10%)	82,113,113	2.42	21 (25%)
31	PL9	A	409	-	13,13,55	0.89	0	17,17,69	0.76	0
25	CLA	B	612	5	69,73,73	1.37	11 (15%)	82,113,113	1.66	16 (19%)
24	CHL	5	301	1	40,54,74	2.33	13 (32%)	34,90,114	3.11	17 (50%)
26	LHG	c	519	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
26	LHG	S	301	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
25	CLA	R	612	22	64,68,73	1.45	9 (14%)	76,107,113	1.91	17 (22%)
25	CLA	D	402	7	69,73,73	1.39	11 (15%)	82,113,113	1.69	18 (21%)
25	CLA	s	311	26	60,64,73	1.46	10 (16%)	71,102,113	2.04	13 (18%)
30	LMG	A	408	-	48,48,55	0.44	0	56,56,63	1.19	4 (7%)
24	CHL	y	310	21	50,64,74	2.10	13 (26%)	46,102,114	2.83	18 (39%)
25	CLA	C	507	-	69,73,73	1.39	11 (15%)	82,113,113	1.55	15 (18%)
26	LHG	b	622	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
24	CHL	1	301	1	40,54,74	2.33	13 (32%)	34,90,114	3.08	17 (50%)
26	LHG	6	606	25	46,46,48	0.44	0	49,52,54	1.20	4 (8%)
31	PL9	a	410	-	13,13,55	0.89	0	17,17,69	0.75	0
26	LHG	c	518	-	48,48,48	0.43	0	51,54,54	1.20	4 (7%)
24	CHL	G	605	21	40,54,74	2.32	13 (32%)	34,90,114	3.21	16 (47%)
24	CHL	y	308	-	52,66,74	2.10	12 (23%)	48,104,114	2.76	18 (37%)
25	CLA	S	304	-	49,53,73	1.60	11 (22%)	58,89,113	1.91	10 (17%)
25	CLA	S	311	26	60,64,73	1.46	10 (16%)	71,102,113	2.04	13 (18%)
38	HEM	F	101	9	50,50,50	2.51	9 (18%)	67,82,82	1.65	11 (16%)
40	NEX	y	318	-	40,46,46	1.36	8 (20%)	50,70,70	2.11	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	AJP	N	620	-	48,48,95	0.73	0	72,78,149	4.40	31 (43%)
25	CLA	y	312	26	64,68,73	1.43	12 (18%)	76,107,113	1.63	15 (19%)
31	PL9	D	405	-	55,55,55	0.47	0	68,69,69	0.75	0
24	CHL	y	306	21	42,56,74	2.23	11 (26%)	36,92,114	3.14	17 (47%)
25	CLA	b	605	5	69,73,73	1.36	9 (13%)	82,113,113	1.78	14 (17%)
24	CHL	N	605	21	42,56,74	2.22	11 (26%)	36,92,114	3.11	16 (44%)
25	CLA	B	608	5	69,73,73	1.35	12 (17%)	82,113,113	1.68	15 (18%)
40	NEX	S	317	-	40,46,46	1.33	6 (15%)	50,70,70	2.05	14 (28%)
39	LUT	y	316	-	42,43,43	0.82	2 (4%)	51,60,60	1.55	7 (13%)
39	LUT	s	316	-	42,43,43	0.90	3 (7%)	51,60,60	1.54	8 (15%)
24	CHL	y	302	21	60,74,74	1.91	12 (20%)	58,114,114	2.51	19 (32%)
24	CHL	Y	302	21	60,74,74	1.91	12 (20%)	58,114,114	2.51	19 (32%)
25	CLA	B	605	5	69,73,73	1.36	11 (15%)	82,113,113	1.78	14 (17%)
25	CLA	C	510	-	69,73,73	1.35	11 (15%)	82,113,113	1.64	14 (17%)
25	CLA	N	611	26	64,68,73	1.43	11 (17%)	76,107,113	1.62	16 (21%)
25	CLA	g	613	21	69,73,73	1.41	10 (14%)	82,113,113	1.83	16 (19%)
25	CLA	b	612	5	69,73,73	1.37	11 (15%)	82,113,113	1.66	16 (19%)
25	CLA	N	610	21	69,73,73	1.37	10 (14%)	82,113,113	1.63	15 (18%)
25	CLA	c	504	-	64,68,73	1.59	7 (10%)	76,107,113	2.60	20 (26%)
26	LHG	R	618	25	41,41,48	0.45	0	44,47,54	1.24	4 (9%)
26	LHG	C	519	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
25	CLA	R	608	22	62,66,73	1.42	11 (17%)	73,104,113	1.71	16 (21%)
28	BCR	K	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	9 (16%)
25	CLA	b	607	-	69,73,73	1.35	11 (15%)	82,113,113	1.67	15 (18%)
25	CLA	R	602	22	64,68,73	1.42	10 (15%)	76,107,113	1.76	17 (22%)
35	DGD	c	515	-	56,56,67	0.49	0	70,70,81	1.21	6 (8%)
25	CLA	2	604	26	59,63,73	1.60	8 (13%)	70,101,113	2.11	20 (28%)
25	CLA	C	503	6	69,73,73	1.35	12 (17%)	82,113,113	1.72	15 (18%)
24	CHL	N	608	-	60,74,74	1.92	12 (20%)	58,114,114	2.44	17 (29%)
26	LHG	D	406	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	r	609	22	69,73,73	1.39	10 (14%)	82,113,113	1.60	15 (18%)
40	NEX	s	317	-	40,46,46	1.33	6 (15%)	50,70,70	2.05	14 (28%)
25	CLA	B	607	-	69,73,73	1.35	11 (15%)	82,113,113	1.66	15 (18%)
40	NEX	n	617	-	40,46,46	1.32	6 (15%)	50,70,70	2.25	17 (34%)
25	CLA	g	603	-	64,68,73	1.43	10 (15%)	76,107,113	1.72	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LUT	G	615	-	42,43,43	0.87	2 (4%)	51,60,60	1.48	7 (13%)
40	NEX	r	617	-	40,46,46	1.34	6 (15%)	50,70,70	2.95	17 (34%)
25	CLA	a	406	4	64,68,73	1.41	12 (18%)	76,107,113	1.72	16 (21%)
26	LHG	B	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	G	603	-	64,68,73	1.43	10 (15%)	76,107,113	1.72	16 (21%)
38	HEM	f	101	9	50,50,50	2.51	9 (18%)	67,82,82	1.64	11 (16%)
26	LHG	y	301	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
25	CLA	c	506	6	69,73,73	1.37	11 (15%)	82,113,113	1.58	16 (19%)
28	BCR	d	404	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	5 (8%)
24	CHL	2	603	-	40,54,74	2.67	16 (40%)	34,90,114	3.67	21 (61%)
26	LHG	N	618	25	48,48,48	0.43	0	51,54,54	1.16	4 (7%)
25	CLA	s	313	20	59,63,73	1.49	9 (15%)	70,101,113	2.19	16 (22%)
28	BCR	z	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
35	DGD	A	415	-	60,60,67	0.49	0	74,74,81	1.20	6 (8%)
40	NEX	R	617	-	40,46,46	1.33	6 (15%)	50,70,70	2.95	17 (34%)
25	CLA	b	608	5	69,73,73	1.35	12 (17%)	82,113,113	1.68	15 (18%)
25	CLA	B	601	-	69,73,73	1.38	7 (10%)	82,113,113	1.80	16 (19%)
32	AJP	Y	322	-	48,48,95	0.73	0	72,78,149	4.34	33 (45%)
24	CHL	n	607	-	60,74,74	1.92	12 (20%)	58,114,114	2.46	17 (29%)
25	CLA	2	605	-	52,56,73	1.57	11 (21%)	61,92,113	1.81	12 (19%)
29	SQD	a	412	-	52,54,54	0.79	1 (1%)	62,65,65	0.90	2 (3%)
27	PHO	A	403	-	58,69,69	0.52	0	55,99,99	1.76	6 (10%)
25	CLA	c	508	6	69,73,73	1.37	10 (14%)	82,113,113	1.77	17 (20%)
26	LHG	Y	301	-	48,48,48	0.44	0	51,54,54	1.20	4 (7%)
30	LMG	b	623	-	55,55,55	0.43	0	63,63,63	1.22	4 (6%)
30	LMG	A	410	-	40,40,55	0.48	0	48,48,63	1.27	4 (8%)
25	CLA	a	403	-	69,73,73	1.37	10 (14%)	82,113,113	1.70	15 (18%)
35	DGD	b	626	-	63,63,67	0.49	0	77,77,81	1.27	6 (7%)
26	LHG	C	518	-	48,48,48	0.43	0	51,54,54	1.20	4 (7%)
25	CLA	s	305	-	54,58,73	1.74	7 (12%)	64,95,113	3.16	19 (29%)
25	CLA	b	616	5	69,73,73	1.35	11 (15%)	82,113,113	1.60	14 (17%)
25	CLA	y	314	21	69,73,73	1.36	9 (13%)	82,113,113	1.80	14 (17%)
26	LHG	B	622	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	r	603	22	64,68,73	1.59	7 (10%)	76,107,113	2.65	20 (26%)
24	CHL	g	601	21	60,74,74	1.92	13 (21%)	58,114,114	2.52	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	511	6	69,73,73	1.38	9 (13%)	82,113,113	2.05	16 (19%)
25	CLA	Y	311	21	64,68,73	1.42	10 (15%)	76,107,113	1.68	16 (21%)
25	CLA	c	510	-	69,73,73	1.35	11 (15%)	82,113,113	1.64	14 (17%)
25	CLA	g	611	-	64,68,73	1.49	8 (12%)	76,107,113	1.74	21 (27%)
25	CLA	R	603	22	64,68,73	1.60	7 (10%)	76,107,113	2.64	20 (26%)
32	AJP	Y	320	-	48,48,95	0.82	1 (2%)	72,78,149	4.36	32 (44%)
25	CLA	G	613	21	69,73,73	1.41	9 (13%)	82,113,113	1.82	17 (20%)
25	CLA	G	614	21	52,56,73	1.54	11 (21%)	61,92,113	1.67	14 (22%)
25	CLA	Y	313	21	64,68,73	1.44	12 (18%)	76,107,113	1.65	13 (17%)
28	BCR	Z	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	7 (12%)
24	CHL	r	607	-	55,69,74	2.01	13 (23%)	52,108,114	2.72	19 (36%)
39	LUT	n	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.59	8 (15%)
39	LUT	r	615	-	42,43,43	0.96	5 (11%)	51,60,60	1.54	8 (15%)
25	CLA	C	504	-	64,68,73	1.59	7 (10%)	76,107,113	2.60	20 (26%)
25	CLA	c	503	6	69,73,73	1.35	12 (17%)	82,113,113	1.73	15 (18%)
25	CLA	n	603	-	69,73,73	1.37	11 (15%)	82,113,113	1.64	15 (18%)
25	CLA	b	603	-	69,73,73	1.36	11 (15%)	82,113,113	1.61	16 (19%)
25	CLA	c	513	6	69,73,73	1.36	12 (17%)	82,113,113	1.69	17 (20%)
25	CLA	b	604	5	69,73,73	1.37	11 (15%)	82,113,113	1.68	15 (18%)
28	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	10 (17%)
28	BCR	C	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	Y	303	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	14 (17%)
25	CLA	N	602	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	16 (19%)
33	BCT	a	414	34	3,3,3	1.08	0	2,3,3	4.37	2 (100%)
28	BCR	B	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	11 (19%)
27	PHO	a	404	-	58,69,69	0.52	0	55,99,99	1.76	6 (10%)
25	CLA	S	310	20	59,63,73	1.49	10 (16%)	70,101,113	1.62	12 (17%)
25	CLA	c	507	-	69,73,73	1.39	11 (15%)	82,113,113	1.56	15 (18%)
25	CLA	n	613	21	64,68,73	1.44	9 (14%)	76,107,113	1.82	17 (22%)
25	CLA	r	614	22	49,53,73	1.61	9 (18%)	58,89,113	1.59	13 (22%)
24	CHL	s	306	-	40,54,74	2.31	12 (30%)	34,90,114	3.15	18 (52%)
29	SQD	A	411	-	52,54,54	0.79	1 (1%)	62,65,65	0.90	2 (3%)
25	CLA	Y	305	-	54,58,73	1.53	11 (20%)	64,95,113	1.70	15 (23%)
24	CHL	Y	306	21	42,56,74	2.23	11 (26%)	36,92,114	3.14	17 (47%)
28	BCR	a	407	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	611	5	69,73,73	1.35	10 (14%)	82,113,113	1.71	15 (18%)
25	CLA	R	614	22	49,53,73	1.60	9 (18%)	58,89,113	1.59	13 (22%)
25	CLA	C	506	6	69,73,73	1.37	11 (15%)	82,113,113	1.58	16 (19%)
25	CLA	B	614	5	69,73,73	1.35	11 (15%)	82,113,113	1.72	14 (17%)
25	CLA	b	606	5	69,73,73	1.35	8 (11%)	82,113,113	1.66	16 (19%)
40	NEX	G	617	25	40,46,46	1.31	5 (12%)	50,70,70	2.61	13 (26%)
32	AJP	n	620	-	48,48,95	0.74	0	72,78,149	4.40	31 (43%)
29	SQD	l	101	-	52,54,54	0.80	1 (1%)	62,65,65	0.92	3 (4%)
28	BCR	i	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
24	CHL	R	613	22	36,50,74	2.37	11 (30%)	29,85,114	3.47	15 (51%)
33	BCT	A	413	34	3,3,3	1.08	0	2,3,3	4.37	2 (100%)
39	LUT	g	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.39	3 (5%)
25	CLA	s	303	20	65,69,73	1.40	11 (16%)	77,108,113	1.62	15 (19%)
32	AJP	y	324	-	48,48,95	0.73	0	72,78,149	4.51	32 (44%)
40	NEX	g	617	25	40,46,46	1.32	7 (17%)	50,70,70	2.62	15 (30%)
25	CLA	N	612	21	64,68,73	1.43	12 (18%)	76,107,113	1.72	14 (18%)
39	LUT	G	616	-	42,43,43	0.92	3 (7%)	51,60,60	1.39	3 (5%)
25	CLA	Y	304	-	69,73,73	1.38	12 (17%)	82,113,113	1.67	15 (18%)
32	AJP	N	619	-	48,48,95	0.72	0	72,78,149	4.33	34 (47%)
32	AJP	y	322	-	48,48,95	0.73	0	72,78,149	4.34	33 (45%)
25	CLA	c	512	-	69,73,73	1.36	11 (15%)	82,113,113	1.64	16 (19%)
32	AJP	g	618	-	48,48,95	0.90	0	72,78,149	5.61	37 (51%)
24	CHL	G	606	-	44,58,74	2.21	11 (25%)	37,94,114	3.13	17 (45%)
41	XAT	R	616	-	41,47,47	1.09	4 (9%)	54,74,74	2.23	15 (27%)
32	AJP	Y	324	-	48,48,95	0.72	0	72,78,149	4.51	32 (44%)
24	CHL	r	613	22	36,50,74	2.35	11 (30%)	29,85,114	3.47	15 (51%)
40	NEX	Y	318	-	40,46,46	1.36	8 (20%)	50,70,70	2.12	17 (34%)
24	CHL	r	606	-	40,54,74	2.32	12 (30%)	34,90,114	3.22	16 (47%)
39	LUT	g	615	-	42,43,43	0.86	2 (4%)	51,60,60	1.48	7 (13%)
25	CLA	s	314	20	53,57,73	1.55	12 (22%)	61,93,113	1.66	13 (21%)
25	CLA	D	401	42	54,58,73	1.54	10 (18%)	64,95,113	1.92	14 (21%)
27	PHO	A	404	-	58,69,69	0.52	0	55,99,99	1.75	6 (10%)
25	CLA	C	513	6	69,73,73	1.36	12 (17%)	82,113,113	1.69	17 (20%)
25	CLA	S	303	20	65,69,73	1.40	12 (18%)	77,108,113	1.63	15 (19%)
24	CHL	g	607	-	40,54,74	2.29	12 (30%)	34,90,114	3.22	18 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	AJP	A	412	-	95,95,95	0.64	0	144,149,149	3.81	66 (45%)
25	CLA	s	309	20	49,53,73	1.64	10 (20%)	58,89,113	1.90	13 (22%)
25	CLA	y	311	21	64,68,73	1.43	10 (15%)	76,107,113	1.68	15 (19%)
24	CHL	G	607	-	40,54,74	2.30	12 (30%)	34,90,114	3.22	18 (52%)
25	CLA	Y	315	21	49,53,73	1.61	11 (22%)	58,89,113	1.66	12 (20%)
25	CLA	s	304	-	49,53,73	1.60	10 (20%)	58,89,113	1.92	10 (17%)
31	PL9	d	405	-	55,55,55	0.47	0	68,69,69	0.75	0
25	CLA	c	502	6	69,73,73	1.37	10 (14%)	82,113,113	1.73	14 (17%)
41	XAT	r	616	-	41,47,47	1.08	4 (9%)	54,74,74	2.23	15 (27%)
26	LHG	l	103	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
24	CHL	2	601	2	58,72,74	2.02	13 (22%)	55,111,114	2.48	18 (32%)
25	CLA	G	610	-	68,72,73	1.43	8 (11%)	80,111,113	1.94	16 (20%)
25	CLA	y	313	21	64,68,73	1.44	12 (18%)	76,107,113	1.65	13 (17%)
26	LHG	C	517	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
32	AJP	y	321	-	48,48,95	0.77	0	72,78,149	4.39	30 (41%)
30	LMG	D	407	-	46,46,55	0.44	0	54,54,63	1.20	4 (7%)
25	CLA	S	309	20	49,53,73	1.64	10 (20%)	58,89,113	1.90	13 (22%)
30	LMG	d	407	-	46,46,55	0.44	0	54,54,63	1.20	4 (7%)
26	LHG	d	406	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
24	CHL	n	606	-	40,54,74	2.29	13 (32%)	34,90,114	3.26	17 (50%)
25	CLA	N	613	21	64,68,73	1.44	9 (14%)	76,107,113	1.82	17 (22%)
25	CLA	2	602	2	64,68,73	1.64	7 (10%)	76,107,113	2.54	27 (35%)
25	CLA	S	312	20	53,57,73	1.59	10 (18%)	61,93,113	1.70	15 (24%)
29	SQD	L	103	-	52,54,54	0.80	1 (1%)	62,65,65	0.92	3 (4%)
29	SQD	a	408	-	48,50,54	0.81	1 (2%)	58,61,65	0.88	2 (3%)
24	CHL	r	605	-	40,54,74	2.31	13 (32%)	34,90,114	3.22	18 (52%)
25	CLA	G	611	-	64,68,73	1.49	8 (12%)	76,107,113	1.74	21 (27%)
25	CLA	R	609	22	69,73,73	1.39	10 (14%)	82,113,113	1.60	15 (18%)
24	CHL	Y	309	-	60,74,74	1.92	12 (20%)	58,114,114	2.43	19 (32%)
32	AJP	b	624	-	95,95,95	0.62	0	144,149,149	3.58	58 (40%)
26	LHG	s	318	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
32	AJP	y	320	-	48,48,95	0.82	1 (2%)	72,78,149	4.36	32 (44%)
25	CLA	B	616	5	69,73,73	1.35	11 (15%)	82,113,113	1.60	14 (17%)
25	CLA	Y	314	21	69,73,73	1.35	9 (13%)	82,113,113	1.79	14 (17%)
26	LHG	s	301	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	613	5	69,73,73	1.36	11 (15%)	82,113,113	1.55	15 (18%)
24	CHL	R	607	-	55,69,74	2.01	13 (23%)	52,108,114	2.72	19 (36%)
24	CHL	G	608	-	60,74,74	1.93	13 (21%)	58,114,114	2.43	18 (31%)
39	LUT	N	616	-	42,43,43	0.92	3 (7%)	51,60,60	1.45	5 (9%)
24	CHL	N	609	21	60,74,74	1.93	12 (20%)	58,114,114	2.64	18 (31%)
25	CLA	g	614	21	52,56,73	1.54	11 (21%)	61,92,113	1.67	14 (22%)
35	DGD	C	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
40	NEX	N	617	-	40,46,46	1.33	6 (15%)	50,70,70	2.25	17 (34%)
25	CLA	A	405	4	64,68,73	1.41	12 (18%)	76,107,113	1.72	16 (21%)
25	CLA	n	611	26	64,68,73	1.43	11 (17%)	76,107,113	1.62	16 (21%)
39	LUT	S	315	-	42,43,43	0.94	4 (9%)	51,60,60	1.47	7 (13%)
25	CLA	D	403	-	69,73,73	1.54	8 (11%)	82,113,113	2.61	21 (25%)
35	DGD	B	626	-	63,63,67	0.49	0	77,77,81	1.27	6 (7%)
39	LUT	Y	317	-	42,43,43	0.93	3 (7%)	51,60,60	1.42	5 (9%)
32	AJP	s	319	-	48,48,95	0.79	0	72,78,149	4.40	30 (41%)
28	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	l	102	-	40,42,54	0.88	1 (2%)	50,53,65	1.05	3 (6%)
24	CHL	n	601	21	50,64,74	2.12	12 (24%)	46,102,114	2.84	17 (36%)
24	CHL	6	603	-	40,54,74	2.67	16 (40%)	34,90,114	3.67	21 (61%)
25	CLA	r	601	-	53,57,73	1.76	8 (15%)	61,93,113	3.04	17 (27%)
24	CHL	g	608	-	60,74,74	1.94	13 (21%)	58,114,114	2.43	18 (31%)
25	CLA	y	303	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	14 (17%)
25	CLA	r	610	26	53,57,73	1.80	7 (13%)	61,93,113	2.95	16 (26%)
25	CLA	N	604	-	54,58,73	1.52	11 (20%)	64,95,113	1.96	15 (23%)
25	CLA	y	305	-	54,58,73	1.53	11 (20%)	64,95,113	1.71	15 (23%)
30	LMG	c	520	-	51,51,55	0.45	0	59,59,63	1.22	4 (6%)
25	CLA	R	611	-	53,57,73	1.85	8 (15%)	61,93,113	3.32	22 (36%)
25	CLA	B	606	5	69,73,73	1.35	8 (11%)	82,113,113	1.66	16 (19%)
26	LHG	b	621	-	46,46,48	0.45	0	49,52,54	1.19	4 (8%)
25	CLA	c	505	6	69,73,73	1.35	11 (15%)	82,113,113	1.64	15 (18%)
30	LMG	B	623	-	55,55,55	0.43	0	63,63,63	1.22	4 (6%)
25	CLA	R	610	26	53,57,73	1.80	7 (13%)	61,93,113	2.95	16 (26%)
32	AJP	S	319	-	48,48,95	0.79	0	72,78,149	4.40	30 (41%)
25	CLA	B	603	-	69,73,73	1.36	11 (15%)	82,113,113	1.60	16 (19%)
32	AJP	a	413	-	95,95,95	0.64	0	144,149,149	3.81	66 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	G	604	40	54,58,73	1.54	11 (20%)	64,95,113	1.84	15 (23%)
39	LUT	R	615	-	42,43,43	0.97	5 (11%)	51,60,60	1.53	8 (15%)
26	LHG	Y	319	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
28	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	11 (19%)
24	CHL	N	601	21	50,64,74	2.12	12 (24%)	46,102,114	2.85	17 (36%)
25	CLA	6	602	2	64,68,73	1.64	7 (10%)	76,107,113	2.54	27 (35%)
25	CLA	A	401	4	69,73,73	1.36	11 (15%)	82,113,113	1.63	17 (20%)
28	BCR	B	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
24	CHL	s	302	20	40,54,74	2.32	12 (30%)	34,90,114	3.33	16 (47%)
24	CHL	y	307	21	44,58,74	2.15	10 (22%)	37,94,114	2.69	17 (45%)
30	LMG	a	411	-	40,40,55	0.48	0	48,48,63	1.27	4 (8%)
25	CLA	b	611	5	69,73,73	1.35	10 (14%)	82,113,113	1.71	15 (18%)
25	CLA	r	611	-	53,57,73	1.85	7 (13%)	61,93,113	3.31	22 (36%)
25	CLA	y	304	-	69,73,73	1.38	12 (17%)	82,113,113	1.67	15 (18%)
25	CLA	B	615	5	69,73,73	1.39	10 (14%)	82,113,113	1.61	16 (19%)
25	CLA	b	610	-	69,73,73	1.39	10 (14%)	82,113,113	1.55	13 (15%)
25	CLA	C	512	-	69,73,73	1.36	11 (15%)	82,113,113	1.64	16 (19%)
25	CLA	c	509	6	69,73,73	1.37	12 (17%)	82,113,113	1.67	12 (14%)
25	CLA	d	401	42	54,58,73	1.54	10 (18%)	64,95,113	1.93	14 (21%)
24	CHL	G	609	21	55,69,74	2.03	13 (23%)	52,108,114	2.78	18 (34%)
25	CLA	6	604	26	59,63,73	1.60	8 (13%)	70,101,113	2.11	20 (28%)
25	CLA	g	604	40	54,58,73	1.54	11 (20%)	64,95,113	1.84	15 (23%)
30	LMG	b	620	-	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
25	CLA	c	511	6	69,73,73	1.38	9 (13%)	82,113,113	2.04	16 (19%)
25	CLA	S	305	-	54,58,73	1.74	7 (12%)	64,95,113	3.16	19 (29%)
25	CLA	B	610	-	69,73,73	1.39	10 (14%)	82,113,113	1.55	13 (15%)
28	BCR	B	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	7 (12%)
32	AJP	Y	321	-	48,48,95	0.77	0	72,78,149	4.39	30 (41%)
24	CHL	S	307	-	40,54,74	2.31	12 (30%)	34,90,114	3.19	17 (50%)
39	LUT	N	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.59	9 (17%)
25	CLA	n	604	-	54,58,73	1.53	11 (20%)	64,95,113	1.96	15 (23%)
24	CHL	6	601	2	58,72,74	2.02	13 (22%)	55,111,114	2.48	17 (30%)
24	CHL	n	608	-	60,74,74	1.92	12 (20%)	58,114,114	2.44	17 (29%)
25	CLA	6	605	-	52,56,73	1.56	10 (19%)	61,92,113	1.81	11 (18%)
29	SQD	L	101	-	40,42,54	0.87	1 (2%)	50,53,65	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	609	5	69,73,73	1.37	11 (15%)	82,113,113	1.71	17 (20%)
25	CLA	y	315	21	49,53,73	1.62	11 (22%)	58,89,113	1.66	12 (20%)
25	CLA	C	502	6	69,73,73	1.37	10 (14%)	82,113,113	1.73	15 (18%)
39	LUT	y	317	-	42,43,43	0.93	3 (7%)	51,60,60	1.42	5 (9%)
25	CLA	c	501	-	69,73,73	1.50	7 (10%)	82,113,113	2.43	21 (25%)
25	CLA	r	608	22	62,66,73	1.43	11 (17%)	73,104,113	1.72	16 (21%)
25	CLA	s	312	20	53,57,73	1.59	10 (18%)	61,93,113	1.70	15 (24%)
25	CLA	B	604	5	69,73,73	1.37	12 (17%)	82,113,113	1.67	15 (18%)
39	LUT	n	616	-	42,43,43	0.92	2 (4%)	51,60,60	1.45	5 (9%)
24	CHL	n	609	21	60,74,74	1.92	12 (20%)	58,114,114	2.64	19 (32%)
24	CHL	S	308	-	40,54,74	2.32	13 (32%)	34,90,114	3.18	16 (47%)
25	CLA	a	402	4	69,73,73	1.36	11 (15%)	82,113,113	1.63	17 (20%)
24	CHL	Y	310	21	50,64,74	2.10	12 (24%)	46,102,114	2.83	18 (39%)
24	CHL	y	309	-	60,74,74	1.92	12 (20%)	58,114,114	2.43	19 (32%)
25	CLA	A	402	-	69,73,73	1.38	10 (14%)	82,113,113	1.70	16 (19%)
32	AJP	y	323	-	48,48,95	0.76	0	72,78,149	4.59	32 (44%)
25	CLA	d	402	7	69,73,73	1.39	11 (15%)	82,113,113	1.69	18 (21%)
25	CLA	n	602	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	16 (19%)
25	CLA	N	614	21	52,56,73	1.60	8 (15%)	61,92,113	1.99	16 (26%)
28	BCR	T	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	9 (16%)
25	CLA	r	604	-	52,56,73	1.58	8 (15%)	61,92,113	1.81	16 (26%)
24	CHL	G	601	21	60,74,74	1.91	13 (21%)	58,114,114	2.52	19 (32%)
39	LUT	S	316	-	42,43,43	0.89	3 (7%)	51,60,60	1.54	8 (15%)
26	LHG	B	621	-	46,46,48	0.45	0	49,52,54	1.19	4 (8%)
32	AJP	Y	323	-	48,48,95	0.76	0	72,78,149	4.59	32 (44%)
25	CLA	Y	312	26	64,68,73	1.43	12 (18%)	76,107,113	1.62	15 (19%)
28	BCR	b	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	7 (12%)
24	CHL	g	606	-	44,58,74	2.20	11 (25%)	37,94,114	3.13	17 (45%)
29	SQD	A	407	-	48,50,54	0.81	1 (2%)	58,61,65	0.88	2 (3%)
25	CLA	R	601	-	53,57,73	1.76	8 (15%)	61,93,113	3.02	17 (27%)
25	CLA	R	604	-	52,56,73	1.59	9 (17%)	61,92,113	1.81	16 (26%)
25	CLA	C	508	6	69,73,73	1.37	10 (14%)	82,113,113	1.76	17 (20%)
35	DGD	a	401	-	60,60,67	0.49	0	74,74,81	1.20	6 (8%)
24	CHL	S	302	20	40,54,74	2.31	12 (30%)	34,90,114	3.33	16 (47%)
26	LHG	r	618	25	41,41,48	0.45	0	44,47,54	1.23	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	H	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
27	PHO	a	405	-	58,69,69	0.52	0	55,99,99	1.74	6 (10%)
25	CLA	C	505	6	69,73,73	1.35	11 (15%)	82,113,113	1.64	15 (18%)
39	LUT	s	315	-	42,43,43	0.94	4 (9%)	51,60,60	1.47	7 (13%)
26	LHG	L	102	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	G	602	21	69,73,73	1.35	12 (17%)	82,113,113	1.70	16 (19%)
25	CLA	b	601	-	69,73,73	1.38	7 (10%)	82,113,113	1.79	16 (19%)
26	LHG	b	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	G	612	21	64,68,73	1.41	10 (15%)	76,107,113	1.57	12 (15%)
35	DGD	C	515	-	56,56,67	0.49	0	70,70,81	1.21	6 (8%)
25	CLA	r	602	22	64,68,73	1.42	11 (17%)	76,107,113	1.76	17 (22%)
25	CLA	g	610	-	68,72,73	1.44	8 (11%)	80,111,113	1.94	16 (20%)
28	BCR	I	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.30	9 (16%)
25	CLA	C	509	6	69,73,73	1.37	12 (17%)	82,113,113	1.67	12 (14%)
24	CHL	Y	307	21	44,58,74	2.15	10 (22%)	37,94,114	2.69	17 (45%)
35	DGD	c	516	-	63,63,67	0.52	0	77,77,81	1.22	6 (7%)
24	CHL	R	605	-	40,54,74	2.31	13 (32%)	34,90,114	3.23	18 (52%)
25	CLA	b	615	5	69,73,73	1.39	9 (13%)	82,113,113	1.61	16 (19%)
25	CLA	g	602	21	69,73,73	1.35	12 (17%)	82,113,113	1.70	16 (19%)
24	CHL	5	302	1	40,54,74	2.35	14 (35%)	34,90,114	3.27	16 (47%)
25	CLA	n	610	21	69,73,73	1.38	10 (14%)	82,113,113	1.63	15 (18%)
25	CLA	g	612	21	64,68,73	1.42	10 (15%)	76,107,113	1.58	12 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	605	21	3/3/16/26	7/15/113/137	-
30	LMG	a	409	-	-	18/43/63/70	0/1/1/1
28	BCR	D	404	-	-	5/29/63/63	0/2/2/2
30	LMG	B	620	-	-	15/46/66/70	0/1/1/1
28	BCR	t	101	-	-	17/29/63/63	0/2/2/2
26	LHG	2	606	25	-	25/51/51/53	-
24	CHL	Y	308	-	2/2/18/26	7/30/128/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	y	319	25	-	23/53/53/53	-
32	AJP	B	624	-	34/34/38/38	13/28/220/220	0/11/11/11
24	CHL	l	302	1	3/3/16/26	6/15/113/137	-
28	BCR	h	101	-	-	6/29/63/63	0/2/2/2
24	CHL	R	606	-	3/3/16/26	9/15/113/137	-
26	LHG	n	618	25	-	28/53/53/53	-
25	CLA	b	614	5	1/1/15/20	13/39/115/115	-
26	LHG	S	318	25	-	20/53/53/53	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
25	CLA	b	613	5	1/1/15/20	13/39/115/115	-
24	CHL	s	307	-	3/3/16/26	7/15/113/137	-
24	CHL	S	306	-	3/3/16/26	6/15/113/137	-
24	CHL	s	308	-	3/3/16/26	3/15/113/137	-
25	CLA	n	614	21	1/1/11/20	3/19/95/115	-
25	CLA	B	609	5	1/1/15/20	11/39/115/115	-
39	LUT	Y	316	-	-	4/29/67/67	0/2/2/2
25	CLA	S	313	20	1/1/13/20	11/27/103/115	-
25	CLA	s	310	20	1/1/13/20	11/27/103/115	-
25	CLA	B	602	5	1/1/15/20	13/39/115/115	-
25	CLA	S	314	20	1/1/11/20	2/20/96/115	-
25	CLA	b	602	5	1/1/15/20	13/39/115/115	-
24	CHL	N	607	-	2/2/20/26	17/39/137/137	-
25	CLA	d	403	-	1/1/15/20	11/39/115/115	-
32	AJP	G	618	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	b	619	-	-	3/29/63/63	0/2/2/2
24	CHL	n	605	21	3/3/16/26	9/18/116/137	-
26	LHG	c	517	-	-	15/53/53/53	-
25	CLA	n	612	21	1/1/14/20	18/33/109/115	-
25	CLA	r	612	22	1/1/14/20	11/33/109/115	-
24	CHL	N	606	-	2/2/16/26	5/15/113/137	-
24	CHL	g	609	21	3/3/19/26	10/33/131/137	-
32	AJP	n	619	-	15/15/19/38	1/6/117/220	0/7/7/11
30	LMG	C	520	-	-	18/46/66/70	0/1/1/1
25	CLA	N	603	-	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	501	-	1/1/15/20	7/39/115/115	-
31	PL9	A	409	-	-	2/5/18/73	0/1/1/1
25	CLA	B	612	5	1/1/15/20	10/39/115/115	-
24	CHL	5	301	1	3/3/16/26	3/15/113/137	-
26	LHG	c	519	-	-	21/53/53/53	-
26	LHG	S	301	-	-	21/53/53/53	-
25	CLA	R	612	22	1/1/14/20	11/33/109/115	-
25	CLA	D	402	7	1/1/15/20	10/39/115/115	-
25	CLA	s	311	26	1/1/13/20	10/29/105/115	-
30	LMG	A	408	-	-	18/43/63/70	0/1/1/1
24	CHL	y	310	21	3/3/18/26	9/27/125/137	-
25	CLA	C	507	-	1/1/15/20	17/39/115/115	-
26	LHG	b	622	-	-	17/53/53/53	-
24	CHL	1	301	1	3/3/16/26	3/15/113/137	-
26	LHG	6	606	25	-	25/51/51/53	-
31	PL9	a	410	-	-	2/5/18/73	0/1/1/1
26	LHG	c	518	-	-	12/53/53/53	-
24	CHL	G	605	21	3/3/16/26	7/15/113/137	-
24	CHL	y	308	-	2/2/18/26	7/30/128/137	-
25	CLA	S	304	-	1/1/11/20	4/15/91/115	-
25	CLA	S	311	26	1/1/13/20	10/29/105/115	-
38	HEM	F	101	9	-	3/14/54/54	-
40	NEX	y	318	-	-	7/27/83/83	1/3/3/3
32	AJP	N	620	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	y	312	26	1/1/14/20	12/33/109/115	-
31	PL9	D	405	-	-	5/53/73/73	0/1/1/1
24	CHL	y	306	21	3/3/16/26	9/18/116/137	-
25	CLA	b	605	5	1/1/15/20	8/39/115/115	-
24	CHL	N	605	21	3/3/16/26	9/18/116/137	-
25	CLA	B	608	5	1/1/15/20	13/39/115/115	-
40	NEX	S	317	-	-	6/27/83/83	0/3/3/3
39	LUT	y	316	-	-	4/29/67/67	0/2/2/2
39	LUT	s	316	-	-	4/29/67/67	0/2/2/2
24	CHL	y	302	21	2/2/20/26	22/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	Y	302	21	2/2/20/26	22/39/137/137	-
25	CLA	B	605	5	1/1/15/20	8/39/115/115	-
25	CLA	C	510	-	1/1/15/20	13/39/115/115	-
25	CLA	N	611	26	1/1/14/20	14/33/109/115	-
25	CLA	g	613	21	1/1/15/20	15/39/115/115	-
25	CLA	b	612	5	1/1/15/20	10/39/115/115	-
25	CLA	N	610	21	1/1/15/20	16/39/115/115	-
25	CLA	c	504	-	1/1/14/20	13/33/109/115	-
26	LHG	R	618	25	-	11/46/46/53	-
26	LHG	C	519	-	-	21/53/53/53	-
25	CLA	R	608	22	1/1/13/20	16/31/107/115	-
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
25	CLA	b	607	-	1/1/15/20	16/39/115/115	-
25	CLA	R	602	22	1/1/14/20	8/33/109/115	-
35	DGD	c	515	-	-	17/44/84/95	0/2/2/2
25	CLA	2	604	26	1/1/13/20	11/27/103/115	-
25	CLA	C	503	6	1/1/15/20	11/39/115/115	-
24	CHL	N	608	-	3/3/20/26	14/39/137/137	-
26	LHG	D	406	-	-	17/53/53/53	-
25	CLA	r	609	22	1/1/15/20	15/39/115/115	-
40	NEX	s	317	-	-	6/27/83/83	0/3/3/3
25	CLA	B	607	-	1/1/15/20	16/39/115/115	-
40	NEX	n	617	-	-	10/27/83/83	0/3/3/3
25	CLA	g	603	-	1/1/14/20	12/33/109/115	-
39	LUT	G	615	-	-	4/29/67/67	0/2/2/2
40	NEX	r	617	-	-	6/27/83/83	0/3/3/3
25	CLA	a	406	4	1/1/14/20	11/33/109/115	-
26	LHG	B	625	-	-	14/50/50/53	-
25	CLA	G	603	-	1/1/14/20	13/33/109/115	-
38	HEM	f	101	9	-	3/14/54/54	-
26	LHG	y	301	-	-	14/53/53/53	-
25	CLA	c	506	6	1/1/15/20	11/39/115/115	-
28	BCR	d	404	-	-	5/29/63/63	0/2/2/2
24	CHL	2	603	-	3/3/16/26	10/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	N	618	25	-	28/53/53/53	-
25	CLA	s	313	20	1/1/13/20	11/27/103/115	-
28	BCR	z	101	-	-	8/29/63/63	0/2/2/2
35	DGD	A	415	-	-	26/48/88/95	0/2/2/2
40	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	b	608	5	1/1/15/20	13/39/115/115	-
25	CLA	B	601	-	1/1/15/20	15/39/115/115	-
32	AJP	Y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	n	607	-	2/2/20/26	17/39/137/137	-
25	CLA	2	605	-	1/1/11/20	10/19/95/115	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
27	PHO	A	403	-	-	11/37/103/103	0/5/6/6
25	CLA	c	508	6	1/1/15/20	12/39/115/115	-
26	LHG	Y	301	-	-	14/53/53/53	-
30	LMG	b	623	-	-	28/50/70/70	0/1/1/1
30	LMG	A	410	-	-	14/35/55/70	0/1/1/1
25	CLA	a	403	-	1/1/15/20	8/39/115/115	-
35	DGD	b	626	-	-	22/51/91/95	0/2/2/2
26	LHG	C	518	-	-	12/53/53/53	-
25	CLA	s	305	-	1/1/12/20	8/21/97/115	-
25	CLA	b	616	5	1/1/15/20	18/39/115/115	-
25	CLA	y	314	21	1/1/15/20	13/39/115/115	-
26	LHG	B	622	-	-	17/53/53/53	-
25	CLA	r	603	22	1/1/14/20	12/33/109/115	-
24	CHL	g	601	21	2/2/20/26	23/39/137/137	-
25	CLA	C	511	6	1/1/15/20	9/39/115/115	-
25	CLA	Y	311	21	1/1/14/20	11/33/109/115	-
25	CLA	c	510	-	1/1/15/20	13/39/115/115	-
25	CLA	g	611	-	1/1/14/20	15/33/109/115	-
25	CLA	R	603	22	1/1/14/20	12/33/109/115	-
32	AJP	Y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	G	613	21	1/1/15/20	15/39/115/115	-
25	CLA	G	614	21	1/1/11/20	10/19/95/115	-
25	CLA	Y	313	21	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
24	CHL	r	607	-	3/3/19/26	12/33/131/137	-
39	LUT	n	615	-	-	7/29/67/67	0/2/2/2
39	LUT	r	615	-	-	4/29/67/67	0/2/2/2
25	CLA	C	504	-	1/1/14/20	13/33/109/115	-
25	CLA	c	503	6	1/1/15/20	11/39/115/115	-
25	CLA	n	603	-	1/1/15/20	20/39/115/115	-
25	CLA	b	603	-	1/1/15/20	12/39/115/115	-
25	CLA	c	513	6	1/1/15/20	10/39/115/115	-
25	CLA	b	604	5	1/1/15/20	16/39/115/115	-
28	BCR	A	406	-	-	5/29/63/63	0/2/2/2
28	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	CLA	Y	303	21	1/1/15/20	12/39/115/115	-
25	CLA	N	602	21	1/1/15/20	15/39/115/115	-
28	BCR	B	618	-	-	2/29/63/63	0/2/2/2
27	PHO	a	404	-	-	11/37/103/103	0/5/6/6
25	CLA	S	310	20	1/1/13/20	11/27/103/115	-
25	CLA	c	507	-	1/1/15/20	17/39/115/115	-
25	CLA	n	613	21	1/1/14/20	20/33/109/115	-
25	CLA	r	614	22	1/1/11/20	8/15/91/115	-
24	CHL	s	306	-	3/3/16/26	6/15/113/137	-
29	SQD	A	411	-	-	22/49/69/69	0/1/1/1
25	CLA	Y	305	-	1/1/12/20	6/21/97/115	-
24	CHL	Y	306	21	3/3/16/26	9/18/116/137	-
28	BCR	a	407	-	-	5/29/63/63	0/2/2/2
25	CLA	B	611	5	1/1/15/20	11/39/115/115	-
25	CLA	R	614	22	1/1/11/20	8/15/91/115	-
25	CLA	C	506	6	1/1/15/20	11/39/115/115	-
25	CLA	B	614	5	1/1/15/20	13/39/115/115	-
25	CLA	b	606	5	1/1/15/20	13/39/115/115	-
40	NEX	G	617	25	-	11/27/83/83	0/3/3/3
32	AJP	n	620	-	16/16/19/38	4/6/117/220	0/7/7/11
29	SQD	l	101	-	-	27/49/69/69	0/1/1/1
28	BCR	i	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	R	613	22	3/3/15/26	5/10/108/137	-
39	LUT	g	616	-	-	0/29/67/67	0/2/2/2
25	CLA	s	303	20	1/1/14/20	20/35/111/115	-
32	AJP	y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
40	NEX	g	617	25	-	11/27/83/83	0/3/3/3
25	CLA	N	612	21	1/1/14/20	18/33/109/115	-
39	LUT	G	616	-	-	0/29/67/67	0/2/2/2
25	CLA	Y	304	-	1/1/15/20	22/39/115/115	-
32	AJP	N	619	-	15/15/19/38	1/6/117/220	0/7/7/11
32	AJP	y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	c	512	-	1/1/15/20	13/39/115/115	-
32	AJP	g	618	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	G	606	-	3/3/16/26	3/20/118/137	-
41	XAT	R	616	-	-	2/31/93/93	0/4/4/4
32	AJP	Y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	r	613	22	3/3/15/26	5/10/108/137	-
40	NEX	Y	318	-	-	7/27/83/83	1/3/3/3
24	CHL	r	606	-	3/3/16/26	9/15/113/137	-
39	LUT	g	615	-	-	4/29/67/67	0/2/2/2
25	CLA	s	314	20	1/1/11/20	2/20/96/115	-
25	CLA	D	401	42	1/1/12/20	2/21/97/115	-
27	PHO	A	404	-	-	2/37/103/103	0/5/6/6
25	CLA	C	513	6	1/1/15/20	10/39/115/115	-
25	CLA	S	303	20	1/1/14/20	20/35/111/115	-
24	CHL	g	607	-	2/2/16/26	5/15/113/137	-
32	AJP	A	412	-	34/34/38/38	9/28/220/220	0/11/11/11
25	CLA	s	309	20	1/1/11/20	6/15/91/115	-
25	CLA	y	311	21	1/1/14/20	11/33/109/115	-
24	CHL	G	607	-	2/2/16/26	5/15/113/137	-
25	CLA	Y	315	21	1/1/11/20	9/15/91/115	-
25	CLA	s	304	-	1/1/11/20	4/15/91/115	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
25	CLA	c	502	6	1/1/15/20	6/39/115/115	-
41	XAT	r	616	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	l	103	-	-	28/53/53/53	-
24	CHL	2	601	2	3/3/19/26	14/37/135/137	-
25	CLA	G	610	-	1/1/14/20	14/38/114/115	-
25	CLA	y	313	21	1/1/14/20	12/33/109/115	-
26	LHG	C	517	-	-	15/53/53/53	-
32	AJP	y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	S	309	20	1/1/11/20	6/15/91/115	-
30	LMG	D	407	-	-	16/41/61/70	0/1/1/1
30	LMG	d	407	-	-	16/41/61/70	0/1/1/1
26	LHG	d	406	-	-	17/53/53/53	-
24	CHL	n	606	-	2/2/16/26	5/15/113/137	-
25	CLA	N	613	21	1/1/14/20	20/33/109/115	-
25	CLA	2	602	2	1/1/14/20	14/33/109/115	-
25	CLA	S	312	20	1/1/11/20	8/20/96/115	-
29	SQD	L	103	-	-	27/49/69/69	0/1/1/1
29	SQD	a	408	-	-	21/45/65/69	0/1/1/1
24	CHL	r	605	-	3/3/16/26	3/15/113/137	-
25	CLA	G	611	-	1/1/14/20	15/33/109/115	-
25	CLA	R	609	22	1/1/15/20	15/39/115/115	-
24	CHL	Y	309	-	3/3/20/26	19/39/137/137	-
32	AJP	b	624	-	34/34/38/38	13/28/220/220	0/11/11/11
26	LHG	s	318	25	-	20/53/53/53	-
32	AJP	y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	B	616	5	1/1/15/20	18/39/115/115	-
25	CLA	Y	314	21	1/1/15/20	13/39/115/115	-
26	LHG	s	301	-	-	21/53/53/53	-
25	CLA	B	613	5	1/1/15/20	13/39/115/115	-
24	CHL	R	607	-	3/3/19/26	12/33/131/137	-
24	CHL	G	608	-	3/3/20/26	23/39/137/137	-
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
24	CHL	N	609	21	2/2/20/26	13/39/137/137	-
25	CLA	g	614	21	1/1/11/20	10/19/95/115	-
35	DGD	C	516	-	-	27/51/91/95	0/2/2/2
40	NEX	N	617	-	-	10/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	405	4	1/1/14/20	11/33/109/115	-
25	CLA	n	611	26	1/1/14/20	14/33/109/115	-
39	LUT	S	315	-	-	3/29/67/67	0/2/2/2
25	CLA	D	403	-	1/1/15/20	11/39/115/115	-
35	DGD	B	626	-	-	22/51/91/95	0/2/2/2
39	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
32	AJP	s	319	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
29	SQD	l	102	-	-	13/37/57/69	0/1/1/1
24	CHL	n	601	21	2/2/18/26	11/27/125/137	-
24	CHL	6	603	-	3/3/16/26	10/15/113/137	-
25	CLA	r	601	-	1/1/11/20	11/20/96/115	-
24	CHL	g	608	-	3/3/20/26	23/39/137/137	-
25	CLA	y	303	21	1/1/15/20	12/39/115/115	-
25	CLA	r	610	26	1/1/11/20	10/20/96/115	-
25	CLA	N	604	-	1/1/12/20	5/21/97/115	-
25	CLA	y	305	-	1/1/12/20	6/21/97/115	-
30	LMG	c	520	-	-	18/46/66/70	0/1/1/1
25	CLA	R	611	-	1/1/11/20	11/20/96/115	-
25	CLA	B	606	5	1/1/15/20	13/39/115/115	-
26	LHG	b	621	-	-	17/51/51/53	-
25	CLA	c	505	6	1/1/15/20	9/39/115/115	-
30	LMG	B	623	-	-	28/50/70/70	0/1/1/1
25	CLA	R	610	26	1/1/11/20	10/20/96/115	-
32	AJP	S	319	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	B	603	-	1/1/15/20	12/39/115/115	-
32	AJP	a	413	-	34/34/38/38	9/28/220/220	0/11/11/11
25	CLA	G	604	40	1/1/12/20	10/21/97/115	-
39	LUT	R	615	-	-	4/29/67/67	0/2/2/2
26	LHG	Y	319	25	-	23/53/53/53	-
28	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CHL	N	601	21	2/2/18/26	11/27/125/137	-
25	CLA	6	602	2	1/1/14/20	14/33/109/115	-
25	CLA	A	401	4	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	B	619	-	-	3/29/63/63	0/2/2/2
24	CHL	s	302	20	2/2/16/26	3/15/113/137	-
24	CHL	y	307	21	3/3/16/26	4/20/118/137	-
30	LMG	a	411	-	-	14/35/55/70	0/1/1/1
25	CLA	b	611	5	1/1/15/20	11/39/115/115	-
25	CLA	r	611	-	1/1/11/20	11/20/96/115	-
25	CLA	y	304	-	1/1/15/20	22/39/115/115	-
25	CLA	B	615	5	1/1/15/20	10/39/115/115	-
25	CLA	b	610	-	1/1/15/20	7/39/115/115	-
25	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	CLA	c	509	6	1/1/15/20	10/39/115/115	-
25	CLA	d	401	42	1/1/12/20	2/21/97/115	-
24	CHL	G	609	21	3/3/19/26	10/33/131/137	-
25	CLA	6	604	26	1/1/13/20	11/27/103/115	-
25	CLA	g	604	40	1/1/12/20	10/21/97/115	-
30	LMG	b	620	-	-	15/46/66/70	0/1/1/1
25	CLA	c	511	6	1/1/15/20	9/39/115/115	-
25	CLA	S	305	-	1/1/12/20	8/21/97/115	-
25	CLA	B	610	-	1/1/15/20	7/39/115/115	-
28	BCR	B	617	-	-	3/29/63/63	0/2/2/2
32	AJP	Y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
24	CHL	S	307	-	3/3/16/26	7/15/113/137	-
39	LUT	N	615	-	-	7/29/67/67	0/2/2/2
25	CLA	n	604	-	1/1/12/20	5/21/97/115	-
24	CHL	6	601	2	3/3/19/26	14/37/135/137	-
24	CHL	n	608	-	3/3/20/26	15/39/137/137	-
25	CLA	6	605	-	1/1/11/20	10/19/95/115	-
29	SQD	L	101	-	-	13/37/57/69	0/1/1/1
25	CLA	b	609	5	1/1/15/20	11/39/115/115	-
25	CLA	y	315	21	1/1/11/20	9/15/91/115	-
25	CLA	C	502	6	1/1/15/20	6/39/115/115	-
39	LUT	y	317	-	-	4/29/67/67	0/2/2/2
25	CLA	c	501	-	1/1/15/20	7/39/115/115	-
25	CLA	r	608	22	1/1/13/20	16/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	312	20	1/1/11/20	8/20/96/115	-
25	CLA	B	604	5	1/1/15/20	16/39/115/115	-
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
24	CHL	n	609	21	2/2/20/26	13/39/137/137	-
24	CHL	S	308	-	3/3/16/26	3/15/113/137	-
25	CLA	a	402	4	1/1/15/20	7/39/115/115	-
24	CHL	Y	310	21	3/3/18/26	9/27/125/137	-
24	CHL	y	309	-	3/3/20/26	19/39/137/137	-
25	CLA	A	402	-	1/1/15/20	8/39/115/115	-
32	AJP	y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	d	402	7	1/1/15/20	10/39/115/115	-
25	CLA	n	602	21	1/1/15/20	15/39/115/115	-
25	CLA	N	614	21	1/1/11/20	3/19/95/115	-
28	BCR	T	101	-	-	17/29/63/63	0/2/2/2
25	CLA	r	604	-	1/1/11/20	7/19/95/115	-
24	CHL	G	601	21	2/2/20/26	23/39/137/137	-
39	LUT	S	316	-	-	4/29/67/67	0/2/2/2
26	LHG	B	621	-	-	17/51/51/53	-
32	AJP	Y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	Y	312	26	1/1/14/20	12/33/109/115	-
28	BCR	b	617	-	-	3/29/63/63	0/2/2/2
24	CHL	g	606	-	3/3/16/26	3/20/118/137	-
29	SQD	A	407	-	-	21/45/65/69	0/1/1/1
25	CLA	R	601	-	1/1/11/20	11/20/96/115	-
25	CLA	R	604	-	1/1/11/20	7/19/95/115	-
25	CLA	C	508	6	1/1/15/20	12/39/115/115	-
35	DGD	a	401	-	-	26/48/88/95	0/2/2/2
24	CHL	S	302	20	2/2/16/26	3/15/113/137	-
26	LHG	r	618	25	-	11/46/46/53	-
28	BCR	H	101	-	-	6/29/63/63	0/2/2/2
27	PHO	a	405	-	-	2/37/103/103	0/5/6/6
25	CLA	C	505	6	1/1/15/20	9/39/115/115	-
39	LUT	s	315	-	-	3/29/67/67	0/2/2/2
26	LHG	L	102	-	-	28/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	602	21	1/1/15/20	14/39/115/115	-
25	CLA	b	601	-	1/1/15/20	15/39/115/115	-
26	LHG	b	625	-	-	14/50/50/53	-
25	CLA	G	612	21	1/1/14/20	12/33/109/115	-
35	DGD	C	515	-	-	17/44/84/95	0/2/2/2
25	CLA	r	602	22	1/1/14/20	8/33/109/115	-
25	CLA	g	610	-	1/1/14/20	14/38/114/115	-
28	BCR	I	101	-	-	4/29/63/63	0/2/2/2
25	CLA	C	509	6	1/1/15/20	10/39/115/115	-
24	CHL	Y	307	21	3/3/16/26	4/20/118/137	-
35	DGD	c	516	-	-	27/51/91/95	0/2/2/2
24	CHL	R	605	-	3/3/16/26	3/15/113/137	-
25	CLA	b	615	5	1/1/15/20	10/39/115/115	-
25	CLA	g	602	21	1/1/15/20	14/39/115/115	-
24	CHL	5	302	1	3/3/16/26	6/15/113/137	-
25	CLA	n	610	21	1/1/15/20	16/39/115/115	-
25	CLA	g	612	21	1/1/14/20	12/33/109/115	-

All (2571) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	101	HEM	FE-NB	14.55	2.39	1.94
38	f	101	HEM	FE-NB	14.55	2.39	1.94
24	2	603	CHL	C1D-C2D	7.93	1.48	1.39
24	6	603	CHL	C1D-C2D	7.93	1.48	1.39
25	R	611	CLA	MG-ND	-6.76	1.92	2.05
25	r	611	CLA	MG-ND	-6.71	1.92	2.05
25	R	611	CLA	MG-NB	-6.50	1.92	2.05
25	r	611	CLA	MG-NB	-6.50	1.92	2.05
25	r	610	CLA	MG-NB	-6.43	1.93	2.05
25	R	610	CLA	MG-NB	-6.42	1.93	2.05
25	R	610	CLA	MG-ND	-6.29	1.93	2.05
25	R	601	CLA	MG-ND	-6.26	1.93	2.05
25	r	610	CLA	MG-ND	-6.26	1.93	2.05
25	r	601	CLA	MG-ND	-6.23	1.93	2.05
25	2	602	CLA	MG-NB	-6.16	1.93	2.05
25	6	602	CLA	MG-NB	-6.16	1.93	2.05
25	R	603	CLA	MG-ND	-6.12	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	603	CLA	MG-ND	-6.12	1.93	2.05
25	C	504	CLA	MG-NB	-6.12	1.93	2.05
25	c	504	CLA	MG-NB	-6.12	1.93	2.05
25	R	603	CLA	MG-NB	-6.11	1.93	2.05
25	r	601	CLA	MG-NB	-6.08	1.93	2.05
25	S	305	CLA	MG-NB	-6.08	1.93	2.05
25	r	603	CLA	MG-NB	-6.08	1.93	2.05
25	s	305	CLA	MG-NB	-6.07	1.93	2.05
25	S	305	CLA	MG-ND	-6.06	1.93	2.05
25	s	305	CLA	MG-ND	-6.06	1.93	2.05
25	d	403	CLA	MG-ND	-6.06	1.93	2.05
25	D	403	CLA	MG-ND	-6.05	1.93	2.05
25	D	403	CLA	MG-NB	-6.05	1.93	2.05
25	d	403	CLA	MG-NB	-6.05	1.93	2.05
25	R	601	CLA	MG-NB	-6.04	1.93	2.05
25	C	504	CLA	MG-ND	-6.01	1.93	2.05
25	c	504	CLA	MG-ND	-5.99	1.93	2.05
25	2	602	CLA	MG-ND	-5.98	1.93	2.05
25	6	602	CLA	MG-ND	-5.98	1.93	2.05
25	C	501	CLA	MG-NB	-5.93	1.94	2.05
25	c	501	CLA	MG-NB	-5.93	1.94	2.05
24	2	603	CHL	C3B-C4B	5.86	1.47	1.41
24	6	603	CHL	C3B-C4B	5.86	1.47	1.41
24	G	607	CHL	C3B-C4B	5.81	1.47	1.41
25	C	501	CLA	MG-ND	-5.81	1.94	2.05
25	c	501	CLA	MG-ND	-5.81	1.94	2.05
24	2	601	CHL	C3B-C4B	5.75	1.47	1.41
24	6	601	CHL	C3B-C4B	5.75	1.47	1.41
24	Y	308	CHL	CMC-C2C	5.75	1.56	1.44
24	y	308	CHL	CMC-C2C	5.75	1.56	1.44
24	5	302	CHL	CMC-C2C	5.73	1.56	1.44
24	1	301	CHL	C3B-C4B	5.72	1.47	1.41
24	5	301	CHL	C3B-C4B	5.72	1.47	1.41
25	2	604	CLA	MG-ND	-5.71	1.94	2.05
24	G	607	CHL	CMC-C2C	5.71	1.56	1.44
24	g	607	CHL	CMC-C2C	5.71	1.56	1.44
24	6	601	CHL	CMC-C2C	5.71	1.56	1.44
24	R	613	CHL	CMC-C2C	5.71	1.56	1.44
24	R	605	CHL	C3B-C4B	5.70	1.46	1.41
24	n	601	CHL	CMC-C2C	5.70	1.56	1.44
24	N	601	CHL	CMC-C2C	5.70	1.56	1.44
24	r	607	CHL	CMC-C2C	5.69	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	605	CHL	C3B-C4B	5.68	1.46	1.41
24	1	302	CHL	CMC-C2C	5.68	1.56	1.44
24	1	301	CHL	CMC-C2C	5.68	1.56	1.44
24	S	306	CHL	C3B-C4B	5.67	1.46	1.41
24	R	607	CHL	CMC-C2C	5.67	1.56	1.44
24	5	301	CHL	CMC-C2C	5.67	1.56	1.44
25	6	604	CLA	MG-ND	-5.67	1.94	2.05
24	g	609	CHL	CMC-C2C	5.66	1.56	1.44
24	2	601	CHL	CMC-C2C	5.66	1.56	1.44
24	S	308	CHL	CMC-C2C	5.66	1.56	1.44
24	s	308	CHL	CMC-C2C	5.66	1.56	1.44
24	S	308	CHL	C3B-C4B	5.66	1.46	1.41
24	G	606	CHL	C3B-C4B	5.66	1.46	1.41
24	s	308	CHL	C3B-C4B	5.66	1.46	1.41
24	r	606	CHL	CMC-C2C	5.66	1.56	1.44
25	2	604	CLA	MG-NB	-5.65	1.94	2.05
25	6	604	CLA	MG-NB	-5.65	1.94	2.05
24	r	613	CHL	CMC-C2C	5.65	1.56	1.44
24	g	607	CHL	C3B-C4B	5.65	1.46	1.41
24	r	605	CHL	C3B-C4B	5.65	1.46	1.41
24	S	306	CHL	CMC-C2C	5.65	1.56	1.44
24	S	307	CHL	CMC-C2C	5.65	1.56	1.44
24	s	307	CHL	CMC-C2C	5.65	1.56	1.44
24	G	606	CHL	CMC-C2C	5.64	1.56	1.44
24	g	606	CHL	CMC-C2C	5.64	1.56	1.44
24	R	606	CHL	CMC-C2C	5.64	1.56	1.44
24	s	302	CHL	CMC-C2C	5.64	1.56	1.44
24	Y	309	CHL	CMC-C2C	5.64	1.56	1.44
24	s	306	CHL	C3B-C4B	5.63	1.46	1.41
24	r	613	CHL	C3B-C4B	5.63	1.46	1.41
24	N	605	CHL	CMC-C2C	5.63	1.56	1.44
24	n	605	CHL	CMC-C2C	5.63	1.56	1.44
24	G	609	CHL	CMC-C2C	5.63	1.56	1.44
24	n	608	CHL	CMC-C2C	5.63	1.56	1.44
24	N	607	CHL	C3B-C4B	5.63	1.46	1.41
24	n	607	CHL	C3B-C4B	5.63	1.46	1.41
24	G	608	CHL	C3B-C4B	5.62	1.46	1.41
24	N	609	CHL	CMC-C2C	5.62	1.56	1.44
24	n	609	CHL	CMC-C2C	5.62	1.56	1.44
24	Y	306	CHL	CMC-C2C	5.62	1.56	1.44
24	N	606	CHL	CMC-C2C	5.62	1.56	1.44
24	n	606	CHL	CMC-C2C	5.62	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	309	CHL	CMC-C2C	5.62	1.56	1.44
24	R	606	CHL	C3B-C4B	5.62	1.46	1.41
24	g	606	CHL	C3B-C4B	5.62	1.46	1.41
24	r	606	CHL	C3B-C4B	5.62	1.46	1.41
24	N	609	CHL	C3B-C4B	5.62	1.46	1.41
24	n	609	CHL	C3B-C4B	5.62	1.46	1.41
24	s	302	CHL	C3B-C4B	5.62	1.46	1.41
24	G	608	CHL	CMC-C2C	5.62	1.56	1.44
24	g	608	CHL	CMC-C2C	5.62	1.56	1.44
24	y	306	CHL	CMC-C2C	5.62	1.56	1.44
24	R	613	CHL	C3B-C4B	5.61	1.46	1.41
24	s	306	CHL	CMC-C2C	5.61	1.56	1.44
24	N	608	CHL	CMC-C2C	5.61	1.56	1.44
24	G	601	CHL	C3B-C4B	5.61	1.46	1.41
24	N	605	CHL	C3B-C4B	5.61	1.46	1.41
24	n	605	CHL	C3B-C4B	5.61	1.46	1.41
24	Y	302	CHL	CMC-C2C	5.61	1.56	1.44
24	y	302	CHL	CMC-C2C	5.61	1.56	1.44
24	r	605	CHL	CMC-C2C	5.60	1.56	1.44
24	N	607	CHL	CMC-C2C	5.60	1.56	1.44
24	n	607	CHL	CMC-C2C	5.60	1.56	1.44
24	G	605	CHL	CMC-C2C	5.60	1.56	1.44
24	S	302	CHL	CMC-C2C	5.59	1.56	1.44
24	Y	307	CHL	CMC-C2C	5.59	1.56	1.44
24	g	605	CHL	C3B-C4B	5.59	1.46	1.41
24	Y	310	CHL	CMC-C2C	5.59	1.56	1.44
24	y	310	CHL	CMC-C2C	5.59	1.56	1.44
24	y	306	CHL	C3B-C4B	5.58	1.46	1.41
24	R	605	CHL	CMC-C2C	5.58	1.56	1.44
24	N	608	CHL	C3B-C4B	5.58	1.46	1.41
24	n	608	CHL	C3B-C4B	5.58	1.46	1.41
24	G	601	CHL	CMC-C2C	5.58	1.56	1.44
24	g	601	CHL	CMC-C2C	5.58	1.56	1.44
24	y	307	CHL	CMC-C2C	5.58	1.56	1.44
24	g	601	CHL	C3B-C4B	5.57	1.46	1.41
24	g	608	CHL	C3B-C4B	5.56	1.46	1.41
24	S	302	CHL	C3B-C4B	5.55	1.46	1.41
24	G	609	CHL	C3B-C4B	5.55	1.46	1.41
24	n	601	CHL	C3B-C4B	5.55	1.46	1.41
24	g	605	CHL	CMC-C2C	5.54	1.56	1.44
24	N	601	CHL	C3B-C4B	5.54	1.46	1.41
24	Y	306	CHL	C3B-C4B	5.53	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	606	CHL	C3B-C4B	5.52	1.46	1.41
24	S	307	CHL	C3B-C4B	5.52	1.46	1.41
24	s	307	CHL	C3B-C4B	5.52	1.46	1.41
24	n	606	CHL	C3B-C4B	5.52	1.46	1.41
24	y	309	CHL	C3B-C4B	5.52	1.46	1.41
24	Y	309	CHL	C3B-C4B	5.46	1.46	1.41
24	g	609	CHL	C3B-C4B	5.46	1.46	1.41
24	G	607	CHL	C1D-C2D	5.45	1.45	1.39
24	g	607	CHL	C1D-C2D	5.45	1.45	1.39
24	Y	310	CHL	C3B-C4B	5.45	1.46	1.41
24	y	310	CHL	C3B-C4B	5.45	1.46	1.41
24	R	607	CHL	C3B-C4B	5.41	1.46	1.41
24	r	607	CHL	C3B-C4B	5.41	1.46	1.41
24	2	603	CHL	CMC-C2C	5.39	1.56	1.44
24	Y	302	CHL	C3B-C4B	5.37	1.46	1.41
24	y	302	CHL	C3B-C4B	5.37	1.46	1.41
25	2	602	CLA	MG-NA	-5.35	1.93	2.06
25	6	602	CLA	MG-NA	-5.35	1.93	2.06
24	6	603	CHL	CMC-C2C	5.35	1.55	1.44
25	R	611	CLA	MG-NA	-5.32	1.93	2.06
25	r	611	CLA	MG-NA	-5.32	1.93	2.06
25	2	602	CLA	MG-NC	-5.31	1.93	2.06
25	6	602	CLA	MG-NC	-5.31	1.93	2.06
25	R	611	CLA	MG-NC	-5.28	1.93	2.06
25	r	611	CLA	MG-NC	-5.28	1.93	2.06
24	y	308	CHL	C3B-C4B	5.26	1.46	1.41
24	N	601	CHL	C1D-C2D	5.25	1.45	1.39
24	Y	308	CHL	C1D-C2D	5.25	1.45	1.39
24	y	308	CHL	C1D-C2D	5.22	1.45	1.39
24	n	601	CHL	C1D-C2D	5.21	1.45	1.39
24	Y	308	CHL	C3B-C4B	5.21	1.46	1.41
24	G	601	CHL	C1D-C2D	5.19	1.45	1.39
24	g	601	CHL	C1D-C2D	5.19	1.45	1.39
25	G	611	CLA	MG-ND	-5.18	1.95	2.05
25	g	611	CLA	MG-ND	-5.18	1.95	2.05
24	G	608	CHL	C1D-C2D	5.18	1.45	1.39
24	G	606	CHL	C1D-C2D	5.18	1.45	1.39
24	g	606	CHL	C1D-C2D	5.18	1.45	1.39
25	G	610	CLA	MG-NB	-5.17	1.95	2.05
25	g	610	CLA	MG-NB	-5.17	1.95	2.05
25	r	610	CLA	MG-NA	-5.17	1.94	2.06
24	g	608	CHL	C1D-C2D	5.17	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	302	CHL	C1D-C2D	5.16	1.45	1.39
24	R	607	CHL	C1D-C2D	5.16	1.45	1.39
24	r	607	CHL	C1D-C2D	5.16	1.45	1.39
25	G	611	CLA	MG-NB	-5.16	1.95	2.05
25	g	611	CLA	MG-NB	-5.16	1.95	2.05
25	r	604	CLA	MG-NB	-5.15	1.95	2.05
25	g	610	CLA	MG-ND	-5.14	1.95	2.05
24	R	613	CHL	C1D-C2D	5.14	1.45	1.39
24	r	613	CHL	C1D-C2D	5.14	1.45	1.39
24	Y	309	CHL	C1D-C2D	5.14	1.45	1.39
24	y	309	CHL	C1D-C2D	5.14	1.45	1.39
24	Y	302	CHL	C1D-C2D	5.14	1.45	1.39
24	y	302	CHL	C1D-C2D	5.14	1.45	1.39
24	S	306	CHL	C1D-C2D	5.14	1.45	1.39
24	N	607	CHL	C1D-C2D	5.14	1.45	1.39
24	n	607	CHL	C1D-C2D	5.14	1.45	1.39
25	R	604	CLA	MG-NB	-5.13	1.95	2.05
25	R	610	CLA	MG-NA	-5.13	1.94	2.06
24	R	605	CHL	C1D-C2D	5.12	1.45	1.39
24	r	605	CHL	C1D-C2D	5.12	1.45	1.39
25	r	612	CLA	MG-NB	-5.12	1.95	2.05
24	l	302	CHL	C3B-C4B	5.12	1.46	1.41
24	G	605	CHL	C1D-C2D	5.12	1.45	1.39
24	g	605	CHL	C1D-C2D	5.12	1.45	1.39
25	R	612	CLA	MG-NB	-5.11	1.95	2.05
24	s	306	CHL	C1D-C2D	5.11	1.45	1.39
24	N	605	CHL	C1D-C2D	5.10	1.45	1.39
24	n	605	CHL	C1D-C2D	5.10	1.45	1.39
25	G	610	CLA	MG-ND	-5.10	1.95	2.05
24	l	301	CHL	C1D-C2D	5.10	1.45	1.39
24	S	308	CHL	C1D-C2D	5.10	1.45	1.39
24	5	301	CHL	C1D-C2D	5.10	1.45	1.39
24	s	308	CHL	C1D-C2D	5.10	1.45	1.39
24	n	606	CHL	C1D-C2D	5.10	1.45	1.39
24	N	609	CHL	C1D-C2D	5.09	1.45	1.39
24	n	609	CHL	C1D-C2D	5.09	1.45	1.39
24	2	601	CHL	C1D-C2D	5.08	1.45	1.39
24	6	601	CHL	C1D-C2D	5.08	1.45	1.39
24	5	302	CHL	C3B-C4B	5.07	1.46	1.41
24	S	307	CHL	C1D-C2D	5.06	1.45	1.39
24	s	307	CHL	C1D-C2D	5.06	1.45	1.39
24	S	302	CHL	C1D-C2D	5.06	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	305	CLA	MG-NA	-5.06	1.94	2.06
25	s	305	CLA	MG-NA	-5.06	1.94	2.06
24	N	608	CHL	C1D-C2D	5.06	1.45	1.39
24	G	609	CHL	C1D-C2D	5.06	1.45	1.39
24	n	608	CHL	C1D-C2D	5.05	1.45	1.39
24	5	302	CHL	C1D-C2D	5.05	1.45	1.39
24	R	606	CHL	C1D-C2D	5.04	1.45	1.39
24	r	606	CHL	C1D-C2D	5.04	1.45	1.39
24	g	609	CHL	C1D-C2D	5.04	1.45	1.39
24	N	606	CHL	C1D-C2D	5.03	1.45	1.39
24	1	302	CHL	C1B-C2B	5.02	1.45	1.39
24	5	302	CHL	C1B-C2B	5.02	1.45	1.39
24	Y	302	CHL	C1B-C2B	5.02	1.45	1.39
25	N	614	CLA	MG-NB	-5.01	1.95	2.05
24	Y	306	CHL	C1D-C2D	5.01	1.45	1.39
24	y	306	CHL	C1D-C2D	5.01	1.45	1.39
24	y	302	CHL	C1B-C2B	4.99	1.45	1.39
24	G	606	CHL	C1B-C2B	4.99	1.45	1.39
25	R	604	CLA	MG-ND	-4.99	1.95	2.05
24	y	310	CHL	C1D-C2D	4.97	1.45	1.39
24	1	302	CHL	C1D-C2D	4.96	1.45	1.39
25	G	613	CLA	MG-NB	-4.94	1.96	2.05
25	R	610	CLA	MG-NC	-4.94	1.94	2.06
25	n	614	CLA	MG-NB	-4.94	1.96	2.05
25	r	604	CLA	MG-ND	-4.93	1.96	2.05
24	Y	310	CHL	C1D-C2D	4.93	1.45	1.39
25	R	612	CLA	MG-ND	-4.93	1.96	2.05
24	2	603	CHL	OBD-CAD	4.92	1.28	1.22
24	6	603	CHL	OBD-CAD	4.92	1.28	1.22
25	r	610	CLA	MG-NC	-4.92	1.94	2.06
25	S	313	CLA	MG-NB	-4.91	1.96	2.05
25	D	403	CLA	MG-NA	-4.91	1.94	2.06
25	g	613	CLA	MG-NB	-4.91	1.96	2.05
25	c	504	CLA	MG-NA	-4.91	1.94	2.06
25	N	613	CLA	MG-NB	-4.91	1.96	2.05
25	n	613	CLA	MG-NB	-4.91	1.96	2.05
24	2	603	CHL	C1B-C2B	4.90	1.45	1.39
25	r	612	CLA	MG-ND	-4.90	1.96	2.05
24	n	601	CHL	C1B-C2B	4.90	1.45	1.39
25	d	403	CLA	MG-NA	-4.90	1.94	2.06
25	C	504	CLA	MG-NA	-4.89	1.94	2.06
24	G	609	CHL	C1B-C2B	4.89	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	609	CHL	C1B-C2B	4.89	1.45	1.39
25	s	305	CLA	MG-NC	-4.89	1.94	2.06
24	R	613	CHL	C1B-C2B	4.89	1.45	1.39
24	n	606	CHL	C1B-C2B	4.89	1.45	1.39
24	N	606	CHL	C1B-C2B	4.89	1.45	1.39
25	s	313	CLA	MG-NB	-4.88	1.96	2.05
25	r	603	CLA	MG-NA	-4.88	1.94	2.06
24	g	605	CHL	C1B-C2B	4.87	1.45	1.39
25	B	601	CLA	MG-NB	-4.87	1.96	2.05
25	b	601	CLA	MG-NB	-4.87	1.96	2.05
25	R	603	CLA	MG-NA	-4.87	1.94	2.06
24	g	606	CHL	C1B-C2B	4.87	1.45	1.39
25	S	305	CLA	MG-NC	-4.86	1.94	2.06
24	N	601	CHL	C1B-C2B	4.86	1.45	1.39
25	R	601	CLA	MG-NA	-4.85	1.94	2.06
25	r	601	CLA	MG-NA	-4.85	1.94	2.06
24	l	301	CHL	C1B-C2B	4.85	1.45	1.39
24	N	608	CHL	C1B-C2B	4.84	1.45	1.39
24	R	607	CHL	C1B-C2B	4.84	1.45	1.39
24	r	607	CHL	C1B-C2B	4.84	1.45	1.39
24	r	613	CHL	C1B-C2B	4.83	1.45	1.39
24	s	302	CHL	C1B-C2B	4.83	1.45	1.39
25	d	403	CLA	MG-NC	-4.82	1.94	2.06
24	6	603	CHL	C1B-C2B	4.82	1.45	1.39
24	Y	306	CHL	C1B-C2B	4.82	1.45	1.39
24	S	307	CHL	C1B-C2B	4.81	1.45	1.39
24	s	307	CHL	C1B-C2B	4.81	1.45	1.39
24	y	307	CHL	C1B-C2B	4.81	1.45	1.39
24	G	605	CHL	C1B-C2B	4.81	1.45	1.39
24	g	601	CHL	C1B-C2B	4.81	1.45	1.39
24	Y	310	CHL	C1B-C2B	4.81	1.45	1.39
25	r	601	CLA	MG-NC	-4.81	1.94	2.06
25	n	614	CLA	MG-ND	-4.81	1.96	2.05
24	S	302	CHL	C1B-C2B	4.81	1.45	1.39
24	r	606	CHL	C1B-C2B	4.80	1.45	1.39
24	R	606	CHL	C1B-C2B	4.80	1.45	1.39
24	y	309	CHL	C1B-C2B	4.80	1.45	1.39
24	N	609	CHL	C1B-C2B	4.80	1.45	1.39
24	n	609	CHL	C1B-C2B	4.80	1.45	1.39
25	D	403	CLA	MG-NC	-4.79	1.94	2.06
25	N	614	CLA	MG-ND	-4.79	1.96	2.05
24	Y	307	CHL	C1B-C2B	4.79	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	313	CLA	MG-ND	-4.79	1.96	2.05
24	5	301	CHL	C1B-C2B	4.79	1.45	1.39
25	R	601	CLA	MG-NC	-4.78	1.94	2.06
24	g	608	CHL	C1B-C2B	4.78	1.45	1.39
24	y	306	CHL	C1B-C2B	4.78	1.45	1.39
25	B	606	CLA	MG-NB	-4.77	1.96	2.05
25	b	606	CLA	MG-NB	-4.77	1.96	2.05
24	S	308	CHL	C1B-C2B	4.76	1.44	1.39
24	n	608	CHL	C1B-C2B	4.76	1.44	1.39
25	C	504	CLA	MG-NC	-4.76	1.95	2.06
24	N	605	CHL	C1B-C2B	4.76	1.44	1.39
24	n	605	CHL	C1B-C2B	4.76	1.44	1.39
24	G	608	CHL	C1B-C2B	4.76	1.44	1.39
25	g	613	CLA	MG-NA	-4.75	1.95	2.06
25	c	504	CLA	MG-NC	-4.75	1.95	2.06
25	S	313	CLA	MG-ND	-4.75	1.96	2.05
25	R	603	CLA	MG-NC	-4.75	1.95	2.06
25	r	603	CLA	MG-NC	-4.75	1.95	2.06
24	Y	307	CHL	C3B-C4B	4.74	1.46	1.41
24	2	601	CHL	C1B-C2B	4.74	1.44	1.39
24	6	601	CHL	C1B-C2B	4.74	1.44	1.39
24	Y	309	CHL	C1B-C2B	4.74	1.44	1.39
24	y	310	CHL	C1B-C2B	4.73	1.44	1.39
24	S	306	CHL	C1B-C2B	4.72	1.44	1.39
24	s	306	CHL	C1B-C2B	4.72	1.44	1.39
24	G	601	CHL	C1B-C2B	4.72	1.44	1.39
25	B	601	CLA	MG-ND	-4.72	1.96	2.05
25	b	601	CLA	MG-ND	-4.72	1.96	2.05
25	C	508	CLA	MG-NB	-4.71	1.96	2.05
25	c	508	CLA	MG-NB	-4.71	1.96	2.05
25	G	613	CLA	MG-NA	-4.71	1.95	2.06
24	y	307	CHL	C3B-C4B	4.70	1.46	1.41
24	Y	308	CHL	C1B-C2B	4.70	1.44	1.39
24	s	308	CHL	C1B-C2B	4.69	1.44	1.39
24	R	605	CHL	C1B-C2B	4.68	1.44	1.39
24	r	605	CHL	C1B-C2B	4.68	1.44	1.39
25	g	613	CLA	MG-ND	-4.68	1.96	2.05
25	C	501	CLA	MG-NA	-4.67	1.95	2.06
25	c	501	CLA	MG-NA	-4.67	1.95	2.06
25	C	511	CLA	MG-NB	-4.67	1.96	2.05
25	c	511	CLA	MG-NB	-4.67	1.96	2.05
25	G	613	CLA	MG-ND	-4.64	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	604	CLA	MG-NC	-4.62	1.95	2.06
25	6	604	CLA	MG-NC	-4.62	1.95	2.06
24	y	308	CHL	C1B-C2B	4.61	1.44	1.39
25	A	402	CLA	MG-NB	-4.61	1.96	2.05
25	a	403	CLA	MG-NB	-4.61	1.96	2.05
25	C	501	CLA	MG-NC	-4.59	1.95	2.06
25	c	501	CLA	MG-NC	-4.59	1.95	2.06
25	c	507	CLA	MG-ND	-4.58	1.96	2.05
25	C	507	CLA	MG-ND	-4.57	1.96	2.05
25	B	605	CLA	MG-NB	-4.56	1.96	2.05
25	S	311	CLA	MG-NB	-4.55	1.96	2.05
25	s	311	CLA	MG-NB	-4.55	1.96	2.05
25	C	508	CLA	MG-ND	-4.55	1.96	2.05
25	c	508	CLA	MG-ND	-4.55	1.96	2.05
25	A	402	CLA	MG-ND	-4.55	1.96	2.05
25	N	612	CLA	MG-NA	-4.54	1.95	2.06
25	D	401	CLA	MG-NB	-4.54	1.96	2.05
25	d	401	CLA	MG-NB	-4.54	1.96	2.05
25	B	606	CLA	MG-ND	-4.53	1.96	2.05
25	b	606	CLA	MG-ND	-4.53	1.96	2.05
25	a	403	CLA	MG-ND	-4.52	1.96	2.05
25	b	605	CLA	MG-NB	-4.52	1.96	2.05
25	Y	314	CLA	MG-NB	-4.52	1.96	2.05
25	y	314	CLA	MG-NB	-4.52	1.96	2.05
25	C	507	CLA	MG-NB	-4.52	1.96	2.05
25	S	311	CLA	MG-ND	-4.51	1.96	2.05
25	n	612	CLA	MG-NA	-4.51	1.95	2.06
25	c	510	CLA	MG-NB	-4.51	1.96	2.05
25	C	510	CLA	MG-NB	-4.50	1.96	2.05
24	n	607	CHL	C1B-C2B	4.49	1.44	1.39
25	C	512	CLA	MG-ND	-4.49	1.96	2.05
25	c	512	CLA	MG-ND	-4.49	1.96	2.05
25	r	609	CLA	MG-ND	-4.49	1.96	2.05
25	C	511	CLA	MG-ND	-4.49	1.96	2.05
25	c	511	CLA	MG-ND	-4.49	1.96	2.05
25	6	604	CLA	MG-NA	-4.49	1.95	2.06
24	N	607	CHL	C1B-C2B	4.49	1.44	1.39
25	c	510	CLA	MG-ND	-4.49	1.96	2.05
25	2	604	CLA	MG-NA	-4.48	1.95	2.06
25	C	510	CLA	MG-ND	-4.48	1.96	2.05
25	s	311	CLA	MG-ND	-4.47	1.96	2.05
25	D	401	CLA	MG-ND	-4.46	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	CLA	MG-ND	-4.46	1.96	2.05
25	s	304	CLA	MG-NB	-4.46	1.97	2.05
25	6	605	CLA	MG-ND	-4.46	1.97	2.05
25	c	507	CLA	MG-NB	-4.45	1.97	2.05
25	A	401	CLA	MG-ND	-4.45	1.97	2.05
25	a	402	CLA	MG-ND	-4.45	1.97	2.05
25	B	605	CLA	MG-ND	-4.44	1.97	2.05
25	b	605	CLA	MG-ND	-4.44	1.97	2.05
25	A	401	CLA	MG-NB	-4.44	1.97	2.05
25	a	402	CLA	MG-NB	-4.44	1.97	2.05
24	Y	307	CHL	C1D-C2D	4.44	1.44	1.39
24	y	307	CHL	C1D-C2D	4.44	1.44	1.39
25	2	605	CLA	MG-ND	-4.43	1.97	2.05
25	R	609	CLA	MG-ND	-4.43	1.97	2.05
25	C	509	CLA	MG-ND	-4.42	1.97	2.05
25	s	304	CLA	MG-ND	-4.42	1.97	2.05
25	c	509	CLA	MG-ND	-4.41	1.97	2.05
25	C	512	CLA	MG-NB	-4.41	1.97	2.05
25	c	512	CLA	MG-NB	-4.41	1.97	2.05
25	S	312	CLA	MG-NA	-4.41	1.95	2.06
25	s	312	CLA	MG-NA	-4.41	1.95	2.06
25	S	304	CLA	MG-NB	-4.41	1.97	2.05
25	B	612	CLA	MG-ND	-4.41	1.97	2.05
25	b	612	CLA	MG-ND	-4.41	1.97	2.05
25	S	304	CLA	MG-ND	-4.40	1.97	2.05
25	B	604	CLA	MG-NB	-4.40	1.97	2.05
25	b	604	CLA	MG-NB	-4.40	1.97	2.05
25	B	604	CLA	MG-ND	-4.39	1.97	2.05
25	b	604	CLA	MG-ND	-4.39	1.97	2.05
25	C	509	CLA	MG-NB	-4.39	1.97	2.05
25	c	509	CLA	MG-NB	-4.39	1.97	2.05
29	A	411	SQD	O8-S	4.38	1.63	1.47
29	a	412	SQD	O8-S	4.38	1.63	1.47
29	A	407	SQD	O8-S	4.37	1.63	1.47
29	a	408	SQD	O8-S	4.37	1.63	1.47
29	L	103	SQD	O8-S	4.37	1.63	1.47
29	l	101	SQD	O8-S	4.37	1.63	1.47
25	2	605	CLA	MG-NB	-4.37	1.97	2.05
29	l	102	SQD	O8-S	4.37	1.63	1.47
25	S	310	CLA	MG-NB	-4.36	1.97	2.05
25	s	310	CLA	MG-NB	-4.36	1.97	2.05
25	y	304	CLA	MG-ND	-4.36	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	MG-NB	-4.36	1.97	2.05
25	b	612	CLA	MG-NB	-4.36	1.97	2.05
29	L	101	SQD	O8-S	4.35	1.63	1.47
25	n	604	CLA	MG-NB	-4.35	1.97	2.05
25	N	613	CLA	MG-NA	-4.34	1.96	2.06
25	n	613	CLA	MG-NA	-4.34	1.96	2.06
25	n	613	CLA	MG-ND	-4.34	1.97	2.05
25	6	605	CLA	MG-NB	-4.33	1.97	2.05
25	R	609	CLA	MG-NB	-4.32	1.97	2.05
25	B	615	CLA	MG-NA	-4.32	1.96	2.06
25	b	615	CLA	MG-NA	-4.32	1.96	2.06
25	N	604	CLA	MG-NB	-4.32	1.97	2.05
25	D	402	CLA	MG-ND	-4.31	1.97	2.05
25	d	402	CLA	MG-ND	-4.31	1.97	2.05
25	N	613	CLA	MG-ND	-4.31	1.97	2.05
25	c	503	CLA	MG-NB	-4.31	1.97	2.05
25	B	603	CLA	MG-NB	-4.31	1.97	2.05
25	r	609	CLA	MG-NB	-4.31	1.97	2.05
25	Y	304	CLA	MG-ND	-4.30	1.97	2.05
25	Y	304	CLA	MG-NB	-4.30	1.97	2.05
25	C	503	CLA	MG-NB	-4.29	1.97	2.05
25	b	603	CLA	MG-NB	-4.28	1.97	2.05
25	G	603	CLA	MG-NB	-4.28	1.97	2.05
25	g	603	CLA	MG-NB	-4.28	1.97	2.05
25	N	603	CLA	MG-NB	-4.28	1.97	2.05
25	n	603	CLA	MG-NB	-4.28	1.97	2.05
38	F	101	HEM	FE-NC	4.28	2.09	1.95
25	A	405	CLA	MG-ND	-4.28	1.97	2.05
25	a	406	CLA	MG-ND	-4.28	1.97	2.05
25	N	604	CLA	MG-ND	-4.27	1.97	2.05
25	n	604	CLA	MG-ND	-4.27	1.97	2.05
38	f	101	HEM	FE-NC	4.27	2.09	1.95
25	C	513	CLA	MG-ND	-4.27	1.97	2.05
24	G	607	CHL	C1B-C2B	4.26	1.44	1.39
24	g	607	CHL	C1B-C2B	4.26	1.44	1.39
25	G	611	CLA	C1D-C2D	-4.26	1.36	1.45
25	R	612	CLA	MG-NA	-4.26	1.96	2.06
25	A	405	CLA	MG-NB	-4.26	1.97	2.05
25	a	406	CLA	MG-NB	-4.26	1.97	2.05
25	B	611	CLA	MG-NB	-4.26	1.97	2.05
25	b	611	CLA	MG-NB	-4.26	1.97	2.05
25	b	602	CLA	MG-ND	-4.25	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	611	CLA	C1D-C2D	-4.25	1.36	1.45
25	C	503	CLA	MG-ND	-4.25	1.97	2.05
25	c	503	CLA	MG-ND	-4.25	1.97	2.05
25	N	603	CLA	MG-ND	-4.25	1.97	2.05
25	n	603	CLA	MG-ND	-4.25	1.97	2.05
25	S	310	CLA	MG-ND	-4.25	1.97	2.05
25	s	310	CLA	MG-ND	-4.25	1.97	2.05
25	R	608	CLA	MG-ND	-4.25	1.97	2.05
25	r	612	CLA	MG-NA	-4.24	1.96	2.06
25	y	304	CLA	MG-NB	-4.24	1.97	2.05
25	r	608	CLA	MG-ND	-4.24	1.97	2.05
25	b	607	CLA	MG-NB	-4.24	1.97	2.05
25	B	607	CLA	MG-NB	-4.24	1.97	2.05
25	R	602	CLA	MG-NB	-4.23	1.97	2.05
25	c	513	CLA	MG-ND	-4.23	1.97	2.05
25	r	602	CLA	MG-NB	-4.23	1.97	2.05
25	B	611	CLA	MG-ND	-4.23	1.97	2.05
25	b	611	CLA	MG-ND	-4.23	1.97	2.05
25	B	615	CLA	MG-NB	-4.22	1.97	2.05
25	b	615	CLA	MG-NB	-4.22	1.97	2.05
25	b	615	CLA	MG-ND	-4.22	1.97	2.05
25	G	603	CLA	MG-ND	-4.22	1.97	2.05
25	B	602	CLA	MG-ND	-4.22	1.97	2.05
25	c	513	CLA	MG-NB	-4.21	1.97	2.05
25	b	609	CLA	MG-ND	-4.21	1.97	2.05
25	N	611	CLA	MG-ND	-4.20	1.97	2.05
25	D	402	CLA	MG-NA	-4.20	1.96	2.06
25	C	513	CLA	MG-NB	-4.19	1.97	2.05
25	S	309	CLA	MG-ND	-4.19	1.97	2.05
25	d	402	CLA	MG-NA	-4.19	1.96	2.06
25	B	615	CLA	MG-ND	-4.18	1.97	2.05
25	B	609	CLA	MG-NB	-4.18	1.97	2.05
25	S	303	CLA	MG-ND	-4.17	1.97	2.05
25	s	303	CLA	MG-ND	-4.17	1.97	2.05
25	g	603	CLA	MG-ND	-4.17	1.97	2.05
25	S	313	CLA	MG-NA	-4.17	1.96	2.06
25	n	611	CLA	MG-ND	-4.17	1.97	2.05
25	R	602	CLA	MG-ND	-4.16	1.97	2.05
25	b	607	CLA	MG-ND	-4.16	1.97	2.05
25	S	312	CLA	MG-ND	-4.16	1.97	2.05
25	b	603	CLA	MG-ND	-4.16	1.97	2.05
25	G	604	CLA	MG-NB	-4.16	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	604	CLA	MG-NB	-4.16	1.97	2.05
25	s	313	CLA	MG-NA	-4.15	1.96	2.06
25	B	602	CLA	MG-NB	-4.15	1.97	2.05
25	b	602	CLA	MG-NB	-4.15	1.97	2.05
25	b	609	CLA	MG-NB	-4.15	1.97	2.05
25	s	309	CLA	MG-ND	-4.14	1.97	2.05
25	Y	315	CLA	MG-ND	-4.14	1.97	2.05
25	B	607	CLA	MG-ND	-4.14	1.97	2.05
25	b	613	CLA	MG-NB	-4.14	1.97	2.05
28	B	617	BCR	C1-C6	-4.14	1.48	1.53
28	b	617	BCR	C1-C6	-4.14	1.48	1.53
25	B	609	CLA	MG-ND	-4.14	1.97	2.05
25	n	612	CLA	MG-ND	-4.14	1.97	2.05
25	Y	312	CLA	MG-ND	-4.14	1.97	2.05
25	y	315	CLA	MG-ND	-4.14	1.97	2.05
25	r	609	CLA	MG-NA	-4.13	1.96	2.06
25	G	604	CLA	MG-ND	-4.12	1.97	2.05
25	g	604	CLA	MG-ND	-4.12	1.97	2.05
25	B	603	CLA	MG-ND	-4.12	1.97	2.05
25	d	402	CLA	MG-NB	-4.12	1.97	2.05
25	y	312	CLA	MG-ND	-4.12	1.97	2.05
25	B	613	CLA	MG-ND	-4.11	1.97	2.05
25	s	312	CLA	MG-ND	-4.11	1.97	2.05
24	2	601	CHL	CHA-CBD	4.11	1.56	1.51
25	C	502	CLA	MG-NB	-4.11	1.97	2.05
25	c	502	CLA	MG-NB	-4.11	1.97	2.05
25	y	314	CLA	MG-ND	-4.11	1.97	2.05
25	S	309	CLA	MG-NA	-4.11	1.96	2.06
25	s	309	CLA	MG-NA	-4.11	1.96	2.06
25	B	614	CLA	MG-NB	-4.11	1.97	2.05
25	b	614	CLA	MG-NB	-4.11	1.97	2.05
25	B	608	CLA	MG-ND	-4.10	1.97	2.05
25	r	602	CLA	MG-ND	-4.10	1.97	2.05
25	C	502	CLA	MG-ND	-4.10	1.97	2.05
25	c	502	CLA	MG-ND	-4.10	1.97	2.05
25	b	608	CLA	MG-NB	-4.10	1.97	2.05
25	R	609	CLA	MG-NA	-4.10	1.96	2.06
25	B	613	CLA	MG-NB	-4.09	1.97	2.05
25	g	612	CLA	MG-NA	-4.09	1.96	2.06
25	b	608	CLA	MG-ND	-4.09	1.97	2.05
25	R	604	CLA	MG-NA	-4.09	1.96	2.06
25	r	604	CLA	MG-NA	-4.09	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	404	BCR	C1-C6	-4.09	1.48	1.53
28	d	404	BCR	C1-C6	-4.09	1.48	1.53
25	B	608	CLA	MG-NB	-4.08	1.97	2.05
25	c	506	CLA	MG-ND	-4.08	1.97	2.05
25	N	611	CLA	MG-NB	-4.08	1.97	2.05
25	n	611	CLA	MG-NB	-4.08	1.97	2.05
25	D	402	CLA	MG-NB	-4.08	1.97	2.05
25	G	610	CLA	MG-NA	-4.08	1.96	2.06
25	N	612	CLA	MG-ND	-4.07	1.97	2.05
25	g	610	CLA	MG-NA	-4.07	1.96	2.06
25	C	511	CLA	MG-NA	-4.07	1.96	2.06
25	c	511	CLA	MG-NA	-4.07	1.96	2.06
25	Y	314	CLA	MG-ND	-4.07	1.97	2.05
25	S	303	CLA	MG-NB	-4.07	1.97	2.05
25	s	303	CLA	MG-NB	-4.07	1.97	2.05
25	s	312	CLA	MG-NB	-4.06	1.97	2.05
25	b	613	CLA	MG-ND	-4.06	1.97	2.05
25	B	614	CLA	MG-ND	-4.06	1.97	2.05
25	b	614	CLA	MG-ND	-4.06	1.97	2.05
25	B	601	CLA	MG-NA	-4.05	1.96	2.06
25	S	314	CLA	MG-ND	-4.05	1.97	2.05
25	s	314	CLA	MG-ND	-4.05	1.97	2.05
25	G	612	CLA	MG-NA	-4.05	1.96	2.06
25	Y	312	CLA	MG-NB	-4.04	1.97	2.05
25	y	312	CLA	MG-NB	-4.04	1.97	2.05
25	B	610	CLA	MG-ND	-4.04	1.97	2.05
25	g	614	CLA	MG-ND	-4.04	1.97	2.05
25	B	610	CLA	MG-NB	-4.04	1.97	2.05
25	b	610	CLA	MG-NB	-4.04	1.97	2.05
25	s	309	CLA	MG-NB	-4.04	1.97	2.05
25	G	611	CLA	MG-NA	-4.03	1.96	2.06
25	g	611	CLA	MG-NA	-4.03	1.96	2.06
25	C	506	CLA	MG-ND	-4.03	1.97	2.05
24	6	601	CHL	CHA-CBD	4.03	1.56	1.51
25	S	312	CLA	MG-NB	-4.03	1.97	2.05
25	b	616	CLA	MG-ND	-4.03	1.97	2.05
25	r	614	CLA	MG-NA	-4.02	1.96	2.06
25	b	601	CLA	MG-NA	-4.02	1.96	2.06
25	G	614	CLA	MG-ND	-4.02	1.97	2.05
25	R	614	CLA	MG-NA	-4.01	1.96	2.06
25	s	310	CLA	MG-NA	-4.01	1.96	2.06
25	N	602	CLA	MG-ND	-4.01	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	MG-ND	-4.01	1.97	2.05
25	B	616	CLA	MG-NB	-4.01	1.97	2.05
25	b	610	CLA	MG-ND	-4.00	1.97	2.05
25	S	310	CLA	MG-NA	-4.00	1.96	2.06
25	b	616	CLA	MG-NB	-3.99	1.97	2.05
25	S	309	CLA	MG-NB	-3.99	1.97	2.05
24	Y	307	CHL	CHA-CBD	3.98	1.56	1.51
24	y	307	CHL	C3B-C2B	-3.98	1.35	1.40
25	Y	305	CLA	MG-ND	-3.98	1.97	2.05
25	y	305	CLA	MG-ND	-3.98	1.97	2.05
25	n	602	CLA	MG-ND	-3.98	1.97	2.05
25	Y	311	CLA	MG-ND	-3.97	1.97	2.05
25	y	311	CLA	MG-ND	-3.97	1.97	2.05
28	i	101	BCR	C1-C6	-3.97	1.48	1.53
25	N	610	CLA	MG-NB	-3.96	1.97	2.05
25	n	610	CLA	MG-NB	-3.96	1.97	2.05
25	y	312	CLA	C1D-C2D	-3.96	1.37	1.45
25	C	505	CLA	MG-NB	-3.96	1.97	2.05
25	B	610	CLA	MG-NA	-3.96	1.96	2.06
25	b	610	CLA	MG-NA	-3.96	1.96	2.06
25	y	305	CLA	MG-NB	-3.96	1.97	2.05
25	r	608	CLA	MG-NB	-3.95	1.97	2.05
25	y	303	CLA	MG-NA	-3.95	1.96	2.06
25	Y	312	CLA	C1D-C2D	-3.95	1.37	1.45
25	y	311	CLA	MG-NB	-3.95	1.98	2.05
25	G	614	CLA	MG-NB	-3.94	1.98	2.05
25	c	505	CLA	MG-NB	-3.94	1.98	2.05
25	N	610	CLA	MG-ND	-3.94	1.98	2.05
25	n	610	CLA	MG-ND	-3.94	1.98	2.05
24	Y	307	CHL	C3B-C2B	-3.94	1.35	1.40
25	Y	305	CLA	MG-NB	-3.93	1.98	2.05
25	g	614	CLA	MG-NB	-3.93	1.98	2.05
25	Y	313	CLA	MG-ND	-3.93	1.98	2.05
25	Y	303	CLA	MG-NA	-3.93	1.96	2.06
25	c	507	CLA	MG-NA	-3.93	1.96	2.06
25	y	313	CLA	MG-ND	-3.92	1.98	2.05
25	N	612	CLA	MG-NB	-3.92	1.98	2.05
25	n	612	CLA	MG-NB	-3.92	1.98	2.05
25	G	602	CLA	MG-ND	-3.91	1.98	2.05
28	I	101	BCR	C1-C6	-3.91	1.48	1.53
28	T	101	BCR	C1-C6	-3.90	1.48	1.53
28	t	101	BCR	C1-C6	-3.90	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	MG-NA	-3.90	1.97	2.06
24	y	307	CHL	CHA-CBD	3.90	1.56	1.51
25	S	314	CLA	MG-NB	-3.90	1.98	2.05
25	Y	311	CLA	MG-NB	-3.90	1.98	2.05
25	s	314	CLA	MG-NB	-3.90	1.98	2.05
25	g	602	CLA	MG-ND	-3.90	1.98	2.05
24	G	609	CHL	CHA-CBD	3.90	1.56	1.51
24	g	609	CHL	CHA-CBD	3.90	1.56	1.51
25	N	611	CLA	C1D-C2D	-3.89	1.37	1.45
25	n	611	CLA	C1D-C2D	-3.89	1.37	1.45
25	R	608	CLA	MG-NB	-3.89	1.98	2.05
25	C	505	CLA	MG-ND	-3.89	1.98	2.05
25	c	505	CLA	MG-ND	-3.89	1.98	2.05
25	N	602	CLA	MG-NA	-3.88	1.97	2.06
25	n	602	CLA	MG-NA	-3.87	1.97	2.06
28	C	514	BCR	C1-C6	-3.87	1.48	1.53
28	c	514	BCR	C1-C6	-3.87	1.48	1.53
24	5	302	CHL	CHA-CBD	3.87	1.56	1.51
24	l	302	CHL	CHA-CBD	3.87	1.56	1.51
25	Y	303	CLA	MG-ND	-3.87	1.98	2.05
25	y	303	CLA	MG-ND	-3.87	1.98	2.05
25	S	312	CLA	MG-NC	-3.87	1.97	2.06
25	s	312	CLA	MG-NC	-3.87	1.97	2.06
25	n	612	CLA	MG-NC	-3.86	1.97	2.06
25	s	311	CLA	MG-NA	-3.86	1.97	2.06
25	N	612	CLA	MG-NC	-3.86	1.97	2.06
25	S	311	CLA	MG-NA	-3.85	1.97	2.06
25	R	612	CLA	MG-NC	-3.85	1.97	2.06
25	c	506	CLA	MG-NB	-3.85	1.98	2.05
25	g	602	CLA	MG-NA	-3.85	1.97	2.06
25	s	313	CLA	MG-NC	-3.85	1.97	2.06
25	c	508	CLA	MG-NA	-3.84	1.97	2.06
25	B	615	CLA	MG-NC	-3.84	1.97	2.06
25	b	615	CLA	MG-NC	-3.84	1.97	2.06
25	G	612	CLA	MG-ND	-3.83	1.98	2.05
25	C	506	CLA	MG-NB	-3.83	1.98	2.05
25	A	402	CLA	MG-NA	-3.83	1.97	2.06
25	a	403	CLA	MG-NA	-3.83	1.97	2.06
25	g	610	CLA	MG-NC	-3.83	1.97	2.06
25	6	605	CLA	MG-NA	-3.83	1.97	2.06
25	r	612	CLA	MG-NC	-3.82	1.97	2.06
25	G	602	CLA	MG-NA	-3.82	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	MG-NA	-3.82	1.97	2.06
25	S	313	CLA	MG-NC	-3.82	1.97	2.06
25	d	402	CLA	MG-NC	-3.82	1.97	2.06
25	G	610	CLA	MG-NC	-3.82	1.97	2.06
25	C	507	CLA	MG-NC	-3.82	1.97	2.06
25	R	604	CLA	MG-NC	-3.82	1.97	2.06
25	B	604	CLA	MG-NA	-3.81	1.97	2.06
25	D	402	CLA	MG-NC	-3.81	1.97	2.06
25	b	604	CLA	MG-NA	-3.81	1.97	2.06
25	N	614	CLA	MG-NA	-3.81	1.97	2.06
25	n	614	CLA	MG-NA	-3.81	1.97	2.06
28	I	101	BCR	C30-C25	-3.80	1.48	1.53
25	Y	313	CLA	C1D-C2D	-3.80	1.37	1.45
25	y	313	CLA	C1D-C2D	-3.80	1.37	1.45
25	g	612	CLA	MG-ND	-3.79	1.98	2.05
25	c	507	CLA	MG-NC	-3.79	1.97	2.06
25	r	604	CLA	MG-NC	-3.79	1.97	2.06
25	y	313	CLA	MG-NA	-3.79	1.97	2.06
28	k	101	BCR	C30-C25	-3.79	1.48	1.53
38	F	101	HEM	C1B-NB	-3.78	1.33	1.40
28	B	619	BCR	C1-C6	-3.78	1.48	1.53
28	b	619	BCR	C1-C6	-3.78	1.48	1.53
28	i	101	BCR	C30-C25	-3.78	1.48	1.53
25	B	605	CLA	MG-NA	-3.78	1.97	2.06
25	n	614	CLA	MG-NC	-3.77	1.97	2.06
25	N	614	CLA	MG-NC	-3.77	1.97	2.06
25	2	605	CLA	MG-NA	-3.77	1.97	2.06
25	R	614	CLA	MG-ND	-3.77	1.98	2.05
25	D	401	CLA	MG-NA	-3.77	1.97	2.06
25	d	401	CLA	MG-NA	-3.77	1.97	2.06
38	f	101	HEM	C4D-ND	-3.76	1.33	1.40
25	c	506	CLA	MG-NA	-3.76	1.97	2.06
25	R	602	CLA	MG-NA	-3.76	1.97	2.06
25	Y	313	CLA	MG-NA	-3.76	1.97	2.06
25	s	304	CLA	MG-NA	-3.75	1.97	2.06
25	r	614	CLA	MG-ND	-3.75	1.98	2.05
25	R	609	CLA	MG-NC	-3.75	1.97	2.06
28	A	406	BCR	C30-C25	-3.74	1.49	1.53
25	A	401	CLA	MG-NA	-3.74	1.97	2.06
25	a	402	CLA	MG-NA	-3.74	1.97	2.06
25	r	602	CLA	MG-NA	-3.74	1.97	2.06
25	S	304	CLA	MG-NA	-3.74	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	MG-NA	-3.74	1.97	2.06
28	H	101	BCR	C1-C6	-3.74	1.49	1.53
28	h	101	BCR	C1-C6	-3.74	1.49	1.53
25	Y	314	CLA	MG-NA	-3.73	1.97	2.06
25	y	314	CLA	MG-NA	-3.73	1.97	2.06
28	K	101	BCR	C1-C6	-3.73	1.49	1.53
28	k	101	BCR	C1-C6	-3.73	1.49	1.53
25	C	506	CLA	MG-NA	-3.73	1.97	2.06
28	K	101	BCR	C30-C25	-3.72	1.49	1.53
38	f	101	HEM	C1B-NB	-3.72	1.33	1.40
28	B	618	BCR	C1-C6	-3.72	1.49	1.53
28	b	618	BCR	C1-C6	-3.72	1.49	1.53
25	B	606	CLA	MG-NA	-3.72	1.97	2.06
25	b	606	CLA	MG-NA	-3.72	1.97	2.06
25	C	510	CLA	MG-NA	-3.71	1.97	2.06
25	c	510	CLA	MG-NA	-3.71	1.97	2.06
25	r	609	CLA	MG-NC	-3.71	1.97	2.06
24	R	613	CHL	CHA-CBD	3.71	1.56	1.51
28	a	407	BCR	C30-C25	-3.71	1.49	1.53
38	F	101	HEM	C4D-ND	-3.70	1.33	1.40
25	r	614	CLA	MG-NC	-3.70	1.97	2.06
25	C	512	CLA	MG-NA	-3.70	1.97	2.06
25	c	512	CLA	MG-NA	-3.70	1.97	2.06
28	A	406	BCR	C1-C6	-3.70	1.49	1.53
28	a	407	BCR	C1-C6	-3.70	1.49	1.53
25	S	309	CLA	MG-NC	-3.69	1.97	2.06
25	s	309	CLA	MG-NC	-3.69	1.97	2.06
25	R	614	CLA	MG-NC	-3.68	1.97	2.06
25	b	601	CLA	MG-NC	-3.68	1.97	2.06
25	y	315	CLA	MG-NB	-3.68	1.98	2.05
24	y	308	CHL	CHA-CBD	3.67	1.56	1.51
25	C	513	CLA	MG-NA	-3.67	1.97	2.06
25	c	513	CLA	MG-NA	-3.67	1.97	2.06
25	A	405	CLA	MG-NA	-3.67	1.97	2.06
25	a	406	CLA	MG-NA	-3.67	1.97	2.06
24	Y	308	CHL	CHA-CBD	3.66	1.55	1.51
24	R	606	CHL	CHA-CBD	3.66	1.55	1.51
24	r	606	CHL	CHA-CBD	3.66	1.55	1.51
25	B	602	CLA	MG-NA	-3.65	1.97	2.06
25	b	602	CLA	MG-NA	-3.65	1.97	2.06
25	S	314	CLA	MG-NA	-3.65	1.97	2.06
25	s	314	CLA	MG-NA	-3.65	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	614	CLA	MG-NB	-3.64	1.98	2.05
25	Y	315	CLA	MG-NB	-3.64	1.98	2.05
25	B	601	CLA	MG-NC	-3.64	1.97	2.06
25	B	610	CLA	MG-NC	-3.64	1.97	2.06
25	b	610	CLA	MG-NC	-3.64	1.97	2.06
25	B	603	CLA	MG-NA	-3.64	1.97	2.06
25	b	603	CLA	MG-NA	-3.64	1.97	2.06
25	g	603	CLA	MG-NA	-3.63	1.97	2.06
25	B	612	CLA	MG-NA	-3.63	1.97	2.06
28	Z	101	BCR	C1-C6	-3.63	1.49	1.53
24	n	601	CHL	CHA-CBD	3.63	1.55	1.51
25	g	612	CLA	MG-NB	-3.63	1.98	2.05
25	b	612	CLA	MG-NA	-3.63	1.97	2.06
25	C	503	CLA	MG-NA	-3.62	1.97	2.06
25	c	503	CLA	MG-NA	-3.62	1.97	2.06
25	G	612	CLA	MG-NB	-3.62	1.98	2.05
25	G	603	CLA	MG-NA	-3.62	1.97	2.06
25	C	502	CLA	C1D-C2D	-3.61	1.38	1.45
25	c	502	CLA	C1D-C2D	-3.61	1.38	1.45
25	B	610	CLA	C1D-C2D	-3.61	1.38	1.45
25	b	610	CLA	C1D-C2D	-3.61	1.38	1.45
25	C	511	CLA	MG-NC	-3.61	1.97	2.06
25	c	511	CLA	MG-NC	-3.61	1.97	2.06
25	n	610	CLA	C1D-C2D	-3.61	1.38	1.45
25	n	604	CLA	MG-NA	-3.61	1.97	2.06
24	r	613	CHL	CHA-CBD	3.61	1.55	1.51
25	n	603	CLA	MG-NA	-3.60	1.97	2.06
25	g	612	CLA	C1D-C2D	-3.60	1.38	1.45
25	n	610	CLA	MG-NA	-3.60	1.97	2.06
25	N	614	CLA	C1D-C2D	-3.60	1.38	1.45
25	n	614	CLA	C1D-C2D	-3.60	1.38	1.45
24	y	306	CHL	CHA-CBD	3.60	1.55	1.51
25	y	304	CLA	MG-NA	-3.60	1.97	2.06
24	2	601	CHL	C1A-CHA	3.59	1.44	1.40
24	6	601	CHL	C1A-CHA	3.59	1.44	1.40
25	N	604	CLA	MG-NA	-3.59	1.97	2.06
24	5	301	CHL	CHA-CBD	3.59	1.55	1.51
25	N	610	CLA	C1D-C2D	-3.59	1.38	1.45
28	z	101	BCR	C1-C6	-3.59	1.49	1.53
24	G	605	CHL	CHA-CBD	3.59	1.55	1.51
25	Y	311	CLA	C1D-C2D	-3.58	1.38	1.45
25	g	604	CLA	MG-NA	-3.58	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	610	CLA	MG-NA	-3.58	1.97	2.06
24	N	601	CHL	CHA-CBD	3.58	1.55	1.51
25	S	303	CLA	MG-NA	-3.58	1.97	2.06
25	s	303	CLA	MG-NA	-3.58	1.97	2.06
25	y	311	CLA	C1D-C2D	-3.57	1.38	1.45
25	Y	304	CLA	C1D-C2D	-3.57	1.38	1.45
25	Y	311	CLA	MG-NA	-3.57	1.97	2.06
25	y	311	CLA	MG-NA	-3.57	1.97	2.06
25	Y	304	CLA	MG-NA	-3.57	1.97	2.06
24	g	605	CHL	CHA-CBD	3.57	1.55	1.51
25	c	509	CLA	MG-NA	-3.57	1.97	2.06
25	C	509	CLA	MG-NA	-3.57	1.97	2.06
25	N	603	CLA	MG-NA	-3.57	1.97	2.06
25	Y	303	CLA	C1D-C2D	-3.57	1.38	1.45
25	y	303	CLA	C1D-C2D	-3.57	1.38	1.45
25	G	612	CLA	MG-NC	-3.56	1.97	2.06
24	s	302	CHL	CHA-CBD	3.56	1.55	1.51
24	N	607	CHL	O2D-CGD	3.56	1.42	1.33
24	n	607	CHL	O2D-CGD	3.56	1.42	1.33
25	S	310	CLA	C1D-C2D	-3.56	1.38	1.45
24	Y	310	CHL	CHA-CBD	3.56	1.55	1.51
24	y	310	CHL	CHA-CBD	3.56	1.55	1.51
25	G	604	CLA	MG-NA	-3.56	1.97	2.06
24	Y	306	CHL	CHA-CBD	3.56	1.55	1.51
25	R	614	CLA	MG-NB	-3.56	1.98	2.05
24	S	302	CHL	CHA-CBD	3.56	1.55	1.51
25	N	611	CLA	MG-NA	-3.55	1.97	2.06
25	n	611	CLA	MG-NA	-3.55	1.97	2.06
25	2	605	CLA	MG-NC	-3.55	1.97	2.06
25	B	615	CLA	C1D-C2D	-3.55	1.38	1.45
25	b	607	CLA	MG-NA	-3.55	1.97	2.06
25	B	612	CLA	MG-NC	-3.55	1.97	2.06
25	b	612	CLA	MG-NC	-3.55	1.97	2.06
25	s	310	CLA	C1D-C2D	-3.55	1.38	1.45
25	N	612	CLA	C1D-C2D	-3.55	1.38	1.45
24	2	603	CHL	C3B-C2B	-3.55	1.35	1.40
24	6	603	CHL	C3B-C2B	-3.55	1.35	1.40
25	G	603	CLA	C1D-C2D	-3.55	1.38	1.45
25	g	603	CLA	C1D-C2D	-3.55	1.38	1.45
25	B	606	CLA	MG-NC	-3.55	1.97	2.06
25	b	606	CLA	MG-NC	-3.55	1.97	2.06
25	N	602	CLA	C1D-C2D	-3.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	514	BCR	C30-C25	-3.54	1.49	1.53
28	c	514	BCR	C30-C25	-3.54	1.49	1.53
25	B	611	CLA	MG-NA	-3.54	1.97	2.06
25	b	611	CLA	MG-NA	-3.54	1.97	2.06
25	C	508	CLA	MG-NC	-3.54	1.97	2.06
25	A	402	CLA	MG-NC	-3.54	1.97	2.06
25	a	403	CLA	MG-NC	-3.54	1.97	2.06
24	S	307	CHL	CHA-CBD	3.54	1.55	1.51
25	g	614	CLA	MG-NA	-3.54	1.97	2.06
25	B	613	CLA	C1D-C2D	-3.54	1.38	1.45
25	b	613	CLA	C1D-C2D	-3.54	1.38	1.45
24	R	607	CHL	CHA-CBD	3.54	1.55	1.51
24	r	607	CHL	CHA-CBD	3.54	1.55	1.51
25	G	614	CLA	MG-NA	-3.54	1.97	2.06
25	y	304	CLA	C1D-C2D	-3.53	1.38	1.45
25	g	612	CLA	MG-NC	-3.53	1.97	2.06
24	G	608	CHL	CHA-CBD	3.53	1.55	1.51
25	S	311	CLA	MG-NC	-3.53	1.97	2.06
24	Y	308	CHL	O2D-CGD	3.53	1.41	1.33
24	y	308	CHL	O2D-CGD	3.53	1.41	1.33
25	c	508	CLA	MG-NC	-3.53	1.97	2.06
25	G	602	CLA	C1D-C2D	-3.53	1.38	1.45
25	g	602	CLA	C1D-C2D	-3.53	1.38	1.45
24	l	301	CHL	CHA-CBD	3.53	1.55	1.51
24	S	308	CHL	CHA-CBD	3.52	1.55	1.51
24	s	308	CHL	CHA-CBD	3.52	1.55	1.51
25	s	311	CLA	MG-NC	-3.52	1.97	2.06
24	s	307	CHL	CHA-CBD	3.52	1.55	1.51
25	b	616	CLA	C1D-C2D	-3.52	1.38	1.45
24	n	607	CHL	CHA-CBD	3.52	1.55	1.51
25	b	604	CLA	MG-NC	-3.52	1.97	2.06
25	B	616	CLA	C1D-C2D	-3.52	1.38	1.45
25	n	602	CLA	C1D-C2D	-3.52	1.38	1.45
25	Y	315	CLA	C1D-C2D	-3.52	1.38	1.45
25	y	315	CLA	C1D-C2D	-3.52	1.38	1.45
24	g	608	CHL	CHA-CBD	3.52	1.55	1.51
25	B	607	CLA	MG-NA	-3.52	1.97	2.06
25	G	612	CLA	C1D-C2D	-3.52	1.38	1.45
25	B	609	CLA	MG-NA	-3.52	1.97	2.06
25	Y	305	CLA	C1D-C2D	-3.51	1.38	1.45
25	y	305	CLA	C1D-C2D	-3.51	1.38	1.45
25	C	509	CLA	MG-NC	-3.51	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	C1D-C2D	-3.51	1.38	1.45
25	n	612	CLA	C1D-C2D	-3.51	1.38	1.45
25	c	510	CLA	MG-NC	-3.51	1.97	2.06
25	6	605	CLA	MG-NC	-3.51	1.97	2.06
25	Y	311	CLA	MG-NC	-3.50	1.97	2.06
25	C	502	CLA	MG-NA	-3.50	1.98	2.06
25	c	502	CLA	MG-NA	-3.50	1.98	2.06
25	B	604	CLA	MG-NC	-3.50	1.98	2.06
25	C	505	CLA	C1D-C2D	-3.50	1.38	1.45
25	c	505	CLA	C1D-C2D	-3.50	1.38	1.45
28	B	618	BCR	C30-C25	-3.50	1.49	1.53
28	b	618	BCR	C30-C25	-3.50	1.49	1.53
24	N	607	CHL	CHA-CBD	3.50	1.55	1.51
24	N	608	CHL	CHA-CBD	3.50	1.55	1.51
24	n	608	CHL	CHA-CBD	3.50	1.55	1.51
25	b	609	CLA	MG-NA	-3.50	1.98	2.06
24	R	613	CHL	C3B-C2B	-3.50	1.35	1.40
25	s	314	CLA	C1D-C2D	-3.50	1.38	1.45
24	Y	306	CHL	C3B-C2B	-3.49	1.35	1.40
25	C	506	CLA	C1D-C2D	-3.49	1.38	1.45
25	c	506	CLA	C1D-C2D	-3.49	1.38	1.45
24	l	301	CHL	O2D-CGD	3.49	1.41	1.33
24	5	301	CHL	O2D-CGD	3.49	1.41	1.33
25	y	305	CLA	MG-NA	-3.49	1.98	2.06
25	R	608	CLA	C1D-C2D	-3.49	1.38	1.45
24	S	306	CHL	C3B-C2B	-3.49	1.35	1.40
24	s	306	CHL	C3B-C2B	-3.49	1.35	1.40
24	g	606	CHL	O2D-CGD	3.49	1.41	1.33
25	c	509	CLA	MG-NC	-3.49	1.98	2.06
25	B	608	CLA	C1D-C2D	-3.49	1.38	1.45
24	S	308	CHL	C3B-C2B	-3.49	1.35	1.40
25	A	405	CLA	C1D-C2D	-3.49	1.38	1.45
25	g	614	CLA	C1D-C2D	-3.49	1.38	1.45
25	Y	305	CLA	MG-NA	-3.49	1.98	2.06
25	y	311	CLA	MG-NC	-3.49	1.98	2.06
25	S	314	CLA	C1D-C2D	-3.49	1.38	1.45
25	A	401	CLA	MG-NC	-3.48	1.98	2.06
25	a	402	CLA	MG-NC	-3.48	1.98	2.06
24	y	310	CHL	O2D-CGD	3.48	1.41	1.33
25	G	614	CLA	C1D-C2D	-3.48	1.38	1.45
25	C	509	CLA	C1D-C2D	-3.48	1.38	1.45
25	c	509	CLA	C1D-C2D	-3.48	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	601	CHL	O2D-CGD	3.48	1.41	1.33
25	B	608	CLA	MG-NA	-3.48	1.98	2.06
25	C	510	CLA	MG-NC	-3.48	1.98	2.06
25	a	406	CLA	C1D-C2D	-3.48	1.38	1.45
24	R	605	CHL	CHA-CBD	3.48	1.55	1.51
24	r	605	CHL	CHA-CBD	3.48	1.55	1.51
25	n	603	CLA	C1D-C2D	-3.48	1.38	1.45
25	R	608	CLA	MG-NA	-3.48	1.98	2.06
25	b	608	CLA	C1D-C2D	-3.48	1.38	1.45
25	G	604	CLA	C1D-C2D	-3.47	1.38	1.45
24	Y	310	CHL	O2D-CGD	3.47	1.41	1.33
25	Y	312	CLA	MG-NA	-3.47	1.98	2.06
25	y	312	CLA	MG-NA	-3.47	1.98	2.06
24	Y	309	CHL	O2D-CGD	3.47	1.41	1.33
25	S	309	CLA	C1D-C2D	-3.47	1.38	1.45
25	b	612	CLA	C1D-C2D	-3.47	1.38	1.45
25	s	309	CLA	C1D-C2D	-3.47	1.38	1.45
24	s	308	CHL	C3B-C2B	-3.47	1.35	1.40
24	6	601	CHL	O2D-CGD	3.47	1.41	1.33
24	G	606	CHL	O2D-CGD	3.47	1.41	1.33
24	y	309	CHL	O2D-CGD	3.47	1.41	1.33
25	B	614	CLA	MG-NA	-3.47	1.98	2.06
25	b	614	CLA	MG-NA	-3.47	1.98	2.06
24	R	613	CHL	O2D-CGD	3.46	1.41	1.33
28	B	619	BCR	C30-C25	-3.46	1.49	1.53
28	b	619	BCR	C30-C25	-3.46	1.49	1.53
25	r	608	CLA	C1D-C2D	-3.46	1.38	1.45
24	G	608	CHL	O2D-CGD	3.46	1.41	1.33
25	N	613	CLA	C1D-C2D	-3.46	1.38	1.45
25	N	610	CLA	MG-NC	-3.46	1.98	2.06
25	n	610	CLA	MG-NC	-3.46	1.98	2.06
24	r	605	CHL	C3B-C2B	-3.46	1.35	1.40
25	C	513	CLA	C1D-C2D	-3.46	1.38	1.45
24	s	308	CHL	O2D-CGD	3.45	1.41	1.33
25	n	613	CLA	C1D-C2D	-3.45	1.38	1.45
24	Y	310	CHL	C3B-C2B	-3.45	1.35	1.40
24	y	310	CHL	C3B-C2B	-3.45	1.35	1.40
25	C	511	CLA	C1D-C2D	-3.45	1.38	1.45
25	c	511	CLA	C1D-C2D	-3.45	1.38	1.45
25	B	609	CLA	C1D-C2D	-3.45	1.38	1.45
24	S	302	CHL	O2D-CGD	3.45	1.41	1.33
24	s	302	CHL	O2D-CGD	3.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	606	CHL	O2D-CGD	3.45	1.41	1.33
24	r	606	CHL	O2D-CGD	3.45	1.41	1.33
24	g	601	CHL	O2D-CGD	3.45	1.41	1.33
24	1	302	CHL	O2D-CGD	3.45	1.41	1.33
24	5	302	CHL	O2D-CGD	3.45	1.41	1.33
24	r	607	CHL	O2D-CGD	3.45	1.41	1.33
24	5	302	CHL	MG-NB	3.45	2.12	2.05
25	C	507	CLA	C1D-C2D	-3.45	1.38	1.45
25	N	603	CLA	C1D-C2D	-3.45	1.38	1.45
25	r	608	CLA	MG-NA	-3.45	1.98	2.06
24	Y	308	CHL	C3B-C2B	-3.45	1.35	1.40
25	R	602	CLA	MG-NC	-3.45	1.98	2.06
24	G	605	CHL	O2D-CGD	3.45	1.41	1.33
24	g	605	CHL	O2D-CGD	3.45	1.41	1.33
24	y	302	CHL	C3B-C2B	-3.45	1.35	1.40
25	D	402	CLA	C1D-C2D	-3.45	1.38	1.45
25	d	402	CLA	C1D-C2D	-3.45	1.38	1.45
24	N	606	CHL	O2D-CGD	3.45	1.41	1.33
24	n	601	CHL	O2D-CGD	3.45	1.41	1.33
25	g	604	CLA	C1D-C2D	-3.45	1.38	1.45
25	C	506	CLA	MG-NC	-3.44	1.98	2.06
25	c	506	CLA	MG-NC	-3.44	1.98	2.06
24	N	605	CHL	C3B-C2B	-3.44	1.35	1.40
24	n	605	CHL	C3B-C2B	-3.44	1.35	1.40
25	B	614	CLA	C1D-C2D	-3.44	1.38	1.45
25	S	312	CLA	C1D-C2D	-3.44	1.38	1.45
25	b	614	CLA	C1D-C2D	-3.44	1.38	1.45
25	s	312	CLA	C1D-C2D	-3.44	1.38	1.45
25	B	613	CLA	MG-NA	-3.44	1.98	2.06
25	b	613	CLA	MG-NA	-3.44	1.98	2.06
24	y	302	CHL	CHA-CBD	3.44	1.55	1.51
24	2	601	CHL	O2D-CGD	3.44	1.41	1.33
24	r	613	CHL	O2D-CGD	3.44	1.41	1.33
24	R	605	CHL	O2D-CGD	3.44	1.41	1.33
24	r	605	CHL	O2D-CGD	3.44	1.41	1.33
24	S	307	CHL	O2D-CGD	3.43	1.41	1.33
24	s	307	CHL	O2D-CGD	3.43	1.41	1.33
24	G	601	CHL	O2D-CGD	3.43	1.41	1.33
25	b	604	CLA	C1D-C2D	-3.43	1.38	1.45
25	c	513	CLA	C1D-C2D	-3.43	1.38	1.45
24	g	608	CHL	O2D-CGD	3.43	1.41	1.33
24	Y	302	CHL	O2D-CGD	3.43	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	302	CHL	O2D-CGD	3.43	1.41	1.33
25	b	608	CLA	MG-NA	-3.43	1.98	2.06
25	B	607	CLA	C1D-C2D	-3.43	1.38	1.45
25	b	607	CLA	C1D-C2D	-3.43	1.38	1.45
25	S	304	CLA	MG-NC	-3.43	1.98	2.06
25	s	304	CLA	MG-NC	-3.43	1.98	2.06
24	n	606	CHL	CHA-CBD	3.43	1.55	1.51
24	Y	302	CHL	CHA-CBD	3.43	1.55	1.51
24	G	601	CHL	CHA-CBD	3.43	1.55	1.51
24	g	601	CHL	CHA-CBD	3.43	1.55	1.51
25	B	605	CLA	MG-NC	-3.43	1.98	2.06
25	b	605	CLA	MG-NC	-3.43	1.98	2.06
25	r	602	CLA	MG-NC	-3.43	1.98	2.06
25	r	608	CLA	MG-NC	-3.43	1.98	2.06
24	y	306	CHL	C3B-C2B	-3.43	1.35	1.40
25	b	609	CLA	C1D-C2D	-3.43	1.38	1.45
24	l	302	CHL	MG-NB	3.43	2.12	2.05
25	b	611	CLA	C1D-C2D	-3.43	1.38	1.45
25	c	507	CLA	C1D-C2D	-3.43	1.38	1.45
24	r	606	CHL	O2A-CGA	3.42	1.42	1.30
24	S	308	CHL	O2D-CGD	3.42	1.41	1.33
25	B	612	CLA	C1D-C2D	-3.42	1.38	1.45
24	Y	306	CHL	O2D-CGD	3.42	1.41	1.33
24	y	306	CHL	O2D-CGD	3.42	1.41	1.33
24	g	607	CHL	O2D-CGD	3.42	1.41	1.33
25	s	314	CLA	MG-NC	-3.42	1.98	2.06
24	N	608	CHL	O2D-CGD	3.42	1.41	1.33
24	n	608	CHL	O2D-CGD	3.42	1.41	1.33
25	D	401	CLA	MG-NC	-3.42	1.98	2.06
25	d	401	CLA	MG-NC	-3.42	1.98	2.06
24	R	605	CHL	O2A-CGA	3.42	1.42	1.30
24	r	605	CHL	O2A-CGA	3.42	1.42	1.30
24	N	605	CHL	CHA-CBD	3.42	1.55	1.51
24	n	605	CHL	CHA-CBD	3.42	1.55	1.51
24	R	607	CHL	O2D-CGD	3.41	1.41	1.33
25	2	605	CLA	C1D-C2D	-3.41	1.38	1.45
25	G	610	CLA	C1D-C2D	-3.41	1.38	1.45
25	6	605	CLA	C1D-C2D	-3.41	1.38	1.45
24	R	605	CHL	C3B-C2B	-3.41	1.35	1.40
24	S	306	CHL	CHA-CBD	3.41	1.55	1.51
24	s	306	CHL	CHA-CBD	3.41	1.55	1.51
24	N	605	CHL	O2D-CGD	3.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	605	CHL	O2D-CGD	3.41	1.41	1.33
24	5	301	CHL	O2A-CGA	3.41	1.42	1.30
25	C	505	CLA	MG-NA	-3.41	1.98	2.06
25	c	505	CLA	MG-NA	-3.41	1.98	2.06
24	1	301	CHL	O2A-CGA	3.41	1.42	1.30
24	N	606	CHL	CHA-CBD	3.41	1.55	1.51
25	S	303	CLA	C1D-C2D	-3.41	1.38	1.45
24	G	605	CHL	O2A-CGA	3.41	1.42	1.30
24	g	605	CHL	O2A-CGA	3.41	1.42	1.30
24	S	307	CHL	O2A-CGA	3.41	1.42	1.30
40	s	317	NEX	C12-C13	-3.40	1.38	1.46
24	y	308	CHL	C3B-C2B	-3.40	1.35	1.40
24	S	302	CHL	O2A-CGA	3.40	1.42	1.30
24	s	302	CHL	O2A-CGA	3.40	1.42	1.30
25	g	610	CLA	C1D-C2D	-3.40	1.38	1.45
25	R	608	CLA	MG-NC	-3.40	1.98	2.06
24	S	306	CHL	O2D-CGD	3.40	1.41	1.33
24	G	606	CHL	CHA-CBD	3.40	1.55	1.51
25	S	311	CLA	C1D-C2D	-3.40	1.38	1.45
24	n	609	CHL	CHA-CBD	3.40	1.55	1.51
24	2	603	CHL	O2A-CGA	3.40	1.42	1.30
24	6	603	CHL	O2A-CGA	3.40	1.42	1.30
25	R	614	CLA	C1D-C2D	-3.40	1.38	1.45
25	r	614	CLA	C1D-C2D	-3.40	1.38	1.45
24	1	302	CHL	O2A-CGA	3.40	1.42	1.30
24	5	302	CHL	O2A-CGA	3.40	1.42	1.30
24	Y	307	CHL	O2D-CGD	3.40	1.41	1.33
24	n	606	CHL	O2D-CGD	3.40	1.41	1.33
24	y	307	CHL	O2D-CGD	3.40	1.41	1.33
24	s	307	CHL	O2A-CGA	3.40	1.42	1.30
25	B	611	CLA	C1D-C2D	-3.40	1.38	1.45
24	n	609	CHL	O2D-CGD	3.40	1.41	1.33
25	b	603	CLA	C1D-C2D	-3.40	1.38	1.45
24	g	609	CHL	C3B-C2B	-3.40	1.35	1.40
24	r	613	CHL	C3B-C2B	-3.40	1.35	1.40
24	G	607	CHL	O2D-CGD	3.40	1.41	1.33
24	N	609	CHL	O2D-CGD	3.40	1.41	1.33
24	S	308	CHL	O2A-CGA	3.39	1.42	1.30
24	s	308	CHL	O2A-CGA	3.39	1.42	1.30
24	R	606	CHL	O2A-CGA	3.39	1.42	1.30
24	N	607	CHL	C3B-C2B	-3.39	1.35	1.40
25	S	314	CLA	MG-NC	-3.39	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	MG-NC	-3.39	1.98	2.06
25	c	513	CLA	MG-NC	-3.39	1.98	2.06
25	Y	314	CLA	C1D-C2D	-3.39	1.38	1.45
25	y	314	CLA	C1D-C2D	-3.39	1.38	1.45
24	N	606	CHL	O2A-CGA	3.39	1.42	1.30
24	G	609	CHL	C3B-C2B	-3.39	1.35	1.40
25	B	604	CLA	C1D-C2D	-3.39	1.38	1.45
24	s	306	CHL	O2D-CGD	3.39	1.41	1.33
24	S	306	CHL	O2A-CGA	3.39	1.42	1.30
24	s	306	CHL	O2A-CGA	3.39	1.42	1.30
25	B	603	CLA	C1D-C2D	-3.39	1.38	1.45
25	c	503	CLA	C1D-C2D	-3.39	1.38	1.45
25	b	616	CLA	MG-NA	-3.38	1.98	2.06
24	G	609	CHL	O2D-CGD	3.38	1.41	1.33
40	S	317	NEX	C12-C13	-3.38	1.38	1.46
25	g	613	CLA	C1D-C2D	-3.38	1.38	1.45
24	2	603	CHL	O2D-CGD	3.38	1.41	1.33
24	6	603	CHL	O2D-CGD	3.38	1.41	1.33
24	g	609	CHL	O2D-CGD	3.38	1.41	1.33
25	n	604	CLA	C1D-C2D	-3.38	1.38	1.45
24	y	309	CHL	C3B-C2B	-3.37	1.35	1.40
25	d	401	CLA	C1D-C2D	-3.37	1.38	1.45
25	r	609	CLA	C1D-C2D	-3.37	1.38	1.45
24	n	606	CHL	O2A-CGA	3.37	1.42	1.30
24	R	607	CHL	C3B-C2B	-3.37	1.35	1.40
24	r	607	CHL	C3B-C2B	-3.37	1.35	1.40
24	n	607	CHL	C3B-C2B	-3.37	1.35	1.40
25	G	613	CLA	C1D-C2D	-3.37	1.38	1.45
25	C	512	CLA	C1D-C2D	-3.37	1.38	1.45
25	c	512	CLA	C1D-C2D	-3.37	1.38	1.45
25	s	303	CLA	C1D-C2D	-3.37	1.38	1.45
24	g	601	CHL	C3B-C2B	-3.37	1.35	1.40
25	D	401	CLA	C1D-C2D	-3.37	1.38	1.45
24	N	609	CHL	CHA-CBD	3.36	1.55	1.51
24	N	609	CHL	C3B-C2B	-3.36	1.35	1.40
24	Y	302	CHL	C3B-C2B	-3.36	1.35	1.40
24	n	609	CHL	C3B-C2B	-3.36	1.35	1.40
25	N	604	CLA	MG-NC	-3.36	1.98	2.06
24	G	607	CHL	CHA-CBD	3.36	1.55	1.51
25	s	311	CLA	C1D-C2D	-3.36	1.38	1.45
25	A	402	CLA	C1D-C2D	-3.36	1.38	1.45
25	a	403	CLA	C1D-C2D	-3.36	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	302	CHL	C3B-C2B	-3.35	1.35	1.40
24	1	301	CHL	C3B-C2B	-3.35	1.35	1.40
24	5	301	CHL	C3B-C2B	-3.35	1.35	1.40
25	R	609	CLA	C1D-C2D	-3.35	1.38	1.45
25	y	313	CLA	MG-NB	-3.35	1.99	2.05
25	B	616	CLA	MG-NA	-3.35	1.98	2.06
24	G	601	CHL	C3B-C2B	-3.35	1.35	1.40
25	B	607	CLA	MG-NC	-3.35	1.98	2.06
25	r	602	CLA	C1D-C2D	-3.35	1.38	1.45
24	S	307	CHL	C3B-C2B	-3.35	1.35	1.40
24	s	307	CHL	C3B-C2B	-3.35	1.35	1.40
25	C	503	CLA	C1D-C2D	-3.34	1.38	1.45
25	S	303	CLA	MG-NC	-3.34	1.98	2.06
25	s	303	CLA	MG-NC	-3.34	1.98	2.06
25	A	401	CLA	C1D-C2D	-3.34	1.38	1.45
25	a	402	CLA	C1D-C2D	-3.34	1.38	1.45
24	g	607	CHL	CHA-CBD	3.34	1.55	1.51
24	g	608	CHL	C3B-C2B	-3.34	1.35	1.40
24	G	605	CHL	C3B-C2B	-3.34	1.35	1.40
24	G	607	CHL	O2A-CGA	3.34	1.41	1.30
25	N	604	CLA	C1D-C2D	-3.34	1.38	1.45
25	C	512	CLA	MG-NC	-3.34	1.98	2.06
25	c	512	CLA	MG-NC	-3.34	1.98	2.06
24	Y	309	CHL	C3B-C2B	-3.34	1.35	1.40
25	g	602	CLA	MG-NB	-3.33	1.99	2.05
25	a	406	CLA	MG-NC	-3.33	1.98	2.06
25	R	602	CLA	C1D-C2D	-3.33	1.38	1.45
25	B	605	CLA	C1D-C2D	-3.33	1.38	1.45
25	b	605	CLA	C1D-C2D	-3.33	1.38	1.45
24	Y	309	CHL	CHA-CBD	3.33	1.55	1.51
40	g	617	NEX	C12-C13	-3.33	1.38	1.46
25	n	604	CLA	MG-NC	-3.33	1.98	2.06
24	g	606	CHL	CHA-CBD	3.33	1.55	1.51
24	G	606	CHL	C3B-C2B	-3.33	1.35	1.40
24	g	606	CHL	C3B-C2B	-3.33	1.35	1.40
24	g	607	CHL	O2A-CGA	3.33	1.41	1.30
25	B	616	CLA	MG-NC	-3.33	1.98	2.06
24	R	606	CHL	C3B-C2B	-3.33	1.35	1.40
24	y	309	CHL	CHA-CBD	3.33	1.55	1.51
25	Y	313	CLA	MG-NB	-3.32	1.99	2.05
25	R	610	CLA	C1D-C2D	-3.32	1.38	1.45
25	r	610	CLA	C1D-C2D	-3.32	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	611	CLA	MG-NC	-3.32	1.98	2.06
25	C	503	CLA	MG-NC	-3.32	1.98	2.06
25	c	503	CLA	MG-NC	-3.32	1.98	2.06
25	C	501	CLA	C1D-C2D	-3.32	1.38	1.45
25	c	501	CLA	C1D-C2D	-3.32	1.38	1.45
25	c	508	CLA	C1D-C2D	-3.32	1.38	1.45
25	B	611	CLA	MG-NC	-3.31	1.98	2.06
28	T	101	BCR	C30-C25	-3.31	1.49	1.53
25	B	602	CLA	MG-NC	-3.31	1.98	2.06
25	b	602	CLA	MG-NC	-3.31	1.98	2.06
25	b	611	CLA	MG-NC	-3.31	1.98	2.06
25	b	607	CLA	MG-NC	-3.31	1.98	2.06
24	G	608	CHL	C3B-C2B	-3.31	1.35	1.40
25	b	616	CLA	MG-NC	-3.31	1.98	2.06
24	g	605	CHL	C3B-C2B	-3.31	1.35	1.40
25	n	611	CLA	MG-NC	-3.31	1.98	2.06
25	G	602	CLA	MG-NB	-3.31	1.99	2.05
28	t	101	BCR	C30-C25	-3.30	1.49	1.53
25	A	405	CLA	MG-NC	-3.30	1.98	2.06
25	n	602	CLA	MG-NB	-3.30	1.99	2.05
25	c	510	CLA	C1D-C2D	-3.30	1.38	1.45
25	B	603	CLA	MG-NC	-3.30	1.98	2.06
25	b	603	CLA	MG-NC	-3.30	1.98	2.06
25	B	606	CLA	C1D-C2D	-3.30	1.38	1.45
25	b	606	CLA	C1D-C2D	-3.30	1.38	1.45
25	C	510	CLA	C1D-C2D	-3.30	1.38	1.45
25	S	304	CLA	C1D-C2D	-3.30	1.38	1.45
25	s	304	CLA	C1D-C2D	-3.30	1.38	1.45
25	C	508	CLA	C1D-C2D	-3.29	1.38	1.45
24	N	606	CHL	C3B-C2B	-3.29	1.35	1.40
24	n	606	CHL	C3B-C2B	-3.29	1.35	1.40
25	N	602	CLA	MG-NB	-3.29	1.99	2.05
25	G	604	CLA	MG-NC	-3.29	1.98	2.06
25	Y	305	CLA	MG-NC	-3.28	1.98	2.06
24	N	601	CHL	C3B-C2B	-3.28	1.35	1.40
25	B	602	CLA	C1D-C2D	-3.28	1.38	1.45
25	b	602	CLA	C1D-C2D	-3.28	1.38	1.45
24	r	606	CHL	C3B-C2B	-3.28	1.35	1.40
28	B	617	BCR	C30-C25	-3.28	1.49	1.53
28	b	617	BCR	C30-C25	-3.28	1.49	1.53
25	S	310	CLA	MG-NC	-3.28	1.98	2.06
25	Y	314	CLA	MG-NC	-3.28	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C1D-C2D	-3.27	1.38	1.45
25	b	601	CLA	C1D-C2D	-3.27	1.38	1.45
25	Y	315	CLA	MG-NA	-3.27	1.98	2.06
25	B	613	CLA	MG-NC	-3.27	1.98	2.06
25	c	505	CLA	MG-NC	-3.27	1.98	2.06
25	b	613	CLA	MG-NC	-3.27	1.98	2.06
25	y	305	CLA	MG-NC	-3.26	1.98	2.06
24	s	302	CHL	C3B-C2B	-3.26	1.36	1.40
25	g	604	CLA	MG-NC	-3.26	1.98	2.06
25	Y	303	CLA	MG-NC	-3.26	1.98	2.06
25	y	303	CLA	MG-NC	-3.26	1.98	2.06
25	s	310	CLA	MG-NC	-3.26	1.98	2.06
25	B	614	CLA	MG-NC	-3.26	1.98	2.06
25	b	614	CLA	MG-NC	-3.26	1.98	2.06
25	C	504	CLA	C1D-C2D	-3.26	1.38	1.45
25	Y	313	CLA	MG-NC	-3.25	1.98	2.06
25	N	602	CLA	MG-NC	-3.25	1.98	2.06
25	C	505	CLA	MG-NC	-3.25	1.98	2.06
25	y	314	CLA	MG-NC	-3.25	1.98	2.06
25	D	403	CLA	C1D-C2D	-3.24	1.38	1.45
25	d	403	CLA	C1D-C2D	-3.24	1.38	1.45
25	n	602	CLA	MG-NC	-3.24	1.98	2.06
24	N	608	CHL	C3B-C2B	-3.24	1.36	1.40
25	y	315	CLA	MG-NA	-3.24	1.98	2.06
24	n	601	CHL	C3B-C2B	-3.24	1.36	1.40
38	F	101	HEM	FE-ND	-3.24	1.84	1.94
38	f	101	HEM	FE-ND	-3.24	1.84	1.94
25	b	608	CLA	MG-NC	-3.24	1.98	2.06
25	b	609	CLA	MG-NC	-3.24	1.98	2.06
25	R	603	CLA	C1D-C2D	-3.23	1.38	1.45
25	y	313	CLA	MG-NC	-3.23	1.98	2.06
24	2	601	CHL	C3B-C2B	-3.23	1.36	1.40
24	6	601	CHL	C3B-C2B	-3.23	1.36	1.40
25	C	502	CLA	MG-NC	-3.23	1.98	2.06
25	c	502	CLA	MG-NC	-3.23	1.98	2.06
28	z	101	BCR	C30-C25	-3.23	1.49	1.53
25	S	313	CLA	C1D-C2D	-3.22	1.39	1.45
25	R	604	CLA	C1D-C2D	-3.21	1.39	1.45
25	r	604	CLA	C1D-C2D	-3.21	1.39	1.45
25	c	504	CLA	C1D-C2D	-3.21	1.39	1.45
25	s	313	CLA	C1D-C2D	-3.21	1.39	1.45
25	B	609	CLA	MG-NC	-3.21	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	C3B-C2B	-3.21	1.36	1.40
25	Y	304	CLA	MG-NC	-3.20	1.98	2.06
25	y	304	CLA	MG-NC	-3.20	1.98	2.06
25	B	608	CLA	MG-NC	-3.20	1.98	2.06
25	G	603	CLA	MG-NC	-3.20	1.98	2.06
25	g	603	CLA	MG-NC	-3.20	1.98	2.06
25	G	611	CLA	MG-NC	-3.19	1.98	2.06
25	g	611	CLA	MG-NC	-3.19	1.98	2.06
25	r	603	CLA	C1D-C2D	-3.19	1.39	1.45
28	Z	101	BCR	C30-C25	-3.18	1.49	1.53
25	N	603	CLA	MG-NC	-3.18	1.98	2.06
25	n	603	CLA	MG-NC	-3.18	1.98	2.06
24	l	302	CHL	C3B-C2B	-3.18	1.36	1.40
24	5	302	CHL	C3B-C2B	-3.18	1.36	1.40
25	R	612	CLA	C1D-C2D	-3.17	1.39	1.45
25	r	612	CLA	C1D-C2D	-3.17	1.39	1.45
25	Y	303	CLA	MG-NB	-3.17	1.99	2.05
25	y	303	CLA	MG-NB	-3.17	1.99	2.05
25	G	614	CLA	MG-NC	-3.16	1.98	2.06
25	g	614	CLA	MG-NC	-3.16	1.98	2.06
25	r	601	CLA	C1D-C2D	-3.15	1.39	1.45
25	G	602	CLA	MG-NC	-3.15	1.98	2.06
25	y	315	CLA	MG-NC	-3.14	1.98	2.06
25	S	305	CLA	C1D-C2D	-3.14	1.39	1.45
25	s	305	CLA	C1D-C2D	-3.14	1.39	1.45
25	g	602	CLA	MG-NC	-3.14	1.98	2.06
28	D	404	BCR	C30-C25	-3.13	1.49	1.53
28	d	404	BCR	C30-C25	-3.13	1.49	1.53
25	Y	312	CLA	MG-NC	-3.12	1.98	2.06
25	y	312	CLA	MG-NC	-3.12	1.98	2.06
24	6	603	CHL	MG-NB	3.11	2.11	2.05
25	R	601	CLA	C1D-C2D	-3.10	1.39	1.45
40	G	617	NEX	C12-C13	-3.10	1.39	1.46
25	Y	315	CLA	MG-NC	-3.09	1.98	2.06
25	6	604	CLA	C1D-C2D	-3.09	1.39	1.45
28	H	101	BCR	C30-C25	-3.08	1.49	1.53
28	h	101	BCR	C30-C25	-3.08	1.49	1.53
40	n	617	NEX	C10-C9	3.08	1.42	1.35
40	N	617	NEX	C10-C9	3.08	1.42	1.35
24	S	302	CHL	C1A-CHA	3.06	1.43	1.40
24	Y	308	CHL	C1A-CHA	3.06	1.43	1.40
24	y	308	CHL	C1A-CHA	3.06	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	604	CLA	C1D-C2D	-3.05	1.39	1.45
24	2	603	CHL	MG-NB	3.04	2.11	2.05
24	5	302	CHL	C1A-CHA	3.04	1.43	1.40
24	n	601	CHL	C1A-CHA	3.03	1.43	1.40
40	G	617	NEX	C11-C12	3.03	1.42	1.34
24	Y	307	CHL	O2A-CGA	3.02	1.42	1.33
40	r	617	NEX	C12-C13	-3.02	1.39	1.46
24	N	601	CHL	C1A-CHA	3.01	1.43	1.40
40	R	617	NEX	C12-C13	-3.01	1.39	1.46
24	G	609	CHL	C1A-CHA	3.01	1.43	1.40
40	y	318	NEX	C10-C9	3.01	1.42	1.35
25	n	613	CLA	MG-NC	-3.00	1.99	2.06
24	s	302	CHL	C1A-CHA	2.99	1.43	1.40
24	y	307	CHL	O2A-CGA	2.99	1.42	1.33
24	N	605	CHL	O2A-CGA	2.98	1.42	1.33
40	N	617	NEX	O24-C25	-2.98	1.42	1.46
24	G	608	CHL	O2A-CGA	2.98	1.42	1.33
24	Y	308	CHL	O2A-CGA	2.98	1.42	1.33
24	g	608	CHL	O2A-CGA	2.98	1.42	1.33
25	2	602	CLA	C1D-C2D	-2.98	1.39	1.45
25	6	602	CLA	C1D-C2D	-2.98	1.39	1.45
40	Y	318	NEX	C10-C9	2.98	1.42	1.35
25	N	613	CLA	MG-NC	-2.97	1.99	2.06
24	y	308	CHL	O2A-CGA	2.97	1.42	1.33
24	n	605	CHL	O2A-CGA	2.97	1.42	1.33
24	r	607	CHL	O2A-CGA	2.97	1.42	1.33
24	2	601	CHL	O2A-CGA	2.97	1.42	1.33
24	6	601	CHL	O2A-CGA	2.97	1.42	1.33
25	g	613	CLA	MG-NC	-2.96	1.99	2.06
24	Y	306	CHL	O2A-CGA	2.96	1.42	1.33
24	Y	310	CHL	O2A-CGA	2.96	1.42	1.33
24	y	310	CHL	O2A-CGA	2.96	1.42	1.33
24	G	606	CHL	O2A-CGA	2.96	1.42	1.33
24	g	606	CHL	O2A-CGA	2.96	1.42	1.33
24	N	601	CHL	O2A-CGA	2.96	1.42	1.33
24	g	609	CHL	C1A-CHA	2.96	1.43	1.40
24	G	607	CHL	C1A-CHA	2.95	1.43	1.40
24	g	607	CHL	C1A-CHA	2.95	1.43	1.40
24	y	306	CHL	O2A-CGA	2.95	1.42	1.33
24	N	608	CHL	O2A-CGA	2.95	1.41	1.33
24	Y	309	CHL	O2A-CGA	2.95	1.41	1.33
24	y	309	CHL	O2A-CGA	2.95	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	O2A-CGA	2.95	1.41	1.33
24	l	302	CHL	C1A-CHA	2.95	1.43	1.40
24	R	607	CHL	O2A-CGA	2.95	1.41	1.33
40	n	617	NEX	O24-C25	-2.95	1.42	1.46
24	G	609	CHL	O2A-CGA	2.94	1.41	1.33
24	g	609	CHL	O2A-CGA	2.94	1.41	1.33
25	G	613	CLA	MG-NC	-2.93	1.99	2.06
24	Y	310	CHL	C1A-CHA	2.93	1.43	1.40
24	n	601	CHL	O2A-CGA	2.93	1.41	1.33
25	N	610	CLA	C1B-NB	2.93	1.41	1.37
24	n	609	CHL	O2A-CGA	2.93	1.41	1.33
40	g	617	NEX	O24-C25	-2.92	1.42	1.46
24	N	609	CHL	O2A-CGA	2.92	1.41	1.33
25	n	610	CLA	C1B-NB	2.91	1.41	1.37
24	Y	302	CHL	O2A-CGA	2.91	1.41	1.33
24	y	302	CHL	O2A-CGA	2.91	1.41	1.33
24	y	307	CHL	MG-NB	2.91	2.11	2.05
24	N	607	CHL	C1A-CHA	2.91	1.43	1.40
24	n	607	CHL	C1A-CHA	2.91	1.43	1.40
24	g	601	CHL	O2A-CGA	2.89	1.41	1.33
40	G	617	NEX	O24-C25	-2.89	1.42	1.46
24	N	609	CHL	C1A-CHA	2.89	1.43	1.40
24	g	605	CHL	C1A-CHA	2.89	1.43	1.40
41	R	616	XAT	O24-C25	-2.89	1.42	1.46
40	y	318	NEX	O24-C25	-2.89	1.42	1.46
40	R	617	NEX	C10-C9	2.88	1.42	1.35
40	r	617	NEX	C10-C9	2.88	1.42	1.35
24	G	601	CHL	O2A-CGA	2.88	1.41	1.33
40	s	317	NEX	O24-C25	-2.87	1.42	1.46
24	l	301	CHL	C1A-CHA	2.87	1.43	1.40
24	2	601	CHL	C2C-C3C	2.87	1.39	1.36
25	y	311	CLA	C1B-NB	2.86	1.41	1.37
25	Y	313	CLA	CHC-C4B	-2.86	1.33	1.39
24	n	607	CHL	O2A-CGA	2.86	1.41	1.33
24	N	607	CHL	O2A-CGA	2.85	1.41	1.33
24	G	605	CHL	C1A-CHA	2.85	1.43	1.40
24	g	606	CHL	C1A-CHA	2.85	1.43	1.40
24	y	310	CHL	C1A-CHA	2.85	1.43	1.40
41	r	616	XAT	O24-C25	-2.85	1.42	1.46
25	s	312	CLA	C1B-NB	2.85	1.41	1.37
40	Y	318	NEX	O24-C25	-2.85	1.42	1.46
24	Y	307	CHL	MG-NB	2.84	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Y	318	NEX	C11-C12	2.84	1.42	1.34
24	6	603	CHL	CHD-C4C	2.84	1.44	1.39
40	S	317	NEX	O24-C25	-2.84	1.42	1.46
40	y	318	NEX	C11-C12	2.84	1.42	1.34
41	R	616	XAT	O4-C5	-2.83	1.42	1.46
41	r	616	XAT	O4-C5	-2.83	1.42	1.46
40	N	617	NEX	C11-C12	2.83	1.42	1.34
24	Y	308	CHL	C2C-C3C	2.83	1.39	1.36
24	y	308	CHL	C2C-C3C	2.83	1.39	1.36
24	G	606	CHL	C1A-CHA	2.82	1.43	1.40
24	y	302	CHL	C1A-CHA	2.82	1.43	1.40
24	n	609	CHL	C1A-CHA	2.81	1.43	1.40
40	n	617	NEX	C11-C12	2.81	1.42	1.34
40	R	617	NEX	O24-C25	-2.81	1.42	1.46
40	r	617	NEX	O24-C25	-2.81	1.42	1.46
25	S	312	CLA	C1B-NB	2.81	1.41	1.37
25	y	313	CLA	CHC-C4B	-2.81	1.33	1.39
25	s	309	CLA	C1B-NB	2.80	1.41	1.37
25	Y	311	CLA	C1B-NB	2.79	1.41	1.37
24	2	603	CHL	CHD-C4C	2.79	1.44	1.39
24	Y	302	CHL	C1A-CHA	2.79	1.43	1.40
40	s	317	NEX	C10-C9	2.79	1.42	1.35
24	6	601	CHL	C2C-C3C	2.78	1.39	1.36
24	5	301	CHL	C1A-CHA	2.78	1.43	1.40
25	r	614	CLA	C1B-NB	2.78	1.41	1.37
40	S	317	NEX	C10-C9	2.78	1.42	1.35
25	r	608	CLA	C1B-NB	2.77	1.41	1.37
24	G	607	CHL	C3B-C2B	-2.77	1.36	1.40
24	g	607	CHL	C3B-C2B	-2.77	1.36	1.40
25	R	611	CLA	C1D-C2D	-2.77	1.39	1.45
24	r	606	CHL	C1A-CHA	2.76	1.43	1.40
25	S	309	CLA	C1B-NB	2.75	1.41	1.37
25	r	611	CLA	C1D-C2D	-2.75	1.39	1.45
25	y	315	CLA	CHC-C4B	-2.74	1.33	1.39
24	R	607	CHL	C1A-CHA	2.74	1.43	1.40
24	N	606	CHL	C1A-CHA	2.74	1.43	1.40
24	n	606	CHL	C1A-CHA	2.74	1.43	1.40
25	N	602	CLA	C4B-NB	2.74	1.41	1.37
25	n	602	CLA	C4B-NB	2.74	1.41	1.37
24	Y	306	CHL	C1A-CHA	2.73	1.43	1.40
25	G	602	CLA	C4B-NB	2.73	1.41	1.37
25	g	602	CLA	C4B-NB	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	617	NEX	C10-C9	2.72	1.42	1.35
24	g	608	CHL	C1A-CHA	2.72	1.43	1.40
24	R	606	CHL	C1A-CHA	2.72	1.43	1.40
24	G	601	CHL	C1A-CHA	2.71	1.43	1.40
24	g	601	CHL	C1A-CHA	2.71	1.43	1.40
24	R	613	CHL	C1A-CHA	2.71	1.43	1.40
24	r	613	CHL	C1A-CHA	2.71	1.43	1.40
25	R	608	CLA	C1B-NB	2.71	1.41	1.37
24	r	607	CHL	C1A-CHA	2.71	1.43	1.40
24	R	605	CHL	C1A-CHA	2.71	1.43	1.40
24	S	307	CHL	C2C-C3C	2.71	1.39	1.36
24	n	605	CHL	C1A-CHA	2.70	1.43	1.40
25	R	614	CLA	C1B-NB	2.70	1.41	1.37
24	y	306	CHL	C1A-CHA	2.70	1.43	1.40
40	S	317	NEX	C32-C33	-2.69	1.40	1.46
40	n	617	NEX	C12-C13	-2.69	1.40	1.46
24	G	608	CHL	C1A-CHA	2.69	1.43	1.40
25	Y	315	CLA	CHC-C4B	-2.69	1.33	1.39
24	s	307	CHL	C1A-CHA	2.69	1.43	1.40
40	N	617	NEX	C12-C13	-2.68	1.40	1.46
24	N	605	CHL	C1A-CHA	2.68	1.43	1.40
24	n	608	CHL	C1A-CHA	2.67	1.43	1.40
40	s	317	NEX	C32-C33	-2.67	1.40	1.46
24	r	605	CHL	C1A-CHA	2.67	1.43	1.40
25	B	609	CLA	CHC-C4B	-2.67	1.33	1.39
25	b	609	CLA	CHC-C4B	-2.67	1.33	1.39
24	N	608	CHL	C1A-CHA	2.66	1.43	1.40
38	F	101	HEM	C1D-ND	-2.66	1.33	1.38
38	f	101	HEM	C1D-ND	-2.66	1.33	1.38
40	y	318	NEX	C12-C13	-2.66	1.40	1.46
24	s	307	CHL	C2C-C3C	2.66	1.38	1.36
40	Y	318	NEX	C12-C13	-2.66	1.40	1.46
25	g	612	CLA	C1B-NB	2.65	1.41	1.37
25	C	506	CLA	C1B-NB	2.65	1.41	1.37
25	c	506	CLA	C1B-NB	2.65	1.41	1.37
25	g	613	CLA	C4C-C3C	-2.65	1.40	1.45
40	R	617	NEX	C11-C12	2.64	1.41	1.34
40	r	617	NEX	C11-C12	2.64	1.41	1.34
25	N	613	CLA	C4C-C3C	-2.64	1.40	1.45
24	n	608	CHL	C2C-C3C	2.63	1.38	1.36
24	g	608	CHL	C2C-C3C	2.63	1.38	1.36
25	C	513	CLA	C4C-C3C	-2.63	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	610	CLA	C4C-C3C	-2.63	1.40	1.45
25	n	610	CLA	C4C-C3C	-2.63	1.40	1.45
24	N	608	CHL	MG-NB	2.62	2.11	2.05
39	R	615	LUT	C23-C24	2.62	1.54	1.50
39	r	615	LUT	C23-C24	2.62	1.54	1.50
24	R	613	CHL	MG-NB	2.62	2.11	2.05
24	S	307	CHL	C1A-CHA	2.62	1.43	1.40
25	c	513	CLA	C4C-C3C	-2.62	1.40	1.45
25	G	603	CLA	CHC-C4B	-2.62	1.33	1.39
25	g	603	CLA	CHC-C4B	-2.62	1.33	1.39
25	g	602	CLA	C4C-C3C	-2.62	1.40	1.45
25	G	602	CLA	C4C-C3C	-2.62	1.40	1.45
25	b	610	CLA	C4C-C3C	-2.62	1.40	1.45
24	S	308	CHL	C1A-CHA	2.61	1.43	1.40
24	s	308	CHL	C1A-CHA	2.61	1.43	1.40
25	y	315	CLA	C4B-NB	2.61	1.41	1.37
24	Y	310	CHL	MG-NB	2.61	2.11	2.05
25	G	612	CLA	C1B-NB	2.61	1.41	1.37
25	G	613	CLA	C4C-C3C	-2.61	1.40	1.45
24	2	603	CHL	CHA-CBD	2.60	1.54	1.51
24	R	607	CHL	C2-C3	2.60	1.39	1.33
25	y	314	CLA	C4C-C3C	-2.60	1.40	1.45
25	r	614	CLA	C4B-NB	2.60	1.41	1.37
25	s	314	CLA	C1B-NB	2.60	1.41	1.37
24	y	308	CHL	C2-C3	2.60	1.39	1.33
25	Y	303	CLA	C4B-NB	2.60	1.41	1.37
25	y	303	CLA	C4B-NB	2.60	1.41	1.37
24	r	613	CHL	MG-NB	2.60	2.10	2.05
24	n	601	CHL	C2-C3	2.60	1.39	1.33
25	b	602	CLA	C1B-NB	2.60	1.41	1.37
25	A	405	CLA	C4C-C3C	-2.59	1.40	1.45
25	a	406	CLA	C4C-C3C	-2.59	1.40	1.45
24	Y	308	CHL	C2-C3	2.59	1.39	1.33
25	C	502	CLA	C4C-C3C	-2.59	1.40	1.45
25	c	502	CLA	C4C-C3C	-2.59	1.40	1.45
25	y	305	CLA	C4C-C3C	-2.59	1.40	1.45
25	B	602	CLA	C1B-NB	2.59	1.41	1.37
25	Y	313	CLA	C1B-NB	2.59	1.41	1.37
25	Y	311	CLA	C4C-C3C	-2.59	1.40	1.45
25	n	613	CLA	C4C-C3C	-2.59	1.40	1.45
25	d	402	CLA	C1B-NB	2.59	1.41	1.37
24	g	608	CHL	C2-C3	2.59	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	CHC-C4B	-2.59	1.33	1.39
25	G	604	CLA	CHC-C4B	-2.58	1.33	1.39
24	N	601	CHL	C2-C3	2.58	1.39	1.33
25	N	613	CLA	CHC-C4B	-2.58	1.33	1.39
25	n	613	CLA	CHC-C4B	-2.58	1.33	1.39
25	Y	314	CLA	C4C-C3C	-2.58	1.40	1.45
25	b	603	CLA	C4C-C3C	-2.58	1.40	1.45
24	n	608	CHL	MG-NB	2.58	2.10	2.05
24	Y	309	CHL	C2C-C3C	2.58	1.38	1.36
25	y	311	CLA	C4C-C3C	-2.58	1.40	1.45
25	B	615	CLA	C1B-NB	2.58	1.41	1.37
25	b	615	CLA	C1B-NB	2.58	1.41	1.37
25	r	609	CLA	C1B-NB	2.58	1.41	1.37
25	G	614	CLA	CHC-C4B	-2.58	1.33	1.39
25	g	604	CLA	CHC-C4B	-2.58	1.33	1.39
25	g	614	CLA	CHC-C4B	-2.58	1.33	1.39
25	B	604	CLA	C4C-C3C	-2.58	1.40	1.45
25	R	614	CLA	C4B-NB	2.58	1.41	1.37
25	y	304	CLA	CHC-C4B	-2.58	1.33	1.39
24	Y	306	CHL	MG-NB	2.58	2.10	2.05
24	y	306	CHL	MG-NB	2.58	2.10	2.05
25	R	609	CLA	C1B-NB	2.57	1.41	1.37
24	N	608	CHL	C2-C3	2.57	1.39	1.33
24	n	608	CHL	C2-C3	2.57	1.39	1.33
25	R	614	CLA	C4C-C3C	-2.57	1.40	1.45
25	B	610	CLA	C4C-C3C	-2.57	1.40	1.45
24	y	309	CHL	C1A-CHA	2.57	1.42	1.40
24	G	608	CHL	C2-C3	2.57	1.39	1.33
25	D	402	CLA	C1B-NB	2.57	1.41	1.37
25	Y	303	CLA	C4C-C3C	-2.57	1.40	1.45
25	r	614	CLA	C4C-C3C	-2.56	1.40	1.45
24	r	607	CHL	C2-C3	2.56	1.39	1.33
25	b	608	CLA	CHC-C4B	-2.56	1.33	1.39
24	Y	309	CHL	C2-C3	2.56	1.39	1.33
24	y	309	CHL	C2-C3	2.56	1.39	1.33
25	B	614	CLA	CHC-C4B	-2.56	1.33	1.39
25	b	614	CLA	CHC-C4B	-2.56	1.33	1.39
25	Y	304	CLA	CHC-C4B	-2.56	1.33	1.39
24	s	306	CHL	MG-NB	2.56	2.10	2.05
25	y	313	CLA	C1B-NB	2.56	1.41	1.37
24	G	606	CHL	MG-NB	2.55	2.10	2.05
24	N	605	CHL	MG-NB	2.55	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	605	CHL	MG-NB	2.55	2.10	2.05
25	y	303	CLA	C4C-C3C	-2.55	1.40	1.45
25	C	509	CLA	C4C-C3C	-2.55	1.40	1.45
25	c	509	CLA	C4C-C3C	-2.55	1.40	1.45
25	C	505	CLA	CHC-C4B	-2.55	1.33	1.39
24	Y	310	CHL	C2-C3	2.55	1.38	1.33
24	y	310	CHL	C2-C3	2.55	1.38	1.33
24	2	601	CHL	C2-C3	2.55	1.38	1.33
24	6	601	CHL	C2-C3	2.55	1.38	1.33
25	B	608	CLA	CHC-C4B	-2.55	1.33	1.39
25	Y	312	CLA	CHC-C4B	-2.55	1.33	1.39
24	6	603	CHL	CHA-CBD	2.55	1.54	1.51
25	B	616	CLA	C4C-C3C	-2.55	1.40	1.45
24	g	606	CHL	MG-NB	2.55	2.10	2.05
24	y	310	CHL	MG-NB	2.55	2.10	2.05
25	n	604	CLA	C4C-C3C	-2.55	1.40	1.45
24	y	302	CHL	C2-C3	2.55	1.38	1.33
25	A	402	CLA	C4C-C3C	-2.54	1.40	1.45
24	G	609	CHL	MG-NB	2.54	2.10	2.05
24	g	609	CHL	MG-NB	2.54	2.10	2.05
24	g	609	CHL	C2-C3	2.54	1.38	1.33
40	Y	318	NEX	C14-C13	2.54	1.41	1.35
24	N	609	CHL	C2-C3	2.54	1.38	1.33
24	n	609	CHL	C2-C3	2.54	1.38	1.33
24	R	605	CHL	MG-NB	2.54	2.10	2.05
25	C	502	CLA	CHC-C4B	-2.54	1.33	1.39
25	c	502	CLA	CHC-C4B	-2.54	1.33	1.39
24	R	606	CHL	MG-NB	2.54	2.10	2.05
24	r	606	CHL	MG-NB	2.54	2.10	2.05
25	B	601	CLA	C4C-C3C	-2.54	1.40	1.45
24	N	608	CHL	C2C-C3C	2.54	1.38	1.36
25	b	604	CLA	C4C-C3C	-2.54	1.40	1.45
25	Y	315	CLA	C4B-NB	2.54	1.41	1.37
24	6	603	CHL	C2C-C3C	2.54	1.38	1.36
25	S	314	CLA	C4C-C3C	-2.54	1.40	1.45
25	N	603	CLA	CHC-C4B	-2.54	1.33	1.39
25	n	603	CLA	CHC-C4B	-2.54	1.33	1.39
25	N	611	CLA	C4C-C3C	-2.53	1.40	1.45
25	n	611	CLA	C4C-C3C	-2.53	1.40	1.45
25	C	505	CLA	C4C-C3C	-2.53	1.40	1.45
25	c	505	CLA	C4C-C3C	-2.53	1.40	1.45
24	S	306	CHL	MG-NB	2.53	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	C4C-C3C	-2.53	1.40	1.45
40	y	318	NEX	C14-C13	2.53	1.41	1.35
25	S	314	CLA	C1B-NB	2.53	1.41	1.37
25	N	602	CLA	C4C-C3C	-2.53	1.40	1.45
25	n	602	CLA	C4C-C3C	-2.53	1.40	1.45
25	B	613	CLA	CHC-C4B	-2.53	1.33	1.39
25	B	609	CLA	C4C-C3C	-2.53	1.40	1.45
25	Y	305	CLA	C4C-C3C	-2.53	1.40	1.45
25	b	609	CLA	C4C-C3C	-2.53	1.40	1.45
25	N	614	CLA	C4C-C3C	-2.53	1.40	1.45
25	B	603	CLA	C4C-C3C	-2.53	1.40	1.45
25	B	614	CLA	C4C-C3C	-2.53	1.40	1.45
25	g	613	CLA	CHC-C4B	-2.53	1.33	1.39
24	G	608	CHL	MG-NB	2.52	2.10	2.05
24	g	608	CHL	MG-NB	2.52	2.10	2.05
25	B	607	CLA	C4C-C3C	-2.52	1.40	1.45
25	y	312	CLA	CHC-C4B	-2.52	1.33	1.39
39	n	616	LUT	C23-C24	2.52	1.53	1.50
25	G	603	CLA	C4C-C3C	-2.52	1.40	1.45
25	n	614	CLA	C4C-C3C	-2.52	1.40	1.45
24	Y	309	CHL	MG-NB	2.52	2.10	2.05
24	y	309	CHL	MG-NB	2.52	2.10	2.05
24	G	609	CHL	C2-C3	2.52	1.38	1.33
25	G	613	CLA	CHC-C4B	-2.52	1.33	1.39
24	S	308	CHL	MG-NB	2.52	2.10	2.05
24	s	308	CHL	MG-NB	2.52	2.10	2.05
24	g	605	CHL	MG-NB	2.52	2.10	2.05
25	g	603	CLA	C4C-C3C	-2.52	1.40	1.45
25	N	604	CLA	C4C-C3C	-2.52	1.40	1.45
25	R	602	CLA	C4C-C3C	-2.52	1.40	1.45
25	r	602	CLA	C4C-C3C	-2.52	1.40	1.45
24	2	603	CHL	C2C-C3C	2.51	1.38	1.36
24	Y	309	CHL	C1A-CHA	2.51	1.42	1.40
25	B	611	CLA	CHC-C4B	-2.51	1.33	1.39
25	b	611	CLA	CHC-C4B	-2.51	1.33	1.39
24	S	306	CHL	C1A-CHA	2.51	1.42	1.40
24	s	306	CHL	C1A-CHA	2.51	1.42	1.40
25	Y	315	CLA	C1B-C2B	-2.51	1.37	1.43
25	y	315	CLA	C1B-C2B	-2.51	1.37	1.43
24	r	605	CHL	MG-NB	2.51	2.10	2.05
25	G	604	CLA	C4C-C3C	-2.51	1.40	1.45
25	B	610	CLA	C1B-NB	2.51	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C1B-NB	2.51	1.41	1.37
25	c	508	CLA	C4C-C3C	-2.51	1.40	1.45
25	G	610	CLA	C4C-C3C	-2.50	1.40	1.45
24	G	608	CHL	C2C-C3C	2.50	1.38	1.36
25	g	610	CLA	C4C-C3C	-2.50	1.40	1.45
25	b	616	CLA	C4C-C3C	-2.50	1.40	1.45
25	Y	305	CLA	CHC-C4B	-2.50	1.33	1.39
25	y	305	CLA	CHC-C4B	-2.50	1.33	1.39
24	G	605	CHL	MG-NB	2.50	2.10	2.05
25	C	508	CLA	C4C-C3C	-2.50	1.40	1.45
25	N	603	CLA	C4C-C3C	-2.50	1.40	1.45
25	n	603	CLA	C4C-C3C	-2.50	1.40	1.45
24	s	307	CHL	MG-NB	2.50	2.10	2.05
25	b	613	CLA	CHC-C4B	-2.50	1.33	1.39
25	y	312	CLA	C4C-C3C	-2.49	1.40	1.45
25	R	609	CLA	C4C-C3C	-2.49	1.40	1.45
25	r	609	CLA	C4C-C3C	-2.49	1.40	1.45
25	b	616	CLA	CHC-C4B	-2.49	1.33	1.39
25	D	401	CLA	C4C-C3C	-2.49	1.40	1.45
25	d	401	CLA	C4C-C3C	-2.49	1.40	1.45
25	N	612	CLA	C1B-NB	2.49	1.41	1.37
25	n	612	CLA	C1B-NB	2.49	1.41	1.37
25	B	615	CLA	C4C-C3C	-2.49	1.40	1.45
25	b	615	CLA	C4C-C3C	-2.49	1.40	1.45
24	R	607	CHL	C2C-C3C	2.49	1.38	1.36
25	Y	314	CLA	CHC-C4B	-2.49	1.33	1.39
25	Y	312	CLA	C4C-C3C	-2.49	1.40	1.45
25	a	403	CLA	C4C-C3C	-2.49	1.40	1.45
24	l	301	CHL	MG-NB	2.49	2.10	2.05
38	F	101	HEM	C4B-NB	-2.49	1.34	1.38
25	b	601	CLA	C4C-C3C	-2.48	1.40	1.45
25	s	314	CLA	C4C-C3C	-2.48	1.40	1.45
25	B	613	CLA	C4C-C3C	-2.48	1.40	1.45
25	b	613	CLA	C4C-C3C	-2.48	1.40	1.45
40	g	617	NEX	C32-C33	-2.48	1.40	1.46
25	A	405	CLA	CHC-C4B	-2.48	1.33	1.39
25	a	406	CLA	CHC-C4B	-2.48	1.33	1.39
38	f	101	HEM	C4B-NB	-2.48	1.34	1.38
25	c	506	CLA	C4C-C3C	-2.48	1.40	1.45
25	b	614	CLA	C4C-C3C	-2.48	1.40	1.45
25	g	604	CLA	C4C-C3C	-2.48	1.40	1.45
24	y	309	CHL	C2C-C3C	2.48	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	C4C-C3C	-2.48	1.40	1.45
24	g	607	CHL	C2C-C3C	2.48	1.38	1.36
24	Y	302	CHL	C2-C3	2.48	1.38	1.33
24	r	613	CHL	C2C-C3C	2.48	1.38	1.36
25	s	310	CLA	C4C-C3C	-2.48	1.40	1.45
25	b	605	CLA	C4C-C3C	-2.48	1.40	1.45
25	D	401	CLA	CHC-C4B	-2.48	1.33	1.39
24	S	307	CHL	MG-NB	2.48	2.10	2.05
24	n	607	CHL	C2-C3	2.48	1.38	1.33
25	C	503	CLA	CHC-C4B	-2.48	1.33	1.39
25	c	503	CLA	CHC-C4B	-2.48	1.33	1.39
24	s	308	CHL	C2C-C3C	2.48	1.38	1.36
25	B	612	CLA	C4C-C3C	-2.47	1.40	1.45
25	b	612	CLA	C4C-C3C	-2.47	1.40	1.45
39	N	616	LUT	C23-C24	2.47	1.53	1.50
40	G	617	NEX	C32-C33	-2.47	1.40	1.46
24	G	601	CHL	C2-C3	2.47	1.38	1.33
25	Y	303	CLA	C1B-NB	2.47	1.41	1.37
25	y	303	CLA	C1B-NB	2.47	1.41	1.37
25	y	314	CLA	CHC-C4B	-2.47	1.33	1.39
25	S	304	CLA	C4C-C3C	-2.47	1.40	1.45
25	B	616	CLA	CHC-C4B	-2.47	1.33	1.39
25	B	605	CLA	C4C-C3C	-2.47	1.40	1.45
24	R	607	CHL	MG-NB	2.47	2.10	2.05
25	S	311	CLA	C4C-C3C	-2.47	1.40	1.45
25	s	311	CLA	C4C-C3C	-2.47	1.40	1.45
24	N	601	CHL	C2C-C3C	2.47	1.38	1.36
24	n	601	CHL	C2C-C3C	2.47	1.38	1.36
25	G	611	CLA	C4C-C3C	-2.47	1.40	1.45
25	g	611	CLA	C4C-C3C	-2.47	1.40	1.45
39	Y	317	LUT	C23-C24	2.47	1.53	1.50
25	B	607	CLA	CHC-C4B	-2.47	1.33	1.39
25	b	607	CLA	CHC-C4B	-2.47	1.33	1.39
25	G	612	CLA	C4B-NB	2.47	1.41	1.37
24	N	606	CHL	MG-NB	2.47	2.10	2.05
24	n	606	CHL	MG-NB	2.47	2.10	2.05
25	b	607	CLA	C4C-C3C	-2.47	1.40	1.45
24	G	607	CHL	C2C-C3C	2.46	1.38	1.36
24	R	605	CHL	CBA-CGA	2.46	1.56	1.50
24	r	605	CHL	CBA-CGA	2.46	1.56	1.50
24	N	607	CHL	C2-C3	2.46	1.38	1.33
25	Y	303	CLA	CHC-C4B	-2.46	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	303	CLA	CHC-C4B	-2.46	1.33	1.39
25	s	304	CLA	C4C-C3C	-2.46	1.40	1.45
24	5	301	CHL	MG-NB	2.46	2.10	2.05
25	R	614	CLA	CHC-C4B	-2.46	1.33	1.39
24	2	603	CHL	CHD-C1D	2.46	1.43	1.39
24	6	603	CHL	CHD-C1D	2.46	1.43	1.39
25	B	611	CLA	C4C-C3C	-2.46	1.40	1.45
25	S	310	CLA	C4C-C3C	-2.46	1.40	1.45
24	g	601	CHL	C2-C3	2.46	1.38	1.33
24	1	301	CHL	CBA-CGA	2.46	1.56	1.50
25	C	503	CLA	C4C-C3C	-2.46	1.40	1.45
25	C	506	CLA	C4C-C3C	-2.46	1.40	1.45
25	c	503	CLA	C4C-C3C	-2.46	1.40	1.45
25	C	512	CLA	CHC-C4B	-2.45	1.33	1.39
25	c	512	CLA	CHC-C4B	-2.45	1.33	1.39
24	5	301	CHL	CBA-CGA	2.45	1.56	1.50
24	Y	310	CHL	C2C-C3C	2.45	1.38	1.36
25	R	608	CLA	CHC-C4B	-2.45	1.33	1.39
25	d	401	CLA	CHC-C4B	-2.45	1.33	1.39
25	S	303	CLA	C4C-C3C	-2.45	1.40	1.45
25	s	303	CLA	C4C-C3C	-2.45	1.40	1.45
25	g	602	CLA	CHC-C4B	-2.45	1.33	1.39
24	S	302	CHL	CBA-CGA	2.45	1.56	1.50
24	s	302	CHL	CBA-CGA	2.45	1.56	1.50
25	b	611	CLA	C4C-C3C	-2.45	1.40	1.45
24	N	609	CHL	MG-NB	2.45	2.10	2.05
24	n	609	CHL	MG-NB	2.45	2.10	2.05
25	Y	313	CLA	C4C-C3C	-2.44	1.40	1.45
25	d	402	CLA	C4C-C3C	-2.44	1.40	1.45
25	y	313	CLA	C4C-C3C	-2.44	1.40	1.45
24	R	606	CHL	CBA-CGA	2.44	1.56	1.50
24	1	301	CHL	C2C-C3C	2.44	1.38	1.36
25	y	303	CLA	CHC-C4B	-2.44	1.33	1.39
25	c	501	CLA	C4C-C3C	-2.44	1.40	1.45
25	B	603	CLA	CHC-C4B	-2.44	1.33	1.39
25	b	603	CLA	CHC-C4B	-2.44	1.33	1.39
24	s	306	CHL	C2C-C3C	2.44	1.38	1.36
24	r	607	CHL	MG-NB	2.44	2.10	2.05
24	1	302	CHL	CBA-CGA	2.44	1.56	1.50
25	R	611	CLA	C3D-C4D	-2.44	1.38	1.44
24	S	308	CHL	CBA-CGA	2.44	1.56	1.50
25	y	311	CLA	CHC-C4B	-2.44	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	303	CLA	CHC-C4B	-2.43	1.34	1.39
25	R	608	CLA	C4C-C3C	-2.43	1.40	1.45
25	r	608	CLA	C4C-C3C	-2.43	1.40	1.45
25	r	612	CLA	C4C-C3C	-2.43	1.40	1.45
32	y	320	AJP	C85-C02	2.43	1.56	1.51
40	R	617	NEX	C32-C33	-2.43	1.40	1.46
40	r	617	NEX	C32-C33	-2.43	1.40	1.46
24	S	307	CHL	CBA-CGA	2.43	1.56	1.50
25	2	605	CLA	C4C-C3C	-2.43	1.40	1.45
25	6	605	CLA	C4C-C3C	-2.43	1.40	1.45
25	N	610	CLA	CHC-C4B	-2.43	1.34	1.39
24	y	302	CHL	MG-NB	2.43	2.10	2.05
24	5	301	CHL	C2C-C3C	2.43	1.38	1.36
25	C	507	CLA	C4C-C3C	-2.43	1.40	1.45
25	c	507	CLA	C4C-C3C	-2.43	1.40	1.45
25	y	305	CLA	C4B-NB	2.43	1.41	1.37
25	Y	311	CLA	CHC-C4B	-2.42	1.34	1.39
24	s	307	CHL	CBA-CGA	2.42	1.56	1.50
24	n	606	CHL	CBA-CGA	2.42	1.56	1.50
40	g	617	NEX	C11-C12	2.42	1.41	1.34
25	N	604	CLA	CHC-C4B	-2.42	1.34	1.39
24	S	306	CHL	CBA-CGA	2.42	1.56	1.50
24	s	306	CHL	CBA-CGA	2.42	1.56	1.50
25	C	506	CLA	CHC-C4B	-2.42	1.34	1.39
25	r	608	CLA	CHC-C4B	-2.42	1.34	1.39
24	N	606	CHL	CBA-CGA	2.42	1.56	1.50
25	Y	305	CLA	C4B-NB	2.42	1.41	1.37
24	S	306	CHL	C2C-C3C	2.42	1.38	1.36
24	G	605	CHL	CBA-CGA	2.42	1.56	1.50
24	g	605	CHL	CBA-CGA	2.42	1.56	1.50
39	y	317	LUT	C23-C24	2.42	1.53	1.50
24	R	605	CHL	C2C-C3C	2.42	1.38	1.36
25	B	608	CLA	C4C-C3C	-2.42	1.40	1.45
25	b	608	CLA	C4C-C3C	-2.42	1.40	1.45
25	g	614	CLA	C4C-C3C	-2.42	1.40	1.45
24	r	606	CHL	CBA-CGA	2.42	1.56	1.50
25	G	602	CLA	CHC-C4B	-2.42	1.34	1.39
25	b	602	CLA	C4B-NB	2.42	1.41	1.37
25	Y	304	CLA	C4C-C3C	-2.42	1.40	1.45
25	r	614	CLA	CHC-C4B	-2.42	1.34	1.39
25	D	402	CLA	C4C-C3C	-2.42	1.40	1.45
24	G	601	CHL	C2C-C3C	2.42	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	601	CHL	C2C-C3C	2.42	1.38	1.36
24	r	607	CHL	C2C-C3C	2.42	1.38	1.36
39	G	616	LUT	C23-C24	2.42	1.53	1.50
39	g	616	LUT	C23-C24	2.42	1.53	1.50
25	a	402	CLA	CHC-C4B	-2.42	1.34	1.39
24	5	302	CHL	CBA-CGA	2.41	1.56	1.50
25	s	314	CLA	CHC-C4B	-2.41	1.34	1.39
24	Y	308	CHL	MG-NB	2.41	2.10	2.05
25	b	605	CLA	CHC-C4B	-2.41	1.34	1.39
25	n	602	CLA	C1B-NB	2.41	1.41	1.37
25	b	602	CLA	C4C-C3C	-2.41	1.40	1.45
25	Y	313	CLA	C4B-NB	2.41	1.41	1.37
25	B	602	CLA	C4B-NB	2.40	1.41	1.37
25	R	612	CLA	C4C-C3C	-2.40	1.41	1.45
24	y	307	CHL	C3D-C2D	-2.40	1.35	1.39
25	B	605	CLA	CHC-C4B	-2.40	1.34	1.39
25	c	505	CLA	C4B-NB	2.40	1.41	1.37
25	r	611	CLA	C3D-C4D	-2.40	1.38	1.44
24	N	607	CHL	C2C-C3C	2.40	1.38	1.36
24	n	607	CHL	C2C-C3C	2.40	1.38	1.36
24	r	605	CHL	C2C-C3C	2.40	1.38	1.36
24	s	308	CHL	CBA-CGA	2.40	1.56	1.50
40	S	317	NEX	C11-C12	2.40	1.40	1.34
40	s	317	NEX	C11-C12	2.40	1.40	1.34
25	G	612	CLA	CHC-C4B	-2.40	1.34	1.39
25	g	612	CLA	CHC-C4B	-2.40	1.34	1.39
25	n	611	CLA	CHC-C4B	-2.40	1.34	1.39
32	Y	320	AJP	C85-C02	2.40	1.56	1.51
25	S	304	CLA	CHC-C4B	-2.40	1.34	1.39
25	s	304	CLA	CHC-C4B	-2.40	1.34	1.39
25	C	501	CLA	C4C-C3C	-2.40	1.41	1.45
25	n	610	CLA	CHC-C4B	-2.40	1.34	1.39
25	S	314	CLA	CHC-C4B	-2.40	1.34	1.39
24	S	308	CHL	C2C-C3C	2.39	1.38	1.36
25	g	612	CLA	C4B-NB	2.39	1.41	1.37
24	y	308	CHL	MG-NB	2.39	2.10	2.05
25	S	310	CLA	CHC-C4B	-2.39	1.34	1.39
25	S	312	CLA	C4C-C3C	-2.39	1.41	1.45
25	R	604	CLA	C4C-C3C	-2.39	1.41	1.45
24	Y	302	CHL	MG-NB	2.39	2.10	2.05
39	N	615	LUT	C5-C6	2.39	1.38	1.34
25	B	604	CLA	CHC-C4B	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	CHC-C4B	-2.39	1.34	1.39
24	g	605	CHL	C2C-C3C	2.39	1.38	1.36
25	c	506	CLA	CHC-C4B	-2.39	1.34	1.39
25	y	313	CLA	C4B-NB	2.39	1.41	1.37
25	s	312	CLA	C4C-C3C	-2.39	1.41	1.45
25	R	602	CLA	CHC-C4B	-2.39	1.34	1.39
25	r	602	CLA	CHC-C4B	-2.39	1.34	1.39
25	A	402	CLA	CHC-C4B	-2.39	1.34	1.39
25	a	403	CLA	CHC-C4B	-2.39	1.34	1.39
25	S	303	CLA	C1B-NB	2.39	1.41	1.37
25	s	303	CLA	C1B-NB	2.39	1.41	1.37
25	n	604	CLA	CHC-C4B	-2.38	1.34	1.39
25	D	403	CLA	C4C-C3C	-2.38	1.41	1.45
25	R	610	CLA	C4C-C3C	-2.38	1.41	1.45
25	d	403	CLA	C4C-C3C	-2.38	1.41	1.45
25	r	610	CLA	C4C-C3C	-2.38	1.41	1.45
24	6	603	CHL	C3D-C4D	2.38	1.45	1.41
40	n	617	NEX	C14-C13	2.38	1.41	1.35
25	A	401	CLA	C4C-C3C	-2.38	1.41	1.45
25	a	402	CLA	C4C-C3C	-2.38	1.41	1.45
25	S	309	CLA	C4C-C3C	-2.38	1.41	1.45
25	c	504	CLA	C4C-C3C	-2.38	1.41	1.45
25	s	309	CLA	C4C-C3C	-2.38	1.41	1.45
25	y	304	CLA	C4C-C3C	-2.38	1.41	1.45
24	2	603	CHL	CBA-CGA	2.38	1.56	1.50
25	C	504	CLA	C4C-C3C	-2.38	1.41	1.45
25	B	616	CLA	C4B-NB	2.38	1.41	1.37
25	b	616	CLA	C4B-NB	2.38	1.41	1.37
24	G	607	CHL	CBA-CGA	2.38	1.56	1.50
40	N	617	NEX	C14-C13	2.38	1.41	1.35
25	y	305	CLA	C1B-NB	2.37	1.41	1.37
25	N	611	CLA	CHC-C4B	-2.37	1.34	1.39
25	Y	315	CLA	C4C-C3C	-2.37	1.41	1.45
24	6	603	CHL	CBA-CGA	2.37	1.56	1.50
24	y	310	CHL	C2C-C3C	2.37	1.38	1.36
25	A	401	CLA	CHC-C4B	-2.37	1.34	1.39
24	Y	307	CHL	C3D-C2D	-2.37	1.35	1.39
25	C	513	CLA	CHC-C4B	-2.37	1.34	1.39
24	N	607	CHL	MG-NB	2.37	2.10	2.05
24	n	607	CHL	MG-NB	2.37	2.10	2.05
39	G	616	LUT	C5-C6	2.37	1.38	1.34
39	g	616	LUT	C5-C6	2.37	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	313	CLA	C1B-C2B	-2.37	1.37	1.43
25	S	310	CLA	C1B-NB	2.36	1.41	1.37
25	s	310	CLA	CHC-C4B	-2.36	1.34	1.39
24	G	609	CHL	C2C-C3C	2.36	1.38	1.36
24	g	609	CHL	C2C-C3C	2.36	1.38	1.36
25	C	512	CLA	C4C-C3C	-2.36	1.41	1.45
25	G	614	CLA	C4C-C3C	-2.36	1.41	1.45
25	c	512	CLA	C4C-C3C	-2.36	1.41	1.45
24	G	605	CHL	C2C-C3C	2.36	1.38	1.36
24	g	601	CHL	MG-NB	2.36	2.10	2.05
25	C	510	CLA	C4C-C3C	-2.36	1.41	1.45
25	c	510	CLA	C4C-C3C	-2.36	1.41	1.45
25	g	602	CLA	C1B-NB	2.35	1.41	1.37
25	B	602	CLA	C4C-C3C	-2.35	1.41	1.45
25	S	313	CLA	C4C-C3C	-2.35	1.41	1.45
25	s	313	CLA	C4C-C3C	-2.35	1.41	1.45
39	n	615	LUT	C5-C6	2.35	1.38	1.34
24	G	601	CHL	MG-NB	2.35	2.10	2.05
25	S	310	CLA	C4B-NB	2.35	1.40	1.37
25	s	310	CLA	C4B-NB	2.35	1.40	1.37
25	G	614	CLA	C4B-NB	2.34	1.40	1.37
25	g	614	CLA	C4B-NB	2.34	1.40	1.37
24	Y	306	CHL	C2C-C3C	2.34	1.38	1.36
24	y	306	CHL	C2C-C3C	2.34	1.38	1.36
25	B	606	CLA	C4C-C3C	-2.34	1.41	1.45
25	b	606	CLA	C4C-C3C	-2.34	1.41	1.45
25	y	315	CLA	C4C-C3C	-2.34	1.41	1.45
24	S	302	CHL	MG-NB	2.34	2.10	2.05
39	s	315	LUT	C23-C24	2.34	1.53	1.50
25	N	610	CLA	C4B-NB	2.34	1.40	1.37
25	n	610	CLA	C4B-NB	2.34	1.40	1.37
25	N	602	CLA	C1B-NB	2.34	1.40	1.37
40	r	617	NEX	C14-C13	2.34	1.41	1.35
25	B	610	CLA	C4B-NB	2.34	1.40	1.37
25	C	508	CLA	CHC-C4B	-2.33	1.34	1.39
25	c	508	CLA	CHC-C4B	-2.33	1.34	1.39
25	C	505	CLA	C4B-NB	2.33	1.40	1.37
25	C	506	CLA	C4B-NB	2.33	1.40	1.37
25	c	513	CLA	CHC-C4B	-2.33	1.34	1.39
39	y	317	LUT	C5-C6	2.33	1.38	1.34
25	n	612	CLA	CHC-C4B	-2.33	1.34	1.39
25	Y	305	CLA	C1B-NB	2.33	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	612	CLA	CHC-C4B	-2.33	1.34	1.39
25	G	612	CLA	C4C-C3C	-2.33	1.41	1.45
25	y	304	CLA	C1B-C2B	-2.33	1.37	1.43
25	c	513	CLA	C4B-NB	2.33	1.40	1.37
25	g	604	CLA	C4B-NB	2.33	1.40	1.37
25	s	311	CLA	CHC-C4B	-2.33	1.34	1.39
25	s	305	CLA	C4C-C3C	-2.33	1.41	1.45
39	S	316	LUT	C23-C24	2.33	1.53	1.50
39	s	316	LUT	C23-C24	2.33	1.53	1.50
24	g	607	CHL	CBA-CGA	2.32	1.56	1.50
40	R	617	NEX	C14-C13	2.32	1.41	1.35
40	N	617	NEX	C32-C33	-2.32	1.41	1.46
25	S	303	CLA	C4B-NB	2.32	1.40	1.37
25	s	303	CLA	C4B-NB	2.32	1.40	1.37
25	S	314	CLA	C4B-NB	2.32	1.40	1.37
25	b	608	CLA	C4B-NB	2.32	1.40	1.37
25	s	314	CLA	C4B-NB	2.32	1.40	1.37
25	b	612	CLA	CHC-C4B	-2.32	1.34	1.39
25	n	611	CLA	C4B-NB	2.32	1.40	1.37
40	n	617	NEX	C32-C33	-2.32	1.41	1.46
25	C	510	CLA	CHC-C4B	-2.31	1.34	1.39
25	c	510	CLA	CHC-C4B	-2.31	1.34	1.39
39	S	315	LUT	C23-C24	2.31	1.53	1.50
25	Y	313	CLA	C1B-C2B	-2.31	1.37	1.43
25	C	513	CLA	C4B-NB	2.31	1.40	1.37
25	B	612	CLA	CHC-C4B	-2.31	1.34	1.39
25	g	612	CLA	C4C-C3C	-2.31	1.41	1.45
24	R	613	CHL	C2C-C3C	2.30	1.38	1.36
25	S	311	CLA	CHC-C4B	-2.30	1.34	1.39
39	G	616	LUT	C1-C6	2.30	1.56	1.53
39	g	616	LUT	C1-C6	2.30	1.56	1.53
25	B	609	CLA	C1B-C2B	-2.30	1.37	1.43
25	Y	304	CLA	C1B-C2B	-2.30	1.37	1.43
25	c	506	CLA	C4B-NB	2.30	1.40	1.37
25	b	609	CLA	C1B-C2B	-2.30	1.37	1.43
25	r	604	CLA	C4C-C3C	-2.30	1.41	1.45
39	S	315	LUT	C5-C6	2.30	1.38	1.34
25	G	602	CLA	C1B-NB	2.30	1.40	1.37
25	s	312	CLA	C4B-NB	2.30	1.40	1.37
24	s	302	CHL	MG-NB	2.30	2.10	2.05
25	s	310	CLA	C1B-NB	2.30	1.40	1.37
39	N	616	LUT	C5-C6	2.30	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	616	LUT	C5-C6	2.30	1.38	1.34
25	R	602	CLA	C4B-NB	2.29	1.40	1.37
25	r	602	CLA	C4B-NB	2.29	1.40	1.37
25	r	603	CLA	C4C-C3C	-2.29	1.41	1.45
25	Y	312	CLA	C4B-NB	2.29	1.40	1.37
25	y	312	CLA	C4B-NB	2.29	1.40	1.37
25	B	613	CLA	C4B-NB	2.29	1.40	1.37
25	b	613	CLA	C4B-NB	2.29	1.40	1.37
24	2	603	CHL	C3D-C4D	2.29	1.45	1.41
25	S	305	CLA	C4C-C3C	-2.29	1.41	1.45
24	N	605	CHL	C2C-C3C	2.29	1.38	1.36
24	n	605	CHL	C2C-C3C	2.29	1.38	1.36
25	b	602	CLA	C1B-C2B	-2.29	1.37	1.43
25	G	604	CLA	C1B-NB	2.29	1.40	1.37
25	b	610	CLA	C4B-NB	2.29	1.40	1.37
25	g	604	CLA	C1B-NB	2.29	1.40	1.37
25	2	604	CLA	C3D-C4D	-2.29	1.39	1.44
25	6	604	CLA	C3D-C4D	-2.29	1.39	1.44
38	F	101	HEM	C1C-C2C	-2.29	1.40	1.45
38	f	101	HEM	C1C-C2C	-2.29	1.40	1.45
41	R	616	XAT	C32-C33	-2.28	1.41	1.46
41	r	616	XAT	C32-C33	-2.28	1.41	1.46
25	N	612	CLA	C4B-NB	2.28	1.40	1.37
25	n	612	CLA	C4B-NB	2.28	1.40	1.37
39	Y	317	LUT	C5-C6	2.28	1.38	1.34
25	C	507	CLA	C4B-NB	2.28	1.40	1.37
25	c	507	CLA	C4B-NB	2.28	1.40	1.37
25	C	509	CLA	C1B-C2B	-2.28	1.37	1.43
25	R	603	CLA	C4C-C3C	-2.28	1.41	1.45
25	c	502	CLA	C4B-NB	2.28	1.40	1.37
25	C	509	CLA	CHC-C4B	-2.28	1.34	1.39
25	c	509	CLA	CHC-C4B	-2.28	1.34	1.39
25	Y	311	CLA	C4B-NB	2.28	1.40	1.37
25	y	311	CLA	C4B-NB	2.28	1.40	1.37
41	R	616	XAT	C12-C13	-2.28	1.41	1.46
41	r	616	XAT	C12-C13	-2.28	1.41	1.46
25	C	505	CLA	C1B-C2B	-2.28	1.37	1.43
25	S	312	CLA	C4B-NB	2.28	1.40	1.37
24	G	606	CHL	C2C-C3C	2.27	1.38	1.36
25	Y	312	CLA	C1B-NB	2.27	1.40	1.37
25	y	312	CLA	C1B-NB	2.27	1.40	1.37
25	B	603	CLA	C1B-C2B	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C1B-C2B	-2.27	1.37	1.43
25	N	603	CLA	C1B-C2B	-2.27	1.37	1.43
25	Y	305	CLA	C1B-C2B	-2.27	1.37	1.43
25	G	611	CLA	CHC-C4B	-2.27	1.34	1.39
25	N	611	CLA	C4B-NB	2.27	1.40	1.37
25	B	608	CLA	C1B-C2B	-2.27	1.37	1.43
25	Y	312	CLA	C1B-C2B	-2.27	1.37	1.43
25	y	312	CLA	C1B-C2B	-2.27	1.37	1.43
25	G	603	CLA	C1B-C2B	-2.27	1.37	1.43
25	g	603	CLA	C1B-C2B	-2.27	1.37	1.43
24	r	606	CHL	C2C-C3C	2.27	1.38	1.36
25	B	602	CLA	C1B-C2B	-2.27	1.37	1.43
25	y	305	CLA	C1B-C2B	-2.27	1.37	1.43
25	R	602	CLA	C1B-NB	2.26	1.40	1.37
25	B	612	CLA	C4B-NB	2.26	1.40	1.37
25	r	608	CLA	C4B-NB	2.26	1.40	1.37
25	b	607	CLA	C4B-NB	2.26	1.40	1.37
25	n	603	CLA	C1B-C2B	-2.26	1.37	1.43
25	R	609	CLA	C4B-NB	2.26	1.40	1.37
25	r	609	CLA	C4B-NB	2.26	1.40	1.37
25	S	309	CLA	C1B-C2B	-2.26	1.37	1.43
25	s	309	CLA	C1B-C2B	-2.26	1.37	1.43
25	y	311	CLA	C1B-C2B	-2.26	1.37	1.43
24	N	609	CHL	C2C-C3C	2.26	1.38	1.36
24	n	609	CHL	C2C-C3C	2.26	1.38	1.36
39	N	615	LUT	C23-C24	2.26	1.53	1.50
39	n	615	LUT	C23-C24	2.26	1.53	1.50
25	G	604	CLA	C4B-NB	2.26	1.40	1.37
25	B	610	CLA	CHC-C4B	-2.26	1.34	1.39
25	c	509	CLA	C1B-C2B	-2.26	1.37	1.43
25	B	616	CLA	C1B-C2B	-2.25	1.37	1.43
25	b	616	CLA	C1B-C2B	-2.25	1.37	1.43
24	G	607	CHL	MG-NB	2.25	2.10	2.05
24	g	607	CHL	MG-NB	2.25	2.10	2.05
25	c	511	CLA	CHC-C4B	-2.25	1.34	1.39
25	r	602	CLA	C1B-NB	2.25	1.40	1.37
25	b	610	CLA	CHC-C4B	-2.25	1.34	1.39
25	B	606	CLA	CHC-C4B	-2.25	1.34	1.39
25	b	606	CLA	CHC-C4B	-2.25	1.34	1.39
25	B	608	CLA	C4B-NB	2.25	1.40	1.37
25	B	607	CLA	C4B-NB	2.25	1.40	1.37
25	c	505	CLA	C1B-C2B	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	601	CLA	C1B-C2B	-2.25	1.37	1.43
25	R	601	CLA	C1B-C2B	-2.25	1.37	1.43
25	Y	315	CLA	C1B-NB	2.25	1.40	1.37
25	y	315	CLA	C1B-NB	2.25	1.40	1.37
25	s	312	CLA	C1B-C2B	-2.24	1.37	1.43
25	B	601	CLA	CHC-C4B	-2.24	1.34	1.39
39	G	615	LUT	C23-C24	2.24	1.53	1.50
39	g	615	LUT	C23-C24	2.24	1.53	1.50
24	2	601	CHL	MG-NB	2.24	2.10	2.05
24	6	601	CHL	MG-NB	2.24	2.10	2.05
39	R	615	LUT	C5-C6	2.24	1.38	1.34
39	g	615	LUT	C5-C6	2.24	1.38	1.34
39	S	316	LUT	C5-C6	2.24	1.38	1.34
39	s	316	LUT	C5-C6	2.24	1.38	1.34
25	C	502	CLA	C1B-C2B	-2.24	1.37	1.43
25	B	609	CLA	C4B-NB	2.24	1.40	1.37
25	b	609	CLA	C4B-NB	2.24	1.40	1.37
25	2	605	CLA	CHC-C4B	-2.24	1.34	1.39
25	C	502	CLA	C4B-NB	2.24	1.40	1.37
25	B	612	CLA	C1B-C2B	-2.24	1.37	1.43
25	b	612	CLA	C1B-C2B	-2.24	1.37	1.43
25	r	602	CLA	C1B-C2B	-2.24	1.37	1.43
39	G	615	LUT	C5-C6	2.24	1.38	1.34
24	R	606	CHL	C2C-C3C	2.24	1.38	1.36
25	C	507	CLA	CHC-C4B	-2.24	1.34	1.39
25	c	507	CLA	CHC-C4B	-2.24	1.34	1.39
25	c	502	CLA	C1B-C2B	-2.24	1.37	1.43
25	C	505	CLA	C1B-NB	2.24	1.40	1.37
25	R	608	CLA	C4B-NB	2.24	1.40	1.37
25	S	303	CLA	C1B-C2B	-2.23	1.37	1.43
25	b	608	CLA	C1B-C2B	-2.23	1.37	1.43
25	s	303	CLA	C1B-C2B	-2.23	1.37	1.43
25	B	603	CLA	C4B-NB	2.23	1.40	1.37
25	N	604	CLA	C1B-C2B	-2.23	1.37	1.43
25	n	604	CLA	C1B-C2B	-2.23	1.37	1.43
25	C	506	CLA	C1B-C2B	-2.23	1.37	1.43
25	c	506	CLA	C1B-C2B	-2.23	1.37	1.43
25	C	513	CLA	C1B-C2B	-2.23	1.37	1.43
25	Y	311	CLA	C1B-C2B	-2.23	1.37	1.43
25	S	309	CLA	C4B-NB	2.23	1.40	1.37
25	B	610	CLA	C1B-C2B	-2.23	1.37	1.43
25	b	610	CLA	C1B-C2B	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	CHC-C4B	-2.23	1.34	1.39
25	N	602	CLA	CHC-C4B	-2.23	1.34	1.39
25	n	602	CLA	CHC-C4B	-2.23	1.34	1.39
39	s	315	LUT	C5-C6	2.22	1.38	1.34
25	d	402	CLA	C4B-NB	2.22	1.40	1.37
24	Y	302	CHL	C2C-C3C	2.22	1.38	1.36
24	y	302	CHL	C2C-C3C	2.22	1.38	1.36
39	r	615	LUT	C5-C6	2.22	1.38	1.34
25	g	611	CLA	CHC-C4B	-2.22	1.34	1.39
25	S	309	CLA	CHC-C4B	-2.22	1.34	1.39
25	g	604	CLA	C1B-C2B	-2.22	1.37	1.43
25	B	614	CLA	C4B-NB	2.22	1.40	1.37
25	b	614	CLA	C4B-NB	2.22	1.40	1.37
25	s	314	CLA	C1B-C2B	-2.22	1.37	1.43
25	b	603	CLA	C4B-NB	2.22	1.40	1.37
25	c	513	CLA	C1B-C2B	-2.22	1.37	1.43
24	S	302	CHL	C2C-C3C	2.22	1.38	1.36
24	s	302	CHL	C2C-C3C	2.22	1.38	1.36
25	S	312	CLA	C1B-C2B	-2.21	1.37	1.43
25	C	511	CLA	CHC-C4B	-2.21	1.34	1.39
25	s	309	CLA	CHC-C4B	-2.21	1.34	1.39
25	G	614	CLA	C1B-C2B	-2.21	1.37	1.43
25	g	614	CLA	C1B-C2B	-2.21	1.37	1.43
25	B	613	CLA	C1B-C2B	-2.21	1.37	1.43
25	b	613	CLA	C1B-C2B	-2.21	1.37	1.43
25	y	314	CLA	C1B-C2B	-2.21	1.37	1.43
25	r	608	CLA	C1B-C2B	-2.21	1.37	1.43
25	R	601	CLA	C4C-C3C	-2.21	1.41	1.45
25	r	601	CLA	C4C-C3C	-2.21	1.41	1.45
25	R	602	CLA	C1B-C2B	-2.21	1.37	1.43
25	b	612	CLA	C4B-NB	2.21	1.40	1.37
25	R	611	CLA	C4C-C3C	-2.21	1.41	1.45
25	r	611	CLA	C4C-C3C	-2.21	1.41	1.45
25	r	609	CLA	CHC-C4B	-2.21	1.34	1.39
25	N	611	CLA	C1B-NB	2.21	1.40	1.37
25	n	611	CLA	C1B-NB	2.21	1.40	1.37
25	N	610	CLA	C1B-C2B	-2.21	1.37	1.43
25	6	605	CLA	CHC-C4B	-2.21	1.34	1.39
25	2	605	CLA	C1B-C2B	-2.21	1.38	1.43
25	6	605	CLA	C1B-C2B	-2.21	1.38	1.43
25	B	615	CLA	C4B-NB	2.20	1.40	1.37
25	b	615	CLA	C4B-NB	2.20	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	606	CHL	C2C-C3C	2.20	1.38	1.36
25	2	602	CLA	C4C-C3C	-2.20	1.41	1.45
25	6	602	CLA	C4C-C3C	-2.20	1.41	1.45
25	N	613	CLA	CHD-C1D	-2.20	1.34	1.38
24	N	601	CHL	MG-NB	2.20	2.10	2.05
24	n	601	CHL	MG-NB	2.20	2.10	2.05
25	D	402	CLA	C1B-C2B	-2.20	1.38	1.43
25	d	402	CLA	C1B-C2B	-2.20	1.38	1.43
25	S	314	CLA	C1B-C2B	-2.20	1.38	1.43
25	c	507	CLA	C1B-C2B	-2.20	1.38	1.43
25	s	309	CLA	C4B-NB	2.20	1.40	1.37
25	B	614	CLA	C1B-C2B	-2.20	1.38	1.43
25	b	614	CLA	C1B-C2B	-2.20	1.38	1.43
25	G	604	CLA	C1B-C2B	-2.20	1.38	1.43
25	b	601	CLA	CHC-C4B	-2.19	1.34	1.39
25	C	509	CLA	C4B-NB	2.19	1.40	1.37
25	c	509	CLA	C4B-NB	2.19	1.40	1.37
25	b	602	CLA	CHC-C4B	-2.19	1.34	1.39
25	Y	314	CLA	C1B-C2B	-2.19	1.38	1.43
25	C	507	CLA	C1B-C2B	-2.19	1.38	1.43
40	Y	318	NEX	C32-C33	-2.19	1.41	1.46
25	G	602	CLA	CHD-C1D	-2.18	1.34	1.38
25	g	602	CLA	CHD-C1D	-2.18	1.34	1.38
25	c	508	CLA	C1B-C2B	-2.18	1.38	1.43
25	2	602	CLA	C3D-C4D	-2.18	1.39	1.44
25	D	402	CLA	C4B-NB	2.18	1.40	1.37
25	y	304	CLA	C4B-NB	2.18	1.40	1.37
25	B	611	CLA	C1B-C2B	-2.18	1.38	1.43
25	b	611	CLA	C1B-C2B	-2.18	1.38	1.43
25	R	608	CLA	C1B-C2B	-2.18	1.38	1.43
25	n	610	CLA	C1B-C2B	-2.18	1.38	1.43
25	B	607	CLA	C1B-C2B	-2.18	1.38	1.43
25	b	607	CLA	C1B-C2B	-2.18	1.38	1.43
25	B	615	CLA	C1B-C2B	-2.18	1.38	1.43
25	b	615	CLA	C1B-C2B	-2.18	1.38	1.43
39	Y	317	LUT	C1-C6	2.18	1.56	1.53
25	g	613	CLA	C1B-C2B	-2.18	1.38	1.43
25	N	611	CLA	C1B-C2B	-2.17	1.38	1.43
25	n	611	CLA	C1B-C2B	-2.17	1.38	1.43
39	S	316	LUT	C1-C6	2.17	1.56	1.53
25	B	604	CLA	C4B-NB	2.17	1.40	1.37
25	b	604	CLA	C4B-NB	2.17	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	609	CLA	CHC-C4B	-2.17	1.34	1.39
25	G	613	CLA	C1B-C2B	-2.17	1.38	1.43
40	Y	318	NEX	C34-C33	2.17	1.40	1.35
25	n	613	CLA	CHD-C1D	-2.17	1.34	1.38
25	2	605	CLA	C4B-NB	2.17	1.40	1.37
25	6	605	CLA	C4B-NB	2.17	1.40	1.37
25	n	612	CLA	C4C-C3C	-2.17	1.41	1.45
25	B	608	CLA	C1C-C2C	-2.17	1.40	1.44
25	B	609	CLA	C1C-C2C	-2.16	1.40	1.44
25	g	612	CLA	C1B-C2B	-2.16	1.38	1.43
25	G	612	CLA	C1B-C2B	-2.16	1.38	1.43
40	G	617	NEX	C11-C10	-2.16	1.36	1.43
25	6	602	CLA	C3D-C4D	-2.16	1.39	1.44
25	g	602	CLA	C1B-C2B	-2.16	1.38	1.43
25	S	313	CLA	C1B-C2B	-2.15	1.38	1.43
25	C	502	CLA	C1C-C2C	-2.15	1.40	1.44
25	B	608	CLA	C1B-NB	2.15	1.40	1.37
25	b	609	CLA	C1C-C2C	-2.15	1.40	1.44
39	Y	316	LUT	C5-C6	2.15	1.38	1.34
25	C	508	CLA	C1B-C2B	-2.15	1.38	1.43
25	C	503	CLA	C1B-C2B	-2.15	1.38	1.43
25	C	511	CLA	C1B-C2B	-2.15	1.38	1.43
25	s	313	CLA	C1B-C2B	-2.15	1.38	1.43
25	N	603	CLA	C4B-NB	2.15	1.40	1.37
25	n	603	CLA	C4B-NB	2.15	1.40	1.37
25	Y	304	CLA	C4B-NB	2.15	1.40	1.37
39	y	317	LUT	C1-C6	2.15	1.56	1.53
40	y	318	NEX	C32-C33	-2.14	1.41	1.46
25	S	310	CLA	C1B-C2B	-2.14	1.38	1.43
25	s	310	CLA	C1B-C2B	-2.14	1.38	1.43
25	N	612	CLA	C1B-C2B	-2.14	1.38	1.43
39	y	316	LUT	C23-C24	2.14	1.53	1.50
25	D	401	CLA	C1B-C2B	-2.14	1.38	1.43
25	a	406	CLA	C1B-C2B	-2.14	1.38	1.43
25	S	305	CLA	C3D-C4D	-2.14	1.39	1.44
25	B	614	CLA	C1C-C2C	-2.14	1.40	1.44
25	A	405	CLA	C1B-C2B	-2.14	1.38	1.43
39	s	316	LUT	C1-C6	2.14	1.56	1.53
25	n	602	CLA	C1B-C2B	-2.14	1.38	1.43
25	y	312	CLA	CHD-C1D	-2.14	1.34	1.38
25	c	505	CLA	C1B-NB	2.14	1.40	1.37
25	B	611	CLA	C1C-C2C	-2.14	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	C1C-C2C	-2.14	1.40	1.44
25	s	305	CLA	C3D-C4D	-2.14	1.39	1.44
25	b	604	CLA	C1B-C2B	-2.13	1.38	1.43
25	c	511	CLA	C1B-C2B	-2.13	1.38	1.43
25	n	612	CLA	C1B-C2B	-2.13	1.38	1.43
25	r	609	CLA	C1B-C2B	-2.13	1.38	1.43
25	R	609	CLA	C1B-C2B	-2.13	1.38	1.43
40	y	318	NEX	C34-C33	2.13	1.40	1.35
25	B	603	CLA	C1B-NB	2.13	1.40	1.37
25	A	401	CLA	C4B-NB	2.13	1.40	1.37
25	a	402	CLA	C4B-NB	2.13	1.40	1.37
25	D	403	CLA	C3D-C4D	-2.13	1.39	1.44
25	B	604	CLA	C1B-C2B	-2.13	1.38	1.43
25	b	608	CLA	C1C-C2C	-2.13	1.40	1.44
25	c	502	CLA	C1C-C2C	-2.13	1.40	1.44
25	G	614	CLA	C1B-NB	2.12	1.40	1.37
25	g	603	CLA	C1C-C2C	-2.12	1.40	1.44
25	C	512	CLA	C1B-C2B	-2.12	1.38	1.43
25	c	512	CLA	C1B-C2B	-2.12	1.38	1.43
25	S	303	CLA	C1C-C2C	-2.12	1.40	1.44
25	s	303	CLA	C1C-C2C	-2.12	1.40	1.44
25	C	505	CLA	C1C-C2C	-2.12	1.40	1.44
25	c	505	CLA	C1C-C2C	-2.12	1.40	1.44
40	Y	318	NEX	C31-C32	2.12	1.40	1.34
25	N	613	CLA	C1B-C2B	-2.12	1.38	1.43
25	A	402	CLA	C1B-C2B	-2.12	1.38	1.43
25	a	403	CLA	C1B-C2B	-2.12	1.38	1.43
39	R	615	LUT	C26-C27	2.12	1.53	1.50
25	N	612	CLA	C4C-C3C	-2.12	1.41	1.45
25	n	613	CLA	C1B-C2B	-2.12	1.38	1.43
39	r	615	LUT	C26-C27	2.12	1.53	1.50
25	N	614	CLA	CHC-C4B	-2.12	1.34	1.39
25	N	603	CLA	C1C-C2C	-2.12	1.40	1.44
25	n	603	CLA	C1C-C2C	-2.12	1.40	1.44
25	c	503	CLA	C1B-C2B	-2.12	1.38	1.43
25	b	614	CLA	C1C-C2C	-2.12	1.40	1.44
39	y	316	LUT	C5-C6	2.12	1.38	1.34
25	c	503	CLA	C1C-C2C	-2.11	1.40	1.44
25	d	403	CLA	C3D-C4D	-2.11	1.39	1.44
25	N	604	CLA	C4B-NB	2.11	1.40	1.37
25	G	602	CLA	C1B-C2B	-2.11	1.38	1.43
25	G	603	CLA	C1C-C2C	-2.11	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	602	CLA	C1B-C2B	-2.11	1.38	1.43
25	G	611	CLA	C1B-C2B	-2.11	1.38	1.43
25	R	604	CLA	C1B-C2B	-2.11	1.38	1.43
25	c	512	CLA	C1C-C2C	-2.11	1.40	1.44
25	Y	304	CLA	C1C-C2C	-2.11	1.40	1.44
25	y	304	CLA	C1C-C2C	-2.11	1.40	1.44
25	B	613	CLA	C1C-C2C	-2.11	1.40	1.44
25	Y	313	CLA	C1C-C2C	-2.11	1.40	1.44
25	b	613	CLA	C1C-C2C	-2.11	1.40	1.44
25	y	313	CLA	C1C-C2C	-2.11	1.40	1.44
25	d	401	CLA	C1B-C2B	-2.11	1.38	1.43
25	R	601	CLA	C3D-C4D	-2.11	1.39	1.44
25	r	601	CLA	C3D-C4D	-2.11	1.39	1.44
38	F	101	HEM	C3B-C4B	2.11	1.49	1.44
38	f	101	HEM	C3B-C4B	2.11	1.49	1.44
25	C	510	CLA	C1B-C2B	-2.11	1.38	1.43
25	c	510	CLA	C1B-C2B	-2.11	1.38	1.43
25	n	614	CLA	CHC-C4B	-2.11	1.34	1.39
25	R	604	CLA	CHC-C4B	-2.10	1.34	1.39
24	5	302	CHL	C3D-C2D	-2.10	1.36	1.39
25	c	503	CLA	C4B-NB	2.10	1.40	1.37
25	Y	312	CLA	CHD-C1D	-2.10	1.34	1.38
25	C	504	CLA	C3D-C4D	-2.10	1.39	1.44
25	c	504	CLA	C3D-C4D	-2.10	1.39	1.44
25	B	611	CLA	C4B-NB	2.10	1.40	1.37
25	b	611	CLA	C4B-NB	2.10	1.40	1.37
25	A	405	CLA	C4B-NB	2.10	1.40	1.37
25	a	406	CLA	C4B-NB	2.10	1.40	1.37
25	C	501	CLA	C3D-C4D	-2.10	1.39	1.44
25	G	604	CLA	C1C-C2C	-2.10	1.40	1.44
25	N	604	CLA	C1C-C2C	-2.10	1.40	1.44
25	g	604	CLA	C1C-C2C	-2.10	1.40	1.44
25	b	603	CLA	C1B-NB	2.10	1.40	1.37
25	n	604	CLA	C4B-NB	2.10	1.40	1.37
25	g	614	CLA	C1B-NB	2.10	1.40	1.37
25	S	313	CLA	C3D-C4D	-2.10	1.39	1.44
25	A	401	CLA	C1B-C2B	-2.09	1.38	1.43
25	a	402	CLA	C1B-C2B	-2.09	1.38	1.43
25	R	612	CLA	C3D-C4D	-2.09	1.39	1.44
25	S	304	CLA	C4B-NB	2.09	1.40	1.37
25	s	304	CLA	C4B-NB	2.09	1.40	1.37
25	B	613	CLA	C1B-NB	2.09	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	613	CLA	C1B-NB	2.09	1.40	1.37
25	Y	315	CLA	C1C-C2C	-2.09	1.40	1.44
25	a	403	CLA	C1C-C2C	-2.09	1.40	1.44
25	y	315	CLA	C1C-C2C	-2.09	1.40	1.44
25	S	311	CLA	C4B-NB	2.09	1.40	1.37
25	C	503	CLA	C1C-C2C	-2.09	1.40	1.44
40	y	318	NEX	C31-C32	2.09	1.40	1.34
25	D	402	CLA	CHC-C4B	-2.09	1.34	1.39
25	B	604	CLA	C1B-NB	2.09	1.40	1.37
25	B	616	CLA	C1B-NB	2.09	1.40	1.37
25	b	604	CLA	C1B-NB	2.09	1.40	1.37
25	b	616	CLA	C1B-NB	2.09	1.40	1.37
25	B	606	CLA	C1B-C2B	-2.09	1.38	1.43
25	b	606	CLA	C1B-C2B	-2.09	1.38	1.43
25	A	401	CLA	C1C-C2C	-2.08	1.40	1.44
25	a	402	CLA	C1C-C2C	-2.08	1.40	1.44
25	c	512	CLA	C3D-C4D	-2.08	1.39	1.44
25	G	602	CLA	C1C-C2C	-2.08	1.40	1.44
25	g	602	CLA	C1C-C2C	-2.08	1.40	1.44
25	d	402	CLA	CHC-C4B	-2.08	1.34	1.39
25	N	602	CLA	CHD-C1D	-2.08	1.34	1.38
25	n	602	CLA	CHD-C1D	-2.08	1.34	1.38
25	A	402	CLA	C3D-C4D	-2.08	1.39	1.44
25	a	403	CLA	C3D-C4D	-2.08	1.39	1.44
24	N	606	CHL	C2C-C3C	2.08	1.38	1.36
25	d	401	CLA	C1C-C2C	-2.08	1.40	1.44
25	C	508	CLA	C1C-C2C	-2.08	1.40	1.44
25	c	508	CLA	C1C-C2C	-2.08	1.40	1.44
25	Y	304	CLA	C1B-NB	2.08	1.40	1.37
25	G	614	CLA	C1C-C2C	-2.08	1.40	1.44
25	g	614	CLA	C1C-C2C	-2.08	1.40	1.44
25	C	507	CLA	C1B-NB	2.08	1.40	1.37
25	g	611	CLA	C1B-C2B	-2.08	1.38	1.43
24	n	606	CHL	C2C-C3C	2.08	1.38	1.36
39	Y	316	LUT	C23-C24	2.08	1.53	1.50
28	T	101	BCR	C33-C5	-2.08	1.47	1.50
25	A	402	CLA	C1C-C2C	-2.08	1.40	1.44
25	r	612	CLA	C3D-C4D	-2.08	1.39	1.44
25	b	608	CLA	C1B-NB	2.08	1.40	1.37
25	r	604	CLA	CHC-C4B	-2.08	1.34	1.39
28	t	101	BCR	C33-C5	-2.08	1.47	1.50
25	S	304	CLA	C1B-C2B	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	304	CLA	C1B-C2B	-2.08	1.38	1.43
25	r	604	CLA	C1B-C2B	-2.08	1.38	1.43
25	S	311	CLA	C1B-C2B	-2.07	1.38	1.43
25	s	311	CLA	C1B-C2B	-2.07	1.38	1.43
24	l	302	CHL	C3D-C2D	-2.07	1.36	1.39
25	C	512	CLA	C1C-C2C	-2.07	1.40	1.44
25	b	603	CLA	C1C-C2C	-2.07	1.40	1.44
25	C	513	CLA	C1B-NB	2.07	1.40	1.37
25	c	513	CLA	C1B-NB	2.07	1.40	1.37
25	r	612	CLA	CHC-C4B	-2.07	1.34	1.39
25	C	509	CLA	C3D-C4D	-2.07	1.39	1.44
25	c	509	CLA	C3D-C4D	-2.07	1.39	1.44
25	c	507	CLA	C1C-C2C	-2.07	1.40	1.44
25	Y	304	CLA	C3D-C4D	-2.06	1.39	1.44
25	c	501	CLA	C3D-C4D	-2.06	1.39	1.44
25	y	304	CLA	C3D-C4D	-2.06	1.39	1.44
25	B	605	CLA	C1B-C2B	-2.06	1.38	1.43
25	b	605	CLA	C1B-C2B	-2.06	1.38	1.43
39	s	315	LUT	C1-C6	2.06	1.56	1.53
25	B	612	CLA	C1C-C2C	-2.06	1.40	1.44
25	b	612	CLA	C1C-C2C	-2.06	1.40	1.44
39	R	615	LUT	C1-C6	2.06	1.56	1.53
25	C	510	CLA	C1C-C2C	-2.06	1.40	1.44
25	b	607	CLA	C1B-NB	2.06	1.40	1.37
25	S	312	CLA	CHC-C4B	-2.06	1.34	1.39
25	B	616	CLA	C1C-C2C	-2.06	1.40	1.44
25	b	616	CLA	C1C-C2C	-2.06	1.40	1.44
39	S	315	LUT	C26-C27	2.06	1.53	1.50
25	R	603	CLA	C3D-C4D	-2.06	1.39	1.44
25	r	603	CLA	C3D-C4D	-2.06	1.39	1.44
25	R	610	CLA	C3D-C4D	-2.06	1.39	1.44
25	Y	303	CLA	CHD-C1D	-2.06	1.34	1.38
25	Y	313	CLA	CHD-C1D	-2.06	1.34	1.38
25	y	303	CLA	CHD-C1D	-2.06	1.34	1.38
25	y	313	CLA	CHD-C1D	-2.06	1.34	1.38
24	2	603	CHL	O1D-CGD	2.06	1.26	1.21
24	6	603	CHL	O1D-CGD	2.06	1.26	1.21
25	S	313	CLA	CHC-C4B	-2.06	1.34	1.39
25	s	313	CLA	CHC-C4B	-2.06	1.34	1.39
25	c	509	CLA	C1B-NB	2.06	1.40	1.37
25	y	304	CLA	C1B-NB	2.06	1.40	1.37
25	c	510	CLA	C4B-NB	2.06	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	C1C-C2C	-2.06	1.40	1.44
25	C	507	CLA	C1C-C2C	-2.06	1.40	1.44
25	b	607	CLA	C1C-C2C	-2.06	1.40	1.44
25	r	612	CLA	C1B-C2B	-2.06	1.38	1.43
25	2	604	CLA	C1B-C2B	-2.06	1.38	1.43
25	6	604	CLA	C1B-C2B	-2.06	1.38	1.43
25	B	614	CLA	C1B-NB	2.05	1.40	1.37
25	b	614	CLA	C1B-NB	2.05	1.40	1.37
25	n	604	CLA	C3D-C4D	-2.05	1.39	1.44
25	b	612	CLA	C3D-C4D	-2.05	1.39	1.44
25	R	612	CLA	C1B-C2B	-2.05	1.38	1.43
25	S	314	CLA	C1C-C2C	-2.05	1.40	1.44
25	N	611	CLA	CHD-C1D	-2.05	1.34	1.38
25	n	611	CLA	CHD-C1D	-2.05	1.34	1.38
25	s	311	CLA	C4B-NB	2.05	1.40	1.37
25	s	313	CLA	C3D-C4D	-2.05	1.39	1.44
39	s	315	LUT	C26-C27	2.05	1.53	1.50
25	C	503	CLA	C4B-NB	2.05	1.40	1.37
25	D	401	CLA	C1C-C2C	-2.05	1.40	1.44
25	D	402	CLA	C3D-C4D	-2.05	1.39	1.44
25	d	402	CLA	C3D-C4D	-2.05	1.39	1.44
25	c	503	CLA	C1B-NB	2.05	1.40	1.37
25	2	604	CLA	C4C-C3C	-2.05	1.41	1.45
25	6	604	CLA	C4C-C3C	-2.05	1.41	1.45
25	A	405	CLA	C1B-NB	2.05	1.40	1.37
25	a	406	CLA	C1B-NB	2.05	1.40	1.37
25	c	507	CLA	C1B-NB	2.05	1.40	1.37
25	D	401	CLA	C3D-C4D	-2.05	1.39	1.44
25	d	401	CLA	C3D-C4D	-2.05	1.39	1.44
25	n	612	CLA	C1C-C2C	-2.05	1.40	1.44
25	c	506	CLA	C1C-C2C	-2.05	1.40	1.44
25	s	312	CLA	CHC-C4B	-2.04	1.34	1.39
25	S	304	CLA	C1C-C2C	-2.04	1.40	1.44
25	A	405	CLA	C1C-C2C	-2.04	1.40	1.44
25	a	406	CLA	C1C-C2C	-2.04	1.40	1.44
25	C	512	CLA	C3D-C4D	-2.04	1.39	1.44
25	B	604	CLA	C3D-C4D	-2.04	1.39	1.44
25	C	512	CLA	C4B-NB	2.04	1.40	1.37
25	c	512	CLA	C4B-NB	2.04	1.40	1.37
24	2	601	CHL	O1D-CGD	2.04	1.26	1.21
24	6	601	CHL	O1D-CGD	2.04	1.26	1.21
25	C	510	CLA	C3D-C4D	-2.04	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	314	CLA	C3D-C4D	-2.04	1.39	1.44
25	B	612	CLA	C3D-C4D	-2.04	1.39	1.44
25	A	405	CLA	C3D-C4D	-2.04	1.39	1.44
25	a	406	CLA	C3D-C4D	-2.04	1.39	1.44
25	G	610	CLA	CHC-C4B	-2.04	1.34	1.39
25	g	610	CLA	CHC-C4B	-2.04	1.34	1.39
25	Y	303	CLA	C1B-C2B	-2.04	1.38	1.43
25	y	303	CLA	C1B-C2B	-2.04	1.38	1.43
25	Y	314	CLA	C1C-C2C	-2.04	1.40	1.44
25	y	314	CLA	C1C-C2C	-2.04	1.40	1.44
25	B	603	CLA	C1C-C2C	-2.04	1.40	1.44
40	S	317	NEX	C11-C10	-2.04	1.36	1.43
40	s	317	NEX	C11-C10	-2.04	1.36	1.43
25	G	610	CLA	C1B-C2B	-2.04	1.38	1.43
25	g	610	CLA	C1B-C2B	-2.04	1.38	1.43
25	N	612	CLA	C1C-C2C	-2.04	1.40	1.44
25	B	607	CLA	C1B-NB	2.03	1.40	1.37
25	c	510	CLA	C3D-C4D	-2.03	1.39	1.44
25	b	605	CLA	C1C-C2C	-2.03	1.40	1.44
25	D	403	CLA	C1B-C2B	-2.03	1.38	1.43
25	d	403	CLA	C1B-C2B	-2.03	1.38	1.43
24	G	609	CHL	O1D-CGD	2.03	1.26	1.21
25	R	608	CLA	C1C-C2C	-2.03	1.40	1.44
25	s	311	CLA	C1C-C2C	-2.03	1.40	1.44
25	n	604	CLA	C1C-C2C	-2.03	1.40	1.44
25	r	608	CLA	C1C-C2C	-2.03	1.40	1.44
25	R	612	CLA	CHC-C4B	-2.03	1.34	1.39
25	c	510	CLA	C1C-C2C	-2.03	1.40	1.44
40	g	617	NEX	C11-C10	-2.03	1.36	1.43
25	C	503	CLA	C1B-NB	2.03	1.40	1.37
25	r	610	CLA	C3D-C4D	-2.03	1.39	1.44
25	N	614	CLA	C1B-C2B	-2.03	1.38	1.43
25	n	614	CLA	C1B-C2B	-2.03	1.38	1.43
25	N	604	CLA	C3D-C4D	-2.03	1.39	1.44
39	N	616	LUT	C1-C6	2.03	1.56	1.53
25	g	613	CLA	CHD-C1D	-2.03	1.34	1.38
25	G	613	CLA	CHD-C1D	-2.03	1.34	1.38
24	g	608	CHL	O1D-CGD	2.03	1.26	1.21
24	l	301	CHL	O1D-CGD	2.03	1.26	1.21
24	S	308	CHL	O1D-CGD	2.03	1.26	1.21
40	g	617	NEX	C14-C13	2.03	1.40	1.35
25	s	304	CLA	C1C-C2C	-2.03	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	605	CHL	O1D-CGD	2.03	1.26	1.21
39	R	615	LUT	C24-C25	2.03	1.35	1.33
39	r	615	LUT	C24-C25	2.03	1.35	1.33
25	B	605	CLA	C1C-C2C	-2.03	1.40	1.44
25	A	401	CLA	C3D-C4D	-2.02	1.39	1.44
25	a	402	CLA	C3D-C4D	-2.02	1.39	1.44
25	b	604	CLA	C1C-C2C	-2.02	1.40	1.44
39	r	615	LUT	C1-C6	2.02	1.56	1.53
25	B	608	CLA	C3D-C4D	-2.02	1.39	1.44
25	S	303	CLA	C3D-C4D	-2.02	1.39	1.44
25	b	608	CLA	C3D-C4D	-2.02	1.39	1.44
24	g	605	CHL	O1D-CGD	2.02	1.26	1.21
25	r	602	CLA	C1C-C2C	-2.02	1.40	1.44
25	c	509	CLA	C1C-C2C	-2.02	1.40	1.44
25	c	513	CLA	C3D-C4D	-2.02	1.39	1.44
24	R	613	CHL	O1D-CGD	2.02	1.26	1.21
24	R	607	CHL	O1D-CGD	2.02	1.26	1.21
24	r	607	CHL	O1D-CGD	2.02	1.26	1.21
25	R	611	CLA	C1B-C2B	-2.02	1.38	1.43
25	C	506	CLA	C1C-C2C	-2.02	1.40	1.44
28	K	101	BCR	C33-C5	-2.02	1.47	1.50
28	k	101	BCR	C33-C5	-2.02	1.47	1.50
25	s	314	CLA	C1C-C2C	-2.02	1.40	1.44
25	Y	312	CLA	C1C-C2C	-2.02	1.40	1.44
25	y	312	CLA	C1C-C2C	-2.02	1.40	1.44
25	s	314	CLA	C3D-C4D	-2.02	1.39	1.44
24	g	601	CHL	O1D-CGD	2.02	1.26	1.21
24	l	302	CHL	C2C-C3C	2.02	1.38	1.36
24	5	302	CHL	C2C-C3C	2.02	1.38	1.36
25	C	513	CLA	C3D-C4D	-2.02	1.39	1.44
25	R	604	CLA	C3D-C4D	-2.01	1.39	1.44
25	B	605	CLA	C4B-NB	2.01	1.40	1.37
25	S	304	CLA	C3D-C4D	-2.01	1.39	1.44
39	S	315	LUT	C1-C6	2.01	1.56	1.53
24	r	613	CHL	O1D-CGD	2.01	1.26	1.21
25	N	603	CLA	C3D-C4D	-2.01	1.39	1.44
25	n	603	CLA	C3D-C4D	-2.01	1.39	1.44
25	B	602	CLA	C1C-C2C	-2.01	1.40	1.44
25	G	603	CLA	C4B-NB	2.01	1.40	1.37
25	g	603	CLA	C4B-NB	2.01	1.40	1.37
25	S	311	CLA	C1C-C2C	-2.01	1.40	1.44
25	g	613	CLA	C1C-C2C	-2.01	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	302	CHL	O1D-CGD	2.01	1.26	1.21
24	5	302	CHL	O1D-CGD	2.01	1.26	1.21
25	N	612	CLA	C3D-C4D	-2.01	1.39	1.44
25	n	612	CLA	C3D-C4D	-2.01	1.39	1.44
24	n	606	CHL	O1D-CGD	2.01	1.26	1.21
25	B	604	CLA	C1C-C2C	-2.01	1.40	1.44
25	C	513	CLA	C1C-C2C	-2.01	1.40	1.44
25	c	513	CLA	C1C-C2C	-2.01	1.40	1.44
25	C	511	CLA	C1C-C2C	-2.01	1.40	1.44
25	c	511	CLA	C1C-C2C	-2.01	1.40	1.44
25	B	605	CLA	C3D-C4D	-2.01	1.39	1.44
24	s	308	CHL	O1D-CGD	2.01	1.26	1.21
25	C	510	CLA	C4B-NB	2.01	1.40	1.37
25	Y	305	CLA	C1C-C2C	-2.01	1.40	1.44
25	y	305	CLA	C1C-C2C	-2.01	1.40	1.44
25	C	509	CLA	C1B-NB	2.01	1.40	1.37
25	2	605	CLA	C1C-C2C	-2.01	1.40	1.44
25	C	503	CLA	C3D-C4D	-2.00	1.39	1.44
25	c	503	CLA	C3D-C4D	-2.00	1.39	1.44
24	y	310	CHL	O1D-CGD	2.00	1.26	1.21
25	B	615	CLA	C3D-C4D	-2.00	1.39	1.44
24	G	601	CHL	O1D-CGD	2.00	1.26	1.21
25	C	508	CLA	C3D-C4D	-2.00	1.39	1.44
25	c	508	CLA	C3D-C4D	-2.00	1.39	1.44
28	I	101	BCR	C33-C5	-2.00	1.47	1.50
25	B	609	CLA	C3D-C4D	-2.00	1.39	1.44
25	b	609	CLA	C3D-C4D	-2.00	1.39	1.44
25	C	509	CLA	C1C-C2C	-2.00	1.40	1.44
24	G	608	CHL	O1D-CGD	2.00	1.26	1.21
25	2	605	CLA	C1B-NB	2.00	1.40	1.37
25	6	605	CLA	C1B-NB	2.00	1.40	1.37
24	R	605	CHL	O1D-CGD	2.00	1.26	1.21
24	5	301	CHL	O1D-CGD	2.00	1.26	1.21
24	r	605	CHL	O1D-CGD	2.00	1.26	1.21

All (5192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	305	CLA	C4A-NA-C1A	-18.47	98.25	106.68
25	S	305	CLA	C4A-NA-C1A	-18.41	98.28	106.68
32	Y	320	AJP	O09-C08-C10	17.50	145.62	110.20
32	y	320	AJP	O09-C08-C10	17.50	145.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	601	CLA	C4A-NA-C1A	-16.99	98.93	106.68
25	R	601	CLA	C4A-NA-C1A	-16.84	99.00	106.68
32	N	620	AJP	O09-C08-C10	16.74	144.09	110.20
32	n	620	AJP	O09-C08-C10	16.74	144.09	110.20
32	Y	323	AJP	O84-C05-C04	16.73	125.34	110.76
32	y	323	AJP	O84-C05-C04	16.70	125.31	110.76
32	G	618	AJP	O09-C08-C10	16.28	143.15	110.20
32	g	618	AJP	O09-C08-C10	16.28	143.15	110.20
32	S	319	AJP	O09-C08-C10	16.22	143.04	110.20
32	s	319	AJP	O09-C08-C10	16.20	142.99	110.20
32	N	619	AJP	O09-C08-C10	16.17	142.93	110.20
32	n	619	AJP	O09-C08-C10	16.16	142.91	110.20
32	A	412	AJP	O84-C05-C04	16.14	124.82	110.76
32	a	413	AJP	O84-C05-C04	16.14	124.82	110.76
25	R	610	CLA	C4A-NA-C1A	-16.04	99.36	106.68
25	r	610	CLA	C4A-NA-C1A	-16.04	99.36	106.68
32	y	323	AJP	O09-C08-C10	15.99	142.56	110.20
32	Y	323	AJP	O09-C08-C10	15.97	142.53	110.20
25	D	403	CLA	C4A-NA-C1A	-15.97	99.40	106.68
25	d	403	CLA	C4A-NA-C1A	-15.97	99.40	106.68
25	R	611	CLA	C4A-NA-C1A	-15.74	99.50	106.68
25	r	611	CLA	C4A-NA-C1A	-15.74	99.50	106.68
32	Y	321	AJP	O09-C08-C10	15.54	141.66	110.20
32	y	321	AJP	O09-C08-C10	15.52	141.61	110.20
32	Y	322	AJP	O09-C08-C10	15.42	141.42	110.20
32	y	322	AJP	O09-C08-C10	15.40	141.38	110.20
32	y	324	AJP	O84-C05-C04	15.37	124.15	110.76
32	Y	324	AJP	O84-C05-C04	15.36	124.14	110.76
32	g	618	AJP	C80-C20-C15	-15.31	90.60	111.18
32	G	618	AJP	C80-C20-C15	-15.31	90.61	111.18
32	Y	324	AJP	O09-C08-C10	15.25	141.06	110.20
32	y	324	AJP	O09-C08-C10	15.23	141.03	110.20
25	r	603	CLA	C4A-NA-C1A	-15.19	99.75	106.68
25	R	603	CLA	C4A-NA-C1A	-15.07	99.80	106.68
32	G	618	AJP	C80-C20-C21	-14.98	87.00	108.99
32	g	618	AJP	C80-C20-C21	-14.98	87.00	108.99
32	A	412	AJP	O09-C08-C10	14.91	140.38	110.20
32	a	413	AJP	O09-C08-C10	14.89	140.34	110.20
32	Y	321	AJP	O84-C05-C04	14.83	123.68	110.76
32	y	321	AJP	O84-C05-C04	14.83	123.68	110.76
32	B	624	AJP	O09-C08-C10	14.80	140.17	110.20
32	b	624	AJP	O09-C08-C10	14.80	140.17	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C4A-NA-C1A	-14.75	99.95	106.68
32	y	322	AJP	O84-C05-C04	14.73	123.60	110.76
25	C	504	CLA	C4A-NA-C1A	-14.70	99.97	106.68
32	Y	322	AJP	O84-C05-C04	14.68	123.55	110.76
32	B	624	AJP	O84-C05-C04	14.26	123.18	110.76
32	b	624	AJP	O84-C05-C04	14.26	123.18	110.76
25	C	501	CLA	C4A-NA-C1A	-14.07	100.26	106.68
25	c	501	CLA	C4A-NA-C1A	-14.07	100.26	106.68
32	g	618	AJP	O84-C05-C04	13.58	122.59	110.76
32	G	618	AJP	O84-C05-C04	13.57	122.59	110.76
32	Y	323	AJP	O09-C05-C04	-13.54	81.05	108.54
32	y	323	AJP	O09-C05-C04	-13.54	81.05	108.54
32	A	412	AJP	O09-C05-C04	-13.27	81.58	108.54
32	a	413	AJP	O09-C05-C04	-13.27	81.58	108.54
32	y	324	AJP	O09-C05-C04	-13.21	81.71	108.54
32	Y	324	AJP	O09-C05-C04	-13.19	81.76	108.54
24	5	302	CHL	C1B-CHB-C4A	13.12	129.76	121.32
24	l	302	CHL	C1B-CHB-C4A	13.11	129.76	121.32
24	S	302	CHL	C1B-CHB-C4A	13.06	129.72	121.32
32	y	321	AJP	O09-C05-C04	-13.05	82.04	108.54
24	s	302	CHL	C1B-CHB-C4A	13.03	129.71	121.32
32	Y	321	AJP	O09-C05-C04	-13.03	82.08	108.54
24	N	609	CHL	C1B-CHB-C4A	13.00	129.69	121.32
24	n	609	CHL	C1B-CHB-C4A	12.93	129.64	121.32
32	G	618	AJP	C21-C20-C19	12.86	119.53	107.23
32	g	618	AJP	C21-C20-C19	12.86	119.53	107.23
32	Y	322	AJP	O09-C05-C04	-12.74	82.67	108.54
32	y	322	AJP	O09-C05-C04	-12.73	82.68	108.54
32	n	619	AJP	O09-C05-C04	-12.72	82.72	108.54
32	N	619	AJP	O09-C05-C04	-12.71	82.72	108.54
32	S	319	AJP	O84-C05-C04	12.68	121.81	110.76
32	s	319	AJP	O84-C05-C04	12.68	121.81	110.76
32	S	319	AJP	O09-C05-C04	-12.64	82.88	108.54
32	s	319	AJP	O09-C05-C04	-12.64	82.88	108.54
24	r	607	CHL	C1B-CHB-C4A	12.61	129.43	121.32
24	R	607	CHL	C1B-CHB-C4A	12.59	129.42	121.32
24	G	609	CHL	C1B-CHB-C4A	12.50	129.37	121.32
24	g	609	CHL	C1B-CHB-C4A	12.50	129.37	121.32
24	N	606	CHL	C1B-CHB-C4A	12.34	129.26	121.32
24	n	606	CHL	C1B-CHB-C4A	12.33	129.26	121.32
24	G	605	CHL	C1B-CHB-C4A	12.24	129.20	121.32
24	r	606	CHL	C1B-CHB-C4A	12.19	129.16	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	605	CHL	C1B-CHB-C4A	12.17	129.15	121.32
24	S	307	CHL	C1B-CHB-C4A	12.17	129.15	121.32
32	G	618	AJP	C80-C20-C19	-12.15	90.14	110.44
32	g	618	AJP	C80-C20-C19	-12.14	90.15	110.44
24	R	606	CHL	C1B-CHB-C4A	12.14	129.13	121.32
32	B	624	AJP	O09-C05-C04	-12.10	83.97	108.54
32	b	624	AJP	O09-C05-C04	-12.10	83.97	108.54
24	r	605	CHL	C1B-CHB-C4A	12.09	129.10	121.32
24	g	605	CHL	C1B-CHB-C4A	12.08	129.09	121.32
24	s	307	CHL	C1B-CHB-C4A	12.07	129.09	121.32
32	Y	320	AJP	O09-C05-C04	-12.05	84.07	108.54
32	y	320	AJP	O09-C05-C04	-12.05	84.07	108.54
24	S	308	CHL	C1B-CHB-C4A	12.05	129.07	121.32
24	s	308	CHL	C1B-CHB-C4A	12.05	129.07	121.32
32	N	619	AJP	O84-C05-C04	12.04	121.25	110.76
32	n	619	AJP	O84-C05-C04	12.04	121.25	110.76
24	Y	306	CHL	C1B-CHB-C4A	12.03	129.06	121.32
24	R	613	CHL	C1B-CHB-C4A	12.01	129.05	121.32
24	Y	310	CHL	C1B-CHB-C4A	12.01	129.05	121.32
24	y	310	CHL	C1B-CHB-C4A	12.01	129.05	121.32
24	r	613	CHL	C1B-CHB-C4A	11.98	129.03	121.32
24	y	306	CHL	C1B-CHB-C4A	11.98	129.03	121.32
24	S	306	CHL	C1B-CHB-C4A	11.88	128.97	121.32
24	s	306	CHL	C1B-CHB-C4A	11.87	128.96	121.32
24	N	605	CHL	C1B-CHB-C4A	11.86	128.95	121.32
24	n	605	CHL	C1B-CHB-C4A	11.86	128.95	121.32
32	N	620	AJP	O84-C05-C04	11.83	121.07	110.76
32	n	620	AJP	O84-C05-C04	11.83	121.07	110.76
24	N	601	CHL	C1B-CHB-C4A	11.79	128.91	121.32
24	n	601	CHL	C1B-CHB-C4A	11.77	128.90	121.32
24	g	601	CHL	C1B-CHB-C4A	11.77	128.89	121.32
32	G	618	AJP	O09-C05-C04	-11.76	84.66	108.54
32	g	618	AJP	O09-C05-C04	-11.76	84.66	108.54
24	G	601	CHL	C1B-CHB-C4A	11.75	128.88	121.32
32	A	412	AJP	O84-C05-O09	-11.72	81.99	109.88
32	a	413	AJP	O84-C05-O09	-11.72	81.99	109.88
24	y	302	CHL	C1B-CHB-C4A	11.68	128.83	121.32
24	5	301	CHL	C1B-CHB-C4A	11.66	128.82	121.32
24	Y	302	CHL	C1B-CHB-C4A	11.62	128.80	121.32
32	y	321	AJP	C24-C23-C22	11.62	123.23	111.07
32	n	620	AJP	O09-C05-C04	-11.61	84.96	108.54
32	Y	321	AJP	C24-C23-C22	11.60	123.21	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	323	AJP	C24-C23-C22	11.59	123.19	111.07
32	N	620	AJP	O09-C05-C04	-11.58	85.02	108.54
32	y	323	AJP	C24-C23-C22	11.57	123.17	111.07
32	Y	322	AJP	O84-C05-O09	-11.56	82.38	109.88
32	y	322	AJP	O84-C05-O09	-11.55	82.39	109.88
32	Y	324	AJP	O84-C05-O09	-11.53	82.44	109.88
32	y	324	AJP	O84-C05-O09	-11.52	82.46	109.88
24	1	301	CHL	C1B-CHB-C4A	11.50	128.72	121.32
32	B	624	AJP	O84-C05-O09	-11.48	82.55	109.88
32	b	624	AJP	O84-C05-O09	-11.48	82.55	109.88
32	B	624	AJP	C24-C23-C22	11.43	123.03	111.07
32	b	624	AJP	C24-C23-C22	11.43	123.03	111.07
24	Y	309	CHL	C1B-CHB-C4A	11.42	128.67	121.32
24	y	309	CHL	C1B-CHB-C4A	11.42	128.67	121.32
32	g	618	AJP	O84-C05-O09	-11.41	82.73	109.88
32	G	618	AJP	O84-C05-O09	-11.41	82.74	109.88
25	C	511	CLA	C4A-NA-C1A	-11.37	101.49	106.68
24	g	606	CHL	C1B-CHB-C4A	11.30	128.59	121.32
32	y	320	AJP	C03-C02-C85	11.29	122.28	108.59
24	n	608	CHL	C1B-CHB-C4A	11.28	128.58	121.32
32	Y	320	AJP	C03-C02-C85	11.27	122.26	108.59
24	G	606	CHL	C1B-CHB-C4A	11.26	128.57	121.32
25	c	511	CLA	C4A-NA-C1A	-11.26	101.54	106.68
24	N	608	CHL	C1B-CHB-C4A	11.22	128.54	121.32
24	g	608	CHL	C1B-CHB-C4A	11.19	128.52	121.32
24	G	608	CHL	C1B-CHB-C4A	11.19	128.52	121.32
24	y	308	CHL	C1B-CHB-C4A	10.90	128.34	121.32
24	Y	308	CHL	C1B-CHB-C4A	10.85	128.30	121.32
32	A	412	AJP	C24-C23-C22	10.70	122.27	111.07
32	Y	321	AJP	O84-C05-O09	-10.67	84.48	109.88
32	y	321	AJP	O84-C05-O09	-10.67	84.49	109.88
32	a	413	AJP	C24-C23-C22	10.67	122.23	111.07
32	S	319	AJP	C24-C23-C22	10.59	122.14	111.07
32	s	319	AJP	C24-C23-C22	10.59	122.14	111.07
32	y	323	AJP	O84-C05-O09	-10.58	84.71	109.88
24	g	607	CHL	C1B-CHB-C4A	10.57	128.12	121.32
32	Y	323	AJP	O84-C05-O09	-10.57	84.73	109.88
32	N	619	AJP	O84-C05-O09	-10.53	84.81	109.88
24	G	607	CHL	C1B-CHB-C4A	10.53	128.10	121.32
32	n	619	AJP	O84-C05-O09	-10.52	84.84	109.88
32	y	324	AJP	C03-C02-C85	10.50	121.33	108.59
32	S	319	AJP	O84-C05-O09	-10.50	84.90	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	s	319	AJP	O84-C05-O09	-10.50	84.90	109.88
32	Y	324	AJP	C03-C02-C85	10.49	121.31	108.59
32	n	620	AJP	O84-C05-O09	-10.46	84.98	109.88
32	N	620	AJP	O84-C05-O09	-10.46	84.99	109.88
24	N	607	CHL	C1B-CHB-C4A	10.45	128.04	121.32
25	S	313	CLA	C4A-NA-C1A	-10.44	101.92	106.68
25	s	313	CLA	C4A-NA-C1A	-10.44	101.92	106.68
24	n	607	CHL	C1B-CHB-C4A	10.41	128.02	121.32
24	6	603	CHL	C1B-CHB-C4A	10.32	127.96	121.32
24	2	603	CHL	C1B-CHB-C4A	10.26	127.92	121.32
24	2	601	CHL	C1B-CHB-C4A	10.23	127.90	121.32
25	2	602	CLA	C4A-NA-C1A	10.16	111.31	106.68
25	6	602	CLA	C4A-NA-C1A	10.16	111.31	106.68
24	6	601	CHL	C1B-CHB-C4A	10.11	127.83	121.32
32	g	618	AJP	C24-C23-C22	9.99	121.52	111.07
32	G	618	AJP	C24-C23-C22	9.94	121.47	111.07
25	S	311	CLA	C4A-NA-C1A	-9.86	102.18	106.68
25	s	311	CLA	C4A-NA-C1A	-9.86	102.18	106.68
40	r	617	NEX	C15-C14-C13	-9.74	113.62	127.28
40	R	617	NEX	C15-C14-C13	-9.73	113.63	127.28
25	R	611	CLA	C4D-CHA-C1A	-9.72	109.64	121.24
25	r	611	CLA	C4D-CHA-C1A	-9.72	109.64	121.24
32	Y	320	AJP	O84-C05-C04	9.66	119.17	110.76
32	y	320	AJP	O84-C05-C04	9.66	119.17	110.76
32	g	618	AJP	C21-C20-C15	9.60	123.00	110.10
32	G	618	AJP	C21-C20-C15	9.58	122.97	110.10
32	N	620	AJP	C26-O31-C30	9.55	123.71	113.13
32	n	620	AJP	C26-O31-C30	9.55	123.71	113.13
32	n	619	AJP	C03-C02-C85	9.55	120.17	108.59
32	N	619	AJP	C03-C02-C85	9.54	120.16	108.59
32	Y	323	AJP	C26-O31-C30	9.48	123.63	113.13
32	y	323	AJP	C26-O31-C30	9.48	123.63	113.13
32	Y	320	AJP	O84-C05-O09	-9.35	87.64	109.88
32	y	320	AJP	O84-C05-O09	-9.35	87.64	109.88
32	Y	322	AJP	C03-C02-C85	9.23	119.79	108.59
32	y	322	AJP	C03-C02-C85	9.20	119.75	108.59
32	Y	320	AJP	O31-C30-C32	9.17	121.53	106.83
32	y	320	AJP	O31-C30-C32	9.16	121.53	106.83
32	b	624	AJP	C03-C02-C85	9.09	119.61	108.59
32	Y	324	AJP	C24-C23-C22	9.08	120.57	111.07
32	s	319	AJP	C03-C02-C85	9.08	119.61	108.59
32	y	324	AJP	C24-C23-C22	9.07	120.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	624	AJP	C03-C02-C85	9.06	119.58	108.59
32	S	319	AJP	C03-C02-C85	9.05	119.57	108.59
40	g	617	NEX	C11-C10-C9	-9.03	114.61	127.28
25	N	614	CLA	C4A-NA-C1A	-8.96	102.59	106.68
25	g	610	CLA	C4A-NA-C1A	-8.90	102.62	106.68
32	Y	321	AJP	C03-C02-C85	8.88	119.36	108.59
32	y	321	AJP	C03-C02-C85	8.88	119.36	108.59
40	G	617	NEX	C11-C10-C9	-8.87	114.84	127.28
32	Y	322	AJP	C24-C23-C22	8.83	120.31	111.07
32	y	322	AJP	C24-C23-C22	8.83	120.31	111.07
25	G	610	CLA	C4A-NA-C1A	-8.81	102.66	106.68
25	n	614	CLA	C4A-NA-C1A	-8.81	102.66	106.68
32	N	620	AJP	C24-C23-C22	8.75	120.23	111.07
32	n	620	AJP	C24-C23-C22	8.75	120.23	111.07
32	Y	324	AJP	C26-O31-C30	8.73	122.80	113.13
32	y	324	AJP	C26-O31-C30	8.73	122.80	113.13
32	n	620	AJP	O09-C05-C06	-8.54	93.20	104.56
32	N	620	AJP	O09-C05-C06	-8.51	93.25	104.56
32	N	619	AJP	C24-C23-C22	8.49	119.95	111.07
32	n	619	AJP	C24-C23-C22	8.49	119.95	111.07
24	N	607	CHL	O2D-CGD-CBD	8.25	120.01	110.95
24	n	607	CHL	O2D-CGD-CBD	8.25	120.01	110.95
27	A	403	PHO	O2D-CGD-CBD	8.23	119.99	110.95
27	a	404	PHO	O2D-CGD-CBD	8.23	119.99	110.95
27	A	404	PHO	O2D-CGD-CBD	8.23	119.99	110.95
24	Y	308	CHL	O2D-CGD-CBD	8.21	119.96	110.95
24	y	308	CHL	O2D-CGD-CBD	8.21	119.96	110.95
27	a	405	PHO	O2D-CGD-CBD	8.18	119.94	110.95
32	A	412	AJP	C03-C02-C85	8.09	118.40	108.59
32	a	413	AJP	C03-C02-C85	8.09	118.40	108.59
40	R	617	NEX	C35-C34-C33	-7.97	116.10	127.28
40	r	617	NEX	C35-C34-C33	-7.97	116.10	127.28
24	G	609	CHL	O2D-CGD-CBD	7.97	119.70	110.95
24	g	609	CHL	O2D-CGD-CBD	7.95	119.69	110.95
32	G	618	AJP	C03-C02-C85	7.94	118.22	108.59
32	g	618	AJP	C03-C02-C85	7.93	118.21	108.59
25	Y	314	CLA	C4A-NA-C1A	-7.86	103.09	106.68
25	y	314	CLA	C4A-NA-C1A	-7.86	103.09	106.68
24	G	607	CHL	O2D-CGD-CBD	7.76	119.47	110.95
24	g	607	CHL	O2D-CGD-CBD	7.75	119.46	110.95
25	N	604	CLA	C4A-NA-C1A	-7.71	103.16	106.68
25	n	604	CLA	C4A-NA-C1A	-7.63	103.20	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	413	AJP	O40-C39-C38	7.56	123.32	109.70
32	A	412	AJP	O40-C39-C38	7.54	123.30	109.70
40	y	318	NEX	C31-C30-C29	-7.51	116.75	127.28
40	Y	318	NEX	C31-C30-C29	-7.51	116.75	127.28
32	N	620	AJP	C03-C02-C85	7.47	117.65	108.59
24	G	606	CHL	O2D-CGD-CBD	7.46	119.14	110.95
24	g	606	CHL	O2D-CGD-CBD	7.45	119.13	110.95
25	g	613	CLA	C4A-NA-C1A	-7.44	103.28	106.68
32	n	620	AJP	C03-C02-C85	7.43	117.60	108.59
32	s	319	AJP	C26-O25-C23	7.42	127.68	115.27
32	S	319	AJP	C26-O25-C23	7.41	127.67	115.27
40	S	317	NEX	O24-C25-C24	7.33	120.36	113.49
25	G	613	CLA	C4A-NA-C1A	-7.33	103.34	106.68
40	s	317	NEX	O24-C25-C24	7.31	120.34	113.49
40	G	617	NEX	C31-C30-C29	-7.15	117.25	127.28
40	g	617	NEX	C27-C28-C29	-7.13	114.47	125.53
25	R	612	CLA	C4A-NA-C1A	-7.12	103.43	106.68
32	N	619	AJP	C26-O31-C30	7.09	120.98	113.13
40	g	617	NEX	C31-C30-C29	-7.08	117.34	127.28
40	G	617	NEX	C27-C28-C29	-7.06	114.57	125.53
25	S	304	CLA	C4A-NA-C1A	-7.04	103.47	106.68
25	s	304	CLA	C4A-NA-C1A	-7.04	103.47	106.68
32	n	619	AJP	C26-O31-C30	7.03	120.92	113.13
24	2	603	CHL	C4D-CHA-CBD	-7.02	101.89	108.97
25	r	612	CLA	C4A-NA-C1A	-7.01	103.48	106.68
40	n	617	NEX	O24-C25-C24	7.01	120.06	113.49
24	6	603	CHL	C4D-CHA-CBD	-6.99	101.92	108.97
24	y	307	CHL	C1B-CHB-C4A	6.97	125.81	121.32
40	N	617	NEX	O24-C25-C24	6.97	120.02	113.49
32	S	319	AJP	C29-C28-C27	6.97	120.71	110.67
32	s	319	AJP	C29-C28-C27	6.97	120.71	110.67
24	Y	307	CHL	C1B-CHB-C4A	6.96	125.80	121.32
25	d	401	CLA	C4A-NA-C1A	-6.95	103.51	106.68
40	G	617	NEX	O24-C25-C24	6.94	120.00	113.49
25	D	401	CLA	C4A-NA-C1A	-6.94	103.51	106.68
40	g	617	NEX	O24-C25-C24	6.91	119.97	113.49
24	N	601	CHL	O2D-CGD-CBD	6.86	118.48	110.95
24	1	302	CHL	O2D-CGD-CBD	6.80	118.41	110.95
24	n	601	CHL	O2D-CGD-CBD	6.78	118.40	110.95
24	5	302	CHL	O2D-CGD-CBD	6.77	118.39	110.95
32	Y	324	AJP	C26-O25-C23	6.77	126.59	115.27
32	y	324	AJP	C26-O25-C23	6.75	126.56	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	310	CHL	O2D-CGD-CBD	6.74	118.35	110.95
24	r	606	CHL	O2D-CGD-CBD	6.72	118.33	110.95
24	R	606	CHL	O2D-CGD-CBD	6.72	118.33	110.95
24	2	603	CHL	OBD-CAD-C3D	6.71	138.36	127.89
24	6	603	CHL	OBD-CAD-C3D	6.71	138.36	127.89
24	Y	310	CHL	O2D-CGD-CBD	6.70	118.31	110.95
25	c	504	CLA	CHB-C1B-NB	-6.69	114.01	124.05
25	C	504	CLA	CHB-C1B-NB	-6.69	114.01	124.05
24	Y	306	CHL	O2D-CGD-CBD	6.68	118.29	110.95
24	y	306	CHL	O2D-CGD-CBD	6.68	118.29	110.95
25	B	605	CLA	C4A-NA-C1A	-6.67	103.63	106.68
25	R	603	CLA	CHB-C1B-NB	-6.66	114.06	124.05
32	B	624	AJP	O50-C45-C46	6.65	120.14	109.99
32	b	624	AJP	O50-C45-C46	6.65	120.14	109.99
25	R	610	CLA	CHB-C1B-NB	-6.65	114.08	124.05
32	Y	320	AJP	C05-C06-C07	6.64	113.15	103.37
32	y	320	AJP	C05-C06-C07	6.64	113.15	103.37
25	r	603	CLA	CHB-C1B-NB	-6.64	114.09	124.05
25	r	610	CLA	CHB-C1B-NB	-6.63	114.11	124.05
32	Y	323	AJP	O09-C05-C06	-6.60	95.78	104.56
32	y	323	AJP	O09-C05-C06	-6.60	95.78	104.56
32	Y	320	AJP	C03-C04-C05	-6.57	101.63	111.93
32	y	320	AJP	C03-C04-C05	-6.57	101.63	111.93
32	g	618	AJP	O09-C05-C06	-6.55	95.85	104.56
32	G	618	AJP	O09-C05-C06	-6.54	95.86	104.56
25	b	605	CLA	C4A-NA-C1A	-6.53	103.70	106.68
24	r	613	CHL	O2D-CGD-CBD	6.52	118.11	110.95
24	g	605	CHL	O2D-CGD-CBD	6.52	118.11	110.95
40	N	617	NEX	C15-C14-C13	-6.51	118.14	127.28
25	S	305	CLA	CHB-C1B-NB	-6.51	114.28	124.05
25	s	305	CLA	CHB-C1B-NB	-6.51	114.28	124.05
24	R	613	CHL	O2D-CGD-CBD	6.50	118.09	110.95
40	n	617	NEX	C15-C14-C13	-6.50	118.17	127.28
24	G	605	CHL	O2D-CGD-CBD	6.49	118.08	110.95
24	n	608	CHL	O2D-CGD-CBD	6.48	118.06	110.95
41	R	616	XAT	C35-C34-C33	-6.48	118.20	127.28
41	r	616	XAT	C35-C34-C33	-6.48	118.20	127.28
25	c	509	CLA	C4A-NA-C1A	-6.47	103.72	106.68
24	N	608	CHL	O2D-CGD-CBD	6.45	118.04	110.95
32	N	619	AJP	C26-O25-C23	6.45	126.05	115.27
32	n	619	AJP	C26-O25-C23	6.45	126.05	115.27
24	N	609	CHL	O2D-CGD-CBD	6.45	118.03	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	605	CHL	O2D-CGD-CBD	6.44	118.02	110.95
24	r	605	CHL	O2D-CGD-CBD	6.44	118.02	110.95
24	n	609	CHL	O2D-CGD-CBD	6.44	118.02	110.95
25	D	403	CLA	CHB-C1B-NB	-6.43	114.40	124.05
25	d	403	CLA	CHB-C1B-NB	-6.43	114.40	124.05
32	G	618	AJP	C15-C20-C19	6.43	117.45	108.51
25	C	509	CLA	C4A-NA-C1A	-6.42	103.75	106.68
32	g	618	AJP	C15-C20-C19	6.41	117.42	108.51
25	g	604	CLA	C4A-NA-C1A	-6.40	103.76	106.68
25	c	501	CLA	CHB-C1B-NB	-6.39	114.46	124.05
25	G	604	CLA	C4A-NA-C1A	-6.38	103.77	106.68
25	C	501	CLA	CHB-C1B-NB	-6.38	114.48	124.05
24	N	605	CHL	O2D-CGD-CBD	6.37	117.95	110.95
24	S	307	CHL	O2D-CGD-CBD	6.35	117.92	110.95
24	s	307	CHL	O2D-CGD-CBD	6.35	117.92	110.95
32	A	412	AJP	O53-C46-C45	6.35	125.19	110.08
32	a	413	AJP	O53-C46-C45	6.34	125.19	110.08
24	n	605	CHL	O2D-CGD-CBD	6.34	117.91	110.95
24	S	308	CHL	O2D-CGD-CBD	6.34	117.91	110.95
25	B	601	CLA	C4A-NA-C1A	-6.32	103.79	106.68
32	n	620	AJP	C01-C02-C85	6.30	120.73	111.03
32	Y	323	AJP	C01-C02-C85	6.29	120.72	111.03
32	y	323	AJP	C01-C02-C85	6.29	120.72	111.03
25	C	502	CLA	C4A-NA-C1A	-6.29	103.81	106.68
25	c	502	CLA	C4A-NA-C1A	-6.29	103.81	106.68
32	N	620	AJP	C01-C02-C85	6.29	120.71	111.03
25	R	602	CLA	C4A-NA-C1A	-6.29	103.81	106.68
25	r	602	CLA	C4A-NA-C1A	-6.29	103.81	106.68
24	s	308	CHL	O2D-CGD-CBD	6.28	117.85	110.95
25	b	601	CLA	C4A-NA-C1A	-6.24	103.83	106.68
24	Y	302	CHL	O2D-CGD-CBD	6.22	117.78	110.95
25	B	614	CLA	C4A-NA-C1A	-6.22	103.84	106.68
32	A	412	AJP	O44-C45-O50	6.22	121.79	108.92
25	6	605	CLA	C4A-NA-C1A	-6.22	103.84	106.68
32	Y	321	AJP	O31-C26-C27	6.21	123.13	110.37
25	r	601	CLA	CHB-C1B-NB	-6.21	114.74	124.05
25	2	605	CLA	C4A-NA-C1A	-6.20	103.85	106.68
25	b	614	CLA	C4A-NA-C1A	-6.20	103.85	106.68
32	y	321	AJP	O31-C26-C27	6.20	123.11	110.37
24	S	302	CHL	O2D-CGD-CBD	6.20	117.76	110.95
32	Y	322	AJP	O25-C23-C24	6.20	121.69	109.64
32	y	322	AJP	O25-C23-C24	6.20	121.69	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	302	CHL	O2D-CGD-CBD	6.19	117.75	110.95
32	G	618	AJP	C20-C15-C16	-6.19	106.14	112.43
24	G	601	CHL	O2D-CGD-CBD	6.19	117.75	110.95
32	A	412	AJP	O44-C45-C46	6.19	123.32	108.09
24	s	302	CHL	O2D-CGD-CBD	6.19	117.74	110.95
32	a	413	AJP	O44-C45-C46	6.18	123.30	108.09
32	a	413	AJP	O44-C45-O50	6.18	121.71	108.92
25	R	601	CLA	CHB-C1B-NB	-6.18	114.78	124.05
25	c	508	CLA	C4A-NA-C1A	-6.18	103.86	106.68
32	g	618	AJP	C20-C15-C16	-6.17	106.17	112.43
24	R	607	CHL	O2D-CGD-CBD	6.16	117.71	110.95
24	g	601	CHL	O2D-CGD-CBD	6.14	117.69	110.95
24	r	607	CHL	O2D-CGD-CBD	6.14	117.69	110.95
25	C	508	CLA	C4A-NA-C1A	-6.13	103.88	106.68
25	n	613	CLA	C4A-NA-C1A	-6.12	103.89	106.68
32	A	412	AJP	O70-C69-C68	6.11	120.71	109.70
32	a	413	AJP	O70-C69-C68	6.11	120.71	109.70
32	N	619	AJP	O25-C23-C24	6.11	121.51	109.64
32	n	619	AJP	O25-C23-C24	6.11	121.51	109.64
25	N	613	CLA	C4A-NA-C1A	-6.10	103.90	106.68
32	A	412	AJP	C01-C02-C85	6.10	120.42	111.03
32	a	413	AJP	C01-C02-C85	6.10	120.42	111.03
25	B	609	CLA	C4A-NA-C1A	-6.08	103.90	106.68
25	b	609	CLA	C4A-NA-C1A	-6.08	103.90	106.68
32	B	624	AJP	O44-C45-O50	6.08	121.49	108.92
32	b	624	AJP	O44-C45-O50	6.08	121.49	108.92
41	R	616	XAT	O24-C25-C24	6.06	119.17	113.49
41	r	616	XAT	O24-C25-C24	6.06	119.17	113.49
32	G	618	AJP	C29-C28-C27	6.05	119.39	110.67
32	g	618	AJP	C29-C28-C27	6.04	119.37	110.67
24	s	306	CHL	O2D-CGD-CBD	6.04	117.58	110.95
24	g	608	CHL	O2D-CGD-CBD	6.02	117.56	110.95
24	S	306	CHL	O2D-CGD-CBD	6.00	117.54	110.95
24	2	603	CHL	CBC-CAC-C3C	-6.00	104.28	112.87
24	6	603	CHL	CBC-CAC-C3C	-6.00	104.28	112.87
25	S	309	CLA	C4A-NA-C1A	-5.99	103.95	106.68
24	G	608	CHL	O2D-CGD-CBD	5.99	117.53	110.95
32	g	618	AJP	C01-C02-C85	5.98	120.23	111.03
25	s	309	CLA	C4A-NA-C1A	-5.97	103.95	106.68
32	G	618	AJP	C01-C02-C85	5.97	120.21	111.03
25	c	503	CLA	C4A-NA-C1A	-5.96	103.96	106.68
32	A	412	AJP	O60-C59-C58	5.96	120.44	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	413	AJP	O60-C59-C58	5.96	120.43	109.70
24	n	606	CHL	O2D-CGD-CBD	5.95	117.49	110.95
32	Y	320	AJP	C28-C29-C30	-5.95	101.12	111.19
32	y	320	AJP	C28-C29-C30	-5.95	101.12	111.19
24	N	606	CHL	O2D-CGD-CBD	5.94	117.47	110.95
32	y	321	AJP	C05-C06-C07	5.91	112.07	103.37
25	C	503	CLA	C4A-NA-C1A	-5.89	103.99	106.68
32	y	324	AJP	O25-C23-C24	5.89	121.09	109.64
32	Y	321	AJP	C05-C06-C07	5.89	112.04	103.37
32	B	624	AJP	O74-C67-C68	5.89	124.25	110.38
32	b	624	AJP	O74-C67-C68	5.89	124.25	110.38
25	2	602	CLA	C4B-CHC-C1C	-5.88	112.43	126.25
25	6	602	CLA	C4D-CHA-C1A	-5.87	114.24	121.24
32	s	319	AJP	C01-C02-C85	5.87	120.07	111.03
32	B	624	AJP	O44-C37-C38	5.87	122.14	107.23
32	b	624	AJP	O44-C37-C38	5.87	122.14	107.23
32	Y	324	AJP	O25-C23-C24	5.87	121.04	109.64
32	S	319	AJP	C01-C02-C85	5.86	120.05	111.03
25	6	602	CLA	C4B-CHC-C1C	-5.86	112.47	126.25
25	2	602	CLA	C4D-CHA-C1A	-5.85	114.27	121.24
40	R	617	NEX	O24-C25-C24	5.84	118.97	113.49
40	r	617	NEX	O24-C25-C24	5.84	118.97	113.49
32	A	412	AJP	C05-C06-C07	5.84	111.97	103.37
32	a	413	AJP	C05-C06-C07	5.84	111.97	103.37
32	y	324	AJP	C05-C06-C07	5.83	111.96	103.37
32	Y	324	AJP	C05-C06-C07	5.82	111.94	103.37
32	n	619	AJP	O09-C05-C06	-5.79	96.86	104.56
32	B	624	AJP	O73-C68-C69	5.78	123.56	109.32
32	b	624	AJP	O73-C68-C69	5.78	123.56	109.32
32	N	619	AJP	O09-C05-C06	-5.78	96.88	104.56
24	5	301	CHL	O2D-CGD-CBD	5.77	117.29	110.95
32	a	413	AJP	O53-C46-C47	5.77	123.97	110.38
24	1	301	CHL	O2D-CGD-CBD	5.77	117.28	110.95
32	A	412	AJP	O53-C46-C47	5.77	123.97	110.38
32	Y	320	AJP	C29-C28-C27	5.76	118.96	110.67
32	y	320	AJP	C29-C28-C27	5.76	118.96	110.67
32	B	624	AJP	C27-C28-C29	5.71	122.63	109.68
32	b	624	AJP	C27-C28-C29	5.71	122.63	109.68
32	A	412	AJP	O31-C26-C27	5.69	122.07	110.37
32	a	413	AJP	O31-C26-C27	5.69	122.07	110.37
33	A	413	BCT	O2-C-O1	5.69	134.22	119.68
33	a	414	BCT	O2-C-O1	5.69	134.22	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	323	AJP	C03-C02-C85	5.66	115.46	108.59
32	G	618	AJP	C05-C06-C07	5.66	111.70	103.37
32	g	618	AJP	C05-C06-C07	5.65	111.70	103.37
32	Y	323	AJP	C03-C02-C85	5.65	115.45	108.59
32	B	624	AJP	C05-C06-C07	5.65	111.69	103.37
32	b	624	AJP	C05-C06-C07	5.65	111.69	103.37
25	B	611	CLA	C4A-NA-C1A	-5.65	104.10	106.68
25	b	611	CLA	C4A-NA-C1A	-5.65	104.10	106.68
32	y	322	AJP	C05-C06-C07	5.63	111.66	103.37
32	Y	322	AJP	C05-C06-C07	5.61	111.64	103.37
32	N	619	AJP	O77-C28-C27	5.61	121.78	110.15
32	n	619	AJP	O77-C28-C27	5.61	121.77	110.15
25	R	610	CLA	C3B-C4B-NB	-5.58	105.55	110.53
25	r	610	CLA	C3B-C4B-NB	-5.58	105.55	110.53
25	r	601	CLA	C2A-C3A-C4A	-5.57	92.87	101.87
32	S	319	AJP	C05-C06-C07	5.57	111.57	103.37
32	s	319	AJP	C05-C06-C07	5.57	111.57	103.37
25	R	601	CLA	C2A-C3A-C4A	-5.56	92.88	101.87
32	N	619	AJP	C05-C06-C07	5.56	111.56	103.37
32	n	619	AJP	C05-C06-C07	5.56	111.56	103.37
32	N	620	AJP	O31-C26-C27	5.55	121.78	110.37
32	n	620	AJP	O31-C26-C27	5.55	121.78	110.37
32	y	324	AJP	O31-C26-C27	5.54	121.75	110.37
32	Y	324	AJP	O31-C26-C27	5.53	121.74	110.37
32	Y	324	AJP	O77-C28-C27	5.52	121.59	110.15
32	y	324	AJP	O77-C28-C27	5.52	121.59	110.15
25	G	603	CLA	C4A-NA-C1A	-5.52	104.16	106.68
25	B	612	CLA	C4A-NA-C1A	-5.51	104.17	106.68
25	b	612	CLA	C4A-NA-C1A	-5.51	104.17	106.68
24	Y	307	CHL	O2D-CGD-CBD	5.51	117.00	110.95
24	y	307	CHL	O2D-CGD-CBD	5.51	117.00	110.95
32	B	624	AJP	C01-C02-C85	5.50	119.50	111.03
32	b	624	AJP	C01-C02-C85	5.50	119.50	111.03
32	y	320	AJP	C29-C30-C32	5.50	122.69	112.50
25	g	603	CLA	C4A-NA-C1A	-5.50	104.17	106.68
39	N	615	LUT	C18-C5-C6	5.49	130.48	124.48
39	n	615	LUT	C18-C5-C6	5.49	130.48	124.48
32	B	624	AJP	C03-C04-C05	-5.49	103.33	111.93
32	Y	320	AJP	C29-C30-C32	5.48	122.65	112.50
32	b	624	AJP	C03-C04-C05	-5.48	103.35	111.93
32	Y	323	AJP	O77-C28-C27	5.48	121.50	110.15
32	y	323	AJP	O77-C28-C27	5.48	121.50	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	612	CLA	C1D-ND-C4D	-5.48	102.47	106.31
25	g	612	CLA	C1D-ND-C4D	-5.48	102.47	106.31
32	Y	321	AJP	O25-C23-C24	5.46	120.25	109.64
32	n	620	AJP	O77-C28-C27	5.46	121.45	110.15
32	y	321	AJP	O25-C23-C24	5.46	120.25	109.64
40	r	617	NEX	C11-C12-C13	-5.44	111.46	126.36
32	N	620	AJP	O77-C28-C27	5.43	121.40	110.15
32	a	413	AJP	O74-C67-C66	5.43	123.18	110.38
32	A	412	AJP	O74-C67-C66	5.43	123.17	110.38
40	R	617	NEX	C11-C12-C13	-5.42	111.49	126.36
32	Y	323	AJP	O31-C26-C27	5.42	121.50	110.37
32	y	323	AJP	O31-C26-C27	5.42	121.50	110.37
32	G	618	AJP	C26-O31-C30	5.42	119.13	113.13
24	Y	309	CHL	O2D-CGD-CBD	5.40	116.88	110.95
32	g	618	AJP	C26-O31-C30	5.39	119.10	113.13
25	r	611	CLA	C3B-C4B-NB	-5.38	105.72	110.53
25	y	313	CLA	C1D-ND-C4D	-5.38	102.53	106.31
25	C	505	CLA	O2D-CGD-CBD	5.38	120.64	111.23
25	c	505	CLA	O2D-CGD-CBD	5.38	120.64	111.23
25	R	611	CLA	C3B-C4B-NB	-5.38	105.73	110.53
25	Y	313	CLA	C1D-ND-C4D	-5.37	102.54	106.31
24	y	309	CHL	O2D-CGD-CBD	5.37	116.85	110.95
24	2	603	CHL	OBD-CAD-CBD	-5.35	117.97	125.82
25	g	611	CLA	O2D-CGD-CBD	5.35	120.58	111.23
32	B	624	AJP	O40-C39-C41	5.35	119.69	106.44
32	b	624	AJP	O40-C39-C41	5.35	119.69	106.44
32	S	319	AJP	O09-C05-C06	-5.34	97.46	104.56
32	s	319	AJP	O09-C05-C06	-5.34	97.46	104.56
32	B	624	AJP	O25-C26-C27	5.34	121.23	108.09
32	b	624	AJP	O25-C26-C27	5.34	121.23	108.09
24	2	601	CHL	C4D-CHA-CBD	-5.34	103.58	108.97
24	6	601	CHL	C4D-CHA-CBD	-5.34	103.58	108.97
25	b	605	CLA	O2D-CGD-CBD	5.34	120.56	111.23
25	R	608	CLA	C4A-NA-C1A	-5.33	104.25	106.68
25	r	608	CLA	C4A-NA-C1A	-5.33	104.25	106.68
24	6	603	CHL	OBD-CAD-CBD	-5.33	118.00	125.82
40	R	617	NEX	C27-C28-C29	-5.32	117.27	125.53
24	2	601	CHL	O2D-CGD-CBD	5.32	116.80	110.95
25	G	611	CLA	O2D-CGD-CBD	5.32	120.53	111.23
25	B	605	CLA	O2D-CGD-CBD	5.32	120.53	111.23
32	N	620	AJP	C26-O25-C23	5.32	124.16	115.27
32	n	620	AJP	C26-O25-C23	5.32	124.16	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	322	AJP	C01-C02-C85	5.31	119.21	111.03
24	6	601	CHL	O2D-CGD-CBD	5.31	116.78	110.95
40	r	617	NEX	C27-C28-C29	-5.30	117.30	125.53
24	R	613	CHL	CAA-C2A-C3A	-5.30	104.08	116.23
24	r	613	CHL	CAA-C2A-C3A	-5.30	104.08	116.23
32	B	624	AJP	O60-C59-C61	5.30	119.57	106.44
32	b	624	AJP	O60-C59-C61	5.30	119.57	106.44
25	S	304	CLA	O2D-CGD-CBD	5.30	120.49	111.23
25	s	304	CLA	O2D-CGD-CBD	5.30	120.49	111.23
32	a	413	AJP	C26-O25-C23	5.30	124.12	115.27
39	G	616	LUT	C18-C5-C6	5.29	130.26	124.48
39	g	616	LUT	C18-C5-C6	5.29	130.26	124.48
24	Y	308	CHL	C4D-CHA-CBD	-5.29	103.63	108.97
40	s	317	NEX	C27-C28-C29	-5.28	117.34	125.53
32	Y	320	AJP	O31-C26-C27	5.28	121.21	110.37
32	A	412	AJP	C26-O25-C23	5.27	124.08	115.27
40	S	317	NEX	C27-C28-C29	-5.27	117.35	125.53
32	Y	322	AJP	C01-C02-C85	5.27	119.14	111.03
24	y	308	CHL	C4D-CHA-CBD	-5.27	103.66	108.97
32	S	319	AJP	O25-C23-C24	5.27	119.88	109.64
32	s	319	AJP	O25-C23-C24	5.27	119.88	109.64
25	R	611	CLA	CHD-C1D-C2D	5.27	136.44	125.49
25	B	614	CLA	O2D-CGD-CBD	5.26	120.43	111.23
25	b	614	CLA	O2D-CGD-CBD	5.26	120.43	111.23
32	y	320	AJP	O31-C26-C27	5.26	121.18	110.37
25	N	612	CLA	C4D-CHA-C1A	-5.23	115.00	121.24
25	r	611	CLA	CHD-C1D-C2D	5.23	136.37	125.49
32	y	322	AJP	O77-C28-C27	5.22	120.96	110.15
32	Y	322	AJP	O77-C28-C27	5.22	120.96	110.15
41	r	616	XAT	O4-C5-C4	5.21	118.38	113.49
32	y	320	AJP	O82-C10-C08	5.21	125.77	111.19
32	Y	320	AJP	O82-C10-C08	5.21	125.76	111.19
25	n	612	CLA	C4D-CHA-C1A	-5.21	115.03	121.24
41	R	616	XAT	O4-C5-C4	5.20	118.36	113.49
25	G	614	CLA	C4A-NA-C1A	-5.18	104.31	106.68
25	g	614	CLA	C4A-NA-C1A	-5.18	104.31	106.68
25	b	608	CLA	C4A-NA-C1A	-5.17	104.32	106.68
25	2	604	CLA	C4D-CHA-C1A	-5.17	115.08	121.24
25	6	604	CLA	C4D-CHA-C1A	-5.17	115.08	121.24
25	S	305	CLA	C4D-CHA-C1A	-5.16	115.09	121.24
32	B	624	AJP	O74-C67-C66	5.15	122.53	110.38
32	b	624	AJP	O74-C67-C66	5.15	122.53	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	CHD-C1D-ND	-5.15	117.55	124.80
25	b	606	CLA	CHD-C1D-ND	-5.15	117.55	124.80
32	B	624	AJP	O60-C59-C58	5.15	118.98	109.70
32	b	624	AJP	O60-C59-C58	5.15	118.98	109.70
32	N	620	AJP	O25-C26-C27	5.14	120.75	108.09
32	n	620	AJP	O25-C26-C27	5.14	120.75	108.09
25	s	305	CLA	C4D-CHA-C1A	-5.14	115.11	121.24
25	B	608	CLA	C4A-NA-C1A	-5.14	104.34	106.68
25	G	604	CLA	O2D-CGD-CBD	5.14	120.21	111.23
32	y	322	AJP	O25-C26-O31	5.13	124.20	110.69
25	B	601	CLA	O2D-CGD-CBD	5.13	120.20	111.23
32	Y	322	AJP	O25-C26-O31	5.13	124.19	110.69
25	b	601	CLA	O2D-CGD-CBD	5.13	120.20	111.23
25	b	604	CLA	O2D-CGD-CBD	5.13	120.19	111.23
39	N	616	LUT	C18-C5-C6	5.12	130.08	124.48
39	n	616	LUT	C18-C5-C6	5.12	130.08	124.48
25	S	311	CLA	O2D-CGD-CBD	5.12	120.19	111.23
25	B	604	CLA	O2D-CGD-CBD	5.12	120.18	111.23
25	C	510	CLA	O2D-CGD-CBD	5.12	120.17	111.23
25	c	510	CLA	O2D-CGD-CBD	5.12	120.17	111.23
25	s	311	CLA	O2D-CGD-CBD	5.11	120.17	111.23
25	g	604	CLA	O2D-CGD-CBD	5.11	120.17	111.23
32	s	319	AJP	O31-C26-C27	5.11	120.87	110.37
32	S	319	AJP	O25-C26-C27	5.10	120.64	108.09
32	A	412	AJP	O74-C67-C68	5.10	122.40	110.38
32	a	413	AJP	O74-C67-C68	5.10	122.40	110.38
32	y	321	AJP	C26-O31-C30	5.10	118.78	113.13
25	Y	311	CLA	O2D-CGD-CBD	5.10	120.14	111.23
32	s	319	AJP	O25-C26-C27	5.10	120.63	108.09
39	s	315	LUT	C18-C5-C6	5.09	130.04	124.48
39	S	315	LUT	C18-C5-C6	5.09	130.04	124.48
25	r	612	CLA	CHD-C1D-ND	-5.09	117.64	124.80
25	y	311	CLA	O2D-CGD-CBD	5.08	120.11	111.23
32	S	319	AJP	O31-C26-C27	5.08	120.81	110.37
32	Y	321	AJP	C26-O31-C30	5.07	118.75	113.13
32	y	321	AJP	O77-C28-C27	5.07	120.65	110.15
32	Y	321	AJP	O77-C28-C27	5.06	120.64	110.15
25	Y	304	CLA	O2D-CGD-CBD	5.06	120.08	111.23
32	B	624	AJP	O73-C68-C67	5.06	122.30	110.38
32	b	624	AJP	O73-C68-C67	5.06	122.30	110.38
25	R	612	CLA	CHD-C1D-ND	-5.06	117.69	124.80
25	r	604	CLA	CHD-C1D-ND	-5.05	117.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	603	CHL	O1D-CGD-CBD	-5.05	117.06	124.72
25	B	607	CLA	O2D-CGD-CBD	5.05	120.06	111.23
25	b	607	CLA	O2D-CGD-CBD	5.05	120.06	111.23
25	R	604	CLA	CHD-C1D-ND	-5.05	117.70	124.80
25	y	304	CLA	O2D-CGD-CBD	5.04	120.05	111.23
24	6	603	CHL	C3D-CAD-CBD	-5.04	100.97	107.61
39	r	615	LUT	C18-C5-C6	5.04	129.98	124.48
32	A	412	AJP	O60-C59-C61	5.04	118.93	106.44
24	2	603	CHL	O1D-CGD-CBD	-5.03	117.09	124.72
25	B	602	CLA	O2D-CGD-CBD	5.03	120.03	111.23
25	b	602	CLA	O2D-CGD-CBD	5.03	120.03	111.23
24	2	603	CHL	C3D-CAD-CBD	-5.03	100.98	107.61
25	6	605	CLA	C4D-CHA-C1A	-5.03	115.25	121.24
32	Y	320	AJP	C26-O31-C30	-5.02	107.57	113.13
32	N	619	AJP	C01-C02-C85	5.02	118.76	111.03
32	n	619	AJP	C01-C02-C85	5.02	118.76	111.03
32	A	412	AJP	O54-C36-C37	5.02	120.17	107.42
32	a	413	AJP	O60-C59-C61	5.02	118.88	106.44
25	2	605	CLA	C4D-CHA-C1A	-5.01	115.27	121.24
25	D	402	CLA	O2D-CGD-CBD	5.01	119.98	111.23
25	d	402	CLA	O2D-CGD-CBD	5.01	119.98	111.23
32	A	412	AJP	O70-C69-C71	5.00	118.84	106.44
32	a	413	AJP	O70-C69-C71	5.00	118.84	106.44
32	a	413	AJP	O54-C36-C37	5.00	120.11	107.42
39	Y	316	LUT	C18-C5-C6	5.00	129.94	124.48
25	a	406	CLA	O2D-CGD-CBD	4.99	119.96	111.23
32	y	320	AJP	C26-O31-C30	-4.99	107.60	113.13
25	A	405	CLA	O2D-CGD-CBD	4.99	119.95	111.23
25	b	616	CLA	C1D-ND-C4D	-4.99	102.81	106.31
25	R	611	CLA	CHB-C1B-NB	-4.99	116.57	124.05
32	Y	321	AJP	O84-C85-C02	-4.98	105.77	112.17
32	y	321	AJP	O84-C85-C02	-4.98	105.77	112.17
39	R	615	LUT	C18-C5-C6	4.98	129.91	124.48
24	6	601	CHL	C3D-C4D-CHA	4.98	116.10	108.54
32	A	412	AJP	O77-C28-C27	4.98	122.10	110.38
32	a	413	AJP	O77-C28-C27	4.98	122.10	110.38
39	y	316	LUT	C18-C5-C6	4.97	129.91	124.48
25	A	401	CLA	O2D-CGD-CBD	4.97	119.91	111.23
25	a	402	CLA	O2D-CGD-CBD	4.97	119.91	111.23
24	2	601	CHL	C3D-C4D-CHA	4.96	116.08	108.54
25	G	602	CLA	C1D-ND-C4D	-4.96	102.83	106.31
25	g	602	CLA	C1D-ND-C4D	-4.96	102.83	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	C4A-NA-C1A	-4.96	104.42	106.68
25	b	616	CLA	C4A-NA-C1A	-4.96	104.42	106.68
25	B	616	CLA	C1D-ND-C4D	-4.96	102.83	106.31
25	r	611	CLA	CHB-C1B-NB	-4.95	116.62	124.05
25	B	601	CLA	CHD-C1D-ND	-4.95	117.83	124.80
25	Y	312	CLA	O2D-CGD-CBD	4.95	119.88	111.23
25	G	610	CLA	O2D-CGD-CBD	4.94	119.87	111.23
25	R	611	CLA	CHD-C1D-ND	-4.94	117.85	124.80
25	b	601	CLA	CHD-C1D-ND	-4.94	117.86	124.80
25	A	405	CLA	C4A-NA-C1A	-4.93	104.43	106.68
25	a	406	CLA	C4A-NA-C1A	-4.93	104.43	106.68
32	y	323	AJP	O84-C85-C02	-4.93	105.84	112.17
25	r	611	CLA	CHD-C1D-ND	-4.93	117.86	124.80
25	y	312	CLA	O2D-CGD-CBD	4.93	119.85	111.23
25	s	314	CLA	O2D-CGD-CBD	4.93	119.84	111.23
32	A	412	AJP	C65-O70-C69	4.92	123.34	113.72
32	a	413	AJP	C65-O70-C69	4.92	123.34	113.72
25	B	610	CLA	C1D-ND-C4D	-4.92	102.86	106.31
32	Y	323	AJP	O84-C85-C02	-4.92	105.85	112.17
25	C	505	CLA	C1D-ND-C4D	-4.92	102.86	106.31
25	c	505	CLA	C1D-ND-C4D	-4.92	102.86	106.31
25	S	314	CLA	O2D-CGD-CBD	4.91	119.82	111.23
25	g	610	CLA	O2D-CGD-CBD	4.91	119.82	111.23
25	Y	312	CLA	C1D-ND-C4D	-4.91	102.87	106.31
25	S	309	CLA	O2D-CGD-CBD	4.91	119.81	111.23
32	g	618	AJP	O25-C26-C27	4.91	120.17	108.09
32	G	618	AJP	O25-C26-C27	4.91	120.16	108.09
39	G	615	LUT	C18-C5-C6	4.91	129.84	124.48
32	Y	323	AJP	C05-C06-C07	4.91	110.60	103.37
32	y	323	AJP	C05-C06-C07	4.91	110.60	103.37
39	g	615	LUT	C18-C5-C6	4.90	129.83	124.48
25	s	309	CLA	O2D-CGD-CBD	4.90	119.79	111.23
25	B	603	CLA	O2D-CGD-CBD	4.89	119.78	111.23
25	b	603	CLA	O2D-CGD-CBD	4.89	119.78	111.23
25	y	313	CLA	O2D-CGD-CBD	4.89	119.78	111.23
25	Y	313	CLA	O2D-CGD-CBD	4.88	119.77	111.23
25	c	512	CLA	O2D-CGD-CBD	4.87	119.74	111.23
25	C	512	CLA	O2D-CGD-CBD	4.87	119.74	111.23
25	B	606	CLA	O2D-CGD-CBD	4.87	119.74	111.23
25	b	606	CLA	O2D-CGD-CBD	4.87	119.74	111.23
25	C	511	CLA	O2D-CGD-CBD	4.87	119.73	111.23
25	N	613	CLA	O2D-CGD-CBD	4.87	119.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	617	NEX	C35-C15-C14	4.86	133.47	123.52
40	r	617	NEX	C35-C15-C14	4.86	133.47	123.52
25	n	613	CLA	O2D-CGD-CBD	4.86	119.73	111.23
25	b	602	CLA	C4A-NA-C1A	-4.86	104.46	106.68
25	c	511	CLA	O2D-CGD-CBD	4.86	119.72	111.23
25	b	610	CLA	C1D-ND-C4D	-4.85	102.91	106.31
25	S	312	CLA	O2D-CGD-CBD	4.85	119.70	111.23
25	s	312	CLA	O2D-CGD-CBD	4.84	119.70	111.23
25	B	613	CLA	C1D-ND-C4D	-4.84	102.92	106.31
25	b	613	CLA	C1D-ND-C4D	-4.84	102.92	106.31
25	B	602	CLA	C4A-NA-C1A	-4.84	104.47	106.68
39	S	316	LUT	C18-C5-C6	4.83	129.76	124.48
25	R	611	CLA	C2A-C3A-C4A	-4.83	94.06	101.87
25	N	610	CLA	O2D-CGD-CBD	4.83	119.67	111.23
25	n	610	CLA	O2D-CGD-CBD	4.83	119.67	111.23
32	N	620	AJP	C05-C06-C07	4.82	110.47	103.37
25	b	607	CLA	C4A-NA-C1A	-4.82	104.48	106.68
25	y	312	CLA	C1D-ND-C4D	-4.82	102.93	106.31
39	s	316	LUT	C18-C5-C6	4.82	129.74	124.48
25	C	510	CLA	CHD-C1D-ND	-4.81	118.03	124.80
25	c	510	CLA	CHD-C1D-ND	-4.81	118.03	124.80
32	n	620	AJP	C05-C06-C07	4.81	110.46	103.37
32	Y	324	AJP	O77-C28-C29	4.80	121.79	109.86
32	y	324	AJP	O77-C28-C29	4.80	121.79	109.86
25	r	611	CLA	C2A-C3A-C4A	-4.79	94.13	101.87
39	Y	317	LUT	C18-C5-C6	4.79	129.71	124.48
25	c	505	CLA	C4A-NA-C1A	-4.79	104.49	106.68
39	y	317	LUT	C18-C5-C6	4.79	129.71	124.48
25	C	506	CLA	O2D-CGD-CBD	4.78	119.59	111.23
25	c	506	CLA	O2D-CGD-CBD	4.78	119.59	111.23
25	Y	303	CLA	O2D-CGD-CBD	4.78	119.59	111.23
25	y	303	CLA	O2D-CGD-CBD	4.78	119.59	111.23
25	r	611	CLA	C4D-C3D-CAD	-4.78	102.92	108.11
25	r	604	CLA	O2D-CGD-CBD	4.77	119.57	111.23
25	R	604	CLA	O2D-CGD-CBD	4.76	119.56	111.23
25	Y	305	CLA	C1D-ND-C4D	-4.76	102.97	106.31
25	y	305	CLA	C1D-ND-C4D	-4.76	102.97	106.31
25	S	310	CLA	O2D-CGD-CBD	4.76	119.55	111.23
25	s	310	CLA	O2D-CGD-CBD	4.76	119.55	111.23
32	a	413	AJP	C35-C36-C37	4.75	119.97	110.74
25	r	612	CLA	CHB-C1B-NB	-4.75	116.93	124.05
25	R	611	CLA	C2D-C1D-ND	-4.75	105.43	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	611	CLA	C4D-C3D-CAD	-4.75	102.95	108.11
25	r	608	CLA	O2D-CGD-CBD	4.75	119.53	111.23
32	Y	322	AJP	C26-O25-C23	4.75	123.20	115.27
32	y	322	AJP	C26-O25-C23	4.75	123.20	115.27
32	A	412	AJP	C35-C36-C37	4.74	119.97	110.74
25	D	403	CLA	C3B-C4B-NB	-4.74	106.30	110.53
25	R	612	CLA	CHB-C1B-NB	-4.74	116.94	124.05
25	n	611	CLA	O2D-CGD-CBD	4.74	119.51	111.23
25	B	607	CLA	C4A-NA-C1A	-4.73	104.52	106.68
25	2	604	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	S	305	CLA	C3B-C4B-NB	-4.73	106.31	110.53
24	n	601	CHL	C3D-C4D-CHA	4.73	115.73	108.54
32	Y	320	AJP	C01-C02-C85	4.73	118.31	111.03
24	Y	310	CHL	C4D-CHA-CBD	-4.73	104.20	108.97
24	y	310	CHL	C4D-CHA-CBD	-4.73	104.20	108.97
24	s	302	CHL	C3D-C4D-CHA	4.73	115.72	108.54
25	B	615	CLA	O2D-CGD-CBD	4.72	119.49	111.23
25	N	611	CLA	C1D-ND-C4D	-4.72	103.00	106.31
25	b	610	CLA	O2D-CGD-CBD	4.72	119.49	111.23
25	Y	303	CLA	C1D-ND-C4D	-4.72	103.00	106.31
24	N	601	CHL	C3D-C4D-CHA	4.72	115.71	108.54
25	r	603	CLA	C3B-C4B-NB	-4.71	106.32	110.53
25	s	305	CLA	C3B-C4B-NB	-4.71	106.32	110.53
32	y	320	AJP	C01-C02-C85	4.71	118.28	111.03
25	b	615	CLA	O2D-CGD-CBD	4.71	119.46	111.23
25	R	608	CLA	O2D-CGD-CBD	4.71	119.46	111.23
25	y	303	CLA	C1D-ND-C4D	-4.71	103.01	106.31
25	S	313	CLA	CHD-C1D-ND	-4.71	118.18	124.80
25	s	313	CLA	CHD-C1D-ND	-4.71	118.18	124.80
25	6	604	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	B	610	CLA	O2D-CGD-CBD	4.70	119.45	111.23
25	N	611	CLA	O2D-CGD-CBD	4.70	119.45	111.23
25	C	508	CLA	O2D-CGD-CBD	4.70	119.45	111.23
25	c	508	CLA	O2D-CGD-CBD	4.70	119.45	111.23
25	c	508	CLA	CHD-C1D-ND	-4.70	118.19	124.80
24	N	606	CHL	CBC-CAC-C3C	-4.70	106.14	112.87
24	n	606	CHL	CBC-CAC-C3C	-4.70	106.14	112.87
25	y	311	CLA	C1D-ND-C4D	-4.70	103.01	106.31
24	n	609	CHL	C4D-CHA-CBD	-4.70	104.23	108.97
24	S	302	CHL	C3D-C4D-CHA	4.70	115.68	108.54
25	d	403	CLA	C3B-C4B-NB	-4.70	106.34	110.53
32	A	412	AJP	O25-C26-C27	4.70	119.65	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	413	AJP	O25-C26-C27	4.70	119.65	108.09
25	n	610	CLA	C1D-ND-C4D	-4.70	103.02	106.31
25	R	603	CLA	C3B-C4B-NB	-4.69	106.34	110.53
25	r	611	CLA	C2D-C1D-ND	-4.69	105.48	110.13
25	N	610	CLA	C1D-ND-C4D	-4.69	103.02	106.31
25	B	611	CLA	O2D-CGD-CBD	4.69	119.43	111.23
25	b	611	CLA	O2D-CGD-CBD	4.69	119.43	111.23
25	A	402	CLA	O2D-CGD-CBD	4.69	119.42	111.23
25	a	403	CLA	O2D-CGD-CBD	4.69	119.42	111.23
25	R	612	CLA	O2D-CGD-CBD	4.68	119.42	111.23
25	r	612	CLA	O2D-CGD-CBD	4.68	119.42	111.23
25	C	505	CLA	C4A-NA-C1A	-4.68	104.54	106.68
24	n	609	CHL	C3D-C4D-CHA	4.68	115.65	108.54
32	Y	321	AJP	C29-C28-C27	4.67	117.40	110.67
32	y	321	AJP	C29-C28-C27	4.67	117.40	110.67
32	Y	324	AJP	O25-C26-C27	4.67	119.59	108.09
25	n	611	CLA	C1D-ND-C4D	-4.67	103.03	106.31
32	y	324	AJP	O25-C26-C27	4.67	119.58	108.09
32	Y	323	AJP	O77-C28-C29	4.67	121.46	109.86
32	y	323	AJP	O77-C28-C29	4.67	121.46	109.86
32	a	413	AJP	O40-C39-C41	4.67	118.01	106.44
32	n	619	AJP	O31-C26-C27	4.67	119.96	110.37
24	Y	307	CHL	C4D-CHA-CBD	-4.67	104.26	108.97
25	2	602	CLA	O2D-CGD-CBD	4.66	119.39	111.23
25	S	313	CLA	C2A-C3A-C4A	-4.66	94.34	101.87
25	s	313	CLA	C2A-C3A-C4A	-4.66	94.34	101.87
24	G	607	CHL	C4D-CHA-CBD	-4.66	104.27	108.97
24	N	609	CHL	C3D-C4D-CHA	4.66	115.62	108.54
25	6	602	CLA	CHC-C4B-NB	-4.66	117.06	124.05
32	N	619	AJP	O31-C26-C27	4.66	119.94	110.37
25	2	602	CLA	CHC-C4B-NB	-4.66	117.06	124.05
32	Y	324	AJP	C01-C02-C85	4.66	118.20	111.03
32	y	324	AJP	C01-C02-C85	4.66	118.20	111.03
25	C	502	CLA	O2D-CGD-CBD	4.66	119.37	111.23
25	c	502	CLA	O2D-CGD-CBD	4.66	119.37	111.23
32	A	412	AJP	O40-C39-C41	4.65	117.97	106.44
32	G	618	AJP	C24-C19-C20	-4.65	107.71	112.66
32	g	618	AJP	C24-C19-C20	-4.65	107.71	112.66
25	a	403	CLA	C4A-NA-C1A	-4.65	104.56	106.68
24	N	609	CHL	C4D-CHA-CBD	-4.65	104.28	108.97
24	r	607	CHL	C3D-C4D-CHA	4.65	115.60	108.54
24	n	607	CHL	C4D-CHA-CBD	-4.64	104.29	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	602	CLA	C4A-NA-C1A	-4.64	104.56	106.68
25	6	602	CLA	O2D-CGD-CBD	4.64	119.34	111.23
24	y	307	CHL	C4D-CHA-CBD	-4.64	104.29	108.97
25	C	508	CLA	CHD-C1D-ND	-4.64	118.28	124.80
25	c	501	CLA	C1-C2-C3	-4.64	118.60	126.20
25	g	602	CLA	O1D-CGD-CBD	-4.64	115.38	124.52
25	c	507	CLA	CHD-C1D-ND	-4.63	118.28	124.80
32	N	620	AJP	O77-C28-C29	4.63	121.37	109.86
25	A	402	CLA	C4A-NA-C1A	-4.63	104.57	106.68
24	N	607	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
32	Y	321	AJP	O25-C26-C27	4.63	119.48	108.09
25	y	305	CLA	C4A-NA-C1A	-4.63	104.57	106.68
24	g	607	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
32	n	620	AJP	O77-C28-C29	4.63	121.36	109.86
24	Y	302	CHL	C3D-C4D-CHA	4.63	115.57	108.54
24	y	302	CHL	C3D-C4D-CHA	4.63	115.57	108.54
24	R	607	CHL	C3D-C4D-CHA	4.62	115.57	108.54
25	c	513	CLA	O2D-CGD-CBD	4.62	119.31	111.23
32	n	619	AJP	O25-C26-C27	4.62	119.46	108.09
25	S	314	CLA	C1D-ND-C4D	-4.62	103.07	106.31
25	Y	311	CLA	C1D-ND-C4D	-4.62	103.07	106.31
32	N	619	AJP	O25-C26-C27	4.62	119.46	108.09
25	N	603	CLA	O2D-CGD-CBD	4.62	119.31	111.23
25	C	501	CLA	C1-C2-C3	-4.62	118.63	126.20
32	y	321	AJP	O25-C26-C27	4.61	119.44	108.09
25	C	507	CLA	CHD-C1D-ND	-4.61	118.31	124.80
25	B	616	CLA	O2D-CGD-CBD	4.61	119.29	111.23
25	S	313	CLA	O2D-CGD-CBD	4.61	119.29	111.23
25	A	401	CLA	CHD-C1D-ND	-4.61	118.32	124.80
25	a	402	CLA	CHD-C1D-ND	-4.61	118.32	124.80
24	n	606	CHL	C3D-C4D-CHA	4.61	115.54	108.54
25	N	602	CLA	C1D-ND-C4D	-4.61	103.08	106.31
25	R	604	CLA	CHB-C1B-NB	-4.61	117.14	124.05
25	C	513	CLA	O2D-CGD-CBD	4.61	119.28	111.23
25	B	605	CLA	CHD-C1D-ND	-4.60	118.32	124.80
25	b	605	CLA	CHD-C1D-ND	-4.60	118.32	124.80
24	Y	307	CHL	CBC-CAC-C3C	-4.60	106.28	112.87
25	S	310	CLA	CHD-C1D-ND	-4.60	118.33	124.80
24	N	607	CHL	C3D-C4D-CHA	4.60	115.53	108.54
24	n	607	CHL	C3D-C4D-CHA	4.60	115.53	108.54
25	b	616	CLA	O2D-CGD-CBD	4.60	119.27	111.23
25	G	602	CLA	O1D-CGD-CBD	-4.60	115.44	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	624	AJP	C45-C46-C47	4.60	119.69	110.01
32	b	624	AJP	C45-C46-C47	4.60	119.69	110.01
25	r	601	CLA	C3B-C4B-NB	-4.60	106.42	110.53
25	B	608	CLA	O2D-CGD-CBD	4.60	119.27	111.23
25	c	504	CLA	C3B-C4B-NB	-4.60	106.42	110.53
25	C	504	CLA	C3B-C4B-NB	-4.60	106.42	110.53
24	G	606	CHL	C3D-C4D-CHA	4.60	115.53	108.54
24	g	606	CHL	C3D-C4D-CHA	4.60	115.53	108.54
25	s	310	CLA	CHD-C1D-ND	-4.60	118.33	124.80
25	R	614	CLA	C1D-ND-C4D	-4.60	103.09	106.31
25	r	614	CLA	C1D-ND-C4D	-4.59	103.09	106.31
25	S	303	CLA	O2D-CGD-CBD	4.59	119.26	111.23
25	b	608	CLA	O2D-CGD-CBD	4.59	119.26	111.23
25	s	303	CLA	O2D-CGD-CBD	4.59	119.26	111.23
25	s	313	CLA	O2D-CGD-CBD	4.59	119.26	111.23
24	G	609	CHL	C4D-CHA-CBD	-4.59	104.34	108.97
25	r	604	CLA	CHB-C1B-NB	-4.59	117.17	124.05
25	n	603	CLA	O2D-CGD-CBD	4.59	119.25	111.23
24	g	609	CHL	C4D-CHA-CBD	-4.59	104.34	108.97
24	y	307	CHL	CBC-CAC-C3C	-4.59	106.31	112.87
24	G	601	CHL	C3D-C4D-CHA	4.58	115.50	108.54
25	s	314	CLA	C1D-ND-C4D	-4.58	103.10	106.31
25	n	602	CLA	C1D-ND-C4D	-4.58	103.10	106.31
29	l	101	SQD	O8-S-C6	-4.58	97.13	105.97
24	5	301	CHL	C3D-C4D-CHA	4.58	115.50	108.54
25	d	401	CLA	O2D-CGD-CBD	4.58	119.23	111.23
25	G	612	CLA	O2D-CGD-CBD	4.57	119.22	111.23
25	b	609	CLA	O2D-CGD-CBD	4.57	119.22	111.23
25	N	612	CLA	CHD-C1D-ND	-4.57	118.37	124.80
40	R	617	NEX	C12-C13-C14	4.57	126.19	119.01
25	N	602	CLA	C4A-NA-C1A	-4.57	104.60	106.68
25	B	609	CLA	O2D-CGD-CBD	4.57	119.21	111.23
29	L	103	SQD	O8-S-C6	-4.56	97.16	105.97
24	Y	308	CHL	C3D-C4D-CHA	4.56	115.48	108.54
24	y	308	CHL	C3D-C4D-CHA	4.56	115.48	108.54
25	g	610	CLA	CHB-C1B-NB	-4.56	117.20	124.05
24	g	601	CHL	C3D-C4D-CHA	4.56	115.47	108.54
24	s	302	CHL	C4D-CHA-CBD	-4.56	104.37	108.97
24	N	606	CHL	C3D-C4D-CHA	4.56	115.47	108.54
25	S	305	CLA	O2D-CGD-CBD	4.56	119.20	111.23
25	c	503	CLA	O2D-CGD-CBD	4.56	119.20	111.23
25	s	304	CLA	CHD-C1D-ND	-4.56	118.39	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	617	NEX	C12-C13-C14	4.56	126.17	119.01
25	n	612	CLA	CHD-C1D-ND	-4.55	118.40	124.80
25	R	601	CLA	C3B-C4B-NB	-4.55	106.47	110.53
32	Y	320	AJP	O25-C26-C27	4.55	119.27	108.09
25	s	305	CLA	O2D-CGD-CBD	4.54	119.17	111.23
25	b	604	CLA	CHD-C1D-ND	-4.54	118.41	124.80
24	G	605	CHL	C3D-C4D-CHA	4.54	115.44	108.54
32	y	320	AJP	O25-C26-C27	4.54	119.27	108.09
25	C	503	CLA	O2D-CGD-CBD	4.54	119.17	111.23
25	2	604	CLA	C4B-CHC-C1C	-4.54	115.57	126.25
25	g	612	CLA	O2D-CGD-CBD	4.54	119.17	111.23
25	y	304	CLA	C4A-NA-C1A	-4.54	104.61	106.68
41	r	616	XAT	C31-C30-C29	-4.54	120.91	127.28
25	6	604	CLA	C4B-CHC-C1C	-4.54	115.58	126.25
25	D	401	CLA	O2D-CGD-CBD	4.54	119.16	111.23
32	Y	320	AJP	O77-C28-C27	4.53	119.53	110.15
32	y	320	AJP	O77-C28-C27	4.53	119.53	110.15
25	R	609	CLA	CHD-C1D-ND	-4.52	118.44	124.80
40	y	318	NEX	C5-C6-C1	-4.52	115.21	119.70
32	G	618	AJP	O77-C28-C27	4.52	119.52	110.15
24	1	301	CHL	C3D-C4D-CHA	4.52	115.41	108.54
24	y	306	CHL	C3D-C4D-CHA	4.52	115.41	108.54
24	Y	307	CHL	C3D-C4D-CHA	4.52	115.41	108.54
24	G	607	CHL	O1D-CGD-CBD	-4.52	117.87	124.72
24	S	307	CHL	C3D-C4D-CHA	4.52	115.41	108.54
25	c	506	CLA	C1D-ND-C4D	-4.52	103.14	106.31
32	Y	321	AJP	C01-C02-C85	4.52	117.98	111.03
32	y	321	AJP	C01-C02-C85	4.52	117.98	111.03
32	g	618	AJP	O77-C28-C27	4.52	119.51	110.15
25	g	602	CLA	O2D-CGD-CBD	4.51	119.12	111.23
24	S	302	CHL	C4D-CHA-CBD	-4.51	104.42	108.97
24	Y	310	CHL	C3D-C4D-CHA	4.51	115.40	108.54
24	g	605	CHL	C3D-C4D-CHA	4.51	115.40	108.54
24	y	310	CHL	C3D-C4D-CHA	4.51	115.40	108.54
24	R	606	CHL	C3D-C4D-CHA	4.51	115.40	108.54
25	G	610	CLA	CHB-C1B-NB	-4.51	117.28	124.05
25	g	614	CLA	O2D-CGD-CBD	4.51	119.12	111.23
41	R	616	XAT	C31-C30-C29	-4.51	120.95	127.28
25	r	609	CLA	CHD-C1D-ND	-4.51	118.45	124.80
40	Y	318	NEX	C5-C6-C1	-4.51	115.22	119.70
24	Y	306	CHL	C3D-C4D-CHA	4.51	115.39	108.54
24	s	307	CHL	C3D-C4D-CHA	4.51	115.39	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	609	CHL	C3D-C4D-CHA	4.51	115.39	108.54
25	S	304	CLA	CHD-C1D-ND	-4.50	118.46	124.80
24	G	609	CHL	C3D-C4D-CHA	4.50	115.38	108.54
25	N	614	CLA	CHB-C1B-NB	-4.50	117.30	124.05
24	s	308	CHL	C3D-C4D-CHA	4.50	115.38	108.54
25	R	610	CLA	O2D-CGD-CBD	4.50	119.09	111.23
25	r	610	CLA	O2D-CGD-CBD	4.50	119.09	111.23
25	B	604	CLA	CHD-C1D-ND	-4.50	118.47	124.80
24	y	307	CHL	C3D-C4D-CHA	4.50	115.38	108.54
24	r	606	CHL	C3D-C4D-CHA	4.50	115.38	108.54
24	N	601	CHL	C4D-CHA-CBD	-4.49	104.44	108.97
24	Y	309	CHL	C3D-C4D-CHA	4.49	115.37	108.54
24	y	309	CHL	C3D-C4D-CHA	4.49	115.37	108.54
24	G	608	CHL	C3D-C4D-CHA	4.49	115.37	108.54
24	g	608	CHL	C3D-C4D-CHA	4.49	115.36	108.54
25	G	614	CLA	O2D-CGD-CBD	4.49	119.07	111.23
32	A	412	AJP	O77-C28-C29	4.48	121.43	109.94
32	a	413	AJP	O77-C28-C29	4.48	121.43	109.94
24	N	605	CHL	C3D-C4D-CHA	4.48	115.35	108.54
24	n	605	CHL	C3D-C4D-CHA	4.48	115.35	108.54
25	G	602	CLA	O2D-CGD-CBD	4.48	119.06	111.23
24	s	306	CHL	C3D-C4D-CHA	4.48	115.34	108.54
24	S	308	CHL	C3D-C4D-CHA	4.48	115.34	108.54
25	S	309	CLA	C4D-CHA-C1A	-4.47	115.91	121.24
24	n	601	CHL	C4D-CHA-CBD	-4.47	104.46	108.97
25	6	602	CLA	C3B-C4B-NB	-4.47	106.54	110.53
24	S	306	CHL	C3D-C4D-CHA	4.47	115.33	108.54
24	N	608	CHL	C3D-C4D-CHA	4.47	115.33	108.54
25	n	614	CLA	CHB-C1B-NB	-4.47	117.34	124.05
25	s	309	CLA	C4D-CHA-C1A	-4.47	115.91	121.24
25	B	612	CLA	O2D-CGD-CBD	4.47	119.04	111.23
25	b	612	CLA	O2D-CGD-CBD	4.47	119.04	111.23
25	Y	305	CLA	C4A-NA-C1A	-4.47	104.64	106.68
25	c	513	CLA	C4A-NA-C1A	-4.46	104.64	106.68
25	c	507	CLA	O2D-CGD-CBD	4.46	119.03	111.23
32	B	624	AJP	O25-C26-O31	4.46	122.44	110.69
32	b	624	AJP	O25-C26-O31	4.46	122.44	110.69
24	g	607	CHL	O1D-CGD-CBD	-4.46	117.95	124.72
25	A	402	CLA	CHD-C1D-ND	-4.46	118.52	124.80
25	S	313	CLA	CHB-C1B-NB	-4.46	117.36	124.05
25	C	513	CLA	C4A-NA-C1A	-4.46	104.64	106.68
25	c	509	CLA	O2D-CGD-CBD	4.45	119.02	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	605	CHL	C4D-CHA-CBD	-4.45	104.48	108.97
24	r	605	CHL	C4D-CHA-CBD	-4.45	104.48	108.97
25	C	509	CLA	O2D-CGD-CBD	4.45	119.01	111.23
32	B	624	AJP	O40-C39-C38	4.45	117.72	109.70
32	b	624	AJP	O40-C39-C38	4.45	117.72	109.70
32	Y	322	AJP	C21-C22-C23	4.45	116.41	110.46
32	y	322	AJP	C21-C22-C23	4.45	116.41	110.46
24	G	605	CHL	C4D-CHA-CBD	-4.45	104.48	108.97
25	6	605	CLA	O2D-CGD-CBD	4.45	119.01	111.23
25	2	602	CLA	C3B-C4B-NB	-4.45	106.56	110.53
25	C	507	CLA	O2D-CGD-CBD	4.45	119.00	111.23
25	S	305	CLA	C1-C2-C3	-4.45	119.57	126.76
25	a	403	CLA	CHD-C1D-ND	-4.44	118.55	124.80
32	S	319	AJP	C03-C04-C05	-4.44	104.97	111.93
32	s	319	AJP	C03-C04-C05	-4.44	104.97	111.93
25	6	604	CLA	O2D-CGD-CBD	4.44	119.00	111.23
24	n	608	CHL	C3D-C4D-CHA	4.44	115.30	108.54
25	s	313	CLA	CHB-C1B-NB	-4.44	117.38	124.05
25	Y	303	CLA	O1D-CGD-CBD	-4.44	115.75	124.52
25	y	303	CLA	O1D-CGD-CBD	-4.44	115.75	124.52
25	2	604	CLA	O2D-CGD-CBD	4.44	118.99	111.23
24	g	605	CHL	C4D-CHA-CBD	-4.44	104.49	108.97
32	N	619	AJP	O77-C28-C29	4.44	120.90	109.86
40	S	317	NEX	C35-C34-C33	-4.44	121.05	127.28
40	s	317	NEX	C35-C34-C33	-4.44	121.05	127.28
25	2	605	CLA	O2D-CGD-CBD	4.44	118.99	111.23
24	r	613	CHL	C3D-C4D-CHA	4.44	115.28	108.54
25	C	512	CLA	CHD-C1D-ND	-4.43	118.56	124.80
32	Y	322	AJP	O77-C28-C29	4.43	120.88	109.86
32	y	322	AJP	O77-C28-C29	4.43	120.87	109.86
24	R	613	CHL	C3D-C4D-CHA	4.43	115.27	108.54
25	B	604	CLA	C1-C2-C3	-4.43	118.94	126.20
25	b	604	CLA	C1-C2-C3	-4.43	118.94	126.20
32	n	619	AJP	O77-C28-C29	4.43	120.87	109.86
25	c	512	CLA	CHD-C1D-ND	-4.43	118.57	124.80
25	C	506	CLA	C1D-ND-C4D	-4.43	103.21	106.31
25	s	305	CLA	C1-C2-C3	-4.42	119.60	126.76
25	G	614	CLA	C1D-ND-C4D	-4.42	103.21	106.31
25	g	614	CLA	C1D-ND-C4D	-4.42	103.21	106.31
24	l	302	CHL	C4D-CHA-CBD	-4.42	104.51	108.97
25	c	503	CLA	CHD-C1D-ND	-4.42	118.58	124.80
25	C	513	CLA	C4D-CHA-C1A	-4.42	115.97	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	C4D-CHA-C1A	-4.42	115.97	121.24
25	B	601	CLA	CHB-C1B-NB	-4.41	117.43	124.05
25	b	601	CLA	CHB-C1B-NB	-4.41	117.43	124.05
40	Y	318	NEX	C15-C14-C13	-4.41	121.09	127.28
25	Y	305	CLA	O2D-CGD-CBD	4.41	118.94	111.23
24	5	301	CHL	C4D-CHA-CBD	-4.41	104.52	108.97
25	y	305	CLA	O2D-CGD-CBD	4.41	118.94	111.23
25	N	602	CLA	O2D-CGD-CBD	4.41	118.94	111.23
25	Y	304	CLA	C4A-NA-C1A	-4.41	104.67	106.68
25	n	602	CLA	O2D-CGD-CBD	4.41	118.94	111.23
24	R	605	CHL	C3D-C4D-CHA	4.41	115.24	108.54
24	r	605	CHL	C3D-C4D-CHA	4.41	115.24	108.54
25	2	602	CLA	CHD-C1D-C2D	4.41	134.65	125.49
25	6	602	CLA	CHD-C1D-C2D	4.41	134.65	125.49
24	1	302	CHL	C3D-C4D-CHA	4.41	115.24	108.54
32	s	319	AJP	C21-C22-C23	4.40	116.35	110.46
25	g	611	CLA	CHB-C1B-NB	-4.40	117.45	124.05
25	R	611	CLA	O2D-CGD-CBD	4.40	118.91	111.23
38	F	101	HEM	C1B-NB-C4B	4.39	110.41	105.21
25	C	503	CLA	CHD-C1D-ND	-4.39	118.62	124.80
41	r	616	XAT	C15-C14-C13	-4.39	121.12	127.28
25	S	311	CLA	CHD-C1D-ND	-4.39	118.62	124.80
25	D	403	CLA	O2D-CGD-CBD	4.39	118.90	111.23
32	S	319	AJP	C21-C22-C23	4.38	116.32	110.46
41	R	616	XAT	C15-C14-C13	-4.38	121.13	127.28
25	r	611	CLA	O2D-CGD-CBD	4.38	118.89	111.23
25	d	403	CLA	O2D-CGD-CBD	4.38	118.89	111.23
24	G	607	CHL	C3D-C4D-CHA	4.38	115.19	108.54
24	5	302	CHL	C4D-CHA-CBD	-4.37	104.56	108.97
25	n	610	CLA	C4A-NA-C1A	-4.37	104.68	106.68
25	C	501	CLA	C3B-C4B-NB	-4.37	106.63	110.53
25	G	611	CLA	CHB-C1B-NB	-4.37	117.49	124.05
40	y	318	NEX	C15-C14-C13	-4.37	121.15	127.28
24	5	302	CHL	C3D-C4D-CHA	4.37	115.18	108.54
25	r	602	CLA	C1-C2-C3	-4.37	119.04	126.20
25	y	315	CLA	C1D-ND-C4D	-4.37	103.25	106.31
24	g	607	CHL	C3D-C4D-CHA	4.36	115.17	108.54
24	1	301	CHL	C4D-CHA-CBD	-4.36	104.57	108.97
32	Y	323	AJP	C01-C02-C03	4.35	121.60	112.08
25	c	501	CLA	C3B-C4B-NB	-4.35	106.65	110.53
32	y	323	AJP	C01-C02-C03	4.35	121.58	112.08
32	s	319	AJP	C21-C20-C19	4.35	111.38	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	g	616	LUT	C38-C25-C24	-4.35	113.08	123.36
25	s	311	CLA	CHD-C1D-ND	-4.34	118.69	124.80
38	f	101	HEM	C1B-NB-C4B	4.34	110.35	105.21
24	g	606	CHL	C4D-CHA-CBD	-4.34	104.59	108.97
39	G	616	LUT	C38-C25-C24	-4.34	113.08	123.36
25	N	604	CLA	C1-C2-C3	-4.34	119.74	126.76
24	G	606	CHL	C4D-CHA-CBD	-4.34	104.59	108.97
25	Y	315	CLA	C1D-ND-C4D	-4.34	103.27	106.31
25	n	604	CLA	C1-C2-C3	-4.34	119.75	126.76
25	A	405	CLA	CHD-C1D-ND	-4.34	118.70	124.80
27	A	403	PHO	C1-C2-C3	-4.33	119.10	126.20
27	a	404	PHO	C1-C2-C3	-4.33	119.10	126.20
25	R	602	CLA	C1-C2-C3	-4.33	119.10	126.20
24	r	607	CHL	C4D-CHA-CBD	-4.33	104.61	108.97
25	a	406	CLA	CHD-C1D-ND	-4.32	118.72	124.80
32	S	319	AJP	C21-C20-C19	4.32	111.36	107.23
24	G	601	CHL	C4D-CHA-CBD	-4.32	104.61	108.97
24	g	601	CHL	C4D-CHA-CBD	-4.32	104.61	108.97
32	a	413	AJP	O54-C36-C35	4.32	119.36	108.47
25	N	610	CLA	C4A-NA-C1A	-4.31	104.71	106.68
25	g	613	CLA	C4D-CHA-C1A	-4.31	116.11	121.24
39	S	315	LUT	C38-C25-C24	-4.31	113.17	123.36
25	b	609	CLA	C1D-ND-C4D	-4.30	103.29	106.31
32	A	412	AJP	O54-C36-C35	4.30	119.33	108.47
39	s	315	LUT	C38-C25-C24	-4.30	113.18	123.36
24	R	607	CHL	C4D-CHA-CBD	-4.29	104.64	108.97
29	A	411	SQD	O8-S-C6	-4.29	97.69	105.97
29	a	412	SQD	O8-S-C6	-4.29	97.69	105.97
25	G	613	CLA	CHD-C1D-ND	-4.29	118.77	124.80
25	G	613	CLA	C4D-CHA-C1A	-4.28	116.13	121.24
25	C	501	CLA	O2D-CGD-CBD	4.28	118.72	111.23
25	c	501	CLA	O2D-CGD-CBD	4.28	118.72	111.23
32	G	618	AJP	C12-C07-C06	4.28	133.15	120.50
32	N	619	AJP	C03-C04-C05	-4.28	105.23	111.93
32	g	618	AJP	C12-C07-C06	4.28	133.14	120.50
25	R	609	CLA	O2D-CGD-CBD	4.27	118.70	111.23
24	R	606	CHL	C4D-CHA-CBD	-4.27	104.66	108.97
24	r	606	CHL	C4D-CHA-CBD	-4.27	104.66	108.97
25	r	609	CLA	O2D-CGD-CBD	4.27	118.69	111.23
25	C	511	CLA	CHB-C1B-NB	-4.27	117.65	124.05
40	r	617	NEX	C15-C35-C34	4.26	132.24	123.52
25	g	613	CLA	CHD-C1D-ND	-4.26	118.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	CHB-C1B-NB	-4.26	117.66	124.05
40	R	617	NEX	C15-C35-C34	4.26	132.23	123.52
25	C	504	CLA	C1-C2-C3	-4.26	119.22	126.20
24	Y	302	CHL	C4D-CHA-CBD	-4.26	104.68	108.97
25	g	604	CLA	C1D-ND-C4D	-4.25	103.33	106.31
32	n	619	AJP	C03-C04-C05	-4.25	105.27	111.93
25	B	609	CLA	C1D-ND-C4D	-4.25	103.33	106.31
24	G	606	CHL	CBC-CAC-C3C	-4.25	106.79	112.87
25	c	504	CLA	C1-C2-C3	-4.25	119.24	126.20
25	g	613	CLA	O2D-CGD-CBD	4.25	118.66	111.23
39	s	316	LUT	C38-C25-C24	-4.24	113.31	123.36
25	y	314	CLA	O2D-CGD-CBD	4.24	118.65	111.23
25	G	613	CLA	O2D-CGD-CBD	4.24	118.65	111.23
25	B	614	CLA	C1D-ND-C4D	-4.24	103.33	106.31
25	b	614	CLA	C1D-ND-C4D	-4.24	103.33	106.31
24	g	606	CHL	CBC-CAC-C3C	-4.24	106.80	112.87
25	b	607	CLA	CHD-C1D-ND	-4.24	118.83	124.80
24	y	302	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
32	n	619	AJP	O31-C30-C29	4.24	116.60	110.14
25	Y	313	CLA	C1-C2-C3	-4.24	119.26	126.20
25	D	401	CLA	C4D-CHA-C1A	-4.24	116.19	121.24
25	d	401	CLA	C4D-CHA-C1A	-4.24	116.19	121.24
24	N	608	CHL	C4D-CHA-CBD	-4.23	104.70	108.97
39	S	316	LUT	C38-C25-C24	-4.23	113.35	123.36
25	Y	314	CLA	O2D-CGD-CBD	4.23	118.62	111.23
29	l	102	SQD	O8-S-C6	-4.22	97.81	105.97
39	n	616	LUT	C38-C25-C24	-4.22	113.36	123.36
32	G	618	AJP	O25-C23-C24	4.22	117.85	109.64
25	D	401	CLA	C1-C2-C3	-4.22	119.93	126.76
24	r	613	CHL	C4D-CHA-CBD	-4.22	104.72	108.97
25	d	401	CLA	C1-C2-C3	-4.22	119.94	126.76
24	y	306	CHL	C4D-CHA-CBD	-4.22	104.72	108.97
32	N	619	AJP	O31-C30-C29	4.21	116.56	110.14
32	g	618	AJP	O84-C05-C06	4.21	119.82	107.26
26	R	618	LHG	O7-C7-C8	4.21	120.59	111.48
25	G	603	CLA	O2D-CGD-CBD	4.21	118.59	111.23
25	g	603	CLA	O2D-CGD-CBD	4.21	118.59	111.23
25	2	602	CLA	CHD-C1D-ND	-4.21	118.88	124.80
25	6	602	CLA	CHD-C1D-ND	-4.21	118.88	124.80
25	B	607	CLA	CHD-C1D-ND	-4.21	118.88	124.80
29	L	101	SQD	O8-S-C6	-4.21	97.84	105.97
32	G	618	AJP	O84-C05-C06	4.21	119.80	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	606	CHL	C4D-CHA-CBD	-4.21	104.73	108.97
39	N	616	LUT	C38-C25-C24	-4.21	113.40	123.36
25	y	313	CLA	C1-C2-C3	-4.21	119.31	126.20
24	R	613	CHL	C4D-CHA-CBD	-4.20	104.73	108.97
40	r	617	NEX	C28-C29-C30	4.20	125.62	119.01
25	r	601	CLA	O2D-CGD-CBD	4.20	118.57	111.23
25	b	603	CLA	C1D-ND-C4D	-4.20	103.37	106.31
40	R	617	NEX	C28-C29-C30	4.20	125.61	119.01
24	Y	306	CHL	C4D-CHA-CBD	-4.20	104.74	108.97
38	f	101	HEM	C4D-ND-C1D	4.20	110.18	105.21
32	g	618	AJP	O25-C23-C24	4.20	117.80	109.64
26	r	618	LHG	O7-C7-C8	4.19	120.56	111.48
25	G	604	CLA	C1D-ND-C4D	-4.19	103.37	106.31
24	n	608	CHL	C4D-CHA-CBD	-4.19	104.74	108.97
32	Y	320	AJP	O77-C28-C29	4.19	120.28	109.86
32	y	320	AJP	O77-C28-C29	4.19	120.28	109.86
24	s	308	CHL	C4D-CHA-CBD	-4.19	104.74	108.97
25	r	603	CLA	C1-C2-C3	-4.19	119.34	126.20
32	N	620	AJP	C12-C07-C06	4.18	132.87	120.50
25	B	608	CLA	C1D-ND-C4D	-4.18	103.38	106.31
25	b	608	CLA	C1D-ND-C4D	-4.18	103.38	106.31
32	Y	321	AJP	O77-C28-C29	4.18	120.25	109.86
32	A	412	AJP	C03-C04-C05	-4.18	105.38	111.93
32	a	413	AJP	C03-C04-C05	-4.18	105.38	111.93
24	S	307	CHL	C4D-CHA-CBD	-4.18	104.75	108.97
25	C	511	CLA	CHD-C1D-ND	-4.18	118.92	124.80
25	c	511	CLA	CHD-C1D-ND	-4.18	118.92	124.80
25	R	601	CLA	O2D-CGD-CBD	4.18	118.53	111.23
39	R	615	LUT	C38-C25-C24	-4.18	113.47	123.36
32	y	321	AJP	O77-C28-C29	4.18	120.24	109.86
32	N	620	AJP	O25-C23-C24	4.18	117.76	109.64
32	n	620	AJP	O25-C23-C24	4.18	117.76	109.64
32	n	620	AJP	C12-C07-C06	4.17	132.84	120.50
25	S	303	CLA	C1D-ND-C4D	-4.17	103.38	106.31
25	s	303	CLA	C1D-ND-C4D	-4.17	103.38	106.31
40	G	617	NEX	C38-C25-C26	-4.17	115.44	122.30
39	g	615	LUT	C38-C25-C24	-4.17	113.50	123.36
39	r	615	LUT	C38-C25-C24	-4.17	113.50	123.36
25	N	613	CLA	CHD-C1D-ND	-4.17	118.94	124.80
38	F	101	HEM	C4D-ND-C1D	4.16	110.14	105.21
25	n	613	CLA	CHD-C1D-ND	-4.16	118.94	124.80
24	N	605	CHL	C4D-CHA-CBD	-4.16	104.77	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	605	CHL	C4D-CHA-CBD	-4.16	104.77	108.97
25	r	603	CLA	O2D-CGD-CBD	4.16	118.50	111.23
39	G	615	LUT	C38-C25-C24	-4.16	113.52	123.36
25	R	603	CLA	O2D-CGD-CBD	4.15	118.49	111.23
25	R	603	CLA	C1-C2-C3	-4.15	119.39	126.20
24	S	308	CHL	C4D-CHA-CBD	-4.15	104.78	108.97
24	s	307	CHL	C4D-CHA-CBD	-4.15	104.78	108.97
40	g	617	NEX	C38-C25-C26	-4.15	115.47	122.30
32	A	412	AJP	C04-C03-C02	-4.15	103.38	111.67
32	a	413	AJP	C04-C03-C02	-4.15	103.38	111.67
24	G	608	CHL	C4D-CHA-CBD	-4.15	104.78	108.97
24	G	607	CHL	OBD-CAD-CBD	-4.14	119.74	125.82
24	y	309	CHL	C4D-CHA-CBD	-4.14	104.79	108.97
32	N	620	AJP	O84-C05-C06	4.14	119.60	107.26
32	n	620	AJP	O84-C05-C06	4.14	119.60	107.26
24	N	606	CHL	C4D-CHA-CBD	-4.14	104.80	108.97
25	B	615	CLA	C1-C2-C3	-4.14	119.42	126.20
25	b	615	CLA	C1-C2-C3	-4.14	119.42	126.20
25	C	508	CLA	CHB-C1B-NB	-4.13	117.85	124.05
25	c	508	CLA	CHB-C1B-NB	-4.13	117.85	124.05
39	N	615	LUT	C38-C25-C24	-4.13	113.57	123.36
32	s	319	AJP	O77-C28-C27	4.13	118.71	110.15
39	n	615	LUT	C38-C25-C24	-4.13	113.58	123.36
25	D	402	CLA	C4A-NA-C1A	-4.13	104.79	106.68
25	B	603	CLA	C1D-ND-C4D	-4.13	103.42	106.31
25	n	611	CLA	C1-C2-C3	-4.13	119.44	126.20
39	y	317	LUT	C38-C25-C24	-4.13	113.59	123.36
25	D	403	CLA	C2A-C3A-C4A	-4.13	95.20	101.87
25	d	403	CLA	C2A-C3A-C4A	-4.13	95.20	101.87
24	g	608	CHL	C4D-CHA-CBD	-4.13	104.81	108.97
32	S	319	AJP	O77-C28-C27	4.12	118.69	110.15
26	C	517	LHG	O7-C7-C8	4.12	120.40	111.48
26	c	517	LHG	O7-C7-C8	4.12	120.40	111.48
25	2	604	CLA	C1-C2-C3	-4.12	119.44	126.20
25	6	604	CLA	C1-C2-C3	-4.12	119.44	126.20
39	Y	317	LUT	C38-C25-C24	-4.12	113.61	123.36
35	C	516	DGD	C1D-O6D-C5D	-4.12	105.68	113.72
35	c	516	DGD	C1D-O6D-C5D	-4.12	105.68	113.72
25	N	611	CLA	C1-C2-C3	-4.12	119.45	126.20
35	B	626	DGD	C3G-O3G-C1D	-4.12	104.97	113.80
35	b	626	DGD	C3G-O3G-C1D	-4.12	104.97	113.80
25	D	401	CLA	CHD-C1D-ND	-4.12	119.01	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	608	CLA	CHD-C1D-ND	-4.12	119.01	124.80
25	d	401	CLA	CHD-C1D-ND	-4.12	119.01	124.80
25	D	403	CLA	C1-C2-C3	-4.11	119.46	126.20
25	d	403	CLA	C1-C2-C3	-4.11	119.46	126.20
25	R	602	CLA	C1D-ND-C4D	-4.11	103.43	106.31
24	g	607	CHL	OBD-CAD-CBD	-4.11	119.79	125.82
25	Y	311	CLA	C4A-NA-C1A	-4.11	104.80	106.68
25	C	504	CLA	CHD-C1D-ND	-4.11	119.02	124.80
24	Y	309	CHL	C4D-CHA-CBD	-4.11	104.83	108.97
25	c	505	CLA	CHD-C1D-ND	-4.10	119.03	124.80
25	S	311	CLA	CHB-C1B-NB	-4.10	117.90	124.05
25	2	604	CLA	CHD-C1D-ND	-4.10	119.03	124.80
25	6	604	CLA	CHD-C1D-ND	-4.10	119.03	124.80
25	r	601	CLA	C4D-CHA-C1A	-4.10	116.35	121.24
29	A	407	SQD	O8-S-C6	-4.10	98.06	105.97
29	a	408	SQD	O8-S-C6	-4.10	98.06	105.97
32	B	624	AJP	C26-O25-C23	4.10	122.12	115.27
32	b	624	AJP	C26-O25-C23	4.10	122.12	115.27
25	c	504	CLA	CHD-C1D-ND	-4.10	119.04	124.80
25	r	608	CLA	CHD-C1D-ND	-4.10	119.04	124.80
25	C	502	CLA	C1-C2-C3	-4.10	119.49	126.20
24	Y	302	CHL	CBC-CAC-C3C	-4.09	107.01	112.87
25	C	502	CLA	C1D-ND-C4D	-4.09	103.44	106.31
25	c	502	CLA	C1D-ND-C4D	-4.09	103.44	106.31
25	R	601	CLA	C4D-CHA-C1A	-4.09	116.36	121.24
30	C	520	LMG	O7-C10-C11	4.09	120.33	111.48
30	c	520	LMG	O7-C10-C11	4.09	120.33	111.48
25	c	513	CLA	CHD-C1D-ND	-4.09	119.05	124.80
25	n	612	CLA	O2D-CGD-CBD	4.09	118.38	111.23
25	r	602	CLA	C1D-ND-C4D	-4.09	103.44	106.31
25	B	611	CLA	CHD-C1D-ND	-4.09	119.05	124.80
25	b	611	CLA	CHD-C1D-ND	-4.09	119.05	124.80
25	D	403	CLA	CHD-C1D-ND	-4.08	119.06	124.80
25	R	602	CLA	CHD-C1D-ND	-4.08	119.06	124.80
25	d	403	CLA	CHD-C1D-ND	-4.08	119.06	124.80
25	s	311	CLA	CHB-C1B-NB	-4.08	117.93	124.05
25	B	605	CLA	CHB-C1B-NB	-4.08	117.93	124.05
24	S	306	CHL	C4D-CHA-CBD	-4.08	104.86	108.97
24	s	306	CHL	C4D-CHA-CBD	-4.08	104.86	108.97
32	n	620	AJP	C03-C04-C05	-4.08	105.55	111.93
32	Y	320	AJP	O84-C05-C06	4.08	119.41	107.26
32	y	320	AJP	O84-C05-C06	4.08	119.41	107.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	CHD-C1D-ND	-4.07	119.07	124.80
25	d	402	CLA	C4A-NA-C1A	-4.07	104.82	106.68
25	r	602	CLA	CHD-C1D-ND	-4.07	119.07	124.80
25	c	502	CLA	C1-C2-C3	-4.07	119.53	126.20
25	C	513	CLA	C1-C2-C3	-4.07	119.53	126.20
25	c	513	CLA	C1-C2-C3	-4.07	119.53	126.20
25	r	601	CLA	CHD-C1D-C2D	4.07	133.95	125.49
24	y	302	CHL	CBC-CAC-C3C	-4.07	107.05	112.87
25	r	612	CLA	CHD-C1D-C2D	4.07	133.95	125.49
25	N	612	CLA	O2D-CGD-CBD	4.06	118.34	111.23
26	B	622	LHG	O7-C7-C8	4.06	120.27	111.48
26	b	622	LHG	O7-C7-C8	4.06	120.27	111.48
25	C	505	CLA	CHD-C1D-ND	-4.06	119.08	124.80
25	y	304	CLA	C1-C2-C3	-4.06	119.55	126.20
25	b	605	CLA	CHB-C1B-NB	-4.06	117.96	124.05
25	C	504	CLA	O2D-CGD-CBD	4.06	118.32	111.23
32	Y	323	AJP	C12-C07-C06	4.05	132.49	120.50
25	N	604	CLA	C4D-CHA-C1A	-4.05	116.41	121.24
25	c	504	CLA	O2D-CGD-CBD	4.05	118.32	111.23
25	b	603	CLA	CHD-C1D-ND	-4.05	119.10	124.80
39	y	316	LUT	C38-C25-C24	-4.05	113.77	123.36
32	y	323	AJP	C12-C07-C06	4.05	132.47	120.50
32	N	620	AJP	C03-C04-C05	-4.05	105.59	111.93
32	a	413	AJP	C35-O40-C39	4.05	121.63	113.72
25	R	601	CLA	CHD-C1D-C2D	4.05	133.91	125.49
25	n	604	CLA	C4D-CHA-C1A	-4.05	116.42	121.24
25	y	311	CLA	C4A-NA-C1A	-4.05	104.83	106.68
32	A	412	AJP	C35-O40-C39	4.05	121.63	113.72
25	S	303	CLA	C1-C2-C3	-4.05	119.57	126.20
25	r	608	CLA	C1-C2-C3	-4.04	119.57	126.20
25	C	511	CLA	C2A-C3A-C4A	-4.04	95.34	101.87
39	n	615	LUT	C18-C5-C4	-4.04	106.99	114.42
39	Y	316	LUT	C38-C25-C24	-4.04	113.79	123.36
25	R	612	CLA	CHD-C1D-C2D	4.04	133.89	125.49
25	G	602	CLA	C4A-NA-C1A	-4.04	104.83	106.68
25	g	602	CLA	C4A-NA-C1A	-4.04	104.83	106.68
25	S	303	CLA	CHD-C1D-ND	-4.04	119.12	124.80
25	n	603	CLA	C4A-NA-C1A	-4.04	104.84	106.68
32	B	624	AJP	C12-C07-C06	4.04	132.43	120.50
32	b	624	AJP	C12-C07-C06	4.04	132.43	120.50
26	Y	301	LHG	O7-C7-C8	4.04	120.21	111.48
39	N	615	LUT	C18-C5-C4	-4.04	107.00	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	608	CLA	C1-C2-C3	-4.04	119.59	126.20
25	C	506	CLA	C1-C2-C3	-4.03	119.59	126.20
25	c	506	CLA	C1-C2-C3	-4.03	119.59	126.20
25	B	606	CLA	CHB-C1B-NB	-4.03	118.00	124.05
25	b	606	CLA	CHB-C1B-NB	-4.03	118.00	124.05
26	B	621	LHG	O7-C7-C8	4.03	120.20	111.48
26	b	621	LHG	O7-C7-C8	4.03	120.20	111.48
25	N	604	CLA	CHD-C1D-ND	-4.03	119.13	124.80
26	Y	319	LHG	O7-C7-C8	4.03	120.19	111.48
32	g	618	AJP	O31-C26-C27	4.03	118.64	110.37
25	n	604	CLA	CHD-C1D-ND	-4.02	119.14	124.80
25	6	604	CLA	CHC-C4B-NB	-4.02	118.01	124.05
26	y	301	LHG	O7-C7-C8	4.02	120.18	111.48
25	B	603	CLA	CHD-C1D-ND	-4.02	119.14	124.80
25	s	303	CLA	C1-C2-C3	-4.02	119.61	126.20
25	G	603	CLA	C1D-ND-C4D	-4.02	103.49	106.31
25	g	603	CLA	C1D-ND-C4D	-4.02	103.49	106.31
32	Y	320	AJP	C12-C07-C06	4.02	132.38	120.50
32	y	320	AJP	C12-C07-C06	4.02	132.38	120.50
32	G	618	AJP	O31-C26-C27	4.02	118.63	110.37
26	y	319	LHG	O7-C7-C8	4.02	120.17	111.48
39	Y	317	LUT	C18-C5-C4	-4.01	107.04	114.42
25	R	603	CLA	CHD-C1D-ND	-4.01	119.15	124.80
24	n	601	CHL	CBC-CAC-C3C	-4.01	107.13	112.87
25	r	604	CLA	CHD-C1D-C2D	4.01	133.83	125.49
25	S	305	CLA	CHD-C1D-C2D	4.01	133.83	125.49
25	s	305	CLA	CHD-C1D-C2D	4.01	133.83	125.49
25	s	303	CLA	CHD-C1D-ND	-4.01	119.16	124.80
24	N	601	CHL	CBC-CAC-C3C	-4.01	107.14	112.87
25	c	511	CLA	C2A-C3A-C4A	-4.01	95.40	101.87
39	y	317	LUT	C18-C5-C4	-4.00	107.06	114.42
25	2	604	CLA	CHC-C4B-NB	-4.00	118.05	124.05
32	y	322	AJP	C29-C28-C27	4.00	116.43	110.67
25	Y	304	CLA	C1-C2-C3	-4.00	119.65	126.20
25	R	604	CLA	CHD-C1D-C2D	4.00	133.80	125.49
32	A	412	AJP	C26-O31-C30	4.00	121.52	113.72
32	a	413	AJP	C26-O31-C30	4.00	121.52	113.72
24	2	601	CHL	CAA-C2A-C3A	-3.99	102.20	113.00
25	G	603	CLA	C1-C2-C3	-3.99	119.66	126.20
25	D	402	CLA	C1-C2-C3	-3.99	119.66	126.20
25	y	305	CLA	C1-C2-C3	-3.99	120.31	126.76
25	S	304	CLA	CHB-C1B-NB	-3.99	118.06	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	304	CLA	CHB-C1B-NB	-3.99	118.06	124.05
25	C	501	CLA	CHD-C1D-ND	-3.99	119.19	124.80
25	c	501	CLA	CHD-C1D-ND	-3.99	119.19	124.80
25	s	314	CLA	C4A-NA-C1A	-3.99	104.86	106.68
25	b	612	CLA	CHD-C1D-ND	-3.99	119.19	124.80
32	N	620	AJP	O31-C30-C29	3.99	116.22	110.14
32	n	620	AJP	O31-C30-C29	3.99	116.22	110.14
39	n	616	LUT	C18-C5-C4	-3.98	107.09	114.42
25	n	614	CLA	O2D-CGD-CBD	3.98	118.19	111.23
25	R	610	CLA	CHD-C1D-ND	-3.98	119.20	124.80
25	B	614	CLA	CHD-C1D-ND	-3.98	119.20	124.80
25	b	614	CLA	CHD-C1D-ND	-3.98	119.20	124.80
25	R	610	CLA	CHD-C1D-C2D	3.98	133.77	125.49
25	r	610	CLA	CHD-C1D-C2D	3.98	133.77	125.49
32	Y	322	AJP	C29-C28-C27	3.98	116.40	110.67
25	s	305	CLA	CHD-C1D-ND	-3.98	119.20	124.80
25	6	602	CLA	C1-C2-C3	-3.98	119.68	126.20
39	N	616	LUT	C18-C5-C4	-3.98	107.11	114.42
30	b	623	LMG	O7-C10-C11	3.98	120.08	111.48
24	g	606	CHL	O1D-CGD-CBD	-3.97	118.70	124.72
24	6	601	CHL	CAA-C2A-C3A	-3.97	102.26	113.00
25	S	305	CLA	CHD-C1D-ND	-3.97	119.21	124.80
25	S	312	CLA	C1D-ND-C4D	-3.97	103.53	106.31
25	S	314	CLA	C4A-NA-C1A	-3.97	104.87	106.68
25	6	604	CLA	CHD-C1D-C2D	3.97	133.75	125.49
25	2	602	CLA	C1-C2-C3	-3.97	119.69	126.20
25	r	603	CLA	CHD-C1D-ND	-3.97	119.22	124.80
25	R	610	CLA	CHB-C1B-C2B	3.97	138.95	127.43
25	d	402	CLA	C1-C2-C3	-3.97	119.69	126.20
25	R	603	CLA	CHD-C1D-C2D	3.97	133.74	125.49
26	B	625	LHG	O7-C7-C8	3.97	120.06	111.48
26	b	625	LHG	O7-C7-C8	3.97	120.06	111.48
25	N	614	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	g	603	CLA	C1-C2-C3	-3.97	119.70	126.20
24	G	606	CHL	O1D-CGD-CBD	-3.97	118.71	124.72
25	2	604	CLA	CHD-C1D-C2D	3.96	133.73	125.49
25	r	610	CLA	CHD-C1D-ND	-3.96	119.22	124.80
40	n	617	NEX	C12-C13-C14	3.96	125.24	119.01
39	g	615	LUT	C18-C5-C4	-3.96	107.14	114.42
32	S	319	AJP	O84-C05-C06	3.96	119.07	107.26
32	s	319	AJP	O84-C05-C06	3.96	119.07	107.26
25	Y	305	CLA	C1-C2-C3	-3.96	120.35	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	615	LUT	C18-C5-C4	-3.96	107.14	114.42
25	r	610	CLA	CHB-C1B-C2B	3.96	138.92	127.43
25	R	614	CLA	O2D-CGD-CBD	3.96	118.15	111.23
30	A	410	LMG	O7-C10-C11	3.96	120.04	111.48
30	a	411	LMG	O7-C10-C11	3.96	120.04	111.48
25	r	614	CLA	O2D-CGD-CBD	3.96	118.15	111.23
30	B	623	LMG	O7-C10-C11	3.96	120.04	111.48
25	g	610	CLA	C1-C2-C3	-3.96	119.72	126.20
25	B	605	CLA	C1-C2-C3	-3.96	119.72	126.20
25	2	602	CLA	CHB-C1B-NB	-3.95	118.12	124.05
25	6	602	CLA	CHB-C1B-NB	-3.95	118.12	124.05
25	D	401	CLA	CHB-C1B-NB	-3.95	118.12	124.05
25	d	401	CLA	CHB-C1B-NB	-3.95	118.12	124.05
32	y	321	AJP	C21-C22-C23	3.95	115.75	110.46
25	s	313	CLA	C1-C2-C3	-3.95	119.72	126.20
25	B	615	CLA	C1D-ND-C4D	-3.95	103.54	106.31
25	2	602	CLA	C2D-C1D-ND	-3.95	106.22	110.13
25	6	602	CLA	C2D-C1D-ND	-3.95	106.22	110.13
25	n	603	CLA	C1D-ND-C4D	-3.95	103.54	106.31
25	N	603	CLA	C4A-NA-C1A	-3.95	104.88	106.68
25	G	610	CLA	C1-C2-C3	-3.95	119.73	126.20
25	r	609	CLA	C1-C2-C3	-3.94	119.73	126.20
25	n	613	CLA	C1-C2-C3	-3.94	119.74	126.20
32	Y	322	AJP	O31-C26-C27	3.94	118.47	110.37
40	N	617	NEX	C38-C25-C26	-3.94	115.81	122.30
25	r	603	CLA	CHD-C1D-C2D	3.94	133.69	125.49
32	B	624	AJP	O53-C46-C47	3.94	119.67	110.38
32	b	624	AJP	O53-C46-C47	3.94	119.67	110.38
32	N	619	AJP	O84-C05-C06	3.94	119.01	107.26
32	n	619	AJP	O84-C05-C06	3.94	119.01	107.26
26	l	103	LHG	O7-C7-C8	3.94	120.00	111.48
32	Y	322	AJP	O09-C05-C06	-3.94	99.32	104.56
32	Y	321	AJP	C21-C22-C23	3.94	115.73	110.46
25	B	612	CLA	CHD-C1D-ND	-3.94	119.26	124.80
32	y	322	AJP	O31-C26-C27	3.94	118.46	110.37
25	D	403	CLA	CHD-C1D-C2D	3.94	133.68	125.49
25	d	403	CLA	CHD-C1D-C2D	3.94	133.68	125.49
25	N	613	CLA	C1-C2-C3	-3.94	119.75	126.20
25	A	402	CLA	CHB-C1B-NB	-3.93	118.15	124.05
25	a	403	CLA	CHB-C1B-NB	-3.93	118.15	124.05
25	C	504	CLA	CHD-C1D-C2D	3.93	133.67	125.49
25	c	504	CLA	CHD-C1D-C2D	3.93	133.67	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	313	CLA	C1-C2-C3	-3.93	119.75	126.20
32	y	322	AJP	O09-C05-C06	-3.93	99.33	104.56
25	b	605	CLA	C1-C2-C3	-3.93	119.76	126.20
25	R	609	CLA	C1-C2-C3	-3.93	119.76	126.20
40	n	617	NEX	C38-C25-C26	-3.93	115.84	122.30
25	A	401	CLA	C1-C2-C3	-3.93	119.77	126.20
26	L	102	LHG	O7-C7-C8	3.93	119.97	111.48
40	Y	318	NEX	C38-C25-C26	-3.92	115.84	122.30
40	y	318	NEX	C38-C25-C26	-3.92	115.84	122.30
40	N	617	NEX	C12-C13-C14	3.92	125.18	119.01
32	Y	323	AJP	O25-C26-O31	3.92	121.01	110.69
32	y	323	AJP	O25-C26-O31	3.92	121.01	110.69
25	S	310	CLA	C1D-ND-C4D	-3.92	103.56	106.31
25	N	603	CLA	C1D-ND-C4D	-3.92	103.56	106.31
30	A	408	LMG	O7-C10-C11	3.92	119.96	111.48
25	b	612	CLA	C1D-ND-C4D	-3.92	103.56	106.31
26	d	406	LHG	O7-C7-C8	3.92	119.95	111.48
32	A	412	AJP	C67-C68-C69	-3.92	103.13	110.23
32	a	413	AJP	C67-C68-C69	-3.92	103.13	110.23
39	r	615	LUT	C18-C5-C4	-3.92	107.22	114.42
30	B	620	LMG	O7-C10-C11	3.91	119.95	111.48
30	b	620	LMG	O7-C10-C11	3.91	119.95	111.48
25	n	603	CLA	CHD-C1D-ND	-3.91	119.30	124.80
25	a	402	CLA	C1-C2-C3	-3.91	119.79	126.20
25	c	509	CLA	C1D-ND-C4D	-3.91	103.57	106.31
26	D	406	LHG	O7-C7-C8	3.91	119.94	111.48
25	C	509	CLA	C1D-ND-C4D	-3.91	103.57	106.31
39	R	615	LUT	C18-C5-C4	-3.91	107.23	114.42
25	s	310	CLA	C1D-ND-C4D	-3.91	103.57	106.31
32	Y	323	AJP	O25-C23-C24	3.91	117.23	109.64
32	y	323	AJP	O25-C23-C24	3.91	117.23	109.64
25	b	615	CLA	C1D-ND-C4D	-3.90	103.58	106.31
25	B	612	CLA	C1-C2-C3	-3.90	119.81	126.20
25	b	612	CLA	C1-C2-C3	-3.90	119.81	126.20
25	B	613	CLA	O2D-CGD-CBD	3.90	118.05	111.23
25	b	613	CLA	O2D-CGD-CBD	3.90	118.05	111.23
25	r	610	CLA	C4D-CHA-C1A	-3.90	116.59	121.24
32	y	322	AJP	C03-C04-C05	-3.90	105.83	111.93
39	y	316	LUT	C18-C5-C4	-3.89	107.26	114.42
25	s	312	CLA	C1D-ND-C4D	-3.89	103.58	106.31
32	A	412	AJP	C26-C27-C28	-3.89	101.82	110.01
32	a	413	AJP	C26-C27-C28	-3.89	101.82	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	409	LMG	O7-C10-C11	3.89	119.90	111.48
25	N	603	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	y	314	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	G	602	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
39	Y	316	LUT	C18-C5-C4	-3.89	107.27	114.42
25	B	608	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	b	608	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	Y	304	CLA	C1D-ND-C4D	-3.89	103.58	106.31
32	Y	322	AJP	C03-C04-C05	-3.88	105.85	111.93
25	Y	314	CLA	CHD-C1D-ND	-3.88	119.34	124.80
32	Y	320	AJP	O82-C10-C11	3.88	127.07	113.68
25	g	602	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
32	y	320	AJP	O82-C10-C11	3.88	127.06	113.68
25	G	604	CLA	C4D-CHA-C1A	-3.88	116.62	121.24
25	B	608	CLA	C1-C2-C3	-3.88	119.84	126.20
25	b	608	CLA	C1-C2-C3	-3.88	119.84	126.20
25	r	601	CLA	CHD-C1D-ND	-3.88	119.35	124.80
32	Y	324	AJP	C12-C07-C06	3.88	131.96	120.50
25	B	603	CLA	C4A-NA-C1A	-3.87	104.91	106.68
25	b	603	CLA	C4A-NA-C1A	-3.87	104.91	106.68
25	B	606	CLA	C1-C2-C3	-3.87	119.86	126.20
25	b	606	CLA	C1-C2-C3	-3.87	119.86	126.20
25	b	609	CLA	C1-C2-C3	-3.87	119.86	126.20
25	B	612	CLA	C1D-ND-C4D	-3.87	103.60	106.31
40	S	317	NEX	C38-C25-C26	-3.87	115.94	122.30
40	s	317	NEX	C38-C25-C26	-3.87	115.94	122.30
25	R	610	CLA	C4D-CHA-C1A	-3.87	116.63	121.24
25	B	609	CLA	C1-C2-C3	-3.87	119.86	126.20
26	s	301	LHG	O7-C7-C8	3.87	119.84	111.48
25	Y	312	CLA	C1-C2-C3	-3.86	119.86	126.20
25	y	312	CLA	C1-C2-C3	-3.86	119.86	126.20
32	A	412	AJP	C12-C07-C06	3.86	131.92	120.50
32	a	413	AJP	C12-C07-C06	3.86	131.92	120.50
32	y	324	AJP	C12-C07-C06	3.86	131.92	120.50
26	c	518	LHG	O7-C7-C8	3.86	119.83	111.48
25	y	311	CLA	CHD-C1D-ND	-3.86	119.37	124.80
26	S	301	LHG	O7-C7-C8	3.86	119.83	111.48
25	b	613	CLA	C4A-NA-C1A	-3.86	104.92	106.68
32	y	322	AJP	C12-C07-C06	3.86	131.90	120.50
26	C	518	LHG	O7-C7-C8	3.86	119.82	111.48
25	R	601	CLA	CHD-C1D-ND	-3.85	119.38	124.80
27	A	404	PHO	C1-C2-C3	-3.85	119.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	405	PHO	C1-C2-C3	-3.85	119.89	126.20
25	B	607	CLA	C1D-ND-C4D	-3.85	103.61	106.31
25	b	607	CLA	C1D-ND-C4D	-3.85	103.61	106.31
25	Y	311	CLA	CHD-C1D-ND	-3.85	119.39	124.80
25	g	604	CLA	C4D-CHA-C1A	-3.85	116.66	121.24
32	a	413	AJP	C17-C16-C11	-3.85	106.86	112.29
32	B	624	AJP	C17-C16-C11	-3.84	106.87	112.29
32	b	624	AJP	C17-C16-C11	-3.84	106.87	112.29
25	c	509	CLA	CHD-C1D-ND	-3.84	119.40	124.80
25	C	509	CLA	CHD-C1D-ND	-3.84	119.40	124.80
30	D	407	LMG	O7-C10-C11	3.84	119.78	111.48
30	d	407	LMG	O7-C10-C11	3.84	119.78	111.48
25	y	304	CLA	C1D-ND-C4D	-3.84	103.62	106.31
32	Y	322	AJP	C12-C07-C06	3.84	131.84	120.50
25	N	613	CLA	CHB-C1B-NB	-3.83	118.30	124.05
25	n	604	CLA	C1D-ND-C4D	-3.83	103.62	106.31
40	n	617	NEX	C27-C28-C29	-3.83	119.58	125.53
25	B	611	CLA	C1-C2-C3	-3.83	119.92	126.20
25	b	611	CLA	C1-C2-C3	-3.83	119.92	126.20
25	R	603	CLA	CHB-C1B-C2B	3.83	138.54	127.43
25	g	613	CLA	CHB-C1B-NB	-3.83	118.31	124.05
25	y	312	CLA	C4A-NA-C1A	-3.83	104.93	106.68
25	N	612	CLA	C1-C2-C3	-3.83	119.93	126.20
25	n	612	CLA	C1-C2-C3	-3.83	119.93	126.20
25	c	503	CLA	CHB-C1B-NB	-3.83	118.31	124.05
25	c	504	CLA	CHB-C1B-C2B	3.83	138.53	127.43
25	C	504	CLA	CHB-C1B-C2B	3.82	138.53	127.43
32	A	412	AJP	C17-C16-C11	-3.82	106.89	112.29
25	n	602	CLA	C1-C2-C3	-3.82	119.93	126.20
25	b	609	CLA	CHD-C1D-ND	-3.82	119.42	124.80
25	B	604	CLA	C4A-NA-C1A	-3.82	104.94	106.68
25	b	604	CLA	C4A-NA-C1A	-3.82	104.94	106.68
39	s	315	LUT	C18-C5-C4	-3.82	107.40	114.42
25	Y	314	CLA	C1-C2-C3	-3.81	119.95	126.20
25	C	503	CLA	CHB-C1B-NB	-3.81	118.33	124.05
25	n	613	CLA	CHB-C1B-NB	-3.81	118.33	124.05
25	s	311	CLA	C1-C2-C3	-3.81	119.95	126.20
32	n	619	AJP	C12-C07-C06	3.81	131.76	120.50
32	N	619	AJP	C12-C07-C06	3.81	131.76	120.50
40	N	617	NEX	C27-C28-C29	-3.81	119.62	125.53
32	S	319	AJP	C12-C07-C06	3.81	131.76	120.50
32	s	319	AJP	C12-C07-C06	3.81	131.76	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	314	CLA	C1-C2-C3	-3.81	119.96	126.20
39	S	315	LUT	C18-C5-C4	-3.81	107.42	114.42
25	C	509	CLA	C1-C2-C3	-3.81	119.96	126.20
25	S	312	CLA	C2A-C3A-C4A	-3.80	95.72	101.87
25	r	603	CLA	CHB-C1B-C2B	3.80	138.47	127.43
25	G	613	CLA	CHB-C1B-NB	-3.80	118.34	124.05
26	2	606	LHG	O7-C7-C8	3.80	119.70	111.48
25	G	611	CLA	C1-C2-C3	-3.80	119.97	126.20
26	6	606	LHG	O7-C7-C8	3.80	119.70	111.48
25	A	405	CLA	C1-C2-C3	-3.80	119.97	126.20
25	a	406	CLA	C1-C2-C3	-3.80	119.97	126.20
32	y	324	AJP	C03-C04-C05	-3.80	105.98	111.93
25	N	602	CLA	C1-C2-C3	-3.80	119.97	126.20
25	B	609	CLA	CHD-C1D-ND	-3.80	119.46	124.80
25	B	613	CLA	C4A-NA-C1A	-3.80	104.95	106.68
25	s	312	CLA	C2A-C3A-C4A	-3.79	95.74	101.87
32	B	624	AJP	O53-C46-C45	3.79	119.12	110.08
32	b	624	AJP	O53-C46-C45	3.79	119.12	110.08
32	y	323	AJP	C21-C22-C23	3.79	115.53	110.46
25	n	610	CLA	CHD-C1D-ND	-3.79	119.47	124.80
35	c	515	DGD	O2G-C1B-C2B	3.79	119.69	111.48
32	g	618	AJP	O77-C28-C29	3.79	119.28	109.86
25	G	610	CLA	C4D-CHA-C1A	-3.79	116.72	121.24
32	G	618	AJP	O77-C28-C29	3.79	119.28	109.86
32	Y	324	AJP	C03-C04-C05	-3.79	106.00	111.93
41	r	616	XAT	C18-C5-C6	-3.79	116.07	122.30
25	C	503	CLA	C1D-ND-C4D	-3.78	103.66	106.31
25	b	602	CLA	CHD-C1D-ND	-3.78	119.48	124.80
35	C	515	DGD	O2G-C1B-C2B	3.78	119.66	111.48
25	g	611	CLA	C1-C2-C3	-3.78	120.00	126.20
25	B	614	CLA	C1-C2-C3	-3.78	120.01	126.20
25	R	612	CLA	C1-C2-C3	-3.78	120.01	126.20
25	c	509	CLA	C1-C2-C3	-3.78	120.01	126.20
26	s	318	LHG	O7-C7-C8	3.78	119.65	111.48
25	N	604	CLA	O2D-CGD-CBD	3.78	117.83	111.23
24	G	601	CHL	CBC-CAC-C3C	-3.78	107.47	112.87
25	S	309	CLA	C1D-ND-C4D	-3.77	103.67	106.31
25	N	610	CLA	CHD-C1D-ND	-3.77	119.50	124.80
26	S	318	LHG	O7-C7-C8	3.77	119.64	111.48
25	S	311	CLA	C1-C2-C3	-3.77	120.02	126.20
41	R	616	XAT	C18-C5-C6	-3.77	116.10	122.30
25	B	606	CLA	CHD-C1D-C2D	3.77	133.33	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	CHD-C1D-C2D	3.77	133.33	125.49
25	n	604	CLA	O2D-CGD-CBD	3.77	117.82	111.23
25	C	512	CLA	C1-C2-C3	-3.77	120.02	126.20
25	c	512	CLA	C1-C2-C3	-3.77	120.02	126.20
25	r	612	CLA	C1-C2-C3	-3.77	120.03	126.20
25	2	602	CLA	C2B-C1B-NB	-3.77	106.42	110.33
25	6	602	CLA	C2B-C1B-NB	-3.77	106.42	110.33
25	B	603	CLA	C1-C2-C3	-3.76	120.03	126.20
25	b	614	CLA	C1-C2-C3	-3.76	120.03	126.20
25	y	303	CLA	C1-C2-C3	-3.76	120.03	126.20
25	Y	303	CLA	C1-C2-C3	-3.76	120.03	126.20
32	y	321	AJP	C12-C07-C06	3.76	131.61	120.50
25	N	604	CLA	C1D-ND-C4D	-3.76	103.67	106.31
25	B	602	CLA	CHD-C1D-ND	-3.76	119.51	124.80
25	s	313	CLA	CHD-C1D-C2D	3.76	133.31	125.49
25	g	610	CLA	C4D-CHA-C1A	-3.76	116.77	121.24
25	B	601	CLA	CHD-C1D-C2D	3.75	133.29	125.49
32	Y	323	AJP	C21-C22-C23	3.75	115.48	110.46
25	S	313	CLA	CHD-C1D-C2D	3.75	133.28	125.49
32	Y	321	AJP	C12-C07-C06	3.75	131.58	120.50
25	G	610	CLA	CHD-C1D-ND	-3.75	119.53	124.80
25	b	603	CLA	C1-C2-C3	-3.75	120.06	126.20
24	g	601	CHL	CBC-CAC-C3C	-3.75	107.51	112.87
32	N	619	AJP	O25-C26-O31	3.74	120.54	110.69
25	A	405	CLA	C1D-ND-C4D	-3.74	103.69	106.31
25	n	604	CLA	CHB-C1B-NB	-3.74	118.44	124.05
25	b	601	CLA	CHD-C1D-C2D	3.74	133.27	125.49
25	B	611	CLA	C1D-ND-C4D	-3.74	103.69	106.31
32	Y	322	AJP	C21-C20-C19	3.74	110.80	107.23
25	C	501	CLA	CHD-C1D-C2D	3.73	133.25	125.49
25	c	501	CLA	CHD-C1D-C2D	3.73	133.25	125.49
32	n	619	AJP	O25-C26-O31	3.73	120.52	110.69
25	c	503	CLA	C1D-ND-C4D	-3.73	103.69	106.31
32	a	413	AJP	C45-O44-C37	-3.73	109.13	117.98
32	n	619	AJP	C29-C28-C27	3.73	116.04	110.67
32	A	412	AJP	C45-O44-C37	-3.73	109.13	117.98
25	b	611	CLA	C1D-ND-C4D	-3.73	103.70	106.31
25	6	604	CLA	C3B-C4B-NB	-3.73	107.20	110.53
25	A	402	CLA	C1-C2-C3	-3.73	120.09	126.20
25	a	403	CLA	C1-C2-C3	-3.73	120.09	126.20
25	b	601	CLA	C1-C2-C3	-3.72	120.09	126.20
35	c	516	DGD	O2G-C1B-C2B	3.72	119.54	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	C1D-ND-C4D	-3.72	103.70	106.31
25	A	401	CLA	CHB-C1B-NB	-3.72	118.47	124.05
25	a	402	CLA	CHB-C1B-NB	-3.72	118.47	124.05
25	g	610	CLA	CHD-C1D-ND	-3.72	119.57	124.80
35	C	516	DGD	O2G-C1B-C2B	3.72	119.53	111.48
25	2	604	CLA	C3B-C4B-NB	-3.72	107.21	110.53
25	y	314	CLA	C1D-ND-C4D	-3.72	103.70	106.31
32	B	624	AJP	C65-O70-C69	3.72	120.98	113.72
25	N	604	CLA	CHB-C1B-NB	-3.71	118.48	124.05
25	c	510	CLA	CHB-C1B-NB	-3.71	118.48	124.05
32	N	619	AJP	C29-C28-C27	3.71	116.02	110.67
25	R	614	CLA	CHD-C1D-ND	-3.71	119.58	124.80
25	r	614	CLA	CHD-C1D-ND	-3.71	119.58	124.80
32	b	624	AJP	C65-O70-C69	3.71	120.97	113.72
24	2	603	CHL	O2D-CGD-O1D	-3.71	116.62	123.85
24	6	603	CHL	O2D-CGD-O1D	-3.71	116.62	123.85
25	B	601	CLA	C1-C2-C3	-3.71	120.12	126.20
25	r	601	CLA	C2D-C1D-ND	-3.71	106.45	110.13
25	Y	312	CLA	C4A-NA-C1A	-3.71	104.99	106.68
25	G	604	CLA	CHD-C1D-ND	-3.70	119.59	124.80
25	S	305	CLA	CHB-C1B-C2B	3.70	138.17	127.43
25	s	305	CLA	CHB-C1B-C2B	3.70	138.17	127.43
25	R	601	CLA	C2D-C1D-ND	-3.70	106.46	110.13
25	R	603	CLA	C2A-C3A-C4A	-3.70	95.89	101.87
25	r	603	CLA	C2A-C3A-C4A	-3.70	95.89	101.87
32	y	322	AJP	C21-C20-C19	3.70	110.77	107.23
25	C	510	CLA	CHB-C1B-NB	-3.70	118.50	124.05
32	B	624	AJP	C38-C37-C36	3.70	120.04	111.72
32	b	624	AJP	C38-C37-C36	3.70	120.04	111.72
25	C	503	CLA	C1-C2-C3	-3.70	120.14	126.20
25	c	503	CLA	C1-C2-C3	-3.70	120.14	126.20
39	Y	317	LUT	C11-C10-C9	-3.69	122.10	127.28
25	B	613	CLA	C1-C2-C3	-3.69	120.15	126.20
25	b	613	CLA	C1-C2-C3	-3.69	120.15	126.20
25	C	513	CLA	C1D-ND-C4D	-3.69	103.72	106.31
39	y	317	LUT	C11-C10-C9	-3.69	122.10	127.28
25	s	309	CLA	C1D-ND-C4D	-3.69	103.72	106.31
25	2	604	CLA	C4D-C3D-CAD	-3.69	104.10	108.11
25	6	604	CLA	C4D-C3D-CAD	-3.69	104.10	108.11
32	Y	321	AJP	C04-C05-C06	3.68	122.33	115.66
25	g	604	CLA	CHD-C1D-ND	-3.68	119.63	124.80
39	S	316	LUT	C18-C5-C4	-3.68	107.66	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	316	LUT	C18-C5-C4	-3.67	107.66	114.42
25	Y	311	CLA	C4D-CHA-C1A	-3.67	116.87	121.24
25	y	311	CLA	C4D-CHA-C1A	-3.67	116.87	121.24
25	c	513	CLA	C1D-ND-C4D	-3.67	103.74	106.31
32	y	321	AJP	C04-C05-C06	3.67	122.30	115.66
25	g	603	CLA	CHD-C1D-ND	-3.66	119.65	124.80
25	Y	304	CLA	CHD-C1D-ND	-3.66	119.65	124.80
32	N	620	AJP	C06-C07-C08	-3.66	98.40	104.28
25	S	309	CLA	C3A-C2A-C1A	-3.66	95.86	101.34
32	B	624	AJP	O09-C05-C06	-3.65	99.70	104.56
32	b	624	AJP	O09-C05-C06	-3.65	99.70	104.56
25	Y	314	CLA	C1D-ND-C4D	-3.65	103.75	106.31
40	N	617	NEX	C35-C34-C33	-3.65	122.16	127.28
32	n	620	AJP	C04-C03-C02	-3.65	104.38	111.67
25	G	603	CLA	CHD-C1D-ND	-3.65	119.67	124.80
25	s	309	CLA	C3A-C2A-C1A	-3.65	95.88	101.34
32	B	624	AJP	O44-C37-C36	3.65	116.68	107.42
32	b	624	AJP	O44-C37-C36	3.65	116.68	107.42
32	n	620	AJP	C06-C07-C08	-3.64	98.43	104.28
41	r	616	XAT	C11-C10-C9	-3.64	122.17	127.28
39	G	616	LUT	C18-C5-C4	-3.64	107.73	114.42
35	b	626	DGD	O2G-C1B-C2B	3.64	119.35	111.48
24	y	310	CHL	CBC-CAC-C3C	-3.64	107.67	112.87
24	Y	310	CHL	CBC-CAC-C3C	-3.63	107.67	112.87
32	N	620	AJP	C04-C03-C02	-3.63	104.42	111.67
25	R	602	CLA	C4D-CHA-C1A	-3.63	116.91	121.24
24	1	302	CHL	CMA-C3A-C4A	-3.63	106.79	114.61
25	D	403	CLA	CHB-C1B-C2B	3.63	137.96	127.43
25	d	403	CLA	CHB-C1B-C2B	3.63	137.96	127.43
25	C	512	CLA	CHB-C1B-NB	-3.63	118.61	124.05
25	c	512	CLA	CHB-C1B-NB	-3.63	118.61	124.05
25	2	602	CLA	CHC-C1C-NC	-3.63	118.85	124.31
25	6	602	CLA	CHC-C1C-NC	-3.63	118.85	124.31
32	Y	323	AJP	O25-C26-C27	3.62	117.01	108.09
32	y	323	AJP	O25-C26-C27	3.62	117.01	108.09
39	g	616	LUT	C18-C5-C4	-3.62	107.76	114.42
35	B	626	DGD	O2G-C1B-C2B	3.62	119.31	111.48
25	Y	314	CLA	C4D-CHA-C1A	-3.62	116.93	121.24
25	y	314	CLA	C4D-CHA-C1A	-3.62	116.93	121.24
25	G	612	CLA	CHD-C1D-ND	-3.61	119.72	124.80
25	g	612	CLA	CHD-C1D-ND	-3.61	119.72	124.80
24	5	302	CHL	CMA-C3A-C4A	-3.61	106.83	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	624	AJP	O44-C45-C46	3.61	116.97	108.09
32	b	624	AJP	O44-C45-C46	3.61	116.97	108.09
25	C	501	CLA	CHB-C1B-C2B	3.61	137.90	127.43
25	c	501	CLA	CHB-C1B-C2B	3.61	137.90	127.43
25	G	613	CLA	C1-C2-C3	-3.61	120.29	126.20
25	r	602	CLA	C4D-CHA-C1A	-3.61	116.94	121.24
25	g	613	CLA	C1-C2-C3	-3.61	120.29	126.20
25	B	611	CLA	CHB-C1B-NB	-3.60	118.64	124.05
25	b	611	CLA	CHB-C1B-NB	-3.60	118.64	124.05
25	y	304	CLA	CHD-C1D-ND	-3.60	119.73	124.80
25	b	612	CLA	CHB-C1B-NB	-3.60	118.64	124.05
25	n	610	CLA	C4D-CHA-C1A	-3.60	116.95	121.24
24	2	603	CHL	CMA-C3A-C4A	-3.60	106.85	114.61
25	Y	315	CLA	O2D-CGD-CBD	3.60	117.52	111.23
25	y	315	CLA	O2D-CGD-CBD	3.60	117.52	111.23
40	n	617	NEX	C35-C34-C33	-3.60	122.23	127.28
41	R	616	XAT	C11-C10-C9	-3.60	122.23	127.28
25	A	405	CLA	CHB-C1B-NB	-3.60	118.65	124.05
25	N	602	CLA	O1D-CGD-CBD	-3.60	117.42	124.52
40	r	617	NEX	C20-C13-C14	-3.60	116.99	122.82
25	Y	304	CLA	C4D-CHA-C1A	-3.60	116.95	121.24
25	y	304	CLA	C4D-CHA-C1A	-3.60	116.95	121.24
32	y	322	AJP	O84-C05-C06	3.59	117.97	107.26
40	R	617	NEX	C20-C13-C14	-3.59	117.00	122.82
24	y	302	CHL	CMA-C3A-C4A	-3.59	106.87	114.61
24	G	609	CHL	CBC-CAC-C3C	-3.59	107.73	112.87
24	Y	302	CHL	CMA-C3A-C4A	-3.59	106.87	114.61
24	6	603	CHL	CMA-C3A-C4A	-3.59	106.88	114.61
30	B	623	LMG	C1-O6-C5	-3.59	106.71	113.72
40	R	617	NEX	C11-C10-C9	3.59	132.31	127.28
40	r	617	NEX	C11-C10-C9	3.59	132.31	127.28
25	c	511	CLA	C1-C2-C3	-3.59	120.32	126.20
25	S	305	CLA	C2A-C3A-C4A	-3.59	96.07	101.87
25	N	610	CLA	C4D-CHA-C1A	-3.59	116.97	121.24
32	Y	322	AJP	O84-C05-C06	3.59	117.95	107.26
25	a	406	CLA	CHB-C1B-NB	-3.58	118.67	124.05
25	D	402	CLA	C4D-CHA-C1A	-3.58	116.97	121.24
25	d	402	CLA	C4D-CHA-C1A	-3.58	116.97	121.24
25	n	612	CLA	C1D-ND-C4D	-3.58	103.80	106.31
24	g	601	CHL	CMA-C3A-C4A	-3.58	106.89	114.61
25	c	506	CLA	CHD-C1D-ND	-3.58	119.77	124.80
25	B	612	CLA	CHB-C1B-NB	-3.58	118.68	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C1-C2-C3	-3.58	120.34	126.20
25	b	602	CLA	C1-C2-C3	-3.58	120.34	126.20
24	G	605	CHL	CMA-C3A-C4A	-3.58	106.91	114.61
25	C	511	CLA	C1-C2-C3	-3.58	120.34	126.20
25	s	305	CLA	C2A-C3A-C4A	-3.58	96.09	101.87
30	b	623	LMG	C1-O6-C5	-3.57	106.74	113.72
25	B	616	CLA	CHD-C1D-ND	-3.57	119.77	124.80
25	b	616	CLA	CHD-C1D-ND	-3.57	119.77	124.80
32	S	319	AJP	O77-C28-C29	3.57	118.74	109.86
24	G	601	CHL	CMA-C3A-C4A	-3.57	106.92	114.61
25	G	614	CLA	CHD-C1D-ND	-3.57	119.78	124.80
25	g	614	CLA	CHD-C1D-ND	-3.57	119.78	124.80
25	S	310	CLA	C1-C2-C3	-3.57	120.35	126.20
25	n	602	CLA	O1D-CGD-CBD	-3.57	117.48	124.52
25	y	314	CLA	CHB-C1B-NB	-3.57	118.69	124.05
35	A	415	DGD	O2G-C1B-C2B	3.57	119.20	111.48
35	a	401	DGD	O2G-C1B-C2B	3.57	119.20	111.48
32	s	319	AJP	O77-C28-C29	3.57	118.73	109.86
32	b	624	AJP	C04-C03-C02	-3.57	104.55	111.67
24	g	605	CHL	CMA-C3A-C4A	-3.57	106.93	114.61
25	Y	305	CLA	CHD-C1D-ND	-3.56	119.79	124.80
25	y	305	CLA	CHD-C1D-ND	-3.56	119.79	124.80
25	C	510	CLA	CHD-C1D-C2D	3.56	132.90	125.49
24	2	603	CHL	C3C-C4C-NC	-3.56	105.95	114.65
25	C	506	CLA	CHD-C1D-ND	-3.56	119.79	124.80
25	Y	311	CLA	C1-C2-C3	-3.56	120.37	126.20
25	y	311	CLA	C1-C2-C3	-3.56	120.37	126.20
32	B	624	AJP	C04-C03-C02	-3.56	104.57	111.67
25	c	510	CLA	CHD-C1D-C2D	3.56	132.88	125.49
25	s	310	CLA	C1-C2-C3	-3.55	120.38	126.20
24	Y	307	CHL	CMA-C3A-C4A	-3.55	106.96	114.61
24	y	307	CHL	CMA-C3A-C4A	-3.55	106.96	114.61
24	2	603	CHL	C1A-CHA-C4D	3.55	124.90	118.98
24	2	603	CHL	C3D-C4D-CHA	3.55	113.93	108.54
24	6	603	CHL	C3C-C4C-NC	-3.55	105.98	114.65
24	R	607	CHL	CMA-C3A-C4A	-3.55	106.97	114.61
32	Y	322	AJP	O25-C26-C27	3.54	116.81	108.09
32	y	322	AJP	O25-C26-C27	3.54	116.81	108.09
26	C	519	LHG	O7-C7-C8	3.54	119.14	111.48
26	c	519	LHG	O7-C7-C8	3.54	119.14	111.48
24	2	601	CHL	CBC-CAC-C3C	-3.54	107.80	112.87
24	6	601	CHL	CBC-CAC-C3C	-3.54	107.80	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	612	CLA	C1-C2-C3	-3.54	120.40	126.20
35	A	415	DGD	C6D-O5D-C1E	-3.54	106.21	113.80
35	a	401	DGD	C6D-O5D-C1E	-3.54	106.21	113.80
38	f	101	HEM	CHD-C4C-NC	3.54	128.31	124.45
25	A	402	CLA	C4D-CHA-C1A	-3.54	117.02	121.24
25	a	403	CLA	C4D-CHA-C1A	-3.54	117.02	121.24
24	n	605	CHL	CAA-C2A-C3A	-3.54	103.44	113.00
24	N	605	CHL	CAA-C2A-C3A	-3.54	103.44	113.00
38	F	101	HEM	CHD-C4C-NC	3.53	128.30	124.45
25	R	602	CLA	O2D-CGD-CBD	3.53	117.41	111.23
24	g	609	CHL	CBC-CAC-C3C	-3.53	107.81	112.87
25	Y	314	CLA	CHB-C1B-NB	-3.53	118.75	124.05
24	r	607	CHL	CMA-C3A-C4A	-3.53	107.00	114.61
32	A	412	AJP	C49-C48-C47	3.53	114.78	109.64
24	6	603	CHL	C1A-CHA-C4D	3.53	124.87	118.98
25	r	602	CLA	O2D-CGD-CBD	3.53	117.40	111.23
25	N	613	CLA	C1D-ND-C4D	-3.53	103.84	106.31
25	n	613	CLA	C1D-ND-C4D	-3.53	103.84	106.31
32	Y	321	AJP	O09-C05-C06	-3.53	99.87	104.56
24	R	605	CHL	CMA-C3A-C4A	-3.52	107.02	114.61
32	a	413	AJP	C21-C22-C23	3.52	115.17	110.46
32	a	413	AJP	C49-C48-C47	3.52	114.77	109.64
25	r	608	CLA	C1D-ND-C4D	-3.52	103.84	106.31
24	6	603	CHL	C3D-C4D-CHA	3.52	113.89	108.54
25	N	612	CLA	C1D-ND-C4D	-3.52	103.84	106.31
25	G	612	CLA	C1-C2-C3	-3.52	120.43	126.20
25	B	607	CLA	C1-C2-C3	-3.52	120.43	126.20
32	G	618	AJP	O25-C26-O31	3.52	119.94	110.69
25	g	611	CLA	C3D-C2D-C1D	3.52	110.63	105.83
32	g	618	AJP	O25-C26-O31	3.51	119.94	110.69
24	N	601	CHL	CMA-C3A-C4A	-3.51	107.04	114.61
24	r	607	CHL	CBC-CAC-C3C	-3.51	107.84	112.87
24	r	605	CHL	CBC-CAC-C3C	-3.51	107.84	112.87
25	S	314	CLA	CHD-C1D-ND	-3.51	119.86	124.80
25	s	314	CLA	CHD-C1D-ND	-3.51	119.86	124.80
32	y	321	AJP	O09-C05-C06	-3.51	99.89	104.56
24	S	302	CHL	CBC-CAC-C3C	-3.51	107.85	112.87
24	s	302	CHL	CBC-CAC-C3C	-3.51	107.85	112.87
24	r	605	CHL	CMA-C3A-C4A	-3.50	107.06	114.61
24	y	306	CHL	CBC-CAC-C3C	-3.50	107.86	112.87
24	R	605	CHL	CBC-CAC-C3C	-3.50	107.86	112.87
25	c	508	CLA	C1-C2-C3	-3.50	120.46	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	502	CLA	C4D-CHA-C1A	-3.50	117.07	121.24
25	G	611	CLA	C3D-C2D-C1D	3.50	110.60	105.83
24	n	601	CHL	CMA-C3A-C4A	-3.49	107.08	114.61
24	R	607	CHL	CBC-CAC-C3C	-3.49	107.87	112.87
24	Y	306	CHL	CBC-CAC-C3C	-3.49	107.87	112.87
32	A	412	AJP	C21-C22-C23	3.49	115.13	110.46
25	C	508	CLA	C1-C2-C3	-3.49	120.48	126.20
25	b	607	CLA	C1-C2-C3	-3.49	120.48	126.20
25	S	303	CLA	C2A-C1A-CHA	-3.49	117.82	123.87
40	n	617	NEX	C20-C13-C14	-3.49	117.17	122.82
25	s	309	CLA	CHB-C4A-NA	-3.49	119.37	124.40
25	c	502	CLA	C4D-CHA-C1A	-3.49	117.09	121.24
25	S	309	CLA	CHB-C4A-NA	-3.48	119.37	124.40
25	R	608	CLA	C1D-ND-C4D	-3.48	103.87	106.31
40	Y	318	NEX	C27-C28-C29	-3.48	120.13	125.53
25	y	315	CLA	C4D-CHA-C1A	-3.48	117.09	121.24
25	c	508	CLA	CHD-C1D-C2D	3.48	132.72	125.49
25	s	303	CLA	C2A-C1A-CHA	-3.47	117.84	123.87
25	C	507	CLA	C1-C2-C3	-3.47	120.51	126.20
25	c	507	CLA	C1-C2-C3	-3.47	120.51	126.20
40	N	617	NEX	C20-C13-C14	-3.47	117.19	122.82
24	N	605	CHL	CBC-CAC-C3C	-3.47	107.90	112.87
24	n	605	CHL	CBC-CAC-C3C	-3.47	107.90	112.87
25	G	611	CLA	C4D-CHA-C1A	-3.47	117.10	121.24
25	g	611	CLA	C4D-CHA-C1A	-3.47	117.10	121.24
25	C	509	CLA	CHB-C1B-NB	-3.47	118.84	124.05
25	r	611	CLA	C1D-ND-C4D	3.47	108.75	106.31
40	y	318	NEX	C27-C28-C29	-3.47	120.15	125.53
24	y	309	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
25	c	509	CLA	CHB-C1B-NB	-3.47	118.85	124.05
24	r	613	CHL	CBC-CAC-C3C	-3.47	107.91	112.87
26	n	618	LHG	O7-C7-C8	3.46	118.97	111.48
24	s	307	CHL	CMA-C3A-C4A	-3.46	107.15	114.61
24	Y	309	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
25	N	614	CLA	C2A-C1A-CHA	-3.46	117.87	123.87
25	B	602	CLA	CHB-C4A-NA	-3.46	119.41	124.40
25	C	508	CLA	CHD-C1D-C2D	3.46	132.68	125.49
25	r	611	CLA	C2B-C1B-NB	-3.46	106.74	110.33
25	R	611	CLA	C2B-C1B-NB	-3.45	106.75	110.33
24	y	306	CHL	CMA-C3A-C4A	-3.45	107.17	114.61
24	r	613	CHL	CMA-C3A-C4A	-3.45	107.17	114.61
24	R	613	CHL	CMA-C3A-C4A	-3.45	107.18	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	CHB-C4A-NA	-3.45	119.42	124.40
25	r	601	CLA	CHB-C1B-C2B	3.45	137.43	127.43
30	B	623	LMG	C7-O1-C1	-3.45	106.41	113.80
30	b	623	LMG	C7-O1-C1	-3.45	106.41	113.80
25	D	402	CLA	C1D-ND-C4D	-3.45	103.89	106.31
25	d	402	CLA	C1D-ND-C4D	-3.45	103.89	106.31
24	S	307	CHL	CMA-C3A-C4A	-3.45	107.19	114.61
24	Y	306	CHL	CMA-C3A-C4A	-3.44	107.19	114.61
24	G	609	CHL	CMA-C3A-C4A	-3.44	107.19	114.61
24	R	606	CHL	CBC-CAC-C3C	-3.44	107.94	112.87
24	r	606	CHL	CBC-CAC-C3C	-3.44	107.94	112.87
32	Y	320	AJP	O31-C30-C29	3.44	115.38	110.14
41	R	616	XAT	C38-C25-C26	-3.44	116.64	122.30
24	R	613	CHL	CBC-CAC-C3C	-3.43	107.96	112.87
26	N	618	LHG	O7-C7-C8	3.43	118.91	111.48
40	n	617	NEX	C11-C12-C13	-3.43	116.95	126.36
25	B	604	CLA	CHB-C1B-NB	-3.43	118.90	124.05
25	b	604	CLA	CHB-C1B-NB	-3.43	118.90	124.05
41	r	616	XAT	C38-C25-C26	-3.43	116.65	122.30
40	N	617	NEX	C11-C12-C13	-3.43	116.95	126.36
24	g	609	CHL	CMA-C3A-C4A	-3.43	107.22	114.61
40	r	617	NEX	C39-C29-C30	-3.43	117.26	122.82
25	2	602	CLA	C3D-C2D-C1D	3.43	110.51	105.83
25	6	602	CLA	C3D-C2D-C1D	3.43	110.51	105.83
40	R	617	NEX	C39-C29-C30	-3.43	117.26	122.82
25	R	611	CLA	C1D-ND-C4D	3.43	108.72	106.31
25	S	305	CLA	C2D-C1D-ND	-3.43	106.73	110.13
24	5	301	CHL	CMA-C3A-C4A	-3.42	107.23	114.61
24	N	607	CHL	CMA-C3A-C4A	-3.42	107.23	114.61
24	n	606	CHL	CMA-C3A-C4A	-3.42	107.24	114.61
25	R	601	CLA	CHB-C1B-C2B	3.42	137.36	127.43
25	G	611	CLA	C4A-NA-C1A	-3.42	105.12	106.68
25	g	611	CLA	C4A-NA-C1A	-3.42	105.12	106.68
25	Y	315	CLA	C4D-CHA-C1A	-3.42	117.17	121.24
25	s	305	CLA	C2D-C1D-ND	-3.42	106.74	110.13
24	1	301	CHL	CMA-C3A-C4A	-3.42	107.25	114.61
32	y	320	AJP	O31-C30-C29	3.42	115.35	110.14
41	R	616	XAT	C6-C7-C8	-3.42	118.77	125.99
24	S	306	CHL	CMA-C3A-C4A	-3.42	107.25	114.61
41	r	616	XAT	C6-C7-C8	-3.41	118.77	125.99
39	Y	316	LUT	C3-C4-C5	3.41	120.68	112.18
25	n	614	CLA	C2A-C1A-CHA	-3.41	117.94	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	609	CHL	CAA-C2A-C3A	-3.41	103.77	113.00
24	n	609	CHL	CAA-C2A-C3A	-3.41	103.77	113.00
24	R	607	CHL	C1-C2-C3	3.41	131.79	126.20
25	n	603	CLA	C1-C2-C3	-3.41	120.61	126.20
25	2	605	CLA	CHD-C1D-ND	-3.41	120.00	124.80
39	G	615	LUT	C3-C4-C5	3.41	120.67	112.18
39	g	615	LUT	C3-C4-C5	3.41	120.67	112.18
24	N	606	CHL	CMA-C3A-C4A	-3.41	107.27	114.61
24	Y	310	CHL	CAA-C2A-C3A	-3.41	103.79	113.00
39	y	316	LUT	C3-C4-C5	3.41	120.66	112.18
35	A	415	DGD	C1E-O6E-C5E	-3.41	107.07	113.72
35	a	401	DGD	C1E-O6E-C5E	-3.41	107.07	113.72
25	6	605	CLA	CHD-C1D-ND	-3.40	120.01	124.80
24	R	606	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	S	308	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	n	607	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	2	601	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	6	601	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	s	306	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
24	y	310	CHL	CAA-C2A-C3A	-3.40	103.81	113.00
25	6	602	CLA	C4D-C3D-CAD	-3.39	104.42	108.11
24	N	605	CHL	CMA-C3A-C4A	-3.39	107.30	114.61
24	s	308	CHL	CMA-C3A-C4A	-3.39	107.31	114.61
25	y	315	CLA	CHD-C1D-ND	-3.39	120.04	124.80
32	A	412	AJP	O84-C05-C06	3.39	117.36	107.26
32	a	413	AJP	O84-C05-C06	3.39	117.36	107.26
25	b	610	CLA	C1-C2-C3	-3.38	120.65	126.20
24	g	605	CHL	CBC-CAC-C3C	-3.38	108.03	112.87
24	S	302	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
24	s	302	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
24	r	606	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
24	G	608	CHL	CAA-C2A-C3A	-3.38	103.86	113.00
32	B	624	AJP	C41-C39-C38	3.38	121.32	113.02
32	b	624	AJP	C41-C39-C38	3.38	121.32	113.02
24	r	607	CHL	C1-C2-C3	3.38	131.74	126.20
24	n	605	CHL	CMA-C3A-C4A	-3.38	107.33	114.61
25	6	605	CLA	CHB-C1B-NB	-3.38	118.98	124.05
25	Y	315	CLA	CHD-C1D-ND	-3.38	120.05	124.80
24	s	306	CHL	CBC-CAC-C3C	-3.38	108.04	112.87
25	N	603	CLA	C1-C2-C3	-3.38	120.67	126.20
38	F	101	HEM	C3B-C4B-NB	-3.37	107.04	109.47
24	S	306	CHL	CBC-CAC-C3C	-3.37	108.04	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	609	CHL	CBC-CAC-C3C	-3.37	108.04	112.87
24	n	609	CHL	CBC-CAC-C3C	-3.37	108.04	112.87
32	B	624	AJP	O25-C23-C24	3.37	116.19	109.64
32	b	624	AJP	O25-C23-C24	3.37	116.19	109.64
24	g	608	CHL	CAA-C2A-C3A	-3.37	103.89	113.00
25	B	610	CLA	C1-C2-C3	-3.37	120.67	126.20
24	g	606	CHL	CAA-C2A-C3A	-3.37	103.89	113.00
24	Y	308	CHL	CMA-C3A-C4A	-3.37	107.35	114.61
25	Y	303	CLA	C4A-NA-C1A	-3.37	105.14	106.68
24	y	307	CHL	O1D-CGD-CBD	-3.37	119.61	124.72
25	r	610	CLA	C2D-C1D-ND	-3.37	106.79	110.13
24	y	308	CHL	CMA-C3A-C4A	-3.36	107.36	114.61
32	Y	320	AJP	O09-C05-C06	-3.36	100.09	104.56
32	y	320	AJP	O09-C05-C06	-3.36	100.09	104.56
32	N	620	AJP	C21-C22-C23	3.36	114.96	110.46
32	n	620	AJP	C21-C22-C23	3.36	114.96	110.46
24	G	606	CHL	CAA-C2A-C3A	-3.36	103.91	113.00
24	S	302	CHL	CAA-C2A-C3A	-3.36	103.92	113.00
24	G	605	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
32	Y	321	AJP	C01-C02-C03	3.36	119.42	112.08
32	y	321	AJP	C01-C02-C03	3.36	119.42	112.08
24	N	608	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
25	C	510	CLA	C1-C2-C3	-3.36	120.70	126.20
24	Y	307	CHL	O1D-CGD-CBD	-3.36	119.63	124.72
25	2	605	CLA	CHB-C1B-NB	-3.36	119.01	124.05
32	N	620	AJP	C17-C16-C15	-3.35	106.50	110.52
32	n	620	AJP	C17-C16-C15	-3.35	106.50	110.52
25	2	602	CLA	C4D-C3D-CAD	-3.35	104.47	108.11
39	N	615	LUT	C3-C4-C5	3.35	120.52	112.18
39	n	615	LUT	C3-C4-C5	3.35	120.52	112.18
25	R	610	CLA	C4D-C3D-CAD	-3.35	104.47	108.11
24	2	601	CHL	O1D-CGD-CBD	-3.35	119.64	124.72
24	6	601	CHL	O1D-CGD-CBD	-3.35	119.64	124.72
24	R	606	CHL	CAA-C2A-C3A	-3.35	103.95	113.00
24	S	307	CHL	CAA-C2A-C3A	-3.35	103.96	113.00
24	s	307	CHL	CAA-C2A-C3A	-3.35	103.96	113.00
24	n	608	CHL	CBC-CAC-C3C	-3.34	108.08	112.87
25	Y	315	CLA	C4A-NA-C1A	-3.34	105.15	106.68
25	c	510	CLA	C1-C2-C3	-3.34	120.72	126.20
24	N	608	CHL	CMA-C3A-C4A	-3.34	107.41	114.61
24	n	607	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
25	C	502	CLA	CHD-C1D-ND	-3.34	120.11	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	CHD-C1D-ND	-3.34	120.11	124.80
24	y	306	CHL	CAA-C2A-C3A	-3.34	103.98	113.00
25	R	610	CLA	C2D-C1D-ND	-3.34	106.82	110.13
24	N	607	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
24	y	310	CHL	CMA-C3A-C4A	-3.34	107.42	114.61
25	A	401	CLA	CHD-C1D-C2D	3.34	132.43	125.49
25	a	402	CLA	CHD-C1D-C2D	3.34	132.43	125.49
24	s	302	CHL	CAA-C2A-C3A	-3.33	103.99	113.00
32	y	324	AJP	O09-C05-C06	-3.33	100.13	104.56
25	Y	303	CLA	CHD-C1D-ND	-3.33	120.11	124.80
25	y	303	CLA	CHD-C1D-ND	-3.33	120.11	124.80
24	r	606	CHL	CAA-C2A-C3A	-3.33	104.00	113.00
40	R	617	NEX	C10-C11-C12	3.33	132.85	123.20
40	r	617	NEX	C10-C11-C12	3.33	132.85	123.20
35	C	515	DGD	C6D-O5D-C1E	-3.33	106.66	113.80
35	c	515	DGD	C6D-O5D-C1E	-3.33	106.66	113.80
25	s	314	CLA	C4D-CHA-C1A	-3.33	117.27	121.24
25	s	304	CLA	C1D-ND-C4D	-3.33	103.98	106.31
30	C	520	LMG	C1-O6-C5	-3.33	107.22	113.72
30	c	520	LMG	C1-O6-C5	-3.33	107.22	113.72
25	G	602	CLA	CHD-C1D-ND	-3.33	120.12	124.80
25	g	602	CLA	CHD-C1D-ND	-3.33	120.12	124.80
24	Y	307	CHL	CHA-C1A-C2A	-3.32	125.50	133.31
24	n	608	CHL	CMA-C3A-C4A	-3.32	107.45	114.61
24	y	307	CHL	CHA-C1A-C2A	-3.32	125.50	133.31
25	B	605	CLA	CHD-C1D-C2D	3.32	132.40	125.49
25	b	605	CLA	CHD-C1D-C2D	3.32	132.40	125.49
24	Y	310	CHL	CMA-C3A-C4A	-3.32	107.45	114.61
24	Y	306	CHL	CAA-C2A-C3A	-3.32	104.02	113.00
32	Y	324	AJP	O09-C05-C06	-3.32	100.14	104.56
30	A	410	LMG	C1-O6-C5	-3.32	107.24	113.72
30	a	411	LMG	C1-O6-C5	-3.32	107.24	113.72
32	Y	323	AJP	C26-O25-C23	3.32	120.81	115.27
32	y	323	AJP	C26-O25-C23	3.32	120.81	115.27
38	f	101	HEM	C3B-C4B-NB	-3.32	107.09	109.47
24	6	603	CHL	C4C-CHD-C1D	3.31	127.92	116.07
24	2	603	CHL	C4C-CHD-C1D	3.31	127.92	116.07
25	S	314	CLA	C4D-CHA-C1A	-3.31	117.29	121.24
24	r	605	CHL	CAA-C2A-C3A	-3.31	104.05	113.00
32	y	324	AJP	O84-C05-C06	3.31	117.13	107.26
24	y	308	CHL	O1D-CGD-CBD	-3.31	119.70	124.72
24	g	606	CHL	CMA-C3A-C4A	-3.31	107.48	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	603	CLA	C2D-C1D-ND	-3.31	106.85	110.13
24	R	605	CHL	CAA-C2A-C3A	-3.31	104.06	113.00
25	R	611	CLA	CHB-C4A-NA	-3.31	119.63	124.40
25	r	611	CLA	CHB-C4A-NA	-3.31	119.63	124.40
25	r	610	CLA	C4D-C3D-CAD	-3.31	104.52	108.11
25	s	312	CLA	C4A-NA-C1A	-3.31	105.17	106.68
24	G	606	CHL	CMA-C3A-C4A	-3.30	107.49	114.61
25	n	610	CLA	C1-C2-C3	-3.30	120.78	126.20
25	g	604	CLA	C1-C2-C3	-3.30	121.42	126.76
25	R	609	CLA	CHD-C1D-C2D	3.30	132.35	125.49
32	Y	324	AJP	O84-C05-C06	3.30	117.11	107.26
25	y	303	CLA	C4A-NA-C1A	-3.30	105.17	106.68
25	b	604	CLA	CHD-C1D-C2D	3.30	132.35	125.49
24	Y	308	CHL	O1D-CGD-CBD	-3.30	119.72	124.72
32	N	620	AJP	C29-C28-C27	3.30	115.42	110.67
25	R	603	CLA	C2D-C1D-ND	-3.29	106.86	110.13
40	g	617	NEX	C40-C33-C32	3.29	123.12	118.09
25	N	610	CLA	C1-C2-C3	-3.29	120.80	126.20
24	S	306	CHL	CAA-C2A-C3A	-3.29	104.11	113.00
25	R	601	CLA	C4D-C3D-CAD	-3.29	104.53	108.11
40	r	617	NEX	C38-C25-C26	-3.29	116.89	122.30
24	s	308	CHL	CBC-CAC-C3C	-3.29	108.17	112.87
25	S	312	CLA	C4A-NA-C1A	-3.29	105.18	106.68
39	r	615	LUT	C3-C4-C5	3.29	120.36	112.18
32	B	624	AJP	O77-C28-C27	3.29	118.12	110.38
32	b	624	AJP	O77-C28-C27	3.29	118.12	110.38
39	R	615	LUT	C3-C4-C5	3.28	120.36	112.18
24	R	607	CHL	CAA-C2A-C3A	-3.28	104.12	113.00
24	s	306	CHL	CAA-C2A-C3A	-3.28	104.13	113.00
24	S	308	CHL	CBC-CAC-C3C	-3.28	108.17	112.87
25	r	601	CLA	C4D-C3D-CAD	-3.28	104.54	108.11
40	G	617	NEX	C40-C33-C32	3.28	123.10	118.09
25	R	610	CLA	C2B-C1B-NB	-3.28	106.92	110.33
25	r	610	CLA	C2B-C1B-NB	-3.28	106.92	110.33
25	g	611	CLA	CHD-C1D-ND	-3.28	120.19	124.80
25	y	315	CLA	C4A-NA-C1A	-3.28	105.18	106.68
30	A	410	LMG	C7-O1-C1	-3.28	106.77	113.80
30	a	411	LMG	C7-O1-C1	-3.28	106.77	113.80
25	G	611	CLA	CHD-C1D-ND	-3.28	120.19	124.80
25	r	609	CLA	CHD-C1D-C2D	3.28	132.30	125.49
32	a	413	AJP	O50-C45-C46	3.28	114.99	109.99
25	G	604	CLA	C1-C2-C3	-3.27	121.47	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	309	CLA	CHD-C1D-ND	-3.27	120.20	124.80
25	B	604	CLA	CHD-C1D-C2D	3.27	132.29	125.49
40	R	617	NEX	C38-C25-C26	-3.27	116.92	122.30
32	Y	323	AJP	C83-C06-C05	-3.27	109.67	114.94
32	y	323	AJP	C83-C06-C05	-3.27	109.67	114.94
25	D	402	CLA	CHD-C1D-ND	-3.27	120.20	124.80
25	d	402	CLA	CHD-C1D-ND	-3.27	120.20	124.80
25	G	603	CLA	CHB-C1B-NB	-3.27	119.15	124.05
24	S	308	CHL	CAA-C2A-C3A	-3.27	104.17	113.00
24	s	308	CHL	CAA-C2A-C3A	-3.27	104.17	113.00
24	r	607	CHL	CAA-C2A-C3A	-3.26	104.18	113.00
25	S	304	CLA	C1D-ND-C4D	-3.26	104.02	106.31
32	n	620	AJP	C29-C28-C27	3.26	115.37	110.67
25	b	602	CLA	C1D-ND-C4D	-3.26	104.02	106.31
35	B	626	DGD	C6D-O5D-C1E	-3.26	106.81	113.80
35	b	626	DGD	C6D-O5D-C1E	-3.26	106.81	113.80
24	n	609	CHL	C1A-CHA-C4D	3.26	124.42	118.98
25	a	403	CLA	CHD-C1D-C2D	3.26	132.26	125.49
35	b	626	DGD	C1D-O6D-C5D	-3.26	107.36	113.72
24	y	307	CHL	O2A-CGA-CBA	3.26	121.77	111.83
24	Y	307	CHL	O2A-CGA-CBA	3.26	121.76	111.83
25	g	603	CLA	CHB-C1B-NB	-3.26	119.17	124.05
25	s	309	CLA	CHD-C1D-ND	-3.25	120.22	124.80
24	G	608	CHL	CMA-C3A-C4A	-3.25	107.60	114.61
32	y	320	AJP	O25-C26-O31	3.25	119.25	110.69
25	A	402	CLA	CHD-C1D-C2D	3.25	132.25	125.49
24	Y	309	CHL	CAA-C2A-C3A	-3.25	104.22	113.00
25	b	607	CLA	CHB-C1B-NB	-3.25	119.18	124.05
24	N	608	CHL	CAA-C2A-C3A	-3.25	104.22	113.00
35	B	626	DGD	C1D-O6D-C5D	-3.25	107.38	113.72
32	A	412	AJP	O34-C35-C36	-3.25	102.78	109.09
32	a	413	AJP	O34-C35-C36	-3.25	102.78	109.09
24	N	609	CHL	C1A-CHA-C4D	3.24	124.40	118.98
24	n	606	CHL	CAA-C2A-C3A	-3.24	104.23	113.00
24	g	608	CHL	CMA-C3A-C4A	-3.24	107.62	114.61
38	f	101	HEM	CHC-C1C-NC	3.24	127.98	124.45
24	y	309	CHL	CBC-CAC-C3C	-3.24	108.23	112.87
24	y	309	CHL	CAA-C2A-C3A	-3.24	104.24	113.00
25	B	607	CLA	CHB-C1B-NB	-3.24	119.19	124.05
25	R	611	CLA	C3D-C2D-C1D	3.24	110.25	105.83
24	N	609	CHL	CMA-C3A-C4A	-3.24	107.64	114.61
32	Y	320	AJP	O25-C26-O31	3.24	119.21	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	CHD-C1D-C2D	3.24	132.22	125.49
32	Y	321	AJP	C28-C29-C30	-3.24	105.72	111.19
32	y	321	AJP	C28-C29-C30	-3.24	105.72	111.19
39	y	316	LUT	C35-C15-C14	-3.24	116.90	123.52
38	F	101	HEM	CHC-C1C-NC	3.24	127.98	124.45
24	Y	310	CHL	OBD-CAD-CBD	-3.24	121.08	125.82
24	y	310	CHL	OBD-CAD-CBD	-3.24	121.08	125.82
24	Y	309	CHL	CBC-CAC-C3C	-3.24	108.24	112.87
25	s	304	CLA	CHD-C1D-C2D	3.23	132.21	125.49
24	N	606	CHL	CAA-C2A-C3A	-3.23	104.27	113.00
24	n	601	CHL	C1A-CHA-C4D	3.23	124.37	118.98
24	n	608	CHL	CAA-C2A-C3A	-3.23	104.28	113.00
25	r	601	CLA	C3D-C2D-C1D	3.22	110.23	105.83
25	6	604	CLA	C2D-C1D-ND	-3.22	106.94	110.13
28	z	101	BCR	C2-C1-C6	3.22	115.12	110.44
25	C	507	CLA	CHD-C1D-C2D	3.22	132.18	125.49
25	C	512	CLA	CHD-C1D-C2D	3.22	132.18	125.49
30	D	407	LMG	C7-O1-C1	-3.22	106.90	113.80
30	d	407	LMG	C7-O1-C1	-3.22	106.90	113.80
25	N	613	CLA	C4D-CHA-C1A	-3.21	117.41	121.24
25	N	603	CLA	CHB-C1B-NB	-3.21	119.23	124.05
39	Y	316	LUT	C35-C15-C14	-3.21	116.94	123.52
28	Z	101	BCR	C2-C1-C6	3.21	115.11	110.44
32	N	620	AJP	C01-C02-C03	3.21	119.10	112.08
32	n	620	AJP	C01-C02-C03	3.21	119.10	112.08
25	2	604	CLA	C2D-C1D-ND	-3.21	106.95	110.13
32	A	412	AJP	O50-C45-C46	3.21	114.89	109.99
25	c	512	CLA	CHD-C1D-C2D	3.21	132.17	125.49
25	n	603	CLA	CHB-C1B-NB	-3.21	119.23	124.05
24	n	609	CHL	CMA-C3A-C4A	-3.21	107.70	114.61
25	g	610	CLA	C4-C3-C5	3.21	120.80	115.23
25	R	603	CLA	O1D-CGD-CBD	-3.21	118.19	124.52
25	r	603	CLA	O1D-CGD-CBD	-3.21	118.19	124.52
25	S	304	CLA	CHD-C1D-C2D	3.21	132.15	125.49
25	S	311	CLA	CHD-C1D-C2D	3.21	132.15	125.49
24	y	307	CHL	OMC-CMC-C2C	-3.20	119.56	125.12
25	n	613	CLA	C4D-CHA-C1A	-3.20	117.42	121.24
25	Y	303	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	y	303	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	B	613	CLA	CHD-C1D-ND	-3.20	120.30	124.80
25	b	613	CLA	CHD-C1D-ND	-3.20	120.30	124.80
24	g	608	CHL	C1-C2-C3	3.20	131.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	610	CLA	C3D-C2D-C1D	3.20	110.20	105.83
28	A	406	BCR	C15-C14-C13	-3.20	122.79	127.28
28	a	407	BCR	C15-C14-C13	-3.20	122.79	127.28
25	r	611	CLA	C3D-C2D-C1D	3.20	110.20	105.83
32	Y	323	AJP	C29-C28-C27	3.20	115.28	110.67
32	y	323	AJP	C29-C28-C27	3.20	115.28	110.67
25	y	304	CLA	C3D-C2D-C1D	3.20	110.19	105.83
24	N	601	CHL	C1A-CHA-C4D	3.20	124.31	118.98
35	C	515	DGD	C3G-O3G-C1D	-3.19	106.95	113.80
35	c	515	DGD	C3G-O3G-C1D	-3.19	106.95	113.80
25	S	305	CLA	C3D-C2D-C1D	3.19	110.19	105.83
25	s	305	CLA	C3D-C2D-C1D	3.19	110.19	105.83
25	2	604	CLA	CHB-C1B-NB	-3.19	119.26	124.05
25	6	604	CLA	CHB-C1B-NB	-3.19	119.26	124.05
24	g	601	CHL	O1D-CGD-CBD	-3.19	119.88	124.72
25	Y	304	CLA	C2A-C1A-CHA	-3.19	118.33	123.87
25	y	304	CLA	C2A-C1A-CHA	-3.19	118.33	123.87
25	s	305	CLA	C4D-C3D-CAD	-3.19	104.64	108.11
25	R	601	CLA	C3D-C2D-C1D	3.19	110.18	105.83
32	B	624	AJP	O84-C05-C06	3.19	116.77	107.26
32	b	624	AJP	O84-C05-C06	3.19	116.77	107.26
25	B	602	CLA	C1D-ND-C4D	-3.19	104.08	106.31
25	y	315	CLA	O1D-CGD-CBD	-3.19	118.23	124.52
24	G	608	CHL	C1-C2-C3	3.18	131.41	126.20
24	y	309	CHL	C1-C2-C3	3.18	131.41	126.20
25	G	610	CLA	C4-C3-C5	3.18	120.75	115.23
25	R	611	CLA	CHB-C1B-C2B	3.18	136.67	127.43
25	Y	304	CLA	C3D-C2D-C1D	3.18	110.17	105.83
25	S	305	CLA	C4D-C3D-CAD	-3.18	104.65	108.11
24	Y	309	CHL	C1-C2-C3	3.18	131.41	126.20
25	n	612	CLA	CHD-C1D-C2D	3.18	132.10	125.49
24	G	601	CHL	O1D-CGD-CBD	-3.18	119.90	124.72
25	B	616	CLA	C1-C2-C3	-3.18	120.99	126.20
25	b	616	CLA	C1-C2-C3	-3.18	120.99	126.20
25	s	311	CLA	CHD-C1D-C2D	3.18	132.09	125.49
32	A	412	AJP	O09-C05-C06	-3.17	100.34	104.56
32	a	413	AJP	O09-C05-C06	-3.17	100.34	104.56
25	R	610	CLA	C3D-C2D-C1D	3.17	110.16	105.83
25	S	312	CLA	CHD-C1D-ND	-3.17	120.34	124.80
25	Y	313	CLA	CHD-C1D-ND	-3.17	120.34	124.80
25	y	313	CLA	CHD-C1D-ND	-3.17	120.34	124.80
25	R	603	CLA	C3D-C2D-C1D	3.17	110.16	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	609	CHL	CAA-C2A-C3A	-3.17	104.43	113.00
24	G	609	CHL	CAA-C2A-C3A	-3.17	104.44	113.00
40	S	317	NEX	C19-C9-C10	-3.17	117.68	122.82
24	Y	308	CHL	C1-C2-C3	3.17	131.39	126.20
25	Y	315	CLA	O1D-CGD-CBD	-3.17	118.27	124.52
25	N	612	CLA	CHD-C1D-C2D	3.17	132.07	125.49
25	r	611	CLA	CHB-C1B-C2B	3.17	136.62	127.43
24	N	609	CHL	CHA-C1A-C2A	-3.16	125.88	133.31
24	n	609	CHL	CHA-C1A-C2A	-3.16	125.88	133.31
25	c	504	CLA	O1D-CGD-CBD	-3.16	118.28	124.52
24	R	607	CHL	O1D-CGD-CBD	-3.16	119.93	124.72
24	r	607	CHL	O1D-CGD-CBD	-3.16	119.93	124.72
32	N	620	AJP	C17-C16-C11	-3.16	107.82	112.29
32	n	620	AJP	C17-C16-C11	-3.16	107.82	112.29
32	B	624	AJP	O77-C28-C29	3.16	118.04	109.94
32	b	624	AJP	O77-C28-C29	3.16	118.04	109.94
24	g	607	CHL	CMA-C3A-C4A	-3.16	107.80	114.61
40	s	317	NEX	C19-C9-C10	-3.16	117.69	122.82
25	s	312	CLA	CHD-C1D-ND	-3.16	120.36	124.80
25	r	603	CLA	C3D-C2D-C1D	3.16	110.14	105.83
32	A	412	AJP	O31-C30-C29	3.16	116.25	109.72
32	a	413	AJP	O31-C30-C29	3.16	116.25	109.72
32	Y	320	AJP	C04-C05-C06	3.16	121.38	115.66
32	y	320	AJP	C04-C05-C06	3.16	121.38	115.66
24	y	308	CHL	C1-C2-C3	3.16	131.37	126.20
25	s	312	CLA	C3D-C2D-C1D	3.16	110.14	105.83
38	F	101	HEM	CHC-C4B-NB	3.15	127.82	124.42
25	d	403	CLA	C3D-C2D-C1D	3.15	110.13	105.83
24	G	607	CHL	CMA-C3A-C4A	-3.15	107.82	114.61
25	C	504	CLA	O1D-CGD-CBD	-3.15	118.31	124.52
25	D	403	CLA	C3D-C2D-C1D	3.15	110.12	105.83
24	s	306	CHL	O1D-CGD-CBD	-3.14	119.95	124.72
24	S	306	CHL	O1D-CGD-CBD	-3.14	119.96	124.72
27	A	403	PHO	O1D-CGD-CBD	-3.14	119.96	124.72
27	a	404	PHO	O1D-CGD-CBD	-3.14	119.96	124.72
24	Y	307	CHL	OMC-CMC-C2C	-3.14	119.67	125.12
25	N	614	CLA	C4D-CHA-C1A	-3.14	117.50	121.24
25	c	501	CLA	C4D-CHA-C1A	-3.14	117.50	121.24
24	y	302	CHL	C1A-CHA-C4D	3.14	124.22	118.98
25	C	512	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
25	n	614	CLA	CHD-C1D-ND	-3.14	120.39	124.80
25	B	608	CLA	C2A-C1A-CHA	-3.14	118.42	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
24	G	608	CHL	CBC-CAC-C3C	-3.14	108.38	112.87
25	B	608	CLA	C4D-CHA-C1A	-3.13	117.51	121.24
25	b	608	CLA	C4D-CHA-C1A	-3.13	117.51	121.24
25	B	610	CLA	CHD-C1D-ND	-3.13	120.39	124.80
24	Y	308	CHL	CAA-C2A-C3A	-3.13	104.54	113.00
25	n	612	CLA	C3D-C2D-C1D	3.13	110.10	105.83
24	Y	302	CHL	C1A-CHA-C4D	3.13	124.20	118.98
25	N	611	CLA	C4A-NA-C1A	-3.13	105.25	106.68
25	S	312	CLA	C3D-C2D-C1D	3.13	110.10	105.83
24	n	609	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
25	n	611	CLA	C4A-NA-C1A	-3.13	105.25	106.68
25	D	403	CLA	C2D-C1D-ND	-3.13	107.03	110.13
25	d	403	CLA	C2D-C1D-ND	-3.13	107.03	110.13
24	N	601	CHL	C1-C2-C3	3.12	131.31	126.20
25	b	615	CLA	C2A-C3A-C4A	-3.12	96.83	101.87
25	N	614	CLA	CHD-C1D-ND	-3.12	120.41	124.80
25	b	610	CLA	CHD-C1D-ND	-3.12	120.41	124.80
40	y	318	NEX	O24-C25-C24	3.12	116.42	113.49
24	n	609	CHL	OBD-CAD-CBD	-3.12	121.24	125.82
32	S	319	AJP	C04-C03-C02	-3.12	105.44	111.67
32	s	319	AJP	C04-C03-C02	-3.12	105.44	111.67
24	N	609	CHL	O1D-CGD-CBD	-3.12	119.99	124.72
24	y	308	CHL	CAA-C2A-C3A	-3.12	104.57	113.00
24	G	601	CHL	C1A-CHA-C4D	3.12	124.18	118.98
24	g	601	CHL	C1A-CHA-C4D	3.12	124.18	118.98
25	C	501	CLA	C4D-CHA-C1A	-3.12	117.53	121.24
24	Y	309	CHL	OBD-CAD-CBD	-3.12	121.25	125.82
25	B	615	CLA	C2A-C3A-C4A	-3.12	96.84	101.87
30	B	620	LMG	C1-O6-C5	-3.11	107.64	113.72
30	b	620	LMG	C1-O6-C5	-3.11	107.64	113.72
25	6	604	CLA	C3D-C2D-C1D	3.11	110.08	105.83
24	N	609	CHL	OBD-CAD-CBD	-3.11	121.26	125.82
25	c	512	CLA	C2A-C1A-CHA	-3.11	118.47	123.87
30	B	620	LMG	C7-O1-C1	-3.11	107.13	113.80
30	b	620	LMG	C7-O1-C1	-3.11	107.13	113.80
25	s	313	CLA	C3D-C2D-C1D	3.11	110.07	105.83
24	y	309	CHL	OBD-CAD-CBD	-3.11	121.27	125.82
24	S	302	CHL	C1A-CHA-C4D	3.11	124.17	118.98
25	N	602	CLA	C4D-CHA-C1A	-3.11	117.54	121.24
32	B	624	AJP	C55-O60-C59	3.11	119.78	113.72
32	b	624	AJP	C55-O60-C59	3.11	119.78	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	614	CLA	C4D-CHA-C1A	-3.11	117.54	121.24
24	s	302	CHL	C1A-CHA-C4D	3.10	124.16	118.98
25	2	604	CLA	C3D-C2D-C1D	3.10	110.06	105.83
25	c	504	CLA	C3D-C2D-C1D	3.10	110.06	105.83
25	c	504	CLA	C2D-C1D-ND	-3.10	107.06	110.13
24	G	605	CHL	CAA-C2A-C3A	-3.10	104.62	113.00
24	g	605	CHL	CAA-C2A-C3A	-3.10	104.62	113.00
25	R	603	CLA	C4D-C3D-CAD	-3.10	104.74	108.11
25	r	603	CLA	C4D-C3D-CAD	-3.10	104.74	108.11
25	N	602	CLA	CHD-C1D-ND	-3.10	120.44	124.80
24	g	608	CHL	CBC-CAC-C3C	-3.10	108.44	112.87
25	C	504	CLA	C3D-C2D-C1D	3.10	110.06	105.83
32	Y	324	AJP	C29-C28-C27	3.10	115.13	110.67
32	y	324	AJP	C29-C28-C27	3.10	115.13	110.67
27	A	404	PHO	O1D-CGD-CBD	-3.10	120.03	124.72
25	B	615	CLA	CHD-C1D-ND	-3.10	120.44	124.80
24	n	601	CHL	C1-C2-C3	3.09	131.27	126.20
35	C	516	DGD	C1E-O6E-C5E	-3.09	107.68	113.72
35	c	516	DGD	C1E-O6E-C5E	-3.09	107.68	113.72
25	B	603	CLA	C2A-C1A-CHA	-3.09	118.50	123.87
25	b	603	CLA	C2A-C1A-CHA	-3.09	118.50	123.87
25	Y	313	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	y	313	CLA	C3D-C2D-C1D	3.09	110.05	105.83
27	a	405	PHO	O1D-CGD-CBD	-3.09	120.03	124.72
25	C	501	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	N	612	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	c	501	CLA	C3D-C2D-C1D	3.09	110.05	105.83
24	g	608	CHL	O1D-CGD-CBD	-3.09	120.04	124.72
38	f	101	HEM	CHC-C4B-NB	3.09	127.75	124.42
25	c	505	CLA	C2A-C1A-CHA	-3.09	118.51	123.87
25	C	505	CLA	C1-C2-C3	-3.09	121.14	126.20
25	c	505	CLA	C1-C2-C3	-3.09	121.14	126.20
25	n	602	CLA	CHD-C1D-ND	-3.09	120.46	124.80
25	6	604	CLA	CHC-C1C-NC	-3.09	119.66	124.31
24	5	301	CHL	CAA-C2A-C3A	-3.08	104.67	113.00
25	n	602	CLA	C4D-CHA-C1A	-3.08	117.57	121.24
25	R	614	CLA	CHB-C1B-NB	-3.08	119.43	124.05
25	2	604	CLA	CHC-C1C-NC	-3.08	119.68	124.31
24	G	608	CHL	O2A-CGA-CBA	3.08	121.22	111.83
24	g	608	CHL	O2A-CGA-CBA	3.08	121.22	111.83
25	D	402	CLA	C3D-C2D-C1D	3.07	110.03	105.83
25	b	615	CLA	C3D-C2D-C1D	3.07	110.03	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	CLA	C3D-C2D-C1D	3.07	110.03	105.83
25	C	504	CLA	C2D-C1D-ND	-3.07	107.08	110.13
24	l	301	CHL	CAA-C2A-C3A	-3.07	104.69	113.00
32	y	324	AJP	O31-C30-C29	3.07	114.83	110.14
25	B	610	CLA	C4A-NA-C1A	-3.07	105.28	106.68
25	b	610	CLA	C4A-NA-C1A	-3.07	105.28	106.68
25	C	505	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
25	N	604	CLA	O1D-CGD-CBD	-3.07	118.46	124.52
25	n	611	CLA	O1D-CGD-CBD	-3.07	118.47	124.52
32	Y	324	AJP	O31-C30-C29	3.07	114.82	110.14
25	r	614	CLA	CHB-C1B-NB	-3.07	119.45	124.05
25	S	313	CLA	C3D-C2D-C1D	3.07	110.02	105.83
25	N	603	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
25	n	603	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
24	G	609	CHL	O2A-CGA-CBA	3.06	121.18	111.83
35	B	626	DGD	C1E-O6E-C5E	-3.06	107.74	113.72
35	b	626	DGD	C1E-O6E-C5E	-3.06	107.74	113.72
25	n	604	CLA	O1D-CGD-CBD	-3.06	118.48	124.52
24	l	302	CHL	CAA-C2A-C3A	-3.06	104.73	113.00
24	5	302	CHL	CAA-C2A-C3A	-3.06	104.73	113.00
25	B	614	CLA	CHB-C1B-NB	-3.06	119.46	124.05
25	b	614	CLA	CHB-C1B-NB	-3.06	119.46	124.05
24	n	608	CHL	C1-C2-C3	3.06	131.20	126.20
25	B	615	CLA	C3D-C2D-C1D	3.05	110.00	105.83
41	R	616	XAT	C26-C27-C28	-3.05	119.54	125.99
24	l	302	CHL	CBC-CAC-C3C	-3.05	108.50	112.87
24	5	302	CHL	CBC-CAC-C3C	-3.05	108.50	112.87
25	D	401	CLA	C1D-ND-C4D	-3.05	104.17	106.31
25	d	401	CLA	C1D-ND-C4D	-3.05	104.17	106.31
24	g	609	CHL	O2A-CGA-CBA	3.05	121.14	111.83
25	G	613	CLA	CHD-C1D-C2D	3.05	131.83	125.49
25	y	312	CLA	C3D-C2D-C1D	3.05	109.99	105.83
25	N	611	CLA	O1D-CGD-CBD	-3.05	118.50	124.52
24	G	608	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
25	c	503	CLA	CHD-C1D-C2D	3.05	131.82	125.49
24	G	605	CHL	OMC-CMC-C2C	-3.05	119.83	125.12
25	b	615	CLA	CHD-C1D-ND	-3.05	120.52	124.80
24	n	608	CHL	O2A-CGA-CBA	3.04	121.12	111.83
25	C	504	CLA	C4D-CHA-C1A	-3.04	117.61	121.24
25	C	511	CLA	CHD-C1D-C2D	3.04	131.82	125.49
25	c	511	CLA	CHD-C1D-C2D	3.04	131.82	125.49
32	Y	323	AJP	C17-C16-C11	-3.04	107.99	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	323	AJP	C17-C16-C11	-3.04	107.99	112.29
24	N	608	CHL	O2A-CGA-CBA	3.04	121.11	111.83
32	y	322	AJP	C29-C30-C32	-3.04	106.86	112.50
24	N	608	CHL	C1-C2-C3	3.04	131.18	126.20
24	S	308	CHL	OBD-CAD-CBD	-3.04	121.36	125.82
24	6	601	CHL	O2A-CGA-CBA	3.04	121.10	111.83
25	y	315	CLA	C2A-C1A-CHA	-3.04	118.59	123.87
41	r	616	XAT	C26-C27-C28	-3.04	119.57	125.99
24	s	308	CHL	OBD-CAD-CBD	-3.04	121.37	125.82
25	s	309	CLA	C2A-C3A-C4A	-3.04	96.97	101.87
39	S	316	LUT	C22-C23-C24	3.03	115.69	111.18
24	2	601	CHL	O2A-CGA-CBA	3.03	121.08	111.83
40	Y	318	NEX	O24-C25-C24	3.03	116.33	113.49
38	F	101	HEM	CHD-C1D-ND	3.03	127.68	124.42
38	f	101	HEM	CHD-C1D-ND	3.03	127.68	124.42
24	Y	302	CHL	O1D-CGD-CBD	-3.03	120.13	124.72
25	n	614	CLA	C1D-ND-C4D	-3.03	104.19	106.31
32	Y	322	AJP	C29-C30-C32	-3.03	106.89	112.50
24	N	605	CHL	O1D-CGD-CBD	-3.03	120.13	124.72
24	y	302	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
28	b	617	BCR	C15-C14-C13	-3.02	123.04	127.28
25	S	309	CLA	C2A-C3A-C4A	-3.02	96.99	101.87
25	g	613	CLA	CHD-C1D-C2D	3.02	131.77	125.49
24	g	605	CHL	OMC-CMC-C2C	-3.02	119.88	125.12
25	C	503	CLA	CHD-C1D-C2D	3.02	131.76	125.49
39	s	316	LUT	C22-C23-C24	3.02	115.67	111.18
25	B	607	CLA	C4-C3-C5	3.01	120.46	115.23
28	B	617	BCR	C15-C14-C13	-3.01	123.05	127.28
24	y	309	CHL	O2A-CGA-CBA	3.01	121.02	111.83
25	n	611	CLA	C3D-C2D-C1D	3.01	109.94	105.83
24	n	601	CHL	CAA-C2A-C3A	-3.01	104.86	113.00
25	c	504	CLA	C4D-CHA-C1A	-3.01	117.65	121.24
25	s	310	CLA	CHD-C1D-C2D	3.01	131.74	125.49
24	Y	309	CHL	O2A-CGA-CBA	3.01	121.00	111.83
32	g	618	AJP	C01-C02-C03	3.01	118.65	112.08
25	Y	312	CLA	C3D-C2D-C1D	3.01	109.93	105.83
24	N	601	CHL	CAA-C2A-C3A	-3.01	104.88	113.00
25	R	612	CLA	C3D-C2D-C1D	3.01	109.93	105.83
25	r	612	CLA	C3D-C2D-C1D	3.01	109.93	105.83
25	b	607	CLA	C4-C3-C5	3.00	120.44	115.23
32	G	618	AJP	C01-C02-C03	3.00	118.65	112.08
25	A	401	CLA	C1D-ND-C4D	-3.00	104.20	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	402	CLA	C1D-ND-C4D	-3.00	104.20	106.31
25	C	513	CLA	CHB-C1B-NB	-3.00	119.55	124.05
25	c	513	CLA	CHB-C1B-NB	-3.00	119.55	124.05
24	r	606	CHL	OBD-CAD-CBD	-3.00	121.42	125.82
24	2	601	CHL	C1-C2-C3	3.00	131.11	126.20
24	6	601	CHL	C1-C2-C3	3.00	131.11	126.20
24	g	605	CHL	OBD-CAD-CBD	-3.00	121.42	125.82
24	R	605	CHL	OBD-CAD-CBD	-3.00	121.42	125.82
24	1	301	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
25	Y	315	CLA	C2A-C1A-CHA	-3.00	118.66	123.87
25	B	605	CLA	C1D-ND-C4D	-3.00	104.21	106.31
24	n	605	CHL	O1D-CGD-CBD	-3.00	120.18	124.72
24	N	607	CHL	OMC-CMC-C2C	-3.00	119.92	125.12
24	n	601	CHL	OBD-CAD-CBD	-3.00	121.43	125.82
25	N	614	CLA	C1D-ND-C4D	-3.00	104.21	106.31
24	Y	309	CHL	O1D-CGD-CBD	-3.00	120.18	124.72
25	C	507	CLA	CHB-C1B-NB	-2.99	119.56	124.05
24	Y	307	CHL	OBD-CAD-CBD	-2.99	121.43	125.82
40	g	617	NEX	C19-C9-C10	-2.99	117.97	122.82
24	n	607	CHL	OMC-CMC-C2C	-2.99	119.92	125.12
25	N	603	CLA	C3D-C2D-C1D	2.99	109.91	105.83
25	N	611	CLA	C3D-C2D-C1D	2.99	109.91	105.83
25	b	604	CLA	C1D-ND-C4D	-2.99	104.21	106.31
25	Y	311	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
25	y	311	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
24	y	309	CHL	O1D-CGD-CBD	-2.99	120.19	124.72
25	2	602	CLA	CHA-C1A-NA	-2.99	119.62	126.39
25	n	603	CLA	C3D-C2D-C1D	2.99	109.91	105.83
24	r	605	CHL	OBD-CAD-CBD	-2.99	121.44	125.82
32	Y	324	AJP	O25-C26-O31	2.99	118.55	110.69
32	y	324	AJP	O25-C26-O31	2.99	118.55	110.69
25	C	510	CLA	C2A-C1A-CHA	-2.98	118.69	123.87
24	y	307	CHL	CAA-C2A-C3A	-2.98	104.94	113.00
25	S	311	CLA	C3D-C2D-C1D	2.98	109.90	105.83
28	T	101	BCR	C15-C16-C17	-2.98	117.42	123.52
24	5	301	CHL	O1D-CGD-CBD	-2.98	120.20	124.72
25	S	314	CLA	C2A-C1A-CHA	-2.98	118.69	123.87
25	s	314	CLA	C2A-C1A-CHA	-2.98	118.69	123.87
32	y	323	AJP	C06-C07-C08	-2.98	99.49	104.28
25	b	604	CLA	C3D-C2D-C1D	2.98	109.90	105.83
25	6	602	CLA	CHA-C1A-NA	-2.98	119.64	126.39
24	n	605	CHL	O2A-CGA-CBA	2.98	120.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	323	AJP	C06-C07-C08	-2.98	99.49	104.28
32	Y	323	AJP	C04-C03-C02	-2.98	105.72	111.67
24	R	606	CHL	OBD-CAD-CBD	-2.98	121.45	125.82
32	A	412	AJP	C01-C02-C03	2.98	118.59	112.08
32	a	413	AJP	C01-C02-C03	2.98	118.59	112.08
32	y	323	AJP	C04-C03-C02	-2.98	105.73	111.67
24	n	609	CHL	O2A-CGA-CBA	2.98	120.91	111.83
28	t	101	BCR	C15-C16-C17	-2.98	117.43	123.52
25	b	605	CLA	C1D-ND-C4D	-2.98	104.22	106.31
30	C	520	LMG	C7-O1-C1	-2.98	107.42	113.80
24	Y	307	CHL	CAA-C2A-C3A	-2.98	104.96	113.00
25	S	310	CLA	CHD-C1D-C2D	2.97	131.67	125.49
25	d	401	CLA	CHD-C1D-C2D	2.97	131.67	125.49
24	N	605	CHL	O2A-CGA-CBA	2.97	120.90	111.83
32	Y	323	AJP	O31-C30-C29	2.97	114.67	110.14
32	y	323	AJP	O31-C30-C29	2.97	114.67	110.14
32	B	624	AJP	C83-C06-C05	-2.97	110.15	114.94
32	b	624	AJP	C83-C06-C05	-2.97	110.15	114.94
24	s	307	CHL	C1A-CHA-C4D	2.97	123.94	118.98
25	s	311	CLA	C3D-C2D-C1D	2.97	109.88	105.83
25	C	508	CLA	O1D-CGD-CBD	-2.97	118.67	124.52
25	c	508	CLA	O1D-CGD-CBD	-2.97	118.67	124.52
24	r	606	CHL	CHA-C1A-C2A	-2.97	126.34	133.31
24	N	609	CHL	O2A-CGA-CBA	2.97	120.88	111.83
25	G	610	CLA	CHD-C1D-C2D	2.97	131.65	125.49
25	c	507	CLA	CHB-C1B-NB	-2.96	119.60	124.05
35	C	516	DGD	C3G-O3G-C1D	-2.96	107.44	113.80
25	D	401	CLA	CHD-C1D-C2D	2.96	131.65	125.49
25	G	610	CLA	C3D-C2D-C1D	2.96	109.87	105.83
28	B	617	BCR	C33-C5-C6	-2.96	121.25	124.48
28	b	617	BCR	C33-C5-C6	-2.96	121.25	124.48
24	S	307	CHL	C1A-CHA-C4D	2.96	123.92	118.98
25	C	511	CLA	C3D-C2D-C1D	2.96	109.87	105.83
25	c	511	CLA	C3D-C2D-C1D	2.96	109.87	105.83
25	C	508	CLA	C3D-C2D-C1D	2.96	109.87	105.83
24	R	606	CHL	CHA-C1A-C2A	-2.96	126.36	133.31
24	N	601	CHL	OBD-CAD-CBD	-2.96	121.48	125.82
24	6	601	CHL	OBD-CAD-CBD	-2.96	121.48	125.82
24	n	606	CHL	C1A-CHA-C4D	2.96	123.92	118.98
25	2	605	CLA	C1D-ND-C4D	-2.96	104.24	106.31
24	R	605	CHL	O1D-CGD-CBD	-2.96	120.24	124.72
24	r	605	CHL	O1D-CGD-CBD	-2.96	120.24	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	605	CHL	OBD-CAD-CBD	-2.96	121.48	125.82
32	N	619	AJP	C19-C24-C23	-2.96	105.57	112.87
32	n	619	AJP	C19-C24-C23	-2.96	105.57	112.87
24	y	307	CHL	OBD-CAD-CBD	-2.96	121.49	125.82
25	G	603	CLA	C3D-C2D-C1D	2.96	109.86	105.83
25	g	603	CLA	C3D-C2D-C1D	2.96	109.86	105.83
25	C	510	CLA	C3D-C2D-C1D	2.95	109.86	105.83
25	r	601	CLA	O1D-CGD-CBD	-2.95	118.69	124.52
24	5	301	CHL	OBD-CAD-CBD	-2.95	121.49	125.82
28	D	404	BCR	C33-C5-C6	-2.95	121.26	124.48
28	d	404	BCR	C33-C5-C6	-2.95	121.26	124.48
25	B	604	CLA	C1D-ND-C4D	-2.95	104.24	106.31
40	s	317	NEX	C15-C14-C13	-2.95	123.14	127.28
25	C	504	CLA	C4D-C3D-CAD	-2.95	104.90	108.11
25	c	504	CLA	C4D-C3D-CAD	-2.95	104.90	108.11
28	A	406	BCR	C27-C26-C25	2.95	126.69	122.70
28	a	407	BCR	C27-C26-C25	2.95	126.69	122.70
24	2	601	CHL	OBD-CAD-CBD	-2.95	121.50	125.82
32	B	624	AJP	C06-C07-C08	-2.95	99.54	104.28
32	b	624	AJP	C06-C07-C08	-2.95	99.54	104.28
25	g	613	CLA	O1D-CGD-CBD	-2.95	118.70	124.52
30	c	520	LMG	C7-O1-C1	-2.95	107.48	113.80
25	B	606	CLA	C1D-CHD-C4C	-2.95	119.76	126.02
25	b	606	CLA	C1D-CHD-C4C	-2.95	119.76	126.02
35	c	516	DGD	C3G-O3G-C1D	-2.95	107.48	113.80
32	y	321	AJP	C83-C06-C05	-2.95	110.19	114.94
24	n	608	CHL	OBD-CAD-CBD	-2.95	121.50	125.82
24	N	605	CHL	OBD-CAD-CBD	-2.95	121.50	125.82
24	n	605	CHL	OBD-CAD-CBD	-2.95	121.50	125.82
25	c	510	CLA	C2A-C1A-CHA	-2.95	118.75	123.87
24	N	608	CHL	OBD-CAD-CBD	-2.94	121.50	125.82
25	a	406	CLA	CHD-C1D-C2D	2.94	131.61	125.49
25	c	510	CLA	C3D-C2D-C1D	2.94	109.85	105.83
25	G	613	CLA	O1D-CGD-CBD	-2.94	118.72	124.52
40	S	317	NEX	C15-C14-C13	-2.94	123.15	127.28
25	g	603	CLA	O1D-CGD-CBD	-2.94	118.72	124.52
24	g	601	CHL	CAA-C2A-C3A	-2.94	105.06	113.00
28	I	101	BCR	C15-C16-C17	-2.94	117.50	123.52
25	g	614	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	r	609	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	B	604	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	r	609	CLA	C4-C3-C5	2.94	120.33	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	405	CLA	CHD-C1D-C2D	2.94	131.60	125.49
25	g	610	CLA	CHD-C1D-C2D	2.94	131.60	125.49
25	g	610	CLA	C3D-C2D-C1D	2.94	109.84	105.83
24	N	606	CHL	C1A-CHA-C4D	2.94	123.88	118.98
25	R	601	CLA	O1D-CGD-CBD	-2.94	118.73	124.52
25	6	605	CLA	C1D-ND-C4D	-2.94	104.25	106.31
25	A	401	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	a	402	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	Y	311	CLA	C4-C3-C5	2.94	120.32	115.23
32	g	618	AJP	C06-C07-C08	-2.93	99.56	104.28
25	s	309	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	R	608	CLA	C4D-CHA-C1A	-2.93	117.75	121.24
25	A	402	CLA	C1D-ND-C4D	-2.93	104.25	106.31
24	N	601	CHL	O2A-CGA-CBA	2.93	120.78	111.83
28	b	617	BCR	C15-C16-C17	-2.93	117.52	123.52
25	C	513	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	y	311	CLA	C4-C3-C5	2.93	120.32	115.23
24	n	601	CHL	O2A-CGA-CBA	2.93	120.77	111.83
24	1	301	CHL	OBD-CAD-CBD	-2.93	121.52	125.82
28	I	101	BCR	C27-C26-C25	2.93	126.66	122.70
25	2	605	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	6	605	CLA	C3D-C2D-C1D	2.93	109.83	105.83
28	B	617	BCR	C15-C16-C17	-2.93	117.53	123.52
24	G	601	CHL	CAA-C2A-C3A	-2.93	105.09	113.00
32	G	618	AJP	C06-C07-C08	-2.93	99.58	104.28
32	B	624	AJP	C61-C59-C58	2.93	120.21	113.02
32	b	624	AJP	C61-C59-C58	2.93	120.21	113.02
25	c	508	CLA	C3D-C2D-C1D	2.93	109.83	105.83
27	A	404	PHO	C4-C3-C5	2.93	120.31	115.23
27	a	405	PHO	C4-C3-C5	2.93	120.31	115.23
24	G	608	CHL	OBD-CAD-CBD	-2.93	121.53	125.82
24	s	308	CHL	C1A-CHA-C4D	2.93	123.86	118.98
25	d	401	CLA	C3D-C2D-C1D	2.93	109.82	105.83
24	n	606	CHL	O1D-CGD-CBD	-2.93	120.29	124.72
32	Y	321	AJP	C83-C06-C05	-2.92	110.22	114.94
25	C	507	CLA	C1D-ND-C4D	-2.92	104.26	106.31
28	i	101	BCR	C27-C26-C25	2.92	126.66	122.70
25	S	309	CLA	C3D-C2D-C1D	2.92	109.82	105.83
28	i	101	BCR	C15-C16-C17	-2.92	117.54	123.52
24	y	306	CHL	C1A-CHA-C4D	2.92	123.86	118.98
25	s	314	CLA	C3D-C2D-C1D	2.92	109.82	105.83
25	G	603	CLA	O1D-CGD-CBD	-2.92	118.76	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	306	CHL	C1A-CHA-C4D	2.92	123.86	118.98
24	s	306	CHL	C1A-CHA-C4D	2.92	123.86	118.98
24	g	609	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
25	R	609	CLA	C3D-C2D-C1D	2.92	109.82	105.83
25	y	312	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
25	c	512	CLA	C1D-ND-C4D	-2.92	104.26	106.31
25	B	614	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
25	b	614	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
25	r	609	CLA	C1D-ND-C4D	-2.92	104.27	106.31
25	Y	305	CLA	C2A-C1A-CHA	-2.92	118.81	123.87
24	s	308	CHL	O1D-CGD-CBD	-2.92	120.30	124.72
32	a	413	AJP	C55-O54-C36	-2.92	111.07	117.98
25	d	403	CLA	C4D-C3D-CAD	-2.92	104.94	108.11
25	B	609	CLA	C3D-C2D-C1D	2.91	109.81	105.83
32	Y	322	AJP	C04-C03-C02	-2.91	105.85	111.67
25	A	402	CLA	C3D-C2D-C1D	2.91	109.81	105.83
25	a	403	CLA	C3D-C2D-C1D	2.91	109.81	105.83
25	g	613	CLA	C3D-C2D-C1D	2.91	109.81	105.83
32	y	322	AJP	C04-C03-C02	-2.91	105.86	111.67
24	S	307	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
24	G	609	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
25	n	604	CLA	C3D-C2D-C1D	2.91	109.80	105.83
24	S	308	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
25	r	602	CLA	C3D-C2D-C1D	2.91	109.80	105.83
25	Y	312	CLA	C2A-C1A-CHA	-2.91	118.82	123.87
25	R	602	CLA	C3D-C2D-C1D	2.91	109.80	105.83
32	S	319	AJP	O25-C26-O31	2.91	118.34	110.69
28	K	101	BCR	C27-C26-C25	2.91	126.63	122.70
24	Y	306	CHL	C1A-CHA-C4D	2.90	123.83	118.98
24	S	308	CHL	C1A-CHA-C4D	2.90	123.83	118.98
25	S	304	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	s	304	CLA	C3D-C2D-C1D	2.90	109.79	105.83
32	A	412	AJP	C55-O54-C36	-2.90	111.10	117.98
25	D	401	CLA	C3D-C2D-C1D	2.90	109.79	105.83
32	g	618	AJP	O31-C30-C32	2.90	111.48	106.83
25	B	601	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	N	604	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	b	601	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	S	305	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
25	S	313	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
25	s	305	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
25	g	602	CLA	C1-C2-C3	-2.90	121.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	b	610	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	R	609	CLA	C4-C3-C5	2.90	120.26	115.23
25	S	303	CLA	C4A-NA-C1A	-2.90	105.36	106.68
24	s	307	CHL	O1D-CGD-CBD	-2.90	120.33	124.72
30	A	408	LMG	C7-O1-C1	-2.90	107.58	113.80
30	a	409	LMG	C7-O1-C1	-2.90	107.58	113.80
25	6	604	CLA	CHA-C1A-NA	-2.90	119.83	126.39
32	n	620	AJP	C83-C06-C05	-2.90	110.27	114.94
24	Y	308	CHL	C4C-CHD-C1D	2.90	126.43	116.07
25	y	305	CLA	C4D-CHA-C1A	-2.89	117.79	121.24
32	g	618	AJP	C04-C03-C02	-2.89	105.89	111.67
25	S	311	CLA	C1D-ND-C4D	-2.89	104.28	106.31
25	c	507	CLA	C1D-ND-C4D	-2.89	104.28	106.31
25	G	613	CLA	C3D-C2D-C1D	2.89	109.78	105.83
24	Y	306	CHL	O2A-CGA-CBA	2.89	120.66	111.83
40	G	617	NEX	C19-C9-C10	-2.89	118.13	122.82
25	Y	312	CLA	CHD-C1D-ND	-2.89	120.73	124.80
24	y	308	CHL	C4C-CHD-C1D	2.89	126.42	116.07
30	D	407	LMG	C1-O6-C5	-2.89	108.07	113.72
30	d	407	LMG	C1-O6-C5	-2.89	108.07	113.72
25	B	605	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	B	608	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	b	605	CLA	C3D-C2D-C1D	2.89	109.78	105.83
32	s	319	AJP	O25-C26-O31	2.89	118.30	110.69
24	Y	302	CHL	O2A-CGA-CBA	2.89	120.65	111.83
24	y	302	CHL	O2A-CGA-CBA	2.89	120.65	111.83
25	R	604	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	r	604	CLA	C3D-C2D-C1D	2.89	109.78	105.83
32	S	319	AJP	C19-C24-C23	-2.89	105.73	112.87
32	s	319	AJP	C19-C24-C23	-2.89	105.73	112.87
32	G	618	AJP	C04-C03-C02	-2.89	105.90	111.67
25	S	314	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	G	602	CLA	C4-C3-C5	2.89	120.24	115.23
25	a	403	CLA	C1D-ND-C4D	-2.89	104.29	106.31
25	B	607	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	C	512	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	b	607	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	c	512	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	s	313	CLA	O1D-CGD-CBD	-2.89	118.83	124.52
28	C	514	BCR	C33-C5-C6	-2.89	121.34	124.48
40	n	617	NEX	C39-C29-C30	-2.88	118.14	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	605	CLA	O1D-CGD-CBD	-2.88	118.83	124.52
25	y	305	CLA	C2A-C1A-CHA	-2.88	118.86	123.87
28	k	101	BCR	C27-C26-C25	2.88	126.60	122.70
25	2	604	CLA	CHA-C1A-NA	-2.88	119.86	126.39
25	2	605	CLA	O1D-CGD-CBD	-2.88	118.83	124.52
25	g	602	CLA	C4-C3-C5	2.88	120.23	115.23
24	R	613	CHL	CMA-C3A-C2A	-2.88	109.62	116.23
24	r	613	CHL	CMA-C3A-C2A	-2.88	109.62	116.23
25	N	610	CLA	C2A-C1A-CHA	-2.88	118.87	123.87
39	S	315	LUT	C3-C4-C5	2.88	119.35	112.18
39	s	315	LUT	C3-C4-C5	2.88	119.35	112.18
25	Y	305	CLA	C4D-CHA-C1A	-2.88	117.81	121.24
25	G	604	CLA	C3D-C2D-C1D	2.88	109.76	105.83
24	G	609	CHL	OMC-CMC-C2C	-2.88	120.12	125.12
25	b	607	CLA	CHD-C1D-C2D	2.88	131.47	125.49
25	G	614	CLA	C3D-C2D-C1D	2.88	109.76	105.83
32	G	618	AJP	O31-C30-C32	2.88	111.45	106.83
25	C	502	CLA	C3D-C2D-C1D	2.88	109.76	105.83
32	N	620	AJP	C83-C06-C05	-2.88	110.30	114.94
25	D	403	CLA	C4D-C3D-CAD	-2.88	104.98	108.11
24	N	609	CHL	C1-C2-C3	2.88	130.91	126.20
24	n	609	CHL	C1-C2-C3	2.88	130.91	126.20
25	B	616	CLA	O2A-CGA-CBA	2.88	120.60	111.83
25	b	616	CLA	O2A-CGA-CBA	2.88	120.60	111.83
24	r	605	CHL	C1A-CHA-C4D	2.88	123.78	118.98
25	n	610	CLA	C2A-C1A-CHA	-2.88	118.88	123.87
25	R	604	CLA	O2A-CGA-CBA	2.88	120.60	111.83
25	r	604	CLA	O2A-CGA-CBA	2.88	120.60	111.83
25	C	505	CLA	C3D-C2D-C1D	2.87	109.75	105.83
40	N	617	NEX	C39-C29-C30	-2.87	118.16	122.82
24	y	306	CHL	O2A-CGA-CBA	2.87	120.59	111.83
25	b	608	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	S	303	CLA	C3D-C2D-C1D	2.87	109.75	105.83
24	y	306	CHL	OMC-CMC-C2C	-2.87	120.13	125.12
25	b	611	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	G	602	CLA	C1-C2-C3	-2.87	121.49	126.20
25	C	512	CLA	C1D-ND-C4D	-2.87	104.30	106.31
24	G	607	CHL	CHA-C1A-C2A	-2.87	126.57	133.31
25	c	502	CLA	C3D-C2D-C1D	2.87	109.75	105.83
32	B	624	AJP	C85-O84-C05	2.87	118.64	113.69
32	b	624	AJP	C85-O84-C05	2.87	118.64	113.69
25	d	402	CLA	CHB-C1B-NB	-2.87	119.75	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	302	CHL	CAA-C2A-C3A	-2.87	105.25	113.00
24	y	302	CHL	CAA-C2A-C3A	-2.87	105.25	113.00
25	N	611	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
25	n	611	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
25	c	503	CLA	C3D-C2D-C1D	2.87	109.75	105.83
32	y	321	AJP	C21-C20-C15	-2.87	106.24	110.10
32	Y	321	AJP	C21-C20-C15	-2.87	106.24	110.10
25	B	601	CLA	C4-C3-C5	2.87	120.20	115.23
25	b	601	CLA	C4-C3-C5	2.87	120.20	115.23
28	H	101	BCR	C2-C1-C6	2.87	114.60	110.44
24	N	606	CHL	OMC-CMC-C2C	-2.87	120.14	125.12
25	B	602	CLA	C3D-C2D-C1D	2.87	109.74	105.83
25	b	609	CLA	C3D-C2D-C1D	2.87	109.74	105.83
24	S	307	CHL	OBD-CAD-CBD	-2.86	121.62	125.82
25	C	508	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
25	c	508	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	l	301	CHL	C1A-CHA-C4D	2.86	123.76	118.98
32	B	624	AJP	O31-C26-C27	2.86	116.25	110.37
32	b	624	AJP	O31-C26-C27	2.86	116.25	110.37
25	y	312	CLA	CHD-C1D-ND	-2.86	120.77	124.80
25	B	611	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	B	614	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	b	614	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	b	612	CLA	C3D-C2D-C1D	2.86	109.74	105.83
24	g	607	CHL	CHA-C1A-C2A	-2.86	126.59	133.31
24	g	609	CHL	OMC-CMC-C2C	-2.86	120.15	125.12
25	y	313	CLA	O1D-CGD-CBD	-2.86	118.88	124.52
24	n	606	CHL	OMC-CMC-C2C	-2.86	120.15	125.12
28	c	514	BCR	C33-C5-C6	-2.86	121.36	124.48
25	r	611	CLA	CHD-C4C-C3C	2.86	128.94	124.77
24	G	607	CHL	CBC-CAC-C3C	-2.86	108.78	112.87
28	T	101	BCR	C11-C10-C9	-2.86	123.27	127.28
25	B	612	CLA	C3D-C2D-C1D	2.86	109.73	105.83
25	s	311	CLA	C1D-ND-C4D	-2.86	104.31	106.31
28	K	101	BCR	C2-C1-C6	2.86	114.59	110.44
28	k	101	BCR	C2-C1-C6	2.86	114.59	110.44
25	B	607	CLA	CHD-C1D-C2D	2.86	131.43	125.49
25	c	513	CLA	C3D-C2D-C1D	2.86	109.73	105.83
25	G	603	CLA	C4D-CHA-C1A	-2.86	117.84	121.24
25	g	603	CLA	C4D-CHA-C1A	-2.86	117.84	121.24
24	g	608	CHL	OBD-CAD-CBD	-2.86	121.63	125.82
25	r	608	CLA	C4D-CHA-C1A	-2.86	117.84	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	604	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	R	603	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
25	r	603	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
25	c	506	CLA	C3D-C2D-C1D	2.85	109.73	105.83
24	R	605	CHL	C1A-CHA-C4D	2.85	123.75	118.98
24	5	301	CHL	C1A-CHA-C4D	2.85	123.75	118.98
35	C	516	DGD	C6D-O5D-C1E	-2.85	107.68	113.80
25	n	602	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
25	C	503	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	C	506	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	b	602	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	c	505	CLA	C3D-C2D-C1D	2.85	109.72	105.83
24	Y	306	CHL	OMC-CMC-C2C	-2.85	120.17	125.12
25	s	303	CLA	C3D-C2D-C1D	2.85	109.72	105.83
24	Y	302	CHL	CHA-C1A-C2A	-2.85	126.62	133.31
25	r	612	CLA	C3B-C4B-NB	-2.85	107.99	110.53
24	N	606	CHL	O1D-CGD-CBD	-2.85	120.41	124.72
28	h	101	BCR	C2-C1-C6	2.85	114.58	110.44
25	r	603	CLA	C4D-CHA-C1A	-2.85	117.85	121.24
35	c	516	DGD	C6D-O5D-C1E	-2.85	107.69	113.80
24	y	302	CHL	CHA-C1A-C2A	-2.85	126.62	133.31
24	G	601	CHL	O2A-CGA-CBA	2.85	120.51	111.83
24	g	601	CHL	O2A-CGA-CBA	2.85	120.51	111.83
25	R	609	CLA	C1D-ND-C4D	-2.84	104.32	106.31
25	c	508	CLA	C4-C3-C5	2.84	120.16	115.23
25	s	303	CLA	C4A-NA-C1A	-2.84	105.38	106.68
41	R	616	XAT	C27-C28-C29	-2.84	121.12	125.53
24	n	605	CHL	C1A-CHA-C4D	2.84	123.72	118.98
24	g	607	CHL	CBC-CAC-C3C	-2.84	108.80	112.87
25	R	614	CLA	O1D-CGD-CBD	-2.84	118.91	124.52
25	R	608	CLA	O2A-CGA-CBA	2.84	120.50	111.83
25	R	608	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	b	603	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	R	603	CLA	C4D-CHA-C1A	-2.84	117.86	121.24
25	c	501	CLA	C4D-C3D-CAD	-2.84	105.02	108.11
25	a	406	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	C	501	CLA	C2D-C1D-ND	-2.84	107.31	110.13
25	c	501	CLA	C2D-C1D-ND	-2.84	107.31	110.13
25	N	602	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	N	613	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	R	603	CLA	C2B-C1B-NB	-2.84	107.38	110.33
25	r	614	CLA	O1D-CGD-CBD	-2.84	118.92	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	608	CLA	O2A-CGA-CBA	2.84	120.49	111.83
32	y	322	AJP	C06-C07-C08	-2.84	99.72	104.28
25	B	608	CLA	CHB-C1B-NB	-2.84	119.80	124.05
25	B	609	CLA	CHB-C1B-NB	-2.84	119.80	124.05
25	b	609	CLA	CHB-C1B-NB	-2.84	119.80	124.05
25	D	402	CLA	CHB-C1B-NB	-2.83	119.80	124.05
25	A	405	CLA	C3D-C2D-C1D	2.83	109.70	105.83
25	A	405	CLA	C4-C3-C5	2.83	120.15	115.23
25	a	406	CLA	C4-C3-C5	2.83	120.15	115.23
25	B	613	CLA	O1D-CGD-CBD	-2.83	118.93	124.52
25	b	613	CLA	O1D-CGD-CBD	-2.83	118.93	124.52
32	Y	322	AJP	C06-C07-C08	-2.83	99.73	104.28
25	n	613	CLA	C4-C3-C5	2.83	120.14	115.23
25	g	604	CLA	C3D-C2D-C1D	2.83	109.69	105.83
25	R	611	CLA	CHD-C4C-C3C	2.83	128.90	124.77
25	y	305	CLA	C3D-C2D-C1D	2.83	109.69	105.83
25	Y	313	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
24	N	605	CHL	C1A-CHA-C4D	2.83	123.70	118.98
25	2	602	CLA	CHD-C4C-C3C	2.83	128.90	124.77
25	6	602	CLA	CHD-C4C-C3C	2.83	128.90	124.77
25	B	616	CLA	C2A-C1A-CHA	-2.83	118.96	123.87
25	b	616	CLA	C2A-C1A-CHA	-2.83	118.96	123.87
25	b	614	CLA	C4-C3-C5	2.83	120.13	115.23
28	B	617	BCR	C11-C10-C9	-2.83	123.31	127.28
28	b	617	BCR	C11-C10-C9	-2.83	123.31	127.28
25	g	612	CLA	C3D-C2D-C1D	2.83	109.69	105.83
25	Y	305	CLA	C3D-C2D-C1D	2.82	109.69	105.83
25	B	607	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
25	b	607	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
25	B	614	CLA	C4-C3-C5	2.82	120.13	115.23
25	r	604	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	S	302	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
25	C	509	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	Y	314	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	c	509	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	y	314	CLA	C3D-C2D-C1D	2.82	109.68	105.83
32	B	624	AJP	C01-C02-C03	2.82	118.25	112.08
25	C	506	CLA	C4A-NA-C1A	-2.82	105.39	106.68
25	c	506	CLA	C4A-NA-C1A	-2.82	105.39	106.68
25	r	608	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	D	403	CLA	C4D-CHA-C1A	-2.82	117.88	121.24
25	c	507	CLA	C4D-CHA-C1A	-2.82	117.88	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	CLA	C4D-CHA-C1A	-2.82	117.88	121.24
35	c	515	DGD	C1E-O6E-C5E	-2.82	108.21	113.72
35	C	515	DGD	C1E-O6E-C5E	-2.82	108.21	113.72
25	Y	315	CLA	C3D-C2D-C1D	2.82	109.68	105.83
24	g	609	CHL	C1-C2-C3	2.82	130.82	126.20
24	s	306	CHL	OBD-CAD-CBD	-2.82	121.69	125.82
24	R	607	CHL	O2A-CGA-CBA	2.82	120.43	111.83
28	t	101	BCR	C11-C10-C9	-2.82	123.32	127.28
26	s	318	LHG	O8-C23-C24	2.82	120.43	111.83
24	N	605	CHL	OMC-CMC-C2C	-2.82	120.23	125.12
24	n	605	CHL	OMC-CMC-C2C	-2.82	120.23	125.12
25	B	603	CLA	C3D-C2D-C1D	2.82	109.68	105.83
24	s	307	CHL	OBD-CAD-CBD	-2.82	121.69	125.82
25	b	608	CLA	CHB-C1B-NB	-2.82	119.83	124.05
32	a	413	AJP	O25-C23-C24	2.81	115.11	109.64
25	r	608	CLA	CHD-C1D-C2D	2.81	131.34	125.49
26	S	318	LHG	O8-C23-C24	2.81	120.42	111.83
25	C	508	CLA	C4-C3-C5	2.81	120.11	115.23
25	R	608	CLA	CHD-C1D-C2D	2.81	131.34	125.49
25	B	616	CLA	CHB-C1B-NB	-2.81	119.83	124.05
25	b	616	CLA	CHB-C1B-NB	-2.81	119.83	124.05
25	N	613	CLA	C4-C3-C5	2.81	120.11	115.23
25	y	305	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
24	s	302	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
40	G	617	NEX	C10-C11-C12	2.81	131.34	123.20
30	C	520	LMG	O8-C28-C29	2.81	120.40	111.83
25	y	311	CLA	C3D-C2D-C1D	2.81	109.66	105.83
25	Y	305	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
25	b	608	CLA	C4-C3-C5	2.81	120.10	115.23
32	b	624	AJP	C01-C02-C03	2.81	118.22	112.08
25	B	606	CLA	C3D-C2D-C1D	2.81	109.66	105.83
25	b	606	CLA	C3D-C2D-C1D	2.81	109.66	105.83
25	R	612	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	C	513	CLA	CHD-C1D-C2D	2.81	131.32	125.49
25	S	312	CLA	O2A-CGA-CBA	2.81	120.39	111.83
25	B	603	CLA	C4-C3-C5	2.81	120.10	115.23
24	g	606	CHL	O2A-CGA-CBA	2.80	120.39	111.83
32	Y	322	AJP	C01-C02-C03	2.80	118.21	112.08
30	c	520	LMG	O8-C28-C29	2.80	120.38	111.83
25	C	512	CLA	O1D-CGD-CBD	-2.80	118.99	124.52
25	c	512	CLA	O1D-CGD-CBD	-2.80	118.99	124.52
25	G	610	CLA	C2A-C1A-CHA	-2.80	119.00	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	C4-C3-C5	2.80	120.09	115.23
24	G	607	CHL	CMB-C2B-C3B	2.80	130.28	124.68
26	Y	301	LHG	O8-C23-C24	2.80	120.38	111.83
24	G	601	CHL	CHA-C1A-C2A	-2.80	126.73	133.31
24	g	601	CHL	CHA-C1A-C2A	-2.80	126.73	133.31
25	R	612	CLA	C4-C3-C5	2.80	120.09	115.23
25	r	603	CLA	C2B-C1B-NB	-2.80	107.42	110.33
24	r	607	CHL	O2A-CGA-CBA	2.80	120.38	111.83
24	Y	302	CHL	C1-C2-C3	2.80	130.79	126.20
24	y	302	CHL	C1-C2-C3	2.80	130.79	126.20
28	K	101	BCR	C15-C16-C17	-2.80	117.79	123.52
24	S	306	CHL	OBD-CAD-CBD	-2.80	121.71	125.82
32	Y	321	AJP	C21-C20-C19	2.80	109.91	107.23
32	y	321	AJP	C21-C20-C19	2.80	109.91	107.23
32	n	619	AJP	C06-C07-C08	-2.80	99.78	104.28
24	G	609	CHL	C1-C2-C3	2.80	130.78	126.20
25	G	612	CLA	C3D-C2D-C1D	2.80	109.65	105.83
25	y	315	CLA	C3D-C2D-C1D	2.80	109.65	105.83
41	r	616	XAT	C27-C28-C29	-2.80	121.19	125.53
24	y	307	CHL	C4D-ND-C1D	-2.80	103.09	105.22
24	g	607	CHL	C1C-CHC-C4B	2.80	126.08	116.07
25	C	501	CLA	C4D-C3D-CAD	-2.80	105.07	108.11
32	Y	324	AJP	C17-C16-C11	-2.80	108.34	112.29
25	C	506	CLA	CHB-C4A-NA	-2.80	120.36	124.40
25	c	506	CLA	CHB-C4A-NA	-2.80	120.36	124.40
28	T	101	BCR	C33-C5-C6	-2.80	121.43	124.48
25	B	613	CLA	C3D-C2D-C1D	2.80	109.65	105.83
24	G	606	CHL	O2A-CGA-CBA	2.80	120.36	111.83
32	Y	322	AJP	C26-O31-C30	2.80	116.23	113.13
26	y	301	LHG	O8-C23-C24	2.79	120.36	111.83
25	Y	311	CLA	C3D-C2D-C1D	2.79	109.64	105.83
25	Y	314	CLA	C4-C3-C5	2.79	120.08	115.23
32	Y	321	AJP	C85-O84-C05	-2.79	108.87	113.69
32	y	321	AJP	C85-O84-C05	-2.79	108.87	113.69
25	c	513	CLA	CHD-C1D-C2D	2.79	131.29	125.49
25	N	611	CLA	CHD-C1D-ND	-2.79	120.87	124.80
24	r	605	CHL	OMC-CMC-C2C	-2.79	120.27	125.12
35	c	515	DGD	C1D-O6D-C5D	-2.79	108.27	113.72
32	y	322	AJP	C01-C02-C03	2.79	118.18	112.08
32	N	619	AJP	C06-C07-C08	-2.79	99.80	104.28
24	R	605	CHL	OMC-CMC-C2C	-2.79	120.28	125.12
25	C	504	CLA	C2B-C1B-NB	-2.79	107.43	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	k	101	BCR	C15-C16-C17	-2.79	117.81	123.52
28	Z	101	BCR	C24-C23-C22	-2.79	122.11	126.23
28	z	101	BCR	C24-C23-C22	-2.79	122.11	126.23
25	c	503	CLA	O1D-CGD-CBD	-2.79	119.02	124.52
28	A	406	BCR	C33-C5-C6	-2.79	121.44	124.48
28	a	407	BCR	C33-C5-C6	-2.79	121.44	124.48
25	g	610	CLA	C2A-C1A-CHA	-2.79	119.03	123.87
24	g	607	CHL	CMB-C2B-C3B	2.79	130.25	124.68
25	b	610	CLA	C4-C3-C5	2.79	120.06	115.23
25	y	314	CLA	C4-C3-C5	2.79	120.06	115.23
25	n	611	CLA	CHD-C1D-ND	-2.79	120.88	124.80
24	G	607	CHL	C1C-CHC-C4B	2.79	126.03	116.07
25	c	504	CLA	C2B-C1B-NB	-2.78	107.44	110.33
25	B	611	CLA	CHD-C1D-C2D	2.78	131.28	125.49
25	B	615	CLA	C4A-NA-C1A	-2.78	105.41	106.68
25	b	615	CLA	C4A-NA-C1A	-2.78	105.41	106.68
25	s	312	CLA	O2A-CGA-CBA	2.78	120.32	111.83
25	B	610	CLA	C4-C3-C5	2.78	120.06	115.23
28	t	101	BCR	C33-C5-C6	-2.78	121.45	124.48
40	S	317	NEX	C39-C29-C30	-2.78	118.31	122.82
25	b	611	CLA	CHD-C1D-C2D	2.78	131.27	125.49
25	B	611	CLA	C4D-CHA-C1A	-2.78	117.93	121.24
25	c	507	CLA	O2A-CGA-CBA	2.78	120.31	111.83
25	n	610	CLA	C3D-C2D-C1D	2.78	109.62	105.83
25	b	603	CLA	C4-C3-C5	2.78	120.05	115.23
28	B	619	BCR	C24-C23-C22	-2.78	122.13	126.23
28	b	619	BCR	C24-C23-C22	-2.78	122.13	126.23
24	G	608	CHL	C4C-CHD-C1D	2.78	126.00	116.07
24	g	608	CHL	C4C-CHD-C1D	2.78	126.00	116.07
25	n	613	CLA	C3D-C2D-C1D	2.78	109.62	105.83
25	c	504	CLA	C4-C3-C5	2.78	120.05	115.23
40	s	317	NEX	C39-C29-C30	-2.78	118.32	122.82
25	R	610	CLA	C2A-C3A-C4A	-2.77	97.39	101.87
35	C	515	DGD	C1D-O6D-C5D	-2.77	108.31	113.72
25	6	602	CLA	O1D-CGD-CBD	-2.77	119.05	124.52
25	r	610	CLA	C2A-C3A-C4A	-2.77	97.39	101.87
24	Y	306	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
25	C	507	CLA	C4D-CHA-C1A	-2.77	117.94	121.24
24	y	306	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
32	A	412	AJP	O25-C23-C24	2.77	115.03	109.64
24	g	605	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
24	g	608	CHL	OMC-CMC-C2C	-2.77	120.31	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	303	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
25	r	612	CLA	C4-C3-C5	2.77	120.03	115.23
28	B	619	BCR	C33-C5-C6	-2.77	121.46	124.48
28	b	619	BCR	C33-C5-C6	-2.77	121.46	124.48
25	b	613	CLA	C3D-C2D-C1D	2.77	109.61	105.83
25	B	616	CLA	C3D-C2D-C1D	2.77	109.61	105.83
25	b	611	CLA	C4D-CHA-C1A	-2.77	117.94	121.24
25	s	303	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
25	N	612	CLA	C4A-NA-C1A	-2.77	105.42	106.68
25	n	612	CLA	C4A-NA-C1A	-2.77	105.42	106.68
32	B	624	AJP	C24-C19-C18	-2.77	106.94	111.73
32	b	624	AJP	C24-C19-C18	-2.77	106.94	111.73
25	C	507	CLA	O2A-CGA-CBA	2.77	120.27	111.83
24	R	607	CHL	C4C-CHD-C1D	2.77	125.96	116.07
24	r	607	CHL	C4C-CHD-C1D	2.77	125.96	116.07
25	b	609	CLA	C4-C3-C5	2.77	120.03	115.23
25	G	604	CLA	C2A-C1A-CHA	-2.77	119.07	123.87
25	2	602	CLA	CHB-C1B-C2B	2.77	135.45	127.43
25	6	602	CLA	CHB-C1B-C2B	2.77	135.45	127.43
25	B	604	CLA	C4D-CHA-C1A	-2.76	117.95	121.24
25	b	604	CLA	C4D-CHA-C1A	-2.76	117.95	121.24
28	K	101	BCR	C33-C5-C6	-2.76	121.47	124.48
28	k	101	BCR	C33-C5-C6	-2.76	121.47	124.48
25	R	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	r	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	D	402	CLA	C2A-C3A-C4A	-2.76	97.41	101.87
25	d	402	CLA	C2A-C3A-C4A	-2.76	97.41	101.87
32	y	322	AJP	C26-O31-C30	2.76	116.19	113.13
32	y	324	AJP	C17-C16-C11	-2.76	108.39	112.29
25	b	609	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
24	y	302	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
24	5	302	CHL	OMC-CMC-C2C	-2.76	120.33	125.12
25	2	602	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
24	Y	310	CHL	C1-C2-C3	2.76	130.72	126.20
24	y	310	CHL	C1-C2-C3	2.76	130.72	126.20
25	G	614	CLA	CHB-C1B-NB	-2.76	119.91	124.05
25	N	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	n	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	N	610	CLA	C3D-C2D-C1D	2.76	109.59	105.83
25	C	504	CLA	C4-C3-C5	2.76	120.01	115.23
25	y	312	CLA	O2A-CGA-CBA	2.76	120.24	111.83
24	G	608	CHL	OMC-CMC-C2C	-2.76	120.33	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	303	CLA	C3D-C2D-C1D	2.76	109.59	105.83
24	N	607	CHL	C1A-CHA-C4D	2.76	123.58	118.98
24	n	607	CHL	C1A-CHA-C4D	2.76	123.58	118.98
25	y	304	CLA	CHB-C1B-NB	-2.76	119.92	124.05
25	c	502	CLA	C4-C3-C5	2.76	120.01	115.23
25	y	303	CLA	C4-C3-C5	2.76	120.01	115.23
25	N	604	CLA	CHD-C1D-C2D	2.76	131.22	125.49
24	Y	309	CHL	C4C-CHD-C1D	2.76	125.93	116.07
24	5	301	CHL	C1C-CHC-C4B	2.76	125.93	116.07
25	C	506	CLA	O2A-CGA-CBA	2.75	120.23	111.83
25	c	506	CLA	O2A-CGA-CBA	2.75	120.23	111.83
25	Y	303	CLA	C4-C3-C5	2.75	120.01	115.23
24	n	607	CHL	O2A-CGA-O1A	-2.75	116.74	123.63
25	2	604	CLA	C2B-C1B-NB	-2.75	107.47	110.33
25	6	604	CLA	C2B-C1B-NB	-2.75	107.47	110.33
25	b	616	CLA	C3D-C2D-C1D	2.75	109.59	105.83
24	N	607	CHL	O2A-CGA-O1A	-2.75	116.74	123.63
25	B	609	CLA	C4-C3-C5	2.75	120.01	115.23
24	n	607	CHL	CAA-C2A-C3A	-2.75	105.57	113.00
25	b	612	CLA	CHD-C1D-C2D	2.75	131.21	125.49
24	N	608	CHL	C1A-CHA-C4D	2.75	123.57	118.98
24	l	301	CHL	C1C-CHC-C4B	2.75	125.90	116.07
25	n	604	CLA	CHD-C1D-C2D	2.75	131.20	125.49
25	A	405	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
25	a	406	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
24	y	309	CHL	C4C-CHD-C1D	2.75	125.90	116.07
27	A	403	PHO	O2A-CGA-CBA	2.75	120.22	111.83
25	Y	313	CLA	O2A-CGA-CBA	2.75	120.21	111.83
25	B	609	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
25	g	612	CLA	C4-C3-C5	2.75	120.00	115.23
25	b	611	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
25	C	510	CLA	O2A-CGA-CBA	2.75	120.21	111.83
24	Y	302	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
25	c	510	CLA	O2A-CGA-CBA	2.75	120.21	111.83
25	Y	303	CLA	C3D-C2D-C1D	2.74	109.58	105.83
28	A	406	BCR	C11-C10-C9	-2.74	123.43	127.28
28	a	407	BCR	C11-C10-C9	-2.74	123.43	127.28
25	N	613	CLA	CHD-C1D-C2D	2.74	131.19	125.49
27	a	404	PHO	O2A-CGA-CBA	2.74	120.20	111.83
24	l	302	CHL	OMC-CMC-C2C	-2.74	120.36	125.12
24	N	607	CHL	CAA-C2A-C3A	-2.74	105.59	113.00
25	C	502	CLA	C4-C3-C5	2.74	119.99	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	310	CLA	C4-C3-C5	2.74	119.99	115.23
25	B	611	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
24	G	605	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
25	B	604	CLA	C4-C3-C5	2.74	119.99	115.23
25	b	604	CLA	C4-C3-C5	2.74	119.99	115.23
32	N	619	AJP	C01-C02-C03	2.74	118.07	112.08
32	Y	320	AJP	C83-C06-C05	-2.74	110.52	114.94
24	g	607	CHL	C4C-CHD-C1D	2.74	125.87	116.07
40	N	617	NEX	C10-C11-C12	2.74	131.14	123.20
32	y	322	AJP	C83-C06-C05	-2.74	110.52	114.94
24	g	601	CHL	C1C-CHC-C4B	2.74	125.87	116.07
24	r	613	CHL	C1A-CHA-C4D	2.74	123.55	118.98
40	n	617	NEX	C10-C11-C12	2.74	131.14	123.20
24	Y	307	CHL	C4D-ND-C1D	-2.74	103.14	105.22
32	A	412	AJP	C58-C57-C56	2.74	114.66	110.86
32	a	413	AJP	C58-C57-C56	2.74	114.66	110.86
25	C	503	CLA	O1D-CGD-CBD	-2.74	119.12	124.52
25	Y	312	CLA	O2A-CGA-CBA	2.74	120.18	111.83
32	S	319	AJP	C20-C21-C22	2.74	118.67	114.17
25	S	305	CLA	C2B-C1B-NB	-2.74	107.49	110.33
25	s	305	CLA	C2B-C1B-NB	-2.74	107.49	110.33
25	R	602	CLA	CHD-C1D-C2D	2.74	131.18	125.49
25	g	614	CLA	CHB-C1B-NB	-2.74	119.95	124.05
32	n	619	AJP	C01-C02-C03	2.73	118.06	112.08
25	d	403	CLA	C4-C3-C5	2.73	119.97	115.23
24	g	609	CHL	C4C-CHD-C1D	2.73	125.84	116.07
24	S	308	CHL	C1C-CHC-C4B	2.73	125.84	116.07
24	s	308	CHL	C1C-CHC-C4B	2.73	125.84	116.07
25	b	606	CLA	O2A-CGA-CBA	2.73	120.16	111.83
32	N	619	AJP	C83-C06-C05	-2.73	110.53	114.94
24	n	608	CHL	C4C-CHD-C1D	2.73	125.84	116.07
25	n	612	CLA	C1D-CHD-C4C	-2.73	120.22	126.02
32	Y	322	AJP	C83-C06-C05	-2.73	110.53	114.94
32	G	618	AJP	C21-C22-C23	2.73	114.11	110.46
25	G	612	CLA	C4-C3-C5	2.73	119.97	115.23
25	s	310	CLA	C4-C3-C5	2.73	119.97	115.23
26	C	518	LHG	O8-C23-C24	2.73	120.16	111.83
28	H	101	BCR	C24-C23-C22	-2.73	122.20	126.23
24	g	601	CHL	C1-C2-C3	2.73	130.67	126.20
25	r	602	CLA	CHD-C1D-C2D	2.73	131.16	125.49
24	G	607	CHL	OMC-CMC-C2C	-2.73	120.38	125.12
24	g	607	CHL	OMC-CMC-C2C	-2.73	120.38	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	602	CLA	C4-C3-C5	2.73	119.97	115.23
24	g	606	CHL	OBD-CAD-CBD	-2.73	121.82	125.82
24	R	613	CHL	C1A-CHA-C4D	2.73	123.53	118.98
25	B	612	CLA	CHD-C1D-C2D	2.73	131.16	125.49
32	y	320	AJP	C83-C06-C05	-2.73	110.54	114.94
39	r	615	LUT	C1-C2-C3	2.73	119.58	113.59
24	s	307	CHL	CHA-C1A-C2A	-2.73	126.90	133.31
25	C	510	CLA	C1D-ND-C4D	-2.73	104.40	106.31
25	c	510	CLA	C1D-ND-C4D	-2.73	104.40	106.31
25	R	602	CLA	C4-C3-C5	2.73	119.96	115.23
32	g	618	AJP	C21-C22-C23	2.73	114.11	110.46
25	g	604	CLA	C2A-C1A-CHA	-2.73	119.14	123.87
28	I	101	BCR	C33-C5-C6	-2.73	121.51	124.48
24	N	608	CHL	C4C-CHD-C1D	2.72	125.82	116.07
25	B	613	CLA	C4-C3-C5	2.72	119.96	115.23
25	b	613	CLA	C4-C3-C5	2.72	119.96	115.23
24	N	607	CHL	C1C-CHC-C4B	2.72	125.81	116.07
32	A	412	AJP	O25-C26-O31	2.72	117.86	110.69
32	a	413	AJP	O25-C26-O31	2.72	117.86	110.69
25	C	507	CLA	C3D-C2D-C1D	2.72	109.55	105.83
32	n	619	AJP	C83-C06-C05	-2.72	110.55	114.94
24	n	607	CHL	C1C-CHC-C4B	2.72	125.81	116.07
25	Y	315	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	S	307	CHL	CHA-C1A-C2A	-2.72	126.91	133.31
25	n	613	CLA	CHD-C1D-C2D	2.72	131.15	125.49
25	C	511	CLA	C1D-ND-C4D	-2.72	104.40	106.31
25	c	511	CLA	C1D-ND-C4D	-2.72	104.40	106.31
25	A	402	CLA	C4-C3-C5	2.72	119.95	115.23
25	a	403	CLA	C4-C3-C5	2.72	119.95	115.23
24	l	301	CHL	C4C-CHD-C1D	2.72	125.81	116.07
24	G	601	CHL	C1C-CHC-C4B	2.72	125.81	116.07
24	G	607	CHL	C4C-CHD-C1D	2.72	125.81	116.07
25	C	501	CLA	O2A-CGA-CBA	2.72	120.13	111.83
30	a	409	LMG	C1-O6-C5	-2.72	108.41	113.72
25	B	606	CLA	O2A-CGA-CBA	2.72	120.13	111.83
25	g	612	CLA	O2A-CGA-CBA	2.72	120.13	111.83
25	r	609	CLA	O2A-CGA-CBA	2.72	120.13	111.83
25	D	403	CLA	C4-C3-C5	2.72	119.95	115.23
25	n	610	CLA	C4-C3-C5	2.72	119.95	115.23
25	b	615	CLA	C4D-CHA-C1A	-2.72	118.00	121.24
24	G	609	CHL	C4C-CHD-C1D	2.72	125.80	116.07
24	l	302	CHL	O1D-CGD-CBD	-2.72	120.60	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	610	CLA	C4-C3-C5	2.72	119.95	115.23
24	s	302	CHL	OMC-CMC-C2C	-2.72	120.40	125.12
30	A	408	LMG	C1-O6-C5	-2.72	108.41	113.72
24	N	606	CHL	C1C-CHC-C4B	2.72	125.80	116.07
24	n	606	CHL	C1C-CHC-C4B	2.72	125.80	116.07
25	g	613	CLA	C1D-ND-C4D	-2.72	104.41	106.31
24	G	606	CHL	OBD-CAD-CBD	-2.72	121.84	125.82
39	R	615	LUT	C1-C2-C3	2.72	119.55	113.59
28	h	101	BCR	C24-C23-C22	-2.72	122.22	126.23
24	5	301	CHL	C4C-CHD-C1D	2.72	125.79	116.07
24	Y	302	CHL	OMC-CMC-C2C	-2.72	120.40	125.12
24	y	302	CHL	OMC-CMC-C2C	-2.72	120.40	125.12
25	y	313	CLA	O2A-CGA-CBA	2.72	120.12	111.83
25	G	611	CLA	C4-C3-C5	2.72	119.94	115.23
25	A	402	CLA	O2A-CGA-CBA	2.72	120.11	111.83
24	n	608	CHL	C1A-CHA-C4D	2.72	123.51	118.98
24	r	607	CHL	C1A-CHA-C4D	2.72	123.51	118.98
24	2	603	CHL	CAA-C2A-C3A	-2.72	105.66	113.00
25	a	403	CLA	O2A-CGA-CBA	2.72	120.11	111.83
26	c	518	LHG	O8-C23-C24	2.72	120.11	111.83
25	Y	313	CLA	C4-C3-C5	2.72	119.94	115.23
24	6	603	CHL	CAA-C2A-C3A	-2.71	105.66	113.00
25	C	506	CLA	C4-C3-C5	2.71	119.94	115.23
25	b	605	CLA	C4-C3-C5	2.71	119.94	115.23
25	c	506	CLA	C4-C3-C5	2.71	119.94	115.23
25	R	609	CLA	O2A-CGA-CBA	2.71	120.11	111.83
32	s	319	AJP	C20-C21-C22	2.71	118.63	114.17
25	c	507	CLA	C3D-C2D-C1D	2.71	109.53	105.83
25	Y	304	CLA	CHB-C1B-NB	-2.71	119.98	124.05
40	y	318	NEX	C30-C31-C32	2.71	131.06	123.20
25	g	603	CLA	C4-C3-C5	2.71	119.94	115.23
25	N	612	CLA	C1D-CHD-C4C	-2.71	120.25	126.02
24	r	606	CHL	C1A-CHA-C4D	2.71	123.51	118.98
25	N	612	CLA	C4-C3-C5	2.71	119.93	115.23
25	y	315	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
24	R	605	CHL	C1C-CHC-C4B	2.71	125.77	116.07
24	r	605	CHL	C1C-CHC-C4B	2.71	125.77	116.07
32	A	412	AJP	C18-C17-C16	-2.71	107.84	112.16
40	Y	318	NEX	C30-C31-C32	2.71	131.05	123.20
24	s	306	CHL	C1C-CHC-C4B	2.71	125.77	116.07
24	G	605	CHL	C4C-CHD-C1D	2.71	125.76	116.07
24	g	605	CHL	C4C-CHD-C1D	2.71	125.76	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	LHG	O8-C23-C24	2.71	120.09	111.83
26	l	103	LHG	O8-C23-C24	2.71	120.09	111.83
25	G	612	CLA	O2A-CGA-CBA	2.71	120.08	111.83
26	2	606	LHG	P-O6-C4	-2.71	105.85	121.35
25	c	505	CLA	C4-C3-C5	2.71	119.92	115.23
25	s	313	CLA	C3B-C4B-NB	-2.70	108.12	110.53
32	a	413	AJP	C18-C17-C16	-2.70	107.85	112.16
26	D	406	LHG	P-O6-C4	-2.70	105.86	121.35
26	d	406	LHG	P-O6-C4	-2.70	105.86	121.35
26	6	606	LHG	P-O6-C4	-2.70	105.86	121.35
25	G	602	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
25	g	602	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
25	S	303	CLA	CHD-C1D-C2D	2.70	131.11	125.49
25	n	612	CLA	C4-C3-C5	2.70	119.92	115.23
32	y	324	AJP	C21-C20-C19	2.70	109.81	107.23
25	S	313	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	Y	308	CHL	C1C-CHC-C4B	2.70	125.74	116.07
24	y	308	CHL	C1C-CHC-C4B	2.70	125.74	116.07
24	G	601	CHL	C1-C2-C3	2.70	130.62	126.20
25	Y	312	CLA	C4-C3-C5	2.70	119.92	115.23
25	g	611	CLA	C4-C3-C5	2.70	119.92	115.23
24	n	609	CHL	C4C-CHD-C1D	2.70	125.73	116.07
24	y	310	CHL	C1A-CHA-C4D	2.70	123.49	118.98
24	N	609	CHL	C1C-CHC-C4B	2.70	125.73	116.07
24	n	609	CHL	C1C-CHC-C4B	2.70	125.73	116.07
25	G	613	CLA	C1D-ND-C4D	-2.70	104.42	106.31
24	S	306	CHL	C1C-CHC-C4B	2.70	125.73	116.07
25	c	501	CLA	O2A-CGA-CBA	2.70	120.07	111.83
24	2	601	CHL	C3C-C4C-NC	-2.70	108.05	114.65
24	6	601	CHL	C3C-C4C-NC	-2.70	108.05	114.65
25	G	603	CLA	C4-C3-C5	2.70	119.92	115.23
24	5	302	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
24	R	606	CHL	C1A-CHA-C4D	2.70	123.49	118.98
25	B	602	CLA	CHD-C1D-C2D	2.70	131.10	125.49
25	b	602	CLA	CHD-C1D-C2D	2.70	131.10	125.49
24	g	606	CHL	C1C-CHC-C4B	2.70	125.72	116.07
32	Y	324	AJP	C21-C20-C19	2.70	109.81	107.23
24	S	307	CHL	C1C-CHC-C4B	2.70	125.72	116.07
24	s	307	CHL	C1C-CHC-C4B	2.70	125.72	116.07
25	C	504	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	S	311	CLA	C4D-CHA-C1A	-2.70	118.03	121.24
25	s	311	CLA	C4D-CHA-C1A	-2.70	118.03	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	313	CLA	C4-C3-C5	2.70	119.91	115.23
25	S	313	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	s	313	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
28	T	101	BCR	C27-C26-C25	2.70	126.35	122.70
28	t	101	BCR	C27-C26-C25	2.70	126.35	122.70
25	N	602	CLA	C3D-C2D-C1D	2.70	109.51	105.83
24	Y	310	CHL	C1A-CHA-C4D	2.70	123.48	118.98
24	g	606	CHL	C4C-CHD-C1D	2.69	125.71	116.07
32	N	619	AJP	C18-C17-C16	-2.69	107.86	112.16
24	R	606	CHL	C1C-CHC-C4B	2.69	125.71	116.07
32	n	619	AJP	C04-C03-C02	-2.69	106.29	111.67
28	B	618	BCR	C33-C5-C6	-2.69	121.55	124.48
28	b	618	BCR	C33-C5-C6	-2.69	121.55	124.48
25	N	614	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
24	G	606	CHL	C1C-CHC-C4B	2.69	125.70	116.07
25	B	615	CLA	C4D-CHA-C1A	-2.69	118.03	121.24
25	G	614	CLA	O2A-CGA-CBA	2.69	120.04	111.83
25	g	614	CLA	O2A-CGA-CBA	2.69	120.04	111.83
24	S	306	CHL	OMC-CMC-C2C	-2.69	120.44	125.12
24	s	308	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
24	g	601	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
24	G	601	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
24	R	613	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
25	D	402	CLA	CHB-C4A-NA	-2.69	120.52	124.40
25	y	312	CLA	C4-C3-C5	2.69	119.90	115.23
25	B	615	CLA	CHB-C1B-NB	-2.69	120.01	124.05
25	C	502	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
24	s	306	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
32	Y	320	AJP	C26-O25-C23	-2.69	110.77	115.27
24	G	606	CHL	C4C-CHD-C1D	2.69	125.69	116.07
25	b	603	CLA	CHD-C1D-C2D	2.69	131.08	125.49
26	n	618	LHG	O8-C23-C24	2.69	120.03	111.83
24	r	606	CHL	C1C-CHC-C4B	2.69	125.69	116.07
32	N	620	AJP	C21-C20-C19	2.69	109.80	107.23
25	b	615	CLA	CHB-C1B-NB	-2.69	120.02	124.05
24	G	608	CHL	C1A-CHA-C4D	2.69	123.47	118.98
25	N	611	CLA	C4-C3-C5	2.69	119.89	115.23
35	B	626	DGD	O1G-C1A-C2A	2.69	120.03	111.83
25	N	603	CLA	C4-C3-C5	2.69	119.89	115.23
25	6	604	CLA	C4-C3-C5	2.69	119.89	115.23
25	s	312	CLA	CHB-C1B-NB	-2.69	120.02	124.05
24	N	609	CHL	C4C-CHD-C1D	2.68	125.67	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	O1D-CGD-CBD	-2.68	119.22	124.52
25	b	610	CLA	O1D-CGD-CBD	-2.68	119.22	124.52
24	S	302	CHL	OMC-CMC-C2C	-2.68	120.46	125.12
32	n	620	AJP	C21-C20-C19	2.68	109.79	107.23
25	n	603	CLA	C4-C3-C5	2.68	119.89	115.23
24	R	607	CHL	C1A-CHA-C4D	2.68	123.46	118.98
24	s	307	CHL	OMC-CMC-C2C	-2.68	120.46	125.12
25	c	509	CLA	C4-C3-C5	2.68	119.88	115.23
24	Y	306	CHL	C1C-CHC-C4B	2.68	125.66	116.07
32	y	323	AJP	C21-C20-C19	2.68	109.79	107.23
24	5	301	CHL	CBC-CAC-C3C	-2.68	109.03	112.87
25	n	611	CLA	C4-C3-C5	2.68	119.88	115.23
28	Z	101	BCR	C28-C27-C26	-2.68	109.28	114.06
24	S	302	CHL	C1C-CHC-C4B	2.68	125.66	116.07
24	g	601	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
25	C	505	CLA	C4-C3-C5	2.68	119.88	115.23
40	g	617	NEX	C20-C13-C12	2.68	122.18	118.09
28	A	406	BCR	C24-C23-C22	-2.68	122.27	126.23
28	a	407	BCR	C24-C23-C22	-2.68	122.27	126.23
35	c	516	DGD	O1G-C1A-C2A	2.68	120.00	111.83
24	l	301	CHL	CBC-CAC-C3C	-2.68	109.04	112.87
25	y	312	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
32	A	412	AJP	O40-C35-C36	2.68	114.70	109.49
24	Y	306	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
24	y	306	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
32	n	619	AJP	C18-C17-C16	-2.68	107.89	112.16
25	B	605	CLA	C4-C3-C5	2.68	119.88	115.23
24	g	608	CHL	C1A-CHA-C4D	2.68	123.45	118.98
24	Y	302	CHL	C1C-CHC-C4B	2.68	125.65	116.07
24	y	302	CHL	C1C-CHC-C4B	2.68	125.65	116.07
35	b	626	DGD	O1G-C1A-C2A	2.68	120.00	111.83
25	G	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	g	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	N	605	CHL	C1C-CHC-C4B	2.67	125.64	116.07
24	n	605	CHL	C1C-CHC-C4B	2.67	125.64	116.07
28	k	101	BCR	C24-C23-C22	-2.67	122.28	126.23
25	b	609	CLA	O1D-CGD-CBD	-2.67	119.24	124.52
25	n	614	CLA	O1D-CGD-CBD	-2.67	119.24	124.52
24	G	601	CHL	OBD-CAD-CBD	-2.67	121.90	125.82
24	r	613	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
25	N	614	CLA	CBA-CAA-C2A	-2.67	105.84	113.79
25	c	502	CLA	O1D-CGD-CBD	-2.67	119.25	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	413	AJP	O40-C35-C36	2.67	114.69	109.49
24	Y	310	CHL	O2A-CGA-CBA	2.67	119.98	111.83
24	y	310	CHL	O2A-CGA-CBA	2.67	119.98	111.83
24	6	601	CHL	C1C-CHC-C4B	2.67	125.63	116.07
24	r	613	CHL	OMC-CMC-C2C	-2.67	120.48	125.12
25	C	513	CLA	C4-C3-C5	2.67	119.87	115.23
26	2	606	LHG	O8-C23-C24	2.67	119.98	111.83
25	c	510	CLA	C4-C3-C5	2.67	119.86	115.23
25	2	602	CLA	C3C-C4C-NC	-2.67	107.01	110.43
25	6	602	CLA	C3C-C4C-NC	-2.67	107.01	110.43
24	y	309	CHL	OMC-CMC-C2C	-2.67	120.48	125.12
25	s	303	CLA	CHD-C1D-C2D	2.67	131.04	125.49
24	S	308	CHL	OMC-CMC-C2C	-2.67	120.48	125.12
40	y	318	NEX	C12-C13-C14	2.67	123.21	119.01
25	A	405	CLA	C4D-CHA-C1A	-2.67	118.06	121.24
25	a	406	CLA	C4D-CHA-C1A	-2.67	118.06	121.24
25	G	611	CLA	C3B-C4B-NB	-2.67	108.15	110.53
25	c	504	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
24	S	307	CHL	OMC-CMC-C2C	-2.67	120.48	125.12
25	n	602	CLA	C3D-C2D-C1D	2.67	109.47	105.83
25	2	605	CLA	O2A-CGA-CBA	2.67	119.97	111.83
25	6	605	CLA	O2A-CGA-CBA	2.67	119.97	111.83
24	N	601	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
25	n	603	CLA	CHD-C1D-C2D	2.67	131.04	125.49
25	c	502	CLA	CHB-C1B-NB	-2.67	120.05	124.05
25	n	603	CLA	O2A-CGA-CBA	2.67	119.97	111.83
26	N	618	LHG	O8-C23-C24	2.67	119.97	111.83
25	B	602	CLA	C4-C3-C5	2.67	119.86	115.23
25	c	513	CLA	C4-C3-C5	2.67	119.86	115.23
35	C	516	DGD	O1G-C1A-C2A	2.67	119.96	111.83
28	B	619	BCR	C2-C1-C6	2.67	114.31	110.44
28	b	619	BCR	C2-C1-C6	2.67	114.31	110.44
24	y	306	CHL	C1C-CHC-C4B	2.67	125.61	116.07
24	R	607	CHL	CHA-C1A-C2A	-2.66	127.05	133.31
25	C	509	CLA	C4-C3-C5	2.66	119.85	115.23
25	B	609	CLA	O1D-CGD-CBD	-2.66	119.26	124.52
40	Y	318	NEX	C12-C13-C14	2.66	123.20	119.01
40	s	317	NEX	C28-C29-C30	2.66	123.20	119.01
32	N	619	AJP	C04-C03-C02	-2.66	106.36	111.67
25	N	603	CLA	CHD-C1D-C2D	2.66	131.02	125.49
25	C	502	CLA	CHB-C1B-NB	-2.66	120.06	124.05
24	N	606	CHL	C4C-CHD-C1D	2.66	125.59	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	609	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
24	g	609	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
24	N	601	CHL	C4C-CHD-C1D	2.66	125.59	116.07
24	n	601	CHL	C4C-CHD-C1D	2.66	125.59	116.07
32	n	619	AJP	C17-C16-C15	-2.66	107.33	110.52
24	S	302	CHL	C4C-CHD-C1D	2.66	125.58	116.07
25	B	603	CLA	CHD-C1D-C2D	2.66	131.02	125.49
24	n	606	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
25	n	614	CLA	CBA-CAA-C2A	-2.66	105.89	113.79
24	Y	309	CHL	OMC-CMC-C2C	-2.66	120.51	125.12
25	s	311	CLA	C4-C3-C5	2.66	119.84	115.23
39	G	615	LUT	C35-C15-C14	-2.66	118.08	123.52
39	g	615	LUT	C35-C15-C14	-2.66	118.08	123.52
24	n	606	CHL	C4C-CHD-C1D	2.66	125.57	116.07
40	S	317	NEX	C28-C29-C30	2.66	123.19	119.01
24	G	606	CHL	OMC-CMC-C2C	-2.66	120.51	125.12
26	d	406	LHG	O8-C23-C24	2.66	119.93	111.83
28	K	101	BCR	C24-C23-C22	-2.66	122.31	126.23
25	S	312	CLA	CHB-C1B-NB	-2.66	120.06	124.05
25	Y	312	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
25	b	612	CLA	O2A-CGA-CBA	2.66	119.93	111.83
24	N	606	CHL	OBD-CAD-CBD	-2.66	121.93	125.82
32	G	618	AJP	C03-C04-C05	-2.66	107.77	111.93
25	2	604	CLA	C4-C3-C5	2.66	119.84	115.23
25	N	603	CLA	O2A-CGA-CBA	2.66	119.93	111.83
28	z	101	BCR	C28-C27-C26	-2.65	109.32	114.06
24	s	302	CHL	C1C-CHC-C4B	2.65	125.57	116.07
25	N	604	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
26	D	406	LHG	O8-C23-C24	2.65	119.93	111.83
25	G	602	CLA	C3D-C2D-C1D	2.65	109.45	105.83
25	g	602	CLA	C3D-C2D-C1D	2.65	109.45	105.83
25	d	402	CLA	CHB-C4A-NA	-2.65	120.57	124.40
25	g	604	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
24	2	601	CHL	C1C-CHC-C4B	2.65	125.56	116.07
24	n	607	CHL	C4C-CHD-C1D	2.65	125.56	116.07
28	B	618	BCR	C15-C16-C17	-2.65	118.09	123.52
28	b	618	BCR	C15-C16-C17	-2.65	118.09	123.52
32	y	320	AJP	C26-O25-C23	-2.65	110.83	115.27
25	S	313	CLA	C4-C3-C5	2.65	119.83	115.23
25	s	313	CLA	C4-C3-C5	2.65	119.83	115.23
24	Y	308	CHL	C3C-C4C-NC	-2.65	108.17	114.65
26	6	606	LHG	O8-C23-C24	2.65	119.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	607	CHL	C4C-CHD-C1D	2.65	125.55	116.07
24	Y	309	CHL	C1A-CHA-C4D	2.65	123.41	118.98
25	B	602	CLA	O2A-CGA-CBA	2.65	119.92	111.83
24	g	605	CHL	C1A-CHA-C4D	2.65	123.40	118.98
28	i	101	BCR	C33-C5-C6	-2.65	121.59	124.48
24	g	606	CHL	OMC-CMC-C2C	-2.65	120.52	125.12
25	B	612	CLA	O2A-CGA-CBA	2.65	119.91	111.83
24	R	613	CHL	O1D-CGD-CBD	-2.65	120.71	124.72
24	s	302	CHL	C4C-CHD-C1D	2.65	125.55	116.07
24	y	308	CHL	C3C-C4C-NC	-2.65	108.18	114.65
24	n	601	CHL	O1D-CGD-CBD	-2.65	120.71	124.72
25	B	613	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	b	613	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	N	605	CHL	C4C-CHD-C1D	2.65	125.54	116.07
24	n	605	CHL	C4C-CHD-C1D	2.65	125.54	116.07
25	b	602	CLA	O2A-CGA-CBA	2.65	119.91	111.83
25	n	604	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
24	n	607	CHL	OBD-CAD-CBD	-2.65	121.94	125.82
25	b	602	CLA	C4-C3-C5	2.65	119.82	115.23
25	R	602	CLA	CHB-C1B-NB	-2.65	120.08	124.05
25	G	613	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
26	S	318	LHG	P-O6-C4	-2.65	106.19	121.35
25	S	311	CLA	C4-C3-C5	2.64	119.82	115.23
24	R	613	CHL	C1C-CHC-C4B	2.64	125.53	116.07
24	r	613	CHL	C1C-CHC-C4B	2.64	125.53	116.07
26	Y	301	LHG	P-O3-C3	-2.64	106.20	121.35
26	y	301	LHG	P-O3-C3	-2.64	106.20	121.35
25	A	401	CLA	C4A-NA-C1A	-2.64	105.47	106.68
24	y	309	CHL	C1A-CHA-C4D	2.64	123.39	118.98
28	D	404	BCR	C28-C27-C26	-2.64	109.34	114.06
24	Y	302	CHL	C4C-CHD-C1D	2.64	125.52	116.07
24	y	302	CHL	C4C-CHD-C1D	2.64	125.52	116.07
25	r	601	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	N	608	CHL	C1C-CHC-C4B	2.64	125.52	116.07
25	r	602	CLA	CHB-C1B-NB	-2.64	120.09	124.05
32	g	618	AJP	C03-C04-C05	-2.64	107.79	111.93
25	a	402	CLA	C4A-NA-C1A	-2.64	105.47	106.68
32	N	619	AJP	C17-C16-C15	-2.64	107.35	110.52
25	C	510	CLA	C4-C3-C5	2.64	119.81	115.23
25	C	509	CLA	CHD-C1D-C2D	2.64	130.98	125.49
25	S	310	CLA	CHB-C1B-NB	-2.64	120.09	124.05
40	N	617	NEX	C2-C1-C6	2.64	111.78	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	609	CHL	C1A-CHA-C4D	2.64	123.38	118.98
32	Y	323	AJP	C21-C20-C19	2.64	109.75	107.23
26	s	318	LHG	P-O6-C4	-2.64	106.24	121.35
26	B	625	LHG	P-O6-C4	-2.64	106.24	121.35
24	Y	306	CHL	C4C-CHD-C1D	2.64	125.50	116.07
24	y	306	CHL	C4C-CHD-C1D	2.64	125.50	116.07
30	A	408	LMG	O8-C28-C29	2.64	119.87	111.83
24	n	608	CHL	C1C-CHC-C4B	2.64	125.50	116.07
25	S	310	CLA	C1D-CHD-C4C	-2.64	120.42	126.02
25	G	604	CLA	O1D-CGD-CBD	-2.64	119.32	124.52
25	c	509	CLA	CHD-C1D-C2D	2.63	130.97	125.49
25	c	508	CLA	C1D-ND-C4D	-2.63	104.46	106.31
24	r	607	CHL	CHA-C1A-C2A	-2.63	127.12	133.31
30	A	410	LMG	O8-C28-C29	2.63	119.86	111.83
30	a	411	LMG	O8-C28-C29	2.63	119.86	111.83
24	g	607	CHL	O2D-CGD-O1D	-2.63	118.72	123.85
25	C	511	CLA	C4D-CHA-C1A	-2.63	118.11	121.24
24	y	310	CHL	OMC-CMC-C2C	-2.63	120.55	125.12
25	G	613	CLA	O2A-CGA-CBA	2.63	119.86	111.83
25	R	601	CLA	O2A-CGA-CBA	2.63	119.86	111.83
28	k	101	BCR	C15-C14-C13	-2.63	123.59	127.28
24	N	607	CHL	OBD-CAD-CBD	-2.63	121.97	125.82
30	a	409	LMG	O8-C28-C29	2.63	119.85	111.83
32	y	323	AJP	C17-C16-C15	-2.63	107.37	110.52
24	G	601	CHL	C4C-CHD-C1D	2.63	125.47	116.07
24	r	606	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
24	G	605	CHL	C1A-CHA-C4D	2.63	123.37	118.98
24	G	607	CHL	C1A-CHA-C4D	2.63	123.37	118.98
24	g	607	CHL	C1A-CHA-C4D	2.63	123.37	118.98
26	b	625	LHG	P-O6-C4	-2.63	106.30	121.35
24	R	613	CHL	OBD-CAD-CBD	-2.63	121.97	125.82
25	Y	314	CLA	CHD-C1D-C2D	2.63	130.95	125.49
25	y	314	CLA	CHD-C1D-C2D	2.63	130.95	125.49
25	g	613	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
28	A	406	BCR	C2-C1-C6	2.63	114.25	110.44
28	a	407	BCR	C2-C1-C6	2.63	114.25	110.44
24	n	608	CHL	OMC-CMC-C2C	-2.62	120.56	125.12
26	B	625	LHG	O8-C23-C24	2.62	119.84	111.83
26	b	625	LHG	O8-C23-C24	2.62	119.84	111.83
24	Y	309	CHL	C1C-CHC-C4B	2.62	125.46	116.07
24	S	302	CHL	OBD-CAD-CBD	-2.62	121.97	125.82
24	s	302	CHL	OBD-CAD-CBD	-2.62	121.97	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	C2B-C1B-NB	-2.62	107.61	110.33
24	Y	310	CHL	C1C-CHC-C4B	2.62	125.46	116.07
25	B	610	CLA	C4D-CHA-C1A	-2.62	118.11	121.24
25	b	610	CLA	C4D-CHA-C1A	-2.62	118.11	121.24
24	y	310	CHL	C1C-CHC-C4B	2.62	125.45	116.07
25	d	403	CLA	C2B-C1B-NB	-2.62	107.61	110.33
25	c	511	CLA	C4D-CHA-C1A	-2.62	118.12	121.24
24	r	613	CHL	OBD-CAD-CBD	-2.62	121.98	125.82
28	K	101	BCR	C15-C14-C13	-2.62	123.60	127.28
24	Y	310	CHL	OMC-CMC-C2C	-2.62	120.57	125.12
30	d	407	LMG	O8-C28-C29	2.62	119.82	111.83
25	D	403	CLA	C2B-C1B-NB	-2.62	107.61	110.33
24	R	607	CHL	OBD-CAD-CBD	-2.62	121.98	125.82
24	r	607	CHL	OMC-CMC-C2C	-2.62	120.57	125.12
32	Y	323	AJP	C17-C16-C15	-2.62	107.38	110.52
25	a	402	CLA	C4-C3-C5	2.62	119.77	115.23
25	R	609	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
24	g	601	CHL	C4C-CHD-C1D	2.62	125.44	116.07
25	c	511	CLA	C4-C3-C5	2.62	119.77	115.23
24	y	309	CHL	C1C-CHC-C4B	2.62	125.43	116.07
25	B	615	CLA	CHC-C4B-NB	-2.62	120.12	124.05
25	b	615	CLA	CHC-C4B-NB	-2.62	120.12	124.05
25	r	609	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
28	Z	101	BCR	C33-C5-C6	-2.62	121.63	124.48
24	Y	306	CHL	CHA-C1A-C2A	-2.62	127.17	133.31
25	g	611	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	A	401	CLA	C4-C3-C5	2.61	119.77	115.23
28	d	404	BCR	C28-C27-C26	-2.61	109.39	114.06
40	n	617	NEX	C2-C1-C6	2.61	111.75	109.21
24	r	606	CHL	OMC-CMC-C2C	-2.61	120.58	125.12
24	5	301	CHL	OMC-CMC-C2C	-2.61	120.58	125.12
25	B	614	CLA	CHD-C1D-C2D	2.61	130.92	125.49
25	b	614	CLA	CHD-C1D-C2D	2.61	130.92	125.49
30	D	407	LMG	O8-C28-C29	2.61	119.80	111.83
25	s	310	CLA	C1D-CHD-C4C	-2.61	120.47	126.02
24	G	609	CHL	C1A-CHA-C4D	2.61	123.34	118.98
24	S	307	CHL	C4C-CHD-C1D	2.61	125.41	116.07
25	R	611	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
25	c	501	CLA	C2B-C1B-NB	-2.61	107.62	110.33
24	r	613	CHL	C4C-CHD-C1D	2.61	125.41	116.07
25	c	504	CLA	C2A-C3A-C4A	-2.61	97.65	101.87
24	Y	308	CHL	OMC-CMC-C2C	-2.61	120.59	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	602	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
25	r	602	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
24	N	609	CHL	OMC-CMC-C2C	-2.61	120.59	125.12
24	n	609	CHL	OMC-CMC-C2C	-2.61	120.59	125.12
24	N	608	CHL	OMC-CMC-C2C	-2.61	120.59	125.12
25	r	611	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
28	I	101	BCR	C15-C14-C13	-2.61	123.62	127.28
24	y	306	CHL	CHA-C1A-C2A	-2.61	127.19	133.31
25	C	511	CLA	C4-C3-C5	2.61	119.75	115.23
32	S	319	AJP	C01-C02-C03	2.61	117.78	112.08
24	y	308	CHL	OMC-CMC-C2C	-2.60	120.60	125.12
28	B	618	BCR	C15-C14-C13	-2.60	123.62	127.28
28	b	618	BCR	C15-C14-C13	-2.60	123.62	127.28
25	C	512	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
28	z	101	BCR	C33-C5-C6	-2.60	121.64	124.48
30	B	620	LMG	O8-C28-C29	2.60	119.78	111.83
25	C	510	CLA	O1D-CGD-CBD	-2.60	119.38	124.52
25	c	510	CLA	O1D-CGD-CBD	-2.60	119.38	124.52
25	g	613	CLA	O2A-CGA-CBA	2.60	119.77	111.83
24	s	307	CHL	C4C-CHD-C1D	2.60	125.38	116.07
25	C	501	CLA	C4-C3-C5	2.60	119.75	115.23
24	S	302	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
25	Y	304	CLA	C4-C3-C5	2.60	119.74	115.23
27	A	403	PHO	C4-C3-C5	2.60	119.74	115.23
27	a	404	PHO	C4-C3-C5	2.60	119.74	115.23
25	c	512	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
24	2	603	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
24	6	603	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
25	y	304	CLA	C4-C3-C5	2.60	119.74	115.23
24	R	613	CHL	C4C-CHD-C1D	2.60	125.38	116.07
25	S	303	CLA	C4-C3-C5	2.60	119.74	115.23
25	s	310	CLA	CHB-C1B-NB	-2.60	120.15	124.05
26	n	618	LHG	P-O6-C4	-2.60	106.45	121.35
25	s	314	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
26	Y	319	LHG	P-O3-C3	-2.60	106.46	121.35
26	y	319	LHG	P-O3-C3	-2.60	106.46	121.35
30	b	620	LMG	O8-C28-C29	2.60	119.76	111.83
24	Y	310	CHL	C4C-CHD-C1D	2.60	125.37	116.07
25	D	401	CLA	O2A-CGA-CBA	2.60	119.76	111.83
25	d	401	CLA	O2A-CGA-CBA	2.60	119.76	111.83
24	r	607	CHL	OBD-CAD-CBD	-2.60	122.01	125.82
24	6	603	CHL	C1C-CHC-C4B	2.60	125.36	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	517	LHG	O8-C23-C24	2.60	119.75	111.83
26	c	517	LHG	O8-C23-C24	2.60	119.75	111.83
24	R	606	CHL	O1D-CGD-CBD	-2.60	120.78	124.72
25	n	611	CLA	O2A-CGA-CBA	2.60	119.75	111.83
24	R	607	CHL	OMC-CMC-C2C	-2.60	120.61	125.12
24	R	605	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
25	s	310	CLA	C3D-C2D-C1D	2.59	109.37	105.83
25	C	504	CLA	C2A-C3A-C4A	-2.59	97.68	101.87
25	r	604	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
26	b	621	LHG	O8-C23-C24	2.59	119.74	111.83
24	y	310	CHL	C4C-CHD-C1D	2.59	125.35	116.07
26	N	618	LHG	P-O6-C4	-2.59	106.50	121.35
26	b	621	LHG	P-O3-C3	-2.59	106.50	121.35
26	B	621	LHG	P-O3-C3	-2.59	106.50	121.35
24	2	603	CHL	C1C-CHC-C4B	2.59	125.34	116.07
26	C	519	LHG	O8-C23-C24	2.59	119.73	111.83
26	c	519	LHG	O8-C23-C24	2.59	119.73	111.83
25	N	603	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
25	N	603	CLA	C4D-CHA-C1A	-2.59	118.15	121.24
25	n	603	CLA	C4D-CHA-C1A	-2.59	118.15	121.24
40	y	318	NEX	C24-C23-C22	-2.59	105.94	110.79
25	N	611	CLA	O2A-CGA-CBA	2.59	119.73	111.83
32	N	620	AJP	C19-C24-C23	-2.59	106.47	112.87
32	n	620	AJP	C19-C24-C23	-2.59	106.47	112.87
32	s	319	AJP	C01-C02-C03	2.59	117.74	112.08
24	Y	302	CHL	C3C-C4C-NC	-2.59	108.32	114.65
24	y	302	CHL	C3C-C4C-NC	-2.59	108.32	114.65
25	N	612	CLA	O2A-CGA-CBA	2.59	119.73	111.83
40	y	318	NEX	C20-C13-C14	-2.59	118.62	122.82
26	C	518	LHG	P-O3-C3	-2.59	106.51	121.35
24	G	608	CHL	C1C-CHC-C4B	2.59	125.33	116.07
24	R	606	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
32	B	624	AJP	C21-C22-C23	2.59	113.92	110.46
32	b	624	AJP	C21-C22-C23	2.59	113.92	110.46
24	g	609	CHL	C1C-CHC-C4B	2.59	125.33	116.07
24	s	302	CHL	CHA-C1A-C2A	-2.59	127.23	133.31
25	2	602	CLA	O2A-CGA-CBA	2.59	119.73	111.83
25	6	602	CLA	O2A-CGA-CBA	2.59	119.73	111.83
24	G	601	CHL	C3C-C4C-NC	-2.59	108.32	114.65
26	c	518	LHG	P-O3-C3	-2.59	106.52	121.35
28	i	101	BCR	C15-C14-C13	-2.59	123.65	127.28
24	2	601	CHL	C1A-CHA-C4D	2.59	123.30	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	601	CHL	C1A-CHA-C4D	2.59	123.30	118.98
25	R	604	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
24	G	607	CHL	O2D-CGD-O1D	-2.59	118.81	123.85
39	S	315	LUT	C1-C2-C3	2.59	119.27	113.59
32	A	412	AJP	C85-O84-C05	2.59	118.15	113.69
32	a	413	AJP	C85-O84-C05	2.59	118.15	113.69
28	B	618	BCR	C27-C26-C25	2.59	126.20	122.70
28	b	618	BCR	C27-C26-C25	2.59	126.20	122.70
40	Y	318	NEX	C20-C13-C14	-2.59	118.63	122.82
25	R	611	CLA	O2A-CGA-CBA	2.59	119.72	111.83
25	B	606	CLA	C4-C3-C5	2.58	119.72	115.23
25	b	606	CLA	C4-C3-C5	2.58	119.72	115.23
25	c	501	CLA	C4-C3-C5	2.58	119.72	115.23
25	S	311	CLA	O2A-CGA-CBA	2.58	119.72	111.83
26	B	621	LHG	O8-C23-C24	2.58	119.72	111.83
24	G	609	CHL	C1C-CHC-C4B	2.58	125.32	116.07
25	r	611	CLA	O2A-CGA-CBA	2.58	119.71	111.83
25	g	613	CLA	C4-C3-C5	2.58	119.71	115.23
39	s	315	LUT	C1-C2-C3	2.58	119.26	113.59
39	G	615	LUT	C1-C2-C3	2.58	119.26	113.59
24	g	608	CHL	C1C-CHC-C4B	2.58	125.31	116.07
24	G	608	CHL	C3C-C4C-NC	-2.58	108.34	114.65
24	r	606	CHL	C4C-CHD-C1D	2.58	125.30	116.07
24	r	605	CHL	CHA-C1A-C2A	-2.58	127.25	133.31
40	Y	318	NEX	C24-C23-C22	-2.58	105.97	110.79
25	C	508	CLA	C1D-ND-C4D	-2.58	104.50	106.31
25	s	303	CLA	C4-C3-C5	2.58	119.70	115.23
25	Y	304	CLA	CHD-C1D-C2D	2.58	130.85	125.49
25	C	509	CLA	O2A-CGA-CBA	2.58	119.69	111.83
25	s	311	CLA	O2A-CGA-CBA	2.58	119.69	111.83
32	Y	324	AJP	C17-C16-C15	-2.58	107.43	110.52
32	y	324	AJP	C17-C16-C15	-2.58	107.43	110.52
32	a	413	AJP	C61-C59-C58	2.58	119.34	113.02
26	s	301	LHG	P-O6-C4	-2.58	106.59	121.35
32	a	413	AJP	C24-C19-C18	-2.57	107.28	111.73
24	s	306	CHL	C4C-CHD-C1D	2.57	125.28	116.07
32	S	319	AJP	C83-C06-C05	-2.57	110.79	114.94
25	n	603	CLA	O1D-CGD-CBD	-2.57	119.44	124.52
39	g	615	LUT	C1-C2-C3	2.57	119.23	113.59
25	n	612	CLA	O2A-CGA-CBA	2.57	119.67	111.83
25	B	608	CLA	CHD-C1D-C2D	2.57	130.83	125.49
25	c	509	CLA	O2A-CGA-CBA	2.57	119.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	303	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
24	S	306	CHL	C4C-CHD-C1D	2.57	125.26	116.07
26	B	622	LHG	P-O6-C4	-2.57	106.63	121.35
26	b	622	LHG	P-O6-C4	-2.57	106.63	121.35
24	R	606	CHL	C4C-CHD-C1D	2.57	125.26	116.07
25	B	603	CLA	CHB-C1B-NB	-2.57	120.20	124.05
24	N	601	CHL	C3C-C4C-NC	-2.57	108.37	114.65
26	l	103	LHG	P-O6-C4	-2.57	106.64	121.35
25	c	512	CLA	C4-C3-C5	2.57	119.69	115.23
25	b	608	CLA	CHD-C1D-C2D	2.57	130.83	125.49
30	B	623	LMG	O8-C28-C29	2.57	119.66	111.83
30	b	623	LMG	O8-C28-C29	2.57	119.66	111.83
25	y	304	CLA	CHD-C1D-C2D	2.57	130.82	125.49
26	S	301	LHG	P-O3-C3	-2.57	106.64	121.35
26	s	301	LHG	P-O3-C3	-2.57	106.64	121.35
35	A	415	DGD	C3G-O3G-C1D	-2.57	108.29	113.80
35	a	401	DGD	C3G-O3G-C1D	-2.57	108.29	113.80
26	S	301	LHG	P-O6-C4	-2.57	106.65	121.35
24	G	606	CHL	C1A-CHA-C4D	2.57	123.26	118.98
24	n	601	CHL	C3C-C4C-NC	-2.57	108.38	114.65
25	b	611	CLA	C4-C3-C5	2.56	119.68	115.23
25	C	502	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
28	H	101	BCR	C29-C30-C25	2.56	114.16	110.44
28	h	101	BCR	C29-C30-C25	2.56	114.16	110.44
24	l	301	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
26	L	102	LHG	P-O6-C4	-2.56	106.66	121.35
25	D	403	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
28	I	101	BCR	C11-C10-C9	-2.56	123.69	127.28
28	i	101	BCR	C11-C10-C9	-2.56	123.69	127.28
25	a	402	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
25	s	310	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
25	S	314	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
24	N	601	CHL	C1C-CHC-C4B	2.56	125.23	116.07
24	g	601	CHL	C3C-C4C-NC	-2.56	108.39	114.65
40	N	617	NEX	C28-C29-C30	2.56	123.04	119.01
26	y	319	LHG	O8-C23-C24	2.56	119.64	111.83
24	n	601	CHL	C1C-CHC-C4B	2.56	125.23	116.07
25	b	603	CLA	CHB-C1B-NB	-2.56	120.21	124.05
25	R	614	CLA	C4D-C3D-CAD	-2.56	105.33	108.11
40	n	617	NEX	C28-C29-C30	2.56	123.03	119.01
24	S	307	CHL	CBC-CAC-C3C	-2.56	109.21	112.87
24	Y	309	CHL	C3C-C4C-NC	-2.56	108.40	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	306	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
40	R	617	NEX	C40-C33-C34	-2.56	118.67	122.82
24	s	308	CHL	C4C-CHD-C1D	2.56	125.22	116.07
28	H	101	BCR	C33-C5-C6	-2.56	121.69	124.48
28	h	101	BCR	C33-C5-C6	-2.56	121.69	124.48
25	y	304	CLA	O2A-CGA-CBA	2.56	119.63	111.83
25	n	613	CLA	O1D-CGD-CBD	-2.56	119.48	124.52
24	y	309	CHL	C3C-C4C-NC	-2.56	108.41	114.65
27	A	404	PHO	O2A-CGA-CBA	2.55	119.62	111.83
27	a	405	PHO	O2A-CGA-CBA	2.55	119.62	111.83
26	b	621	LHG	P-O6-C4	-2.55	106.71	121.35
32	y	323	AJP	O84-C05-C06	2.55	114.88	107.26
32	A	412	AJP	C61-C59-C58	2.55	119.29	113.02
25	s	309	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
32	s	319	AJP	C83-C06-C05	-2.55	110.82	114.94
26	R	618	LHG	O8-C23-C24	2.55	119.62	111.83
39	y	316	LUT	C1-C2-C3	2.55	119.19	113.59
25	d	403	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
25	S	310	CLA	C3D-C2D-C1D	2.55	109.31	105.83
26	Y	319	LHG	O8-C23-C24	2.55	119.62	111.83
25	S	303	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
25	Y	313	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
25	B	616	CLA	C4-C3-C5	2.55	119.66	115.23
25	b	616	CLA	C4-C3-C5	2.55	119.66	115.23
25	G	613	CLA	C4-C3-C5	2.55	119.66	115.23
25	Y	304	CLA	O2A-CGA-CBA	2.55	119.62	111.83
25	S	309	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
24	g	606	CHL	C1A-CHA-C4D	2.55	123.24	118.98
24	s	306	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
39	Y	316	LUT	C1-C2-C3	2.55	119.19	113.59
25	N	613	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
25	c	505	CLA	CHD-C1D-C2D	2.55	130.79	125.49
24	G	606	CHL	C3C-C4C-NC	-2.55	108.42	114.65
24	g	606	CHL	C3C-C4C-NC	-2.55	108.42	114.65
24	S	308	CHL	C4C-CHD-C1D	2.55	125.19	116.07
32	n	619	AJP	C17-C16-C11	-2.55	108.69	112.29
25	r	608	CLA	C4-C3-C5	2.55	119.65	115.23
25	B	611	CLA	C4-C3-C5	2.55	119.65	115.23
25	C	512	CLA	C4-C3-C5	2.55	119.65	115.23
24	G	605	CHL	C1C-CHC-C4B	2.55	125.18	116.07
24	s	307	CHL	CBC-CAC-C3C	-2.55	109.23	112.87
39	y	317	LUT	C3-C4-C5	2.55	118.52	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	310	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
24	g	606	CHL	CHA-C1A-C2A	-2.55	127.33	133.31
25	R	608	CLA	C4-C3-C5	2.55	119.65	115.23
39	n	616	LUT	C3-C4-C5	2.55	118.52	112.18
32	B	624	AJP	O34-C29-C28	-2.55	100.76	107.23
32	b	624	AJP	O34-C29-C28	-2.55	100.76	107.23
25	B	601	CLA	O2A-CGA-CBA	2.55	119.60	111.83
25	b	601	CLA	O2A-CGA-CBA	2.55	119.60	111.83
39	N	616	LUT	C3-C4-C5	2.55	118.52	112.18
26	B	621	LHG	P-O6-C4	-2.54	106.77	121.35
32	Y	324	AJP	C01-C02-C03	2.54	117.64	112.08
32	Y	323	AJP	O84-C05-C06	2.54	114.85	107.26
24	g	608	CHL	C3C-C4C-NC	-2.54	108.43	114.65
25	c	502	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
25	r	614	CLA	C4D-C3D-CAD	-2.54	105.34	108.11
39	Y	317	LUT	C3-C4-C5	2.54	118.51	112.18
24	y	310	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
25	y	313	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
26	s	301	LHG	O8-C23-C24	2.54	119.58	111.83
25	C	506	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
25	c	506	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
24	6	601	CHL	OMC-CMC-C2C	-2.54	120.71	125.12
32	A	412	AJP	C24-C19-C18	-2.54	107.34	111.73
25	B	615	CLA	O2A-CGA-CBA	2.54	119.58	111.83
25	b	615	CLA	O2A-CGA-CBA	2.54	119.58	111.83
25	G	603	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
24	Y	310	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
24	N	608	CHL	C3C-C4C-NC	-2.54	108.44	114.65
32	y	324	AJP	C01-C02-C03	2.54	117.63	112.08
24	g	605	CHL	C1C-CHC-C4B	2.54	125.15	116.07
25	A	401	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	Y	308	CHL	CHA-C1A-C2A	-2.54	127.35	133.31
38	f	101	HEM	CHA-C4D-ND	2.54	127.51	124.37
40	Y	318	NEX	O24-C25-C38	2.54	117.88	115.05
25	R	602	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
25	S	312	CLA	C4D-CHA-C1A	-2.54	118.22	121.24
25	s	312	CLA	C4D-CHA-C1A	-2.54	118.22	121.24
24	5	302	CHL	CHA-C1A-C2A	-2.54	127.35	133.31
24	y	308	CHL	CHA-C1A-C2A	-2.54	127.35	133.31
25	B	613	CLA	CHB-C1B-NB	-2.54	120.24	124.05
25	b	613	CLA	CHB-C1B-NB	-2.54	120.24	124.05
25	B	612	CLA	C4-C3-C5	2.54	119.63	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	C4-C3-C5	2.54	119.63	115.23
24	n	607	CHL	C3C-C4C-NC	-2.54	108.45	114.65
32	y	324	AJP	C83-C06-C05	-2.54	110.85	114.94
40	y	318	NEX	C39-C29-C30	-2.54	118.71	122.82
24	N	607	CHL	C3C-C4C-NC	-2.53	108.46	114.65
25	R	609	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	r	609	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
24	N	601	CHL	OMC-CMC-C2C	-2.53	120.72	125.12
25	Y	314	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
25	y	314	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
24	G	605	CHL	C3C-C4C-NC	-2.53	108.46	114.65
24	g	605	CHL	C3C-C4C-NC	-2.53	108.46	114.65
32	N	619	AJP	C17-C16-C11	-2.53	108.72	112.29
25	B	608	CLA	O2A-CGA-CBA	2.53	119.55	111.83
25	b	608	CLA	O2A-CGA-CBA	2.53	119.55	111.83
25	R	604	CLA	CAA-CBA-CGA	-2.53	106.03	113.21
25	r	604	CLA	CAA-CBA-CGA	-2.53	106.03	113.21
25	Y	311	CLA	O2A-CGA-CBA	2.53	119.55	111.83
25	y	311	CLA	O2A-CGA-CBA	2.53	119.55	111.83
25	S	313	CLA	O2A-CGA-CBA	2.53	119.54	111.83
24	1	301	CHL	C3C-C4C-NC	-2.53	108.47	114.65
24	G	606	CHL	CHA-C1A-C2A	-2.53	127.37	133.31
24	2	601	CHL	OMC-CMC-C2C	-2.53	120.73	125.12
40	r	617	NEX	C40-C33-C34	-2.53	118.72	122.82
24	R	607	CHL	C3C-C4C-NC	-2.53	108.47	114.65
24	r	607	CHL	C3C-C4C-NC	-2.53	108.47	114.65
39	S	316	LUT	C3-C4-C5	2.53	118.47	112.18
24	n	608	CHL	C3C-C4C-NC	-2.53	108.47	114.65
25	R	601	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
26	c	519	LHG	P-O3-C3	-2.52	106.89	121.35
25	C	505	CLA	CHD-C1D-C2D	2.52	130.74	125.49
25	r	614	CLA	C4D-CHA-C1A	-2.52	118.23	121.24
26	2	606	LHG	P-O3-C3	-2.52	106.89	121.35
25	s	313	CLA	O2A-CGA-CBA	2.52	119.53	111.83
26	r	618	LHG	O8-C23-C24	2.52	119.53	111.83
25	B	607	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
25	b	607	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
26	S	318	LHG	P-O3-C3	-2.52	106.90	121.35
26	s	318	LHG	P-O3-C3	-2.52	106.90	121.35
25	2	604	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	6	604	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	y	303	CLA	O2A-CGA-CBA	2.52	119.52	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	606	LHG	P-O3-C3	-2.52	106.90	121.35
26	C	517	LHG	P-O6-C4	-2.52	106.91	121.35
25	g	603	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	A	401	CLA	O2A-CGA-CBA	2.52	119.52	111.83
25	a	402	CLA	O2A-CGA-CBA	2.52	119.52	111.83
28	B	619	BCR	C27-C26-C25	2.52	126.11	122.70
28	H	101	BCR	C27-C26-C25	2.52	126.11	122.70
25	r	614	CLA	C4A-NA-C1A	-2.52	105.53	106.68
26	C	519	LHG	P-O3-C3	-2.52	106.92	121.35
26	S	301	LHG	O8-C23-C24	2.52	119.51	111.83
26	c	517	LHG	P-O6-C4	-2.52	106.92	121.35
25	r	601	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
24	S	308	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
24	s	308	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
26	c	517	LHG	P-O3-C3	-2.52	106.93	121.35
28	C	514	BCR	C15-C16-C17	-2.52	118.37	123.52
28	c	514	BCR	C15-C16-C17	-2.52	118.37	123.52
25	g	604	CLA	CHB-C1B-NB	-2.52	120.28	124.05
25	G	603	CLA	O2A-CGA-CBA	2.52	119.50	111.83
25	G	612	CLA	C4D-CHA-C1A	-2.52	118.24	121.24
39	s	316	LUT	C3-C4-C5	2.51	118.44	112.18
26	C	517	LHG	P-O3-C3	-2.51	106.94	121.35
24	n	606	CHL	C3C-C4C-NC	-2.51	108.51	114.65
24	n	601	CHL	OMC-CMC-C2C	-2.51	120.76	125.12
25	N	602	CLA	O2A-CGA-CBA	2.51	119.50	111.83
26	B	625	LHG	P-O3-C3	-2.51	106.95	121.35
26	b	625	LHG	P-O3-C3	-2.51	106.95	121.35
26	d	406	LHG	P-O3-C3	-2.51	106.95	121.35
24	R	607	CHL	C1C-CHC-C4B	2.51	125.06	116.07
25	B	606	CLA	C1D-ND-C4D	-2.51	104.55	106.31
25	b	606	CLA	C1D-ND-C4D	-2.51	104.55	106.31
25	r	602	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
32	Y	320	AJP	O84-C85-C02	2.51	115.39	112.17
25	n	611	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	Y	308	CHL	C1A-CHA-C4D	2.51	123.17	118.98
24	y	308	CHL	C1A-CHA-C4D	2.51	123.17	118.98
40	Y	318	NEX	C39-C29-C30	-2.51	118.75	122.82
32	g	618	AJP	C83-C06-C05	-2.51	110.89	114.94
25	Y	303	CLA	O2A-CGA-CBA	2.51	119.49	111.83
24	l	302	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
32	Y	324	AJP	C83-C06-C05	-2.51	110.89	114.94
25	C	508	CLA	O2A-CGA-CBA	2.51	119.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	O2A-CGA-CBA	2.51	119.49	111.83
25	n	602	CLA	O2A-CGA-CBA	2.51	119.48	111.83
26	D	406	LHG	P-O3-C3	-2.51	106.97	121.35
24	R	605	CHL	C4C-CHD-C1D	2.51	125.04	116.07
35	A	415	DGD	O1G-C1A-C2A	2.51	119.48	111.83
35	a	401	DGD	O1G-C1A-C2A	2.51	119.48	111.83
32	a	413	AJP	C57-C58-C59	2.51	114.91	109.57
28	b	619	BCR	C27-C26-C25	2.51	126.09	122.70
25	B	609	CLA	CHD-C1D-C2D	2.51	130.70	125.49
25	y	305	CLA	O2A-CGA-CBA	2.50	119.47	111.83
40	S	317	NEX	C1-C2-C3	-2.50	108.10	113.59
24	n	608	CHL	O1D-CGD-CBD	-2.50	120.92	124.72
25	N	611	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
26	B	622	LHG	P-O3-C3	-2.50	107.00	121.35
26	b	622	LHG	P-O3-C3	-2.50	107.00	121.35
25	6	602	CLA	C4-C3-C5	2.50	119.57	115.23
38	F	101	HEM	CHB-C4A-NA	2.50	128.40	123.86
38	f	101	HEM	CHB-C4A-NA	2.50	128.40	123.86
24	r	607	CHL	C1C-CHC-C4B	2.50	125.02	116.07
25	g	603	CLA	O2A-CGA-CBA	2.50	119.47	111.83
24	N	605	CHL	C3C-C4C-NC	-2.50	108.54	114.65
24	n	605	CHL	C3C-C4C-NC	-2.50	108.54	114.65
25	S	312	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
25	b	605	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
25	Y	305	CLA	O2A-CGA-CBA	2.50	119.46	111.83
26	C	518	LHG	P-O6-C4	-2.50	107.02	121.35
26	c	518	LHG	P-O6-C4	-2.50	107.02	121.35
25	2	602	CLA	C4-C3-C5	2.50	119.57	115.23
25	s	312	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
25	R	609	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
25	g	604	CLA	O2A-CGA-CBA	2.50	119.46	111.83
40	R	617	NEX	C1-C2-C3	-2.50	108.11	113.59
26	N	618	LHG	P-O3-C3	-2.50	107.04	121.35
26	n	618	LHG	P-O3-C3	-2.50	107.05	121.35
40	s	317	NEX	C1-C2-C3	-2.50	108.12	113.59
25	C	503	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
25	B	609	CLA	O2A-CGA-CBA	2.50	119.44	111.83
25	b	609	CLA	O2A-CGA-CBA	2.50	119.44	111.83
25	G	604	CLA	O2A-CGA-CBA	2.50	119.44	111.83
28	h	101	BCR	C27-C26-C25	2.49	126.08	122.70
40	n	617	NEX	C26-C27-C28	-2.49	120.72	125.99
32	a	413	AJP	O50-C49-C48	2.49	116.74	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	301	CHL	C3C-C4C-NC	-2.49	108.56	114.65
25	C	503	CLA	C4-C3-C5	2.49	119.56	115.23
25	c	503	CLA	C4-C3-C5	2.49	119.56	115.23
25	C	510	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	c	510	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	n	614	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	B	608	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
40	y	318	NEX	O24-C25-C38	2.49	117.83	115.05
24	r	605	CHL	C4C-CHD-C1D	2.49	124.98	116.07
24	Y	308	CHL	O2A-CGA-CBA	2.49	119.43	111.83
28	B	617	BCR	C28-C27-C26	-2.49	109.61	114.06
28	b	617	BCR	C28-C27-C26	-2.49	109.61	114.06
32	y	320	AJP	O84-C85-C02	2.49	115.37	112.17
32	A	412	AJP	C57-C58-C59	2.49	114.88	109.57
25	B	611	CLA	O2A-CGA-CBA	2.49	119.43	111.83
25	b	611	CLA	O2A-CGA-CBA	2.49	119.43	111.83
24	5	301	CHL	CHA-C1A-C2A	-2.49	127.46	133.31
25	r	601	CLA	C2B-C1B-NB	-2.49	107.74	110.33
25	G	604	CLA	CHB-C1B-NB	-2.49	120.31	124.05
25	b	609	CLA	CHD-C1D-C2D	2.49	130.66	125.49
32	A	412	AJP	O50-C49-C48	2.49	116.73	110.79
25	b	608	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
25	B	605	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
39	n	616	LUT	C11-C10-C9	-2.49	123.79	127.28
24	N	606	CHL	C3C-C4C-NC	-2.49	108.57	114.65
24	g	609	CHL	C3C-C4C-NC	-2.49	108.57	114.65
25	B	607	CLA	C4D-CHA-C1A	-2.49	118.28	121.24
25	b	607	CLA	C4D-CHA-C1A	-2.49	118.28	121.24
26	L	102	LHG	P-O3-C3	-2.49	107.10	121.35
39	s	315	LUT	C22-C23-C24	2.49	114.88	111.18
26	l	103	LHG	P-O3-C3	-2.49	107.11	121.35
40	r	617	NEX	C1-C2-C3	-2.48	108.15	113.59
38	F	101	HEM	CHA-C4D-ND	2.48	127.44	124.37
24	y	310	CHL	O2A-CGA-O1A	-2.48	117.42	123.63
25	r	609	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
39	S	315	LUT	C22-C23-C24	2.48	114.87	111.18
25	2	605	CLA	CHD-C1D-C2D	2.48	130.65	125.49
25	S	311	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
24	Y	310	CHL	O2A-CGA-O1A	-2.48	117.42	123.63
32	G	618	AJP	C83-C06-C05	-2.48	110.94	114.94
25	r	609	CLA	CHB-C1B-NB	-2.48	120.33	124.05
24	y	308	CHL	O2A-CGA-CBA	2.48	119.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	622	LHG	O8-C23-C24	2.48	119.39	111.83
26	b	622	LHG	O8-C23-C24	2.48	119.39	111.83
25	R	609	CLA	CHB-C1B-NB	-2.48	120.33	124.05
24	y	306	CHL	C3C-C4C-NC	-2.48	108.59	114.65
41	r	616	XAT	C31-C32-C33	-2.48	119.57	126.36
25	C	503	CLA	O2A-CGA-CBA	2.48	119.39	111.83
24	Y	306	CHL	C3C-C4C-NC	-2.48	108.60	114.65
25	g	611	CLA	CHD-C1D-C2D	2.48	130.64	125.49
28	A	406	BCR	C15-C16-C17	-2.48	118.45	123.52
28	a	407	BCR	C15-C16-C17	-2.48	118.45	123.52
25	c	503	CLA	O2A-CGA-CBA	2.48	119.39	111.83
24	N	609	CHL	C3C-C4C-NC	-2.48	108.60	114.65
24	n	609	CHL	C3C-C4C-NC	-2.48	108.60	114.65
25	R	610	CLA	O2A-CGA-CBA	2.48	119.38	111.83
35	c	515	DGD	O1G-C1A-C2A	2.48	119.38	111.83
25	C	512	CLA	C4D-CHA-C1A	-2.47	118.29	121.24
40	N	617	NEX	C26-C27-C28	-2.47	120.76	125.99
25	A	402	CLA	C2A-C1A-CHA	-2.47	119.57	123.87
25	a	403	CLA	C2A-C1A-CHA	-2.47	119.57	123.87
25	r	610	CLA	O2A-CGA-CBA	2.47	119.38	111.83
24	S	308	CHL	C3C-C4C-NC	-2.47	108.61	114.65
32	A	412	AJP	C71-C69-C68	2.47	119.09	113.02
32	a	413	AJP	C71-C69-C68	2.47	119.09	113.02
25	n	602	CLA	C4-C3-C5	2.47	119.52	115.23
25	6	605	CLA	CHD-C1D-C2D	2.47	130.63	125.49
25	c	507	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
25	s	311	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
25	D	402	CLA	C4-C3-C5	2.47	119.52	115.23
25	B	611	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
25	B	615	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
25	b	611	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
28	B	618	BCR	C2-C1-C6	2.47	114.03	110.44
28	b	618	BCR	C2-C1-C6	2.47	114.03	110.44
35	C	515	DGD	O1G-C1A-C2A	2.47	119.36	111.83
41	R	616	XAT	C31-C32-C33	-2.47	119.59	126.36
25	g	614	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
25	c	503	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	g	612	CLA	C4D-CHA-C1A	-2.47	118.30	121.24
28	B	618	BCR	C24-C23-C22	-2.46	122.59	126.23
28	b	618	BCR	C24-C23-C22	-2.46	122.59	126.23
24	l	301	CHL	CHA-C1A-C2A	-2.46	127.52	133.31
25	C	507	CLA	O1D-CGD-CBD	-2.46	119.66	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	CLA	C4-C3-C5	2.46	119.50	115.23
32	N	619	AJP	C21-C20-C19	2.46	109.58	107.23
32	n	619	AJP	C21-C20-C19	2.46	109.58	107.23
24	N	607	CHL	O2A-CGA-CBA	2.46	119.34	111.83
26	r	618	LHG	P-O3-C3	-2.46	107.24	121.35
24	G	609	CHL	C3C-C4C-NC	-2.46	108.63	114.65
25	N	602	CLA	C4-C3-C5	2.46	119.50	115.23
39	N	616	LUT	C11-C10-C9	-2.46	123.83	127.28
25	R	601	CLA	C2B-C1B-NB	-2.46	107.77	110.33
25	N	610	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
25	n	610	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
25	c	505	CLA	CHB-C1B-NB	-2.46	120.36	124.05
25	r	608	CLA	C2A-C3A-C4A	-2.46	97.89	101.87
25	R	614	CLA	C4D-CHA-C1A	-2.46	118.31	121.24
25	g	611	CLA	CMD-C2D-C1D	-2.46	120.40	124.73
24	n	607	CHL	O2A-CGA-CBA	2.46	119.33	111.83
24	s	308	CHL	C3C-C4C-NC	-2.46	108.65	114.65
28	B	617	BCR	C7-C8-C9	-2.46	122.60	126.23
28	b	617	BCR	C7-C8-C9	-2.46	122.60	126.23
25	b	615	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
24	S	306	CHL	C3C-C4C-NC	-2.45	108.65	114.65
25	A	401	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
25	a	402	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
25	c	512	CLA	C4A-NA-C1A	-2.45	105.56	106.68
25	R	612	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	N	608	CHL	O1D-CGD-CBD	-2.45	121.00	124.72
24	G	607	CHL	C3C-C4C-NC	-2.45	108.66	114.65
32	N	620	AJP	O25-C26-O31	2.45	117.14	110.69
32	n	620	AJP	O25-C26-O31	2.45	117.14	110.69
25	G	611	CLA	CHD-C1D-C2D	2.45	130.59	125.49
26	R	618	LHG	P-O3-C3	-2.45	107.31	121.35
25	r	612	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	R	613	CHL	C3C-C4C-NC	-2.45	108.66	114.65
25	N	604	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	g	607	CHL	C3C-C4C-NC	-2.45	108.67	114.65
25	C	507	CLA	C4D-C3D-CAD	-2.45	105.45	108.11
24	R	606	CHL	C3C-C4C-NC	-2.45	108.67	114.65
32	B	624	AJP	C26-O31-C30	-2.45	108.94	113.72
32	b	624	AJP	C26-O31-C30	-2.45	108.94	113.72
25	n	604	CLA	O2A-CGA-CBA	2.45	119.30	111.83
25	R	608	CLA	C2A-C3A-C4A	-2.45	97.92	101.87
28	K	101	BCR	C38-C26-C25	-2.45	121.81	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	324	AJP	C18-C17-C16	-2.45	108.26	112.16
25	C	505	CLA	CHB-C1B-NB	-2.45	120.38	124.05
24	r	613	CHL	C3C-C4C-NC	-2.44	108.67	114.65
25	G	611	CLA	CMD-C2D-C1D	-2.44	120.42	124.73
24	s	306	CHL	C3C-C4C-NC	-2.44	108.68	114.65
32	A	412	AJP	C83-C06-C05	-2.44	111.00	114.94
32	a	413	AJP	C83-C06-C05	-2.44	111.00	114.94
27	A	403	PHO	CBC-CAC-C3C	-2.44	109.38	112.87
27	a	404	PHO	CBC-CAC-C3C	-2.44	109.38	112.87
24	Y	310	CHL	C3C-C4C-NC	-2.44	108.68	114.65
25	6	602	CLA	C1D-ND-C4D	2.44	108.03	106.31
25	G	611	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
24	r	606	CHL	C3C-C4C-NC	-2.44	108.69	114.65
24	R	605	CHL	C3C-C4C-NC	-2.44	108.69	114.65
25	B	601	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
25	N	610	CLA	O2A-CGA-CBA	2.44	119.28	111.83
25	n	610	CLA	O2A-CGA-CBA	2.44	119.28	111.83
25	N	614	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
25	b	601	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
25	C	512	CLA	C4A-NA-C1A	-2.44	105.57	106.68
25	g	611	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
32	y	324	AJP	C18-C17-C16	-2.44	108.27	112.16
25	c	512	CLA	C4D-CHA-C1A	-2.44	118.34	121.24
25	D	402	CLA	O2A-CGA-CBA	2.43	119.26	111.83
32	Y	321	AJP	C17-C16-C11	-2.43	108.85	112.29
32	y	321	AJP	C17-C16-C11	-2.43	108.85	112.29
25	G	614	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
24	r	605	CHL	C3C-C4C-NC	-2.43	108.70	114.65
25	G	603	CLA	C2A-C1A-CHA	-2.43	119.64	123.87
25	g	603	CLA	C2A-C1A-CHA	-2.43	119.64	123.87
25	c	507	CLA	C4D-C3D-CAD	-2.43	105.46	108.11
25	b	610	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
25	G	612	CLA	CHB-C1B-NB	-2.43	120.40	124.05
33	A	413	BCT	O3-C-O1	-2.43	113.46	119.68
33	a	414	BCT	O3-C-O1	-2.43	113.46	119.68
25	d	402	CLA	O2A-CGA-CBA	2.43	119.24	111.83
39	S	316	LUT	C37-C21-C22	-2.43	104.88	109.41
39	s	316	LUT	C37-C21-C22	-2.43	104.88	109.41
25	R	614	CLA	C4A-NA-C1A	-2.43	105.57	106.68
25	B	612	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
25	b	612	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
25	s	304	CLA	O1D-CGD-CBD	-2.43	119.73	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	305	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
38	F	101	HEM	CHB-C1B-NB	2.43	127.37	124.37
24	S	302	CHL	C3C-C4C-NC	-2.43	108.72	114.65
24	s	302	CHL	C3C-C4C-NC	-2.43	108.72	114.65
24	y	310	CHL	C3C-C4C-NC	-2.43	108.72	114.65
24	2	601	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
24	1	302	CHL	C4C-CHD-C1D	2.42	124.74	116.07
25	S	304	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
24	g	607	CHL	CAA-C2A-C3A	-2.42	106.46	113.00
25	S	305	CLA	O2A-CGA-CBA	2.42	119.22	111.83
25	s	305	CLA	O2A-CGA-CBA	2.42	119.22	111.83
24	5	302	CHL	C4C-CHD-C1D	2.42	124.73	116.07
25	B	610	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	b	610	CLA	O2A-CGA-CBA	2.42	119.21	111.83
25	R	611	CLA	C3C-C4C-NC	-2.42	107.33	110.43
25	r	611	CLA	C3C-C4C-NC	-2.42	107.33	110.43
25	g	603	CLA	CHD-C1D-C2D	2.42	130.52	125.49
28	k	101	BCR	C38-C26-C25	-2.42	121.85	124.48
25	G	604	CLA	CHD-C1D-C2D	2.42	130.51	125.49
25	g	612	CLA	CHB-C1B-NB	-2.42	120.43	124.05
32	Y	322	AJP	C20-C21-C22	2.41	118.14	114.17
25	s	305	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
24	6	601	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
25	B	616	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
25	b	616	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
25	d	401	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
25	2	605	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
25	6	605	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
25	G	614	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
25	Y	314	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
25	y	311	CLA	CHD-C1D-C2D	2.41	130.50	125.49
32	y	322	AJP	C20-C21-C22	2.41	118.13	114.17
32	G	618	AJP	C18-C17-C16	2.41	116.00	112.16
25	B	615	CLA	C4-C3-C5	2.41	119.41	115.23
25	b	615	CLA	C4-C3-C5	2.41	119.41	115.23
25	G	603	CLA	CHD-C1D-C2D	2.41	130.50	125.49
25	S	314	CLA	C3D-C4D-ND	2.41	113.90	109.99
24	y	307	CHL	C1C-CHC-C4B	2.41	124.69	116.07
25	c	505	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
24	G	607	CHL	CAA-C2A-C3A	-2.41	106.49	113.00
32	A	412	AJP	C27-C28-C29	2.41	115.14	109.68
32	a	413	AJP	C27-C28-C29	2.41	115.14	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	O2A-CGA-CBA	2.41	119.17	111.83
26	r	618	LHG	P-O6-C4	-2.41	107.56	121.35
26	R	618	LHG	P-O6-C4	-2.41	107.57	121.35
24	S	307	CHL	C3C-C4C-NC	-2.41	108.77	114.65
25	Y	303	CLA	CHB-C1B-NB	-2.40	120.44	124.05
25	y	303	CLA	CHB-C1B-NB	-2.40	120.44	124.05
24	s	307	CHL	C3C-C4C-NC	-2.40	108.77	114.65
24	N	601	CHL	CHA-C1A-C2A	-2.40	127.66	133.31
25	c	505	CLA	C3D-C4D-ND	2.40	113.89	109.99
25	R	609	CLA	C4D-CHA-C1A	-2.40	118.38	121.24
25	y	314	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
25	Y	311	CLA	CHD-C1D-C2D	2.40	130.48	125.49
32	A	412	AJP	C48-C47-C46	-2.40	106.64	110.86
32	a	413	AJP	C48-C47-C46	-2.40	106.64	110.86
32	g	618	AJP	C18-C17-C16	2.40	115.99	112.16
25	B	610	CLA	O2A-CGA-CBA	2.40	119.15	111.83
28	B	618	BCR	C11-C10-C9	-2.40	123.91	127.28
28	b	618	BCR	C11-C10-C9	-2.40	123.91	127.28
25	r	608	CLA	CHB-C1B-NB	-2.40	120.45	124.05
25	b	604	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
25	2	602	CLA	C1D-ND-C4D	2.40	107.99	106.31
25	C	505	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
25	A	401	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
25	a	402	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
25	r	608	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
25	C	513	CLA	O2A-CGA-CBA	2.40	119.14	111.83
25	c	513	CLA	O2A-CGA-CBA	2.40	119.14	111.83
25	r	612	CLA	CHB-C1B-C2B	2.40	134.38	127.43
25	B	613	CLA	O2A-CGA-CBA	2.39	119.14	111.83
25	B	604	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
24	N	606	CHL	CHA-C1A-C2A	-2.39	127.69	133.31
25	g	614	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	C	505	CLA	C3D-C4D-ND	2.39	113.88	109.99
25	A	402	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
25	a	403	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
24	n	606	CHL	CHA-C1A-C2A	-2.39	127.69	133.31
25	r	604	CLA	C4D-C3D-CAD	-2.39	105.51	108.11
25	B	603	CLA	O2A-CGA-CBA	2.39	119.12	111.83
25	b	603	CLA	O2A-CGA-CBA	2.39	119.12	111.83
25	R	612	CLA	CHB-C1B-C2B	2.39	134.36	127.43
25	2	602	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	Y	307	CHL	C1C-CHC-C4B	2.39	124.61	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	615	LUT	C31-C30-C29	-2.39	123.93	127.28
39	r	615	LUT	C31-C30-C29	-2.39	123.93	127.28
25	g	604	CLA	C5-C3-C4	2.39	120.08	114.59
25	b	609	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
25	r	609	CLA	C4D-CHA-C1A	-2.38	118.40	121.24
25	R	608	CLA	CHB-C1B-NB	-2.38	120.47	124.05
24	N	607	CHL	CHA-C1A-C2A	-2.38	127.71	133.31
32	a	413	AJP	C06-C07-C08	-2.38	100.45	104.28
25	D	402	CLA	C3A-C2A-C1A	-2.38	97.77	101.34
25	d	402	CLA	C3A-C2A-C1A	-2.38	97.77	101.34
24	n	607	CHL	CHA-C1A-C2A	-2.38	127.71	133.31
25	R	612	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
25	g	604	CLA	CHD-C1D-C2D	2.38	130.44	125.49
25	G	604	CLA	C5-C3-C4	2.38	120.07	114.59
25	D	402	CLA	CHD-C1D-C2D	2.38	130.44	125.49
25	d	402	CLA	CHD-C1D-C2D	2.38	130.44	125.49
25	B	609	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
25	R	604	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
26	y	319	LHG	P-O6-C4	-2.38	107.72	121.35
25	r	604	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
25	B	606	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
25	s	314	CLA	C3D-C4D-ND	2.38	113.85	109.99
26	y	301	LHG	P-O6-C4	-2.38	107.73	121.35
38	f	101	HEM	CHB-C1B-NB	2.38	127.31	124.37
25	D	401	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
32	Y	320	AJP	O09-C08-C07	2.37	109.55	104.08
32	y	320	AJP	O09-C08-C07	2.37	109.55	104.08
32	S	319	AJP	C06-C07-C08	-2.37	100.47	104.28
40	S	317	NEX	C5-C6-C1	-2.37	117.34	119.70
25	r	614	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	n	601	CHL	CHA-C1A-C2A	-2.37	127.73	133.31
25	N	611	CLA	CHB-C1B-NB	-2.37	120.49	124.05
25	n	611	CLA	CHB-C1B-NB	-2.37	120.49	124.05
25	r	614	CLA	C3D-C4D-ND	2.37	113.84	109.99
26	Y	301	LHG	P-O6-C4	-2.37	107.76	121.35
26	Y	319	LHG	P-O6-C4	-2.37	107.76	121.35
40	Y	318	NEX	C40-C33-C32	2.37	121.71	118.09
25	R	608	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	R	614	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
32	Y	324	AJP	C19-C24-C23	-2.37	107.01	112.87
25	r	612	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	Y	305	CLA	O2D-CGD-O1D	-2.37	119.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
28	H	101	BCR	C11-C10-C9	-2.37	123.95	127.28
28	h	101	BCR	C11-C10-C9	-2.37	123.95	127.28
25	S	310	CLA	O2A-CGA-CBA	2.37	119.06	111.83
25	y	304	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
25	g	610	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
25	R	614	CLA	C3D-C4D-ND	2.37	113.83	109.99
40	n	617	NEX	C5-C6-C1	-2.36	117.35	119.70
32	A	412	AJP	C06-C07-C08	-2.36	100.48	104.28
28	A	406	BCR	C38-C26-C25	-2.36	121.91	124.48
28	a	407	BCR	C38-C26-C25	-2.36	121.91	124.48
25	B	615	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
25	b	615	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
25	s	309	CLA	CHB-C1B-NB	-2.36	120.50	124.05
25	y	312	CLA	C4D-CHA-C1A	-2.36	118.43	121.24
32	y	324	AJP	C19-C24-C23	-2.36	107.04	112.87
28	I	101	BCR	C38-C26-C25	-2.36	121.91	124.48
25	c	513	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
25	Y	304	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
25	6	602	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
25	G	602	CLA	C3D-C4D-ND	2.36	113.82	109.99
25	g	602	CLA	C3D-C4D-ND	2.36	113.82	109.99
25	B	614	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
25	b	614	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
25	C	513	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
25	s	310	CLA	O2A-CGA-CBA	2.36	119.02	111.83
32	S	319	AJP	C17-C16-C11	-2.36	108.96	112.29
32	s	319	AJP	C17-C16-C11	-2.36	108.96	112.29
25	y	305	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
25	b	606	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
28	C	514	BCR	C2-C1-C6	2.35	113.86	110.44
40	N	617	NEX	C5-C6-C1	-2.35	117.36	119.70
32	G	618	AJP	C85-O84-C05	2.35	117.75	113.69
28	i	101	BCR	C38-C26-C25	-2.35	121.92	124.48
25	Y	312	CLA	C3D-C4D-ND	2.35	113.81	109.99
25	C	513	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
25	c	513	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
32	s	319	AJP	C06-C07-C08	-2.35	100.50	104.28
24	N	605	CHL	CHA-C1A-C2A	-2.35	127.78	133.31
40	s	317	NEX	C5-C6-C1	-2.35	117.36	119.70
25	d	402	CLA	CHC-C4B-NB	-2.35	120.52	124.05
25	B	611	CLA	O2D-CGD-O1D	-2.35	119.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	611	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
24	l	302	CHL	C1C-CHC-C4B	2.35	124.47	116.07
24	5	302	CHL	C1C-CHC-C4B	2.35	124.47	116.07
25	B	606	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
28	c	514	BCR	C2-C1-C6	2.35	113.85	110.44
25	S	305	CLA	C5-C3-C4	2.35	119.99	114.59
25	Y	305	CLA	C5-C3-C4	2.35	119.99	114.59
25	G	610	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
25	Y	311	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
24	l	302	CHL	O2A-CGA-CBA	2.34	121.41	114.00
25	S	309	CLA	CHB-C1B-NB	-2.34	120.53	124.05
25	s	305	CLA	C5-C3-C4	2.34	119.98	114.59
25	A	405	CLA	O2A-CGA-CBA	2.34	118.98	111.83
25	a	406	CLA	O2A-CGA-CBA	2.34	118.98	111.83
25	D	402	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
25	d	402	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
25	N	612	CLA	CHB-C1B-NB	-2.34	120.54	124.05
32	g	618	AJP	C85-O84-C05	2.34	117.73	113.69
41	R	616	XAT	C40-C33-C34	-2.34	119.03	122.82
32	G	618	AJP	C17-C18-C19	2.34	116.36	111.84
32	g	618	AJP	C17-C18-C19	2.34	116.36	111.84
25	y	311	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
25	R	604	CLA	C4D-C3D-CAD	-2.34	105.57	108.11
25	n	612	CLA	CHB-C1B-NB	-2.34	120.54	124.05
24	5	302	CHL	O2A-CGA-CBA	2.34	121.38	114.00
25	n	604	CLA	C5-C3-C4	2.33	119.96	114.59
25	c	501	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
40	R	617	NEX	C32-C33-C34	2.33	122.68	119.01
41	r	616	XAT	C40-C33-C34	-2.33	119.03	122.82
25	N	604	CLA	C5-C3-C4	2.33	119.96	114.59
24	n	605	CHL	CHA-C1A-C2A	-2.33	127.83	133.31
25	y	305	CLA	C5-C3-C4	2.33	119.96	114.59
40	y	318	NEX	C40-C33-C32	2.33	121.65	118.09
25	y	312	CLA	C3D-C4D-ND	2.33	113.78	109.99
25	B	601	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	B	607	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	b	607	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	n	604	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
25	R	604	CLA	C4D-CHA-C1A	-2.33	118.47	121.24
25	r	604	CLA	C4D-CHA-C1A	-2.33	118.47	121.24
39	R	615	LUT	C35-C34-C33	-2.33	124.02	127.28
25	n	613	CLA	O2A-CGA-CBA	2.33	118.93	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	611	CLA	C2C-C1C-NC	-2.33	107.54	109.98
25	Y	305	CLA	C3D-C4D-ND	2.33	113.77	109.99
25	n	610	CLA	CHD-C1D-C2D	2.33	130.32	125.49
25	C	507	CLA	C1D-CHD-C4C	-2.32	121.08	126.02
25	c	507	CLA	C1D-CHD-C4C	-2.32	121.08	126.02
25	S	303	CLA	C3D-C4D-ND	2.32	113.77	109.99
25	g	612	CLA	C3D-C4D-ND	2.32	113.77	109.99
25	r	603	CLA	O2A-CGA-CBA	2.32	118.92	111.83
40	r	617	NEX	C32-C33-C34	2.32	122.67	119.01
25	B	602	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
25	b	602	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
25	C	502	CLA	O2A-CGA-CBA	2.32	118.92	111.83
25	c	502	CLA	O2A-CGA-CBA	2.32	118.92	111.83
25	N	614	CLA	O2A-CGA-CBA	2.32	118.92	111.83
25	S	303	CLA	CHB-C1B-NB	-2.32	120.57	124.05
25	s	303	CLA	CHB-C1B-NB	-2.32	120.57	124.05
25	B	608	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
25	n	614	CLA	O2A-CGA-CBA	2.32	118.91	111.83
25	s	303	CLA	C3D-C4D-ND	2.32	113.76	109.99
25	g	610	CLA	O2A-CGA-CBA	2.32	118.91	111.83
40	G	617	NEX	C20-C13-C12	2.32	121.63	118.09
25	G	610	CLA	O2A-CGA-CBA	2.32	118.91	111.83
25	D	402	CLA	CHC-C4B-NB	-2.32	120.57	124.05
32	B	624	AJP	C04-C05-C06	2.32	119.86	115.66
32	b	624	AJP	C04-C05-C06	2.32	119.86	115.66
25	N	613	CLA	CHD-C4C-C3C	-2.32	121.39	124.77
25	N	613	CLA	O2A-CGA-CBA	2.32	118.89	111.83
25	y	313	CLA	C4A-NA-C1A	-2.31	105.62	106.68
25	G	612	CLA	C3D-C4D-ND	2.31	113.75	109.99
25	s	312	CLA	CHC-C4B-NB	-2.31	120.58	124.05
25	G	604	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
25	b	608	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
25	Y	313	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
24	6	603	CHL	O2D-CGD-CBD	2.31	113.48	110.95
25	b	609	CLA	C3D-C4D-ND	2.31	113.74	109.99
25	R	604	CLA	CHB-C1B-C2B	2.31	134.13	127.43
25	n	602	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
25	B	609	CLA	C3D-C4D-ND	2.31	113.74	109.99
25	y	305	CLA	C3D-C4D-ND	2.31	113.74	109.99
25	B	614	CLA	O2A-CGA-CBA	2.31	118.87	111.83
25	b	614	CLA	O2A-CGA-CBA	2.31	118.87	111.83
25	Y	303	CLA	C2A-C1A-CHA	-2.31	119.86	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	303	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
25	r	604	CLA	CHB-C1B-C2B	2.31	134.12	127.43
40	g	617	NEX	C10-C11-C12	2.31	129.88	123.20
25	r	610	CLA	CHC-C4B-NB	-2.31	120.59	124.05
25	a	402	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
25	R	603	CLA	CHC-C4B-NB	-2.31	120.59	124.05
38	f	101	HEM	CHA-C1A-NA	2.30	128.04	123.86
25	b	613	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
25	c	502	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
29	l	101	SQD	O9-S-O7	2.30	121.32	113.82
39	r	615	LUT	C35-C34-C33	-2.30	124.05	127.28
25	D	401	CLA	C5-C3-C4	2.30	119.89	114.59
25	d	401	CLA	C5-C3-C4	2.30	119.89	114.59
25	C	506	CLA	CHD-C1D-C2D	2.30	130.28	125.49
25	c	506	CLA	CHD-C1D-C2D	2.30	130.28	125.49
25	c	506	CLA	C3D-C4D-ND	2.30	113.73	109.99
25	C	501	CLA	C2A-C3A-C4A	-2.30	98.15	101.87
25	G	611	CLA	C4D-C3D-CAD	-2.30	105.61	108.11
25	g	611	CLA	C4D-C3D-CAD	-2.30	105.61	108.11
25	n	602	CLA	CHB-C1B-NB	-2.30	120.60	124.05
25	r	611	CLA	C2C-C1C-NC	-2.30	107.56	109.98
25	B	610	CLA	CHB-C1B-NB	-2.30	120.60	124.05
25	b	610	CLA	CHB-C1B-NB	-2.30	120.60	124.05
32	a	413	AJP	O70-C65-C66	2.30	115.10	110.37
25	C	505	CLA	O2A-CGA-CBA	2.30	118.85	111.83
25	S	312	CLA	CHB-C4A-NA	-2.30	121.08	124.40
38	F	101	HEM	CHA-C1A-NA	2.30	128.03	123.86
28	T	101	BCR	C38-C26-C25	-2.30	121.97	124.48
28	t	101	BCR	C38-C26-C25	-2.30	121.97	124.48
24	G	609	CHL	CHA-C1A-C2A	-2.30	127.91	133.31
25	c	505	CLA	O2A-CGA-CBA	2.30	118.84	111.83
39	n	615	LUT	C1-C2-C3	2.30	118.63	113.59
25	N	610	CLA	CHD-C1D-C2D	2.30	130.26	125.49
25	N	604	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
25	N	602	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
25	R	603	CLA	O2A-CGA-CBA	2.29	118.83	111.83
29	L	103	SQD	O9-S-O7	2.29	121.28	113.82
25	s	312	CLA	CHB-C4A-NA	-2.29	121.09	124.40
25	A	401	CLA	C4D-CHA-C1A	-2.29	118.51	121.24
32	Y	324	AJP	C85-O84-C05	2.29	117.64	113.69
32	y	324	AJP	C85-O84-C05	2.29	117.64	113.69
24	l	302	CHL	OBD-CAD-CBD	-2.29	122.46	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	102	SQD	O9-S-O7	2.29	121.28	113.82
25	n	613	CLA	CHD-C4C-C3C	-2.29	121.43	124.77
25	r	603	CLA	CHC-C4B-NB	-2.29	120.61	124.05
29	A	411	SQD	O9-S-O7	2.29	121.27	113.82
29	a	412	SQD	O9-S-O7	2.29	121.27	113.82
25	Y	312	CLA	C4D-CHA-C1A	-2.29	118.51	121.24
24	5	302	CHL	OBD-CAD-CBD	-2.29	122.46	125.82
25	g	614	CLA	CHD-C1D-C2D	2.29	130.25	125.49
32	A	412	AJP	O70-C65-C66	2.29	115.07	110.37
25	R	610	CLA	CHC-C4B-NB	-2.29	120.61	124.05
25	B	605	CLA	O2A-CGA-CBA	2.29	118.81	111.83
25	b	605	CLA	O2A-CGA-CBA	2.29	118.81	111.83
25	B	601	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
25	b	601	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
39	N	615	LUT	C1-C2-C3	2.29	118.61	113.59
24	Y	308	CHL	O2D-CGD-O1D	-2.29	119.40	123.85
25	c	507	CLA	C4-C3-C5	2.28	119.19	115.23
25	C	502	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
29	L	101	SQD	O9-S-O7	2.28	121.25	113.82
25	G	612	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
25	g	612	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
24	l	301	CHL	O2A-CGA-CBA	2.28	121.21	114.00
24	5	301	CHL	O2A-CGA-CBA	2.28	121.21	114.00
25	b	616	CLA	C3D-C4D-ND	2.28	113.70	109.99
28	T	101	BCR	C15-C14-C13	-2.28	124.08	127.28
28	z	101	BCR	C29-C30-C25	2.28	113.75	110.44
25	R	603	CLA	C4-C3-C5	2.28	119.19	115.23
25	r	603	CLA	C4-C3-C5	2.28	119.19	115.23
25	S	312	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
25	S	312	CLA	CHC-C4B-NB	-2.28	120.63	124.05
25	c	503	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
25	g	604	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
25	B	613	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
24	2	603	CHL	O2D-CGD-CBD	2.28	113.45	110.95
25	C	503	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
25	r	602	CLA	C3D-C4D-ND	2.28	113.69	109.99
25	C	504	CLA	CHC-C4B-NB	-2.27	120.64	124.05
24	y	308	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
25	N	602	CLA	CHB-C1B-NB	-2.27	120.64	124.05
25	y	314	CLA	O2A-CGA-CBA	2.27	118.77	111.83
28	D	404	BCR	C29-C30-C25	2.27	113.74	110.44
28	d	404	BCR	C29-C30-C25	2.27	113.74	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	313	CLA	C4D-CHA-C1A	-2.27	118.53	121.24
24	G	606	CHL	O2A-CGA-O1A	-2.27	117.94	123.63
25	G	614	CLA	CHD-C1D-C2D	2.27	130.21	125.49
25	B	606	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
25	b	606	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
25	D	403	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	d	403	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
28	D	404	BCR	C7-C8-C9	-2.27	122.88	126.23
28	d	404	BCR	C7-C8-C9	-2.27	122.88	126.23
25	R	602	CLA	C3D-C4D-ND	2.27	113.68	109.99
25	c	501	CLA	CHC-C4B-NB	-2.27	120.64	124.05
25	N	611	CLA	C3D-C4D-ND	2.27	113.67	109.99
25	D	401	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
25	d	401	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
25	B	605	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	b	605	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	C	507	CLA	C4-C3-C5	2.27	119.17	115.23
25	n	614	CLA	CHD-C1D-C2D	2.27	130.20	125.49
25	c	504	CLA	CHC-C4B-NB	-2.27	120.65	124.05
25	Y	314	CLA	O2A-CGA-CBA	2.27	118.75	111.83
25	s	312	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
25	y	311	CLA	C3D-C4D-ND	2.27	113.67	109.99
25	S	311	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
25	s	311	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
28	h	101	BCR	C38-C26-C25	-2.26	122.01	124.48
25	b	613	CLA	C4D-CHA-C1A	-2.26	118.54	121.24
24	2	603	CHL	OMC-CMC-C2C	-2.26	121.19	125.12
25	C	511	CLA	O2A-CGA-CBA	2.26	118.74	111.83
25	c	511	CLA	O2A-CGA-CBA	2.26	118.74	111.83
28	H	101	BCR	C38-C26-C25	-2.26	122.01	124.48
25	C	506	CLA	C3D-C4D-ND	2.26	113.67	109.99
32	Y	322	AJP	C19-C24-C23	-2.26	107.28	112.87
32	y	322	AJP	C19-C24-C23	-2.26	107.28	112.87
24	g	606	CHL	O2A-CGA-O1A	-2.26	117.97	123.63
25	s	314	CLA	CHD-C1D-C2D	2.26	130.19	125.49
28	I	101	BCR	C7-C8-C9	-2.26	122.89	126.23
25	G	602	CLA	O2A-CGA-CBA	2.26	118.73	111.83
32	B	624	AJP	O60-C55-C56	2.26	115.02	110.37
32	b	624	AJP	O60-C55-C56	2.26	115.02	110.37
28	A	406	BCR	C7-C8-C9	-2.26	122.89	126.23
28	a	407	BCR	C7-C8-C9	-2.26	122.89	126.23
24	g	609	CHL	CHA-C1A-C2A	-2.26	128.00	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	614	CLA	CHD-C1D-C2D	2.26	130.19	125.49
25	N	603	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	B	613	CLA	C4D-CHA-C1A	-2.26	118.55	121.24
28	Z	101	BCR	C29-C30-C25	2.26	113.72	110.44
25	b	601	CLA	C3B-C4B-NB	-2.26	108.52	110.53
25	B	604	CLA	O2A-CGA-CBA	2.26	118.72	111.83
25	g	602	CLA	O2A-CGA-CBA	2.26	118.71	111.83
25	6	604	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
25	2	604	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
25	C	506	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
25	c	506	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
25	C	501	CLA	C2A-C1A-CHA	-2.25	119.95	123.87
25	c	501	CLA	C2A-C1A-CHA	-2.25	119.95	123.87
25	S	309	CLA	CHD-C1D-C2D	2.25	130.17	125.49
25	s	309	CLA	CHD-C1D-C2D	2.25	130.17	125.49
25	b	604	CLA	O2A-CGA-CBA	2.25	118.70	111.83
25	B	612	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
25	S	314	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	R	614	CLA	CHD-C1D-C2D	2.25	130.17	125.49
25	r	614	CLA	CHD-C1D-C2D	2.25	130.17	125.49
25	Y	303	CLA	C3D-C4D-ND	2.25	113.65	109.99
40	g	617	NEX	C39-C29-C30	-2.25	119.17	122.82
32	Y	324	AJP	C04-C03-C02	-2.25	107.18	111.67
24	Y	309	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
27	A	404	PHO	CBC-CAC-C3C	-2.25	109.66	112.87
27	a	405	PHO	CBC-CAC-C3C	-2.25	109.66	112.87
28	C	514	BCR	C27-C26-C25	2.25	125.74	122.70
28	c	514	BCR	C27-C26-C25	2.25	125.74	122.70
25	S	314	CLA	CHD-C1D-C2D	2.25	130.16	125.49
28	i	101	BCR	C7-C8-C9	-2.25	122.91	126.23
32	y	324	AJP	C04-C03-C02	-2.25	107.19	111.67
25	d	403	CLA	CHC-C4B-NB	-2.25	120.68	124.05
25	C	509	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
28	t	101	BCR	C15-C14-C13	-2.25	124.13	127.28
25	y	303	CLA	C3D-C4D-ND	2.25	113.64	109.99
25	Y	313	CLA	C4A-NA-C1A	-2.24	105.66	106.68
25	b	603	CLA	C3D-C4D-ND	2.24	113.63	109.99
25	C	509	CLA	C2A-C1A-CHA	-2.24	119.97	123.87
25	c	509	CLA	C2A-C1A-CHA	-2.24	119.97	123.87
25	n	614	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	C	514	BCR	C8-C7-C6	-2.24	121.01	127.00
25	C	512	CLA	O2A-CGA-CBA	2.24	118.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	619	AJP	C29-C30-C32	-2.24	108.34	112.50
25	n	611	CLA	C3D-C4D-ND	2.24	113.63	109.99
25	r	608	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
24	S	306	CHL	O2D-CGD-O1D	-2.24	119.48	123.85
25	n	603	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
25	r	602	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
25	Y	312	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
41	r	616	XAT	C20-C13-C14	-2.24	119.19	122.82
25	c	512	CLA	O2A-CGA-CBA	2.24	118.66	111.83
28	B	619	BCR	C15-C16-C17	-2.24	118.94	123.52
28	b	619	BCR	C15-C16-C17	-2.24	118.94	123.52
24	s	306	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
24	y	309	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
25	R	608	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
24	6	603	CHL	OMC-CMC-C2C	-2.24	121.24	125.12
24	R	607	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
32	n	619	AJP	C29-C30-C32	-2.23	108.36	112.50
25	Y	304	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	y	304	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	B	616	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	N	603	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	n	603	CLA	C3D-C4D-ND	2.23	113.61	109.99
24	G	601	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
25	R	611	CLA	CHA-C4D-ND	-2.23	127.94	132.55
25	Y	313	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	r	612	CLA	C4D-CHA-C1A	-2.23	118.58	121.24
28	B	618	BCR	C29-C30-C25	2.23	113.68	110.44
28	b	618	BCR	C29-C30-C25	2.23	113.68	110.44
25	Y	311	CLA	C3D-C4D-ND	2.23	113.61	109.99
25	s	314	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
25	s	310	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
25	G	610	CLA	C4D-C3D-CAD	-2.23	105.69	108.11
25	g	610	CLA	C4D-C3D-CAD	-2.23	105.69	108.11
25	B	603	CLA	C3D-C4D-ND	2.23	113.61	109.99
28	c	514	BCR	C15-C14-C13	-2.23	124.15	127.28
25	S	310	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
25	N	612	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
28	c	514	BCR	C8-C7-C6	-2.23	121.05	127.00
25	y	313	CLA	C3D-C4D-ND	2.22	113.60	109.99
25	B	603	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	b	603	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	S	312	CLA	CHD-C1D-C2D	2.22	130.11	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	312	CLA	CHD-C1D-C2D	2.22	130.11	125.49
25	d	401	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
28	D	404	BCR	C11-C10-C9	-2.22	124.16	127.28
28	d	404	BCR	C11-C10-C9	-2.22	124.16	127.28
25	C	501	CLA	CHC-C4B-NB	-2.22	120.71	124.05
25	D	401	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
41	R	616	XAT	C20-C13-C14	-2.22	119.21	122.82
25	D	403	CLA	CHC-C4B-NB	-2.22	120.71	124.05
25	B	608	CLA	C3D-C4D-ND	2.22	113.60	109.99
25	b	608	CLA	C3D-C4D-ND	2.22	113.60	109.99
25	B	605	CLA	CBA-CAA-C2A	-2.22	107.18	113.79
25	b	605	CLA	CBA-CAA-C2A	-2.22	107.18	113.79
25	S	314	CLA	O2A-CGA-CBA	2.22	118.61	111.83
25	s	314	CLA	O2A-CGA-CBA	2.22	118.61	111.83
25	n	604	CLA	C3D-C4D-ND	2.22	113.60	109.99
24	r	607	CHL	O2D-CGD-O1D	-2.22	119.52	123.85
25	c	509	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	n	612	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	b	612	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
25	n	612	CLA	CHB-C4A-NA	-2.22	121.19	124.40
25	N	610	CLA	C3D-C4D-ND	2.22	113.60	109.99
25	n	610	CLA	C3D-C4D-ND	2.22	113.60	109.99
24	6	603	CHL	CAC-C3C-C4C	2.22	129.73	124.03
32	S	319	AJP	C21-C20-C15	-2.22	107.11	110.10
25	N	614	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	r	611	CLA	CHA-C4D-ND	-2.21	127.98	132.55
28	K	101	BCR	C8-C7-C6	-2.21	121.08	127.00
25	N	612	CLA	CHB-C4A-NA	-2.21	121.20	124.40
25	R	602	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
32	s	319	AJP	C21-C20-C15	-2.21	107.12	110.10
25	r	612	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
28	k	101	BCR	C8-C7-C6	-2.21	121.09	127.00
28	B	618	BCR	C38-C26-C25	-2.21	122.07	124.48
28	b	618	BCR	C38-C26-C25	-2.21	122.07	124.48
24	G	605	CHL	O2A-CGA-CBA	2.21	120.98	114.00
24	g	605	CHL	O2A-CGA-CBA	2.21	120.98	114.00
29	l	101	SQD	O7-S-C6	2.21	110.06	106.76
40	n	617	NEX	C17-C1-C6	-2.21	108.50	110.47
24	2	603	CHL	CAC-C3C-C4C	2.21	129.71	124.03
25	r	602	CLA	O2A-CGA-CBA	2.21	118.56	111.83
25	Y	305	CLA	CHD-C1D-C2D	2.20	130.07	125.49
25	y	305	CLA	CHD-C1D-C2D	2.20	130.07	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	610	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
25	r	610	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
25	s	312	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
40	g	617	NEX	C32-C33-C34	-2.20	115.54	119.01
28	C	514	BCR	C15-C14-C13	-2.20	124.19	127.28
25	B	614	CLA	C3D-C4D-ND	2.20	113.57	109.99
25	b	614	CLA	C3D-C4D-ND	2.20	113.57	109.99
25	y	315	CLA	C3D-C4D-ND	2.20	113.57	109.99
32	y	321	AJP	O84-C05-C06	2.20	113.83	107.26
40	G	617	NEX	C32-C33-C34	-2.20	115.55	119.01
25	R	612	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	y	312	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
25	g	604	CLA	C3D-C4D-ND	2.20	113.56	109.99
28	B	619	BCR	C38-C26-C25	-2.20	122.08	124.48
28	b	619	BCR	C38-C26-C25	-2.20	122.08	124.48
25	a	406	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
28	Z	101	BCR	C8-C7-C6	-2.20	121.12	127.00
24	g	601	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
29	L	103	SQD	O7-S-C6	2.20	110.04	106.76
25	B	616	CLA	CHD-C1D-C2D	2.20	130.06	125.49
25	C	505	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
28	I	101	BCR	C2-C1-C6	2.20	113.63	110.44
25	r	604	CLA	C2A-C1A-CHA	-2.20	120.06	123.87
25	R	608	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
25	A	405	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
29	A	407	SQD	O9-S-O7	2.20	120.96	113.82
29	a	408	SQD	O9-S-O7	2.20	120.96	113.82
32	B	624	AJP	O09-C08-C07	2.19	109.13	104.08
32	b	624	AJP	O09-C08-C07	2.19	109.13	104.08
24	l	302	CHL	C1A-CHA-C4D	2.19	122.64	118.98
25	S	312	CLA	C3A-C2A-C1A	-2.19	98.05	101.34
25	r	614	CLA	C2A-C1A-CHA	-2.19	120.06	123.87
25	B	601	CLA	C4D-C3D-CAD	-2.19	105.72	108.11
25	b	601	CLA	C4D-C3D-CAD	-2.19	105.72	108.11
24	Y	308	CHL	O2A-CGA-O1A	-2.19	118.14	123.63
24	y	308	CHL	O2A-CGA-O1A	-2.19	118.14	123.63
25	N	604	CLA	C3D-C4D-ND	2.19	113.55	109.99
24	N	606	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
40	s	317	NEX	C35-C15-C14	-2.19	119.03	123.52
32	Y	322	AJP	C85-O84-C05	2.19	117.47	113.69
25	R	604	CLA	C2A-C1A-CHA	-2.19	120.06	123.87
40	G	617	NEX	C39-C29-C30	-2.19	119.27	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	y	322	AJP	C85-O84-C05	2.19	117.47	113.69
25	c	504	CLA	O2A-CGA-CBA	2.19	118.51	111.83
25	R	602	CLA	O2A-CGA-CBA	2.19	118.51	111.83
32	Y	321	AJP	O84-C05-C06	2.19	113.79	107.26
25	g	614	CLA	C3D-C4D-ND	2.19	113.55	109.99
25	g	611	CLA	CHB-C1B-C2B	2.19	133.78	127.43
25	C	501	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
25	c	501	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
25	Y	315	CLA	C3D-C4D-ND	2.19	113.54	109.99
29	l	102	SQD	C1-C2-C3	2.19	114.61	110.01
24	R	606	CHL	O2A-CGA-CBA	2.19	120.91	114.00
25	G	611	CLA	O2A-CGA-CBA	2.19	118.50	111.83
25	c	505	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
25	g	611	CLA	O2A-CGA-CBA	2.18	118.50	111.83
24	2	601	CHL	C4C-CHD-C1D	2.18	123.89	116.07
24	6	601	CHL	C4C-CHD-C1D	2.18	123.89	116.07
28	z	101	BCR	C8-C7-C6	-2.18	121.16	127.00
25	Y	312	CLA	CHB-C1B-NB	-2.18	120.77	124.05
25	y	312	CLA	CHB-C1B-NB	-2.18	120.77	124.05
25	C	504	CLA	O2A-CGA-CBA	2.18	118.50	111.83
40	S	317	NEX	C35-C15-C14	-2.18	119.05	123.52
25	A	401	CLA	C11-C12-C13	-2.18	108.71	115.97
25	b	616	CLA	CHD-C1D-C2D	2.18	130.03	125.49
29	L	101	SQD	C1-C2-C3	2.18	114.60	110.01
24	N	606	CHL	O2A-CGA-CBA	2.18	120.89	114.00
25	y	314	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
25	y	315	CLA	CHD-C1D-C2D	2.18	130.02	125.49
41	r	616	XAT	C11-C12-C13	-2.18	120.38	126.36
24	G	608	CHL	O2D-CGD-O1D	-2.18	119.60	123.85
28	i	101	BCR	C2-C1-C6	2.18	113.61	110.44
25	r	608	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
24	n	606	CHL	O2A-CGA-CBA	2.18	120.88	114.00
24	r	606	CHL	O2A-CGA-CBA	2.18	120.88	114.00
24	g	608	CHL	O2D-CGD-O1D	-2.18	119.61	123.85
25	s	313	CLA	C4D-C3D-CAD	-2.18	105.74	108.11
25	a	402	CLA	C11-C12-C13	-2.18	108.73	115.97
25	A	402	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
25	a	403	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
25	y	311	CLA	CHB-C1B-NB	-2.18	120.79	124.05
25	G	610	CLA	C1D-ND-C4D	-2.17	104.79	106.31
25	g	610	CLA	C1D-ND-C4D	-2.17	104.79	106.31
25	N	613	CLA	O2D-CGD-O1D	-2.17	119.62	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	315	CLA	CHD-C1D-C2D	2.17	130.01	125.49
39	n	615	LUT	C15-C35-C34	-2.17	119.07	123.52
25	B	607	CLA	O2A-CGA-CBA	2.17	118.46	111.83
25	b	607	CLA	O2A-CGA-CBA	2.17	118.46	111.83
25	G	614	CLA	C3D-C4D-ND	2.17	113.52	109.99
25	R	612	CLA	C4D-CHA-C1A	-2.17	118.65	121.24
41	R	616	XAT	C11-C12-C13	-2.17	120.41	126.36
39	N	615	LUT	C15-C35-C34	-2.17	119.08	123.52
25	G	602	CLA	C6-C7-C8	-2.17	108.75	115.97
25	Y	314	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
32	Y	320	AJP	C24-C23-C22	2.17	113.34	111.07
25	g	602	CLA	C6-C7-C8	-2.17	108.75	115.97
32	y	320	AJP	C24-C23-C22	2.17	113.34	111.07
25	n	613	CLA	C6-C7-C8	-2.17	108.75	115.97
25	B	602	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
25	b	602	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
24	s	307	CHL	O2A-CGA-CBA	2.17	120.85	114.00
25	g	611	CLA	C11-C10-C8	-2.17	108.76	115.97
25	C	503	CLA	C3D-C4D-ND	2.17	113.51	109.99
24	N	607	CHL	C1-C2-C3	2.17	129.75	126.20
25	R	614	CLA	C2A-C1A-CHA	-2.17	120.11	123.87
24	5	302	CHL	C1A-CHA-C4D	2.17	122.60	118.98
25	S	303	CLA	O2A-CGA-CBA	2.17	118.44	111.83
25	s	303	CLA	O2A-CGA-CBA	2.17	118.44	111.83
40	N	617	NEX	C17-C1-C6	-2.17	108.53	110.47
40	N	617	NEX	C40-C33-C34	-2.17	119.31	122.82
25	G	604	CLA	C3D-C4D-ND	2.17	113.51	109.99
25	G	611	CLA	C11-C10-C8	-2.16	108.77	115.97
28	c	514	BCR	C24-C23-C22	-2.16	123.03	126.23
25	C	502	CLA	CHD-C1D-C2D	2.16	129.99	125.49
25	c	502	CLA	CHD-C1D-C2D	2.16	129.99	125.49
32	Y	320	AJP	C11-C16-C15	-2.16	105.35	109.17
32	y	320	AJP	C11-C16-C15	-2.16	105.35	109.17
24	S	307	CHL	O2A-CGA-CBA	2.16	120.83	114.00
24	g	601	CHL	O2A-CGA-O1A	-2.16	118.22	123.63
25	G	611	CLA	CHB-C1B-C2B	2.16	133.70	127.43
25	r	602	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
25	B	612	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
25	b	612	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
28	B	619	BCR	C8-C7-C6	-2.16	121.22	127.00
28	b	619	BCR	C8-C7-C6	-2.16	121.22	127.00
25	R	609	CLA	CAA-CBA-CGA	-2.16	107.07	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
25	B	604	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
25	b	604	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
25	C	506	CLA	CHB-C1B-NB	-2.16	120.81	124.05
25	c	506	CLA	CHB-C1B-NB	-2.16	120.81	124.05
25	D	403	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
25	d	403	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
24	G	601	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
25	B	613	CLA	C3D-C4D-ND	2.16	113.49	109.99
25	N	613	CLA	C6-C7-C8	-2.16	108.80	115.97
25	D	403	CLA	CAA-CBA-CGA	-2.16	107.09	113.21
25	d	403	CLA	CAA-CBA-CGA	-2.16	107.09	113.21
28	C	514	BCR	C24-C23-C22	-2.15	123.05	126.23
25	n	613	CLA	O2D-CGD-O1D	-2.15	119.65	123.85
25	b	613	CLA	C3D-C4D-ND	2.15	113.49	109.99
32	y	320	AJP	C01-C02-C03	2.15	116.79	112.08
25	R	602	CLA	CAA-CBA-CGA	-2.15	107.09	113.21
25	C	513	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
25	N	602	CLA	C3D-C4D-ND	2.15	113.49	109.99
25	R	601	CLA	CHC-C4B-NB	-2.15	120.82	124.05
32	Y	320	AJP	C01-C02-C03	2.15	116.78	112.08
25	C	511	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
25	c	511	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
25	G	611	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
25	g	611	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
25	n	602	CLA	C3D-C4D-ND	2.15	113.48	109.99
25	N	611	CLA	C4D-CHA-C1A	-2.15	118.68	121.24
25	n	611	CLA	C4D-CHA-C1A	-2.15	118.68	121.24
24	Y	306	CHL	O2A-CGA-O1A	-2.15	118.25	123.63
24	2	603	CHL	C1C-C2C-CMC	-2.15	122.93	126.80
24	S	308	CHL	O2A-CGA-CBA	2.15	120.79	114.00
25	B	615	CLA	CHD-C1D-C2D	2.15	129.96	125.49
25	r	612	CLA	C4D-C3D-CAD	-2.15	105.77	108.11
24	s	308	CHL	O2A-CGA-CBA	2.15	120.78	114.00
40	Y	318	NEX	C28-C29-C30	2.15	122.39	119.01
25	C	504	CLA	C6-C7-C8	-2.15	108.83	115.97
40	y	318	NEX	C11-C12-C13	-2.15	120.48	126.36
39	N	615	LUT	C7-C8-C9	2.15	129.41	126.23
25	c	503	CLA	C3D-C4D-ND	2.15	113.47	109.99
25	A	405	CLA	C3D-C4D-ND	2.14	113.47	109.99
25	a	406	CLA	C3D-C4D-ND	2.14	113.47	109.99
25	C	508	CLA	C2A-C1A-CHA	-2.14	120.15	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	603	CHL	O2A-CGA-CBA	2.14	120.77	114.00
25	R	612	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
40	G	617	NEX	C15-C35-C34	-2.14	119.14	123.52
24	6	603	CHL	O2A-CGA-CBA	2.14	120.77	114.00
25	r	609	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
25	B	614	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	b	614	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	c	508	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
25	Y	305	CLA	CHB-C1B-NB	-2.14	120.84	124.05
40	Y	318	NEX	C11-C12-C13	-2.14	120.49	126.36
25	R	611	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	G	614	CLA	C4D-CHA-C1A	-2.14	118.69	121.24
25	g	614	CLA	C4D-CHA-C1A	-2.14	118.69	121.24
25	G	603	CLA	C3D-C4D-ND	2.14	113.46	109.99
25	g	603	CLA	C3D-C4D-ND	2.14	113.46	109.99
25	Y	311	CLA	CHB-C1B-NB	-2.14	120.84	124.05
40	g	617	NEX	C15-C35-C34	-2.14	119.14	123.52
39	n	615	LUT	C7-C8-C9	2.14	129.40	126.23
25	c	504	CLA	C6-C7-C8	-2.14	108.86	115.97
25	r	601	CLA	CHC-C4B-NB	-2.14	120.84	124.05
24	n	606	CHL	O2D-CGD-O1D	-2.14	119.69	123.85
28	h	101	BCR	C16-C15-C14	-2.14	119.15	123.52
25	B	616	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
25	B	601	CLA	CHB-C1B-C2B	2.13	133.62	127.43
25	b	601	CLA	CHB-C1B-C2B	2.13	133.62	127.43
40	y	318	NEX	C28-C29-C30	2.13	122.36	119.01
25	2	602	CLA	CHC-C1C-C2C	2.13	133.01	126.95
25	6	602	CLA	CHC-C1C-C2C	2.13	133.01	126.95
24	6	603	CHL	C1C-C2C-CMC	-2.13	122.96	126.80
25	G	603	CLA	C11-C10-C8	-2.13	108.88	115.97
25	g	602	CLA	CHB-C1B-NB	-2.13	120.85	124.05
25	b	616	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
25	r	611	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
32	A	412	AJP	C17-C16-C15	-2.13	107.97	110.52
32	a	413	AJP	C17-C16-C15	-2.13	107.97	110.52
25	y	305	CLA	CHB-C1B-NB	-2.13	120.86	124.05
24	n	607	CHL	C1-C2-C3	2.13	129.68	126.20
40	n	617	NEX	C40-C33-C34	-2.13	119.37	122.82
24	y	306	CHL	O2A-CGA-O1A	-2.13	118.31	123.63
25	g	611	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
25	S	305	CLA	CHC-C4B-NB	-2.13	120.86	124.05
25	s	305	CLA	CHC-C4B-NB	-2.13	120.86	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	CHD-C1D-C2D	2.13	129.91	125.49
25	Y	312	CLA	C11-C10-C8	-2.13	108.90	115.97
25	y	312	CLA	C11-C10-C8	-2.13	108.90	115.97
40	n	617	NEX	C11-C10-C9	2.12	130.26	127.28
24	5	301	CHL	O2D-CGD-O1D	-2.12	119.71	123.85
25	S	313	CLA	CHB-C1B-C2B	2.12	133.59	127.43
28	H	101	BCR	C16-C15-C14	-2.12	119.17	123.52
25	C	513	CLA	C3D-C4D-ND	2.12	113.44	109.99
24	N	608	CHL	CHA-C1A-C2A	-2.12	128.32	133.31
25	N	610	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
25	n	610	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
25	A	401	CLA	C11-C10-C8	-2.12	108.91	115.97
25	a	402	CLA	C11-C10-C8	-2.12	108.91	115.97
28	H	101	BCR	C8-C7-C6	-2.12	121.33	127.00
28	h	101	BCR	C8-C7-C6	-2.12	121.33	127.00
25	6	602	CLA	C6-C7-C8	-2.12	108.91	115.97
25	c	507	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
25	G	614	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
40	S	317	NEX	C10-C11-C12	-2.12	117.06	123.20
40	s	317	NEX	C10-C11-C12	-2.12	117.06	123.20
24	g	608	CHL	CHA-C1A-C2A	-2.12	128.33	133.31
24	G	608	CHL	CHA-C1A-C2A	-2.12	128.33	133.31
24	R	607	CHL	O2A-CGA-O1A	-2.12	118.33	123.63
24	G	605	CHL	CHA-C1A-C2A	-2.12	128.33	133.31
25	2	602	CLA	C6-C7-C8	-2.12	108.93	115.97
25	g	603	CLA	C11-C10-C8	-2.12	108.93	115.97
40	y	318	NEX	C31-C32-C33	2.12	132.17	126.36
24	S	302	CHL	O2A-CGA-CBA	2.12	120.69	114.00
24	s	302	CHL	O2A-CGA-CBA	2.12	120.69	114.00
25	g	614	CLA	C2A-C1A-CHA	-2.12	120.20	123.87
25	B	607	CLA	C3D-C4D-ND	2.11	113.42	109.99
25	b	607	CLA	C3D-C4D-ND	2.11	113.42	109.99
24	n	608	CHL	CHA-C1A-C2A	-2.11	128.34	133.31
25	r	612	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
25	B	613	CLA	C6-C7-C8	-2.11	108.95	115.97
25	b	613	CLA	C6-C7-C8	-2.11	108.95	115.97
28	K	101	BCR	C11-C10-C9	-2.11	124.32	127.28
25	G	611	CLA	C1D-ND-C4D	-2.11	104.83	106.31
24	r	607	CHL	O2A-CGA-O1A	-2.11	118.35	123.63
28	T	101	BCR	C24-C23-C22	-2.11	123.11	126.23
28	t	101	BCR	C24-C23-C22	-2.11	123.11	126.23
25	S	313	CLA	C4D-C3D-CAD	-2.11	105.81	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	S	315	LUT	C37-C21-C22	-2.11	105.47	109.41
39	s	315	LUT	C37-C21-C22	-2.11	105.47	109.41
24	R	605	CHL	O2A-CGA-CBA	2.11	120.66	114.00
24	r	605	CHL	O2A-CGA-CBA	2.11	120.66	114.00
24	l	301	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
25	s	313	CLA	CHB-C1B-C2B	2.11	133.54	127.43
25	G	602	CLA	CHB-C1B-NB	-2.11	120.89	124.05
25	R	612	CLA	C2A-C3A-C4A	-2.11	98.47	101.87
40	N	617	NEX	C11-C10-C9	2.11	130.23	127.28
28	B	619	BCR	C15-C14-C13	-2.11	124.33	127.28
28	b	619	BCR	C15-C14-C13	-2.11	124.33	127.28
32	Y	323	AJP	C21-C20-C15	-2.11	107.27	110.10
25	C	507	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
25	b	602	CLA	C11-C10-C8	-2.10	108.97	115.97
25	S	304	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
25	b	611	CLA	C3D-C4D-ND	2.10	113.41	109.99
25	c	513	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
25	C	513	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
25	G	611	CLA	C6-C7-C8	-2.10	108.98	115.97
25	N	602	CLA	C16-C15-C13	-2.10	108.98	115.97
25	G	611	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
25	s	313	CLA	C4D-CHA-C1A	-2.10	118.74	121.24
24	g	605	CHL	CHA-C1A-C2A	-2.10	128.38	133.31
25	n	602	CLA	C16-C15-C13	-2.10	108.99	115.97
25	s	304	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
25	s	314	CLA	CHB-C1B-NB	-2.10	120.90	124.05
39	s	316	LUT	C12-C13-C14	-2.10	115.71	119.01
25	b	601	CLA	C1D-CHD-C4C	-2.10	121.56	126.02
40	Y	318	NEX	C31-C32-C33	2.10	132.11	126.36
25	B	603	CLA	C4D-CHA-C1A	-2.10	118.75	121.24
25	b	603	CLA	C4D-CHA-C1A	-2.10	118.75	121.24
25	S	313	CLA	C4D-CHA-C1A	-2.09	118.75	121.24
39	N	615	LUT	C35-C34-C33	2.09	130.22	127.28
25	B	611	CLA	C3D-C4D-ND	2.09	113.39	109.99
25	B	604	CLA	CBA-CAA-C2A	-2.09	107.57	113.79
25	b	604	CLA	CBA-CAA-C2A	-2.09	107.57	113.79
24	Y	310	CHL	CHA-C1A-C2A	-2.09	128.39	133.31
25	c	512	CLA	CBA-CAA-C2A	-2.09	107.57	113.79
25	g	611	CLA	C6-C7-C8	-2.09	109.01	115.97
25	B	601	CLA	C1D-CHD-C4C	-2.09	121.57	126.02
25	B	610	CLA	C3D-C4D-ND	2.09	113.38	109.99
25	B	602	CLA	C11-C10-C8	-2.09	109.02	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	617	BCR	C29-C30-C25	2.09	113.47	110.44
28	b	617	BCR	C29-C30-C25	2.09	113.47	110.44
28	k	101	BCR	C11-C10-C9	-2.09	124.35	127.28
25	G	602	CLA	CHD-C4C-C3C	-2.09	121.73	124.77
25	G	611	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
25	g	611	CLA	C1D-ND-C4D	-2.09	104.85	106.31
39	S	316	LUT	C12-C13-C14	-2.09	115.73	119.01
32	y	321	AJP	O25-C26-O31	2.08	116.18	110.69
25	R	608	CLA	C2A-C1A-CHA	-2.08	120.25	123.87
25	s	304	CLA	C3D-C4D-ND	2.08	113.37	109.99
25	C	511	CLA	C11-C12-C13	-2.08	109.05	115.97
26	c	519	LHG	P-O6-C4	-2.08	109.42	121.35
32	N	619	AJP	C21-C20-C15	-2.08	107.30	110.10
32	n	619	AJP	C21-C20-C15	-2.08	107.30	110.10
25	g	611	CLA	CAA-CBA-CGA	-2.08	107.30	113.21
40	G	617	NEX	C35-C15-C14	-2.08	119.26	123.52
26	C	519	LHG	P-O6-C4	-2.08	109.43	121.35
24	y	302	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
32	y	323	AJP	C21-C20-C15	-2.08	107.30	110.10
25	c	513	CLA	C3D-C4D-ND	2.08	113.37	109.99
25	G	602	CLA	C16-C15-C13	-2.08	109.06	115.97
25	B	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
25	C	512	CLA	CBA-CAA-C2A	-2.08	107.61	113.79
25	c	508	CLA	C4D-CHA-C1A	-2.08	118.77	121.24
24	Y	302	CHL	O2D-CGD-O1D	-2.08	119.81	123.85
25	c	511	CLA	C11-C12-C13	-2.08	109.06	115.97
24	y	307	CHL	C4C-CHD-C1D	2.08	123.50	116.07
25	n	613	CLA	C11-C10-C8	-2.08	109.07	115.97
25	g	602	CLA	C16-C15-C13	-2.08	109.07	115.97
32	B	624	AJP	C24-C19-C20	2.07	114.87	112.66
32	b	624	AJP	C24-C19-C20	2.07	114.87	112.66
25	N	611	CLA	C6-C7-C8	-2.07	109.07	115.97
25	n	611	CLA	C6-C7-C8	-2.07	109.07	115.97
24	Y	307	CHL	O2A-CGA-O1A	-2.07	118.44	123.63
25	b	610	CLA	C3D-C4D-ND	2.07	113.36	109.99
25	g	612	CLA	CHD-C1D-C2D	2.07	129.80	125.49
25	S	314	CLA	CHB-C1B-NB	-2.07	120.94	124.05
25	G	612	CLA	CHD-C1D-C2D	2.07	129.80	125.49
24	y	307	CHL	O2A-CGA-O1A	-2.07	118.44	123.63
25	g	613	CLA	C3B-C4B-NB	-2.07	108.68	110.53
24	g	607	CHL	O2A-CGA-O1A	-2.07	118.00	123.33
25	b	606	CLA	C3B-C4B-NB	-2.07	108.68	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	310	CHL	CHA-C1A-C2A	-2.07	128.44	133.31
25	S	304	CLA	C3D-C4D-ND	2.07	113.35	109.99
32	a	413	AJP	O09-C08-C07	2.07	108.84	104.08
24	Y	307	CHL	C4C-CHD-C1D	2.07	123.47	116.07
25	C	506	CLA	C11-C12-C13	-2.07	109.09	115.97
25	c	506	CLA	C11-C12-C13	-2.07	109.09	115.97
25	R	612	CLA	C11-C10-C8	-2.07	109.09	115.97
25	A	405	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
25	a	406	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
39	n	615	LUT	C35-C34-C33	2.07	130.18	127.28
25	N	613	CLA	CBA-CAA-C2A	-2.07	107.64	113.79
25	R	604	CLA	C4A-NA-C1A	-2.06	105.74	106.68
25	r	604	CLA	C4A-NA-C1A	-2.06	105.74	106.68
25	B	604	CLA	C16-C15-C13	-2.06	109.11	115.97
25	b	604	CLA	C16-C15-C13	-2.06	109.11	115.97
28	b	618	BCR	C8-C7-C6	-2.06	121.48	127.00
40	Y	318	NEX	C19-C9-C10	-2.06	119.47	122.82
40	g	617	NEX	C35-C15-C14	-2.06	119.30	123.52
32	A	412	AJP	O09-C08-C07	2.06	108.83	104.08
32	N	619	AJP	C04-C05-C06	2.06	119.39	115.66
32	n	619	AJP	C04-C05-C06	2.06	119.39	115.66
25	r	608	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
24	S	306	CHL	O2A-CGA-CBA	2.06	120.51	114.00
24	s	306	CHL	O2A-CGA-CBA	2.06	120.51	114.00
25	B	602	CLA	C4D-C3D-CAD	-2.06	105.87	108.11
25	c	510	CLA	C11-C10-C8	-2.06	109.12	115.97
24	Y	309	CHL	O2A-CGA-O1A	-2.06	118.48	123.63
24	y	309	CHL	O2A-CGA-O1A	-2.06	118.48	123.63
32	Y	321	AJP	O25-C26-O31	2.06	116.11	110.69
40	S	317	NEX	C30-C31-C32	-2.06	117.23	123.20
40	s	317	NEX	C30-C31-C32	-2.06	117.23	123.20
25	C	510	CLA	C11-C10-C8	-2.06	109.12	115.97
25	N	614	CLA	CHB-C1B-C2B	2.06	133.40	127.43
25	N	613	CLA	C11-C10-C8	-2.06	109.13	115.97
25	n	602	CLA	C11-C12-C13	-2.06	109.13	115.97
28	B	618	BCR	C8-C7-C6	-2.06	121.50	127.00
25	c	513	CLA	C6-C7-C8	-2.06	109.13	115.97
25	Y	304	CLA	C16-C15-C13	-2.06	109.13	115.97
25	C	508	CLA	C4D-CHA-C1A	-2.05	118.79	121.24
25	c	511	CLA	C6-C7-C8	-2.05	109.14	115.97
28	T	101	BCR	C8-C7-C6	-2.05	121.51	127.00
25	r	612	CLA	C11-C10-C8	-2.05	109.14	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	602	CLA	C11-C12-C13	-2.05	109.14	115.97
32	B	624	AJP	C35-O34-C29	2.05	122.85	117.98
32	b	624	AJP	C35-O34-C29	2.05	122.85	117.98
25	b	612	CLA	C3D-C4D-ND	2.05	113.33	109.99
24	G	607	CHL	O2A-CGA-O1A	-2.05	118.05	123.33
40	y	318	NEX	C19-C9-C10	-2.05	119.49	122.82
25	n	614	CLA	CHB-C1B-C2B	2.05	133.39	127.43
25	C	510	CLA	CAC-C3C-C4C	2.05	127.46	124.79
25	n	613	CLA	CBA-CAA-C2A	-2.05	107.69	113.79
25	C	511	CLA	C6-C7-C8	-2.05	109.14	115.97
25	C	513	CLA	C6-C7-C8	-2.05	109.14	115.97
25	B	602	CLA	C2A-C1A-CHA	-2.05	120.31	123.87
24	Y	308	CHL	C1-O2A-CGA	2.05	121.61	116.65
28	t	101	BCR	C8-C7-C6	-2.05	121.52	127.00
32	Y	324	AJP	C21-C22-C23	2.05	113.20	110.46
25	B	601	CLA	C1D-ND-C4D	-2.05	104.87	106.31
25	b	601	CLA	C1D-ND-C4D	-2.05	104.87	106.31
25	g	602	CLA	CHD-C4C-C3C	-2.05	121.79	124.77
25	G	614	CLA	C2C-C1C-NC	2.05	112.13	109.98
25	g	610	CLA	CHB-C1B-C2B	2.05	133.37	127.43
28	I	101	BCR	C8-C7-C6	-2.05	121.53	127.00
25	c	512	CLA	C11-C12-C13	-2.05	109.16	115.97
40	g	617	NEX	C12-C13-C14	-2.05	115.79	119.01
25	B	612	CLA	C3D-C4D-ND	2.05	113.31	109.99
25	y	315	CLA	C2C-C1C-NC	2.05	112.13	109.98
25	y	304	CLA	C16-C15-C13	-2.05	109.17	115.97
32	y	324	AJP	C21-C22-C23	2.05	113.19	110.46
24	y	307	CHL	CMD-C2D-C3D	2.04	128.77	124.68
24	N	609	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
25	B	602	CLA	C4D-CHA-C1A	-2.04	118.81	121.24
25	D	402	CLA	C16-C15-C13	-2.04	109.17	115.97
25	d	402	CLA	C16-C15-C13	-2.04	109.17	115.97
40	g	617	NEX	C39-C29-C28	2.04	121.21	118.09
25	C	512	CLA	C11-C12-C13	-2.04	109.18	115.97
28	A	406	BCR	C20-C21-C22	-2.04	124.42	127.28
28	a	407	BCR	C20-C21-C22	-2.04	124.42	127.28
28	z	101	BCR	C16-C15-C14	-2.04	119.34	123.52
39	S	316	LUT	C1-C2-C3	2.04	118.07	113.59
39	s	316	LUT	C1-C2-C3	2.04	118.07	113.59
39	R	615	LUT	C22-C23-C24	2.04	114.21	111.18
39	r	615	LUT	C22-C23-C24	2.04	114.21	111.18
25	N	610	CLA	CHB-C1B-NB	-2.04	120.99	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	313	CLA	CHB-C1B-NB	-2.04	120.99	124.05
32	y	322	AJP	O79-C22-C23	-2.04	105.85	110.08
25	R	609	CLA	C11-C12-C13	-2.04	109.19	115.97
25	c	508	CLA	C16-C15-C13	-2.04	109.19	115.97
32	y	321	AJP	O09-C08-C07	2.04	108.77	104.08
24	Y	302	CHL	O2A-CGA-O1A	-2.04	118.53	123.63
24	y	302	CHL	O2A-CGA-O1A	-2.04	118.53	123.63
25	6	602	CLA	CHC-C4B-C3B	2.04	136.22	127.37
24	n	609	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
25	C	503	CLA	C11-C10-C8	-2.04	109.19	115.97
25	c	503	CLA	C11-C10-C8	-2.04	109.19	115.97
24	y	308	CHL	C1-O2A-CGA	2.04	121.58	116.65
25	B	606	CLA	C11-C10-C8	-2.04	109.19	115.97
25	b	606	CLA	C11-C10-C8	-2.04	109.19	115.97
25	n	614	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
25	C	511	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
25	n	611	CLA	C11-C10-C8	-2.04	109.19	115.97
25	d	403	CLA	C6-C7-C8	-2.04	109.19	115.97
25	R	602	CLA	C11-C10-C8	-2.04	109.19	115.97
25	S	309	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
28	i	101	BCR	C8-C7-C6	-2.04	121.56	127.00
25	2	602	CLA	CHC-C4B-C3B	2.04	136.21	127.37
25	r	609	CLA	C11-C12-C13	-2.04	109.20	115.97
24	S	306	CHL	O2A-CGA-O1A	-2.03	118.10	123.33
25	A	405	CLA	C6-C7-C8	-2.03	109.20	115.97
25	C	501	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	c	501	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	C	508	CLA	C16-C15-C13	-2.03	109.21	115.97
32	Y	322	AJP	O79-C22-C23	-2.03	105.86	110.08
25	g	613	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
25	N	611	CLA	C11-C10-C8	-2.03	109.21	115.97
25	B	603	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	b	603	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	B	609	CLA	C11-C12-C13	-2.03	109.21	115.97
25	b	609	CLA	C11-C12-C13	-2.03	109.21	115.97
40	s	317	NEX	C8-C7-C6	-2.03	175.26	177.66
25	c	511	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	C	508	CLA	C3B-C4B-NB	-2.03	108.72	110.53
32	A	412	AJP	C65-O64-C57	-2.03	113.16	117.98
32	a	413	AJP	C65-O64-C57	-2.03	113.16	117.98
25	G	610	CLA	CHB-C1B-C2B	2.03	133.32	127.43
25	B	609	CLA	C16-C15-C13	-2.03	109.22	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	C16-C15-C13	-2.03	109.22	115.97
25	n	610	CLA	CHB-C1B-NB	-2.03	121.00	124.05
28	T	101	BCR	C7-C8-C9	-2.03	123.23	126.23
25	C	506	CLA	C4D-CHA-C1A	-2.03	118.82	121.24
25	c	506	CLA	C4D-CHA-C1A	-2.03	118.82	121.24
25	R	604	CLA	C1D-CHD-C4C	-2.03	121.71	126.02
24	G	609	CHL	O2D-CGD-O1D	-2.03	119.90	123.85
25	a	406	CLA	C6-C7-C8	-2.03	109.22	115.97
28	t	101	BCR	C7-C8-C9	-2.03	123.23	126.23
25	Y	313	CLA	CHB-C1B-NB	-2.03	121.00	124.05
25	C	505	CLA	C4D-CHA-C1A	-2.03	118.82	121.24
25	s	309	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
25	c	508	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	s	306	CHL	O2A-CGA-O1A	-2.03	118.12	123.33
25	g	614	CLA	C2C-C1C-NC	2.03	112.11	109.98
25	a	403	CLA	C6-C7-C8	-2.03	109.23	115.97
28	Z	101	BCR	C16-C15-C14	-2.03	119.37	123.52
25	B	603	CLA	C6-C7-C8	-2.03	109.23	115.97
25	b	603	CLA	C6-C7-C8	-2.03	109.23	115.97
25	c	501	CLA	C6-C7-C8	-2.03	109.23	115.97
25	D	403	CLA	C6-C7-C8	-2.03	109.23	115.97
32	B	624	AJP	C15-C20-C19	-2.03	105.70	108.51
32	b	624	AJP	C15-C20-C19	-2.03	105.70	108.51
25	c	505	CLA	C4D-CHA-C1A	-2.02	118.83	121.24
25	C	507	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
25	c	507	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
25	r	602	CLA	C11-C10-C8	-2.02	109.24	115.97
25	b	602	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
25	c	510	CLA	CAC-C3C-C4C	2.02	127.42	124.79
24	s	307	CHL	O2D-CGD-O1D	-2.02	119.91	123.85
25	A	402	CLA	C6-C7-C8	-2.02	109.25	115.97
25	r	603	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
32	Y	321	AJP	O09-C08-C07	2.02	108.73	104.08
25	B	609	CLA	C11-C10-C8	-2.02	109.25	115.97
25	C	501	CLA	C6-C7-C8	-2.02	109.25	115.97
25	b	612	CLA	C11-C10-C8	-2.02	109.25	115.97
32	B	624	AJP	C35-O40-C39	-2.02	109.78	113.72
32	b	624	AJP	C35-O40-C39	-2.02	109.78	113.72
25	S	303	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
25	s	303	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
39	G	615	LUT	C37-C21-C22	-2.02	105.64	109.41
39	g	615	LUT	C37-C21-C22	-2.02	105.64	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	C11-C10-C8	-2.02	109.26	115.97
25	Y	315	CLA	C2C-C1C-NC	2.02	112.10	109.98
24	R	605	CHL	O2D-CGD-O1D	-2.02	119.92	123.85
24	r	605	CHL	O2D-CGD-O1D	-2.02	119.92	123.85
25	N	614	CLA	C4D-C3D-CAD	-2.02	105.92	108.11
25	b	602	CLA	C4D-CHA-C1A	-2.02	118.84	121.24
39	Y	316	LUT	C37-C21-C22	-2.02	105.65	109.41
25	G	613	CLA	C4D-C3D-CAD	-2.02	105.92	108.11
25	Y	303	CLA	CHD-C1D-C2D	2.02	129.68	125.49
25	y	303	CLA	CHD-C1D-C2D	2.02	129.68	125.49
24	2	601	CHL	CHA-C1A-C2A	-2.02	128.57	133.31
25	B	615	CLA	C11-C12-C13	-2.02	109.27	115.97
25	b	615	CLA	C11-C12-C13	-2.02	109.27	115.97
39	N	615	LUT	C37-C21-C22	-2.02	105.65	109.41
24	R	605	CHL	O2A-CGA-O1A	-2.01	118.15	123.33
24	r	605	CHL	O2A-CGA-O1A	-2.01	118.15	123.33
24	n	609	CHL	O2A-CGA-O1A	-2.01	118.59	123.63
25	B	602	CLA	C11-C12-C13	-2.01	109.27	115.97
25	B	612	CLA	C16-C15-C13	-2.01	109.27	115.97
25	b	612	CLA	C16-C15-C13	-2.01	109.27	115.97
25	g	613	CLA	C11-C10-C8	-2.01	109.27	115.97
25	r	604	CLA	C1D-CHD-C4C	-2.01	121.74	126.02
25	2	604	CLA	CHB-C1B-C2B	2.01	133.27	127.43
25	6	604	CLA	CHB-C1B-C2B	2.01	133.27	127.43
35	A	415	DGD	C1D-O6D-C5D	-2.01	109.79	113.72
35	a	401	DGD	C1D-O6D-C5D	-2.01	109.79	113.72
25	G	613	CLA	C11-C10-C8	-2.01	109.28	115.97
24	y	309	CHL	CHA-C1A-C2A	-2.01	128.58	133.31
25	C	508	CLA	C6-C7-C8	-2.01	109.28	115.97
39	y	316	LUT	C37-C21-C22	-2.01	105.66	109.41
24	Y	307	CHL	CMD-C2D-C3D	2.01	128.70	124.68
25	B	605	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
25	b	605	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
25	b	602	CLA	CHB-C1B-NB	-2.01	121.03	124.05
24	g	609	CHL	O2D-CGD-O1D	-2.01	119.94	123.85
25	G	613	CLA	CHC-C4B-NB	-2.01	121.03	124.05
25	B	606	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
25	b	606	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
28	b	618	BCR	C7-C8-C9	-2.01	123.26	126.23
40	S	317	NEX	C8-C7-C6	-2.01	175.29	177.66
25	2	605	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
25	A	402	CLA	CAA-CBA-CGA	-2.01	107.51	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	309	CHL	CHA-C1A-C2A	-2.01	128.59	133.31
25	D	402	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
25	Y	311	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
25	d	402	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
25	b	602	CLA	C11-C12-C13	-2.01	109.30	115.97
25	G	613	CLA	C3B-C4B-NB	-2.01	108.74	110.53
24	5	302	CHL	C3C-C4C-NC	-2.01	109.75	114.65
25	A	401	CLA	CAC-C3C-C4C	2.01	127.40	124.79
25	a	402	CLA	CAC-C3C-C4C	2.01	127.40	124.79
25	b	609	CLA	C11-C10-C8	-2.01	109.30	115.97
25	c	508	CLA	C6-C7-C8	-2.00	109.30	115.97
25	C	502	CLA	C3D-C4D-ND	2.00	113.24	109.99
24	S	307	CHL	O2D-CGD-O1D	-2.00	119.95	123.85
25	Y	311	CLA	C6-C7-C8	-2.00	109.31	115.97
25	y	311	CLA	C6-C7-C8	-2.00	109.31	115.97
28	B	618	BCR	C7-C8-C9	-2.00	123.27	126.23
25	R	603	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
32	Y	322	AJP	C17-C16-C11	-2.00	109.46	112.29
32	y	322	AJP	C17-C16-C11	-2.00	109.46	112.29
25	b	602	CLA	C4D-C3D-CAD	-2.00	105.93	108.11
32	Y	323	AJP	C18-C17-C16	-2.00	108.97	112.16
32	y	323	AJP	C18-C17-C16	-2.00	108.97	112.16

All (734) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	301	CHL	ND
24	1	301	CHL	NA
24	1	301	CHL	NC
24	1	302	CHL	ND
24	1	302	CHL	NA
24	1	302	CHL	NC
24	2	601	CHL	ND
24	2	601	CHL	NA
24	2	601	CHL	NC
24	2	603	CHL	ND
24	2	603	CHL	NA
24	2	603	CHL	NC
24	S	302	CHL	ND
24	S	302	CHL	NC
24	S	306	CHL	ND
24	S	306	CHL	NA

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Mol	Chain	Res	Type	Atom
24	S	306	CHL	NC
24	S	307	CHL	ND
24	S	307	CHL	NA
24	S	307	CHL	NC
24	S	308	CHL	ND
24	S	308	CHL	NA
24	S	308	CHL	NC
24	G	601	CHL	ND
24	G	601	CHL	NC
24	G	605	CHL	ND
24	G	605	CHL	NA
24	G	605	CHL	NC
24	G	606	CHL	ND
24	G	606	CHL	NA
24	G	606	CHL	NC
24	G	607	CHL	ND
24	G	607	CHL	NC
24	G	608	CHL	ND
24	G	608	CHL	NA
24	G	608	CHL	NC
24	G	609	CHL	ND
24	G	609	CHL	NA
24	G	609	CHL	NC
24	N	601	CHL	ND
24	N	601	CHL	NC
24	N	605	CHL	ND
24	N	605	CHL	NA
24	N	605	CHL	NC
24	N	606	CHL	ND
24	N	606	CHL	NC
24	N	607	CHL	ND
24	N	607	CHL	NC
24	N	608	CHL	ND
24	N	608	CHL	NA
24	N	608	CHL	NC
24	N	609	CHL	ND
24	N	609	CHL	NC
24	Y	302	CHL	ND
24	Y	302	CHL	NC
24	Y	306	CHL	ND
24	Y	306	CHL	NA
24	Y	306	CHL	NC

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Mol	Chain	Res	Type	Atom
24	Y	307	CHL	ND
24	Y	307	CHL	NA
24	Y	307	CHL	NC
24	Y	308	CHL	ND
24	Y	308	CHL	NC
24	Y	309	CHL	ND
24	Y	309	CHL	NA
24	Y	309	CHL	NC
24	Y	310	CHL	ND
24	Y	310	CHL	NA
24	Y	310	CHL	NC
24	R	605	CHL	ND
24	R	605	CHL	NA
24	R	605	CHL	NC
24	R	606	CHL	ND
24	R	606	CHL	NA
24	R	606	CHL	NC
24	R	607	CHL	ND
24	R	607	CHL	NA
24	R	607	CHL	NC
24	R	613	CHL	ND
24	R	613	CHL	NA
24	R	613	CHL	NC
24	5	301	CHL	ND
24	5	301	CHL	NA
24	5	301	CHL	NC
24	5	302	CHL	ND
24	5	302	CHL	NA
24	5	302	CHL	NC
24	6	601	CHL	ND
24	6	601	CHL	NA
24	6	601	CHL	NC
24	6	603	CHL	ND
24	6	603	CHL	NA
24	6	603	CHL	NC
24	s	302	CHL	ND
24	s	302	CHL	NC
24	s	306	CHL	ND
24	s	306	CHL	NA
24	s	306	CHL	NC
24	s	307	CHL	ND
24	s	307	CHL	NA

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Mol	Chain	Res	Type	Atom
24	s	307	CHL	NC
24	s	308	CHL	ND
24	s	308	CHL	NA
24	s	308	CHL	NC
24	g	601	CHL	ND
24	g	601	CHL	NC
24	g	605	CHL	ND
24	g	605	CHL	NA
24	g	605	CHL	NC
24	g	606	CHL	ND
24	g	606	CHL	NA
24	g	606	CHL	NC
24	g	607	CHL	ND
24	g	607	CHL	NC
24	g	608	CHL	ND
24	g	608	CHL	NA
24	g	608	CHL	NC
24	g	609	CHL	ND
24	g	609	CHL	NA
24	g	609	CHL	NC
24	n	601	CHL	ND
24	n	601	CHL	NC
24	n	605	CHL	ND
24	n	605	CHL	NA
24	n	605	CHL	NC
24	n	606	CHL	ND
24	n	606	CHL	NC
24	n	607	CHL	ND
24	n	607	CHL	NC
24	n	608	CHL	ND
24	n	608	CHL	NA
24	n	608	CHL	NC
24	n	609	CHL	ND
24	n	609	CHL	NC
24	y	302	CHL	ND
24	y	302	CHL	NC
24	y	306	CHL	ND
24	y	306	CHL	NA
24	y	306	CHL	NC
24	y	307	CHL	ND
24	y	307	CHL	NA
24	y	307	CHL	NC

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Mol	Chain	Res	Type	Atom
24	y	308	CHL	ND
24	y	308	CHL	NC
24	y	309	CHL	ND
24	y	309	CHL	NA
24	y	309	CHL	NC
24	y	310	CHL	ND
24	y	310	CHL	NA
24	y	310	CHL	NC
24	r	605	CHL	ND
24	r	605	CHL	NA
24	r	605	CHL	NC
24	r	606	CHL	ND
24	r	606	CHL	NA
24	r	606	CHL	NC
24	r	607	CHL	ND
24	r	607	CHL	NA
24	r	607	CHL	NC
24	r	613	CHL	ND
24	r	613	CHL	NA
24	r	613	CHL	NC
25	2	602	CLA	ND
25	2	604	CLA	ND
25	2	605	CLA	ND
25	A	401	CLA	ND
25	A	402	CLA	ND
25	A	405	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND

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Mol	Chain	Res	Type	Atom
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	401	CLA	ND
25	D	402	CLA	ND
25	D	403	CLA	ND
25	S	303	CLA	ND
25	S	304	CLA	ND
25	S	305	CLA	ND
25	S	309	CLA	ND
25	S	310	CLA	ND
25	S	311	CLA	ND
25	S	312	CLA	ND
25	S	313	CLA	ND
25	S	314	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	604	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND
25	G	613	CLA	ND
25	G	614	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	610	CLA	ND
25	N	611	CLA	ND
25	N	612	CLA	ND
25	N	613	CLA	ND
25	N	614	CLA	ND
25	Y	303	CLA	ND

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Mol	Chain	Res	Type	Atom
25	Y	304	CLA	ND
25	Y	305	CLA	ND
25	Y	311	CLA	ND
25	Y	312	CLA	ND
25	Y	313	CLA	ND
25	Y	314	CLA	ND
25	Y	315	CLA	ND
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	608	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	R	614	CLA	ND
25	6	602	CLA	ND
25	6	604	CLA	ND
25	6	605	CLA	ND
25	a	402	CLA	ND
25	a	403	CLA	ND
25	a	406	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	402	CLA	ND
25	d	403	CLA	ND
25	s	303	CLA	ND
25	s	304	CLA	ND
25	s	305	CLA	ND
25	s	309	CLA	ND
25	s	310	CLA	ND
25	s	311	CLA	ND
25	s	312	CLA	ND
25	s	313	CLA	ND
25	s	314	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	604	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND
25	g	612	CLA	ND
25	g	613	CLA	ND
25	g	614	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	610	CLA	ND
25	n	611	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	n	614	CLA	ND
25	y	303	CLA	ND
25	y	304	CLA	ND
25	y	305	CLA	ND
25	y	311	CLA	ND

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Mol	Chain	Res	Type	Atom
25	y	312	CLA	ND
25	y	313	CLA	ND
25	y	314	CLA	ND
25	y	315	CLA	ND
25	r	601	CLA	ND
25	r	602	CLA	ND
25	r	603	CLA	ND
25	r	604	CLA	ND
25	r	608	CLA	ND
25	r	609	CLA	ND
25	r	610	CLA	ND
25	r	611	CLA	ND
25	r	612	CLA	ND
25	r	614	CLA	ND
32	A	412	AJP	C68
32	A	412	AJP	C45
32	A	412	AJP	C35
32	A	412	AJP	C56
32	A	412	AJP	C30
32	A	412	AJP	C47
32	A	412	AJP	C48
32	A	412	AJP	C12
32	A	412	AJP	C55
32	A	412	AJP	C67
32	A	412	AJP	C66
32	A	412	AJP	C19
32	A	412	AJP	C07
32	A	412	AJP	C36
32	A	412	AJP	C08
32	A	412	AJP	C28
32	A	412	AJP	C69
32	A	412	AJP	C20
32	A	412	AJP	C37
32	A	412	AJP	C16
32	A	412	AJP	C27
32	A	412	AJP	C23
32	A	412	AJP	C46
32	A	412	AJP	C57
32	A	412	AJP	C10
32	A	412	AJP	C22
32	A	412	AJP	C11
32	A	412	AJP	C26

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Mol	Chain	Res	Type	Atom
32	A	412	AJP	C02
32	A	412	AJP	C59
32	A	412	AJP	C65
32	A	412	AJP	C38
32	A	412	AJP	C39
32	A	412	AJP	C15
32	B	624	AJP	C45
32	B	624	AJP	C35
32	B	624	AJP	C56
32	B	624	AJP	C30
32	B	624	AJP	C68
32	B	624	AJP	C47
32	B	624	AJP	C48
32	B	624	AJP	C12
32	B	624	AJP	C55
32	B	624	AJP	C67
32	B	624	AJP	C66
32	B	624	AJP	C19
32	B	624	AJP	C69
32	B	624	AJP	C36
32	B	624	AJP	C07
32	B	624	AJP	C08
32	B	624	AJP	C28
32	B	624	AJP	C20
32	B	624	AJP	C16
32	B	624	AJP	C27
32	B	624	AJP	C37
32	B	624	AJP	C23
32	B	624	AJP	C46
32	B	624	AJP	C57
32	B	624	AJP	C10
32	B	624	AJP	C22
32	B	624	AJP	C11
32	B	624	AJP	C26
32	B	624	AJP	C02
32	B	624	AJP	C59
32	B	624	AJP	C65
32	B	624	AJP	C38
32	B	624	AJP	C39
32	B	624	AJP	C15
32	S	319	AJP	C22
32	S	319	AJP	C07

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Mol	Chain	Res	Type	Atom
32	S	319	AJP	C11
32	S	319	AJP	C26
32	S	319	AJP	C30
32	S	319	AJP	C02
32	S	319	AJP	C20
32	S	319	AJP	C23
32	S	319	AJP	C12
32	S	319	AJP	C16
32	S	319	AJP	C27
32	S	319	AJP	C15
32	S	319	AJP	C19
32	S	319	AJP	C28
32	S	319	AJP	C10
32	G	618	AJP	C20
32	G	618	AJP	C22
32	G	618	AJP	C07
32	G	618	AJP	C11
32	G	618	AJP	C26
32	G	618	AJP	C30
32	G	618	AJP	C23
32	G	618	AJP	C28
32	G	618	AJP	C02
32	G	618	AJP	C12
32	G	618	AJP	C16
32	G	618	AJP	C27
32	G	618	AJP	C15
32	G	618	AJP	C19
32	G	618	AJP	C10
32	N	619	AJP	C22
32	N	619	AJP	C07
32	N	619	AJP	C11
32	N	619	AJP	C26
32	N	619	AJP	C30
32	N	619	AJP	C28
32	N	619	AJP	C02
32	N	619	AJP	C20
32	N	619	AJP	C23
32	N	619	AJP	C12
32	N	619	AJP	C16
32	N	619	AJP	C27
32	N	619	AJP	C15
32	N	619	AJP	C19

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Mol	Chain	Res	Type	Atom
32	N	619	AJP	C10
32	N	620	AJP	C22
32	N	620	AJP	C07
32	N	620	AJP	C11
32	N	620	AJP	C26
32	N	620	AJP	C30
32	N	620	AJP	C08
32	N	620	AJP	C28
32	N	620	AJP	C02
32	N	620	AJP	C20
32	N	620	AJP	C23
32	N	620	AJP	C12
32	N	620	AJP	C16
32	N	620	AJP	C27
32	N	620	AJP	C15
32	N	620	AJP	C19
32	N	620	AJP	C10
32	Y	320	AJP	C22
32	Y	320	AJP	C10
32	Y	320	AJP	C07
32	Y	320	AJP	C11
32	Y	320	AJP	C26
32	Y	320	AJP	C23
32	Y	320	AJP	C28
32	Y	320	AJP	C02
32	Y	320	AJP	C30
32	Y	320	AJP	C20
32	Y	320	AJP	C12
32	Y	320	AJP	C16
32	Y	320	AJP	C27
32	Y	320	AJP	C15
32	Y	320	AJP	C19
32	Y	321	AJP	C22
32	Y	321	AJP	C07
32	Y	321	AJP	C11
32	Y	321	AJP	C26
32	Y	321	AJP	C30
32	Y	321	AJP	C08
32	Y	321	AJP	C28
32	Y	321	AJP	C02
32	Y	321	AJP	C20
32	Y	321	AJP	C23

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Mol	Chain	Res	Type	Atom
32	Y	321	AJP	C12
32	Y	321	AJP	C16
32	Y	321	AJP	C27
32	Y	321	AJP	C15
32	Y	321	AJP	C19
32	Y	321	AJP	C10
32	Y	322	AJP	C22
32	Y	322	AJP	C07
32	Y	322	AJP	C11
32	Y	322	AJP	C26
32	Y	322	AJP	C30
32	Y	322	AJP	C28
32	Y	322	AJP	C02
32	Y	322	AJP	C20
32	Y	322	AJP	C23
32	Y	322	AJP	C12
32	Y	322	AJP	C16
32	Y	322	AJP	C27
32	Y	322	AJP	C15
32	Y	322	AJP	C19
32	Y	322	AJP	C10
32	Y	323	AJP	C22
32	Y	323	AJP	C07
32	Y	323	AJP	C11
32	Y	323	AJP	C26
32	Y	323	AJP	C30
32	Y	323	AJP	C28
32	Y	323	AJP	C02
32	Y	323	AJP	C20
32	Y	323	AJP	C23
32	Y	323	AJP	C12
32	Y	323	AJP	C16
32	Y	323	AJP	C27
32	Y	323	AJP	C15
32	Y	323	AJP	C19
32	Y	323	AJP	C10
32	Y	324	AJP	C22
32	Y	324	AJP	C07
32	Y	324	AJP	C11
32	Y	324	AJP	C26
32	Y	324	AJP	C30
32	Y	324	AJP	C28

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Mol	Chain	Res	Type	Atom
32	Y	324	AJP	C02
32	Y	324	AJP	C20
32	Y	324	AJP	C23
32	Y	324	AJP	C12
32	Y	324	AJP	C16
32	Y	324	AJP	C27
32	Y	324	AJP	C15
32	Y	324	AJP	C19
32	Y	324	AJP	C10
32	a	413	AJP	C68
32	a	413	AJP	C45
32	a	413	AJP	C35
32	a	413	AJP	C56
32	a	413	AJP	C30
32	a	413	AJP	C47
32	a	413	AJP	C48
32	a	413	AJP	C12
32	a	413	AJP	C55
32	a	413	AJP	C67
32	a	413	AJP	C66
32	a	413	AJP	C19
32	a	413	AJP	C07
32	a	413	AJP	C36
32	a	413	AJP	C08
32	a	413	AJP	C28
32	a	413	AJP	C69
32	a	413	AJP	C20
32	a	413	AJP	C37
32	a	413	AJP	C16
32	a	413	AJP	C27
32	a	413	AJP	C23
32	a	413	AJP	C46
32	a	413	AJP	C57
32	a	413	AJP	C10
32	a	413	AJP	C22
32	a	413	AJP	C11
32	a	413	AJP	C26
32	a	413	AJP	C02
32	a	413	AJP	C59
32	a	413	AJP	C65
32	a	413	AJP	C38
32	a	413	AJP	C39

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Mol	Chain	Res	Type	Atom
32	a	413	AJP	C15
32	b	624	AJP	C45
32	b	624	AJP	C35
32	b	624	AJP	C56
32	b	624	AJP	C30
32	b	624	AJP	C68
32	b	624	AJP	C47
32	b	624	AJP	C48
32	b	624	AJP	C12
32	b	624	AJP	C55
32	b	624	AJP	C67
32	b	624	AJP	C66
32	b	624	AJP	C19
32	b	624	AJP	C69
32	b	624	AJP	C36
32	b	624	AJP	C07
32	b	624	AJP	C08
32	b	624	AJP	C28
32	b	624	AJP	C20
32	b	624	AJP	C16
32	b	624	AJP	C27
32	b	624	AJP	C37
32	b	624	AJP	C23
32	b	624	AJP	C46
32	b	624	AJP	C57
32	b	624	AJP	C10
32	b	624	AJP	C22
32	b	624	AJP	C11
32	b	624	AJP	C26
32	b	624	AJP	C02
32	b	624	AJP	C59
32	b	624	AJP	C65
32	b	624	AJP	C38
32	b	624	AJP	C39
32	b	624	AJP	C15
32	s	319	AJP	C22
32	s	319	AJP	C07
32	s	319	AJP	C11
32	s	319	AJP	C26
32	s	319	AJP	C30
32	s	319	AJP	C28
32	s	319	AJP	C02

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Mol	Chain	Res	Type	Atom
32	s	319	AJP	C20
32	s	319	AJP	C23
32	s	319	AJP	C12
32	s	319	AJP	C16
32	s	319	AJP	C27
32	s	319	AJP	C15
32	s	319	AJP	C19
32	s	319	AJP	C10
32	g	618	AJP	C20
32	g	618	AJP	C22
32	g	618	AJP	C07
32	g	618	AJP	C11
32	g	618	AJP	C26
32	g	618	AJP	C30
32	g	618	AJP	C23
32	g	618	AJP	C28
32	g	618	AJP	C02
32	g	618	AJP	C12
32	g	618	AJP	C16
32	g	618	AJP	C27
32	g	618	AJP	C15
32	g	618	AJP	C19
32	g	618	AJP	C10
32	n	619	AJP	C22
32	n	619	AJP	C07
32	n	619	AJP	C11
32	n	619	AJP	C26
32	n	619	AJP	C30
32	n	619	AJP	C28
32	n	619	AJP	C02
32	n	619	AJP	C20
32	n	619	AJP	C23
32	n	619	AJP	C12
32	n	619	AJP	C16
32	n	619	AJP	C27
32	n	619	AJP	C15
32	n	619	AJP	C19
32	n	619	AJP	C10
32	n	620	AJP	C22
32	n	620	AJP	C07
32	n	620	AJP	C11
32	n	620	AJP	C26

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Mol	Chain	Res	Type	Atom
32	n	620	AJP	C30
32	n	620	AJP	C08
32	n	620	AJP	C28
32	n	620	AJP	C02
32	n	620	AJP	C20
32	n	620	AJP	C23
32	n	620	AJP	C12
32	n	620	AJP	C16
32	n	620	AJP	C27
32	n	620	AJP	C15
32	n	620	AJP	C19
32	n	620	AJP	C10
32	y	320	AJP	C22
32	y	320	AJP	C10
32	y	320	AJP	C07
32	y	320	AJP	C11
32	y	320	AJP	C26
32	y	320	AJP	C23
32	y	320	AJP	C28
32	y	320	AJP	C02
32	y	320	AJP	C30
32	y	320	AJP	C20
32	y	320	AJP	C12
32	y	320	AJP	C16
32	y	320	AJP	C27
32	y	320	AJP	C15
32	y	320	AJP	C19
32	y	321	AJP	C22
32	y	321	AJP	C07
32	y	321	AJP	C11
32	y	321	AJP	C26
32	y	321	AJP	C30
32	y	321	AJP	C08
32	y	321	AJP	C28
32	y	321	AJP	C02
32	y	321	AJP	C20
32	y	321	AJP	C23
32	y	321	AJP	C12
32	y	321	AJP	C16
32	y	321	AJP	C27
32	y	321	AJP	C15
32	y	321	AJP	C19

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Mol	Chain	Res	Type	Atom
32	y	321	AJP	C10
32	y	322	AJP	C22
32	y	322	AJP	C07
32	y	322	AJP	C11
32	y	322	AJP	C26
32	y	322	AJP	C30
32	y	322	AJP	C28
32	y	322	AJP	C02
32	y	322	AJP	C20
32	y	322	AJP	C23
32	y	322	AJP	C12
32	y	322	AJP	C16
32	y	322	AJP	C27
32	y	322	AJP	C15
32	y	322	AJP	C19
32	y	322	AJP	C10
32	y	323	AJP	C22
32	y	323	AJP	C07
32	y	323	AJP	C11
32	y	323	AJP	C26
32	y	323	AJP	C30
32	y	323	AJP	C28
32	y	323	AJP	C02
32	y	323	AJP	C20
32	y	323	AJP	C23
32	y	323	AJP	C12
32	y	323	AJP	C16
32	y	323	AJP	C27
32	y	323	AJP	C15
32	y	323	AJP	C19
32	y	323	AJP	C10
32	y	324	AJP	C22
32	y	324	AJP	C07
32	y	324	AJP	C11
32	y	324	AJP	C26
32	y	324	AJP	C30
32	y	324	AJP	C28
32	y	324	AJP	C02
32	y	324	AJP	C20
32	y	324	AJP	C23
32	y	324	AJP	C12
32	y	324	AJP	C16

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Mol	Chain	Res	Type	Atom
32	y	324	AJP	C27
32	y	324	AJP	C15
32	y	324	AJP	C19
32	y	324	AJP	C10

All (3970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	302	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	CBD-CGD-O2D-CED
24	2	601	CHL	C6-C7-C8-C10
24	2	603	CHL	C1C-C2C-CMC-OMC
24	2	603	CHL	C3C-C2C-CMC-OMC
24	2	603	CHL	C4C-C3C-CAC-CBC
24	2	603	CHL	CAD-CBD-CGD-O1D
24	2	603	CHL	CBD-CGD-O2D-CED
24	S	306	CHL	CAD-CBD-CGD-O1D
24	S	307	CHL	C3A-C2A-CAA-CBA
24	S	307	CHL	C4C-C3C-CAC-CBC
24	S	307	CHL	CHA-CBD-CGD-O1D
24	G	601	CHL	C1C-C2C-CMC-OMC
24	G	601	CHL	C3C-C2C-CMC-OMC
24	G	601	CHL	C4C-C3C-CAC-CBC
24	G	601	CHL	C11-C10-C8-C7
24	G	605	CHL	C3A-C2A-CAA-CBA
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	C4C-C3C-CAC-CBC
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C3A-C2A-CAA-CBA
24	G	608	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	C4C-C3C-CAC-CBC
24	G	608	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC
24	N	601	CHL	C1C-C2C-CMC-OMC
24	N	601	CHL	C3C-C2C-CMC-OMC
24	N	601	CHL	C4C-C3C-CAC-CBC
24	N	605	CHL	C4C-C3C-CAC-CBC
24	N	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	N	608	CHL	C1A-C2A-CAA-CBA
24	N	608	CHL	C1C-C2C-CMC-OMC
24	N	609	CHL	C3A-C2A-CAA-CBA
24	N	609	CHL	C11-C10-C8-C9
24	Y	302	CHL	C1C-C2C-CMC-OMC
24	Y	302	CHL	C3C-C2C-CMC-OMC
24	Y	302	CHL	C4C-C3C-CAC-CBC
24	Y	306	CHL	C4C-C3C-CAC-CBC
24	Y	308	CHL	C4C-C3C-CAC-CBC
24	Y	309	CHL	C1A-C2A-CAA-CBA
24	Y	309	CHL	C1C-C2C-CMC-OMC
24	Y	309	CHL	C4C-C3C-CAC-CBC
24	Y	309	CHL	C14-C13-C15-C16
24	Y	310	CHL	C1A-C2A-CAA-CBA
24	R	605	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	C4C-C3C-CAC-CBC
24	R	607	CHL	CBA-CGA-O2A-C1
24	R	607	CHL	O1A-CGA-O2A-C1
24	R	613	CHL	C4C-C3C-CAC-CBC
24	R	613	CHL	CAD-CBD-CGD-O1D
24	R	613	CHL	CAD-CBD-CGD-O2D
24	5	302	CHL	C3A-C2A-CAA-CBA
24	6	601	CHL	C1C-C2C-CMC-OMC
24	6	601	CHL	C3C-C2C-CMC-OMC
24	6	601	CHL	CBD-CGD-O2D-CED
24	6	601	CHL	C6-C7-C8-C10
24	6	603	CHL	C1C-C2C-CMC-OMC
24	6	603	CHL	C3C-C2C-CMC-OMC
24	6	603	CHL	C4C-C3C-CAC-CBC
24	6	603	CHL	CAD-CBD-CGD-O1D
24	6	603	CHL	CBD-CGD-O2D-CED
24	s	306	CHL	CAD-CBD-CGD-O1D
24	s	307	CHL	C3A-C2A-CAA-CBA
24	s	307	CHL	C4C-C3C-CAC-CBC
24	g	601	CHL	C1C-C2C-CMC-OMC
24	g	601	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C4C-C3C-CAC-CBC
24	g	601	CHL	C11-C10-C8-C7
24	g	605	CHL	C3A-C2A-CAA-CBA
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C3A-C2A-CAA-CBA
24	g	608	CHL	C1C-C2C-CMC-OMC
24	g	608	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	C4C-C3C-CAC-CBC
24	g	608	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	601	CHL	C1C-C2C-CMC-OMC
24	n	601	CHL	C3C-C2C-CMC-OMC
24	n	601	CHL	C4C-C3C-CAC-CBC
24	n	605	CHL	C4C-C3C-CAC-CBC
24	n	607	CHL	C3A-C2A-CAA-CBA
24	n	608	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	C1C-C2C-CMC-OMC
24	n	609	CHL	C3A-C2A-CAA-CBA
24	n	609	CHL	C11-C10-C8-C9
24	y	302	CHL	C1C-C2C-CMC-OMC
24	y	302	CHL	C3C-C2C-CMC-OMC
24	y	302	CHL	C4C-C3C-CAC-CBC
24	y	306	CHL	C4C-C3C-CAC-CBC
24	y	308	CHL	C4C-C3C-CAC-CBC
24	y	309	CHL	C1A-C2A-CAA-CBA
24	y	309	CHL	C1C-C2C-CMC-OMC
24	y	309	CHL	C4C-C3C-CAC-CBC
24	y	309	CHL	C14-C13-C15-C16
24	y	310	CHL	C1A-C2A-CAA-CBA
24	r	605	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	C4C-C3C-CAC-CBC
24	r	607	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	O1A-CGA-O2A-C1
24	r	613	CHL	C4C-C3C-CAC-CBC
24	r	613	CHL	CAD-CBD-CGD-O1D
24	r	613	CHL	CAD-CBD-CGD-O2D
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C3A-C2A-CAA-CBA
25	2	602	CLA	CAD-CBD-CGD-O1D
25	2	602	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	605	CLA	C1A-C2A-CAA-CBA
25	2	605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	602	CLA	C6-C7-C8-C9
25	B	604	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C15
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	609	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C3A-C2A-CAA-CBA
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	C14-C13-C15-C16
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	C11-C10-C8-C9
25	C	512	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	CHA-CBD-CGD-O2D
25	D	402	CLA	C1A-C2A-CAA-CBA
25	D	402	CLA	C3A-C2A-CAA-CBA
25	D	403	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C3A-C2A-CAA-CBA
25	S	303	CLA	C1A-C2A-CAA-CBA
25	S	305	CLA	C3A-C2A-CAA-CBA
25	S	305	CLA	CAD-CBD-CGD-O2D
25	S	305	CLA	CBD-CGD-O2D-CED
25	S	311	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	CAD-CBD-CGD-O1D
25	S	311	CLA	CAD-CBD-CGD-O2D
25	S	312	CLA	C2B-C3B-CAB-CBB
25	S	312	CLA	C4B-C3B-CAB-CBB
25	S	313	CLA	C1A-C2A-CAA-CBA
25	S	313	CLA	C3A-C2A-CAA-CBA
25	G	602	CLA	CHA-CBD-CGD-O2D
25	G	603	CLA	C2B-C3B-CAB-CBB
25	G	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	G	604	CLA	C2B-C3B-CAB-CBB
25	G	604	CLA	C4B-C3B-CAB-CBB
25	G	604	CLA	CBD-CGD-O2D-CED
25	G	610	CLA	CBD-CGD-O2D-CED
25	G	611	CLA	C3A-C2A-CAA-CBA
25	G	611	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	CAD-CBD-CGD-O2D
25	G	611	CLA	C2-C3-C5-C6
25	G	612	CLA	CHA-CBD-CGD-O2D
25	G	613	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C3A-C2A-CAA-CBA
25	G	614	CLA	CAD-CBD-CGD-O1D
25	N	603	CLA	CHA-CBD-CGD-O2D
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C1A-C2A-CAA-CBA
25	N	611	CLA	C1A-C2A-CAA-CBA
25	N	611	CLA	C3A-C2A-CAA-CBA
25	N	611	CLA	C4B-C3B-CAB-CBB
25	N	612	CLA	CHA-CBD-CGD-O2D
25	N	613	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	Y	304	CLA	CHA-CBD-CGD-O1D
25	Y	304	CLA	CHA-CBD-CGD-O2D
25	Y	305	CLA	CBD-CGD-O2D-CED
25	Y	311	CLA	CBD-CGD-O2D-CED
25	Y	312	CLA	CBA-CGA-O2A-C1
25	Y	312	CLA	O1A-CGA-O2A-C1
25	Y	313	CLA	CHA-CBD-CGD-O1D
25	Y	313	CLA	CHA-CBD-CGD-O2D
25	Y	314	CLA	C14-C13-C15-C16
25	Y	315	CLA	C1A-C2A-CAA-CBA
25	Y	315	CLA	CBD-CGD-O2D-CED
25	Y	315	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	C1A-C2A-CAA-CBA
25	R	601	CLA	C3A-C2A-CAA-CBA
25	R	601	CLA	C2B-C3B-CAB-CBB
25	R	601	CLA	C4B-C3B-CAB-CBB
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	C6-C7-C8-C9
25	R	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	R	608	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	C4B-C3B-CAB-CBB
25	R	611	CLA	CBD-CGD-O2D-CED
25	R	614	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C3A-C2A-CAA-CBA
25	6	602	CLA	CAD-CBD-CGD-O1D
25	6	602	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	605	CLA	C1A-C2A-CAA-CBA
25	6	605	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	602	CLA	C6-C7-C8-C9
25	b	604	CLA	C1A-C2A-CAA-CBA
25	b	604	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C15
25	b	605	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C4B-C3B-CAB-CBB
25	b	609	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C3A-C2A-CAA-CBA
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	C14-C13-C15-C16
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	C11-C10-C8-C9
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	CHA-CBD-CGD-O2D
25	d	402	CLA	C1A-C2A-CAA-CBA
25	d	402	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	s	303	CLA	C1A-C2A-CAA-CBA
25	s	305	CLA	C3A-C2A-CAA-CBA
25	s	305	CLA	CAD-CBD-CGD-O2D
25	s	305	CLA	CBD-CGD-O2D-CED
25	s	311	CLA	C1A-C2A-CAA-CBA
25	s	311	CLA	CAD-CBD-CGD-O1D
25	s	311	CLA	CAD-CBD-CGD-O2D
25	s	312	CLA	C2B-C3B-CAB-CBB
25	s	312	CLA	C4B-C3B-CAB-CBB
25	s	313	CLA	C1A-C2A-CAA-CBA
25	s	313	CLA	C3A-C2A-CAA-CBA
25	g	602	CLA	CHA-CBD-CGD-O2D
25	g	603	CLA	C2B-C3B-CAB-CBB
25	g	603	CLA	C4B-C3B-CAB-CBB
25	g	604	CLA	C2B-C3B-CAB-CBB
25	g	604	CLA	C4B-C3B-CAB-CBB
25	g	604	CLA	CBD-CGD-O2D-CED
25	g	610	CLA	CBD-CGD-O2D-CED
25	g	611	CLA	C3A-C2A-CAA-CBA
25	g	611	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	CAD-CBD-CGD-O2D
25	g	611	CLA	C2-C3-C5-C6
25	g	612	CLA	CHA-CBD-CGD-O2D
25	g	613	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C3A-C2A-CAA-CBA
25	g	614	CLA	CAD-CBD-CGD-O1D
25	n	603	CLA	CHA-CBD-CGD-O2D
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C3A-C2A-CAA-CBA
25	n	610	CLA	C1A-C2A-CAA-CBA
25	n	611	CLA	C1A-C2A-CAA-CBA
25	n	611	CLA	C3A-C2A-CAA-CBA
25	n	611	CLA	C4B-C3B-CAB-CBB
25	n	612	CLA	CHA-CBD-CGD-O2D
25	n	613	CLA	CBD-CGD-O2D-CED
25	n	614	CLA	CBD-CGD-O2D-CED
25	y	304	CLA	CHA-CBD-CGD-O1D
25	y	304	CLA	CHA-CBD-CGD-O2D
25	y	305	CLA	CBD-CGD-O2D-CED
25	y	311	CLA	CBD-CGD-O2D-CED
25	y	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	y	312	CLA	O1A-CGA-O2A-C1
25	y	313	CLA	CHA-CBD-CGD-O1D
25	y	313	CLA	CHA-CBD-CGD-O2D
25	y	314	CLA	C14-C13-C15-C16
25	y	315	CLA	C1A-C2A-CAA-CBA
25	y	315	CLA	CBD-CGD-O2D-CED
25	y	315	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	C1A-C2A-CAA-CBA
25	r	601	CLA	C3A-C2A-CAA-CBA
25	r	601	CLA	C2B-C3B-CAB-CBB
25	r	601	CLA	C4B-C3B-CAB-CBB
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	C6-C7-C8-C9
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	608	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	C4B-C3B-CAB-CBB
25	r	611	CLA	CBD-CGD-O2D-CED
25	r	614	CLA	C1A-C2A-CAA-CBA
26	2	606	LHG	C3-O3-P-O4
26	2	606	LHG	C3-O3-P-O6
26	2	606	LHG	O7-C5-C6-O8
26	C	517	LHG	C1-C2-C3-O3
26	C	518	LHG	C3-O3-P-O6
26	C	518	LHG	C8-C7-O7-C5
26	C	519	LHG	C4-O6-P-O3
26	C	519	LHG	C4-O6-P-O4
26	C	519	LHG	C4-O6-P-O5
26	C	519	LHG	C8-C7-O7-C5
26	D	406	LHG	O1-C1-C2-O2
26	D	406	LHG	O1-C1-C2-C3
26	D	406	LHG	C1-C2-C3-O3
26	L	102	LHG	C4-O6-P-O4
26	L	102	LHG	C4-O6-P-O5
26	S	301	LHG	O1-C1-C2-C3
26	S	318	LHG	O1-C1-C2-C3
26	N	618	LHG	O1-C1-C2-C3
26	N	618	LHG	C3-O3-P-O4
26	N	618	LHG	C3-O3-P-O6
26	Y	301	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
26	Y	319	LHG	O1-C1-C2-C3
26	Y	319	LHG	C3-O3-P-O4
26	Y	319	LHG	C3-O3-P-O5
26	Y	319	LHG	C3-O3-P-O6
26	6	606	LHG	C3-O3-P-O4
26	6	606	LHG	C3-O3-P-O6
26	6	606	LHG	O7-C5-C6-O8
26	c	517	LHG	C1-C2-C3-O3
26	c	518	LHG	C3-O3-P-O6
26	c	518	LHG	C8-C7-O7-C5
26	c	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O5
26	c	519	LHG	C8-C7-O7-C5
26	d	406	LHG	O1-C1-C2-O2
26	d	406	LHG	O1-C1-C2-C3
26	d	406	LHG	C1-C2-C3-O3
26	l	103	LHG	C4-O6-P-O4
26	l	103	LHG	C4-O6-P-O5
26	s	301	LHG	O1-C1-C2-C3
26	s	318	LHG	O1-C1-C2-C3
26	n	618	LHG	O1-C1-C2-C3
26	n	618	LHG	C3-O3-P-O4
26	n	618	LHG	C3-O3-P-O6
26	y	301	LHG	C1-C2-C3-O3
26	y	319	LHG	O1-C1-C2-C3
26	y	319	LHG	C3-O3-P-O4
26	y	319	LHG	C3-O3-P-O5
26	y	319	LHG	C3-O3-P-O6
27	A	403	PHO	O1A-CGA-O2A-C1
27	a	404	PHO	O1A-CGA-O2A-C1
28	A	406	BCR	C14-C15-C16-C17
28	A	406	BCR	C16-C17-C18-C19
28	A	406	BCR	C16-C17-C18-C36
28	D	404	BCR	C7-C8-C9-C10
28	H	101	BCR	C7-C8-C9-C10
28	H	101	BCR	C7-C8-C9-C34
28	H	101	BCR	C22-C23-C24-C25
28	I	101	BCR	C20-C21-C22-C37
28	K	101	BCR	C7-C8-C9-C10
28	T	101	BCR	C11-C10-C9-C8
28	T	101	BCR	C11-C10-C9-C34
28	T	101	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
28	T	101	BCR	C13-C14-C15-C16
28	T	101	BCR	C21-C22-C23-C24
28	T	101	BCR	C37-C22-C23-C24
28	T	101	BCR	C22-C23-C24-C25
28	Z	101	BCR	C7-C8-C9-C34
28	Z	101	BCR	C20-C21-C22-C37
28	Z	101	BCR	C21-C22-C23-C24
28	Z	101	BCR	C37-C22-C23-C24
28	a	407	BCR	C14-C15-C16-C17
28	a	407	BCR	C16-C17-C18-C19
28	a	407	BCR	C16-C17-C18-C36
28	d	404	BCR	C7-C8-C9-C10
28	h	101	BCR	C7-C8-C9-C10
28	h	101	BCR	C7-C8-C9-C34
28	h	101	BCR	C22-C23-C24-C25
28	i	101	BCR	C20-C21-C22-C37
28	k	101	BCR	C7-C8-C9-C10
28	t	101	BCR	C11-C10-C9-C8
28	t	101	BCR	C11-C10-C9-C34
28	t	101	BCR	C11-C12-C13-C35
28	t	101	BCR	C13-C14-C15-C16
28	t	101	BCR	C21-C22-C23-C24
28	t	101	BCR	C37-C22-C23-C24
28	t	101	BCR	C22-C23-C24-C25
28	z	101	BCR	C7-C8-C9-C34
28	z	101	BCR	C20-C21-C22-C37
28	z	101	BCR	C21-C22-C23-C24
28	z	101	BCR	C37-C22-C23-C24
29	A	407	SQD	O49-C7-O47-C45
29	A	407	SQD	O5-C5-C6-S
29	A	411	SQD	O5-C1-O6-C44
29	A	411	SQD	O5-C5-C6-S
29	L	101	SQD	O47-C45-C46-O48
29	L	103	SQD	C2-C1-O6-C44
29	L	103	SQD	O5-C1-O6-C44
29	L	103	SQD	O49-C7-O47-C45
29	L	103	SQD	C8-C7-O47-C45
29	L	103	SQD	O5-C5-C6-S
29	a	408	SQD	O49-C7-O47-C45
29	a	408	SQD	O5-C5-C6-S
29	a	412	SQD	O5-C1-O6-C44
29	a	412	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45
29	l	101	SQD	O5-C5-C6-S
29	l	102	SQD	O47-C45-C46-O48
30	A	410	LMG	O7-C8-C9-O8
30	B	623	LMG	O9-C10-O7-C8
30	C	520	LMG	C2-C1-O1-C7
30	C	520	LMG	O9-C10-O7-C8
30	a	411	LMG	O7-C8-C9-O8
30	b	623	LMG	O9-C10-O7-C8
30	c	520	LMG	C2-C1-O1-C7
30	c	520	LMG	O9-C10-O7-C8
32	A	412	AJP	C22-C23-O25-C26
32	B	624	AJP	C30-C29-O34-C35
32	S	319	AJP	C29-C30-C32-O33
32	S	319	AJP	O31-C30-C32-O33
32	N	620	AJP	C22-C23-O25-C26
32	N	620	AJP	C27-C26-O25-C23
32	N	620	AJP	C29-C30-C32-O33
32	N	620	AJP	O31-C30-C32-O33
32	Y	320	AJP	O31-C30-C32-O33
32	Y	321	AJP	C24-C23-O25-C26
32	Y	321	AJP	C29-C30-C32-O33
32	Y	321	AJP	O31-C30-C32-O33
32	Y	324	AJP	C29-C30-C32-O33
32	Y	324	AJP	O31-C30-C32-O33
32	a	413	AJP	C22-C23-O25-C26
32	b	624	AJP	C30-C29-O34-C35
32	s	319	AJP	C29-C30-C32-O33
32	s	319	AJP	O31-C30-C32-O33
32	n	620	AJP	C22-C23-O25-C26
32	n	620	AJP	C27-C26-O25-C23
32	n	620	AJP	C29-C30-C32-O33
32	n	620	AJP	O31-C30-C32-O33
32	y	320	AJP	O31-C30-C32-O33
32	y	321	AJP	C24-C23-O25-C26
32	y	321	AJP	C29-C30-C32-O33
32	y	321	AJP	O31-C30-C32-O33
32	y	324	AJP	C29-C30-C32-O33
32	y	324	AJP	O31-C30-C32-O33

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Mol	Chain	Res	Type	Atoms
35	A	415	DGD	C2A-C1A-O1G-C1G
35	A	415	DGD	O1A-C1A-O1G-C1G
35	A	415	DGD	C2B-C1B-O2G-C2G
35	A	415	DGD	C2D-C1D-O3G-C3G
35	A	415	DGD	O6D-C1D-O3G-C3G
35	C	516	DGD	C2D-C1D-O3G-C3G
35	C	516	DGD	C2E-C1E-O5D-C6D
35	C	516	DGD	O6E-C1E-O5D-C6D
35	a	401	DGD	C2A-C1A-O1G-C1G
35	a	401	DGD	O1A-C1A-O1G-C1G
35	a	401	DGD	C2B-C1B-O2G-C2G
35	a	401	DGD	C2D-C1D-O3G-C3G
35	a	401	DGD	O6D-C1D-O3G-C3G
35	c	516	DGD	C2D-C1D-O3G-C3G
35	c	516	DGD	C2E-C1E-O5D-C6D
35	c	516	DGD	O6E-C1E-O5D-C6D
40	S	317	NEX	C11-C12-C13-C14
40	S	317	NEX	C11-C12-C13-C20
40	G	617	NEX	C9-C10-C11-C12
40	G	617	NEX	C21-C26-C27-C28
40	G	617	NEX	C25-C26-C27-C28
40	G	617	NEX	C27-C28-C29-C30
40	G	617	NEX	C27-C28-C29-C39
40	N	617	NEX	C7-C8-C9-C10
40	N	617	NEX	C27-C28-C29-C30
40	N	617	NEX	C31-C32-C33-C34
40	N	617	NEX	C31-C32-C33-C40
40	Y	318	NEX	C9-C10-C11-C12
40	Y	318	NEX	C21-C26-C27-C28
40	Y	318	NEX	C27-C28-C29-C30
40	Y	318	NEX	C27-C28-C29-C39
40	R	617	NEX	C9-C10-C11-C12
40	R	617	NEX	C11-C12-C13-C14
40	s	317	NEX	C11-C12-C13-C14
40	s	317	NEX	C11-C12-C13-C20
40	g	617	NEX	C9-C10-C11-C12
40	g	617	NEX	C21-C26-C27-C28
40	g	617	NEX	C25-C26-C27-C28
40	g	617	NEX	C27-C28-C29-C30
40	g	617	NEX	C27-C28-C29-C39
40	n	617	NEX	C7-C8-C9-C10
40	n	617	NEX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
40	n	617	NEX	C31-C32-C33-C34
40	n	617	NEX	C31-C32-C33-C40
40	y	318	NEX	C9-C10-C11-C12
40	y	318	NEX	C21-C26-C27-C28
40	y	318	NEX	C27-C28-C29-C30
40	y	318	NEX	C27-C28-C29-C39
40	r	617	NEX	C9-C10-C11-C12
40	r	617	NEX	C11-C12-C13-C14
25	G	614	CLA	C4C-C3C-CAC-CBC
25	N	602	CLA	C4C-C3C-CAC-CBC
25	g	614	CLA	C4C-C3C-CAC-CBC
25	n	602	CLA	C4C-C3C-CAC-CBC
25	2	604	CLA	O1D-CGD-O2D-CED
25	2	605	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
25	S	305	CLA	O1D-CGD-O2D-CED
25	G	604	CLA	O1D-CGD-O2D-CED
25	G	610	CLA	O1D-CGD-O2D-CED
25	Y	311	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	6	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	s	305	CLA	O1D-CGD-O2D-CED
25	g	604	CLA	O1D-CGD-O2D-CED
25	g	610	CLA	O1D-CGD-O2D-CED
25	y	311	CLA	O1D-CGD-O2D-CED
32	B	624	AJP	O70-C65-O64-C57
32	b	624	AJP	O70-C65-O64-C57
24	Y	308	CHL	C2C-C3C-CAC-CBC
24	y	308	CHL	C2C-C3C-CAC-CBC
25	N	602	CLA	C2C-C3C-CAC-CBC
25	n	602	CLA	C2C-C3C-CAC-CBC
24	2	601	CHL	O1D-CGD-O2D-CED
24	N	608	CHL	O1D-CGD-O2D-CED
24	6	601	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
25	A	401	CLA	O1D-CGD-O2D-CED
25	S	313	CLA	O1D-CGD-O2D-CED
25	N	613	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	a	402	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	s	313	CLA	O1D-CGD-O2D-CED
25	n	613	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED
25	r	611	CLA	O1D-CGD-O2D-CED
24	N	607	CHL	CBD-CGD-O2D-CED
24	N	608	CHL	CBD-CGD-O2D-CED
24	Y	309	CHL	CBD-CGD-O2D-CED
24	Y	310	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	n	607	CHL	CBD-CGD-O2D-CED
24	n	608	CHL	CBD-CGD-O2D-CED
24	y	309	CHL	CBD-CGD-O2D-CED
24	y	310	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
25	2	605	CLA	CBD-CGD-O2D-CED
25	A	401	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	S	304	CLA	CBD-CGD-O2D-CED
25	S	309	CLA	CBD-CGD-O2D-CED
25	S	313	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	N	610	CLA	CBD-CGD-O2D-CED
25	N	611	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	CBD-CGD-O2D-CED
25	6	605	CLA	CBD-CGD-O2D-CED
25	a	402	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	s	304	CLA	CBD-CGD-O2D-CED
25	s	309	CLA	CBD-CGD-O2D-CED
25	s	313	CLA	CBD-CGD-O2D-CED
25	g	613	CLA	CBD-CGD-O2D-CED
25	n	610	CLA	CBD-CGD-O2D-CED
25	n	611	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	CBD-CGD-O2D-CED
32	Y	322	AJP	O31-C26-O25-C23
32	y	322	AJP	O31-C26-O25-C23
32	Y	324	AJP	C27-C26-O25-C23
32	y	324	AJP	C27-C26-O25-C23

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Mol	Chain	Res	Type	Atoms
25	2	602	CLA	O1A-CGA-O2A-C1
25	2	604	CLA	O1A-CGA-O2A-C1
25	2	605	CLA	O1A-CGA-O2A-C1
25	G	614	CLA	O1A-CGA-O2A-C1
25	6	602	CLA	O1A-CGA-O2A-C1
25	6	604	CLA	O1A-CGA-O2A-C1
25	6	605	CLA	O1A-CGA-O2A-C1
25	g	614	CLA	O1A-CGA-O2A-C1
25	R	608	CLA	C4C-C3C-CAC-CBC
25	r	608	CLA	C4C-C3C-CAC-CBC
25	G	614	CLA	C2C-C3C-CAC-CBC
24	Y	309	CHL	O1D-CGD-O2D-CED
24	y	309	CHL	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1D-CGD-O2D-CED
25	g	613	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
32	A	412	AJP	O60-C55-O54-C36
32	Y	323	AJP	O31-C26-O25-C23
32	a	413	AJP	O60-C55-O54-C36
32	y	323	AJP	O31-C26-O25-C23
32	B	624	AJP	C66-C65-O64-C57
32	N	619	AJP	C27-C26-O25-C23
32	b	624	AJP	C66-C65-O64-C57
32	n	619	AJP	C27-C26-O25-C23
25	g	614	CLA	C2C-C3C-CAC-CBC
24	G	608	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
25	S	304	CLA	O1D-CGD-O2D-CED
25	R	608	CLA	O1D-CGD-O2D-CED
25	s	304	CLA	O1D-CGD-O2D-CED
25	r	608	CLA	O1D-CGD-O2D-CED
25	2	604	CLA	CBA-CGA-O2A-C1
25	2	605	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	6	604	CLA	CBA-CGA-O2A-C1
25	6	605	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
25	N	604	CLA	CBD-CGD-O2D-CED
25	n	604	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	O1A-CGA-O2A-C1
25	R	608	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	R	610	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
25	r	608	CLA	O1A-CGA-O2A-C1
25	r	610	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
26	L	102	LHG	O10-C23-O8-C6
26	l	103	LHG	O10-C23-O8-C6
24	S	307	CHL	C2C-C3C-CAC-CBC
24	s	307	CHL	C2C-C3C-CAC-CBC
25	N	613	CLA	C4C-C3C-CAC-CBC
25	n	613	CLA	C4C-C3C-CAC-CBC
25	N	610	CLA	O1D-CGD-O2D-CED
25	N	611	CLA	O1D-CGD-O2D-CED
25	n	610	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
32	S	319	AJP	C27-C26-O25-C23
32	s	319	AJP	C27-C26-O25-C23
25	N	613	CLA	C2C-C3C-CAC-CBC
25	R	608	CLA	C2C-C3C-CAC-CBC
25	n	613	CLA	C2C-C3C-CAC-CBC
25	r	608	CLA	C2C-C3C-CAC-CBC
24	2	603	CHL	O1D-CGD-O2D-CED
24	R	606	CHL	O1D-CGD-O2D-CED
24	6	603	CHL	O1D-CGD-O2D-CED
24	r	606	CHL	O1D-CGD-O2D-CED
25	B	613	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	O1D-CGD-O2D-CED
25	S	309	CLA	O1D-CGD-O2D-CED
25	Y	314	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	s	309	CLA	O1D-CGD-O2D-CED
25	y	314	CLA	O1D-CGD-O2D-CED
26	C	518	LHG	O9-C7-O7-C5
26	C	519	LHG	O9-C7-O7-C5
26	c	518	LHG	O9-C7-O7-C5
26	c	519	LHG	O9-C7-O7-C5
35	A	415	DGD	O1B-C1B-O2G-C2G
35	a	401	DGD	O1B-C1B-O2G-C2G
24	G	609	CHL	C3-C5-C6-C7
24	N	608	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	Y	308	CHL	C3-C5-C6-C7
24	g	609	CHL	C3-C5-C6-C7
24	n	608	CHL	C3-C5-C6-C7
24	y	308	CHL	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
25	G	612	CLA	CBA-CGA-O2A-C1
25	R	610	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	g	612	CLA	CBA-CGA-O2A-C1
25	r	610	CLA	CBA-CGA-O2A-C1
25	r	611	CLA	CBA-CGA-O2A-C1
26	L	102	LHG	C24-C23-O8-C6
26	l	103	LHG	C24-C23-O8-C6
27	A	403	PHO	CBA-CGA-O2A-C1
27	a	404	PHO	CBA-CGA-O2A-C1
29	L	103	SQD	C24-C23-O48-C46
29	l	101	SQD	C24-C23-O48-C46
24	R	607	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CBD-CGD-O2D-CED
25	Y	314	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	n	602	CLA	CBD-CGD-O2D-CED
25	y	314	CLA	CBD-CGD-O2D-CED
29	A	407	SQD	C8-C7-O47-C45
29	a	408	SQD	C8-C7-O47-C45
30	B	623	LMG	C11-C10-O7-C8
30	C	520	LMG	C11-C10-O7-C8
30	b	623	LMG	C11-C10-O7-C8
30	c	520	LMG	C11-C10-O7-C8
24	N	601	CHL	C2C-C3C-CAC-CBC
24	n	601	CHL	C2C-C3C-CAC-CBC
25	D	403	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	C	519	LHG	O10-C23-O8-C6
26	c	519	LHG	O10-C23-O8-C6
25	B	616	CLA	C2C-C3C-CAC-CBC
25	b	616	CLA	C2C-C3C-CAC-CBC
24	N	601	CHL	C4-C3-C5-C6
24	N	607	CHL	C4-C3-C5-C6
24	n	601	CHL	C4-C3-C5-C6
24	n	607	CHL	C4-C3-C5-C6
25	2	604	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	S	303	CLA	C4-C3-C5-C6
25	G	611	CLA	C4-C3-C5-C6
25	N	610	CLA	C4-C3-C5-C6
25	6	604	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
25	s	303	CLA	C4-C3-C5-C6
25	g	611	CLA	C4-C3-C5-C6
25	n	610	CLA	C4-C3-C5-C6
24	G	601	CHL	C2-C3-C5-C6
24	N	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C2-C3-C5-C6
24	n	601	CHL	C2-C3-C5-C6
25	2	604	CLA	C2-C3-C5-C6
25	B	602	CLA	C2-C3-C5-C6
25	C	507	CLA	C2-C3-C5-C6
25	S	310	CLA	C2-C3-C5-C6
25	6	604	CLA	C2-C3-C5-C6
25	b	602	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
25	s	310	CLA	C2-C3-C5-C6
25	y	304	CLA	C2C-C3C-CAC-CBC
24	R	606	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
24	G	608	CHL	C3-C5-C6-C7
24	N	601	CHL	C3-C5-C6-C7
24	R	607	CHL	C3-C5-C6-C7
24	g	608	CHL	C3-C5-C6-C7
24	n	601	CHL	C3-C5-C6-C7
24	r	607	CHL	C3-C5-C6-C7
25	C	504	CLA	C3-C5-C6-C7
25	c	504	CLA	C3-C5-C6-C7
25	Y	304	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	S	312	CLA	CBA-CGA-O2A-C1
25	s	312	CLA	CBA-CGA-O2A-C1
30	A	408	LMG	C4-C5-C6-O5
30	a	409	LMG	C4-C5-C6-O5
35	C	515	DGD	C4E-C5E-C6E-O5E
35	c	515	DGD	C4E-C5E-C6E-O5E
39	S	316	LUT	C33-C34-C35-C15
39	s	316	LUT	C33-C34-C35-C15
40	N	617	NEX	C9-C10-C11-C12
40	n	617	NEX	C9-C10-C11-C12
25	B	601	CLA	O1A-CGA-O2A-C1
25	C	504	CLA	O1A-CGA-O2A-C1
25	S	312	CLA	O1A-CGA-O2A-C1
25	b	601	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	O1A-CGA-O2A-C1
25	s	312	CLA	O1A-CGA-O2A-C1
29	L	103	SQD	O10-C23-O48-C46
29	l	101	SQD	O10-C23-O48-C46
32	A	412	AJP	O70-C69-C71-O72
32	a	413	AJP	O70-C69-C71-O72
25	Y	305	CLA	C2C-C3C-CAC-CBC
25	y	305	CLA	C2C-C3C-CAC-CBC
25	N	613	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	608	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	608	CLA	C3-C5-C6-C7
26	B	622	LHG	O2-C2-C3-O3
26	C	517	LHG	O2-C2-C3-O3
26	D	406	LHG	O2-C2-C3-O3
26	S	301	LHG	O2-C2-C3-O3
26	b	622	LHG	O2-C2-C3-O3
26	c	517	LHG	O2-C2-C3-O3
26	d	406	LHG	O2-C2-C3-O3
26	s	301	LHG	O2-C2-C3-O3
24	Y	310	CHL	O1D-CGD-O2D-CED
24	y	310	CHL	O1D-CGD-O2D-CED
24	Y	310	CHL	CBA-CGA-O2A-C1
24	y	310	CHL	CBA-CGA-O2A-C1
25	2	602	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	6	602	CLA	CBA-CGA-O2A-C1
25	b	601	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	C24-C23-O8-C6
26	c	519	LHG	C24-C23-O8-C6
25	C	510	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
32	B	624	AJP	O31-C26-O25-C23
32	b	624	AJP	O31-C26-O25-C23
32	B	624	AJP	C38-C39-C41-O42
32	b	624	AJP	C38-C39-C41-O42
25	G	603	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	CBD-CGD-O2D-CED
26	2	606	LHG	C8-C7-O7-C5
26	C	517	LHG	C8-C7-O7-C5
26	6	606	LHG	C8-C7-O7-C5
26	c	517	LHG	C8-C7-O7-C5
29	L	101	SQD	C8-C7-O47-C45
29	l	102	SQD	C8-C7-O47-C45
25	B	601	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
32	A	412	AJP	C27-C26-O25-C23
32	a	413	AJP	C27-C26-O25-C23
24	N	607	CHL	CBA-CGA-O2A-C1
24	n	607	CHL	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	R	608	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
25	r	608	CLA	CBA-CGA-O2A-C1
24	G	601	CHL	C4-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
25	B	602	CLA	C4-C3-C5-C6
25	C	507	CLA	C4-C3-C5-C6
25	R	609	CLA	C4-C3-C5-C6
25	b	602	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	r	609	CLA	C4-C3-C5-C6
24	2	601	CHL	C2-C3-C5-C6
24	N	607	CHL	C2-C3-C5-C6
24	6	601	CHL	C2-C3-C5-C6
24	n	607	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C2-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
25	G	612	CLA	O1A-CGA-O2A-C1
25	g	612	CLA	O1A-CGA-O2A-C1
24	G	608	CHL	C2C-C3C-CAC-CBC
24	g	608	CHL	C2C-C3C-CAC-CBC
29	L	101	SQD	C10-C11-C12-C13
29	l	102	SQD	C10-C11-C12-C13
35	C	516	DGD	CCA-CDA-CEA-CFA
35	c	516	DGD	CCA-CDA-CEA-CFA
25	B	601	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
27	A	403	PHO	C3-C5-C6-C7
27	a	404	PHO	C3-C5-C6-C7
29	A	407	SQD	O5-C1-O6-C44
29	a	408	SQD	O5-C1-O6-C44
30	A	408	LMG	O6-C1-O1-C7
30	B	623	LMG	O6-C1-O1-C7
30	a	409	LMG	O6-C1-O1-C7
30	b	623	LMG	O6-C1-O1-C7
30	A	408	LMG	O6-C5-C6-O5
30	a	409	LMG	O6-C5-C6-O5
35	B	626	DGD	O6E-C5E-C6E-O5E
35	C	515	DGD	O6E-C5E-C6E-O5E
35	b	626	DGD	O6E-C5E-C6E-O5E
35	c	515	DGD	O6E-C5E-C6E-O5E
32	A	412	AJP	C38-C39-C41-O42
32	a	413	AJP	C38-C39-C41-O42
25	C	504	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	C4C-C3C-CAC-CBC
25	Y	304	CLA	C4C-C3C-CAC-CBC
25	b	616	CLA	C4C-C3C-CAC-CBC
25	y	304	CLA	C4C-C3C-CAC-CBC
39	N	615	LUT	C9-C10-C11-C12
24	Y	302	CHL	C2C-C3C-CAC-CBC
24	y	302	CHL	C2C-C3C-CAC-CBC
25	G	611	CLA	C2C-C3C-CAC-CBC
25	g	611	CLA	C2C-C3C-CAC-CBC
26	C	517	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
26	c	517	LHG	O9-C7-O7-C5
29	L	101	SQD	O49-C7-O47-C45
29	l	102	SQD	O49-C7-O47-C45
26	B	622	LHG	C1-C2-C3-O3
26	L	102	LHG	C1-C2-C3-O3
26	S	301	LHG	C1-C2-C3-O3
26	b	622	LHG	C1-C2-C3-O3
26	l	103	LHG	C1-C2-C3-O3
26	s	301	LHG	C1-C2-C3-O3
25	C	504	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	N	611	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	n	611	CLA	CBA-CGA-O2A-C1
26	B	622	LHG	C24-C23-O8-C6
26	Y	319	LHG	C24-C23-O8-C6
26	b	622	LHG	C24-C23-O8-C6
26	y	319	LHG	C24-C23-O8-C6
29	L	103	SQD	C10-C11-C12-C13
29	l	101	SQD	C10-C11-C12-C13
24	2	601	CHL	C4-C3-C5-C6
24	6	601	CHL	C4-C3-C5-C6
25	N	610	CLA	C2-C3-C5-C6
25	R	609	CLA	C2-C3-C5-C6
25	n	610	CLA	C2-C3-C5-C6
25	r	609	CLA	C2-C3-C5-C6
25	N	604	CLA	C2C-C3C-CAC-CBC
25	n	604	CLA	C2C-C3C-CAC-CBC
25	N	603	CLA	C3-C5-C6-C7
25	n	603	CLA	C3-C5-C6-C7
24	G	601	CHL	C11-C12-C13-C14
24	G	608	CHL	C11-C10-C8-C9
24	G	608	CHL	C14-C13-C15-C16
24	G	609	CHL	C6-C7-C8-C9
24	N	608	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C12-C13-C14
24	Y	302	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	Y	309	CHL	C11-C10-C8-C9
24	g	601	CHL	C11-C12-C13-C14
24	g	608	CHL	C11-C10-C8-C9
24	g	608	CHL	C14-C13-C15-C16
24	g	609	CHL	C6-C7-C8-C9
24	n	608	CHL	C11-C10-C8-C9
24	n	609	CHL	C11-C12-C13-C14
24	y	302	CHL	C11-C12-C13-C14
24	y	309	CHL	C11-C10-C8-C9
25	A	402	CLA	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	602	CLA	C14-C13-C15-C16
25	B	607	CLA	C14-C13-C15-C16
25	B	608	CLA	C14-C13-C15-C16
25	B	609	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C12-C13-C14
25	B	613	CLA	C14-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	509	CLA	C6-C7-C8-C9
25	C	511	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	S	303	CLA	C11-C10-C8-C9
25	N	602	CLA	C6-C7-C8-C9
25	N	612	CLA	C6-C7-C8-C9
25	N	612	CLA	C11-C10-C8-C9
25	Y	303	CLA	C11-C10-C8-C9
25	Y	304	CLA	C11-C10-C8-C9
25	Y	312	CLA	C6-C7-C8-C9
25	Y	314	CLA	C6-C7-C8-C9
25	R	603	CLA	C11-C10-C8-C9
25	R	608	CLA	C6-C7-C8-C9
25	R	612	CLA	C6-C7-C8-C9
25	a	403	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C14
25	b	602	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C14-C13-C15-C16
25	b	609	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	b	613	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	c	501	CLA	C14-C13-C15-C16
25	c	503	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C12-C13-C14
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C11-C10-C8-C9
25	c	513	CLA	C14-C13-C15-C16
25	s	303	CLA	C11-C10-C8-C9
25	n	602	CLA	C6-C7-C8-C9
25	n	612	CLA	C6-C7-C8-C9
25	n	612	CLA	C11-C10-C8-C9
25	y	303	CLA	C11-C10-C8-C9
25	y	304	CLA	C11-C10-C8-C9
25	y	312	CLA	C6-C7-C8-C9
25	y	314	CLA	C6-C7-C8-C9
25	r	603	CLA	C11-C10-C8-C9
25	r	608	CLA	C6-C7-C8-C9
25	r	612	CLA	C6-C7-C8-C9
27	A	403	PHO	C14-C13-C15-C16
27	a	404	PHO	C14-C13-C15-C16
30	B	620	LMG	C39-C40-C41-C42
29	A	407	SQD	C2-C1-O6-C44
29	a	408	SQD	C2-C1-O6-C44
30	A	408	LMG	C2-C1-O1-C7
30	B	623	LMG	C2-C1-O1-C7
30	a	409	LMG	C2-C1-O1-C7
30	b	623	LMG	C2-C1-O1-C7
30	b	620	LMG	C39-C40-C41-C42
26	L	102	LHG	O2-C2-C3-O3
26	l	103	LHG	O2-C2-C3-O3
26	Y	319	LHG	C29-C30-C31-C32
24	n	607	CHL	O1A-CGA-O2A-C1
25	N	611	CLA	O1A-CGA-O2A-C1
25	n	611	CLA	O1A-CGA-O2A-C1
26	y	319	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	N	607	CHL	O1D-CGD-O2D-CED
24	n	607	CHL	O1D-CGD-O2D-CED
28	H	101	BCR	C37-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C34
28	Z	101	BCR	C11-C12-C13-C35
28	h	101	BCR	C37-C22-C23-C24
28	k	101	BCR	C7-C8-C9-C34
28	z	101	BCR	C11-C12-C13-C35
39	N	615	LUT	C11-C12-C13-C20
39	N	616	LUT	C7-C8-C9-C19
39	Y	317	LUT	C7-C8-C9-C19
39	n	615	LUT	C11-C12-C13-C20
39	n	616	LUT	C7-C8-C9-C19
39	y	317	LUT	C7-C8-C9-C19
40	G	617	NEX	C11-C12-C13-C20
40	N	617	NEX	C27-C28-C29-C39
40	R	617	NEX	C11-C12-C13-C20
40	g	617	NEX	C11-C12-C13-C20
40	n	617	NEX	C27-C28-C29-C39
40	r	617	NEX	C11-C12-C13-C20
28	H	101	BCR	C21-C22-C23-C24
28	h	101	BCR	C21-C22-C23-C24
39	N	615	LUT	C11-C12-C13-C14
39	N	616	LUT	C7-C8-C9-C10
39	n	615	LUT	C11-C12-C13-C14
39	n	616	LUT	C7-C8-C9-C10
26	Y	301	LHG	C23-C24-C25-C26
26	R	618	LHG	C23-C24-C25-C26
26	y	301	LHG	C23-C24-C25-C26
26	r	618	LHG	C23-C24-C25-C26
24	N	607	CHL	O1A-CGA-O2A-C1
25	G	612	CLA	C3-C5-C6-C7
26	2	606	LHG	O9-C7-O7-C5
26	6	606	LHG	O9-C7-O7-C5
24	Y	302	CHL	CBA-CGA-O2A-C1
24	y	302	CHL	CBA-CGA-O2A-C1
24	G	609	CHL	C10-C11-C12-C13
24	g	609	CHL	C10-C11-C12-C13
29	L	103	SQD	C23-C24-C25-C26
29	l	101	SQD	C23-C24-C25-C26
24	G	601	CHL	C2C-C3C-CAC-CBC
24	g	601	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	R	614	CLA	C2C-C3C-CAC-CBC
25	r	614	CLA	C2C-C3C-CAC-CBC
24	R	607	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
25	S	303	CLA	C10-C11-C12-C13
25	Y	304	CLA	C13-C15-C16-C17
25	s	303	CLA	C10-C11-C12-C13
25	y	304	CLA	C13-C15-C16-C17
32	A	412	AJP	O40-C35-O34-C29
32	a	413	AJP	O40-C35-O34-C29
26	N	618	LHG	O1-C1-C2-O2
26	n	618	LHG	O1-C1-C2-O2
25	g	612	CLA	C3-C5-C6-C7
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
25	R	602	CLA	CBD-CGD-O2D-CED
25	R	614	CLA	CBD-CGD-O2D-CED
25	r	602	CLA	CBD-CGD-O2D-CED
25	r	614	CLA	CBD-CGD-O2D-CED
24	R	606	CHL	C2C-C3C-CAC-CBC
24	r	606	CHL	C2C-C3C-CAC-CBC
24	G	601	CHL	C12-C13-C15-C16
24	g	601	CHL	C12-C13-C15-C16
25	B	611	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C12-C13-C15
25	D	403	CLA	C12-C13-C15-C16
25	G	603	CLA	C6-C7-C8-C10
25	Y	313	CLA	C6-C7-C8-C10
25	b	611	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C12-C13-C15
25	d	403	CLA	C12-C13-C15-C16
25	g	603	CLA	C6-C7-C8-C10
25	y	313	CLA	C6-C7-C8-C10
39	S	316	LUT	C13-C14-C15-C35
39	s	316	LUT	C13-C14-C15-C35
39	n	615	LUT	C9-C10-C11-C12
40	N	617	NEX	C33-C34-C35-C15
40	n	617	NEX	C33-C34-C35-C15
30	D	407	LMG	O6-C5-C6-O5
30	d	407	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
24	G	608	CHL	C10-C11-C12-C13
24	g	608	CHL	C10-C11-C12-C13
25	B	616	CLA	C5-C6-C7-C8
25	b	616	CLA	C5-C6-C7-C8
35	C	515	DGD	C2A-C3A-C4A-C5A
35	c	515	DGD	C2A-C3A-C4A-C5A
26	B	625	LHG	C7-C8-C9-C10
26	C	518	LHG	C7-C8-C9-C10
26	b	625	LHG	C7-C8-C9-C10
26	c	518	LHG	C7-C8-C9-C10
30	B	620	LMG	C28-C29-C30-C31
30	b	620	LMG	C28-C29-C30-C31
26	Y	319	LHG	O10-C23-O8-C6
26	y	319	LHG	O10-C23-O8-C6
24	2	601	CHL	C10-C11-C12-C13
24	N	607	CHL	C8-C10-C11-C12
24	Y	302	CHL	C8-C10-C11-C12
24	6	601	CHL	C10-C11-C12-C13
24	n	607	CHL	C8-C10-C11-C12
24	y	302	CHL	C8-C10-C11-C12
25	B	611	CLA	C15-C16-C17-C18
25	B	613	CLA	C13-C15-C16-C17
25	N	603	CLA	C10-C11-C12-C13
25	N	613	CLA	C5-C6-C7-C8
25	b	611	CLA	C15-C16-C17-C18
25	b	613	CLA	C13-C15-C16-C17
25	n	603	CLA	C10-C11-C12-C13
25	n	613	CLA	C5-C6-C7-C8
32	B	624	AJP	C38-C37-O44-C45
32	b	624	AJP	C38-C37-O44-C45
25	y	305	CLA	C4C-C3C-CAC-CBC
32	A	412	AJP	C58-C59-C61-O62
32	a	413	AJP	C58-C59-C61-O62
24	G	608	CHL	C2A-CAA-CBA-CGA
24	Y	306	CHL	C2A-CAA-CBA-CGA
24	g	608	CHL	C2A-CAA-CBA-CGA
24	y	306	CHL	C2A-CAA-CBA-CGA
25	2	602	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C2A-CAA-CBA-CGA
25	G	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	Y	304	CLA	C2A-CAA-CBA-CGA
25	R	609	CLA	C2A-CAA-CBA-CGA
25	R	611	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	g	614	CLA	C2A-CAA-CBA-CGA
25	y	304	CLA	C2A-CAA-CBA-CGA
25	r	609	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
25	Y	305	CLA	C4C-C3C-CAC-CBC
24	G	601	CHL	C8-C10-C11-C12
24	G	608	CHL	C13-C15-C16-C17
24	N	609	CHL	C13-C15-C16-C17
24	g	601	CHL	C8-C10-C11-C12
24	g	608	CHL	C13-C15-C16-C17
24	n	609	CHL	C13-C15-C16-C17
25	B	611	CLA	C13-C15-C16-C17
25	G	612	CLA	C10-C11-C12-C13
25	N	603	CLA	C5-C6-C7-C8
25	Y	314	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	g	612	CLA	C10-C11-C12-C13
25	n	603	CLA	C5-C6-C7-C8
25	y	314	CLA	C13-C15-C16-C17
26	C	519	LHG	C23-C24-C25-C26
26	c	519	LHG	C23-C24-C25-C26
29	L	101	SQD	C23-C24-C25-C26
29	l	102	SQD	C23-C24-C25-C26
30	B	623	LMG	C28-C29-C30-C31
30	b	623	LMG	C28-C29-C30-C31
26	B	622	LHG	O10-C23-O8-C6
26	b	622	LHG	O10-C23-O8-C6
25	2	604	CLA	C3-C5-C6-C7
25	B	607	CLA	C3-C5-C6-C7
25	6	604	CLA	C3-C5-C6-C7
25	b	607	CLA	C3-C5-C6-C7
26	S	301	LHG	C14-C15-C16-C17
26	s	301	LHG	C14-C15-C16-C17
24	G	608	CHL	C5-C6-C7-C8
24	N	601	CHL	C5-C6-C7-C8
24	N	607	CHL	C10-C11-C12-C13
24	g	608	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	n	601	CHL	C5-C6-C7-C8
24	n	607	CHL	C10-C11-C12-C13
25	A	405	CLA	C10-C11-C12-C13
25	B	601	CLA	C10-C11-C12-C13
25	B	607	CLA	C8-C10-C11-C12
25	B	614	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8
25	D	403	CLA	C10-C11-C12-C13
25	S	310	CLA	C5-C6-C7-C8
25	N	602	CLA	C5-C6-C7-C8
25	N	602	CLA	C8-C10-C11-C12
25	Y	311	CLA	C8-C10-C11-C12
25	a	406	CLA	C10-C11-C12-C13
25	b	601	CLA	C10-C11-C12-C13
25	b	607	CLA	C8-C10-C11-C12
25	b	614	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
25	d	403	CLA	C10-C11-C12-C13
25	s	310	CLA	C5-C6-C7-C8
25	n	602	CLA	C5-C6-C7-C8
25	n	602	CLA	C8-C10-C11-C12
25	y	311	CLA	C8-C10-C11-C12
26	N	618	LHG	O2-C2-C3-O3
26	n	618	LHG	O2-C2-C3-O3
30	B	623	LMG	C29-C28-O8-C9
30	b	623	LMG	C29-C28-O8-C9
26	2	606	LHG	C23-C24-C25-C26
26	B	622	LHG	C7-C8-C9-C10
26	6	606	LHG	C23-C24-C25-C26
26	b	622	LHG	C7-C8-C9-C10
25	Y	313	CLA	C10-C11-C12-C13
25	y	313	CLA	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
25	S	303	CLA	C8-C10-C11-C12
25	c	507	CLA	C13-C15-C16-C17
25	s	303	CLA	C8-C10-C11-C12
26	B	621	LHG	C7-C8-C9-C10
26	b	621	LHG	C7-C8-C9-C10
26	y	319	LHG	C33-C34-C35-C36
25	Y	305	CLA	O1D-CGD-O2D-CED
25	y	305	CLA	O1D-CGD-O2D-CED
26	Y	319	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C5-C6-C7-C8
25	B	610	CLA	C15-C16-C17-C18
25	C	510	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
25	b	610	CLA	C15-C16-C17-C18
25	c	510	CLA	C13-C15-C16-C17
25	N	612	CLA	CBD-CGD-O2D-CED
25	n	612	CLA	CBD-CGD-O2D-CED
29	A	411	SQD	C8-C7-O47-C45
29	a	412	SQD	C8-C7-O47-C45
35	C	516	DGD	O6D-C5D-C6D-O5D
35	c	516	DGD	O6D-C5D-C6D-O5D
25	G	602	CLA	C10-C11-C12-C13
25	g	602	CLA	C10-C11-C12-C13
29	A	411	SQD	O49-C7-O47-C45
29	a	412	SQD	O49-C7-O47-C45
26	N	618	LHG	C1-C2-C3-O3
26	n	618	LHG	C1-C2-C3-O3
24	1	301	CHL	C2A-CAA-CBA-CGA
24	5	301	CHL	C2A-CAA-CBA-CGA
25	S	303	CLA	C2A-CAA-CBA-CGA
25	N	613	CLA	C2A-CAA-CBA-CGA
25	Y	311	CLA	C2A-CAA-CBA-CGA
25	R	601	CLA	C2A-CAA-CBA-CGA
25	R	602	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	R	614	CLA	C2A-CAA-CBA-CGA
25	s	303	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
25	y	311	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
25	r	610	CLA	C2A-CAA-CBA-CGA
25	r	614	CLA	C2A-CAA-CBA-CGA
24	G	601	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
26	S	301	LHG	C31-C32-C33-C34
26	s	301	LHG	C31-C32-C33-C34
24	Y	310	CHL	C5-C6-C7-C8
24	y	310	CHL	C5-C6-C7-C8
25	D	402	CLA	C15-C16-C17-C18
25	N	613	CLA	C10-C11-C12-C13
25	Y	303	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	Y	304	CLA	C10-C11-C12-C13
25	Y	311	CLA	C5-C6-C7-C8
25	R	603	CLA	C8-C10-C11-C12
25	d	402	CLA	C15-C16-C17-C18
25	n	613	CLA	C10-C11-C12-C13
25	y	303	CLA	C10-C11-C12-C13
25	y	304	CLA	C10-C11-C12-C13
25	y	311	CLA	C5-C6-C7-C8
25	r	603	CLA	C8-C10-C11-C12
25	R	601	CLA	CBD-CGD-O2D-CED
25	r	601	CLA	CBD-CGD-O2D-CED
24	G	601	CHL	C10-C11-C12-C13
24	N	609	CHL	C8-C10-C11-C12
24	Y	309	CHL	C8-C10-C11-C12
24	g	601	CHL	C10-C11-C12-C13
24	n	609	CHL	C8-C10-C11-C12
24	y	309	CHL	C8-C10-C11-C12
25	B	607	CLA	C10-C11-C12-C13
25	B	607	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	C	513	CLA	C8-C10-C11-C12
25	N	612	CLA	C5-C6-C7-C8
25	Y	313	CLA	C8-C10-C11-C12
25	b	607	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
25	b	611	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	c	513	CLA	C8-C10-C11-C12
25	n	612	CLA	C5-C6-C7-C8
25	y	313	CLA	C8-C10-C11-C12
25	A	401	CLA	C2C-C3C-CAC-CBC
25	N	603	CLA	C2C-C3C-CAC-CBC
25	a	402	CLA	C2C-C3C-CAC-CBC
25	n	603	CLA	C2C-C3C-CAC-CBC
32	B	624	AJP	O60-C59-C61-O62
32	b	624	AJP	O60-C59-C61-O62
24	Y	309	CHL	C13-C15-C16-C17
24	y	309	CHL	C13-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
25	B	616	CLA	C13-C15-C16-C17
25	C	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	G	610	CLA	C8-C10-C11-C12
25	R	608	CLA	C8-C10-C11-C12
25	R	612	CLA	C10-C11-C12-C13
25	b	609	CLA	C15-C16-C17-C18
25	b	616	CLA	C13-C15-C16-C17
25	c	510	CLA	C15-C16-C17-C18
25	r	608	CLA	C8-C10-C11-C12
25	r	612	CLA	C10-C11-C12-C13
25	S	310	CLA	C4-C3-C5-C6
25	s	310	CLA	C4-C3-C5-C6
35	C	516	DGD	C4D-C5D-C6D-O5D
35	c	516	DGD	C4D-C5D-C6D-O5D
25	B	604	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
25	g	610	CLA	C8-C10-C11-C12
30	A	410	LMG	O6-C5-C6-O5
30	a	411	LMG	O6-C5-C6-O5
35	C	516	DGD	C8B-C9B-CAB-CBB
35	c	516	DGD	C8B-C9B-CAB-CBB
26	Y	319	LHG	C23-C24-C25-C26
26	y	319	LHG	C23-C24-C25-C26
26	Y	301	LHG	O2-C2-C3-O3
26	Y	319	LHG	O2-C2-C3-O3
26	y	301	LHG	O2-C2-C3-O3
26	y	319	LHG	O2-C2-C3-O3
25	C	504	CLA	C11-C12-C13-C14
25	G	613	CLA	C16-C17-C18-C19
25	R	609	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	g	613	CLA	C16-C17-C18-C19
25	r	609	CLA	C16-C17-C18-C20
30	D	407	LMG	C31-C32-C33-C34
30	d	407	LMG	C31-C32-C33-C34
25	G	613	CLA	C15-C16-C17-C18
28	H	101	BCR	C20-C21-C22-C37
28	T	101	BCR	C35-C13-C14-C15
28	h	101	BCR	C20-C21-C22-C37
28	t	101	BCR	C35-C13-C14-C15
25	g	613	CLA	C15-C16-C17-C18
28	T	101	BCR	C11-C12-C13-C14
28	t	101	BCR	C11-C12-C13-C14
39	Y	317	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
39	y	317	LUT	C7-C8-C9-C10
40	G	617	NEX	C11-C12-C13-C14
40	g	617	NEX	C11-C12-C13-C14
24	Y	310	CHL	O1A-CGA-O2A-C1
24	y	310	CHL	O1A-CGA-O2A-C1
26	c	517	LHG	C10-C11-C12-C13
25	B	606	CLA	C2A-CAA-CBA-CGA
25	S	312	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2A-CAA-CBA-CGA
25	Y	314	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	s	312	CLA	C2A-CAA-CBA-CGA
25	g	611	CLA	C2A-CAA-CBA-CGA
25	y	314	CLA	C2A-CAA-CBA-CGA
25	r	601	CLA	C2A-CAA-CBA-CGA
25	C	504	CLA	C5-C6-C7-C8
25	c	504	CLA	C5-C6-C7-C8
26	C	517	LHG	C10-C11-C12-C13
26	B	621	LHG	O1-C1-C2-C3
26	B	625	LHG	O1-C1-C2-C3
26	C	519	LHG	O1-C1-C2-C3
26	b	621	LHG	O1-C1-C2-C3
26	b	625	LHG	O1-C1-C2-C3
26	c	519	LHG	O1-C1-C2-C3
26	C	519	LHG	C4-C5-O7-C7
26	c	519	LHG	C4-C5-O7-C7
24	Y	302	CHL	C16-C17-C18-C19
24	y	302	CHL	C16-C17-C18-C19
25	B	608	CLA	C16-C17-C18-C19
25	N	612	CLA	C11-C12-C13-C14
25	b	608	CLA	C16-C17-C18-C19
25	n	612	CLA	C11-C12-C13-C14
25	y	313	CLA	C11-C12-C13-C15
24	n	609	CHL	O1D-CGD-O2D-CED
25	B	607	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	O1A-CGA-O2A-C1
28	T	101	BCR	C20-C21-C22-C23
28	t	101	BCR	C20-C21-C22-C23
24	N	609	CHL	O1D-CGD-O2D-CED
30	A	410	LMG	C35-C36-C37-C38
30	a	411	LMG	C35-C36-C37-C38
26	C	517	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	c	517	LHG	C24-C23-O8-C6
24	G	608	CHL	C8-C10-C11-C12
30	C	520	LMG	O6-C5-C6-O5
25	C	503	CLA	O1D-CGD-O2D-CED
25	A	405	CLA	C11-C12-C13-C14
25	B	612	CLA	C16-C17-C18-C20
25	C	504	CLA	C11-C12-C13-C15
25	G	613	CLA	C16-C17-C18-C20
25	Y	313	CLA	C11-C12-C13-C15
25	a	406	CLA	C11-C12-C13-C14
25	b	612	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C15
25	g	613	CLA	C16-C17-C18-C20
24	g	608	CHL	C8-C10-C11-C12
25	c	503	CLA	O1D-CGD-O2D-CED
30	B	623	LMG	C8-C9-O8-C28
30	b	623	LMG	C8-C9-O8-C28
26	B	625	LHG	C25-C26-C27-C28
26	b	625	LHG	C25-C26-C27-C28
25	G	614	CLA	CBD-CGD-O2D-CED
25	g	614	CLA	CBD-CGD-O2D-CED
26	S	301	LHG	C26-C27-C28-C29
29	A	407	SQD	C11-C12-C13-C14
29	L	103	SQD	C11-C10-C9-C8
29	L	103	SQD	C9-C10-C11-C12
29	a	408	SQD	C11-C12-C13-C14
29	l	101	SQD	C9-C10-C11-C12
30	D	407	LMG	C13-C14-C15-C16
30	d	407	LMG	C13-C14-C15-C16
30	c	520	LMG	O6-C5-C6-O5
26	2	606	LHG	C15-C16-C17-C18
26	D	406	LHG	C33-C34-C35-C36
26	L	102	LHG	C27-C28-C29-C30
26	N	618	LHG	C27-C28-C29-C30
26	6	606	LHG	C15-C16-C17-C18
26	d	406	LHG	C33-C34-C35-C36
26	l	103	LHG	C27-C28-C29-C30
26	s	301	LHG	C26-C27-C28-C29
26	n	618	LHG	C26-C27-C28-C29
29	l	101	SQD	C11-C10-C9-C8
30	A	408	LMG	C30-C31-C32-C33
30	a	409	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	B	623	LMG	O10-C28-O8-C9
30	b	623	LMG	O10-C28-O8-C9
26	C	517	LHG	C34-C35-C36-C37
26	N	618	LHG	C26-C27-C28-C29
26	Y	319	LHG	C13-C14-C15-C16
26	c	517	LHG	C34-C35-C36-C37
26	n	618	LHG	C27-C28-C29-C30
26	y	319	LHG	C13-C14-C15-C16
30	A	410	LMG	C37-C38-C39-C40
30	a	411	LMG	C37-C38-C39-C40
35	C	515	DGD	C5A-C6A-C7A-C8A
35	c	515	DGD	C5A-C6A-C7A-C8A
26	S	301	LHG	O1-C1-C2-O2
26	S	318	LHG	O1-C1-C2-O2
26	Y	319	LHG	O1-C1-C2-O2
26	s	301	LHG	O1-C1-C2-O2
26	s	318	LHG	O1-C1-C2-O2
26	y	319	LHG	O1-C1-C2-O2
30	B	623	LMG	C31-C32-C33-C34
30	D	407	LMG	C12-C13-C14-C15
30	b	623	LMG	C31-C32-C33-C34
30	d	407	LMG	C12-C13-C14-C15
35	C	515	DGD	C4A-C5A-C6A-C7A
35	c	515	DGD	C4A-C5A-C6A-C7A
35	c	515	DGD	C7B-C8B-C9B-CAB
32	Y	320	AJP	C27-C26-O25-C23
32	y	320	AJP	C27-C26-O25-C23
25	2	602	CLA	C4B-C3B-CAB-CBB
25	2	604	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C4B-C3B-CAB-CBB
25	C	509	CLA	C4B-C3B-CAB-CBB
25	D	401	CLA	C4B-C3B-CAB-CBB
25	G	602	CLA	C4B-C3B-CAB-CBB
25	N	602	CLA	C4B-C3B-CAB-CBB
25	N	613	CLA	C4B-C3B-CAB-CBB
25	6	602	CLA	C4B-C3B-CAB-CBB
25	6	604	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	c	509	CLA	C4B-C3B-CAB-CBB
25	d	401	CLA	C4B-C3B-CAB-CBB
25	g	602	CLA	C4B-C3B-CAB-CBB
25	n	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	n	613	CLA	C4B-C3B-CAB-CBB
26	D	406	LHG	C7-C8-C9-C10
26	d	406	LHG	C7-C8-C9-C10
35	C	516	DGD	C1A-C2A-C3A-C4A
35	c	516	DGD	C1A-C2A-C3A-C4A
26	Y	319	LHG	C11-C12-C13-C14
26	y	319	LHG	C11-C12-C13-C14
35	C	515	DGD	C7B-C8B-C9B-CAB
25	B	608	CLA	C16-C17-C18-C20
25	b	608	CLA	C16-C17-C18-C20
24	S	307	CHL	O1D-CGD-O2D-CED
24	s	307	CHL	O1D-CGD-O2D-CED
26	Y	301	LHG	C26-C27-C28-C29
26	y	301	LHG	C26-C27-C28-C29
25	2	602	CLA	C8-C10-C11-C12
25	6	602	CLA	C8-C10-C11-C12
26	Y	301	LHG	C8-C7-O7-C5
26	y	301	LHG	C8-C7-O7-C5
35	C	516	DGD	CBB-CCB-CDB-CEB
35	c	516	DGD	CBB-CCB-CDB-CEB
24	2	603	CHL	C2C-C3C-CAC-CBC
24	R	613	CHL	C2C-C3C-CAC-CBC
24	6	603	CHL	C2C-C3C-CAC-CBC
25	B	602	CLA	C11-C12-C13-C15
25	B	610	CLA	C11-C10-C8-C7
25	G	602	CLA	C11-C10-C8-C7
25	Y	304	CLA	C6-C7-C8-C10
25	b	610	CLA	C11-C10-C8-C7
25	g	602	CLA	C11-C10-C8-C7
25	y	304	CLA	C6-C7-C8-C10
26	B	622	LHG	C18-C19-C20-C21
26	b	622	LHG	C18-C19-C20-C21
26	S	318	LHG	O2-C2-C3-O3
26	s	318	LHG	O2-C2-C3-O3
25	C	506	CLA	C13-C15-C16-C17
25	c	506	CLA	C13-C15-C16-C17
26	2	606	LHG	C14-C15-C16-C17
26	6	606	LHG	C14-C15-C16-C17
29	A	411	SQD	C11-C12-C13-C14
29	A	411	SQD	C12-C13-C14-C15
29	a	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	O1A-CGA-O2A-C1
25	b	610	CLA	O1A-CGA-O2A-C1
25	A	405	CLA	C3-C5-C6-C7
25	a	406	CLA	C3-C5-C6-C7
24	2	603	CHL	C3A-C2A-CAA-CBA
24	G	607	CHL	C3A-C2A-CAA-CBA
24	N	608	CHL	C3A-C2A-CAA-CBA
24	Y	309	CHL	C3A-C2A-CAA-CBA
24	R	605	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	6	603	CHL	C3A-C2A-CAA-CBA
24	g	607	CHL	C3A-C2A-CAA-CBA
24	n	608	CHL	C3A-C2A-CAA-CBA
24	y	309	CHL	C3A-C2A-CAA-CBA
24	r	605	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA
25	S	303	CLA	C3A-C2A-CAA-CBA
25	Y	304	CLA	C3A-C2A-CAA-CBA
25	Y	315	CLA	C3A-C2A-CAA-CBA
25	R	609	CLA	C3A-C2A-CAA-CBA
25	R	614	CLA	C3A-C2A-CAA-CBA
25	s	303	CLA	C3A-C2A-CAA-CBA
25	y	304	CLA	C3A-C2A-CAA-CBA
25	y	315	CLA	C3A-C2A-CAA-CBA
25	r	609	CLA	C3A-C2A-CAA-CBA
25	r	614	CLA	C3A-C2A-CAA-CBA
24	r	613	CHL	C2C-C3C-CAC-CBC
26	B	621	LHG	C26-C27-C28-C29
26	b	621	LHG	C26-C27-C28-C29
29	L	101	SQD	C27-C28-C29-C30
29	l	102	SQD	C27-C28-C29-C30
30	B	623	LMG	C32-C33-C34-C35
30	b	623	LMG	C32-C33-C34-C35
25	C	508	CLA	C13-C15-C16-C17
25	D	402	CLA	C13-C15-C16-C17
25	c	508	CLA	C13-C15-C16-C17
25	d	402	CLA	C13-C15-C16-C17
24	Y	306	CHL	C2C-C3C-CAC-CBC
24	y	306	CHL	C2C-C3C-CAC-CBC
25	N	613	CLA	C11-C12-C13-C14
25	n	613	CLA	C11-C12-C13-C14
26	L	102	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	l	103	LHG	C30-C31-C32-C33
24	R	605	CHL	CBD-CGD-O2D-CED
24	r	605	CHL	CBD-CGD-O2D-CED
26	R	618	LHG	C9-C10-C11-C12
26	r	618	LHG	C9-C10-C11-C12
30	C	520	LMG	C16-C17-C18-C19
30	c	520	LMG	C16-C17-C18-C19
26	S	301	LHG	C4-C5-C6-O8
26	s	301	LHG	C4-C5-C6-O8
26	B	622	LHG	C12-C13-C14-C15
26	B	622	LHG	C13-C14-C15-C16
26	C	519	LHG	C28-C29-C30-C31
26	b	622	LHG	C12-C13-C14-C15
26	b	622	LHG	C13-C14-C15-C16
26	c	519	LHG	C28-C29-C30-C31
26	d	406	LHG	C32-C33-C34-C35
25	g	611	CLA	C3-C5-C6-C7
26	S	301	LHG	C7-C8-C9-C10
26	s	301	LHG	C7-C8-C9-C10
26	B	621	LHG	C32-C33-C34-C35
26	D	406	LHG	C32-C33-C34-C35
26	b	621	LHG	C32-C33-C34-C35
29	L	103	SQD	C32-C33-C34-C35
29	l	101	SQD	C32-C33-C34-C35
35	B	626	DGD	CBB-CCB-CDB-CEB
35	b	626	DGD	CBB-CCB-CDB-CEB
26	B	625	LHG	C10-C11-C12-C13
26	b	625	LHG	C10-C11-C12-C13
30	B	620	LMG	C18-C19-C20-C21
30	a	409	LMG	C16-C17-C18-C19
30	b	620	LMG	C18-C19-C20-C21
30	A	408	LMG	C16-C17-C18-C19
35	C	516	DGD	O6E-C5E-C6E-O5E
35	c	516	DGD	O6E-C5E-C6E-O5E
35	B	626	DGD	C4E-C5E-C6E-O5E
35	b	626	DGD	C4E-C5E-C6E-O5E
26	S	318	LHG	C10-C11-C12-C13
26	s	318	LHG	C10-C11-C12-C13
29	A	411	SQD	C16-C17-C18-C19
29	a	412	SQD	C16-C17-C18-C19
35	B	626	DGD	C7B-C8B-C9B-CAB
35	b	626	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
25	R	609	CLA	C16-C17-C18-C19
25	r	609	CLA	C16-C17-C18-C19
29	A	411	SQD	C23-C24-C25-C26
29	a	412	SQD	C23-C24-C25-C26
25	S	309	CLA	C2B-C3B-CAB-CBB
25	N	611	CLA	C2B-C3B-CAB-CBB
25	R	611	CLA	C2B-C3B-CAB-CBB
25	s	309	CLA	C2B-C3B-CAB-CBB
25	n	611	CLA	C2B-C3B-CAB-CBB
25	r	611	CLA	C2B-C3B-CAB-CBB
28	B	617	BCR	C1-C6-C7-C8
28	B	617	BCR	C5-C6-C7-C8
28	T	101	BCR	C23-C24-C25-C26
28	T	101	BCR	C23-C24-C25-C30
28	b	617	BCR	C1-C6-C7-C8
28	b	617	BCR	C5-C6-C7-C8
28	t	101	BCR	C23-C24-C25-C26
28	t	101	BCR	C23-C24-C25-C30
39	N	615	LUT	C1-C6-C7-C8
39	N	615	LUT	C5-C6-C7-C8
39	N	616	LUT	C1-C6-C7-C8
39	n	615	LUT	C1-C6-C7-C8
39	n	615	LUT	C5-C6-C7-C8
39	n	616	LUT	C1-C6-C7-C8
30	A	408	LMG	C34-C35-C36-C37
30	a	409	LMG	C34-C35-C36-C37
30	D	407	LMG	C11-C10-O7-C8
30	d	407	LMG	C11-C10-O7-C8
25	G	611	CLA	C3-C5-C6-C7
26	S	318	LHG	C17-C18-C19-C20
26	6	606	LHG	C30-C31-C32-C33
26	s	318	LHG	C17-C18-C19-C20
26	2	606	LHG	C30-C31-C32-C33
26	S	318	LHG	C33-C34-C35-C36
26	N	618	LHG	C32-C33-C34-C35
26	s	318	LHG	C33-C34-C35-C36
35	C	516	DGD	CAB-CBB-CCB-CDB
35	b	626	DGD	CBA-CCA-CDA-CEA
35	c	516	DGD	CAB-CBB-CCB-CDB
25	C	513	CLA	C2A-CAA-CBA-CGA
25	S	310	CLA	C2A-CAA-CBA-CGA
25	N	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C2A-CAA-CBA-CGA
25	s	310	CLA	C2A-CAA-CBA-CGA
25	n	610	CLA	C2A-CAA-CBA-CGA
30	D	407	LMG	C28-C29-C30-C31
30	d	407	LMG	C28-C29-C30-C31
25	B	610	CLA	C13-C15-C16-C17
25	b	610	CLA	C13-C15-C16-C17
26	B	621	LHG	C27-C28-C29-C30
26	b	621	LHG	C27-C28-C29-C30
26	n	618	LHG	C32-C33-C34-C35
29	L	103	SQD	C13-C14-C15-C16
29	l	101	SQD	C13-C14-C15-C16
35	B	626	DGD	CBA-CCA-CDA-CEA
26	C	517	LHG	O10-C23-O8-C6
26	c	517	LHG	O10-C23-O8-C6
31	D	405	PL9	C4-C3-C7-C8
31	d	405	PL9	C4-C3-C7-C8
30	B	623	LMG	C33-C34-C35-C36
30	b	623	LMG	C33-C34-C35-C36
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
25	G	610	CLA	C2-C3-C5-C6
25	Y	311	CLA	C2-C3-C5-C6
25	g	610	CLA	C2-C3-C5-C6
25	y	311	CLA	C2-C3-C5-C6
31	A	409	PL9	C2-C3-C7-C8
31	a	410	PL9	C2-C3-C7-C8
26	L	102	LHG	C29-C30-C31-C32
26	l	103	LHG	C29-C30-C31-C32
29	L	103	SQD	C26-C27-C28-C29
29	l	101	SQD	C26-C27-C28-C29
24	y	309	CHL	O1A-CGA-O2A-C1
25	N	603	CLA	C6-C7-C8-C9
25	n	603	CLA	C6-C7-C8-C9
25	B	602	CLA	C8-C10-C11-C12
25	b	602	CLA	C8-C10-C11-C12
35	A	415	DGD	C8B-C9B-CAB-CBB
35	a	401	DGD	C8B-C9B-CAB-CBB
30	A	408	LMG	C36-C37-C38-C39
30	a	409	LMG	C36-C37-C38-C39
25	G	603	CLA	C5-C6-C7-C8
25	g	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	Y	309	CHL	O1A-CGA-O2A-C1
26	B	621	LHG	C25-C26-C27-C28
26	C	518	LHG	C32-C33-C34-C35
26	b	621	LHG	C25-C26-C27-C28
26	c	518	LHG	C32-C33-C34-C35
26	n	618	LHG	C15-C16-C17-C18
35	C	516	DGD	C8A-C9A-CAA-CBA
35	c	516	DGD	C8A-C9A-CAA-CBA
26	N	618	LHG	C15-C16-C17-C18
26	S	318	LHG	C12-C13-C14-C15
26	s	318	LHG	C12-C13-C14-C15
25	A	401	CLA	C15-C16-C17-C18
25	B	605	CLA	C5-C6-C7-C8
25	a	402	CLA	C15-C16-C17-C18
25	b	605	CLA	C5-C6-C7-C8
24	R	607	CHL	C11-C12-C13-C14
24	r	607	CHL	C11-C12-C13-C14
25	R	602	CLA	C11-C12-C13-C15
25	r	602	CLA	C11-C12-C13-C15
26	2	606	LHG	C12-C13-C14-C15
26	6	606	LHG	C12-C13-C14-C15
30	B	623	LMG	C16-C17-C18-C19
30	b	623	LMG	C16-C17-C18-C19
26	L	102	LHG	C28-C29-C30-C31
26	l	103	LHG	C28-C29-C30-C31
35	B	626	DGD	CCB-CDB-CEB-CFB
35	C	516	DGD	C3B-C4B-C5B-C6B
35	b	626	DGD	CCB-CDB-CEB-CFB
35	c	516	DGD	C3B-C4B-C5B-C6B
25	G	611	CLA	C4C-C3C-CAC-CBC
25	g	611	CLA	C4C-C3C-CAC-CBC
25	G	603	CLA	C10-C11-C12-C13
25	g	603	CLA	C10-C11-C12-C13
35	A	415	DGD	C1B-C2B-C3B-C4B
35	a	401	DGD	C1B-C2B-C3B-C4B
24	N	605	CHL	C2A-CAA-CBA-CGA
24	n	605	CHL	C2A-CAA-CBA-CGA
25	R	602	CLA	C11-C12-C13-C14
25	R	603	CLA	C11-C12-C13-C14
25	r	602	CLA	C11-C12-C13-C14
25	r	603	CLA	C11-C12-C13-C14
29	A	411	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C29-C30-C31-C32
25	Y	304	CLA	C4-C3-C5-C6
25	Y	312	CLA	C4-C3-C5-C6
25	y	304	CLA	C4-C3-C5-C6
25	y	312	CLA	C4-C3-C5-C6
26	S	318	LHG	C11-C12-C13-C14
25	N	604	CLA	C4C-C3C-CAC-CBC
32	G	618	AJP	C27-C26-O25-C23
32	g	618	AJP	C27-C26-O25-C23
26	s	318	LHG	C11-C12-C13-C14
25	G	613	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
24	Y	309	CHL	C10-C11-C12-C13
24	y	309	CHL	C10-C11-C12-C13
25	C	511	CLA	C10-C11-C12-C13
25	G	611	CLA	C8-C10-C11-C12
25	R	609	CLA	C13-C15-C16-C17
25	c	511	CLA	C10-C11-C12-C13
25	g	611	CLA	C8-C10-C11-C12
25	r	609	CLA	C13-C15-C16-C17
26	L	102	LHG	O6-C4-C5-O7
26	l	103	LHG	O6-C4-C5-O7
26	n	618	LHG	C34-C35-C36-C37
26	y	319	LHG	C24-C25-C26-C27
26	L	102	LHG	C8-C7-O7-C5
26	l	103	LHG	C8-C7-O7-C5
24	N	608	CHL	C15-C16-C17-C18
24	n	608	CHL	C15-C16-C17-C18
25	n	604	CLA	C4C-C3C-CAC-CBC
26	N	618	LHG	C34-C35-C36-C37
26	Y	319	LHG	C24-C25-C26-C27
35	A	415	DGD	C8A-C9A-CAA-CBA
35	a	401	DGD	C8A-C9A-CAA-CBA
26	C	519	LHG	C25-C26-C27-C28
26	c	519	LHG	C25-C26-C27-C28
30	D	407	LMG	C29-C30-C31-C32
30	d	407	LMG	C29-C30-C31-C32
26	s	318	LHG	C23-C24-C25-C26
25	C	513	CLA	C5-C6-C7-C8
25	c	513	CLA	C5-C6-C7-C8
27	A	403	PHO	C13-C15-C16-C17
27	a	404	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	B	621	LHG	C24-C25-C26-C27
26	b	621	LHG	C24-C25-C26-C27
30	B	623	LMG	C11-C12-C13-C14
30	b	623	LMG	C11-C12-C13-C14
26	S	301	LHG	O7-C5-C6-O8
26	s	301	LHG	O7-C5-C6-O8
29	A	411	SQD	O6-C44-C45-O47
29	a	412	SQD	O6-C44-C45-O47
25	r	614	CLA	C4C-C3C-CAC-CBC
30	b	623	LMG	C30-C31-C32-C33
25	C	512	CLA	O1A-CGA-O2A-C1
26	C	517	LHG	C27-C28-C29-C30
26	C	519	LHG	C9-C10-C11-C12
26	c	519	LHG	C9-C10-C11-C12
30	B	623	LMG	C30-C31-C32-C33
26	S	318	LHG	C23-C24-C25-C26
32	A	412	AJP	C68-C69-C71-O72
32	a	413	AJP	C68-C69-C71-O72
26	c	517	LHG	C27-C28-C29-C30
29	L	103	SQD	C12-C13-C14-C15
29	l	101	SQD	C12-C13-C14-C15
35	C	515	DGD	C6B-C7B-C8B-C9B
35	c	515	DGD	C6B-C7B-C8B-C9B
25	R	614	CLA	C4C-C3C-CAC-CBC
26	s	301	LHG	C24-C25-C26-C27
24	N	608	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
25	N	613	CLA	C11-C12-C13-C15
25	n	613	CLA	C11-C12-C13-C15
26	S	301	LHG	C24-C25-C26-C27
32	B	624	AJP	C56-C57-O64-C65
32	b	624	AJP	C56-C57-O64-C65
30	A	408	LMG	C13-C14-C15-C16
30	a	409	LMG	C13-C14-C15-C16
26	Y	301	LHG	O9-C7-O7-C5
26	y	301	LHG	O9-C7-O7-C5
26	S	318	LHG	C1-C2-C3-O3
26	Y	319	LHG	C1-C2-C3-O3
26	s	318	LHG	C1-C2-C3-O3
26	y	319	LHG	C1-C2-C3-O3
24	n	607	CHL	C13-C15-C16-C17
25	n	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	C	518	LHG	C31-C32-C33-C34
26	L	102	LHG	C31-C32-C33-C34
26	c	518	LHG	C31-C32-C33-C34
26	l	103	LHG	C31-C32-C33-C34
25	2	605	CLA	C2A-CAA-CBA-CGA
25	6	605	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
26	L	102	LHG	C34-C35-C36-C37
26	l	103	LHG	C34-C35-C36-C37
24	N	607	CHL	C13-C15-C16-C17
25	C	508	CLA	C15-C16-C17-C18
25	N	602	CLA	C10-C11-C12-C13
25	N	613	CLA	C8-C10-C11-C12
25	n	613	CLA	C8-C10-C11-C12
30	C	520	LMG	C11-C12-C13-C14
30	c	520	LMG	C11-C12-C13-C14
25	c	508	CLA	C15-C16-C17-C18
25	c	512	CLA	O1A-CGA-O2A-C1
24	2	601	CHL	C3-C5-C6-C7
24	G	601	CHL	C3-C5-C6-C7
24	6	601	CHL	C3-C5-C6-C7
24	g	601	CHL	C3-C5-C6-C7
32	B	624	AJP	C58-C57-O64-C65
32	b	624	AJP	C58-C57-O64-C65
25	A	402	CLA	C1A-C2A-CAA-CBA
25	B	611	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C1A-C2A-CAA-CBA
25	S	305	CLA	C1A-C2A-CAA-CBA
25	S	310	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C1A-C2A-CAA-CBA
25	G	610	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	Y	304	CLA	C1A-C2A-CAA-CBA
25	Y	311	CLA	C1A-C2A-CAA-CBA
25	Y	314	CLA	C1A-C2A-CAA-CBA
25	R	604	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C1A-C2A-CAA-CBA
25	a	403	CLA	C1A-C2A-CAA-CBA
25	b	611	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	s	305	CLA	C1A-C2A-CAA-CBA
25	s	310	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C1A-C2A-CAA-CBA
25	g	610	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	y	304	CLA	C1A-C2A-CAA-CBA
25	y	311	CLA	C1A-C2A-CAA-CBA
25	y	314	CLA	C1A-C2A-CAA-CBA
25	r	604	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C1A-C2A-CAA-CBA
30	B	623	LMG	C19-C20-C21-C22
30	b	623	LMG	C19-C20-C21-C22
29	L	103	SQD	C27-C28-C29-C30
29	l	101	SQD	C27-C28-C29-C30
26	D	406	LHG	C26-C27-C28-C29
26	d	406	LHG	C26-C27-C28-C29
25	B	602	CLA	C5-C6-C7-C8
25	b	602	CLA	C5-C6-C7-C8
26	S	301	LHG	O6-C4-C5-C6
26	N	618	LHG	O6-C4-C5-C6
26	s	301	LHG	O6-C4-C5-C6
26	n	618	LHG	O6-C4-C5-C6
30	D	407	LMG	O9-C10-O7-C8
30	d	407	LMG	O9-C10-O7-C8
24	G	608	CHL	C11-C10-C8-C7
24	Y	309	CHL	C12-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C7
24	y	309	CHL	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	B	604	CLA	C6-C7-C8-C10
25	B	613	CLA	C12-C13-C15-C16
25	C	509	CLA	C6-C7-C8-C10
25	C	511	CLA	C11-C10-C8-C7
25	C	511	CLA	C11-C12-C13-C15
25	C	512	CLA	C12-C13-C15-C16
25	S	303	CLA	C6-C7-C8-C10
25	G	610	CLA	C12-C13-C15-C16
25	N	603	CLA	C11-C10-C8-C7
25	R	603	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C6-C7-C8-C10
25	b	613	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
25	c	511	CLA	C11-C10-C8-C7
25	c	511	CLA	C11-C12-C13-C15
25	c	512	CLA	C12-C13-C15-C16
25	s	303	CLA	C6-C7-C8-C10
25	g	610	CLA	C12-C13-C15-C16
25	n	603	CLA	C11-C10-C8-C7
25	r	603	CLA	C6-C7-C8-C10
26	C	519	LHG	C30-C31-C32-C33
26	c	519	LHG	C30-C31-C32-C33
25	B	603	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C20
25	c	513	CLA	C16-C17-C18-C19
24	G	601	CHL	C13-C15-C16-C17
24	g	601	CHL	C13-C15-C16-C17
25	C	506	CLA	C10-C11-C12-C13
25	c	506	CLA	C10-C11-C12-C13
26	C	519	LHG	C12-C13-C14-C15
30	B	623	LMG	C17-C18-C19-C20
30	b	623	LMG	C17-C18-C19-C20
26	c	519	LHG	C12-C13-C14-C15
30	D	407	LMG	C20-C21-C22-C23
30	d	407	LMG	C20-C21-C22-C23
25	R	608	CLA	C4-C3-C5-C6
25	r	608	CLA	C4-C3-C5-C6
24	N	609	CHL	C2-C3-C5-C6
24	n	609	CHL	C2-C3-C5-C6
25	B	606	CLA	C2-C3-C5-C6
25	D	403	CLA	C2-C3-C5-C6
25	N	612	CLA	C2-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
25	d	403	CLA	C2-C3-C5-C6
25	n	612	CLA	C2-C3-C5-C6
26	D	406	LHG	C25-C26-C27-C28
26	d	406	LHG	C25-C26-C27-C28
25	d	403	CLA	C8-C10-C11-C12
24	1	302	CHL	C2A-CAA-CBA-CGA
25	B	603	CLA	C2A-CAA-CBA-CGA
25	B	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	S	305	CLA	C2A-CAA-CBA-CGA
25	S	314	CLA	C2A-CAA-CBA-CGA
25	N	611	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	C2A-CAA-CBA-CGA
25	s	305	CLA	C2A-CAA-CBA-CGA
25	s	314	CLA	C2A-CAA-CBA-CGA
25	n	611	CLA	C2A-CAA-CBA-CGA
25	B	601	CLA	C11-C12-C13-C14
25	C	508	CLA	C14-C13-C15-C16
25	C	512	CLA	C14-C13-C15-C16
25	G	603	CLA	C11-C10-C8-C9
25	N	603	CLA	C14-C13-C15-C16
25	N	610	CLA	C11-C12-C13-C14
25	b	601	CLA	C11-C12-C13-C14
25	c	508	CLA	C14-C13-C15-C16
25	c	512	CLA	C14-C13-C15-C16
25	g	603	CLA	C11-C10-C8-C9
25	n	603	CLA	C14-C13-C15-C16
25	n	610	CLA	C11-C12-C13-C14
27	A	403	PHO	C11-C10-C8-C9
27	a	404	PHO	C11-C10-C8-C9
30	A	408	LMG	C35-C36-C37-C38
30	a	409	LMG	C35-C36-C37-C38
35	B	626	DGD	C3B-C4B-C5B-C6B
35	b	626	DGD	C3B-C4B-C5B-C6B
25	C	513	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
25	D	403	CLA	C8-C10-C11-C12
24	S	306	CHL	O1D-CGD-O2D-CED
24	s	306	CHL	O1D-CGD-O2D-CED
26	C	517	LHG	C14-C15-C16-C17
26	c	517	LHG	C14-C15-C16-C17
35	A	415	DGD	C9B-CAB-CBB-CCB
35	a	401	DGD	C9B-CAB-CBB-CCB
25	Y	312	CLA	C10-C11-C12-C13
25	y	312	CLA	C10-C11-C12-C13
26	B	621	LHG	C4-C5-C6-O8
26	b	621	LHG	C4-C5-C6-O8
30	A	408	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
30	a	409	LMG	C7-C8-C9-O8
35	B	626	DGD	C1G-C2G-C3G-O3G
35	b	626	DGD	C1G-C2G-C3G-O3G
35	A	415	DGD	C7A-C8A-C9A-CAA
35	a	401	DGD	C7A-C8A-C9A-CAA
25	C	504	CLA	C10-C11-C12-C13
25	R	609	CLA	C5-C6-C7-C8
25	c	504	CLA	C10-C11-C12-C13
25	r	609	CLA	C5-C6-C7-C8
30	A	408	LMG	C29-C30-C31-C32
30	B	620	LMG	C37-C38-C39-C40
30	a	409	LMG	C29-C30-C31-C32
35	C	516	DGD	C2A-C1A-O1G-C1G
35	c	516	DGD	C2A-C1A-O1G-C1G
30	B	623	LMG	O6-C5-C6-O5
30	b	623	LMG	O6-C5-C6-O5
25	2	602	CLA	C11-C12-C13-C15
25	N	612	CLA	C11-C12-C13-C15
25	6	602	CLA	C11-C12-C13-C15
25	n	612	CLA	C11-C12-C13-C15
26	B	625	LHG	C32-C33-C34-C35
26	C	518	LHG	C24-C25-C26-C27
26	b	625	LHG	C32-C33-C34-C35
26	c	518	LHG	C24-C25-C26-C27
30	b	620	LMG	C37-C38-C39-C40
24	g	601	CHL	C5-C6-C7-C8
26	S	318	LHG	C31-C32-C33-C34
26	s	318	LHG	C31-C32-C33-C34
29	A	407	SQD	C17-C18-C19-C20
29	a	408	SQD	C17-C18-C19-C20
35	C	516	DGD	CCB-CDB-CEB-CFB
35	c	516	DGD	CCB-CDB-CEB-CFB
24	G	609	CHL	O1D-CGD-O2D-CED
24	S	308	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	CHA-CBD-CGD-O1D
24	G	608	CHL	CHA-CBD-CGD-O2D
24	G	609	CHL	CHA-CBD-CGD-O2D
24	N	608	CHL	CHA-CBD-CGD-O1D
24	N	608	CHL	CHA-CBD-CGD-O2D
24	Y	306	CHL	CHA-CBD-CGD-O1D
24	Y	309	CHL	CHA-CBD-CGD-O2D
24	s	307	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	s	308	CHL	CHA-CBD-CGD-O2D
24	g	601	CHL	CHA-CBD-CGD-O1D
24	g	608	CHL	CHA-CBD-CGD-O2D
24	g	609	CHL	CHA-CBD-CGD-O2D
24	n	608	CHL	CHA-CBD-CGD-O1D
24	n	608	CHL	CHA-CBD-CGD-O2D
24	y	306	CHL	CHA-CBD-CGD-O1D
24	y	309	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	C5-C6-C7-C8
24	Y	302	CHL	O1A-CGA-O2A-C1
24	y	302	CHL	O1A-CGA-O2A-C1
26	B	625	LHG	C15-C16-C17-C18
26	b	625	LHG	C15-C16-C17-C18
25	B	611	CLA	C2-C3-C5-C6
25	S	313	CLA	C2-C3-C5-C6
25	Y	312	CLA	C2-C3-C5-C6
25	b	611	CLA	C2-C3-C5-C6
25	s	313	CLA	C2-C3-C5-C6
25	y	312	CLA	C2-C3-C5-C6
25	B	603	CLA	C15-C16-C17-C18
25	B	606	CLA	C13-C15-C16-C17
25	b	603	CLA	C15-C16-C17-C18
25	b	606	CLA	C13-C15-C16-C17
29	L	103	SQD	C15-C16-C17-C18
29	L	103	SQD	C31-C32-C33-C34
29	l	101	SQD	C15-C16-C17-C18
29	l	101	SQD	C31-C32-C33-C34
25	B	616	CLA	C8-C10-C11-C12
25	b	616	CLA	C8-C10-C11-C12
35	A	415	DGD	CBB-CCB-CDB-CEB
35	a	401	DGD	CBB-CCB-CDB-CEB
24	R	607	CHL	C2A-CAA-CBA-CGA
24	5	302	CHL	C2A-CAA-CBA-CGA
24	r	607	CHL	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	N	614	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
25	n	614	CLA	C2A-CAA-CBA-CGA
26	S	318	LHG	C29-C30-C31-C32
26	Y	319	LHG	C25-C26-C27-C28
26	s	318	LHG	C29-C30-C31-C32
35	B	626	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
35	b	626	DGD	C1A-C2A-C3A-C4A
24	g	609	CHL	O1D-CGD-O2D-CED
25	B	610	CLA	CBA-CGA-O2A-C1
25	N	603	CLA	CBA-CGA-O2A-C1
25	b	610	CLA	CBA-CGA-O2A-C1
25	n	603	CLA	CBA-CGA-O2A-C1
26	y	319	LHG	C25-C26-C27-C28
24	G	605	CHL	C3C-C2C-CMC-OMC
24	N	608	CHL	C3C-C2C-CMC-OMC
24	Y	306	CHL	C3C-C2C-CMC-OMC
24	Y	309	CHL	C3C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	C3C-C2C-CMC-OMC
24	y	306	CHL	C3C-C2C-CMC-OMC
24	y	309	CHL	C3C-C2C-CMC-OMC
28	I	101	BCR	C20-C21-C22-C23
28	i	101	BCR	C20-C21-C22-C23
26	C	517	LHG	O6-C4-C5-O7
26	c	517	LHG	O6-C4-C5-O7
25	C	504	CLA	C8-C10-C11-C12
25	c	504	CLA	C8-C10-C11-C12
35	A	415	DGD	C3B-C4B-C5B-C6B
35	a	401	DGD	C3B-C4B-C5B-C6B
30	B	620	LMG	C17-C18-C19-C20
30	b	620	LMG	C17-C18-C19-C20
25	Y	311	CLA	C4-C3-C5-C6
25	y	311	CLA	C4-C3-C5-C6
25	B	615	CLA	C2-C3-C5-C6
25	b	615	CLA	C2-C3-C5-C6
29	A	407	SQD	C10-C11-C12-C13
29	a	408	SQD	C10-C11-C12-C13
35	A	415	DGD	C6B-C7B-C8B-C9B
35	a	401	DGD	C6B-C7B-C8B-C9B
26	B	621	LHG	O7-C5-C6-O8
26	N	618	LHG	O7-C5-C6-O8
26	b	621	LHG	O7-C5-C6-O8
26	n	618	LHG	O7-C5-C6-O8
29	A	407	SQD	O6-C44-C45-O47
29	a	408	SQD	O6-C44-C45-O47
30	C	520	LMG	O7-C8-C9-O8
30	c	520	LMG	O7-C8-C9-O8
26	R	618	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	r	618	LHG	C28-C29-C30-C31
26	2	606	LHG	C29-C30-C31-C32
26	6	606	LHG	C29-C30-C31-C32
26	Y	319	LHG	C34-C35-C36-C37
25	C	513	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
26	b	622	LHG	C26-C27-C28-C29
26	y	319	LHG	C34-C35-C36-C37
26	B	622	LHG	C26-C27-C28-C29
26	s	318	LHG	C25-C26-C27-C28
24	G	609	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
26	S	318	LHG	C25-C26-C27-C28
25	R	610	CLA	C2C-C3C-CAC-CBC
25	r	610	CLA	C2C-C3C-CAC-CBC
24	Y	310	CHL	C3-C5-C6-C7
24	y	310	CHL	C3-C5-C6-C7
25	C	506	CLA	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
25	A	401	CLA	C4C-C3C-CAC-CBC
25	S	303	CLA	C14-C13-C15-C16
25	a	402	CLA	C4C-C3C-CAC-CBC
25	s	303	CLA	C14-C13-C15-C16
25	Y	312	CLA	C11-C12-C13-C15
25	y	312	CLA	C11-C12-C13-C15
24	N	609	CHL	C4-C3-C5-C6
24	R	607	CHL	C4-C3-C5-C6
24	n	609	CHL	C4-C3-C5-C6
24	r	607	CHL	C4-C3-C5-C6
25	Y	313	CLA	C4-C3-C5-C6
25	n	602	CLA	C4-C3-C5-C6
25	y	313	CLA	C4-C3-C5-C6
25	B	609	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
26	N	618	LHG	C31-C32-C33-C34
26	n	618	LHG	C31-C32-C33-C34
26	Y	301	LHG	C13-C14-C15-C16
26	y	301	LHG	C13-C14-C15-C16
26	C	519	LHG	O1-C1-C2-O2
26	c	519	LHG	O1-C1-C2-O2
24	2	601	CHL	C6-C7-C8-C9
24	6	601	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C14-C13-C15-C16
25	B	605	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	510	CLA	C11-C10-C8-C9
25	C	511	CLA	C11-C12-C13-C14
25	C	513	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	S	303	CLA	C6-C7-C8-C9
25	G	610	CLA	C14-C13-C15-C16
25	Y	313	CLA	C6-C7-C8-C9
25	Y	313	CLA	C11-C10-C8-C9
25	b	601	CLA	C14-C13-C15-C16
25	b	605	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
25	c	511	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C10-C8-C9
25	d	403	CLA	C14-C13-C15-C16
25	s	303	CLA	C6-C7-C8-C9
25	g	610	CLA	C14-C13-C15-C16
25	y	313	CLA	C6-C7-C8-C9
25	y	313	CLA	C11-C10-C8-C9
25	A	405	CLA	C4B-C3B-CAB-CBB
25	B	604	CLA	C4B-C3B-CAB-CBB
25	B	612	CLA	C4B-C3B-CAB-CBB
25	B	616	CLA	C4B-C3B-CAB-CBB
25	S	303	CLA	C4B-C3B-CAB-CBB
25	S	304	CLA	C4B-C3B-CAB-CBB
25	S	309	CLA	C4B-C3B-CAB-CBB
25	N	610	CLA	C4B-C3B-CAB-CBB
25	Y	312	CLA	C4B-C3B-CAB-CBB
25	R	604	CLA	C4B-C3B-CAB-CBB
25	R	609	CLA	C4B-C3B-CAB-CBB
25	R	610	CLA	C4B-C3B-CAB-CBB
25	R	612	CLA	C4B-C3B-CAB-CBB
25	a	406	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	b	608	CLA	C4B-C3B-CAB-CBB
25	b	612	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
25	s	303	CLA	C4B-C3B-CAB-CBB
25	s	304	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	s	309	CLA	C4B-C3B-CAB-CBB
25	n	610	CLA	C4B-C3B-CAB-CBB
25	y	312	CLA	C4B-C3B-CAB-CBB
25	r	604	CLA	C4B-C3B-CAB-CBB
25	r	609	CLA	C4B-C3B-CAB-CBB
25	r	610	CLA	C4B-C3B-CAB-CBB
25	r	612	CLA	C4B-C3B-CAB-CBB
29	a	412	SQD	C30-C31-C32-C33
25	n	603	CLA	C4C-C3C-CAC-CBC
25	R	604	CLA	C2A-CAA-CBA-CGA
25	r	604	CLA	C2A-CAA-CBA-CGA
29	A	411	SQD	C30-C31-C32-C33
25	N	603	CLA	C4C-C3C-CAC-CBC
30	A	410	LMG	C36-C37-C38-C39
30	a	411	LMG	C36-C37-C38-C39
26	L	102	LHG	O6-C4-C5-C6
26	l	103	LHG	O6-C4-C5-C6
26	L	102	LHG	C10-C11-C12-C13
26	l	103	LHG	C10-C11-C12-C13
24	G	608	CHL	C12-C13-C15-C16
24	G	609	CHL	C6-C7-C8-C10
24	N	609	CHL	C11-C10-C8-C7
24	Y	302	CHL	C11-C12-C13-C15
24	Y	302	CHL	C12-C13-C15-C16
24	g	608	CHL	C12-C13-C15-C16
24	g	609	CHL	C6-C7-C8-C10
24	n	609	CHL	C11-C10-C8-C7
24	y	302	CHL	C11-C12-C13-C15
24	y	302	CHL	C12-C13-C15-C16
25	A	402	CLA	C12-C13-C15-C16
25	B	601	CLA	C11-C12-C13-C15
25	B	602	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C12-C13-C15
25	B	614	CLA	C6-C7-C8-C10
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C12-C13-C15-C16
25	C	506	CLA	C12-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	508	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C12-C13-C15
25	N	603	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	N	612	CLA	C11-C10-C8-C7
25	Y	304	CLA	C11-C10-C8-C7
25	Y	313	CLA	C11-C10-C8-C7
25	Y	314	CLA	C6-C7-C8-C10
25	a	403	CLA	C12-C13-C15-C16
25	b	601	CLA	C11-C12-C13-C15
25	b	602	CLA	C6-C7-C8-C10
25	b	613	CLA	C11-C12-C13-C15
25	b	614	CLA	C6-C7-C8-C10
25	b	614	CLA	C12-C13-C15-C16
25	b	615	CLA	C12-C13-C15-C16
25	c	506	CLA	C12-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C10
25	c	507	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C15
25	n	603	CLA	C11-C12-C13-C15
25	n	612	CLA	C11-C10-C8-C7
25	y	304	CLA	C11-C10-C8-C7
25	y	313	CLA	C11-C10-C8-C7
25	y	314	CLA	C6-C7-C8-C10
25	r	612	CLA	C6-C7-C8-C10
25	R	603	CLA	C10-C11-C12-C13
25	R	612	CLA	C5-C6-C7-C8
25	r	603	CLA	C10-C11-C12-C13
25	r	612	CLA	C5-C6-C7-C8
30	B	620	LMG	C22-C23-C24-C25
30	b	620	LMG	C22-C23-C24-C25
35	A	415	DGD	C1A-C2A-C3A-C4A
35	a	401	DGD	C1A-C2A-C3A-C4A
30	A	410	LMG	C40-C41-C42-C43
30	a	411	LMG	C40-C41-C42-C43
35	C	516	DGD	C2B-C3B-C4B-C5B
26	2	606	LHG	C17-C18-C19-C20
26	6	606	LHG	C17-C18-C19-C20
26	C	519	LHG	C34-C35-C36-C37
26	c	519	LHG	C34-C35-C36-C37
35	c	516	DGD	C2B-C3B-C4B-C5B
24	N	601	CHL	C3A-C2A-CAA-CBA
24	Y	306	CHL	C3A-C2A-CAA-CBA
24	R	607	CHL	C3A-C2A-CAA-CBA
24	n	601	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	y	306	CHL	C3A-C2A-CAA-CBA
24	r	607	CHL	C3A-C2A-CAA-CBA
25	S	311	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	C3A-C2A-CAA-CBA
25	G	613	CLA	C3A-C2A-CAA-CBA
25	G	613	CLA	C4-C3-C5-C6
25	N	602	CLA	C4-C3-C5-C6
25	N	613	CLA	C4-C3-C5-C6
25	Y	314	CLA	C3A-C2A-CAA-CBA
25	R	612	CLA	C3A-C2A-CAA-CBA
25	s	311	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	C3A-C2A-CAA-CBA
25	g	613	CLA	C3A-C2A-CAA-CBA
25	g	613	CLA	C4-C3-C5-C6
25	n	613	CLA	C4-C3-C5-C6
25	y	314	CLA	C3A-C2A-CAA-CBA
25	r	612	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C13-C15-C16-C17
29	L	101	SQD	C29-C30-C31-C32
29	l	102	SQD	C29-C30-C31-C32
26	b	625	LHG	C12-C13-C14-C15
32	G	618	AJP	C22-C23-O25-C26
32	g	618	AJP	C22-C23-O25-C26
35	C	516	DGD	O6D-C1D-O3G-C3G
35	c	516	DGD	O6D-C1D-O3G-C3G
25	C	510	CLA	C2C-C3C-CAC-CBC
25	c	510	CLA	C2C-C3C-CAC-CBC
26	B	625	LHG	C12-C13-C14-C15
35	C	516	DGD	O1A-C1A-O1G-C1G
35	c	516	DGD	O1A-C1A-O1G-C1G
25	B	611	CLA	C10-C11-C12-C13
25	b	611	CLA	C10-C11-C12-C13
25	n	610	CLA	C13-C15-C16-C17
24	2	601	CHL	C15-C16-C17-C18
24	6	601	CHL	C15-C16-C17-C18
24	5	301	CHL	C2C-C3C-CAC-CBC
28	T	101	BCR	C19-C20-C21-C22
28	t	101	BCR	C19-C20-C21-C22
26	N	618	LHG	C35-C36-C37-C38
26	n	618	LHG	C35-C36-C37-C38
24	Y	306	CHL	O1A-CGA-O2A-C1
24	y	306	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	R	609	CLA	O1D-CGD-O2D-CED
25	r	609	CLA	O1D-CGD-O2D-CED
26	B	622	LHG	C14-C15-C16-C17
26	b	622	LHG	C14-C15-C16-C17
26	y	301	LHG	C32-C33-C34-C35
35	A	415	DGD	CCB-CDB-CEB-CFB
35	a	401	DGD	CCB-CDB-CEB-CFB
25	B	615	CLA	C8-C10-C11-C12
25	b	615	CLA	C8-C10-C11-C12
26	Y	301	LHG	C32-C33-C34-C35
24	l	301	CHL	C2C-C3C-CAC-CBC
25	c	512	CLA	C2C-C3C-CAC-CBC
26	B	621	LHG	C11-C10-C9-C8
26	b	621	LHG	C11-C10-C9-C8
24	Y	309	CHL	CBA-CGA-O2A-C1
24	y	309	CHL	CBA-CGA-O2A-C1
25	B	608	CLA	CBA-CGA-O2A-C1
35	C	515	DGD	C4B-C5B-C6B-C7B
35	c	515	DGD	C4B-C5B-C6B-C7B
25	C	512	CLA	C2C-C3C-CAC-CBC
29	A	411	SQD	O6-C44-C45-C46
29	a	412	SQD	O6-C44-C45-C46
30	B	623	LMG	C7-C8-C9-O8
30	b	623	LMG	C7-C8-C9-O8
25	B	603	CLA	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C15
25	b	603	CLA	C16-C17-C18-C19
25	r	603	CLA	C11-C12-C13-C15
25	G	610	CLA	C10-C11-C12-C13
25	g	610	CLA	C10-C11-C12-C13
26	N	618	LHG	C16-C17-C18-C19
26	n	618	LHG	C16-C17-C18-C19
29	L	103	SQD	C11-C12-C13-C14
29	l	101	SQD	C11-C12-C13-C14
24	1	302	CHL	C1A-C2A-CAA-CBA
24	2	603	CHL	C1A-C2A-CAA-CBA
24	N	601	CHL	C1A-C2A-CAA-CBA
24	5	302	CHL	C1A-C2A-CAA-CBA
24	6	603	CHL	C1A-C2A-CAA-CBA
24	n	601	CHL	C1A-C2A-CAA-CBA
25	N	603	CLA	C8-C10-C11-C12
25	n	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C4-C3-C5-C6
25	N	612	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
25	n	612	CLA	C4-C3-C5-C6
25	b	608	CLA	CBA-CGA-O2A-C1
25	R	608	CLA	C2-C3-C5-C6
25	r	608	CLA	C2-C3-C5-C6
25	2	602	CLA	C11-C12-C13-C14
25	C	513	CLA	C16-C17-C18-C20
25	N	610	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
25	n	610	CLA	C16-C17-C18-C19
26	B	621	LHG	O6-C4-C5-O7
26	S	301	LHG	O6-C4-C5-O7
26	N	618	LHG	O6-C4-C5-O7
26	b	621	LHG	O6-C4-C5-O7
26	s	301	LHG	O6-C4-C5-O7
26	n	618	LHG	O6-C4-C5-O7
26	2	606	LHG	C35-C36-C37-C38
28	B	618	BCR	C23-C24-C25-C30
28	D	404	BCR	C1-C6-C7-C8
28	Z	101	BCR	C1-C6-C7-C8
28	b	618	BCR	C23-C24-C25-C30
28	d	404	BCR	C1-C6-C7-C8
28	z	101	BCR	C1-C6-C7-C8
39	Y	316	LUT	C1-C6-C7-C8
39	y	316	LUT	C1-C6-C7-C8
35	A	415	DGD	C2A-C3A-C4A-C5A
35	a	401	DGD	C2A-C3A-C4A-C5A
26	6	606	LHG	C35-C36-C37-C38
25	S	311	CLA	C11-C10-C8-C9
25	s	311	CLA	C11-C10-C8-C9
25	R	612	CLA	C3-C5-C6-C7
26	D	406	LHG	C34-C35-C36-C37
25	2	605	CLA	C2C-C3C-CAC-CBC
26	B	625	LHG	C14-C15-C16-C17
26	b	625	LHG	C14-C15-C16-C17
25	C	510	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
26	d	406	LHG	C34-C35-C36-C37
25	2	605	CLA	O2A-C1-C2-C3
25	6	605	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	r	607	CHL	C11-C12-C13-C15
25	6	602	CLA	C11-C12-C13-C14
25	Y	303	CLA	C2A-CAA-CBA-CGA
25	y	303	CLA	C2A-CAA-CBA-CGA
25	6	605	CLA	C2C-C3C-CAC-CBC
25	B	601	CLA	C5-C6-C7-C8
25	b	601	CLA	C5-C6-C7-C8
26	L	102	LHG	O7-C5-C6-O8
26	l	103	LHG	O7-C5-C6-O8
29	A	407	SQD	O47-C45-C46-O48
29	a	408	SQD	O47-C45-C46-O48
30	B	623	LMG	O7-C8-C9-O8
30	b	623	LMG	O7-C8-C9-O8
25	r	612	CLA	C3-C5-C6-C7
29	A	411	SQD	C25-C26-C27-C28
29	a	412	SQD	C25-C26-C27-C28
24	n	606	CHL	O1D-CGD-O2D-CED
26	L	102	LHG	O9-C7-O7-C5
26	l	103	LHG	O9-C7-O7-C5
29	L	103	SQD	C30-C31-C32-C33
29	l	101	SQD	C30-C31-C32-C33
25	S	311	CLA	C11-C10-C8-C7
25	s	311	CLA	C11-C10-C8-C7
25	C	510	CLA	C2-C3-C5-C6
25	S	311	CLA	C2-C3-C5-C6
25	N	613	CLA	C2-C3-C5-C6
25	Y	304	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
25	s	311	CLA	C2-C3-C5-C6
25	n	613	CLA	C2-C3-C5-C6
25	y	304	CLA	C2-C3-C5-C6
35	C	516	DGD	CAA-CBA-CCA-CDA
35	c	516	DGD	CAA-CBA-CCA-CDA
24	N	607	CHL	C1-C2-C3-C5
24	n	607	CHL	C1-C2-C3-C5
25	C	503	CLA	C1-C2-C3-C5
25	c	503	CLA	C1-C2-C3-C5
24	R	607	CHL	C11-C12-C13-C15
26	2	606	LHG	C27-C28-C29-C30
26	6	606	LHG	C27-C28-C29-C30
30	B	623	LMG	C15-C16-C17-C18
30	b	623	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	C10-C11-C12-C13
25	b	612	CLA	C10-C11-C12-C13
24	N	606	CHL	O1D-CGD-O2D-CED
25	B	606	CLA	C11-C10-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	N	602	CLA	C11-C10-C8-C9
25	Y	303	CLA	C11-C12-C13-C14
25	b	606	CLA	C11-C10-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C9
25	c	509	CLA	C11-C10-C8-C9
25	n	602	CLA	C11-C10-C8-C9
25	y	303	CLA	C11-C12-C13-C14
28	D	404	BCR	C22-C23-C24-C25
28	d	404	BCR	C22-C23-C24-C25
35	B	626	DGD	O6D-C1D-O3G-C3G
35	b	626	DGD	O6D-C1D-O3G-C3G
35	A	415	DGD	O6E-C5E-C6E-O5E
35	a	401	DGD	O6E-C5E-C6E-O5E
26	N	618	LHG	C19-C20-C21-C22
26	n	618	LHG	C19-C20-C21-C22
25	A	405	CLA	C11-C12-C13-C15
25	Y	312	CLA	C11-C12-C13-C14
25	Y	313	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C12-C13-C15
25	y	312	CLA	C11-C12-C13-C14
25	y	313	CLA	C11-C12-C13-C14
25	S	312	CLA	O2A-C1-C2-C3
25	s	312	CLA	O2A-C1-C2-C3
25	B	607	CLA	C15-C16-C17-C18
25	b	607	CLA	C15-C16-C17-C18
25	B	607	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
24	Y	302	CHL	C16-C17-C18-C20
24	y	302	CHL	C16-C17-C18-C20
25	B	612	CLA	C16-C17-C18-C19
25	C	503	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	C16-C17-C18-C19
26	N	618	LHG	C8-C7-O7-C5
26	n	618	LHG	C8-C7-O7-C5
25	B	603	CLA	C5-C6-C7-C8
25	b	603	CLA	C5-C6-C7-C8
26	y	301	LHG	C27-C28-C29-C30
35	b	626	DGD	CDB-CEB-CFB-CGB
26	Y	301	LHG	C27-C28-C29-C30
35	B	626	DGD	CDB-CEB-CFB-CGB
25	y	312	CLA	C8-C10-C11-C12
26	B	625	LHG	C1-C2-C3-O3
26	b	625	LHG	C1-C2-C3-O3
29	L	101	SQD	C28-C29-C30-C31
29	l	102	SQD	C28-C29-C30-C31
24	Y	306	CHL	CAA-CBA-CGA-O2A
24	y	306	CHL	CAA-CBA-CGA-O2A
26	Y	319	LHG	C17-C18-C19-C20
26	y	319	LHG	C17-C18-C19-C20
25	Y	312	CLA	C8-C10-C11-C12
25	R	611	CLA	C2C-C3C-CAC-CBC
26	R	618	LHG	C16-C17-C18-C19
26	C	517	LHG	O6-C4-C5-C6
26	c	517	LHG	O6-C4-C5-C6
25	G	602	CLA	C16-C17-C18-C20
25	g	602	CLA	C16-C17-C18-C20
26	N	618	LHG	C10-C11-C12-C13
26	n	618	LHG	C10-C11-C12-C13
26	r	618	LHG	C16-C17-C18-C19
24	n	601	CHL	O1A-CGA-O2A-C1
24	G	601	CHL	C11-C12-C13-C15
24	Y	308	CHL	C6-C7-C8-C10
24	g	601	CHL	C11-C12-C13-C15
24	y	308	CHL	C6-C7-C8-C10
25	B	606	CLA	C11-C10-C8-C7
25	B	615	CLA	C11-C10-C8-C7
25	B	616	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C12-C13-C15
25	C	509	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	N	612	CLA	C6-C7-C8-C10
25	R	612	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C11-C10-C8-C7
25	b	616	CLA	C12-C13-C15-C16
25	c	507	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
25	n	612	CLA	C6-C7-C8-C10
27	A	403	PHO	C12-C13-C15-C16
27	a	404	PHO	C12-C13-C15-C16
29	A	407	SQD	C7-C8-C9-C10
29	a	408	SQD	C7-C8-C9-C10
26	S	301	LHG	C30-C31-C32-C33
26	6	606	LHG	C11-C10-C9-C8
26	s	301	LHG	C30-C31-C32-C33
26	Y	301	LHG	O8-C23-C24-C25
26	y	301	LHG	O8-C23-C24-C25
26	2	606	LHG	C11-C10-C9-C8
26	S	301	LHG	C17-C18-C19-C20
26	s	301	LHG	C17-C18-C19-C20
25	r	611	CLA	C2C-C3C-CAC-CBC
28	A	406	BCR	C17-C18-C19-C20
28	a	407	BCR	C17-C18-C19-C20
26	D	406	LHG	C24-C23-O8-C6
26	d	406	LHG	C24-C23-O8-C6
26	S	301	LHG	C33-C34-C35-C36
26	s	301	LHG	C33-C34-C35-C36
26	l	103	LHG	C16-C17-C18-C19
24	G	608	CHL	C15-C16-C17-C18
24	g	608	CHL	C15-C16-C17-C18
25	B	605	CLA	C15-C16-C17-C18
25	b	605	CLA	C15-C16-C17-C18
26	L	102	LHG	C16-C17-C18-C19
25	S	313	CLA	C6-C7-C8-C10
25	N	610	CLA	C16-C17-C18-C20
25	s	313	CLA	C6-C7-C8-C10
25	n	610	CLA	C16-C17-C18-C20
24	Y	302	CHL	C4-C3-C5-C6
24	y	302	CHL	C4-C3-C5-C6
24	G	601	CHL	O1A-CGA-O2A-C1
24	N	601	CHL	O1A-CGA-O2A-C1
24	Y	310	CHL	C2-C3-C5-C6
24	y	310	CHL	C2-C3-C5-C6
38	F	101	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	f	101	HEM	C2C-C3C-CAC-CBC
24	Y	302	CHL	C10-C11-C12-C13
24	y	302	CHL	C10-C11-C12-C13
26	L	102	LHG	C35-C36-C37-C38
26	l	103	LHG	C35-C36-C37-C38
25	y	314	CLA	C3-C5-C6-C7
26	C	517	LHG	C33-C34-C35-C36
26	c	517	LHG	C33-C34-C35-C36
24	g	601	CHL	O1A-CGA-O2A-C1
25	Y	314	CLA	C8-C10-C11-C12
25	y	314	CLA	C8-C10-C11-C12
28	T	101	BCR	C9-C10-C11-C12
28	t	101	BCR	C9-C10-C11-C12
39	N	615	LUT	C13-C14-C15-C35
39	n	615	LUT	C13-C14-C15-C35
29	A	407	SQD	C13-C14-C15-C16
29	a	408	SQD	C13-C14-C15-C16
25	Y	314	CLA	C3-C5-C6-C7
26	B	625	LHG	O2-C2-C3-O3
26	b	625	LHG	O2-C2-C3-O3
26	y	319	LHG	C35-C36-C37-C38
25	A	405	CLA	C5-C6-C7-C8
25	Y	314	CLA	C5-C6-C7-C8
25	y	314	CLA	C5-C6-C7-C8
26	Y	319	LHG	C35-C36-C37-C38
26	2	606	LHG	C4-C5-C6-O8
26	L	102	LHG	C4-C5-C6-O8
26	6	606	LHG	C4-C5-C6-O8
26	l	103	LHG	C4-C5-C6-O8
29	L	101	SQD	C44-C45-C46-O48
29	L	103	SQD	O6-C44-C45-C46
29	l	101	SQD	O6-C44-C45-C46
29	l	102	SQD	C44-C45-C46-O48
30	A	410	LMG	C7-C8-C9-O8
30	C	520	LMG	O1-C7-C8-C9
30	a	411	LMG	C7-C8-C9-O8
30	c	520	LMG	O1-C7-C8-C9
25	B	613	CLA	C15-C16-C17-C18
25	a	406	CLA	C5-C6-C7-C8
25	b	613	CLA	C15-C16-C17-C18
38	F	101	HEM	C4C-C3C-CAC-CBC
38	f	101	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	N	603	CLA	C16-C17-C18-C20
25	n	603	CLA	C16-C17-C18-C20
30	c	520	LMG	C35-C36-C37-C38
30	C	520	LMG	C35-C36-C37-C38
35	B	626	DGD	C8A-C9A-CAA-CBA
35	b	626	DGD	C8A-C9A-CAA-CBA
35	b	626	DGD	CAB-CBB-CCB-CDB
40	N	617	NEX	C7-C8-C9-C19
40	Y	318	NEX	C7-C8-C9-C19
40	n	617	NEX	C7-C8-C9-C19
40	y	318	NEX	C7-C8-C9-C19
29	A	407	SQD	C30-C31-C32-C33
29	a	408	SQD	C30-C31-C32-C33
25	g	604	CLA	C2C-C3C-CAC-CBC
25	B	606	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13
26	n	618	LHG	C33-C34-C35-C36
30	c	520	LMG	C32-C33-C34-C35
35	B	626	DGD	CAB-CBB-CCB-CDB
30	C	520	LMG	C32-C33-C34-C35
35	A	415	DGD	O1G-C1G-C2G-O2G
35	B	626	DGD	O2G-C2G-C3G-O3G
35	a	401	DGD	O1G-C1G-C2G-O2G
35	b	626	DGD	O2G-C2G-C3G-O3G
24	G	608	CHL	C6-C7-C8-C9
24	g	608	CHL	C6-C7-C8-C9
25	B	607	CLA	C6-C7-C8-C9
25	G	610	CLA	C11-C12-C13-C14
25	b	607	CLA	C6-C7-C8-C9
25	g	610	CLA	C11-C12-C13-C14
27	A	404	PHO	C6-C7-C8-C9
27	a	405	PHO	C6-C7-C8-C9
25	S	313	CLA	C6-C7-C8-C9
25	G	602	CLA	C16-C17-C18-C19
25	s	313	CLA	C6-C7-C8-C9
25	g	602	CLA	C16-C17-C18-C19
25	G	604	CLA	C2C-C3C-CAC-CBC
29	A	411	SQD	C13-C14-C15-C16
29	a	412	SQD	C13-C14-C15-C16
26	D	406	LHG	C30-C31-C32-C33
26	d	406	LHG	C30-C31-C32-C33
30	B	623	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	b	623	LMG	C29-C30-C31-C32
26	N	618	LHG	C33-C34-C35-C36
35	C	516	DGD	C7A-C8A-C9A-CAA
26	C	518	LHG	C18-C19-C20-C21
26	C	519	LHG	C33-C34-C35-C36
26	c	519	LHG	C33-C34-C35-C36
35	c	516	DGD	C7A-C8A-C9A-CAA
26	c	518	LHG	C18-C19-C20-C21
35	B	626	DGD	C2D-C1D-O3G-C3G
35	b	626	DGD	C2D-C1D-O3G-C3G
25	A	402	CLA	C16-C17-C18-C20
25	C	503	CLA	C16-C17-C18-C20
25	a	403	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
30	B	620	LMG	C30-C31-C32-C33
30	B	620	LMG	C4-C5-C6-O5
30	b	620	LMG	C4-C5-C6-O5
30	b	620	LMG	C30-C31-C32-C33
25	A	405	CLA	C8-C10-C11-C12
25	a	406	CLA	C8-C10-C11-C12
25	c	512	CLA	C13-C15-C16-C17
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	C13-C15-C16-C17
26	R	618	LHG	C11-C10-C9-C8
26	r	618	LHG	C11-C10-C9-C8
30	D	407	LMG	C33-C34-C35-C36
30	d	407	LMG	C33-C34-C35-C36
26	y	301	LHG	C7-C8-C9-C10
25	S	303	CLA	CBD-CGD-O2D-CED
25	s	303	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	C2C-C3C-CAC-CBC
25	g	612	CLA	C2C-C3C-CAC-CBC
24	1	302	CHL	C4C-C3C-CAC-CBC
24	S	306	CHL	C4C-C3C-CAC-CBC
24	5	302	CHL	C4C-C3C-CAC-CBC
24	s	306	CHL	C4C-C3C-CAC-CBC
29	A	411	SQD	C4-C5-C6-S
29	L	103	SQD	C4-C5-C6-S
29	a	412	SQD	C4-C5-C6-S
29	l	101	SQD	C4-C5-C6-S
32	Y	321	AJP	C27-C26-O25-C23

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Mol	Chain	Res	Type	Atoms
32	y	321	AJP	C27-C26-O25-C23
28	T	101	BCR	C10-C11-C12-C13
28	t	101	BCR	C10-C11-C12-C13
25	G	612	CLA	C11-C12-C13-C14
25	g	612	CLA	C11-C12-C13-C14
29	A	407	SQD	C12-C13-C14-C15
29	a	408	SQD	C12-C13-C14-C15
26	Y	301	LHG	C7-C8-C9-C10
26	B	625	LHG	O1-C1-C2-O2
26	b	625	LHG	O1-C1-C2-O2
25	Y	304	CLA	C3-C5-C6-C7
25	y	304	CLA	C3-C5-C6-C7
27	A	403	PHO	C10-C11-C12-C13
27	a	404	PHO	C10-C11-C12-C13
28	B	619	BCR	C7-C8-C9-C34
28	b	619	BCR	C7-C8-C9-C34
26	C	519	LHG	C18-C19-C20-C21
25	B	608	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	C4B-C3B-CAB-CBB
25	Y	315	CLA	C4B-C3B-CAB-CBB
25	R	608	CLA	C1A-C2A-CAA-CBA
25	R	608	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	y	315	CLA	C4B-C3B-CAB-CBB
25	r	608	CLA	C1A-C2A-CAA-CBA
25	r	608	CLA	C4B-C3B-CAB-CBB
25	B	603	CLA	CBA-CGA-O2A-C1
25	b	603	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	C18-C19-C20-C21
25	B	608	CLA	C5-C6-C7-C8
28	Z	101	BCR	C7-C8-C9-C10
28	z	101	BCR	C7-C8-C9-C10
25	2	602	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
26	B	621	LHG	C13-C14-C15-C16
26	b	621	LHG	C13-C14-C15-C16
35	C	515	DGD	C4D-C5D-C6D-O5D
35	c	515	DGD	C4D-C5D-C6D-O5D
25	b	608	CLA	C5-C6-C7-C8
26	n	618	LHG	O9-C7-O7-C5
26	S	301	LHG	C32-C33-C34-C35
32	Y	322	AJP	C29-C30-C32-O33

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Mol	Chain	Res	Type	Atoms
32	y	322	AJP	C29-C30-C32-O33
26	s	301	LHG	C32-C33-C34-C35
24	Y	309	CHL	C11-C10-C8-C7
24	y	309	CHL	C11-C10-C8-C7
25	B	609	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	508	CLA	C11-C12-C13-C15
25	D	402	CLA	C11-C12-C13-C15
25	N	613	CLA	C6-C7-C8-C10
25	N	613	CLA	C11-C10-C8-C7
25	Y	312	CLA	C6-C7-C8-C10
25	b	609	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C12-C13-C15
25	d	402	CLA	C11-C12-C13-C15
25	n	613	CLA	C6-C7-C8-C10
25	n	613	CLA	C11-C10-C8-C7
25	y	312	CLA	C6-C7-C8-C10
25	B	616	CLA	C16-C17-C18-C20
25	S	310	CLA	C6-C7-C8-C9
25	Y	304	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C20
25	s	310	CLA	C6-C7-C8-C9
25	y	304	CLA	C16-C17-C18-C19
30	B	620	LMG	C29-C30-C31-C32
30	b	620	LMG	C29-C30-C31-C32
26	D	406	LHG	O10-C23-O8-C6
26	d	406	LHG	O10-C23-O8-C6
26	2	606	LHG	C2-C3-O3-P
26	6	606	LHG	C2-C3-O3-P
25	R	604	CLA	C3A-C2A-CAA-CBA
25	R	608	CLA	C3A-C2A-CAA-CBA
25	r	604	CLA	C3A-C2A-CAA-CBA
25	r	608	CLA	C3A-C2A-CAA-CBA
29	A	411	SQD	C31-C32-C33-C34
29	a	412	SQD	C31-C32-C33-C34
25	Y	313	CLA	C2-C3-C5-C6
25	y	313	CLA	C2-C3-C5-C6
26	N	618	LHG	O9-C7-O7-C5
24	Y	302	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	y	302	CHL	C3-C5-C6-C7
26	2	606	LHG	C13-C14-C15-C16
30	B	623	LMG	C21-C22-C23-C24
30	b	623	LMG	C21-C22-C23-C24
25	C	507	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	D	402	CLA	C11-C12-C13-C14
25	N	603	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	d	402	CLA	C11-C12-C13-C14
25	n	603	CLA	C11-C12-C13-C14
26	6	606	LHG	C13-C14-C15-C16
26	C	518	LHG	C11-C12-C13-C14
35	C	515	DGD	O6D-C5D-C6D-O5D
35	c	515	DGD	O6D-C5D-C6D-O5D
25	D	402	CLA	C10-C11-C12-C13
25	d	402	CLA	C10-C11-C12-C13
26	c	518	LHG	C11-C12-C13-C14
30	B	623	LMG	C35-C36-C37-C38
24	G	606	CHL	C1-C2-C3-C4
24	Y	307	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	y	307	CHL	C1-C2-C3-C4
25	S	312	CLA	C1-C2-C3-C4
25	R	610	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	s	312	CLA	C1-C2-C3-C4
25	r	610	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4
40	G	617	NEX	C7-C8-C9-C10
40	Y	318	NEX	C7-C8-C9-C10
40	g	617	NEX	C7-C8-C9-C10
40	y	318	NEX	C7-C8-C9-C10
30	b	623	LMG	C35-C36-C37-C38
29	A	411	SQD	O47-C45-C46-O48
29	L	103	SQD	O6-C44-C45-O47
29	a	412	SQD	O47-C45-C46-O48
29	l	101	SQD	O6-C44-C45-O47
30	A	408	LMG	O1-C7-C8-O7
30	A	408	LMG	O7-C8-C9-O8
30	C	520	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
30	D	407	LMG	O1-C7-C8-O7
30	a	409	LMG	O1-C7-C8-O7
30	a	409	LMG	O7-C8-C9-O8
30	c	520	LMG	O1-C7-C8-O7
30	d	407	LMG	O1-C7-C8-O7
26	c	518	LHG	C27-C28-C29-C30
26	C	518	LHG	C27-C28-C29-C30
29	A	411	SQD	C44-C45-C46-O48
29	a	412	SQD	C44-C45-C46-O48
30	A	408	LMG	O1-C7-C8-C9
30	a	409	LMG	O1-C7-C8-C9
30	D	407	LMG	C17-C18-C19-C20
30	d	407	LMG	C17-C18-C19-C20
26	C	517	LHG	C30-C31-C32-C33
26	S	301	LHG	C11-C12-C13-C14
26	s	301	LHG	C11-C12-C13-C14
24	S	306	CHL	CAD-CBD-CGD-O2D
24	s	306	CHL	CAD-CBD-CGD-O2D
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	g	614	CLA	CAD-CBD-CGD-O2D
26	c	517	LHG	C30-C31-C32-C33
25	s	310	CLA	O1A-CGA-O2A-C1
30	A	410	LMG	O6-C1-O1-C7
30	a	411	LMG	O6-C1-O1-C7
25	y	315	CLA	C2A-CAA-CBA-CGA
25	N	611	CLA	C10-C11-C12-C13
25	n	611	CLA	C10-C11-C12-C13
25	S	310	CLA	O1A-CGA-O2A-C1
26	N	618	LHG	C24-C25-C26-C27
26	S	318	LHG	C11-C10-C9-C8
26	s	318	LHG	C11-C10-C9-C8
26	s	318	LHG	C9-C10-C11-C12
26	n	618	LHG	C24-C25-C26-C27
29	L	103	SQD	C29-C30-C31-C32
29	l	101	SQD	C29-C30-C31-C32
26	S	318	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	1	301	CHL	CHA-CBD-CGD-O1D
24	2	603	CHL	CHA-CBD-CGD-O1D
24	G	609	CHL	CHA-CBD-CGD-O1D
24	Y	306	CHL	CHA-CBD-CGD-O2D
24	5	301	CHL	CHA-CBD-CGD-O1D
24	6	603	CHL	CHA-CBD-CGD-O1D
24	g	609	CHL	CHA-CBD-CGD-O1D
24	y	306	CHL	CHA-CBD-CGD-O2D
25	2	604	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	610	CLA	CHA-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	S	303	CLA	CHA-CBD-CGD-O2D
25	S	305	CLA	CAD-CBD-CGD-O1D
25	S	312	CLA	CHA-CBD-CGD-O1D
25	G	604	CLA	CAD-CBD-CGD-O1D
25	G	612	CLA	CHA-CBD-CGD-O1D
25	N	603	CLA	CHA-CBD-CGD-O1D
25	N	612	CLA	CHA-CBD-CGD-O1D
25	Y	303	CLA	CHA-CBD-CGD-O2D
25	Y	305	CLA	CAD-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	609	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CHA-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	510	CLA	CHA-CBD-CGD-O2D
25	s	303	CLA	CHA-CBD-CGD-O2D
25	s	305	CLA	CAD-CBD-CGD-O1D
25	s	312	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	g	604	CLA	CAD-CBD-CGD-O1D
25	g	612	CLA	CHA-CBD-CGD-O1D
25	n	603	CLA	CHA-CBD-CGD-O1D
25	n	612	CLA	CHA-CBD-CGD-O1D
25	y	303	CLA	CHA-CBD-CGD-O2D
25	y	305	CLA	CAD-CBD-CGD-O1D
25	r	604	CLA	CHA-CBD-CGD-O2D
25	r	609	CLA	CAD-CBD-CGD-O1D
26	2	606	LHG	C3-O3-P-O5
26	L	102	LHG	C4-O6-P-O3
26	S	318	LHG	C3-O3-P-O5
26	Y	301	LHG	C3-O3-P-O5
26	6	606	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O4
26	l	103	LHG	C4-O6-P-O3
26	s	318	LHG	C3-O3-P-O5
26	y	301	LHG	C3-O3-P-O5
28	A	406	BCR	C13-C14-C15-C16
28	I	101	BCR	C9-C10-C11-C12
28	a	407	BCR	C13-C14-C15-C16
28	i	101	BCR	C9-C10-C11-C12
39	Y	316	LUT	C33-C34-C35-C15
39	y	316	LUT	C33-C34-C35-C15
25	G	603	CLA	C4-C3-C5-C6
25	g	603	CLA	C4-C3-C5-C6
31	D	405	PL9	C20-C19-C21-C22
31	d	405	PL9	C20-C19-C21-C22
25	2	602	CLA	C2B-C3B-CAB-CBB
25	2	604	CLA	C2B-C3B-CAB-CBB
25	C	503	CLA	C2B-C3B-CAB-CBB
25	C	509	CLA	C2B-C3B-CAB-CBB
25	D	401	CLA	C2B-C3B-CAB-CBB
25	N	602	CLA	C2B-C3B-CAB-CBB
25	N	613	CLA	C2B-C3B-CAB-CBB
25	6	602	CLA	C2B-C3B-CAB-CBB
25	6	604	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
25	c	509	CLA	C2B-C3B-CAB-CBB
25	d	401	CLA	C2B-C3B-CAB-CBB
25	n	602	CLA	C2B-C3B-CAB-CBB
25	n	613	CLA	C2B-C3B-CAB-CBB
28	B	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
28	b	619	BCR	C23-C24-C25-C30
25	G	613	CLA	C2-C3-C5-C6
25	g	613	CLA	C2-C3-C5-C6
26	N	618	LHG	C2-C3-O3-P
26	n	618	LHG	C2-C3-O3-P
24	R	607	CHL	C10-C11-C12-C13
24	r	607	CHL	C10-C11-C12-C13
26	B	622	LHG	C23-C24-C25-C26
38	F	101	HEM	C3D-CAD-CBD-CGD
38	f	101	HEM	C3D-CAD-CBD-CGD
26	N	618	LHG	C18-C19-C20-C21
35	B	626	DGD	C5A-C6A-C7A-C8A
35	b	626	DGD	C5A-C6A-C7A-C8A
24	S	307	CHL	C2A-CAA-CBA-CGA
24	s	307	CHL	C2A-CAA-CBA-CGA
25	Y	315	CLA	C2A-CAA-CBA-CGA
26	n	618	LHG	C18-C19-C20-C21
26	b	622	LHG	C23-C24-C25-C26
31	A	409	PL9	C4-C3-C7-C8
31	a	410	PL9	C4-C3-C7-C8
25	N	603	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C19
25	G	613	CLA	C10-C11-C12-C13
25	g	613	CLA	C10-C11-C12-C13
25	S	303	CLA	C12-C13-C15-C16
25	s	303	CLA	C12-C13-C15-C16
26	L	102	LHG	C6-C5-O7-C7
26	l	103	LHG	C6-C5-O7-C7
29	L	103	SQD	C44-C45-O47-C7
29	l	101	SQD	C44-C45-O47-C7
40	G	617	NEX	C10-C11-C12-C13
40	G	617	NEX	C30-C31-C32-C33
40	Y	318	NEX	C30-C31-C32-C33
40	g	617	NEX	C10-C11-C12-C13
40	g	617	NEX	C30-C31-C32-C33
40	y	318	NEX	C30-C31-C32-C33
29	A	411	SQD	C17-C18-C19-C20
29	a	412	SQD	C17-C18-C19-C20
25	R	610	CLA	C4C-C3C-CAC-CBC
25	r	610	CLA	C4C-C3C-CAC-CBC
26	r	618	LHG	C12-C13-C14-C15
25	y	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	Y	308	CHL	C6-C7-C8-C9
24	y	308	CHL	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	B	615	CLA	C14-C13-C15-C16
25	D	402	CLA	C11-C10-C8-C9
25	S	311	CLA	C6-C7-C8-C9
25	N	613	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	b	615	CLA	C14-C13-C15-C16
25	d	402	CLA	C11-C10-C8-C9
25	s	311	CLA	C6-C7-C8-C9
25	n	613	CLA	C6-C7-C8-C9
26	R	618	LHG	C12-C13-C14-C15
24	2	601	CHL	C11-C10-C8-C7
24	6	601	CHL	C11-C10-C8-C7
25	2	602	CLA	C11-C10-C8-C7
25	S	303	CLA	C11-C10-C8-C7
25	6	602	CLA	C11-C10-C8-C7
25	s	303	CLA	C11-C10-C8-C7
26	s	318	LHG	C15-C16-C17-C18
26	S	318	LHG	C15-C16-C17-C18
28	T	101	BCR	C6-C7-C8-C9
28	t	101	BCR	C6-C7-C8-C9
25	a	403	CLA	C16-C17-C18-C19
25	Y	304	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	C2C-C3C-CAC-CBC
29	A	411	SQD	C32-C33-C34-C35
25	r	601	CLA	C2C-C3C-CAC-CBC
29	L	101	SQD	C2-C1-O6-C44
29	l	102	SQD	C2-C1-O6-C44
30	A	410	LMG	C2-C1-O1-C7
30	a	411	LMG	C2-C1-O1-C7
24	Y	310	CHL	C4-C3-C5-C6
24	y	310	CHL	C4-C3-C5-C6
26	2	606	LHG	C9-C10-C11-C12
26	6	606	LHG	C9-C10-C11-C12
35	B	626	DGD	C7A-C8A-C9A-CAA
25	A	402	CLA	C16-C17-C18-C19
24	n	607	CHL	C5-C6-C7-C8
29	a	412	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	Y	323	AJP	O31-C30-C32-O33
32	y	323	AJP	O31-C30-C32-O33
26	L	102	LHG	C26-C27-C28-C29
26	l	103	LHG	C26-C27-C28-C29
24	N	607	CHL	C5-C6-C7-C8
26	S	318	LHG	C2-C3-O3-P
26	s	318	LHG	C2-C3-O3-P
26	B	621	LHG	C30-C31-C32-C33
26	B	621	LHG	C31-C32-C33-C34
26	b	621	LHG	C30-C31-C32-C33
26	b	621	LHG	C31-C32-C33-C34
35	b	626	DGD	C7A-C8A-C9A-CAA
25	R	602	CLA	O1A-CGA-O2A-C1
30	A	408	LMG	C32-C33-C34-C35
30	a	409	LMG	C32-C33-C34-C35
35	B	626	DGD	C6B-C7B-C8B-C9B
29	L	101	SQD	C25-C26-C27-C28
29	l	102	SQD	C25-C26-C27-C28
30	c	520	LMG	C37-C38-C39-C40
30	C	520	LMG	C37-C38-C39-C40
35	b	626	DGD	C6B-C7B-C8B-C9B
24	y	302	CHL	C15-C16-C17-C18
25	Y	303	CLA	C5-C6-C7-C8
25	y	303	CLA	C5-C6-C7-C8
29	l	102	SQD	C11-C12-C13-C14
30	C	520	LMG	C7-C8-C9-O8
30	c	520	LMG	C7-C8-C9-O8
35	A	415	DGD	O1G-C1G-C2G-C3G
35	a	401	DGD	O1G-C1G-C2G-C3G
25	r	602	CLA	O1A-CGA-O2A-C1
24	G	601	CHL	C15-C16-C17-C18
24	Y	302	CHL	C15-C16-C17-C18
24	g	601	CHL	C15-C16-C17-C18
25	B	604	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
25	y	304	CLA	C15-C16-C17-C18
25	r	612	CLA	C8-C10-C11-C12
29	L	101	SQD	C11-C12-C13-C14
25	Y	304	CLA	C15-C16-C17-C18
26	S	301	LHG	C25-C26-C27-C28
26	s	301	LHG	C25-C26-C27-C28
25	R	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	G	605	CHL	C2C-C3C-CAC-CBC
24	g	605	CHL	C2C-C3C-CAC-CBC
30	B	620	LMG	C8-C7-O1-C1
30	b	620	LMG	C8-C7-O1-C1
25	2	605	CLA	C4C-C3C-CAC-CBC
25	6	605	CLA	C4C-C3C-CAC-CBC
26	B	622	LHG	C9-C10-C11-C12
26	L	102	LHG	C17-C18-C19-C20
26	b	622	LHG	C9-C10-C11-C12
25	C	505	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
39	S	316	LUT	C9-C10-C11-C12
39	s	316	LUT	C9-C10-C11-C12
32	B	624	AJP	C36-C35-O34-C29
32	b	624	AJP	C36-C35-O34-C29
26	l	103	LHG	C17-C18-C19-C20
30	B	620	LMG	C36-C37-C38-C39
30	b	620	LMG	C36-C37-C38-C39
25	R	602	CLA	C4-C3-C5-C6
25	r	602	CLA	C4-C3-C5-C6
25	C	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
24	Y	302	CHL	C14-C13-C15-C16
24	y	302	CHL	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	N	613	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	n	613	CLA	C11-C10-C8-C9
24	N	605	CHL	O1D-CGD-O2D-CED
25	N	610	CLA	CBA-CGA-O2A-C1
24	n	605	CHL	O1D-CGD-O2D-CED
25	A	402	CLA	C4B-C3B-CAB-CBB
25	B	611	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	C	506	CLA	C4B-C3B-CAB-CBB
25	C	508	CLA	C4B-C3B-CAB-CBB
25	C	511	CLA	C4B-C3B-CAB-CBB
25	S	310	CLA	C4B-C3B-CAB-CBB
25	S	313	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	a	403	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C4B-C3B-CAB-CBB
25	c	508	CLA	C4B-C3B-CAB-CBB
25	c	511	CLA	C4B-C3B-CAB-CBB
25	s	310	CLA	C4B-C3B-CAB-CBB
25	s	313	CLA	C4B-C3B-CAB-CBB
26	2	606	LHG	C31-C32-C33-C34
26	6	606	LHG	C31-C32-C33-C34
30	D	407	LMG	C21-C22-C23-C24
26	C	518	LHG	C11-C10-C9-C8
26	c	518	LHG	C11-C10-C9-C8
30	d	407	LMG	C21-C22-C23-C24
25	n	610	CLA	CBA-CGA-O2A-C1
31	D	405	PL9	C45-C44-C46-C47
31	d	405	PL9	C45-C44-C46-C47
25	G	611	CLA	CAA-CBA-CGA-O2A
25	g	611	CLA	CAA-CBA-CGA-O2A
24	Y	302	CHL	C2-C3-C5-C6
24	y	302	CHL	C2-C3-C5-C6
26	S	301	LHG	C16-C17-C18-C19
25	R	601	CLA	O1A-CGA-O2A-C1
25	r	601	CLA	O1A-CGA-O2A-C1
25	G	610	CLA	C13-C15-C16-C17
35	A	415	DGD	C5B-C6B-C7B-C8B
35	a	401	DGD	C5B-C6B-C7B-C8B
26	s	301	LHG	C16-C17-C18-C19
25	A	402	CLA	C11-C12-C13-C15
25	B	607	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C10-C8-C7
25	D	402	CLA	C12-C13-C15-C16
25	S	303	CLA	C11-C12-C13-C15
25	N	602	CLA	C6-C7-C8-C10
25	a	403	CLA	C11-C12-C13-C15
25	b	607	CLA	C11-C12-C13-C15
25	c	503	CLA	C11-C10-C8-C7
25	d	402	CLA	C12-C13-C15-C16
25	s	303	CLA	C11-C12-C13-C15
25	n	602	CLA	C6-C7-C8-C10
25	g	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	g	602	CLA	CBD-CGD-O2D-CED
26	c	519	LHG	C14-C15-C16-C17
30	B	620	LMG	C13-C14-C15-C16
30	b	620	LMG	C13-C14-C15-C16
25	B	604	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C4-C3-C5-C6
25	b	604	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C4-C3-C5-C6
26	C	519	LHG	C14-C15-C16-C17
30	C	520	LMG	C31-C32-C33-C34
30	c	520	LMG	C31-C32-C33-C34
25	S	303	CLA	C5-C6-C7-C8
25	s	303	CLA	C5-C6-C7-C8
24	N	605	CHL	C2C-C3C-CAC-CBC
24	n	605	CHL	C2C-C3C-CAC-CBC
39	S	315	LUT	C40-C33-C34-C35
39	R	615	LUT	C20-C13-C14-C15
39	s	315	LUT	C40-C33-C34-C35
39	r	615	LUT	C20-C13-C14-C15
40	S	317	NEX	C11-C10-C9-C19
40	S	317	NEX	C39-C29-C30-C31
40	N	617	NEX	C39-C29-C30-C31
40	R	617	NEX	C39-C29-C30-C31
40	s	317	NEX	C11-C10-C9-C19
40	s	317	NEX	C39-C29-C30-C31
40	n	617	NEX	C39-C29-C30-C31
40	r	617	NEX	C39-C29-C30-C31
41	R	616	XAT	C20-C13-C14-C15
41	r	616	XAT	C20-C13-C14-C15
39	Y	317	LUT	C29-C30-C31-C32
39	y	317	LUT	C29-C30-C31-C32
25	B	609	CLA	C5-C6-C7-C8
25	b	609	CLA	C5-C6-C7-C8
25	G	602	CLA	CBD-CGD-O2D-CED
24	S	308	CHL	CAA-CBA-CGA-O1A
24	s	308	CHL	CAA-CBA-CGA-O1A
27	A	403	PHO	C4-C3-C5-C6
27	a	404	PHO	C4-C3-C5-C6
26	B	625	LHG	C28-C29-C30-C31
26	b	625	LHG	C28-C29-C30-C31
24	R	607	CHL	C2-C3-C5-C6
24	r	607	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	N	602	CLA	C2-C3-C5-C6
25	Y	303	CLA	C2-C3-C5-C6
25	n	602	CLA	C2-C3-C5-C6
25	y	303	CLA	C2-C3-C5-C6
30	B	623	LMG	C18-C19-C20-C21
30	b	623	LMG	C18-C19-C20-C21
24	Y	309	CHL	C2C-C3C-CAC-CBC
25	C	510	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
26	L	102	LHG	C32-C33-C34-C35
26	l	103	LHG	C32-C33-C34-C35
24	y	309	CHL	C2C-C3C-CAC-CBC
29	A	407	SQD	C29-C30-C31-C32
29	a	408	SQD	C29-C30-C31-C32
24	N	607	CHL	C6-C7-C8-C9
24	Y	302	CHL	C6-C7-C8-C9
24	n	607	CHL	C6-C7-C8-C9
24	y	302	CHL	C6-C7-C8-C9
25	A	405	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	C	504	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C12-C13-C14
25	G	602	CLA	C14-C13-C15-C16
25	G	610	CLA	C6-C7-C8-C9
25	a	406	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	c	504	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C12-C13-C14
25	c	510	CLA	C11-C12-C13-C14
25	s	303	CLA	C11-C12-C13-C14
25	g	602	CLA	C14-C13-C15-C16
25	g	610	CLA	C6-C7-C8-C9
26	C	517	LHG	C35-C36-C37-C38
26	c	517	LHG	C35-C36-C37-C38
26	B	622	LHG	C29-C30-C31-C32
26	b	622	LHG	C29-C30-C31-C32
35	b	626	DGD	CCA-CDA-CEA-CFA
29	L	103	SQD	C46-C45-O47-C7
29	l	101	SQD	C46-C45-O47-C7
35	B	626	DGD	CCA-CDA-CEA-CFA
30	B	620	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
30	b	620	LMG	O9-C10-O7-C8
25	N	612	CLA	C3-C5-C6-C7
25	n	612	CLA	C3-C5-C6-C7
24	G	605	CHL	C1A-C2A-CAA-CBA
24	g	605	CHL	C1A-C2A-CAA-CBA
25	S	310	CLA	C1-C2-C3-C4
25	N	610	CLA	C1-C2-C3-C4
25	s	310	CLA	C1-C2-C3-C4
25	n	610	CLA	C1-C2-C3-C4
35	A	415	DGD	C3A-C4A-C5A-C6A
35	a	401	DGD	C3A-C4A-C5A-C6A
25	S	313	CLA	C4-C3-C5-C6
25	s	313	CLA	C4-C3-C5-C6
25	y	311	CLA	C11-C12-C13-C14
25	G	612	CLA	CBD-CGD-O2D-CED
25	G	603	CLA	C2-C3-C5-C6
25	g	603	CLA	C2-C3-C5-C6
26	B	621	LHG	O1-C1-C2-O2
26	b	621	LHG	O1-C1-C2-O2
25	B	616	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C2A-CAA-CBA-CGA
25	b	616	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
24	Y	302	CHL	C5-C6-C7-C8
25	G	602	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C1A-C2A-CAA-CBA
25	Y	303	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	g	603	CLA	C1A-C2A-CAA-CBA
25	y	303	CLA	C1A-C2A-CAA-CBA
39	S	315	LUT	C32-C33-C34-C35
39	R	615	LUT	C12-C13-C14-C15
39	s	315	LUT	C32-C33-C34-C35
39	r	615	LUT	C12-C13-C14-C15
40	S	317	NEX	C11-C10-C9-C8
40	S	317	NEX	C28-C29-C30-C31
40	N	617	NEX	C28-C29-C30-C31
40	R	617	NEX	C28-C29-C30-C31
40	s	317	NEX	C11-C10-C9-C8
40	s	317	NEX	C28-C29-C30-C31
40	n	617	NEX	C28-C29-C30-C31
40	r	617	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
41	R	616	XAT	C12-C13-C14-C15
41	r	616	XAT	C12-C13-C14-C15
32	B	624	AJP	O40-C35-O34-C29
32	b	624	AJP	O40-C35-O34-C29
25	Y	311	CLA	C11-C12-C13-C14
24	1	302	CHL	CAA-CBA-CGA-O2A
24	5	302	CHL	CAA-CBA-CGA-O2A
24	y	302	CHL	C5-C6-C7-C8
25	A	402	CLA	C2B-C3B-CAB-CBB
25	B	611	CLA	C2B-C3B-CAB-CBB
25	B	612	CLA	C2B-C3B-CAB-CBB
25	B	614	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	C	506	CLA	C2B-C3B-CAB-CBB
25	C	507	CLA	C2B-C3B-CAB-CBB
25	C	508	CLA	C2B-C3B-CAB-CBB
25	C	511	CLA	C2B-C3B-CAB-CBB
25	S	304	CLA	C2B-C3B-CAB-CBB
25	S	310	CLA	C2B-C3B-CAB-CBB
25	S	313	CLA	C2B-C3B-CAB-CBB
25	G	602	CLA	C2B-C3B-CAB-CBB
25	N	603	CLA	C2B-C3B-CAB-CBB
25	Y	312	CLA	C2B-C3B-CAB-CBB
25	Y	315	CLA	C2B-C3B-CAB-CBB
25	R	608	CLA	C2B-C3B-CAB-CBB
25	R	612	CLA	C2B-C3B-CAB-CBB
25	a	403	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	b	612	CLA	C2B-C3B-CAB-CBB
25	b	614	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
25	c	506	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
25	c	508	CLA	C2B-C3B-CAB-CBB
25	c	511	CLA	C2B-C3B-CAB-CBB
25	s	304	CLA	C2B-C3B-CAB-CBB
25	s	310	CLA	C2B-C3B-CAB-CBB
25	s	313	CLA	C2B-C3B-CAB-CBB
25	g	602	CLA	C2B-C3B-CAB-CBB
25	n	603	CLA	C2B-C3B-CAB-CBB
25	y	312	CLA	C2B-C3B-CAB-CBB
25	y	315	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	r	608	CLA	C2B-C3B-CAB-CBB
25	r	612	CLA	C2B-C3B-CAB-CBB
28	B	618	BCR	C23-C24-C25-C26
28	D	404	BCR	C5-C6-C7-C8
28	K	101	BCR	C1-C6-C7-C8
28	Z	101	BCR	C5-C6-C7-C8
28	b	618	BCR	C23-C24-C25-C26
28	d	404	BCR	C5-C6-C7-C8
28	k	101	BCR	C1-C6-C7-C8
28	z	101	BCR	C5-C6-C7-C8
39	S	315	LUT	C1-C6-C7-C8
39	G	615	LUT	C5-C6-C7-C8
39	N	616	LUT	C5-C6-C7-C8
39	Y	316	LUT	C5-C6-C7-C8
39	R	615	LUT	C1-C6-C7-C8
39	R	615	LUT	C5-C6-C7-C8
39	s	315	LUT	C1-C6-C7-C8
39	g	615	LUT	C5-C6-C7-C8
39	n	616	LUT	C5-C6-C7-C8
39	y	316	LUT	C5-C6-C7-C8
39	r	615	LUT	C1-C6-C7-C8
39	r	615	LUT	C5-C6-C7-C8
25	g	612	CLA	CBD-CGD-O2D-CED
30	B	620	LMG	C11-C10-O7-C8
30	b	620	LMG	C11-C10-O7-C8
24	r	606	CHL	CAA-CBA-CGA-O2A
26	S	301	LHG	C19-C20-C21-C22
32	B	624	AJP	O40-C39-C41-O42
32	b	624	AJP	O40-C39-C41-O42
25	Y	315	CLA	C2C-C3C-CAC-CBC
25	C	505	CLA	C10-C11-C12-C13
25	c	505	CLA	C10-C11-C12-C13
35	A	415	DGD	CAB-CBB-CCB-CDB
35	a	401	DGD	CAB-CBB-CCB-CDB
24	Y	309	CHL	C3-C5-C6-C7
24	y	309	CHL	C3-C5-C6-C7
25	b	609	CLA	CBD-CGD-O2D-CED
26	s	301	LHG	C19-C20-C21-C22
24	R	606	CHL	CAA-CBA-CGA-O2A
25	B	613	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
31	D	405	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
31	d	405	PL9	C43-C44-C46-C47
25	y	303	CLA	C2C-C3C-CAC-CBC
26	y	319	LHG	C9-C10-C11-C12
24	2	601	CHL	C12-C13-C15-C16
24	N	608	CHL	C12-C13-C15-C16
24	6	601	CHL	C12-C13-C15-C16
24	n	608	CHL	C12-C13-C15-C16
25	A	405	CLA	C6-C7-C8-C10
25	B	602	CLA	C12-C13-C15-C16
25	B	607	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	C	507	CLA	C12-C13-C15-C16
25	G	602	CLA	C12-C13-C15-C16
25	Y	303	CLA	C11-C10-C8-C7
25	Y	314	CLA	C12-C13-C15-C16
25	R	609	CLA	C11-C12-C13-C15
25	a	406	CLA	C6-C7-C8-C10
25	b	602	CLA	C12-C13-C15-C16
25	b	607	CLA	C12-C13-C15-C16
25	c	506	CLA	C6-C7-C8-C10
25	c	507	CLA	C12-C13-C15-C16
25	g	602	CLA	C12-C13-C15-C16
25	y	303	CLA	C11-C10-C8-C7
25	y	314	CLA	C12-C13-C15-C16
25	r	609	CLA	C11-C12-C13-C15
35	C	515	DGD	O2G-C2G-C3G-O3G
35	c	515	DGD	O2G-C2G-C3G-O3G
25	y	315	CLA	C2C-C3C-CAC-CBC
25	Y	303	CLA	C2C-C3C-CAC-CBC
24	S	302	CHL	CAA-CBA-CGA-O1A
24	R	606	CHL	CAA-CBA-CGA-O1A
24	s	302	CHL	CAA-CBA-CGA-O1A
24	r	606	CHL	CAA-CBA-CGA-O1A
25	S	309	CLA	CAA-CBA-CGA-O2A
25	s	309	CLA	CAA-CBA-CGA-O2A
26	Y	319	LHG	C9-C10-C11-C12
25	B	609	CLA	CBD-CGD-O2D-CED
35	A	415	DGD	C7B-C8B-C9B-CAB
35	a	401	DGD	C7B-C8B-C9B-CAB
24	G	601	CHL	C2-C1-O2A-CGA
24	g	601	CHL	C2-C1-O2A-CGA
25	S	310	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	G	612	CLA	C11-C12-C13-C15
25	s	310	CLA	C6-C7-C8-C10
25	g	612	CLA	C11-C12-C13-C15
25	g	604	CLA	C4C-C3C-CAC-CBC
25	A	405	CLA	C6-C7-C8-C9
25	B	607	CLA	C11-C12-C13-C14
25	C	507	CLA	C14-C13-C15-C16
25	S	303	CLA	C11-C12-C13-C14
25	a	406	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	b	602	CLA	C10-C11-C12-C13
25	G	604	CLA	C4C-C3C-CAC-CBC
24	1	302	CHL	CAA-CBA-CGA-O1A
24	5	302	CHL	CAA-CBA-CGA-O1A
25	B	602	CLA	C10-C11-C12-C13
28	B	617	BCR	C22-C23-C24-C25
28	b	617	BCR	C22-C23-C24-C25
25	b	607	CLA	C4-C3-C5-C6
25	B	606	CLA	C16-C17-C18-C19
25	b	606	CLA	C16-C17-C18-C19
25	S	314	CLA	O2A-C1-C2-C3
25	s	314	CLA	O2A-C1-C2-C3
35	B	626	DGD	O2G-C1B-C2B-C3B
30	D	407	LMG	O1-C7-C8-C9
30	d	407	LMG	O1-C7-C8-C9
35	B	626	DGD	O1G-C1G-C2G-C3G
35	b	626	DGD	O1G-C1G-C2G-C3G
25	G	610	CLA	C15-C16-C17-C18
24	Y	302	CHL	C2A-CAA-CBA-CGA
24	y	302	CHL	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
25	R	612	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
25	r	612	CLA	C2A-CAA-CBA-CGA
25	g	610	CLA	C5-C6-C7-C8
26	B	621	LHG	O8-C23-C24-C25
35	b	626	DGD	O2G-C1B-C2B-C3B
24	G	607	CHL	CAA-CBA-CGA-O2A
24	g	607	CHL	CAA-CBA-CGA-O2A
25	g	610	CLA	C15-C16-C17-C18
29	a	412	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	A	412	AJP	O31-C30-C32-O33
32	a	413	AJP	O31-C30-C32-O33
25	B	607	CLA	C4-C3-C5-C6
26	b	621	LHG	O8-C23-C24-C25
29	A	411	SQD	C14-C15-C16-C17
25	G	610	CLA	C5-C6-C7-C8
25	B	603	CLA	C4B-C3B-CAB-CBB
25	N	603	CLA	C4B-C3B-CAB-CBB
25	b	603	CLA	C4B-C3B-CAB-CBB
25	n	603	CLA	C4B-C3B-CAB-CBB
26	b	622	LHG	C25-C26-C27-C28
26	B	622	LHG	C25-C26-C27-C28
24	S	302	CHL	CAA-CBA-CGA-O2A
24	N	606	CHL	CAA-CBA-CGA-O2A
24	s	302	CHL	CAA-CBA-CGA-O2A
24	n	606	CHL	CAA-CBA-CGA-O2A
25	Y	304	CLA	C16-C17-C18-C20
25	y	304	CLA	C16-C17-C18-C20
24	S	302	CHL	CHA-CBD-CGD-O1D
24	S	307	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	CHA-CBD-CGD-O2D
24	G	607	CHL	CHA-CBD-CGD-O2D
24	N	605	CHL	CHA-CBD-CGD-O2D
24	N	606	CHL	CHA-CBD-CGD-O1D
24	Y	302	CHL	CHA-CBD-CGD-O1D
24	Y	307	CHL	CHA-CBD-CGD-O2D
24	s	302	CHL	CHA-CBD-CGD-O1D
24	s	307	CHL	CHA-CBD-CGD-O2D
24	g	601	CHL	CHA-CBD-CGD-O2D
24	g	607	CHL	CHA-CBD-CGD-O2D
24	n	605	CHL	CHA-CBD-CGD-O2D
24	n	606	CHL	CHA-CBD-CGD-O1D
24	y	302	CHL	CHA-CBD-CGD-O1D
24	y	307	CHL	CHA-CBD-CGD-O2D
27	A	403	PHO	CHA-CBD-CGD-O1D
27	a	404	PHO	CHA-CBD-CGD-O1D
28	T	101	BCR	C20-C21-C22-C37
28	t	101	BCR	C20-C21-C22-C37
24	S	308	CHL	CAA-CBA-CGA-O2A
24	s	308	CHL	CAA-CBA-CGA-O2A
25	S	309	CLA	CAA-CBA-CGA-O1A
25	s	309	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	R	601	CLA	C4C-C3C-CAC-CBC
26	B	621	LHG	O6-C4-C5-C6
26	b	621	LHG	O6-C4-C5-C6
25	B	608	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
30	B	623	LMG	O1-C7-C8-O7
30	b	623	LMG	O1-C7-C8-O7
25	Y	315	CLA	CAA-CBA-CGA-O2A
26	B	622	LHG	C32-C33-C34-C35
26	b	622	LHG	C32-C33-C34-C35
30	A	410	LMG	C29-C30-C31-C32
27	A	403	PHO	C2-C3-C5-C6
27	a	404	PHO	C2-C3-C5-C6
29	L	101	SQD	O5-C1-O6-C44
29	l	102	SQD	O5-C1-O6-C44
24	g	607	CHL	O1D-CGD-O2D-CED
24	n	605	CHL	C2-C1-O2A-CGA
26	C	519	LHG	C31-C32-C33-C34
26	c	519	LHG	C31-C32-C33-C34
24	N	607	CHL	C6-C7-C8-C10
24	N	609	CHL	C11-C12-C13-C15
24	n	607	CHL	C6-C7-C8-C10
24	n	609	CHL	C11-C12-C13-C15
30	a	411	LMG	C29-C30-C31-C32
25	R	601	CLA	O2A-C1-C2-C3
25	r	601	CLA	O2A-C1-C2-C3
26	R	618	LHG	C27-C28-C29-C30
24	N	605	CHL	C2-C1-O2A-CGA
26	r	618	LHG	C27-C28-C29-C30
35	C	515	DGD	C8B-C9B-CAB-CBB
35	c	515	DGD	C8B-C9B-CAB-CBB
25	r	601	CLA	C4C-C3C-CAC-CBC
25	y	315	CLA	CAA-CBA-CGA-O2A
24	G	607	CHL	O1D-CGD-O2D-CED
25	B	602	CLA	C11-C10-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	c	510	CLA	C14-C13-C15-C16
30	A	410	LMG	C8-C7-O1-C1
30	a	411	LMG	C8-C7-O1-C1
25	B	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C13-C15-C16-C17
25	B	610	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2-C1-O2A-CGA
25	g	611	CLA	C2-C1-O2A-CGA
30	C	520	LMG	C18-C19-C20-C21
30	c	520	LMG	C18-C19-C20-C21
24	N	605	CHL	C3A-C2A-CAA-CBA
24	n	605	CHL	C3A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	C	505	CLA	C3A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	N	613	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
25	c	505	CLA	C3A-C2A-CAA-CBA
25	g	603	CLA	C3A-C2A-CAA-CBA
25	n	613	CLA	C3A-C2A-CAA-CBA
25	R	602	CLA	CAA-CBA-CGA-O2A
25	r	602	CLA	CAA-CBA-CGA-O2A
31	D	405	PL9	C18-C19-C21-C22
31	d	405	PL9	C18-C19-C21-C22
24	S	306	CHL	CAA-CBA-CGA-O1A
24	s	306	CHL	CAA-CBA-CGA-O1A
30	B	623	LMG	C41-C42-C43-C44
30	b	623	LMG	C41-C42-C43-C44
30	B	620	LMG	O6-C5-C6-O5
30	b	620	LMG	O6-C5-C6-O5
29	A	407	SQD	C18-C19-C20-C21
29	a	408	SQD	C18-C19-C20-C21
24	y	308	CHL	C5-C6-C7-C8
25	B	612	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	s	305	CLA	O1A-CGA-O2A-C1
24	Y	308	CHL	C5-C6-C7-C8
30	C	520	LMG	C39-C40-C41-C42
30	c	520	LMG	C39-C40-C41-C42
35	C	516	DGD	C5A-C6A-C7A-C8A
35	c	516	DGD	C5A-C6A-C7A-C8A
40	G	617	NEX	O24-C26-C27-C28
40	g	617	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	L	103	SQD	C16-C17-C18-C19
29	l	101	SQD	C16-C17-C18-C19
26	2	606	LHG	O6-C4-C5-O7
26	6	606	LHG	O6-C4-C5-O7
25	S	305	CLA	O1A-CGA-O2A-C1
26	N	618	LHG	C4-C5-C6-O8
26	n	618	LHG	C4-C5-C6-O8
29	A	407	SQD	O6-C44-C45-C46
29	a	408	SQD	O6-C44-C45-C46
35	C	515	DGD	C1G-C2G-C3G-O3G
35	c	515	DGD	C1G-C2G-C3G-O3G
24	n	609	CHL	C10-C11-C12-C13
25	N	610	CLA	C8-C10-C11-C12
25	n	610	CLA	C8-C10-C11-C12
24	G	605	CHL	CAA-CBA-CGA-O2A
24	g	605	CHL	CAA-CBA-CGA-O2A
25	Y	303	CLA	C4C-C3C-CAC-CBC
26	b	625	LHG	C11-C12-C13-C14
26	D	406	LHG	C29-C30-C31-C32
26	d	406	LHG	C29-C30-C31-C32
26	B	625	LHG	C11-C12-C13-C14
40	R	617	NEX	C7-C8-C9-C19
40	r	617	NEX	C7-C8-C9-C19
25	y	303	CLA	C4C-C3C-CAC-CBC
24	N	609	CHL	C10-C11-C12-C13
26	n	618	LHG	C29-C30-C31-C32
35	C	515	DGD	O2G-C1B-C2B-C3B
32	G	618	AJP	O31-C30-C32-O33
32	Y	322	AJP	O31-C30-C32-O33
32	g	618	AJP	O31-C30-C32-O33
32	y	322	AJP	O31-C30-C32-O33
25	N	610	CLA	C5-C6-C7-C8
25	n	610	CLA	C5-C6-C7-C8
24	G	601	CHL	C11-C10-C8-C9
24	N	607	CHL	C11-C10-C8-C9
24	g	601	CHL	C11-C10-C8-C9
24	n	607	CHL	C11-C10-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	B	604	CLA	C11-C10-C8-C9
25	C	510	CLA	C14-C13-C15-C16
25	G	603	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C11-C10-C8-C9
25	g	603	CLA	C6-C7-C8-C9
25	B	616	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C19
30	A	410	LMG	C4-C5-C6-O5
30	a	411	LMG	C4-C5-C6-O5
25	B	613	CLA	CAA-CBA-CGA-O2A
25	b	613	CLA	CAA-CBA-CGA-O2A
35	c	515	DGD	O2G-C1B-C2B-C3B
29	A	407	SQD	C14-C15-C16-C17
29	a	408	SQD	C14-C15-C16-C17
26	N	618	LHG	C29-C30-C31-C32
25	B	608	CLA	C10-C11-C12-C13
25	b	608	CLA	C10-C11-C12-C13
35	C	516	DGD	C6A-C7A-C8A-C9A
24	Y	307	CHL	CAA-CBA-CGA-O2A
24	y	307	CHL	CAA-CBA-CGA-O2A
26	N	618	LHG	C9-C10-C11-C12
26	n	618	LHG	C9-C10-C11-C12
24	N	608	CHL	C11-C10-C8-C7
24	n	608	CHL	C11-C10-C8-C7
25	A	401	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C10-C8-C7
25	C	501	CLA	C12-C13-C15-C16
25	R	602	CLA	C11-C10-C8-C7
25	R	608	CLA	C6-C7-C8-C10
25	a	402	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C10-C8-C7
25	c	501	CLA	C12-C13-C15-C16
25	r	602	CLA	C11-C10-C8-C7
25	r	608	CLA	C6-C7-C8-C10
35	c	516	DGD	C6A-C7A-C8A-C9A
26	y	319	LHG	C15-C16-C17-C18
25	A	405	CLA	C2B-C3B-CAB-CBB
25	B	603	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C2B-C3B-CAB-CBB
25	B	608	CLA	C2B-C3B-CAB-CBB
25	B	609	CLA	C2B-C3B-CAB-CBB
25	B	616	CLA	C2B-C3B-CAB-CBB
25	S	303	CLA	C2B-C3B-CAB-CBB
25	N	610	CLA	C2B-C3B-CAB-CBB
25	Y	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	R	604	CLA	C2B-C3B-CAB-CBB
25	R	609	CLA	C2B-C3B-CAB-CBB
25	R	610	CLA	C2B-C3B-CAB-CBB
25	a	406	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	b	608	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	s	303	CLA	C2B-C3B-CAB-CBB
25	n	610	CLA	C2B-C3B-CAB-CBB
25	y	311	CLA	C2B-C3B-CAB-CBB
25	r	604	CLA	C2B-C3B-CAB-CBB
25	r	609	CLA	C2B-C3B-CAB-CBB
25	r	610	CLA	C2B-C3B-CAB-CBB
28	B	619	BCR	C23-C24-C25-C26
28	K	101	BCR	C5-C6-C7-C8
28	b	619	BCR	C23-C24-C25-C26
28	k	101	BCR	C5-C6-C7-C8
39	G	615	LUT	C1-C6-C7-C8
39	g	615	LUT	C1-C6-C7-C8
25	B	616	CLA	CAA-CBA-CGA-O2A
25	b	616	CLA	CAA-CBA-CGA-O2A
35	C	516	DGD	O1B-C1B-O2G-C2G
24	G	608	CHL	C2-C1-O2A-CGA
24	N	609	CHL	C2-C1-O2A-CGA
24	g	608	CHL	C2-C1-O2A-CGA
24	n	609	CHL	C2-C1-O2A-CGA
25	A	401	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	a	402	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
26	6	606	LHG	C24-C25-C26-C27
25	B	606	CLA	C16-C17-C18-C20
25	b	606	CLA	C16-C17-C18-C20
26	2	606	LHG	C24-C25-C26-C27
26	Y	319	LHG	C15-C16-C17-C18
24	S	306	CHL	CAA-CBA-CGA-O2A
24	s	306	CHL	CAA-CBA-CGA-O2A
35	A	415	DGD	O2G-C1B-C2B-C3B
35	a	401	DGD	O2G-C1B-C2B-C3B
25	B	608	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C2-C3-C5-C6
25	C	508	CLA	C2C-C3C-CAC-CBC
30	A	408	LMG	O9-C10-O7-C8
30	a	409	LMG	O9-C10-O7-C8
35	c	516	DGD	O1B-C1B-O2G-C2G
35	C	516	DGD	CBA-CCA-CDA-CEA
24	N	606	CHL	C1C-C2C-CMC-OMC
24	R	613	CHL	C1C-C2C-CMC-OMC
24	n	606	CHL	C1C-C2C-CMC-OMC
24	r	613	CHL	C1C-C2C-CMC-OMC
35	c	516	DGD	CBA-CCA-CDA-CEA
35	C	516	DGD	C2B-C1B-O2G-C2G
35	c	516	DGD	C2B-C1B-O2G-C2G
25	c	508	CLA	C2C-C3C-CAC-CBC
26	2	606	LHG	O10-C23-O8-C6
25	C	512	CLA	CAA-CBA-CGA-O2A
25	Y	304	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	CAA-CBA-CGA-O2A
25	y	304	CLA	CAA-CBA-CGA-O2A
26	D	406	LHG	C13-C14-C15-C16
26	d	406	LHG	C13-C14-C15-C16
24	N	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C20
25	C	507	CLA	C5-C6-C7-C8
25	D	402	CLA	CAA-CBA-CGA-O2A
25	D	403	CLA	CAA-CBA-CGA-O2A
25	S	313	CLA	CAA-CBA-CGA-O2A
25	d	402	CLA	CAA-CBA-CGA-O2A
25	d	403	CLA	CAA-CBA-CGA-O2A
25	s	313	CLA	CAA-CBA-CGA-O2A
26	R	618	LHG	O7-C7-C8-C9
26	r	618	LHG	O7-C7-C8-C9
26	6	606	LHG	O10-C23-O8-C6
30	D	407	LMG	C14-C15-C16-C17
30	d	407	LMG	C14-C15-C16-C17
25	C	501	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
25	c	507	CLA	C5-C6-C7-C8
30	a	411	LMG	C30-C31-C32-C33
24	6	601	CHL	CBA-CGA-O2A-C1
32	B	624	AJP	C28-C29-O34-C35
32	b	624	AJP	C28-C29-O34-C35

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Mol	Chain	Res	Type	Atoms
25	g	602	CLA	C13-C15-C16-C17
30	A	410	LMG	C30-C31-C32-C33
25	G	602	CLA	C13-C15-C16-C17
29	A	407	SQD	O47-C7-C8-C9
29	a	408	SQD	O47-C7-C8-C9
24	2	601	CHL	CBA-CGA-O2A-C1
26	y	301	LHG	O10-C23-C24-C25
25	B	611	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	G	613	CLA	C14-C13-C15-C16
25	N	611	CLA	C6-C7-C8-C9
25	Y	304	CLA	C6-C7-C8-C9
25	b	611	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
25	g	613	CLA	C14-C13-C15-C16
25	n	611	CLA	C6-C7-C8-C9
25	y	304	CLA	C6-C7-C8-C9
28	D	404	BCR	C7-C8-C9-C34
28	I	101	BCR	C7-C8-C9-C34
28	d	404	BCR	C7-C8-C9-C34
25	n	603	CLA	CAA-CBA-CGA-O2A
26	D	406	LHG	O8-C23-C24-C25
26	d	406	LHG	O8-C23-C24-C25
30	C	520	LMG	O8-C28-C29-C30
24	N	605	CHL	O1A-CGA-O2A-C1
26	Y	301	LHG	O10-C23-C24-C25
29	A	407	SQD	C44-C45-C46-O48
29	a	408	SQD	C44-C45-C46-O48
30	B	623	LMG	O1-C7-C8-C9
30	b	623	LMG	O1-C7-C8-C9
25	C	509	CLA	C13-C15-C16-C17
25	c	509	CLA	C13-C15-C16-C17
25	2	604	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C4B-C3B-CAB-CBB
25	N	612	CLA	C1A-C2A-CAA-CBA
25	Y	311	CLA	C4B-C3B-CAB-CBB
25	R	612	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C4B-C3B-CAB-CBB
25	n	612	CLA	C1A-C2A-CAA-CBA
25	y	311	CLA	C4B-C3B-CAB-CBB
25	r	612	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	A	408	LMG	C11-C10-O7-C8
25	B	612	CLA	CAA-CBA-CGA-O2A
25	G	612	CLA	CAA-CBA-CGA-O2A
25	N	612	CLA	CAA-CBA-CGA-O2A
25	g	612	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
30	c	520	LMG	O8-C28-C29-C30
26	B	622	LHG	O7-C5-C6-O8
26	b	622	LHG	O7-C5-C6-O8
26	Y	319	LHG	C27-C28-C29-C30
26	y	319	LHG	C27-C28-C29-C30
39	S	316	LUT	C29-C30-C31-C32
39	G	615	LUT	C33-C34-C35-C15
39	s	316	LUT	C29-C30-C31-C32
39	g	615	LUT	C33-C34-C35-C15
25	g	611	CLA	C11-C12-C13-C14
25	b	612	CLA	CAA-CBA-CGA-O2A
24	g	601	CHL	C2A-CAA-CBA-CGA
35	C	515	DGD	CDB-CEB-CFB-CGB
35	c	515	DGD	CDB-CEB-CFB-CGB
35	C	515	DGD	C5B-C6B-C7B-C8B
24	n	605	CHL	O1A-CGA-O2A-C1
35	c	515	DGD	C5B-C6B-C7B-C8B
25	G	611	CLA	C11-C12-C13-C14
25	N	603	CLA	CAA-CBA-CGA-O2A
26	Y	319	LHG	C28-C29-C30-C31
35	C	516	DGD	C4E-C5E-C6E-O5E
30	a	409	LMG	C11-C10-O7-C8
26	y	319	LHG	C28-C29-C30-C31
32	Y	323	AJP	C29-C30-C32-O33
32	y	323	AJP	C29-C30-C32-O33
25	B	615	CLA	C4-C3-C5-C6
25	b	615	CLA	C4-C3-C5-C6
24	Y	308	CHL	C2-C1-O2A-CGA
24	y	308	CHL	C2-C1-O2A-CGA
25	B	613	CLA	C2-C1-O2A-CGA
25	b	613	CLA	C2-C1-O2A-CGA
24	G	606	CHL	CAA-CBA-CGA-O2A
25	N	611	CLA	CAA-CBA-CGA-O2A
25	n	611	CLA	CAA-CBA-CGA-O2A
26	b	622	LHG	C16-C17-C18-C19
35	c	516	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C6-C7-C8-C10
25	N	603	CLA	C6-C7-C8-C10
25	b	601	CLA	C6-C7-C8-C10
25	n	603	CLA	C6-C7-C8-C10
25	Y	305	CLA	CBA-CGA-O2A-C1
25	y	305	CLA	CBA-CGA-O2A-C1
26	2	606	LHG	C24-C23-O8-C6
26	6	606	LHG	C24-C23-O8-C6
26	B	622	LHG	C16-C17-C18-C19
26	R	618	LHG	C14-C15-C16-C17
26	r	618	LHG	C14-C15-C16-C17
26	L	102	LHG	C23-C24-C25-C26
26	l	103	LHG	C23-C24-C25-C26
26	L	102	LHG	C4-C5-O7-C7
26	l	103	LHG	C4-C5-O7-C7
24	g	606	CHL	CAA-CBA-CGA-O2A
24	G	601	CHL	C2A-CAA-CBA-CGA
26	S	318	LHG	C32-C33-C34-C35
24	G	607	CHL	CAA-CBA-CGA-O1A
24	g	607	CHL	CAA-CBA-CGA-O1A
25	r	614	CLA	CAA-CBA-CGA-O1A
30	A	410	LMG	C34-C35-C36-C37
30	a	411	LMG	C34-C35-C36-C37
26	s	318	LHG	C32-C33-C34-C35
26	B	625	LHG	C31-C32-C33-C34
25	y	303	CLA	C8-C10-C11-C12
25	R	614	CLA	CAA-CBA-CGA-O1A
24	G	608	CHL	C4-C3-C5-C6
25	B	602	CLA	C3A-C2A-CAA-CBA
25	N	612	CLA	C3A-C2A-CAA-CBA
25	b	602	CLA	C3A-C2A-CAA-CBA
25	n	612	CLA	C3A-C2A-CAA-CBA
25	N	612	CLA	O1A-CGA-O2A-C1
25	B	605	CLA	C13-C15-C16-C17
25	b	605	CLA	C13-C15-C16-C17
26	b	625	LHG	C31-C32-C33-C34
25	S	303	CLA	C2-C3-C5-C6
25	s	303	CLA	C2-C3-C5-C6
30	B	623	LMG	C20-C21-C22-C23
30	b	623	LMG	C20-C21-C22-C23
25	C	501	CLA	O1A-CGA-O2A-C1
25	C	507	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	CBA-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
24	y	307	CHL	CAA-CBA-CGA-O1A
35	C	515	DGD	O1B-C1B-C2B-C3B
35	c	515	DGD	O1B-C1B-C2B-C3B
25	n	611	CLA	C11-C12-C13-C15
26	C	518	LHG	C23-C24-C25-C26
25	D	403	CLA	C2A-CAA-CBA-CGA
25	d	403	CLA	C2A-CAA-CBA-CGA
24	n	609	CHL	CAA-CBA-CGA-O2A
24	Y	307	CHL	CAA-CBA-CGA-O1A
25	Y	303	CLA	C8-C10-C11-C12
25	Y	304	CLA	C8-C10-C11-C12
25	c	508	CLA	C5-C6-C7-C8
25	y	304	CLA	C8-C10-C11-C12
25	N	611	CLA	C11-C12-C13-C15
25	C	508	CLA	C5-C6-C7-C8
24	g	608	CHL	C4-C3-C5-C6
25	S	311	CLA	C4-C3-C5-C6
25	G	610	CLA	C4-C3-C5-C6
25	s	311	CLA	C4-C3-C5-C6
25	g	610	CLA	C4-C3-C5-C6
25	R	603	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
25	G	602	CLA	C8-C10-C11-C12
25	g	602	CLA	C8-C10-C11-C12
39	G	615	LUT	C21-C26-C27-C28
39	N	615	LUT	C21-C26-C27-C28
39	Y	316	LUT	C21-C26-C27-C28
39	g	615	LUT	C21-C26-C27-C28
39	n	615	LUT	C21-C26-C27-C28
39	y	316	LUT	C21-C26-C27-C28
39	y	317	LUT	C21-C26-C27-C28
25	n	612	CLA	O1A-CGA-O2A-C1
25	N	612	CLA	CAA-CBA-CGA-O1A
25	n	612	CLA	CAA-CBA-CGA-O1A
35	A	415	DGD	O1B-C1B-C2B-C3B
35	a	401	DGD	O1B-C1B-C2B-C3B
25	B	606	CLA	C15-C16-C17-C18
25	b	606	CLA	C15-C16-C17-C18
25	r	614	CLA	CAA-CBA-CGA-O2A
25	n	611	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	R	614	CLA	CAA-CBA-CGA-O2A
26	s	318	LHG	C34-C35-C36-C37
25	G	613	CLA	CAA-CBA-CGA-O1A
25	N	611	CLA	CAA-CBA-CGA-O1A
25	g	613	CLA	CAA-CBA-CGA-O1A
24	N	609	CHL	CAA-CBA-CGA-O2A
26	S	318	LHG	C34-C35-C36-C37
35	B	626	DGD	C9A-CAA-CBA-CCA
25	C	508	CLA	C4C-C3C-CAC-CBC
24	G	606	CHL	CAA-CBA-CGA-O1A
24	g	606	CHL	CAA-CBA-CGA-O1A
26	c	518	LHG	C23-C24-C25-C26
35	b	626	DGD	C9A-CAA-CBA-CCA
25	B	615	CLA	C13-C15-C16-C17
25	C	501	CLA	C15-C16-C17-C18
25	b	615	CLA	C13-C15-C16-C17
25	c	501	CLA	C15-C16-C17-C18
26	R	618	LHG	O8-C23-C24-C25
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
26	R	618	LHG	O9-C7-C8-C9
26	r	618	LHG	O9-C7-C8-C9
29	A	407	SQD	O49-C7-C8-C9
29	a	408	SQD	O49-C7-C8-C9
30	c	520	LMG	O10-C28-C29-C30
25	c	508	CLA	C4C-C3C-CAC-CBC
24	N	607	CHL	CAD-CBD-CGD-O2D
24	n	607	CHL	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	C	509	CLA	CAD-CBD-CGD-O2D
25	N	602	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	n	602	CLA	CAD-CBD-CGD-O2D
25	g	613	CLA	CAA-CBA-CGA-O2A
24	N	606	CHL	CAA-CBA-CGA-O1A
24	n	606	CHL	CAA-CBA-CGA-O1A
30	D	407	LMG	C22-C23-C24-C25
30	d	407	LMG	C22-C23-C24-C25
25	G	604	CLA	C2-C1-O2A-CGA
25	g	604	CLA	C2-C1-O2A-CGA
25	B	616	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	b	616	CLA	CAA-CBA-CGA-O1A
30	C	520	LMG	O10-C28-C29-C30
25	G	613	CLA	CAA-CBA-CGA-O2A
26	r	618	LHG	O8-C23-C24-C25
25	B	603	CLA	C1-C2-C3-C4
25	B	607	CLA	C1-C2-C3-C4
25	G	612	CLA	C1-C2-C3-C4
25	b	603	CLA	C1-C2-C3-C4
25	b	607	CLA	C1-C2-C3-C4
25	g	612	CLA	C1-C2-C3-C4
35	C	516	DGD	C7B-C8B-C9B-CAB
35	c	516	DGD	C7B-C8B-C9B-CAB
25	g	611	CLA	C10-C11-C12-C13
25	G	603	CLA	CAA-CBA-CGA-O2A
26	Y	301	LHG	O7-C7-C8-C9
26	y	301	LHG	O7-C7-C8-C9
27	A	404	PHO	CAA-CBA-CGA-O2A
27	a	405	PHO	CAA-CBA-CGA-O2A
26	d	406	LHG	O10-C23-C24-C25
29	A	411	SQD	C28-C29-C30-C31
29	a	412	SQD	C28-C29-C30-C31
24	N	605	CHL	CAA-CBA-CGA-O2A
24	n	605	CHL	CAA-CBA-CGA-O2A
24	n	608	CHL	CAA-CBA-CGA-O2A
25	S	311	CLA	CAA-CBA-CGA-O2A
25	s	311	CLA	CAA-CBA-CGA-O2A
25	G	611	CLA	C10-C11-C12-C13
25	C	501	CLA	CAA-CBA-CGA-O1A
25	c	501	CLA	CAA-CBA-CGA-O1A
26	D	406	LHG	O10-C23-C24-C25

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	Y	318	NEX	C1-C2-C3-C4-C5-C6
40	y	318	NEX	C1-C2-C3-C4-C5-C6

356 monomers are involved in 3261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	605	CHL	4	0
30	a	409	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	D	404	BCR	3	0
30	B	620	LMG	5	0
28	t	101	BCR	21	0
26	2	606	LHG	14	0
24	Y	308	CHL	17	0
26	y	319	LHG	8	0
24	l	302	CHL	9	0
28	h	101	BCR	8	0
24	R	606	CHL	2	0
26	n	618	LHG	10	0
25	b	614	CLA	10	0
26	S	318	LHG	5	0
28	k	101	BCR	9	0
25	b	613	CLA	14	0
24	s	307	CHL	7	0
24	S	306	CHL	10	0
24	s	308	CHL	9	0
25	n	614	CLA	6	0
25	B	609	CLA	11	0
39	Y	316	LUT	12	0
25	S	313	CLA	12	0
25	s	310	CLA	15	0
25	B	602	CLA	8	0
25	S	314	CLA	10	0
25	b	602	CLA	9	0
24	N	607	CHL	48	0
25	d	403	CLA	15	0
28	b	619	BCR	4	0
24	n	605	CHL	5	0
26	c	517	LHG	3	0
25	n	612	CLA	10	0
25	r	612	CLA	19	0
24	N	606	CHL	18	0
24	g	609	CHL	10	0
32	n	619	AJP	2	0
30	C	520	LMG	4	0
25	N	603	CLA	33	0
25	C	501	CLA	18	0
31	A	409	PL9	2	0
25	B	612	CLA	6	0
24	5	301	CHL	9	0
26	c	519	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	S	301	LHG	8	0
25	R	612	CLA	19	0
25	D	402	CLA	19	0
25	s	311	CLA	9	0
30	A	408	LMG	3	0
24	y	310	CHL	18	0
25	C	507	CLA	6	0
26	b	622	LHG	8	0
24	l	301	CHL	9	0
26	6	606	LHG	14	0
31	a	410	PL9	2	0
26	c	518	LHG	3	0
24	G	605	CHL	4	0
24	y	308	CHL	14	0
25	S	304	CLA	12	0
25	S	311	CLA	8	0
38	F	101	HEM	7	0
40	y	318	NEX	10	0
32	N	620	AJP	1	0
25	y	312	CLA	11	0
31	D	405	PL9	6	0
24	y	306	CHL	5	0
25	b	605	CLA	9	0
24	N	605	CHL	5	0
25	B	608	CLA	8	0
40	S	317	NEX	6	0
39	y	316	LUT	13	0
39	s	316	LUT	22	0
24	y	302	CHL	31	0
24	Y	302	CHL	30	0
25	B	605	CLA	7	0
25	C	510	CLA	23	0
25	N	611	CLA	7	0
25	g	613	CLA	17	0
25	b	612	CLA	7	0
25	N	610	CLA	34	0
25	c	504	CLA	15	0
26	R	618	LHG	14	0
26	C	519	LHG	4	0
25	R	608	CLA	18	0
28	K	101	BCR	7	0
25	b	607	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	R	602	CLA	15	0
35	c	515	DGD	7	0
25	2	604	CLA	19	0
25	C	503	CLA	4	0
24	N	608	CHL	11	0
26	D	406	LHG	10	0
25	r	609	CLA	7	0
40	s	317	NEX	5	0
25	B	607	CLA	15	0
40	n	617	NEX	13	0
25	g	603	CLA	14	0
39	G	615	LUT	15	0
40	r	617	NEX	10	0
25	a	406	CLA	9	0
26	B	625	LHG	7	0
25	G	603	CLA	12	0
38	f	101	HEM	8	0
26	y	301	LHG	12	0
25	c	506	CLA	10	0
28	d	404	BCR	3	0
24	2	603	CHL	21	0
26	N	618	LHG	11	0
25	s	313	CLA	9	0
28	z	101	BCR	5	0
35	A	415	DGD	3	0
40	R	617	NEX	8	0
25	b	608	CLA	9	0
25	B	601	CLA	10	0
32	Y	322	AJP	2	0
24	n	607	CHL	50	0
25	2	605	CLA	6	0
29	a	412	SQD	6	0
27	A	403	PHO	13	0
25	c	508	CLA	12	0
26	Y	301	LHG	13	0
30	b	623	LMG	5	0
30	A	410	LMG	3	0
25	a	403	CLA	13	0
35	b	626	DGD	6	0
26	C	518	LHG	3	0
25	s	305	CLA	15	0
25	b	616	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	y	314	CLA	17	0
26	B	622	LHG	8	0
25	r	603	CLA	17	0
24	g	601	CHL	15	0
25	C	511	CLA	20	0
25	Y	311	CLA	25	0
25	c	510	CLA	24	0
25	g	611	CLA	14	0
25	R	603	CLA	17	0
32	Y	320	AJP	3	0
25	G	613	CLA	18	0
25	G	614	CLA	5	0
25	Y	313	CLA	9	0
28	Z	101	BCR	5	0
24	r	607	CHL	9	0
39	n	615	LUT	12	0
39	r	615	LUT	8	0
25	C	504	CLA	14	0
25	c	503	CLA	5	0
25	n	603	CLA	33	0
25	b	603	CLA	6	0
25	c	513	CLA	17	0
25	b	604	CLA	14	0
28	A	406	BCR	4	0
28	C	514	BCR	7	0
25	Y	303	CLA	26	0
25	N	602	CLA	22	0
33	a	414	BCT	1	0
28	B	618	BCR	7	0
27	a	404	PHO	14	0
25	S	310	CLA	14	0
25	c	507	CLA	7	0
25	n	613	CLA	28	0
25	r	614	CLA	13	0
24	s	306	CHL	11	0
29	A	411	SQD	5	0
25	Y	305	CLA	4	0
24	Y	306	CHL	6	0
28	a	407	BCR	5	0
25	B	611	CLA	7	0
25	R	614	CLA	11	0
25	C	506	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	614	CLA	12	0
25	b	606	CLA	16	0
40	G	617	NEX	15	0
32	n	620	AJP	1	0
29	l	101	SQD	5	0
28	i	101	BCR	20	0
24	R	613	CHL	4	0
33	A	413	BCT	2	0
39	g	616	LUT	15	0
25	s	303	CLA	15	0
40	g	617	NEX	15	0
25	N	612	CLA	10	0
39	G	616	LUT	15	0
25	Y	304	CLA	23	0
32	N	619	AJP	2	0
32	y	322	AJP	2	0
25	c	512	CLA	12	0
24	G	606	CHL	19	0
41	R	616	XAT	20	0
24	r	613	CHL	4	0
40	Y	318	NEX	7	0
24	r	606	CHL	2	0
39	g	615	LUT	15	0
25	s	314	CLA	10	0
25	D	401	CLA	8	0
27	A	404	PHO	14	0
25	C	513	CLA	15	0
25	S	303	CLA	14	0
24	g	607	CHL	11	0
25	s	309	CLA	3	0
25	y	311	CLA	24	0
24	G	607	CHL	11	0
25	Y	315	CLA	17	0
25	s	304	CLA	12	0
31	d	405	PL9	6	0
25	c	502	CLA	12	0
41	r	616	XAT	22	0
26	l	103	LHG	5	0
24	2	601	CHL	8	0
25	G	610	CLA	37	0
25	y	313	CLA	9	0
26	C	517	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	y	321	AJP	2	0
30	D	407	LMG	3	0
25	S	309	CLA	3	0
30	d	407	LMG	3	0
26	d	406	LHG	10	0
24	n	606	CHL	17	0
25	N	613	CLA	30	0
25	2	602	CLA	8	0
25	S	312	CLA	9	0
29	L	103	SQD	6	0
29	a	408	SQD	6	0
24	r	605	CHL	9	0
25	G	611	CLA	12	0
25	R	609	CLA	5	0
24	Y	309	CHL	14	0
26	s	318	LHG	6	0
32	y	320	AJP	3	0
25	B	616	CLA	14	0
25	Y	314	CLA	15	0
26	s	301	LHG	9	0
25	B	613	CLA	16	0
24	R	607	CHL	9	0
24	G	608	CHL	19	0
39	N	616	LUT	15	0
24	N	609	CHL	26	0
25	g	614	CLA	4	0
35	C	516	DGD	10	0
40	N	617	NEX	15	0
25	A	405	CLA	9	0
25	n	611	CLA	7	0
39	S	315	LUT	7	0
25	D	403	CLA	15	0
35	B	626	DGD	5	0
39	Y	317	LUT	13	0
32	s	319	AJP	2	0
28	c	514	BCR	7	0
29	l	102	SQD	20	0
24	n	601	CHL	16	0
24	6	603	CHL	20	0
25	r	601	CLA	17	0
24	g	608	CHL	20	0
25	y	303	CLA	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	r	610	CLA	11	0
25	N	604	CLA	9	0
25	y	305	CLA	4	0
30	c	520	LMG	4	0
25	R	611	CLA	3	0
25	B	606	CLA	15	0
26	b	621	LHG	3	0
25	c	505	CLA	10	0
30	B	623	LMG	5	0
25	R	610	CLA	11	0
32	S	319	AJP	2	0
25	B	603	CLA	6	0
25	G	604	CLA	12	0
39	R	615	LUT	6	0
26	Y	319	LHG	7	0
28	b	618	BCR	8	0
24	N	601	CHL	18	0
25	6	602	CLA	10	0
25	A	401	CLA	19	0
28	B	619	BCR	4	0
24	s	302	CHL	7	0
24	y	307	CHL	15	0
30	a	411	LMG	3	0
25	b	611	CLA	7	0
25	r	611	CLA	4	0
25	y	304	CLA	20	0
25	B	615	CLA	15	0
25	b	610	CLA	14	0
25	C	512	CLA	12	0
25	c	509	CLA	9	0
25	d	401	CLA	9	0
24	G	609	CHL	10	0
25	6	604	CLA	19	0
25	g	604	CLA	12	0
30	b	620	LMG	5	0
25	c	511	CLA	21	0
25	S	305	CLA	14	0
25	B	610	CLA	14	0
28	B	617	BCR	7	0
32	Y	321	AJP	2	0
24	S	307	CHL	6	0
39	N	615	LUT	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	n	604	CLA	8	0
24	6	601	CHL	10	0
24	n	608	CHL	9	0
25	6	605	CLA	8	0
29	L	101	SQD	19	0
25	b	609	CLA	11	0
25	y	315	CLA	17	0
25	C	502	CLA	12	0
39	y	317	LUT	12	0
25	c	501	CLA	19	0
25	r	608	CLA	17	0
25	s	312	CLA	10	0
25	B	604	CLA	14	0
39	n	616	LUT	15	0
24	n	609	CHL	29	0
24	S	308	CHL	9	0
25	a	402	CLA	19	0
24	Y	310	CHL	17	0
24	y	309	CHL	14	0
25	A	402	CLA	13	0
25	d	402	CLA	19	0
25	n	602	CLA	23	0
25	N	614	CLA	6	0
28	T	101	BCR	20	0
25	r	604	CLA	10	0
24	G	601	CHL	17	0
39	S	316	LUT	20	0
26	B	621	LHG	3	0
25	Y	312	CLA	10	0
28	b	617	BCR	7	0
24	g	606	CHL	19	0
29	A	407	SQD	8	0
25	R	601	CLA	15	0
25	R	604	CLA	8	0
25	C	508	CLA	10	0
35	a	401	DGD	3	0
24	S	302	CHL	4	0
26	r	618	LHG	16	0
28	H	101	BCR	6	0
27	a	405	PHO	14	0
25	C	505	CLA	10	0
39	s	315	LUT	7	0

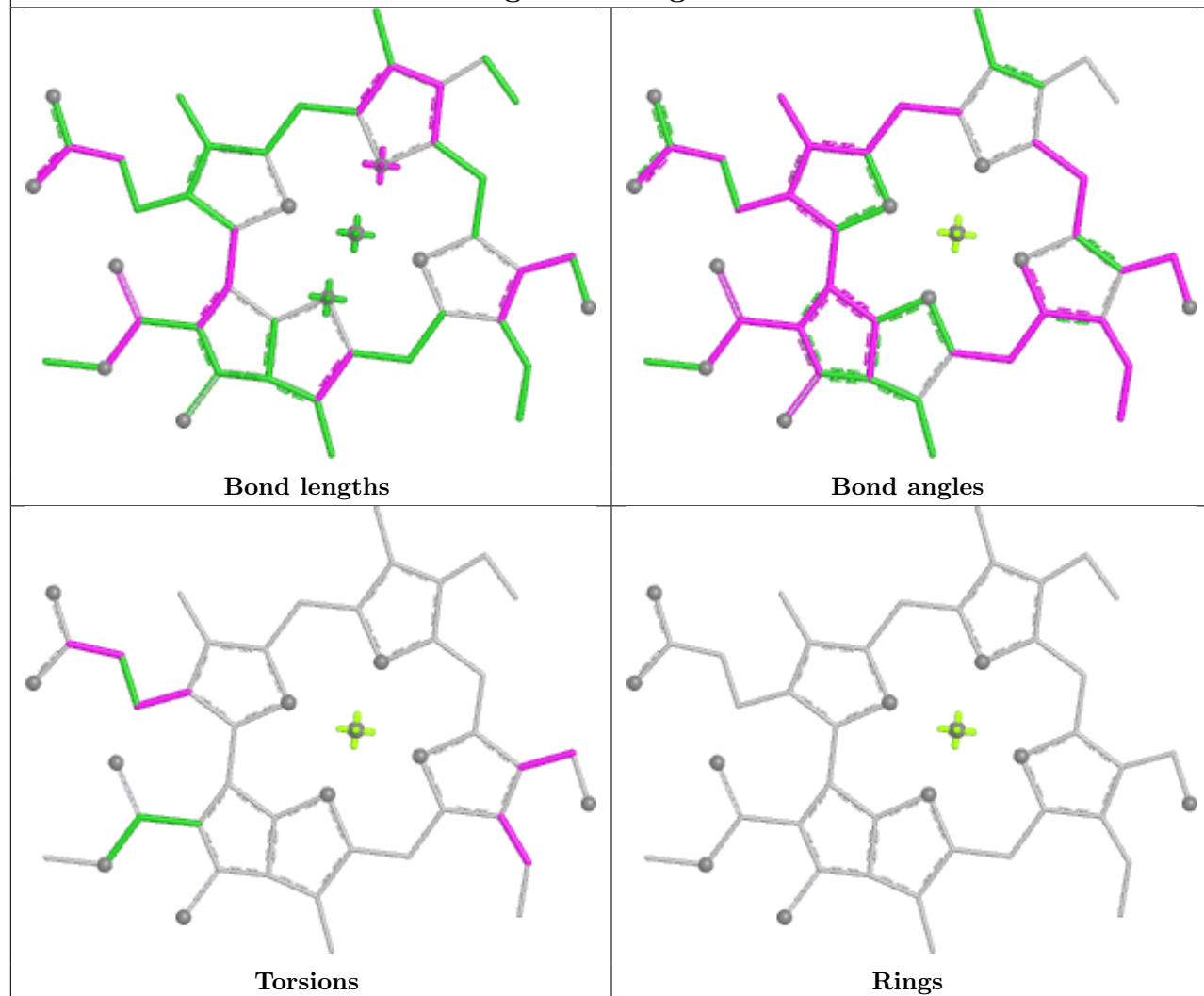
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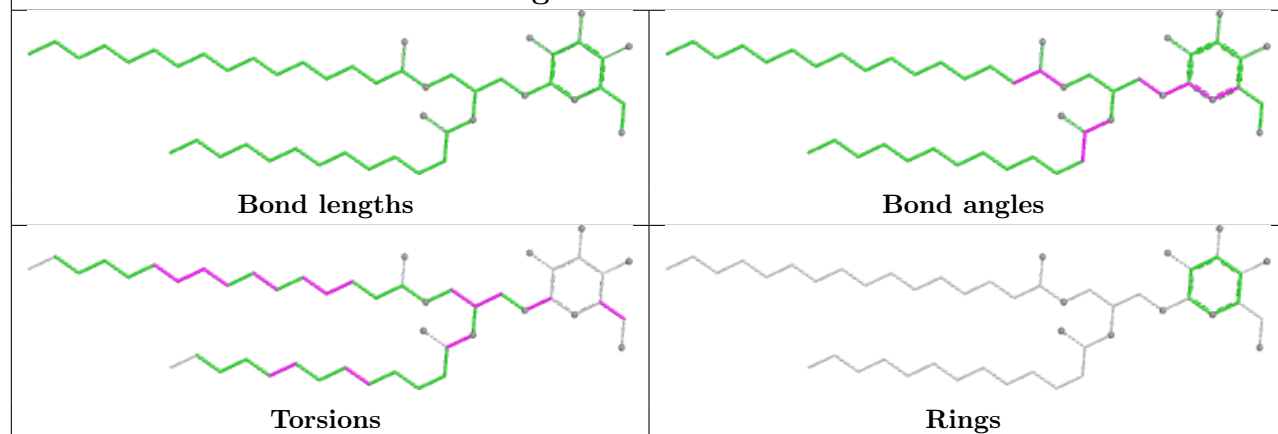
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	L	102	LHG	5	0
25	G	602	CLA	12	0
25	b	601	CLA	9	0
26	b	625	LHG	7	0
25	G	612	CLA	8	0
35	C	515	DGD	8	0
25	r	602	CLA	14	0
25	g	610	CLA	40	0
28	I	101	BCR	20	0
25	C	509	CLA	7	0
24	Y	307	CHL	14	0
35	c	516	DGD	10	0
24	R	605	CHL	8	0
25	b	615	CLA	16	0
25	g	602	CLA	11	0
24	5	302	CHL	8	0
25	n	610	CLA	33	0
25	g	612	CLA	9	0

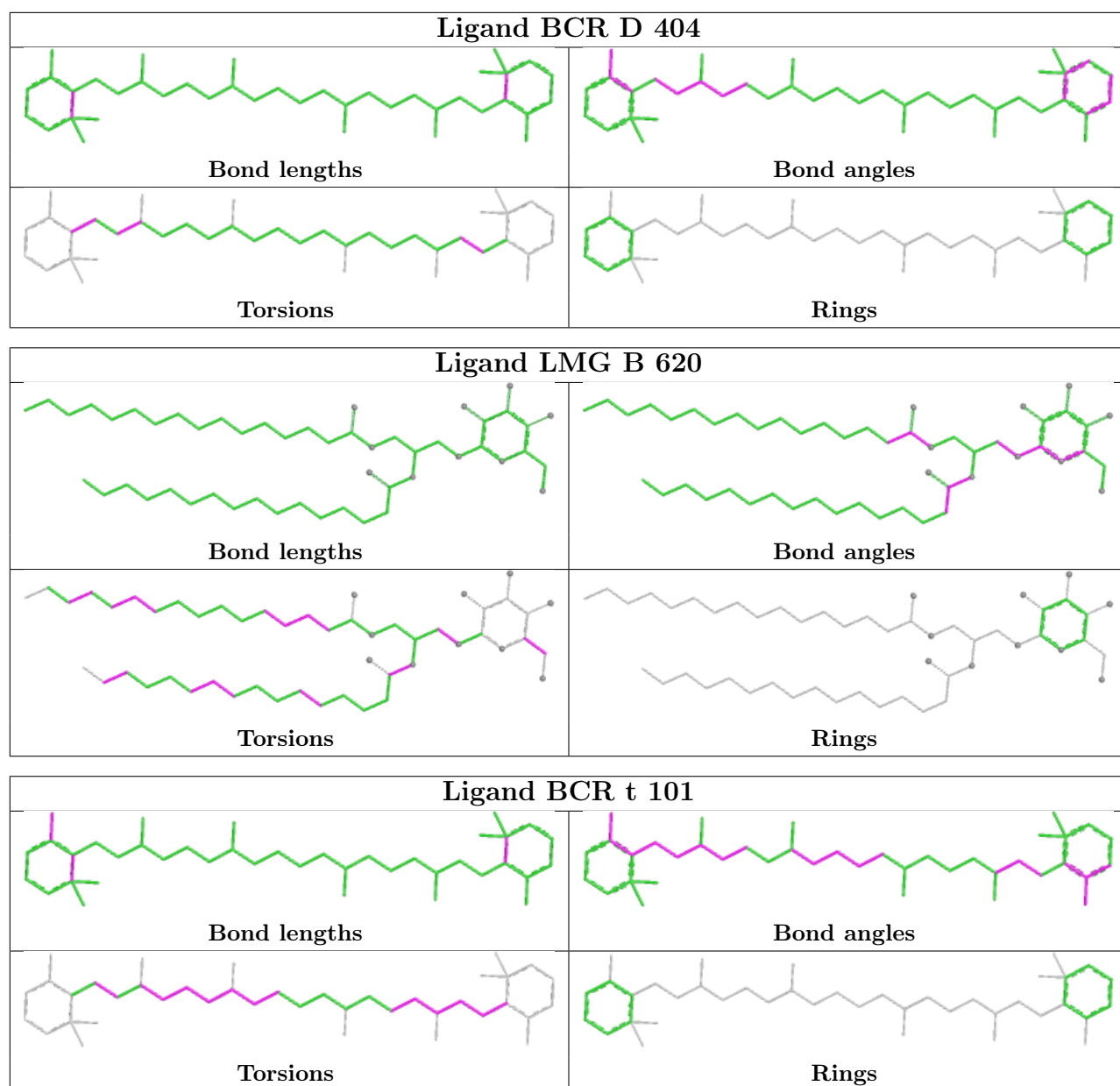
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

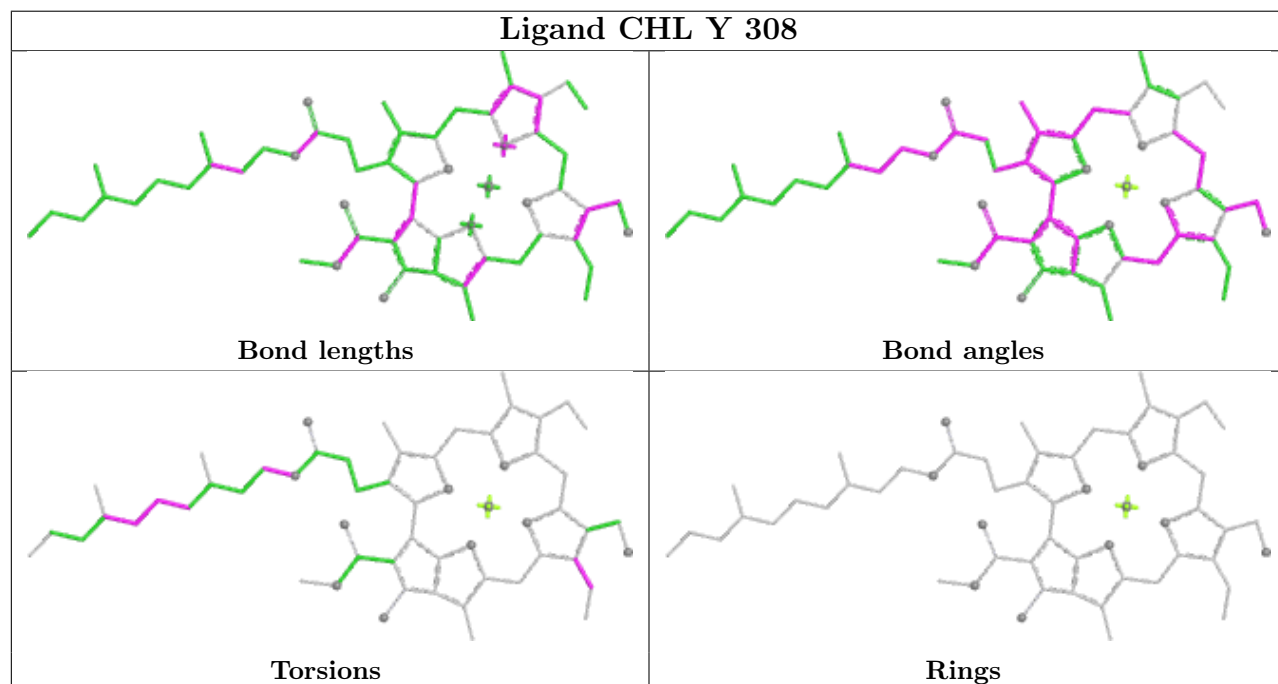
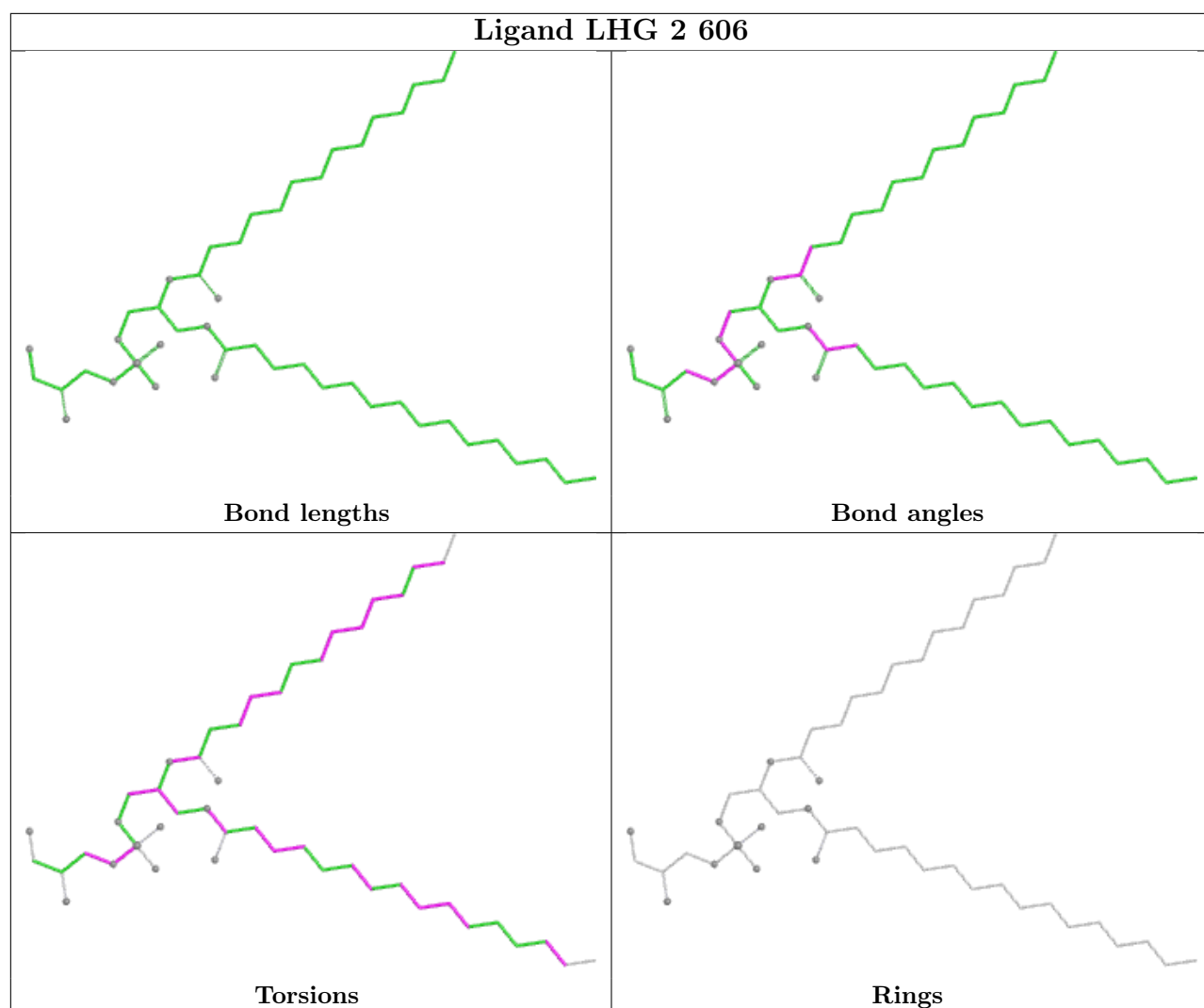
Ligand CHL g 605

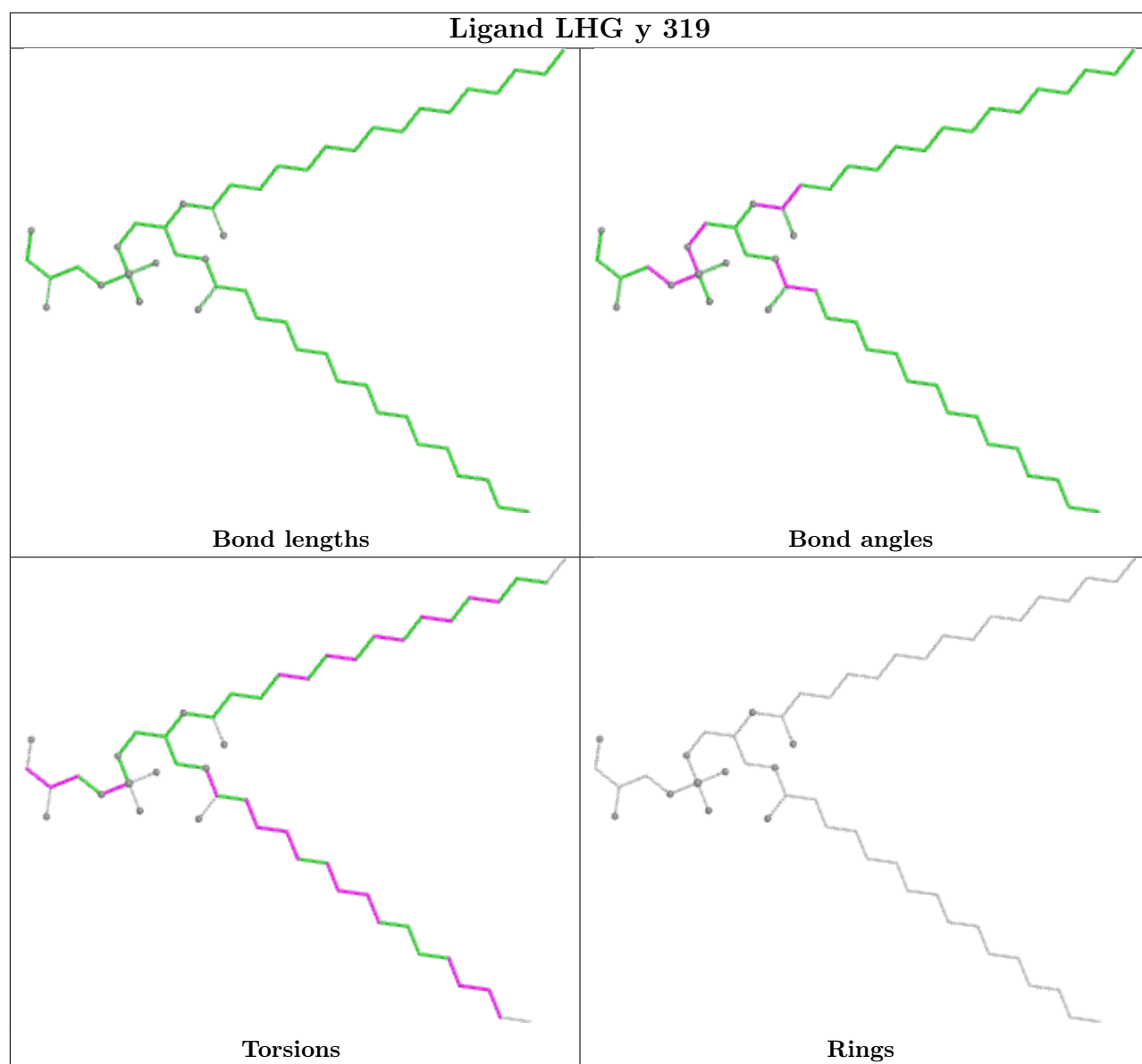


Ligand LMG a 409

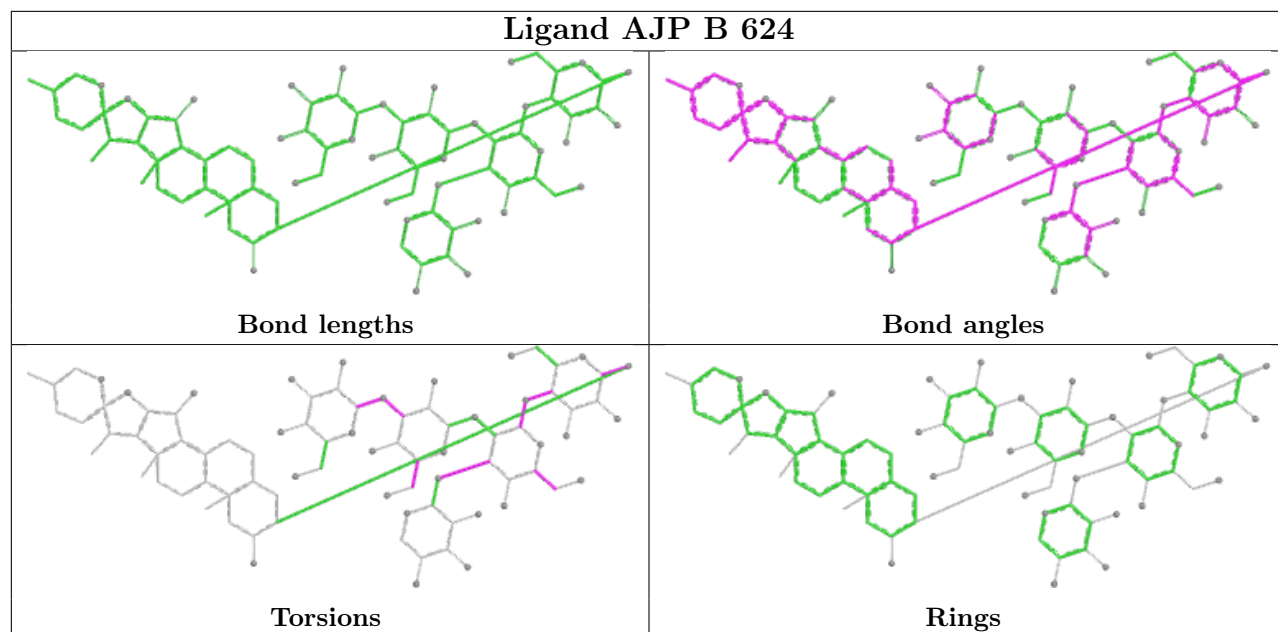




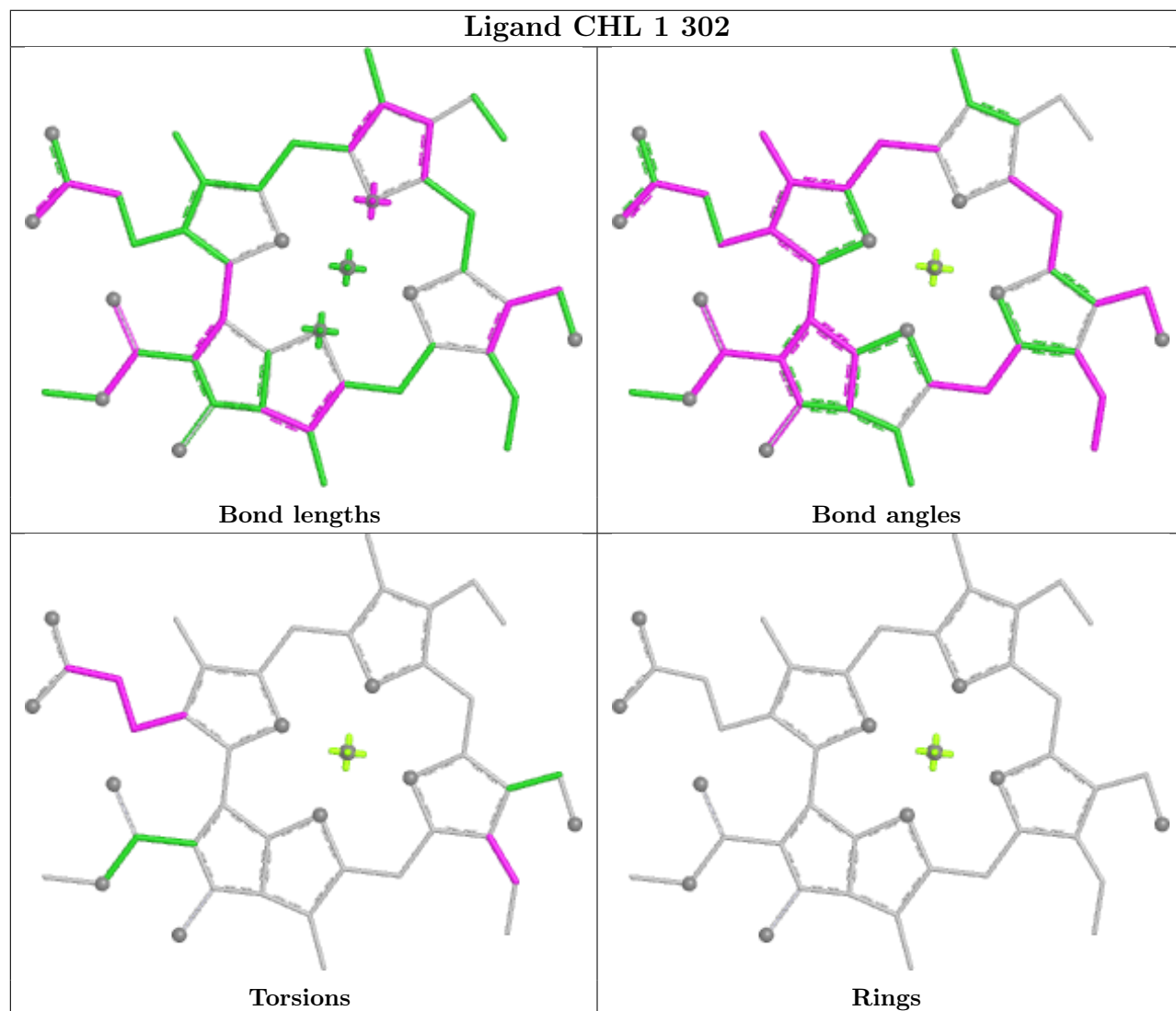


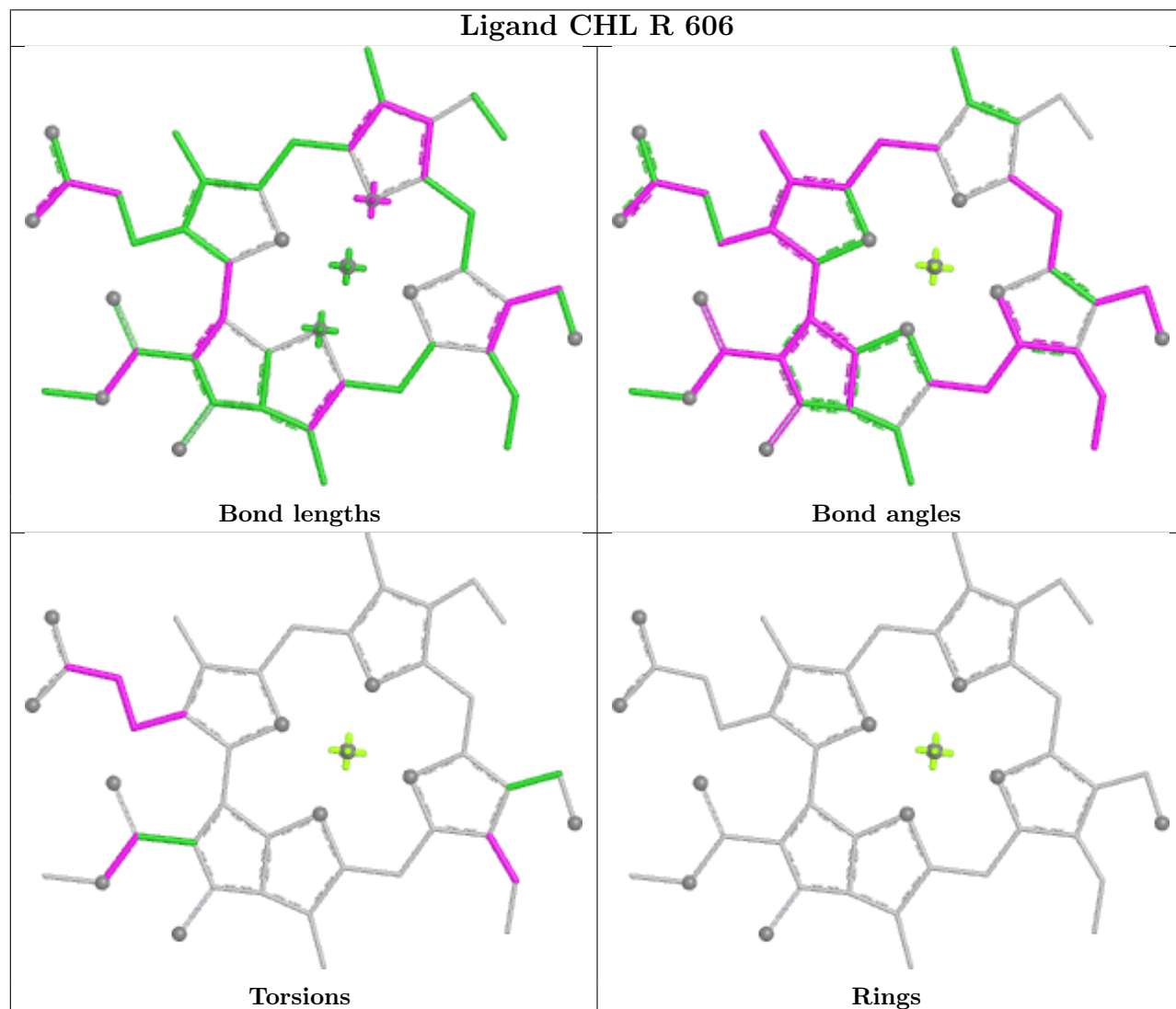
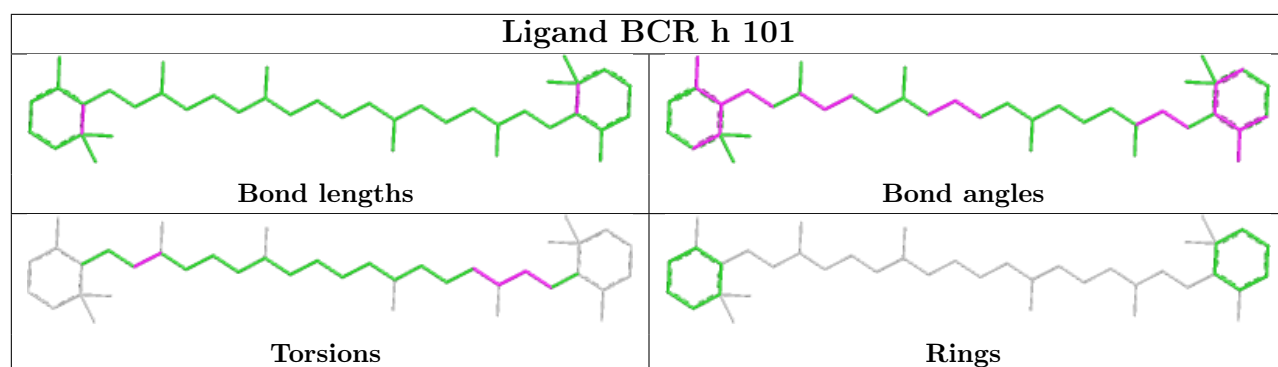


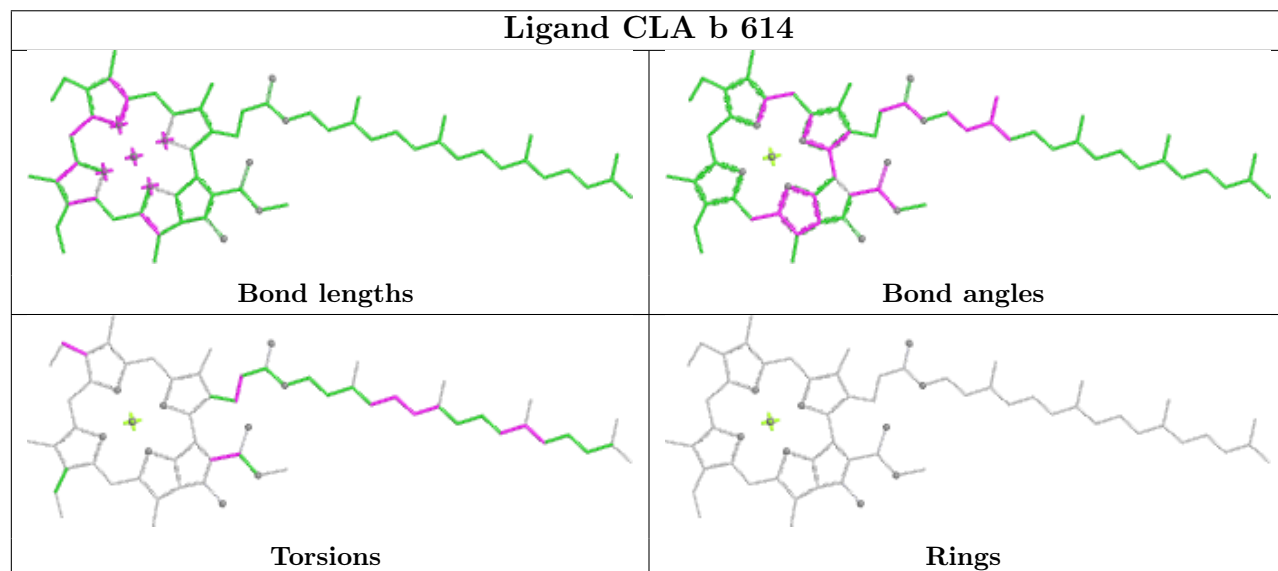
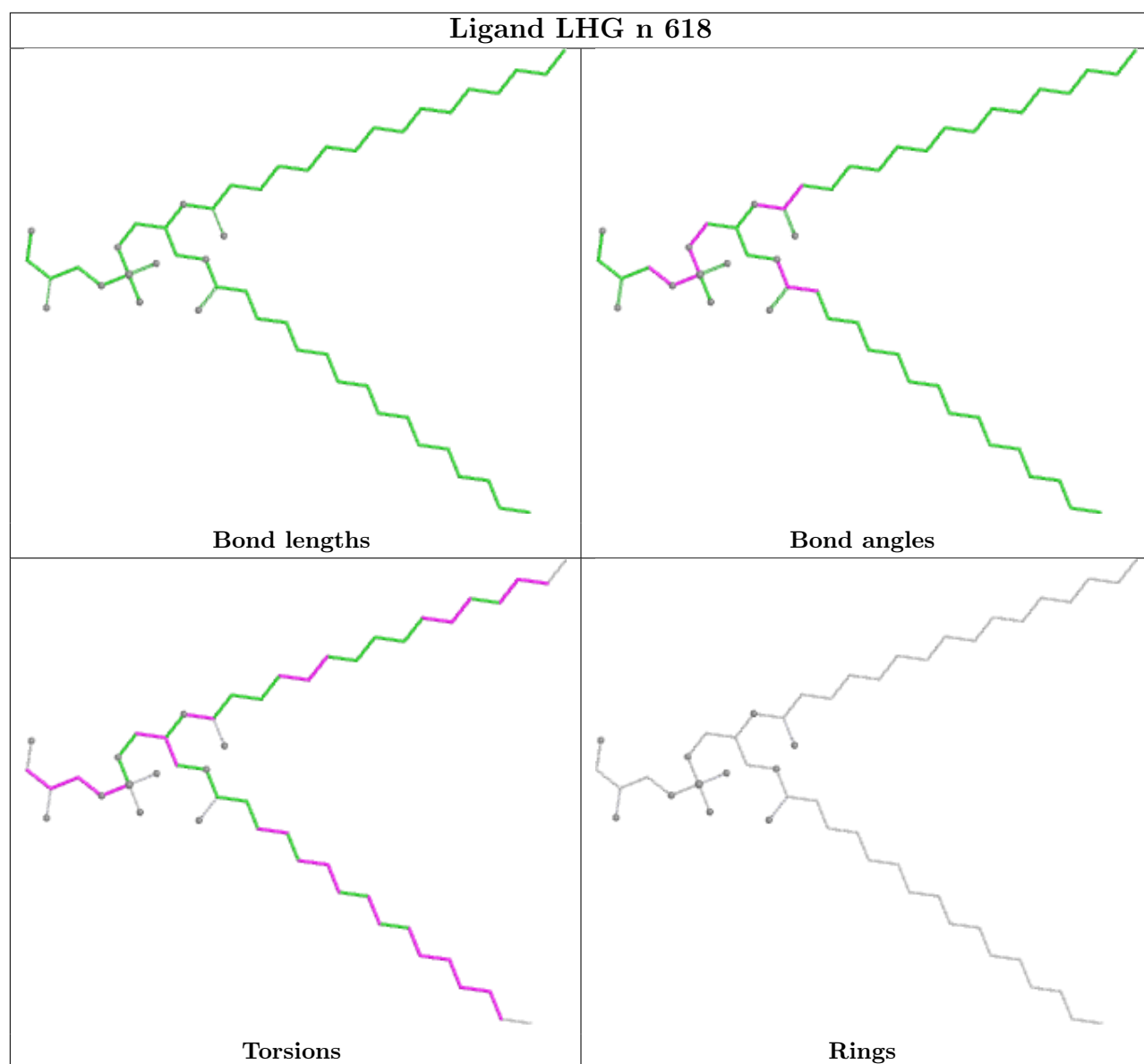
Ligand AJP B 624



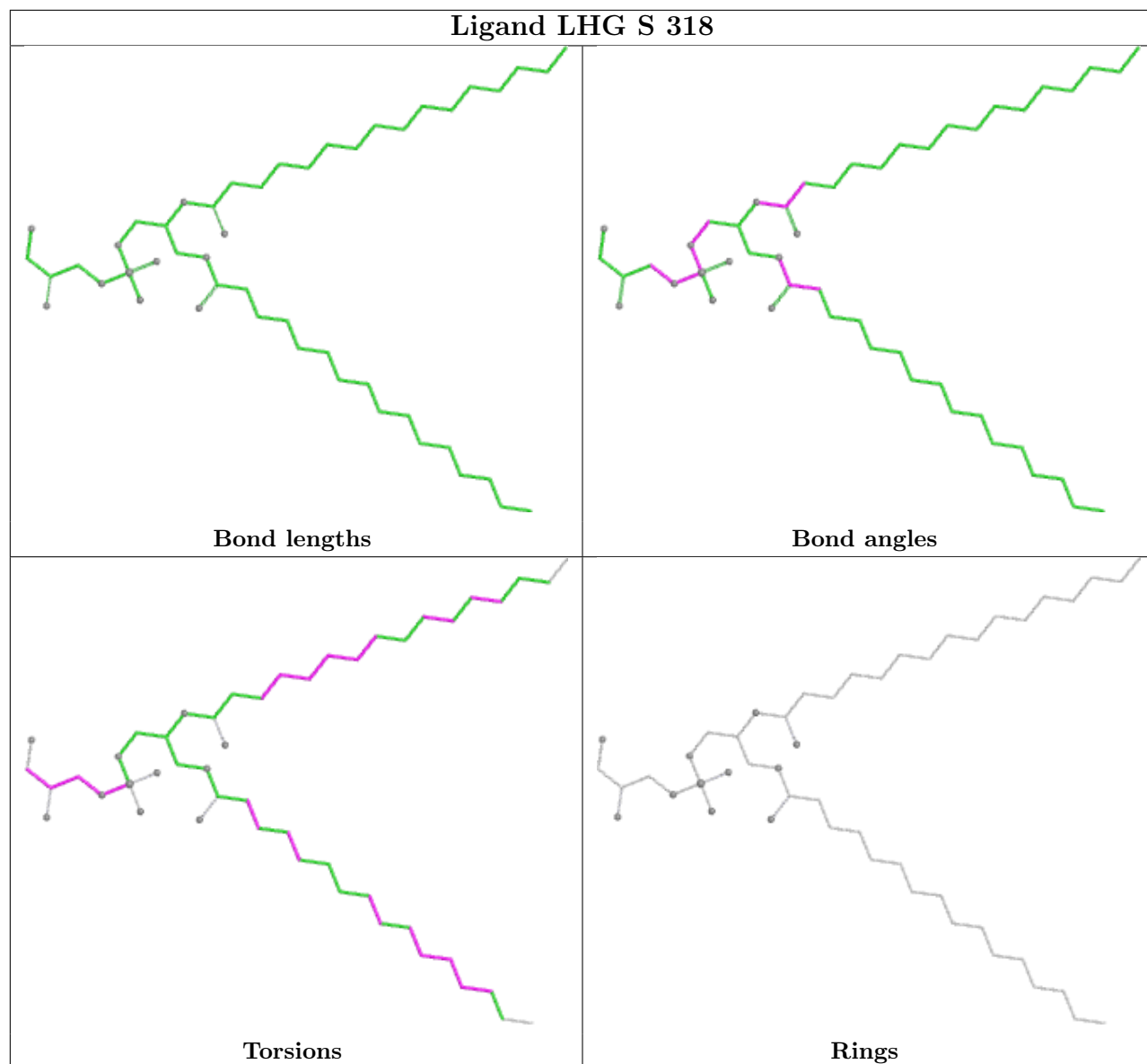
Ligand CHL 1 302



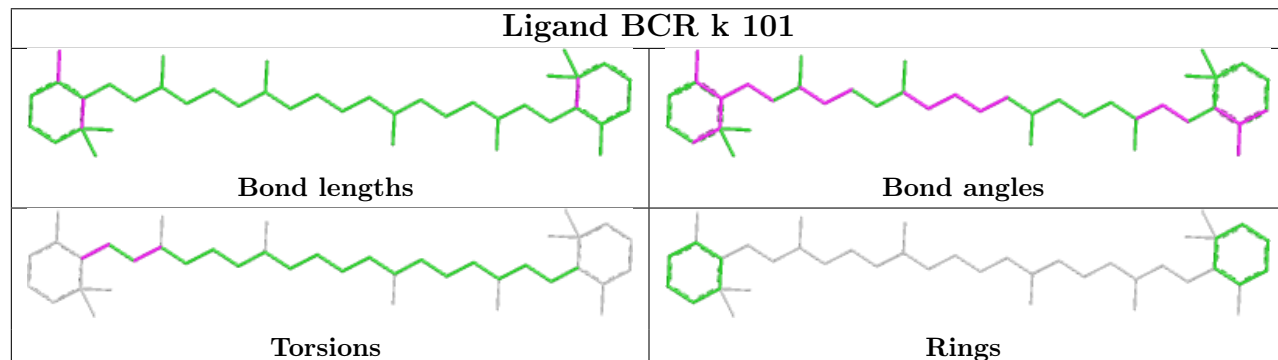




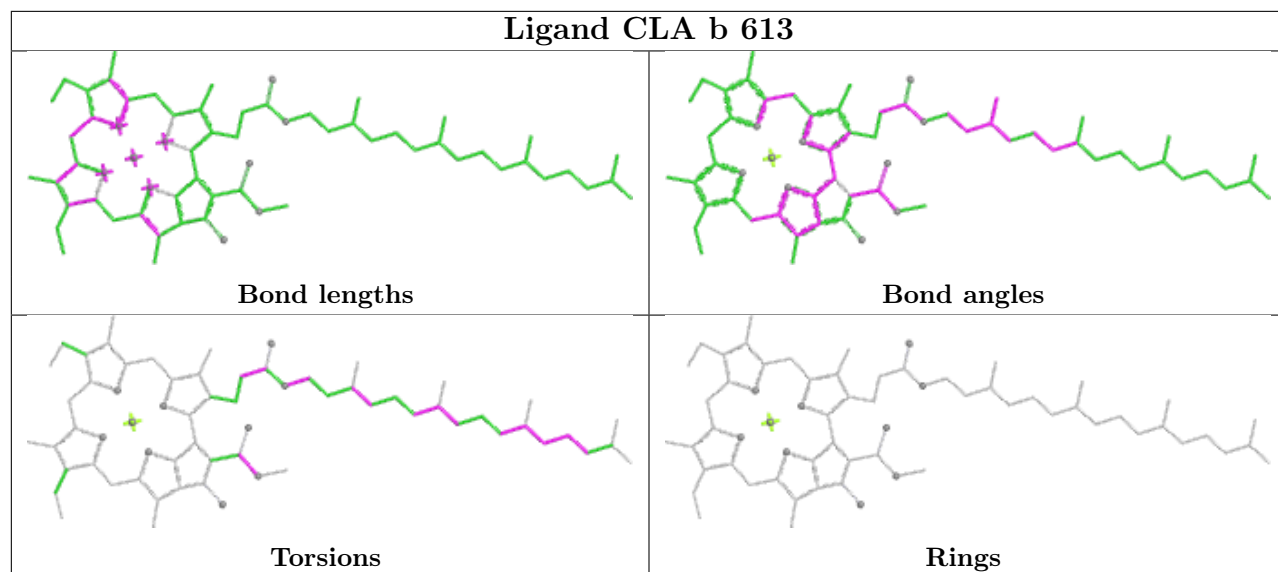
Ligand LHG S 318



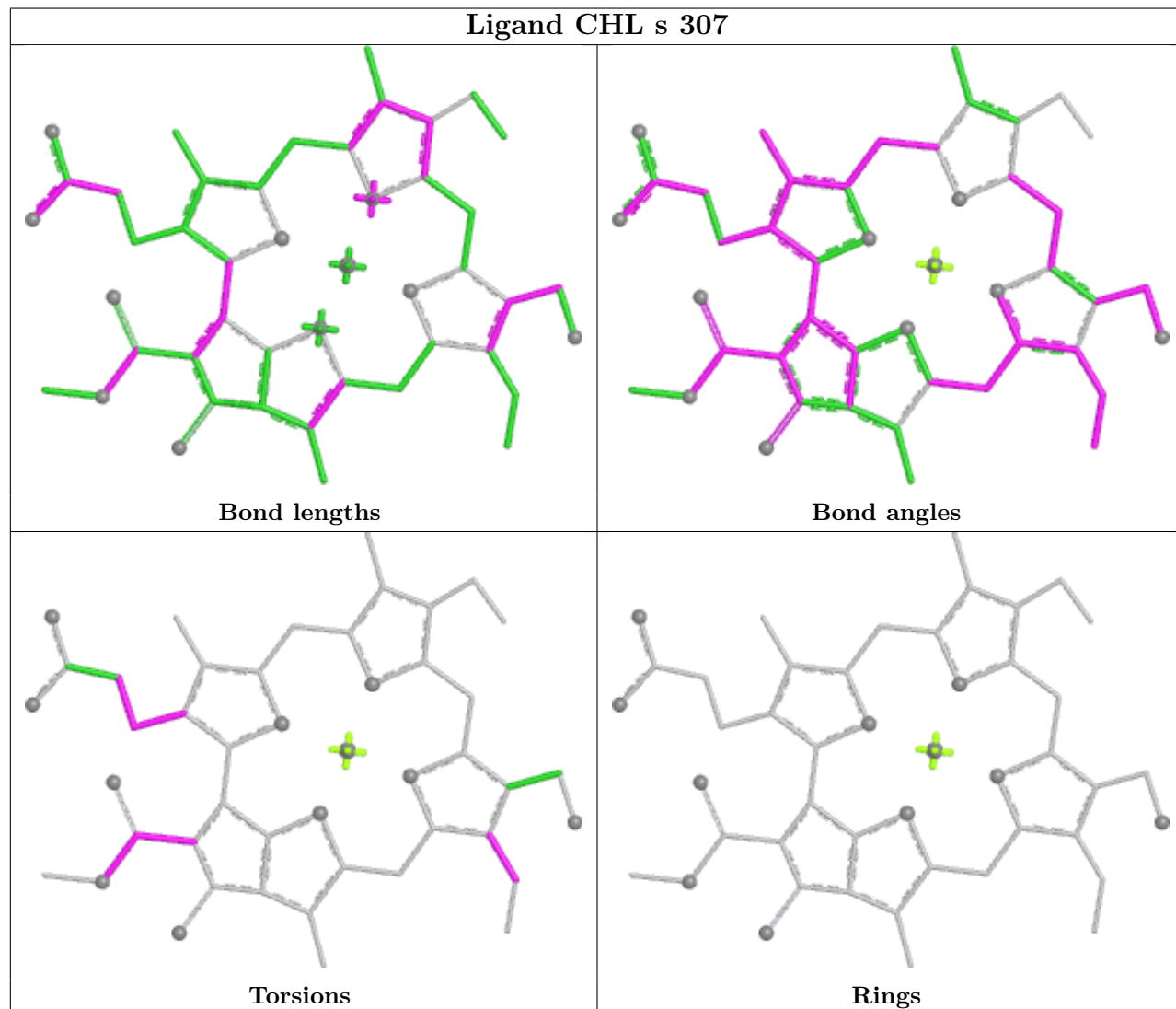
Ligand BCR k 101



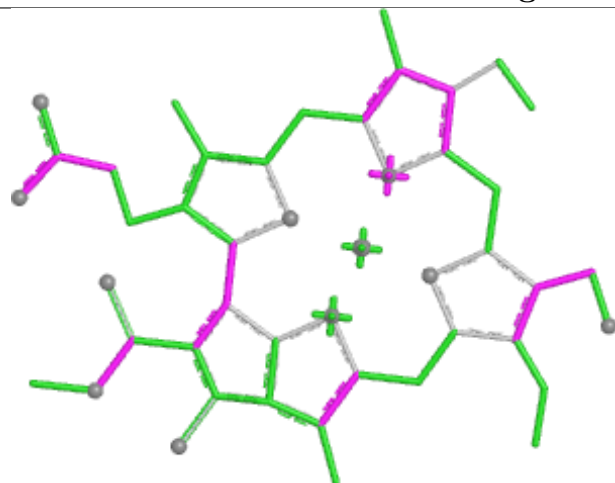
Ligand CLA b 613



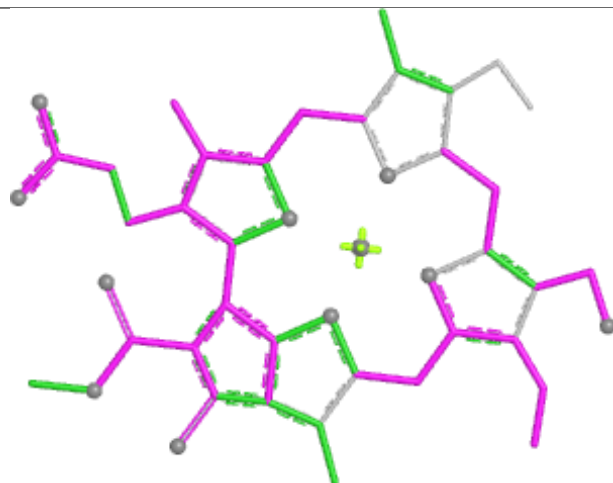
Ligand CHL s 307



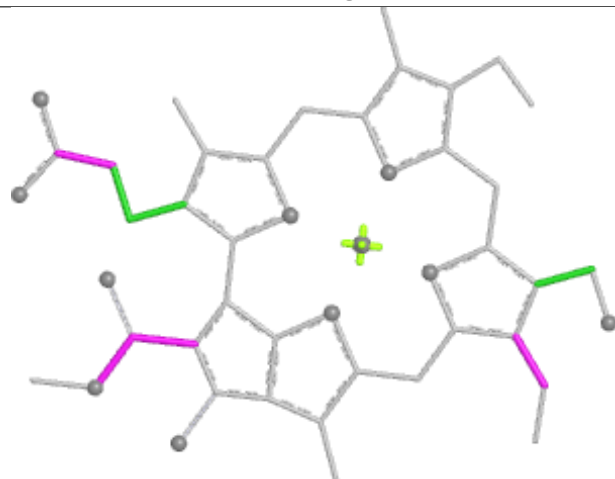
Ligand CHL S 306



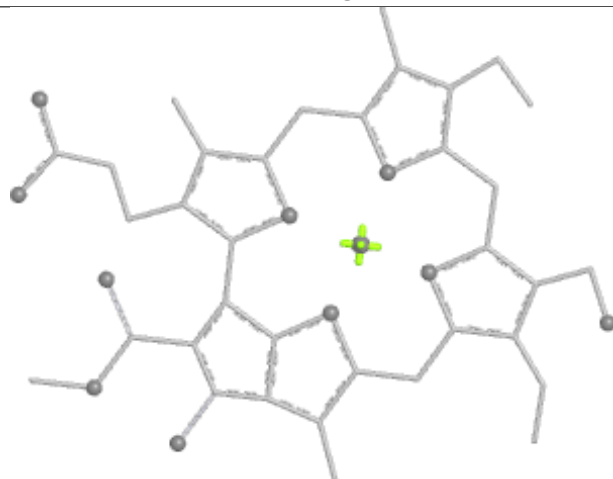
Bond lengths



Bond angles

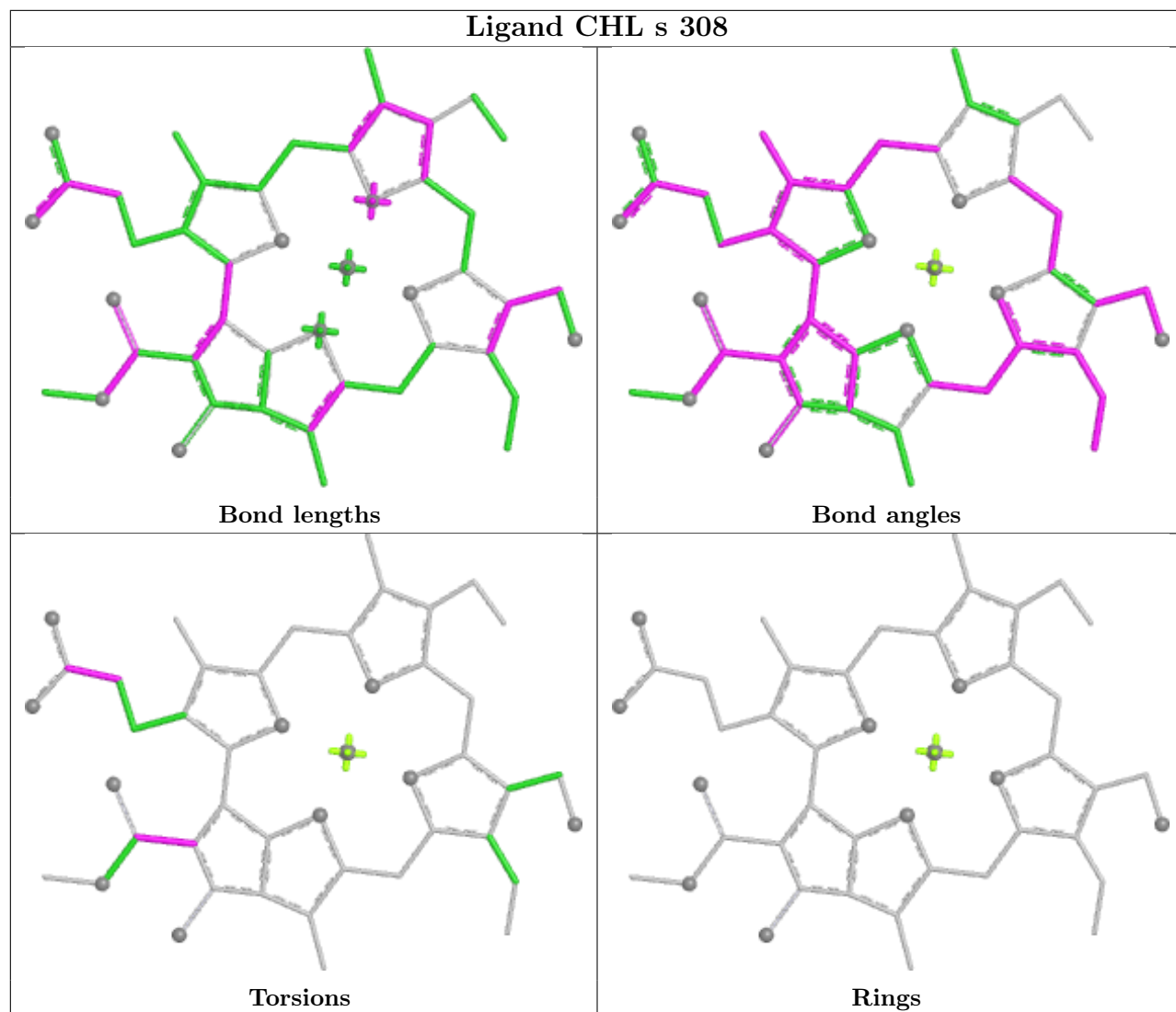


Torsions

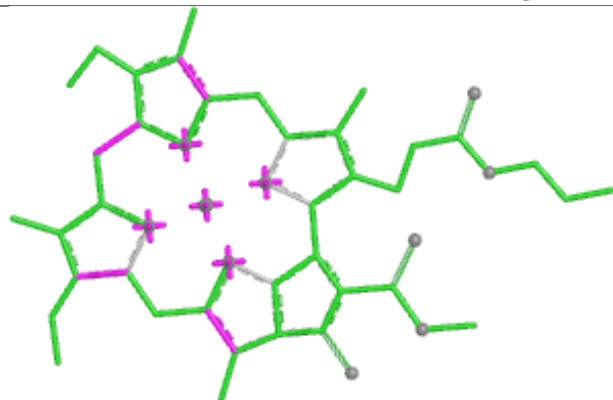


Rings

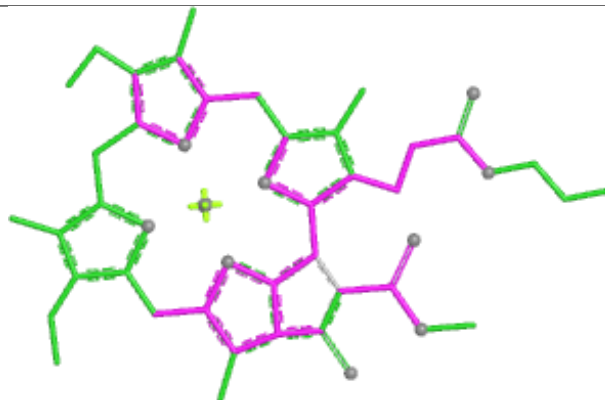
Ligand CHL s 308



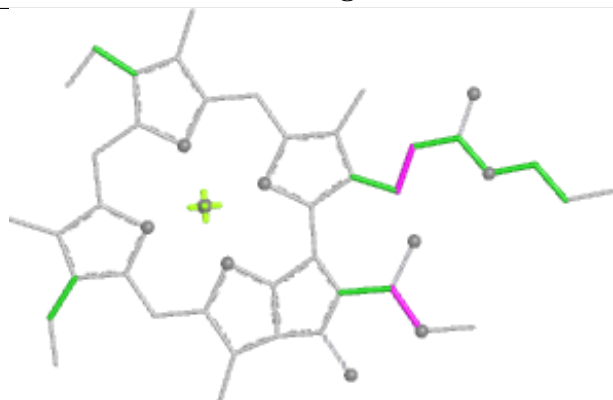
Ligand CLA n 614



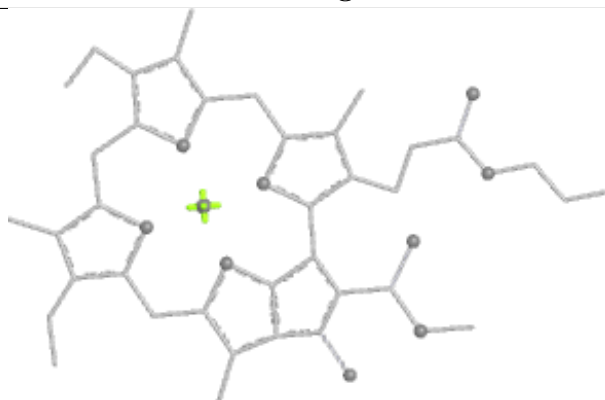
Bond lengths



Bond angles

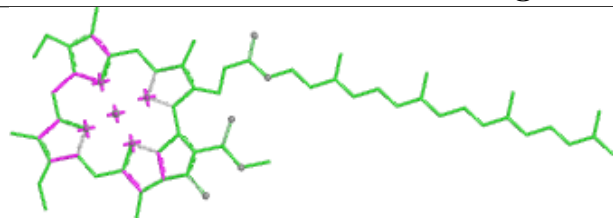


Torsions

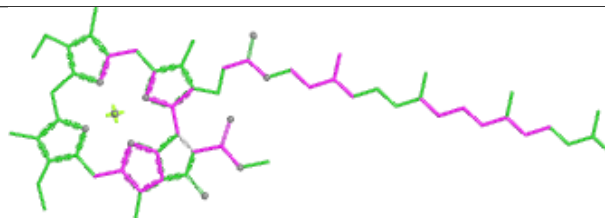


Rings

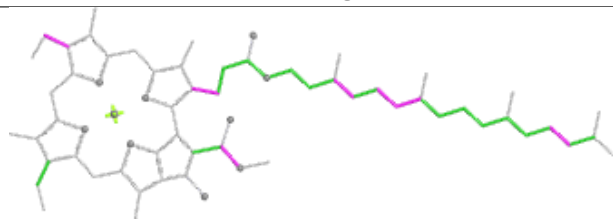
Ligand CLA B 609



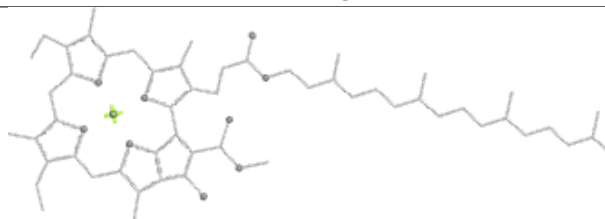
Bond lengths



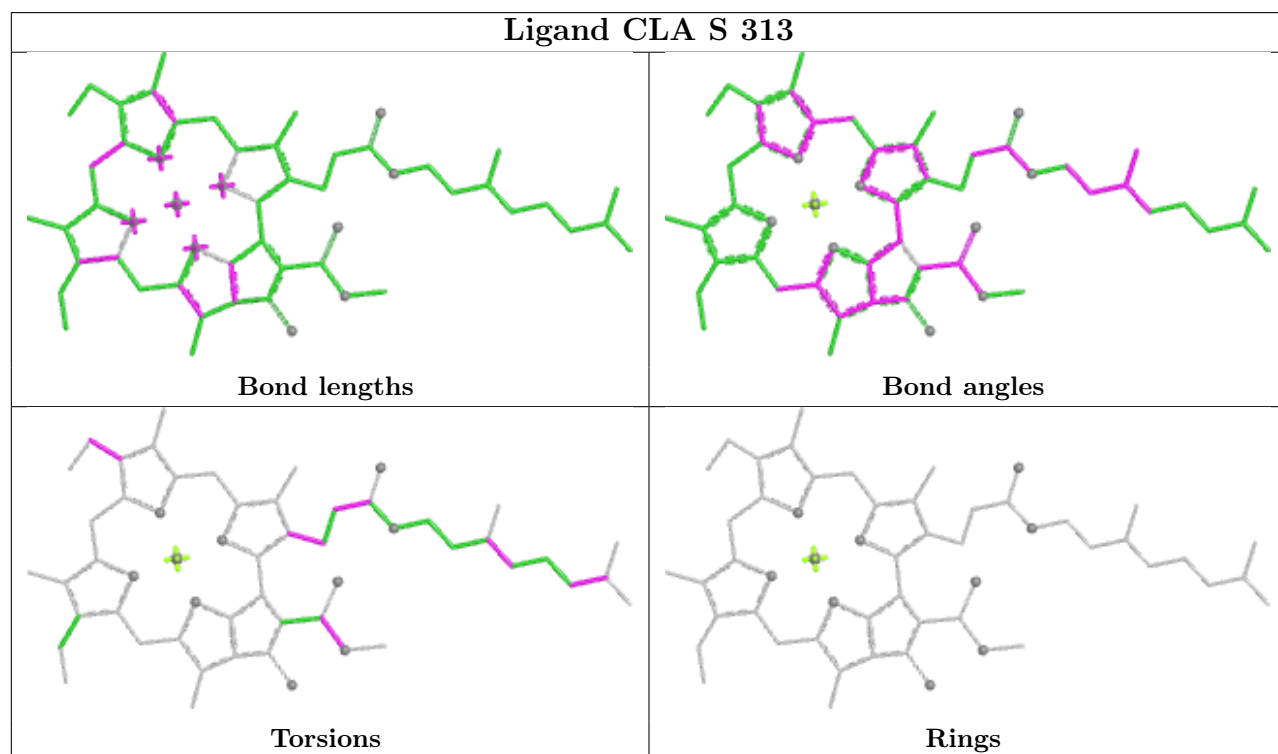
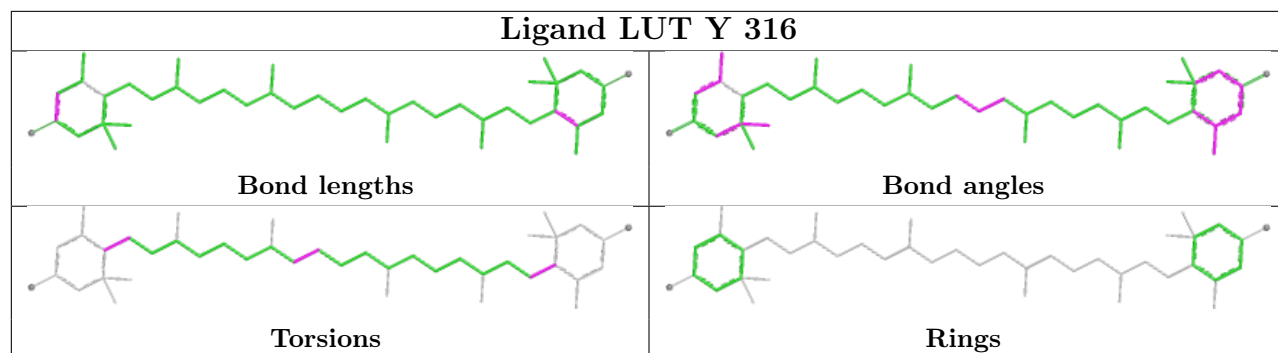
Bond angles



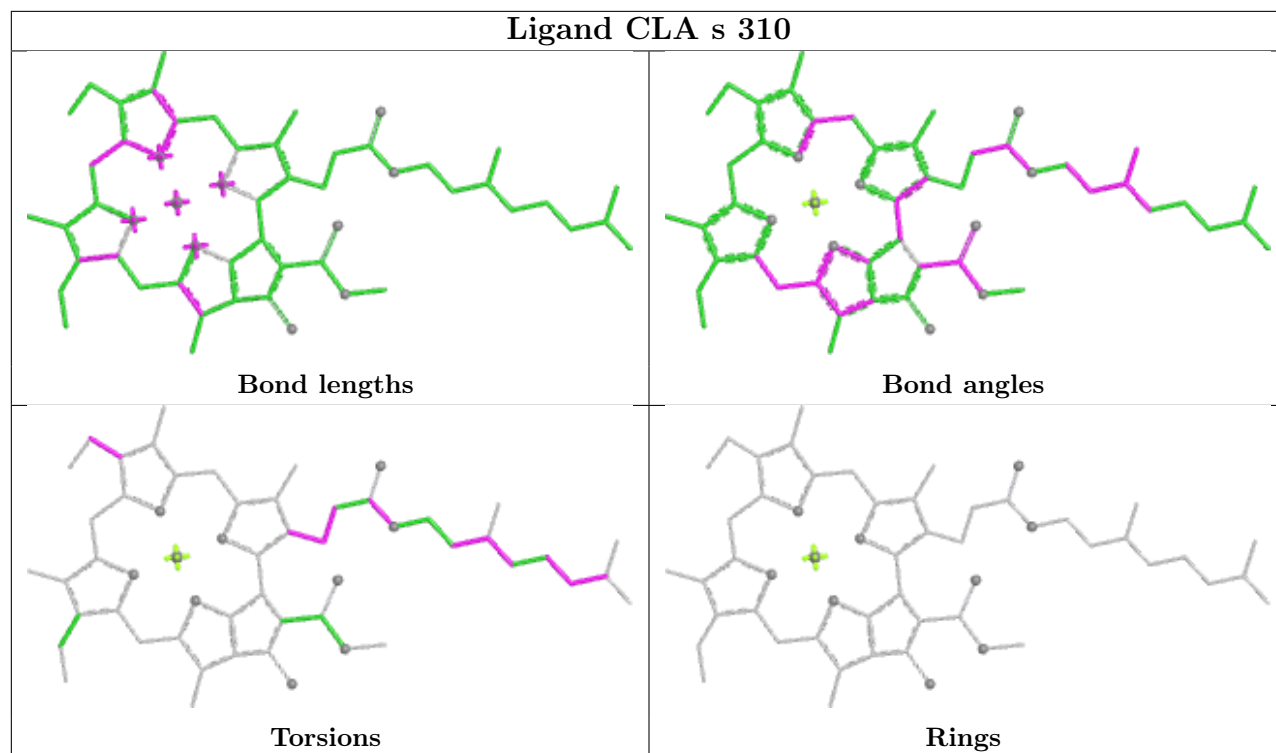
Torsions



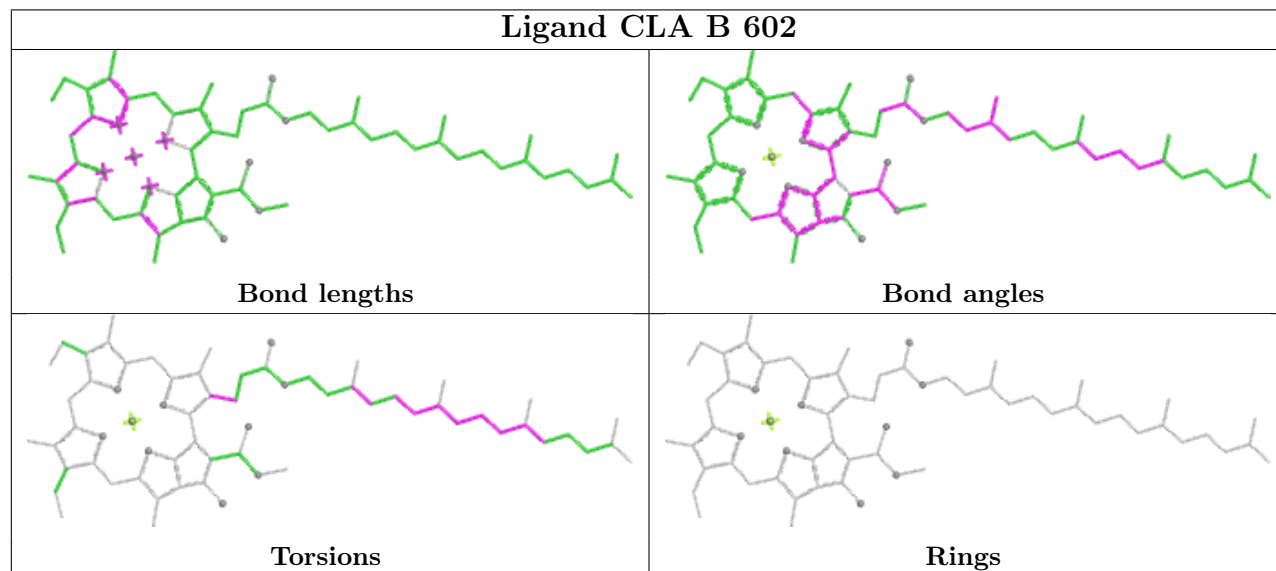
Rings



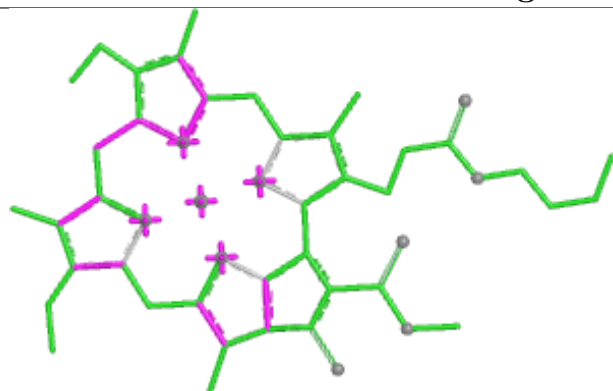
Ligand CLA s 310



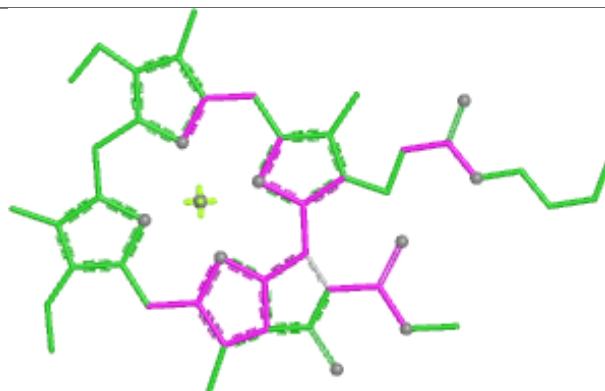
Ligand CLA B 602



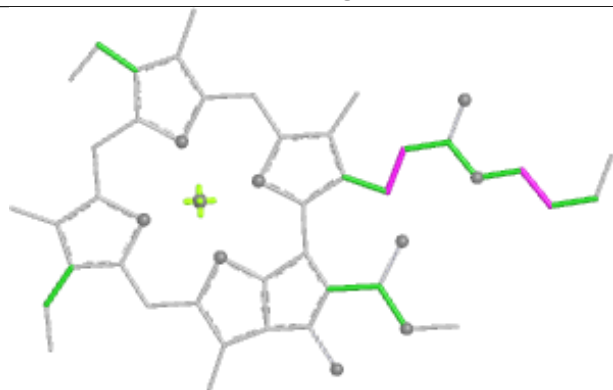
Ligand CLA S 314



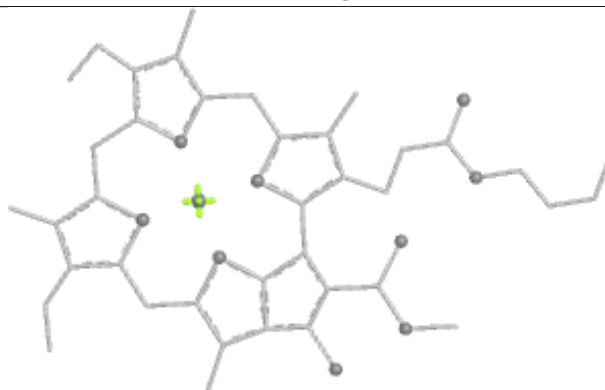
Bond lengths



Bond angles

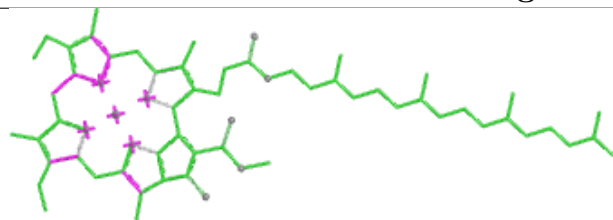


Torsions

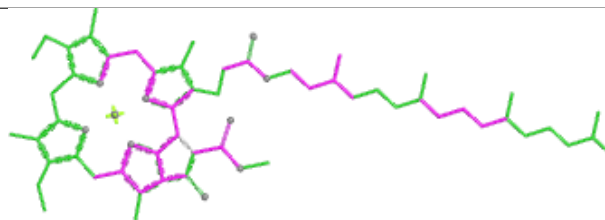


Rings

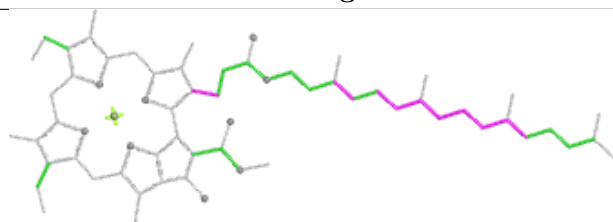
Ligand CLA b 602



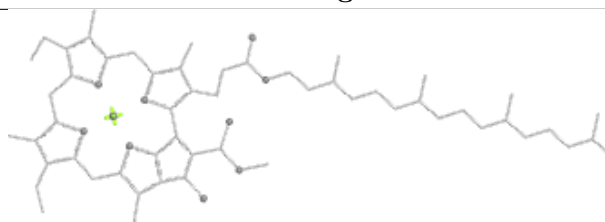
Bond lengths



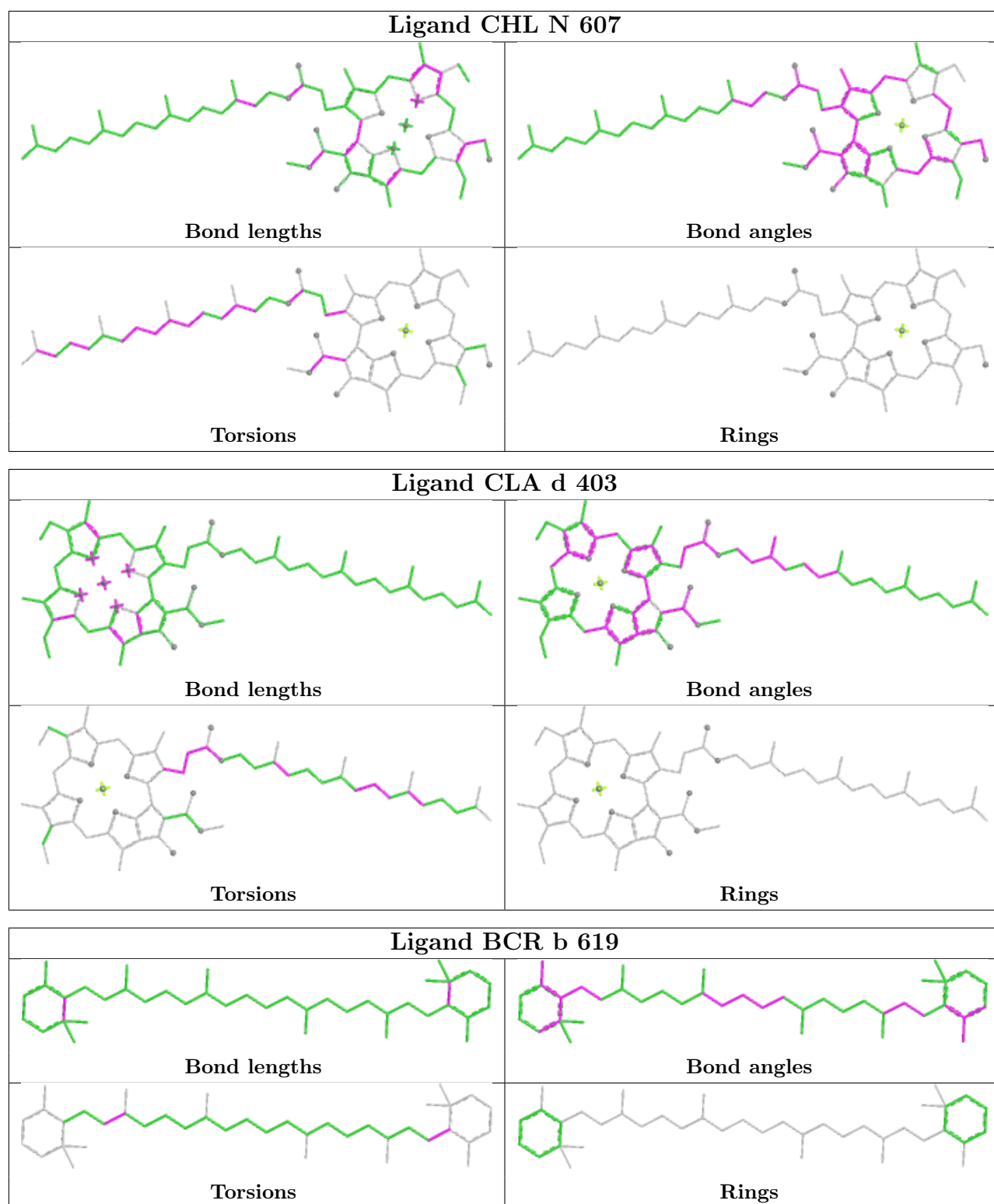
Bond angles

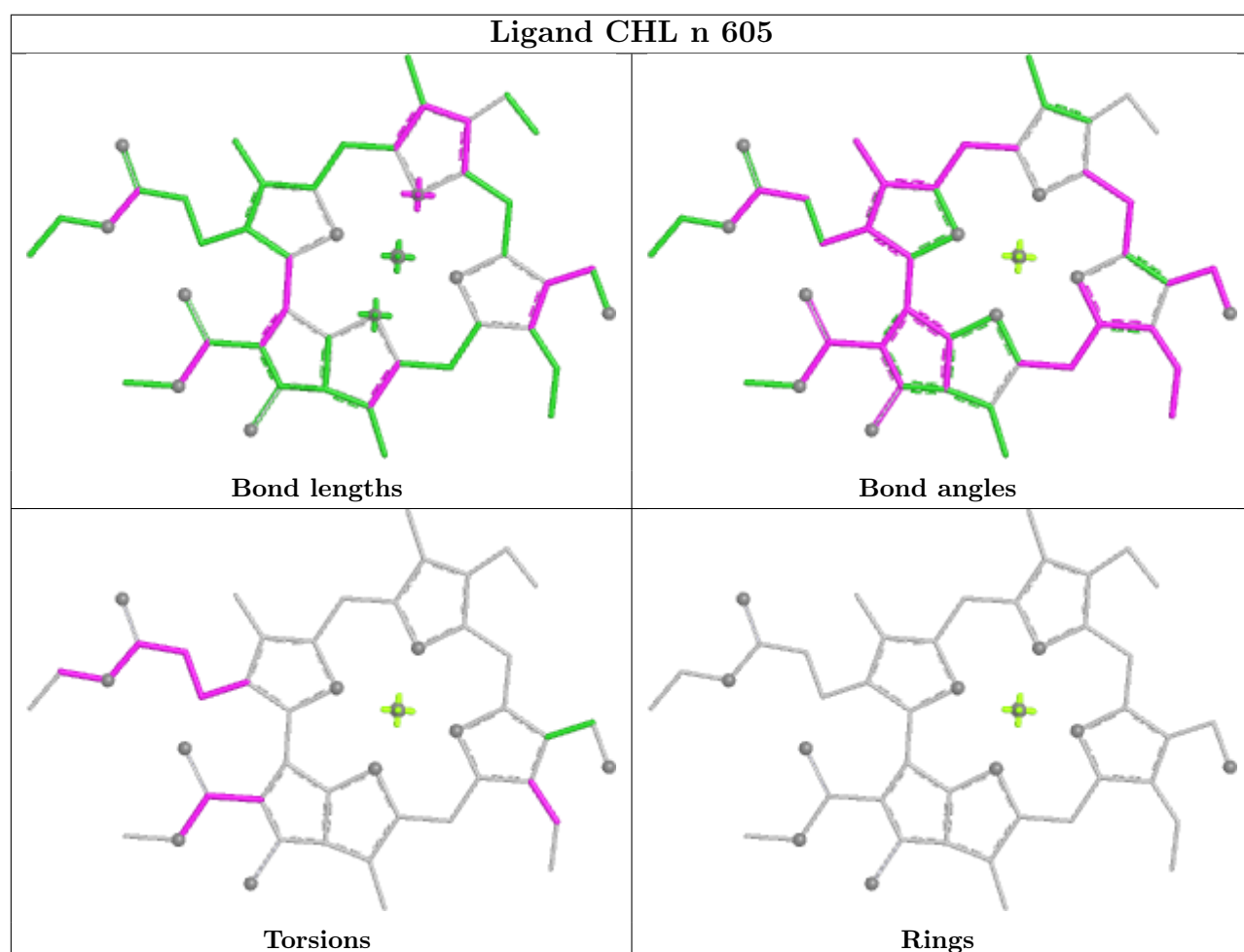
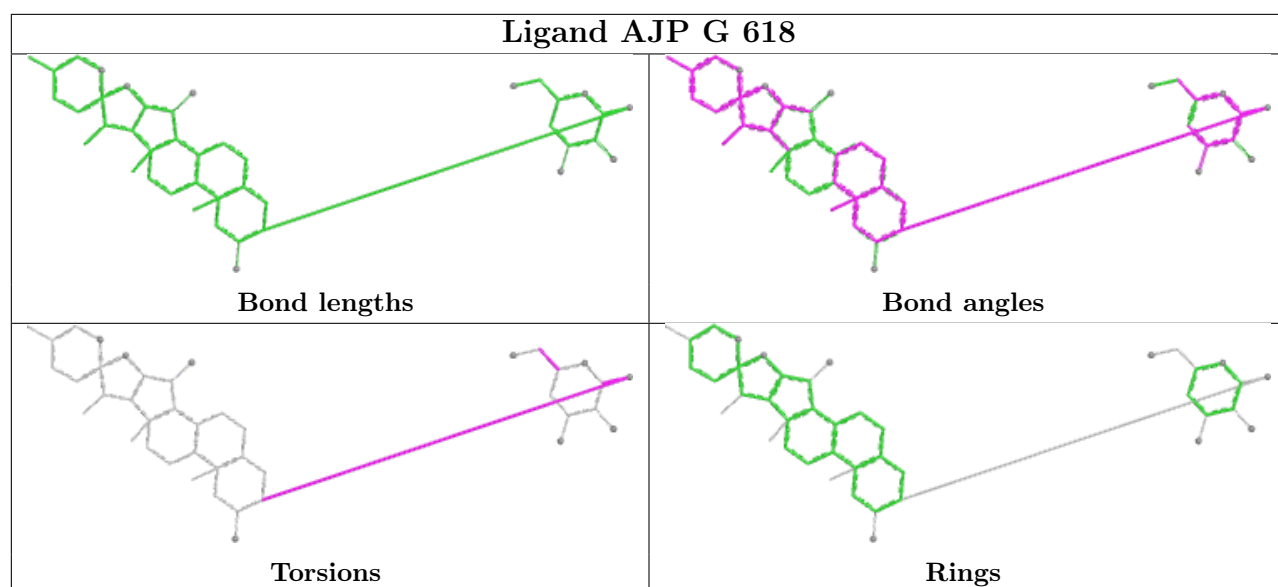


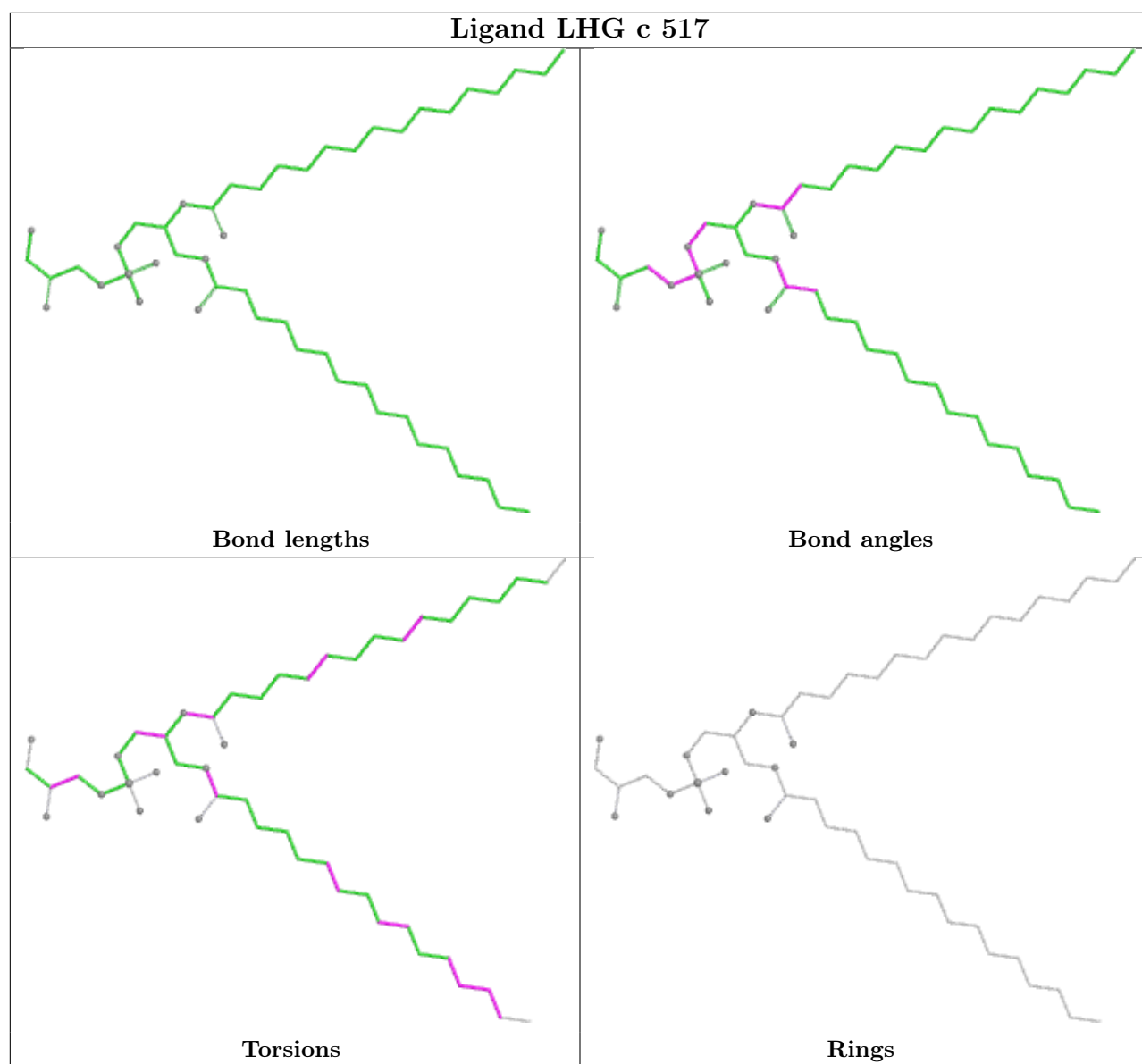
Torsions

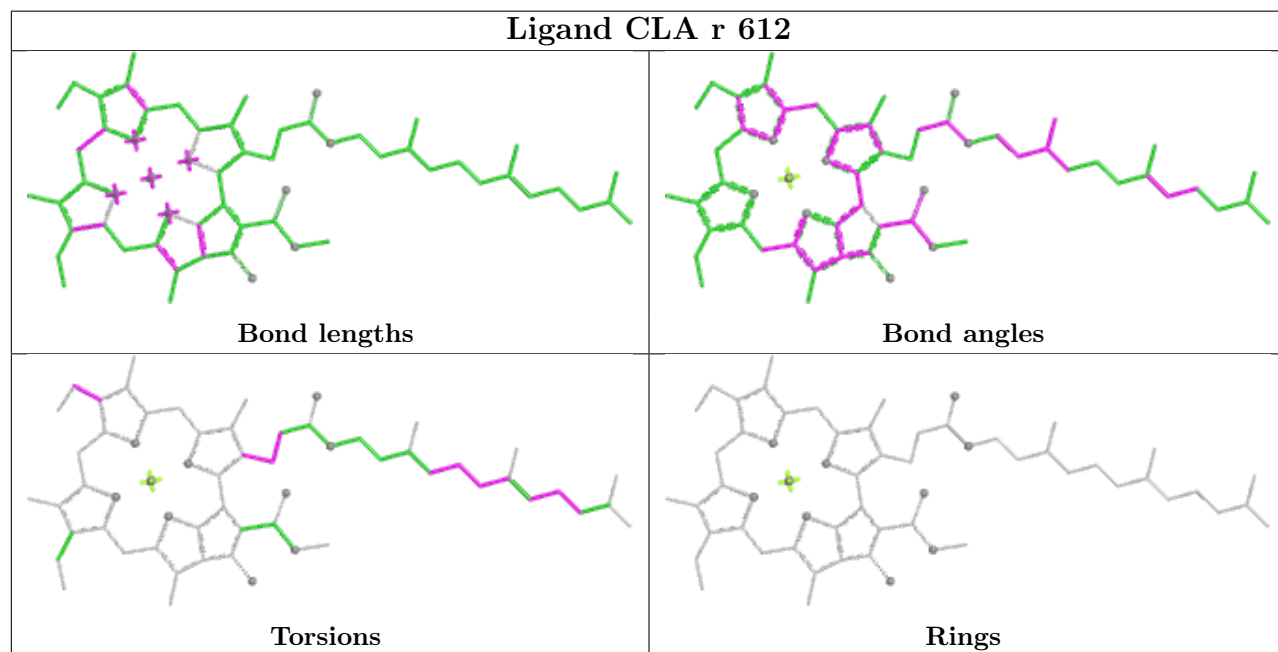
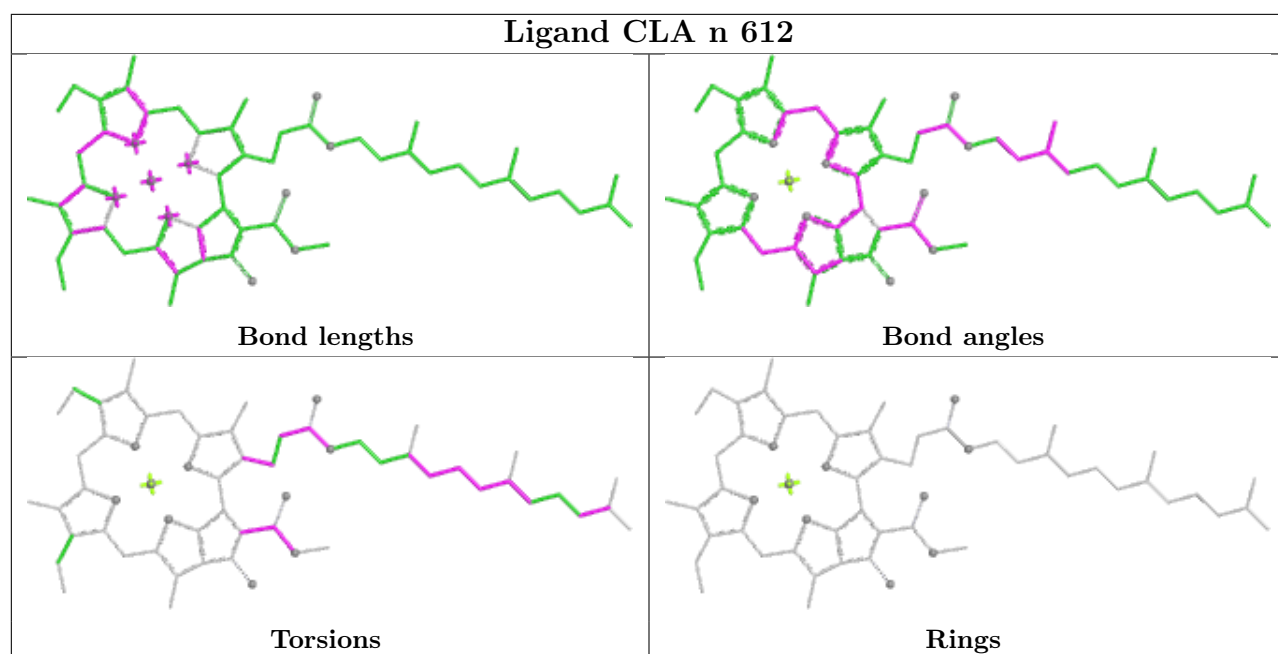


Rings

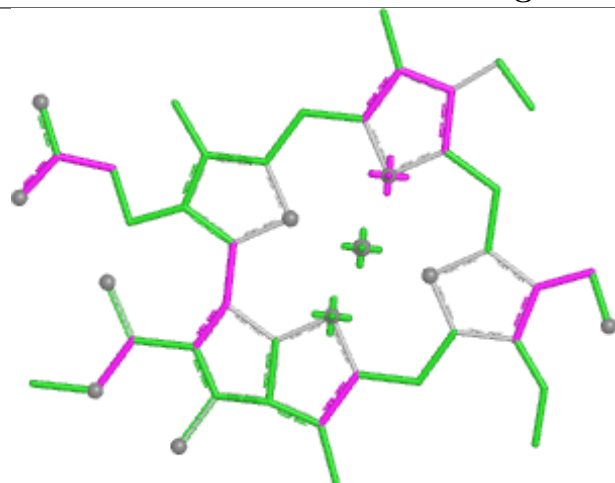




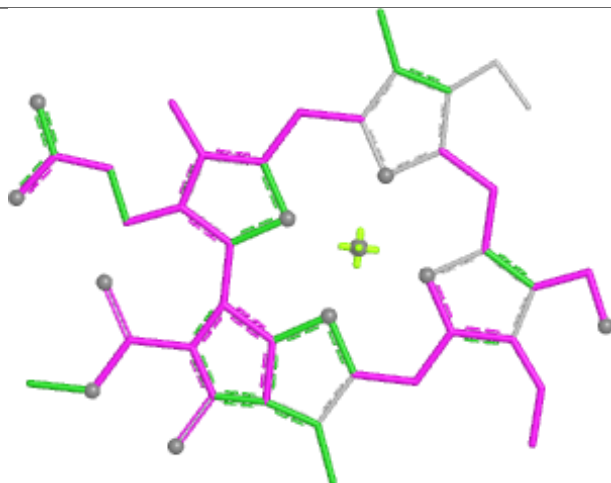




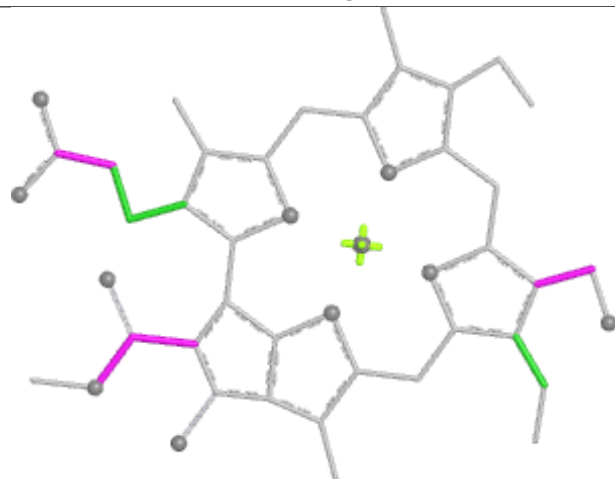
Ligand CHL N 606



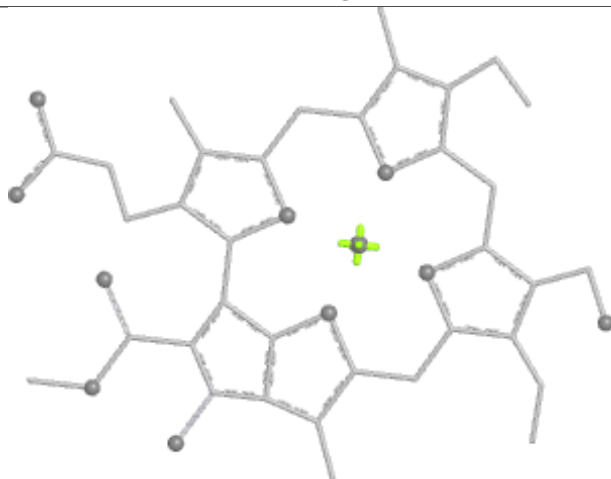
Bond lengths



Bond angles

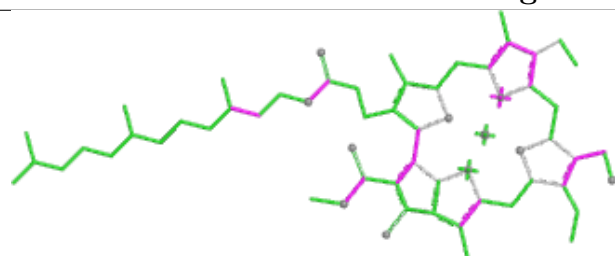


Torsions

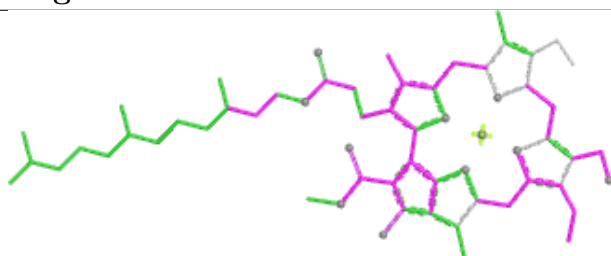


Rings

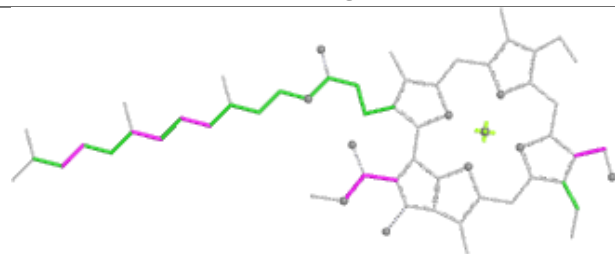
Ligand CHL g 609



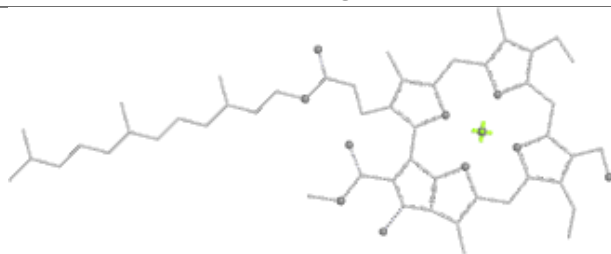
Bond lengths



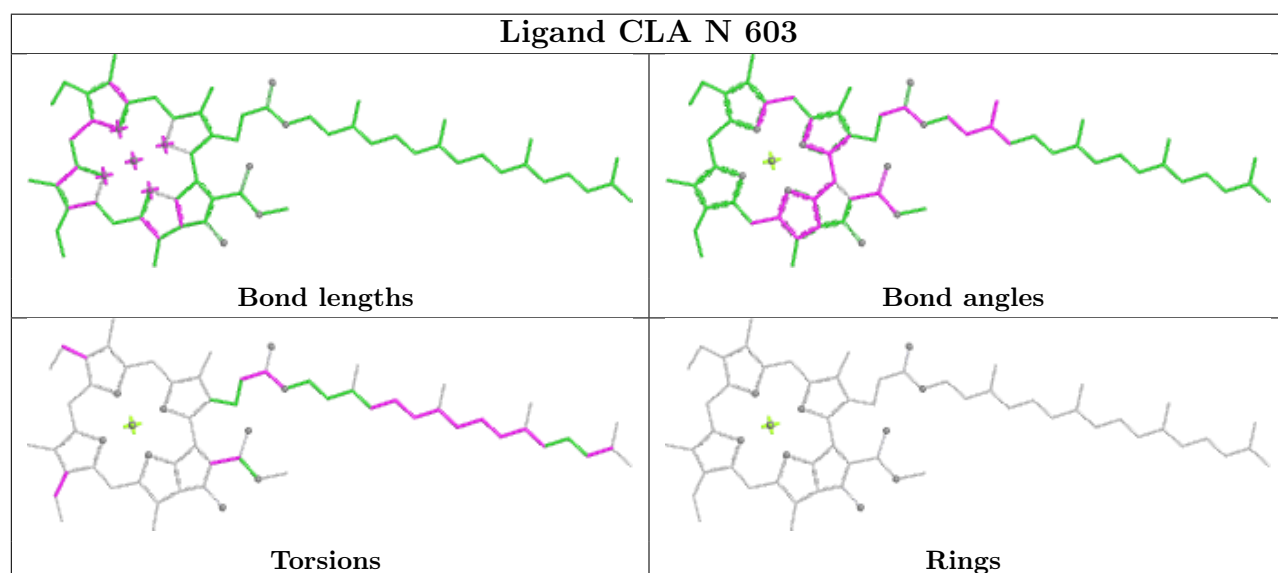
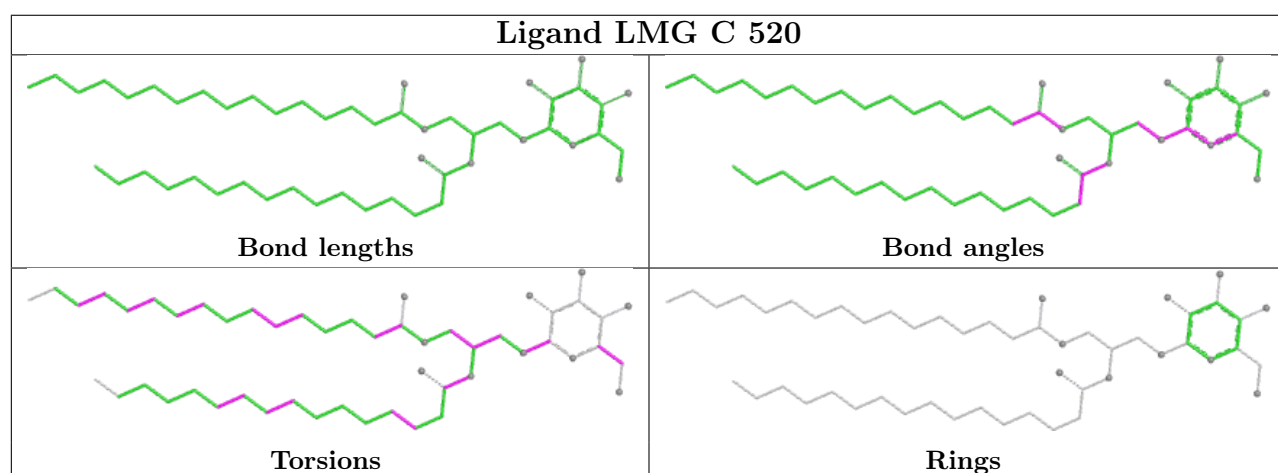
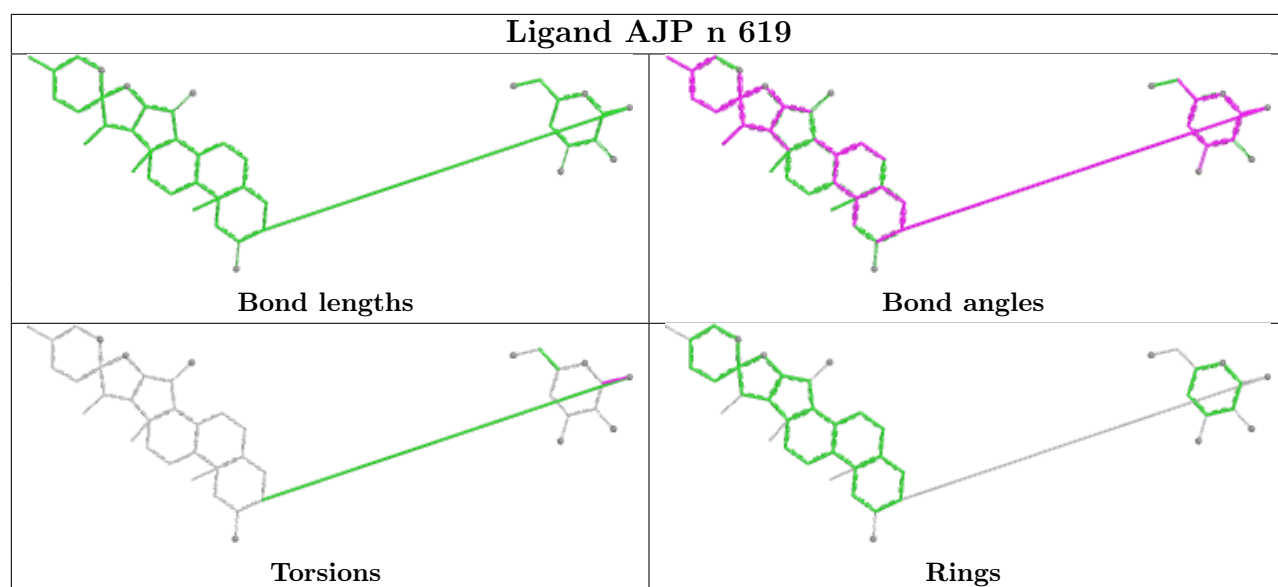
Bond angles

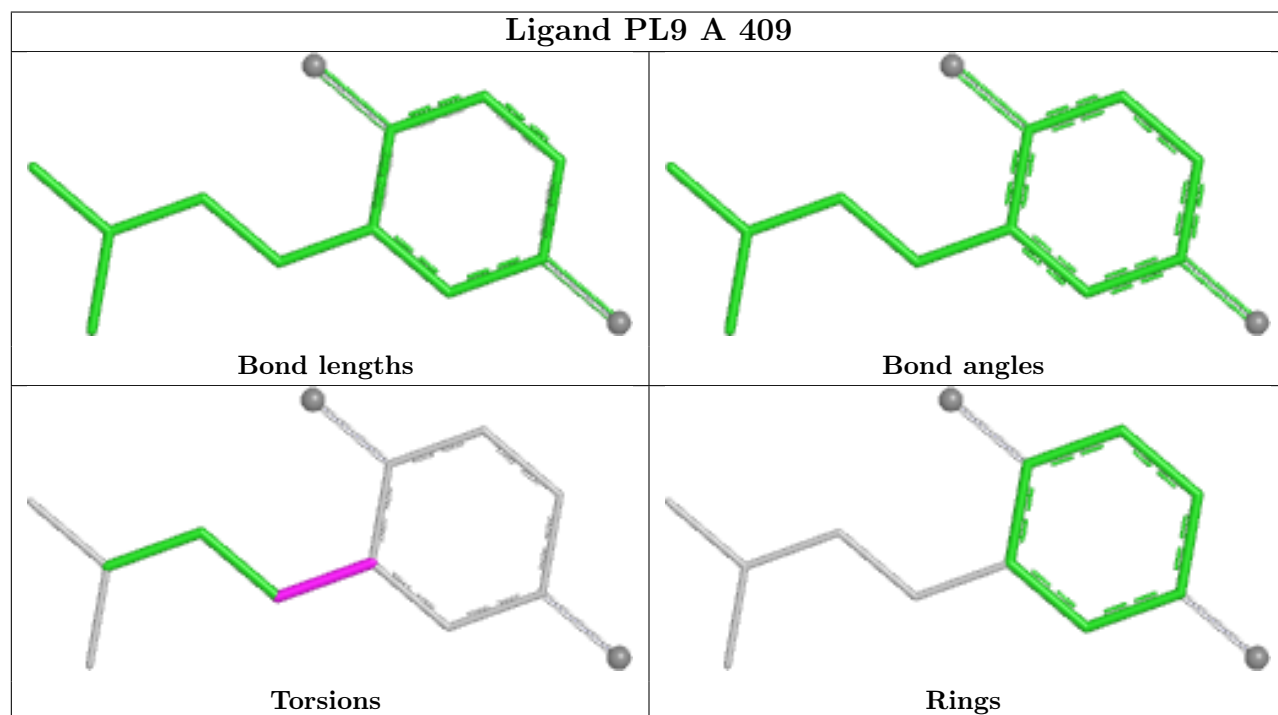
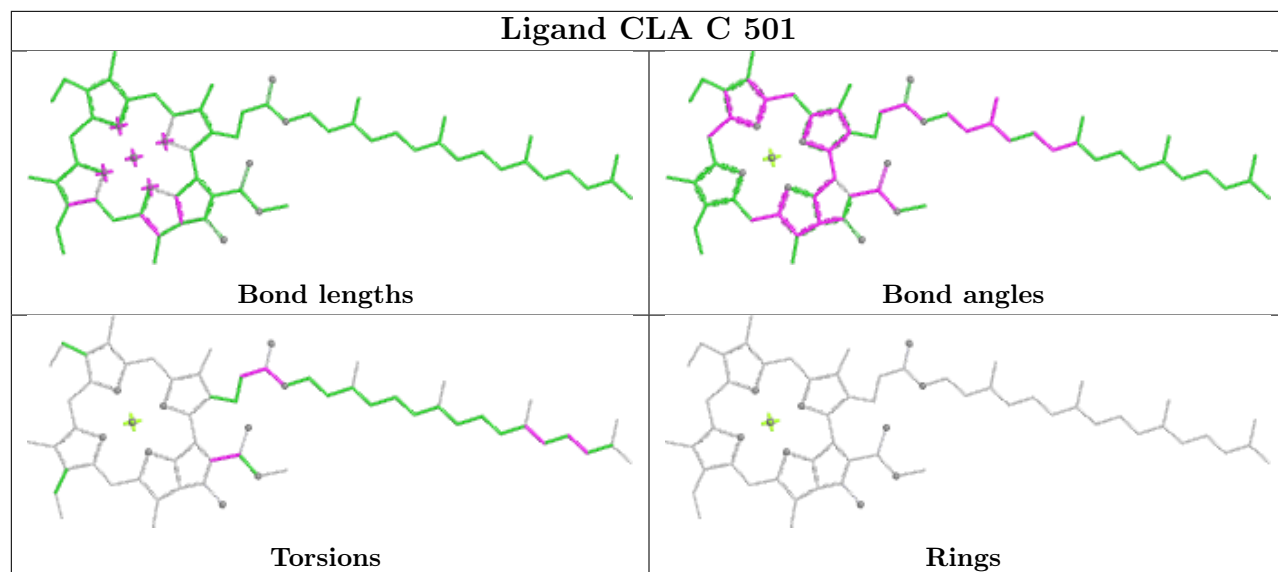


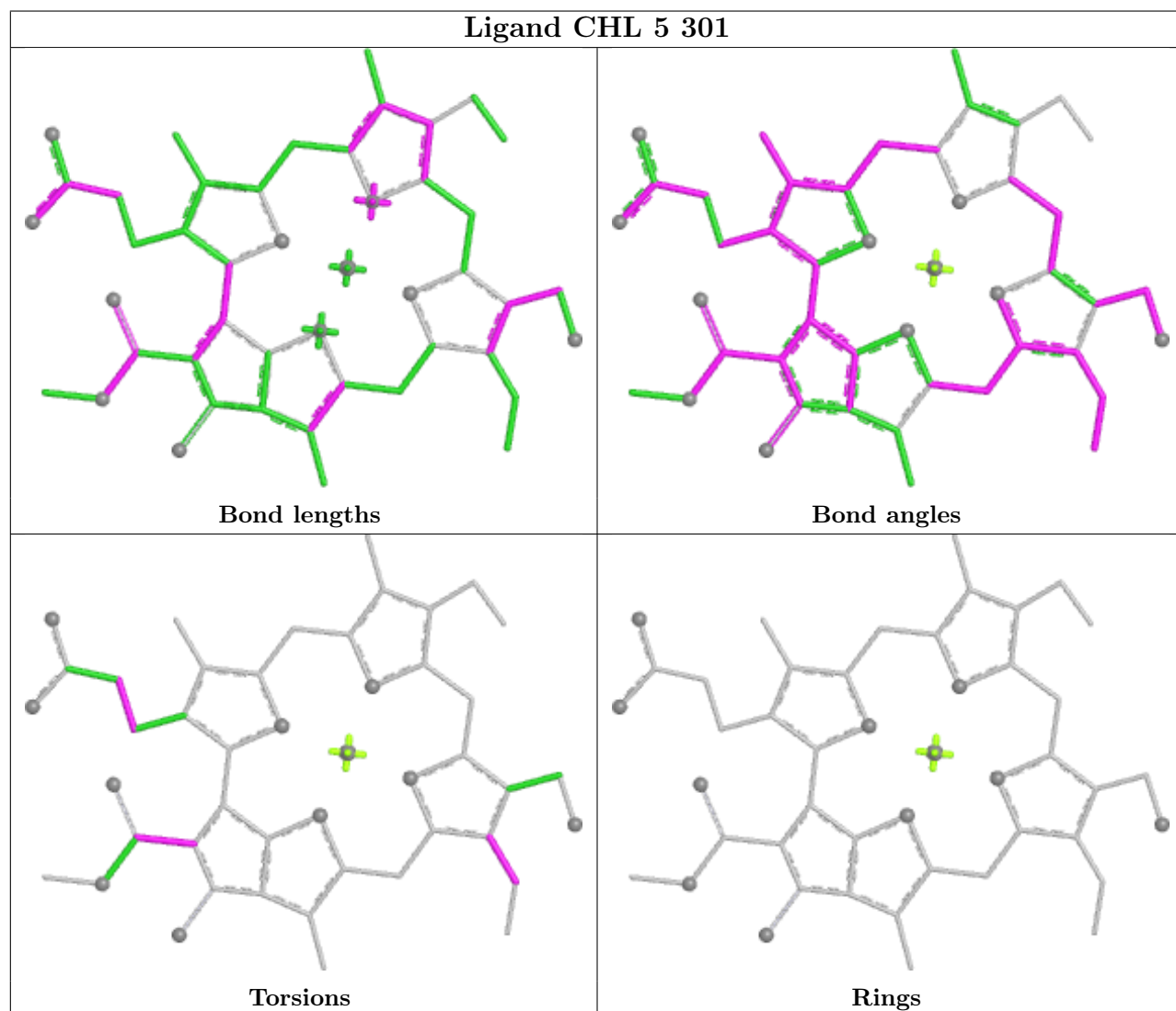
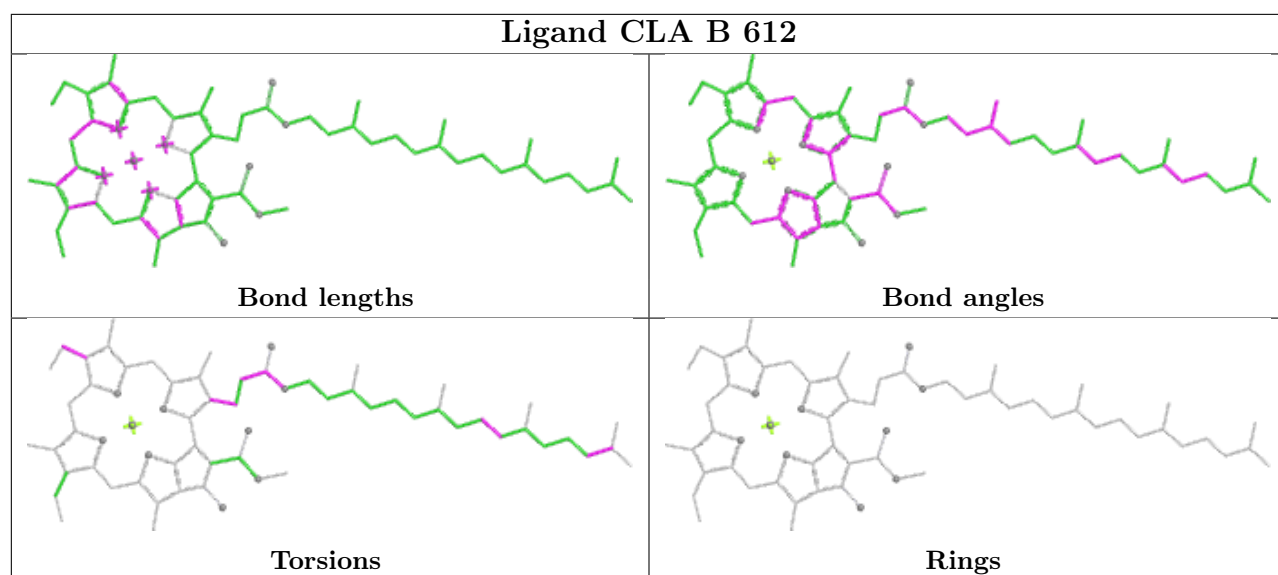
Torsions

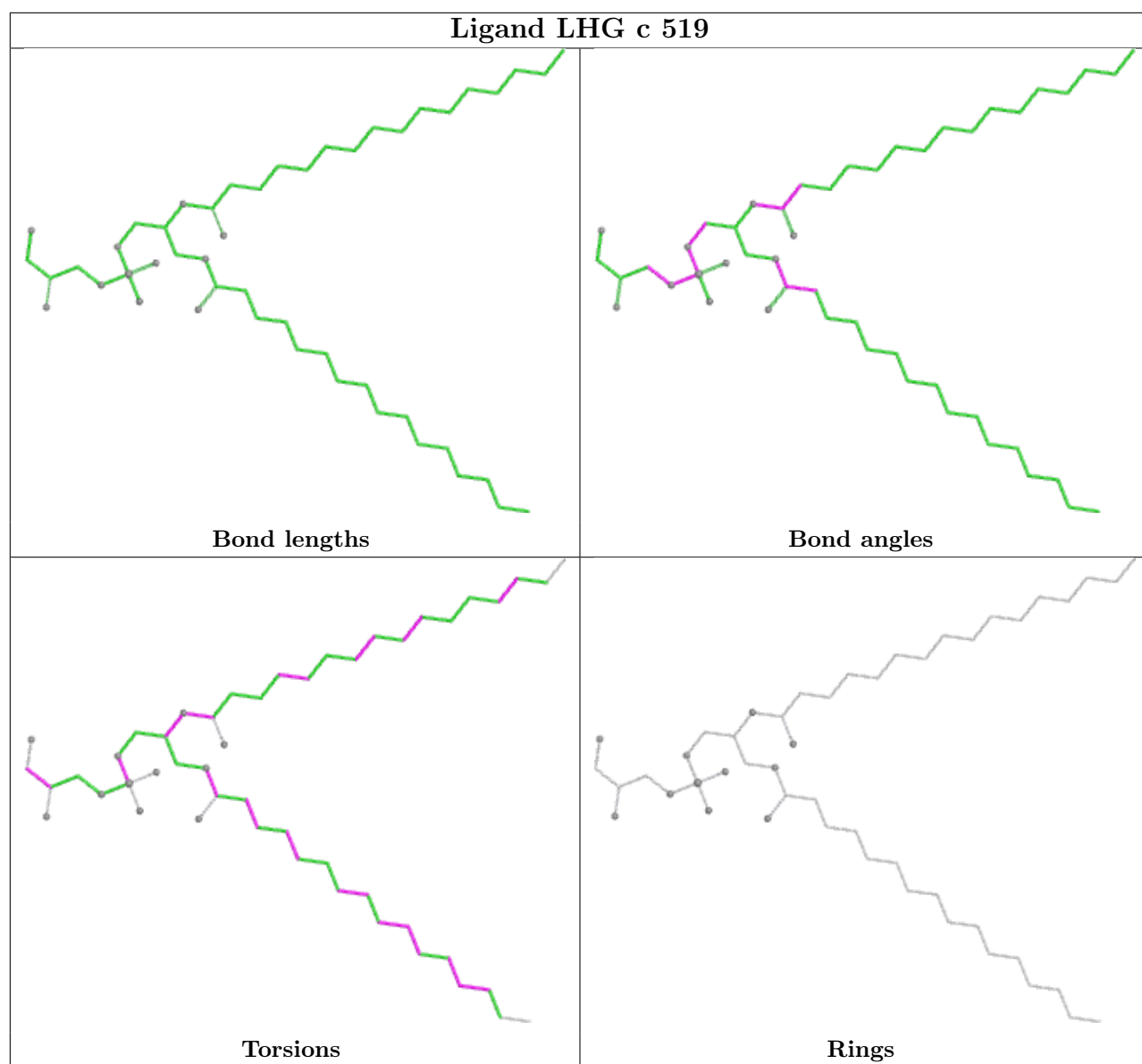


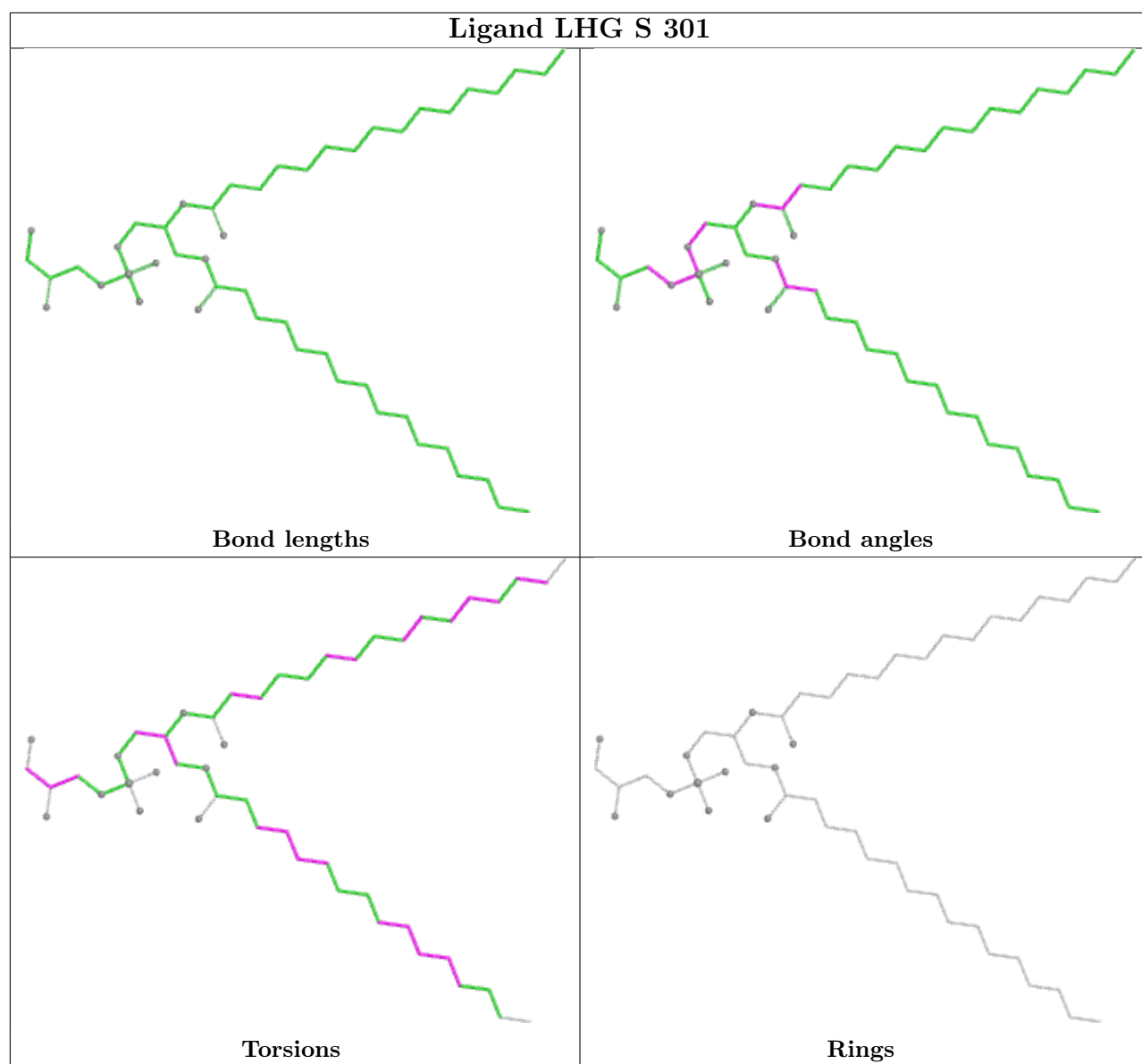
Rings



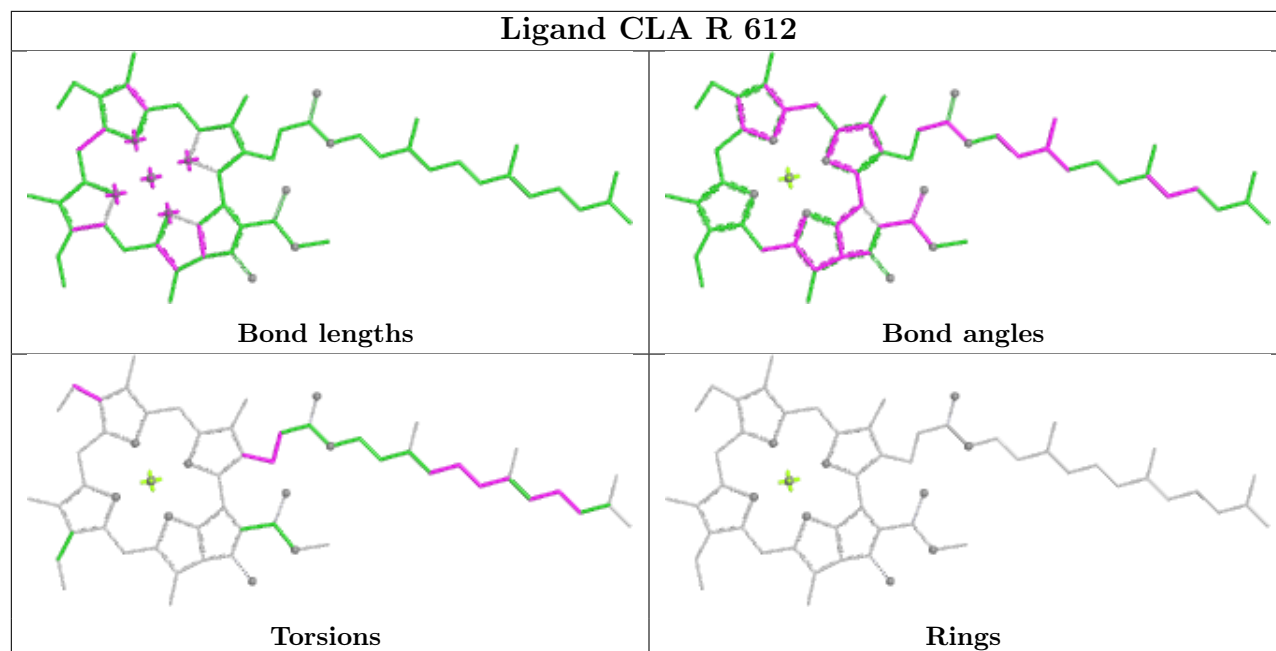




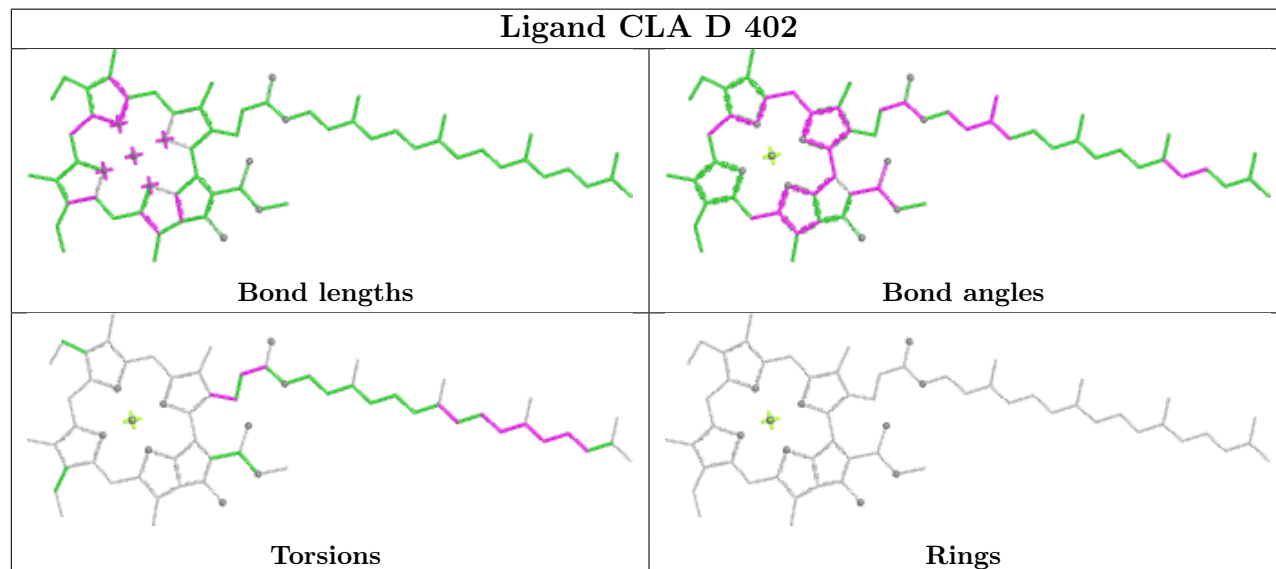


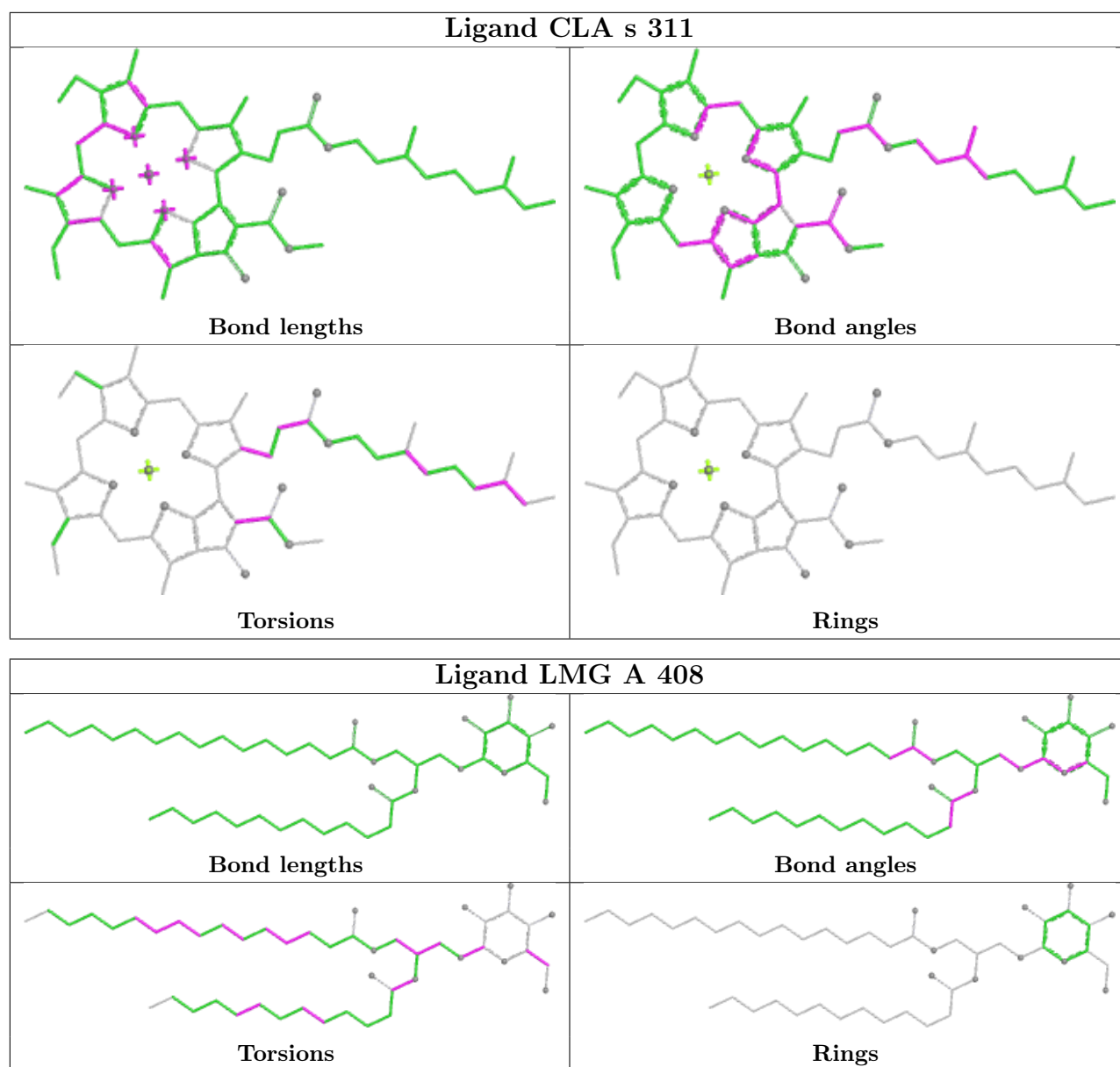


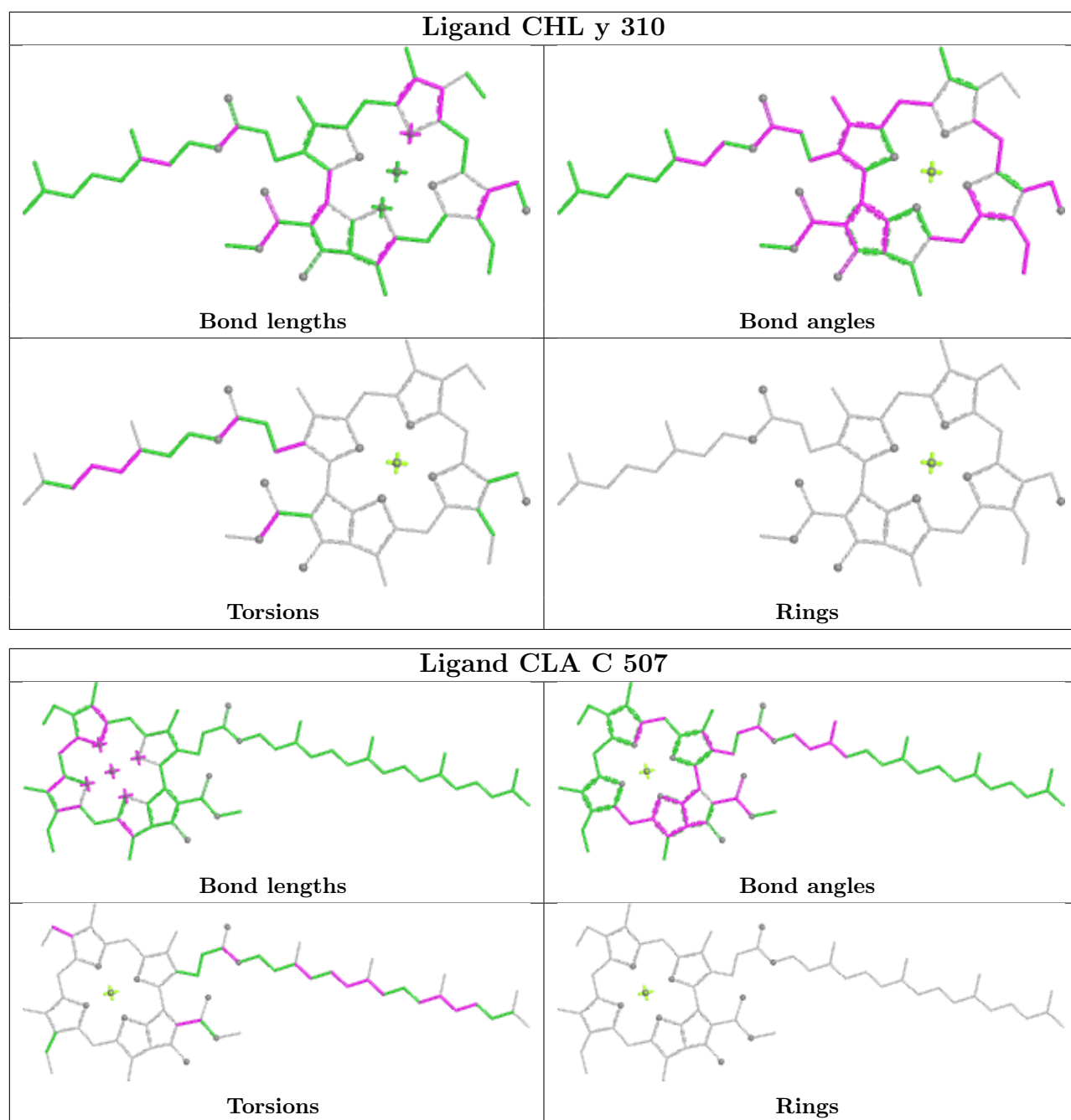
Ligand CLA R 612

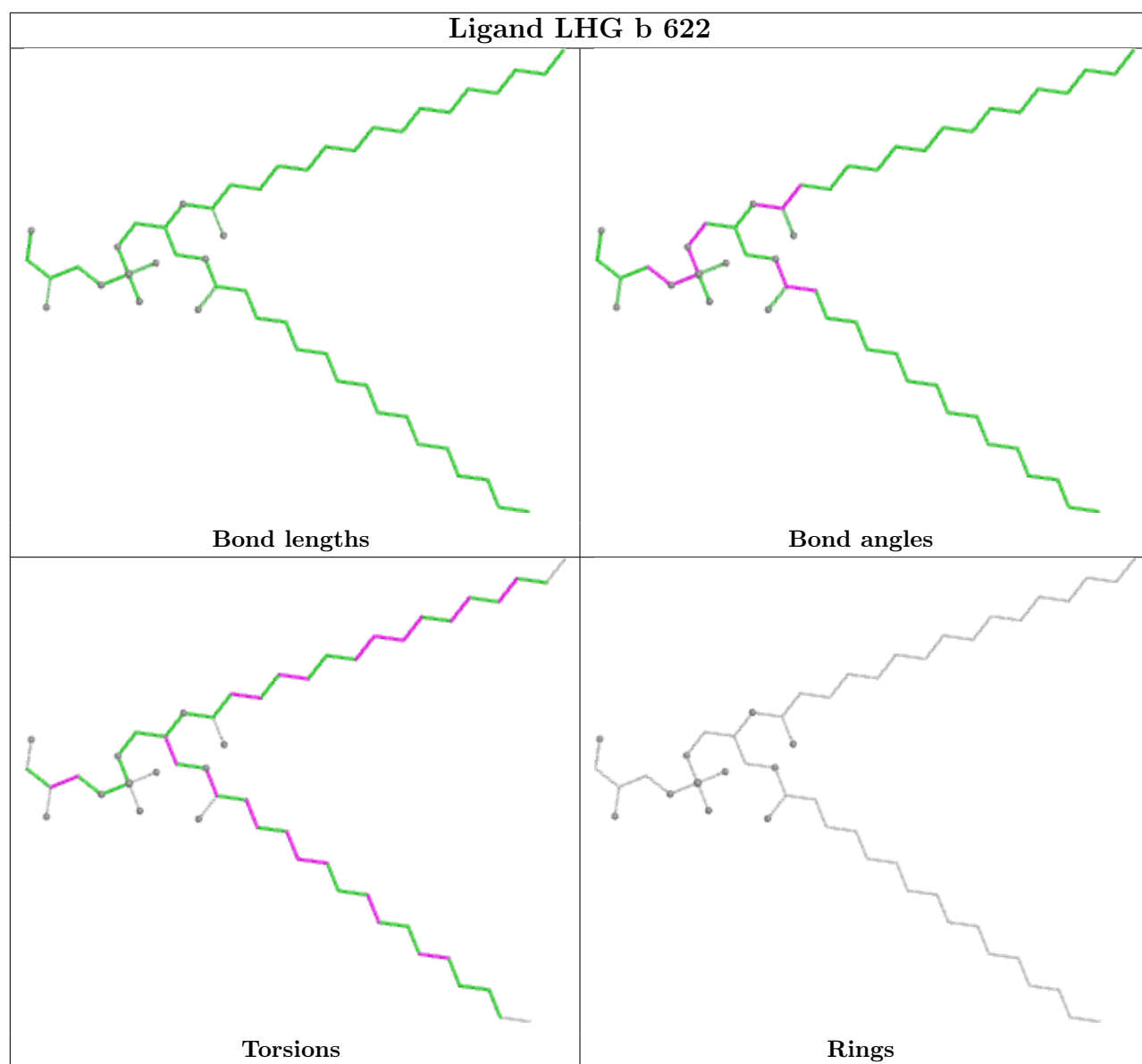


Ligand CLA D 402

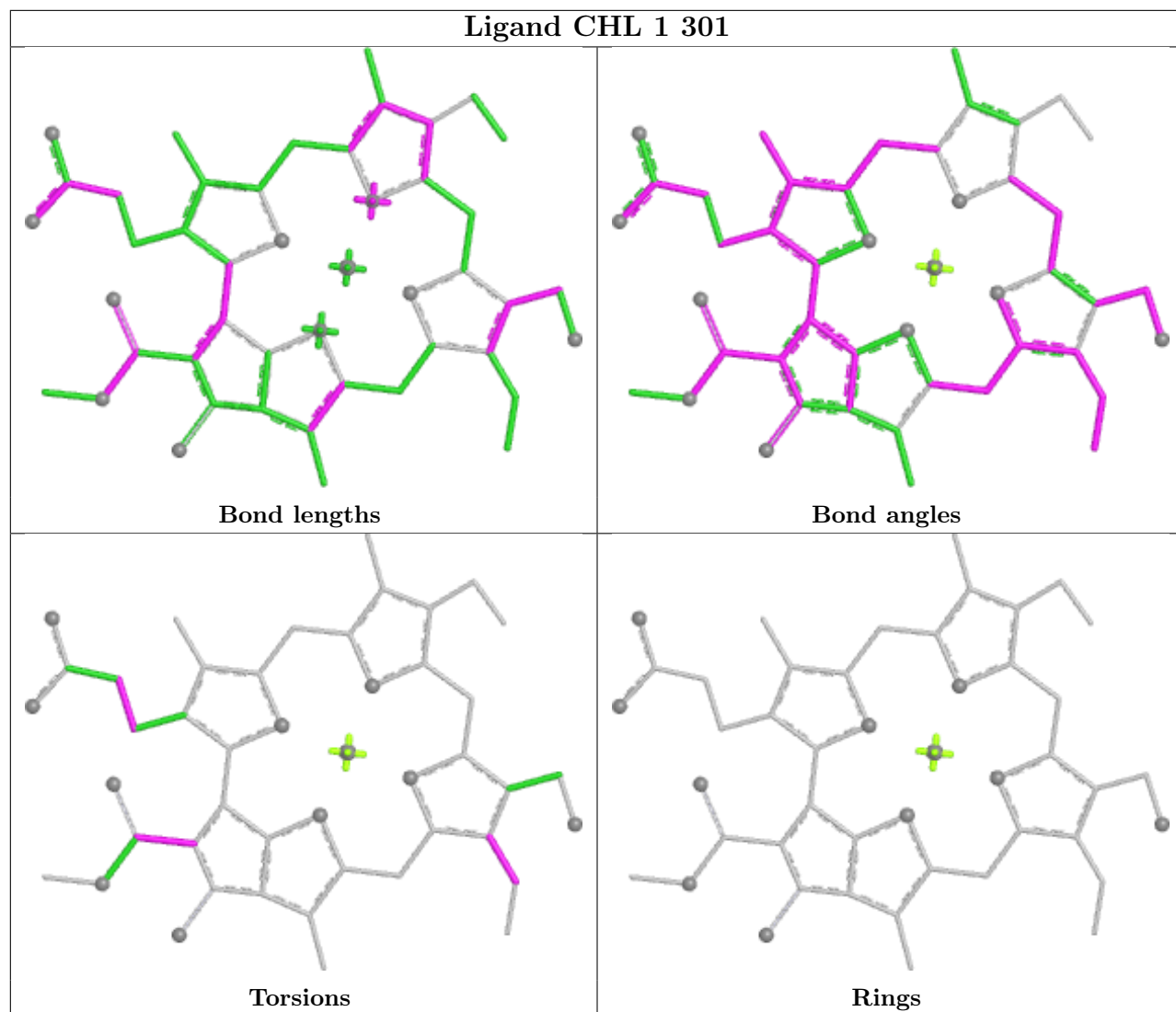


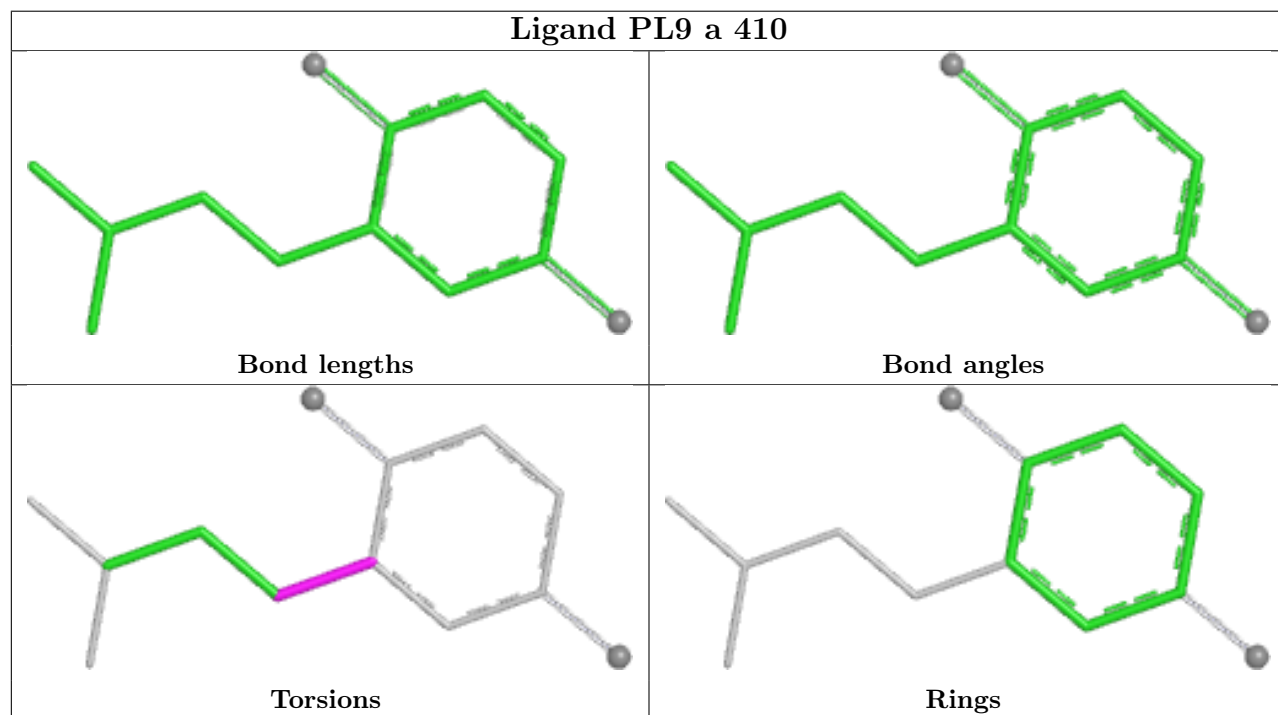
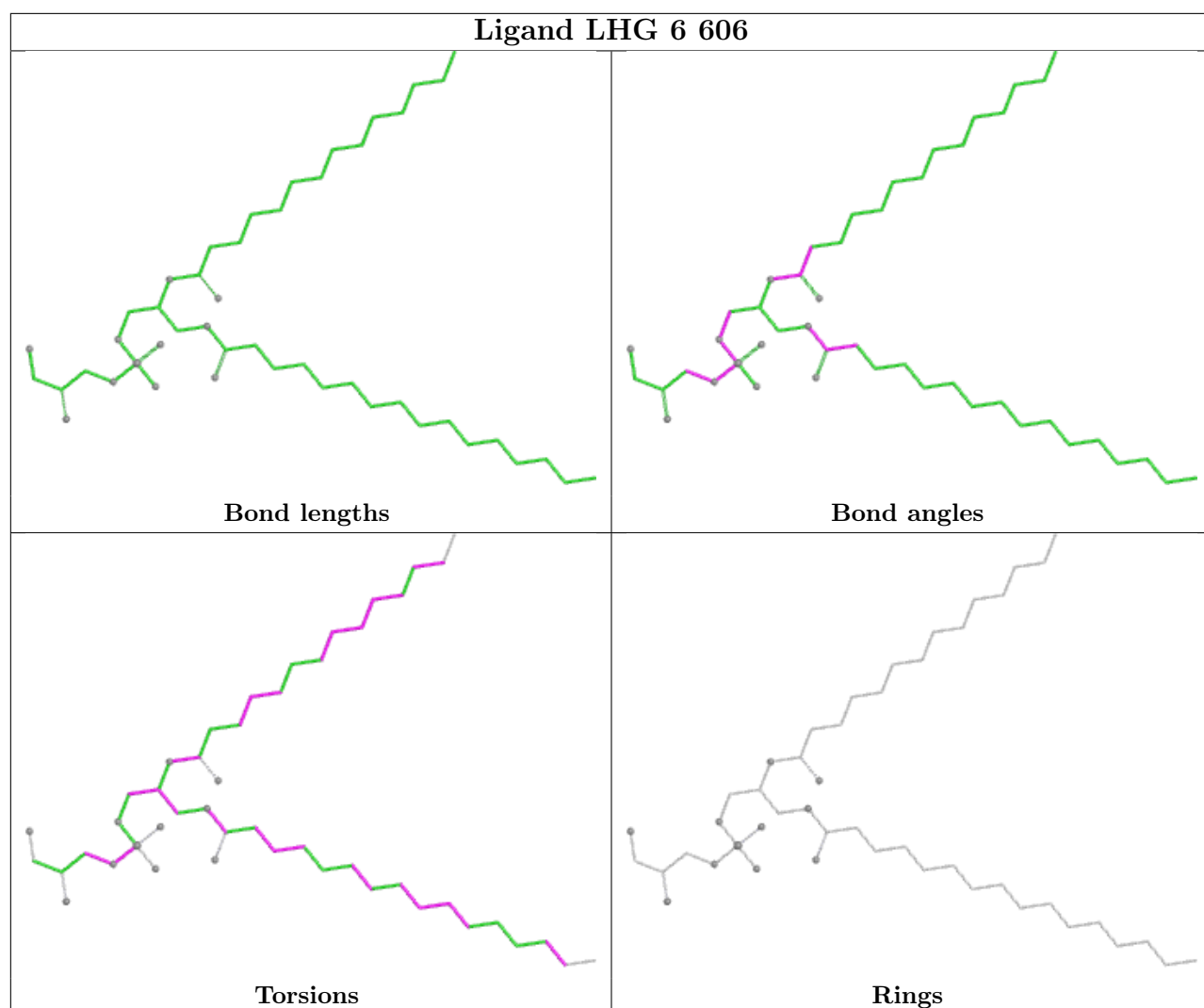


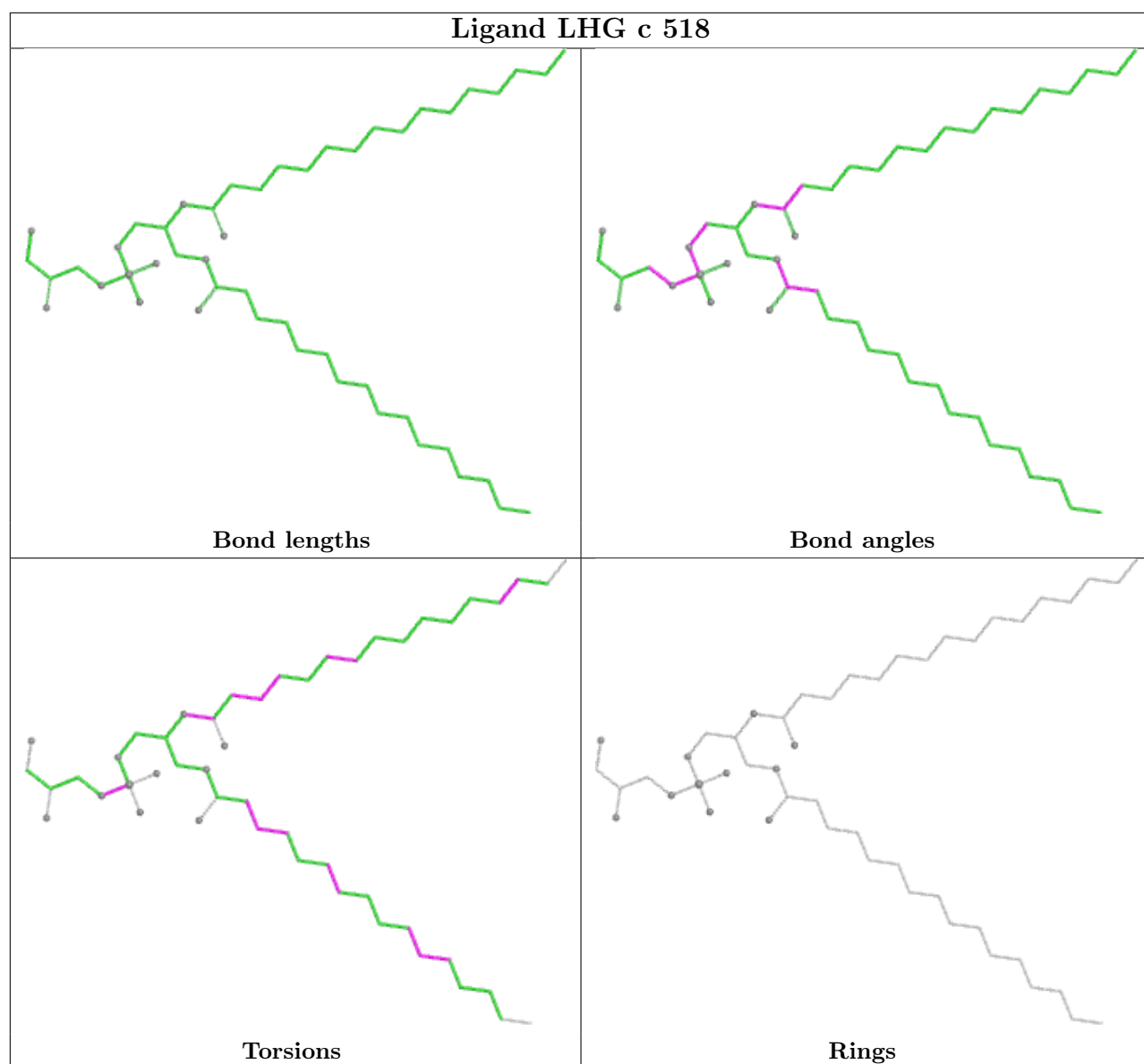


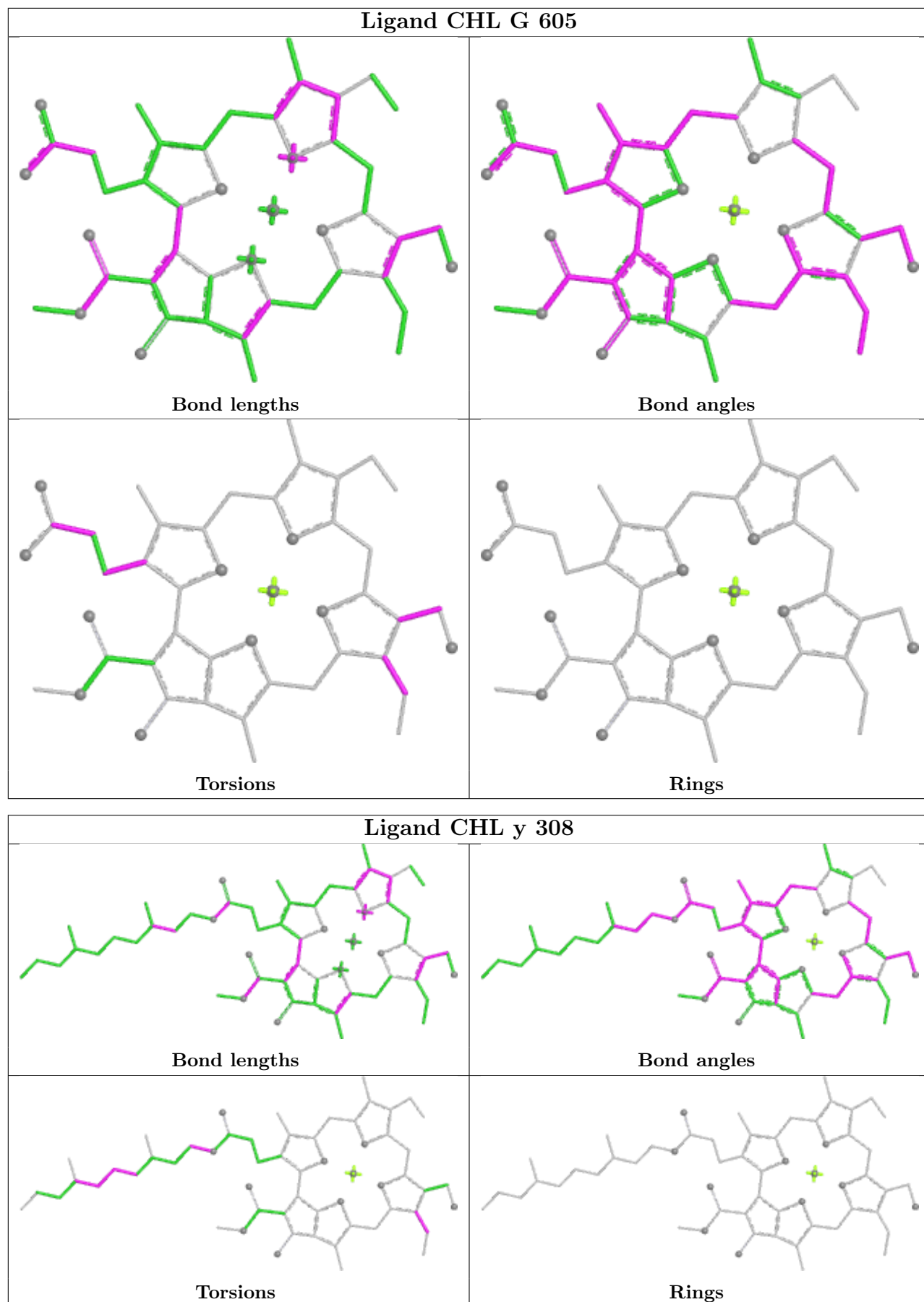


Ligand CHL 1 301

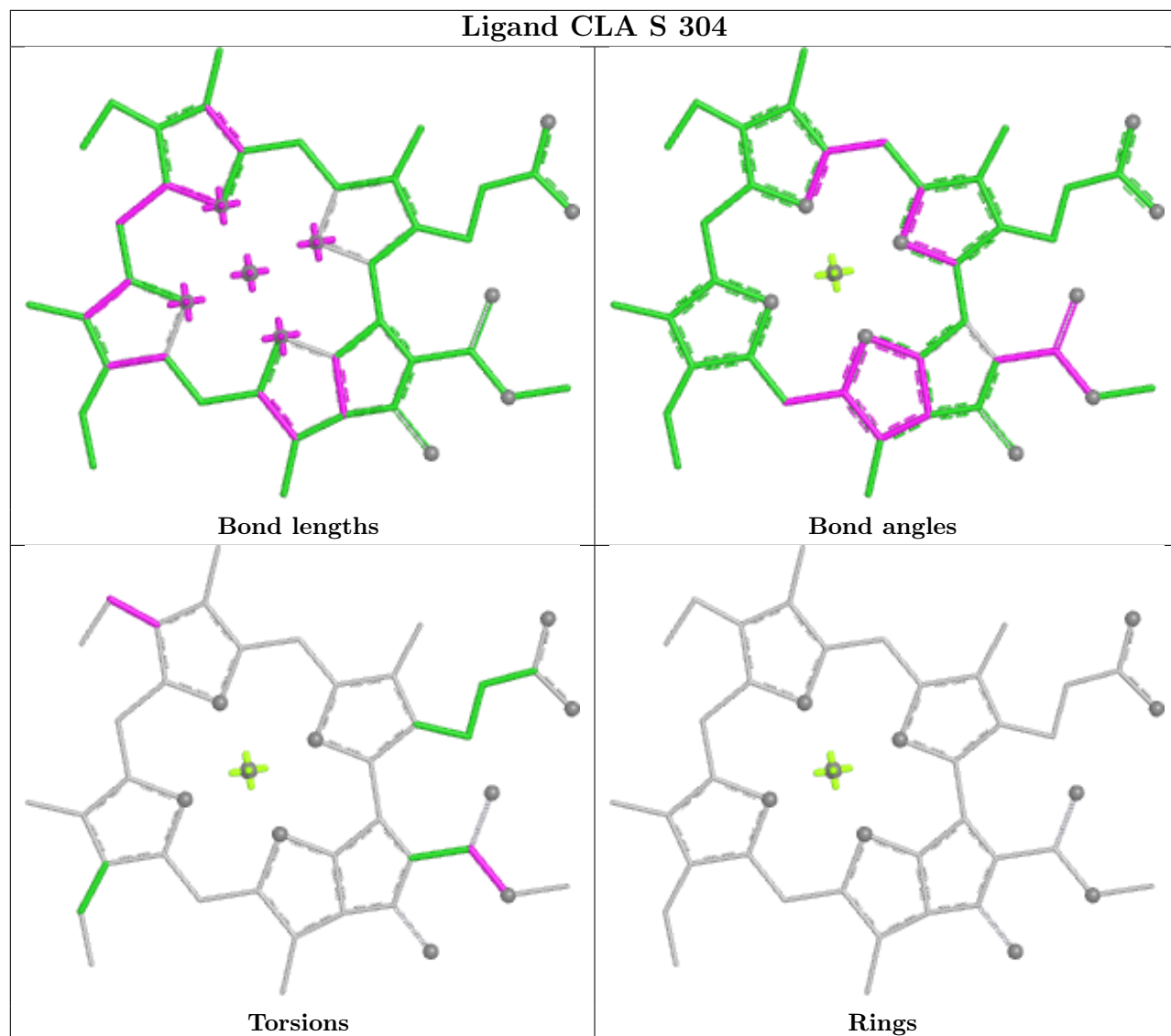




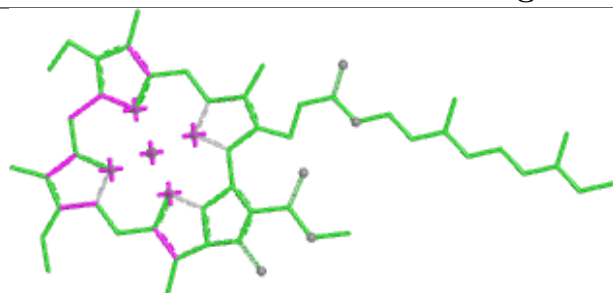




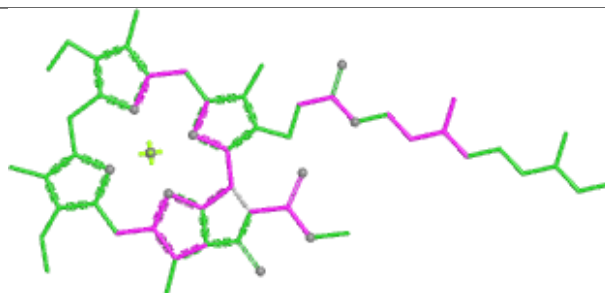
Ligand CLA S 304



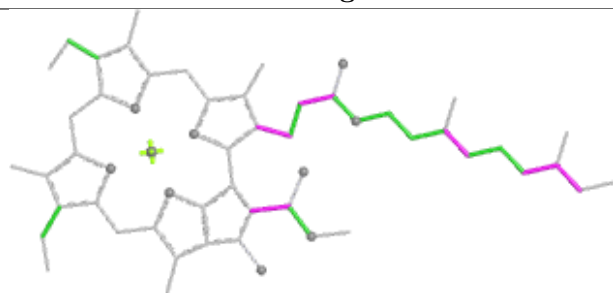
Ligand CLA S 311



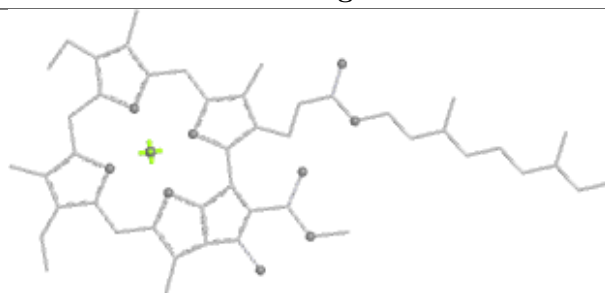
Bond lengths



Bond angles

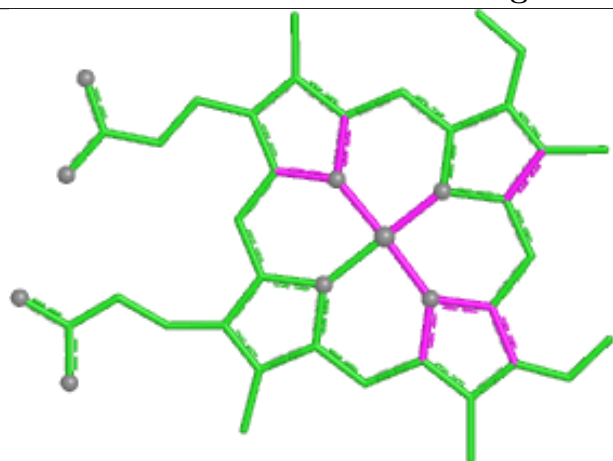


Torsions

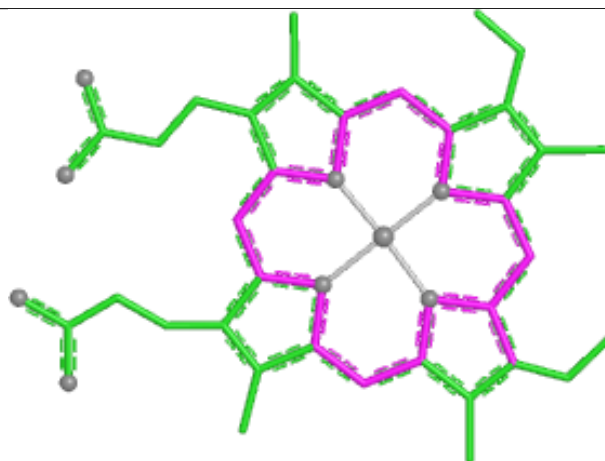


Rings

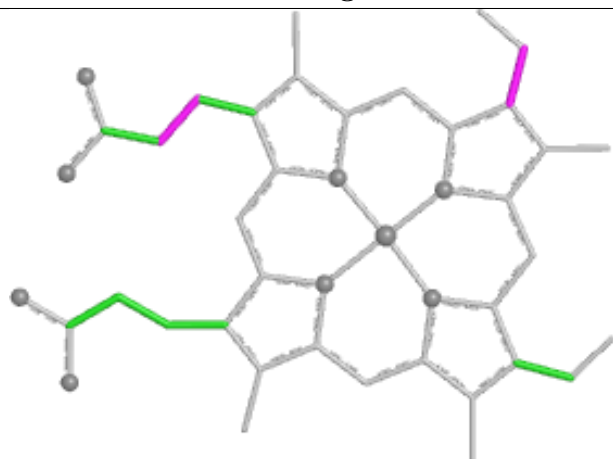
Ligand HEM F 101



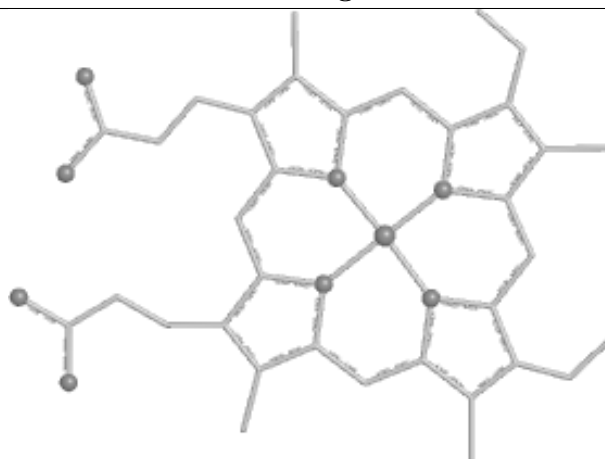
Bond lengths



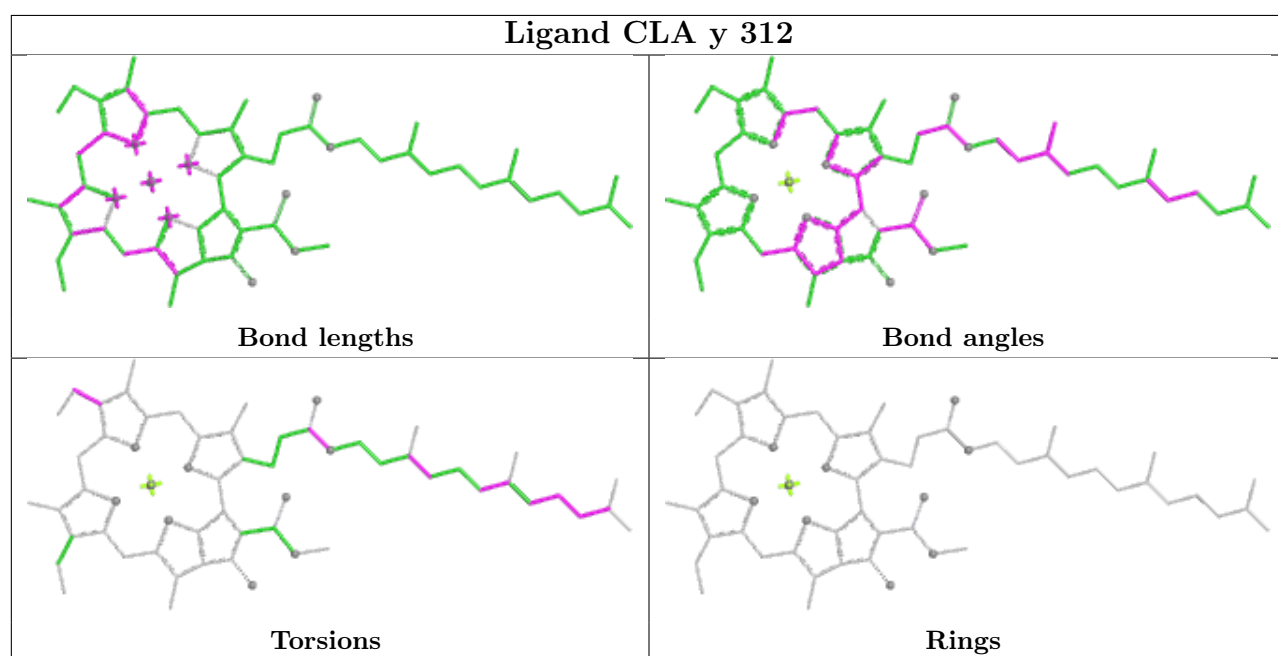
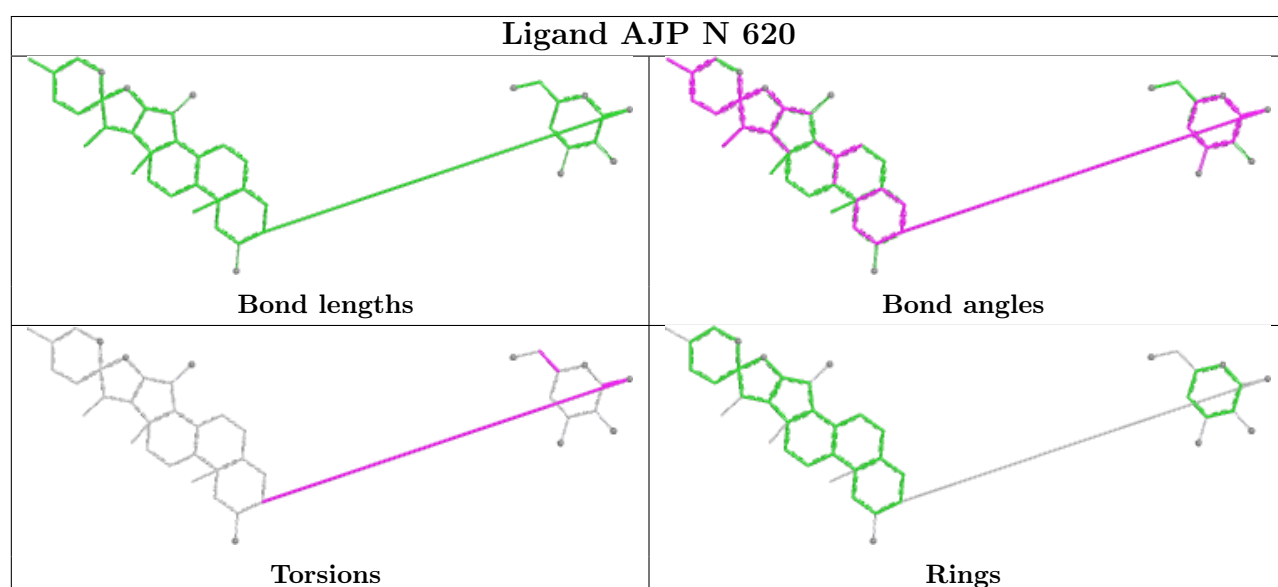
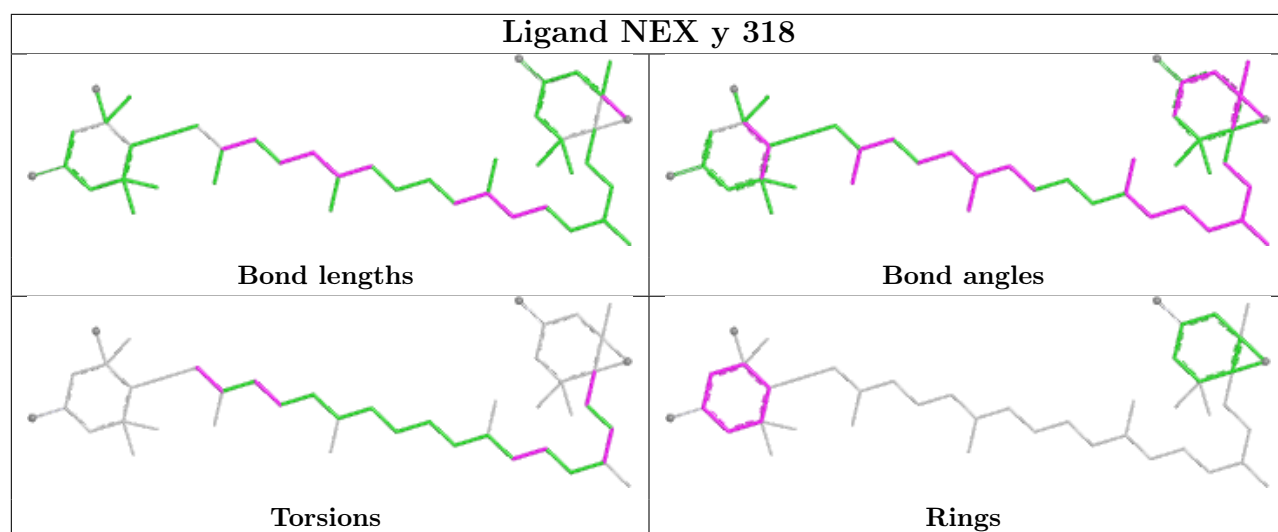
Bond angles

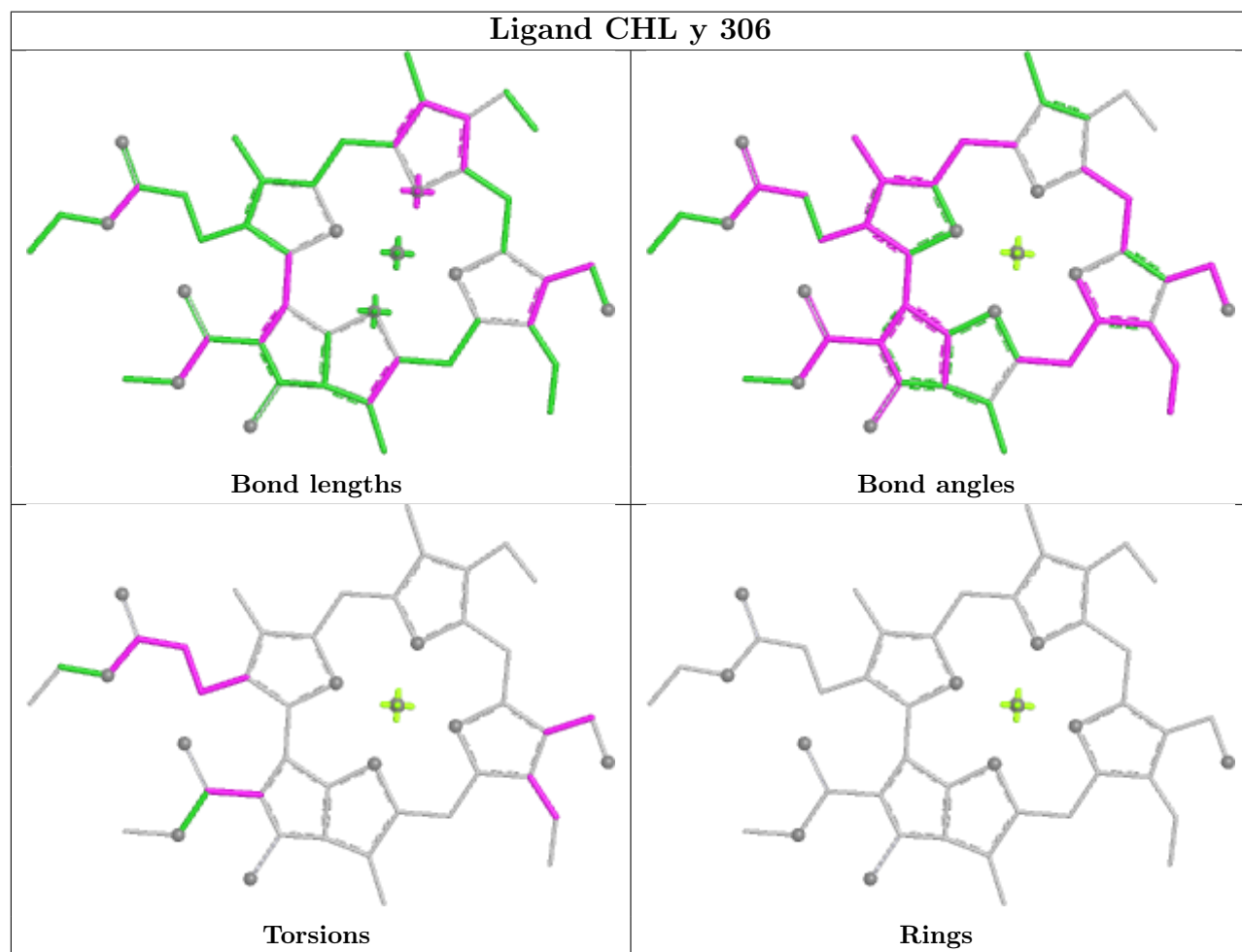
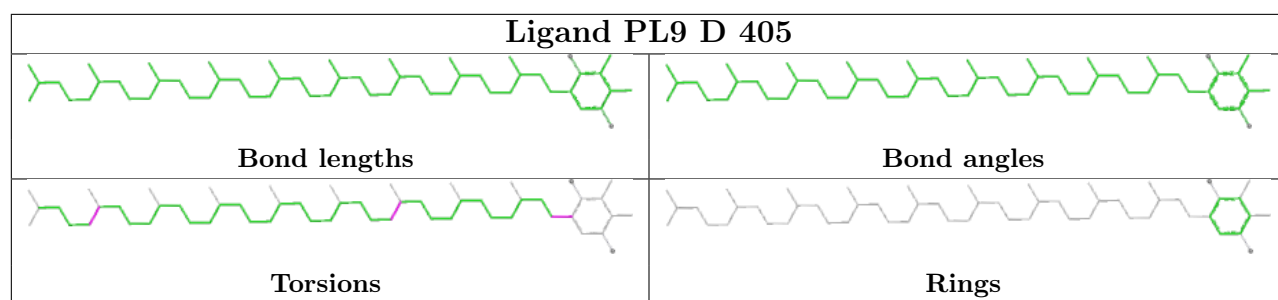


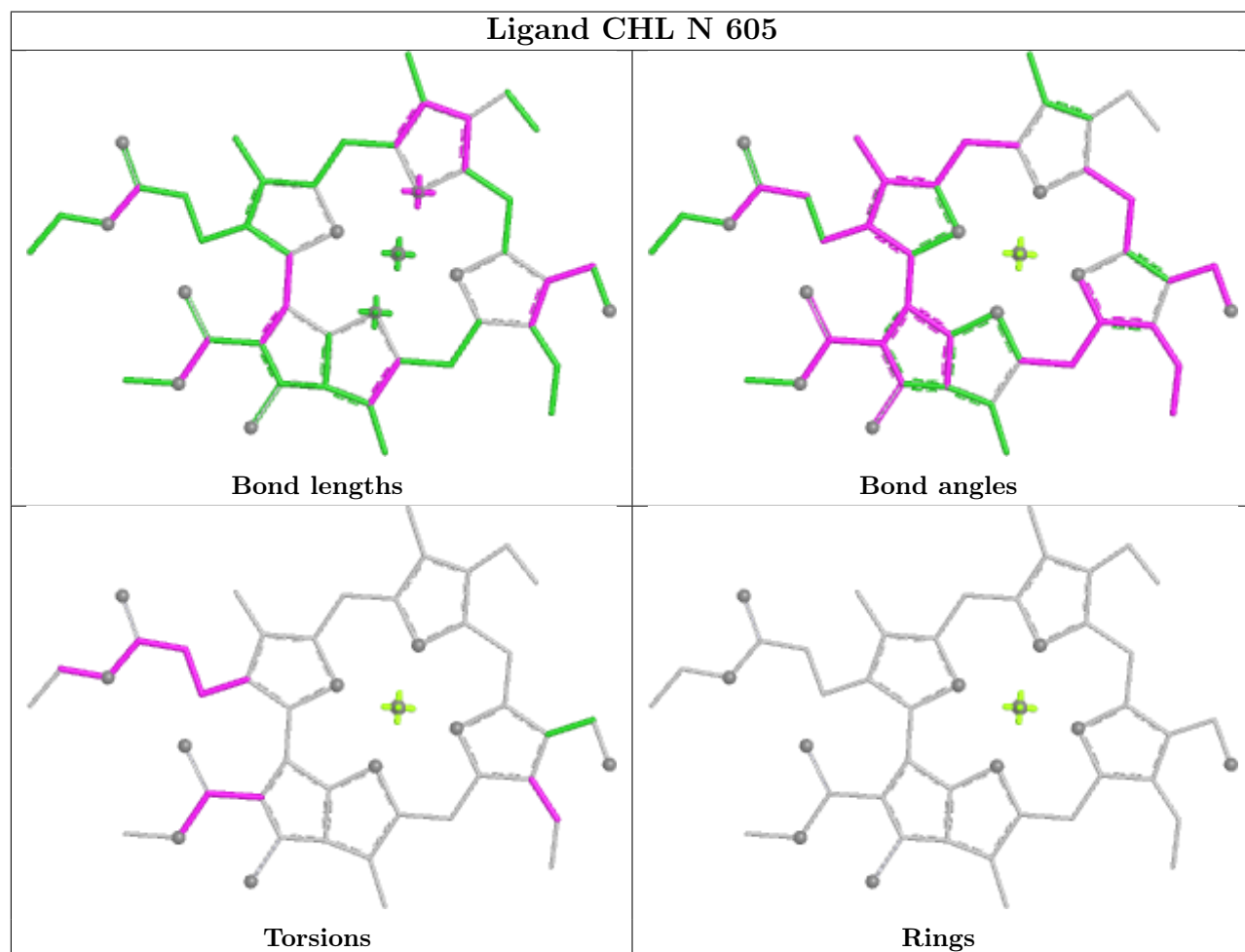
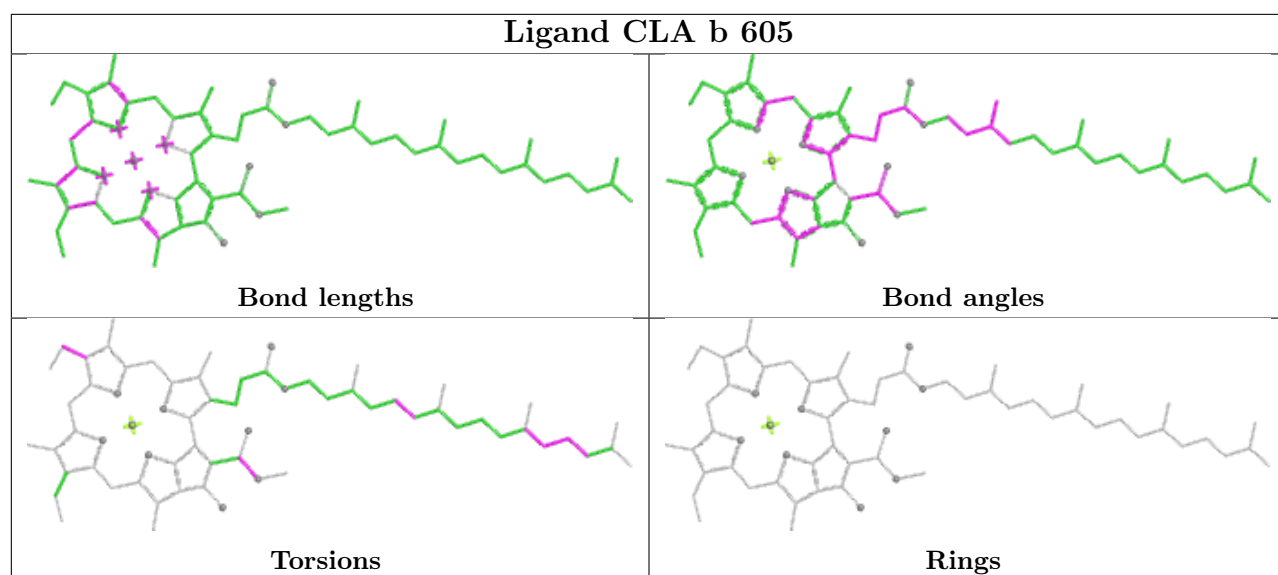
Torsions

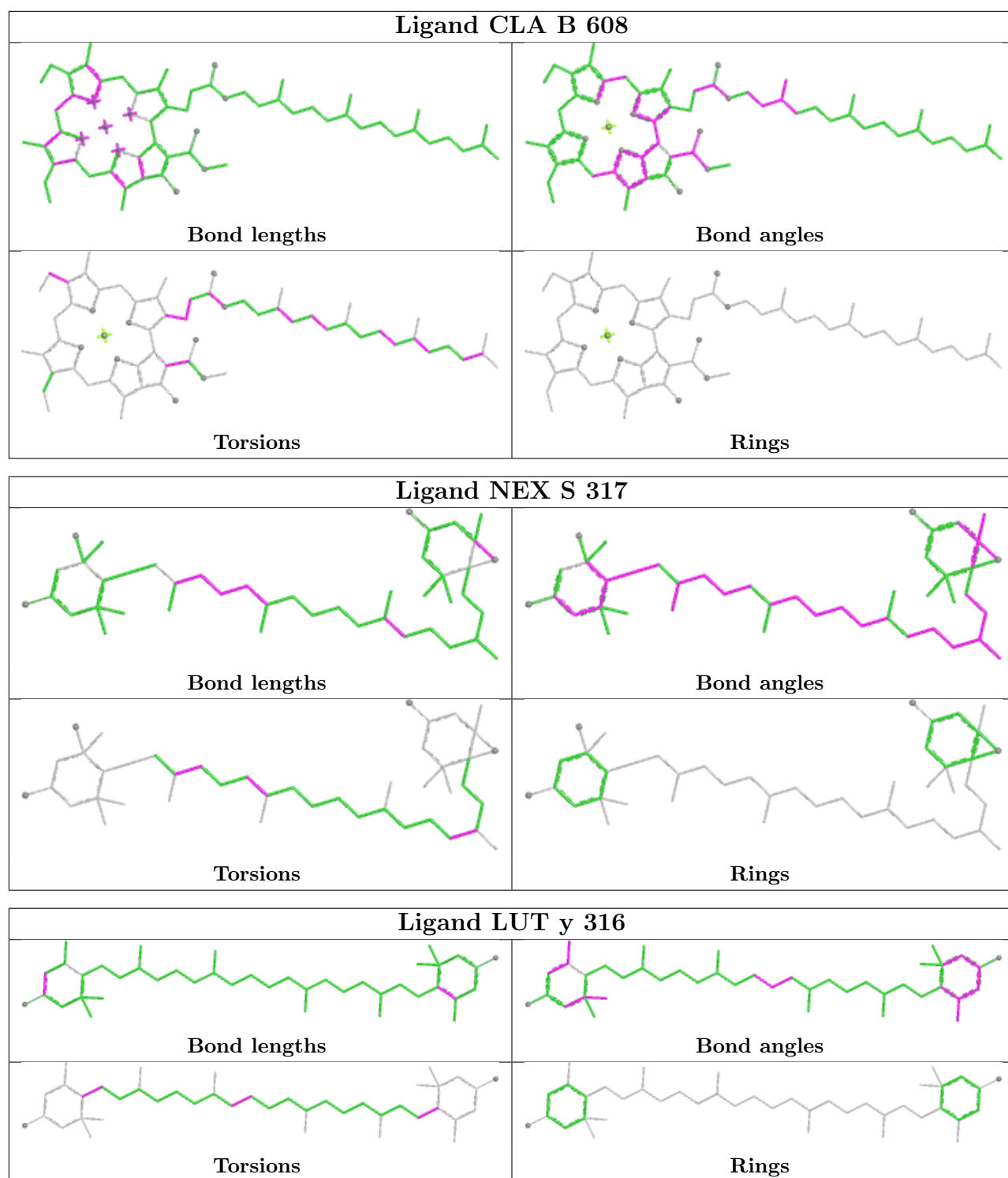


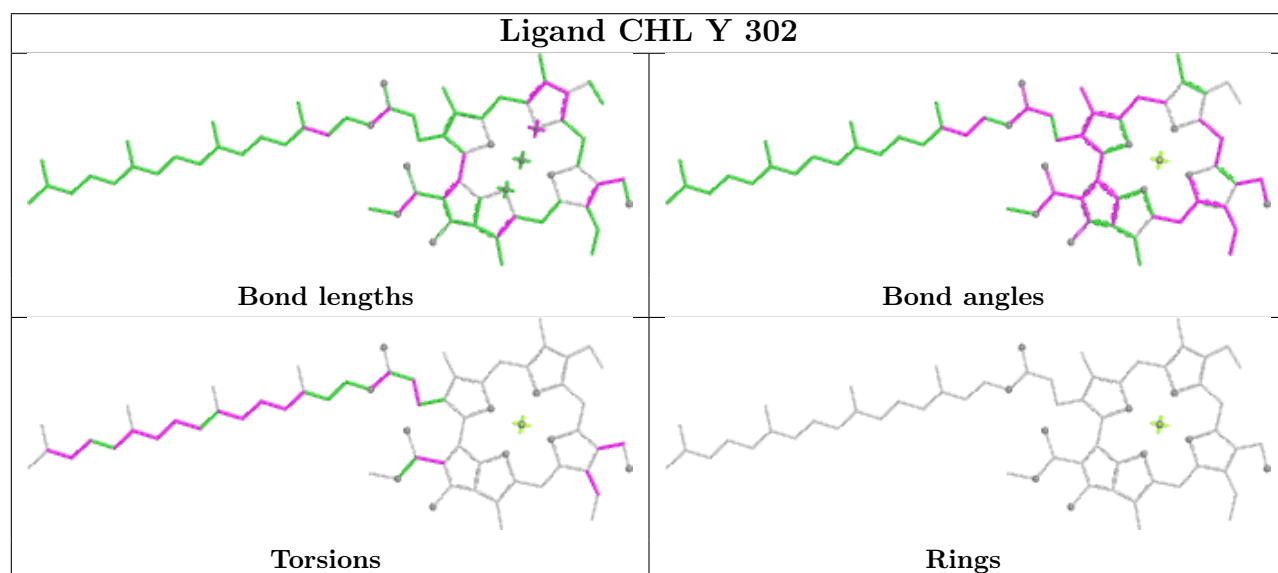
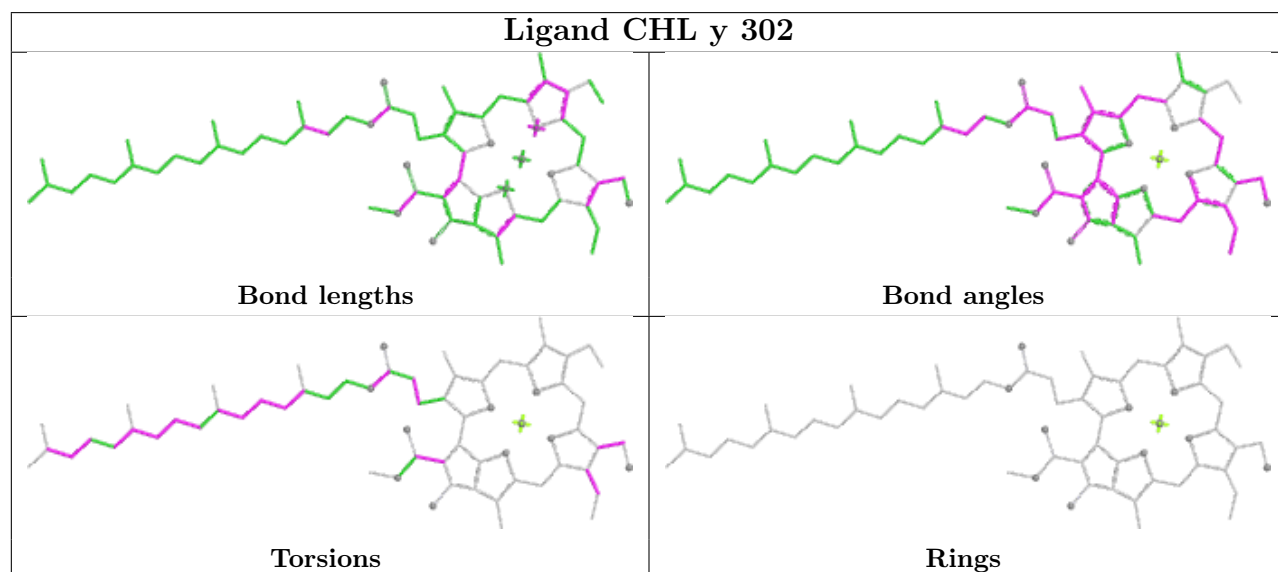
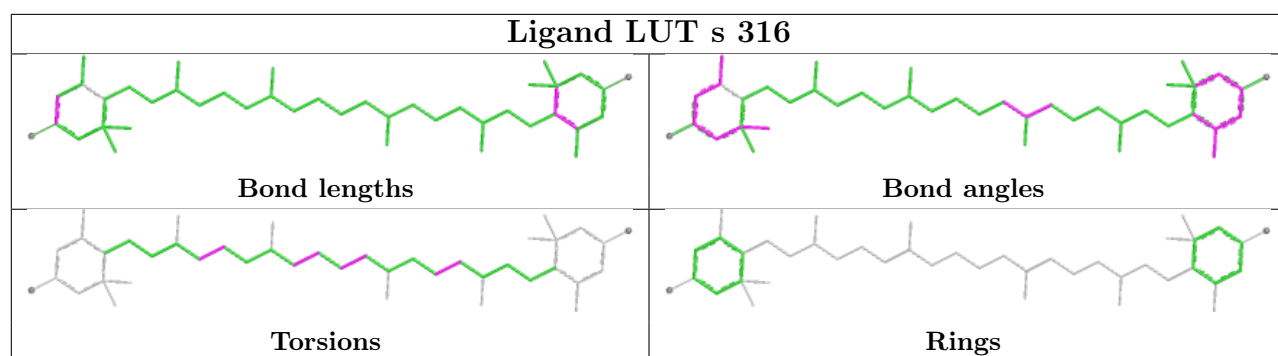
Rings

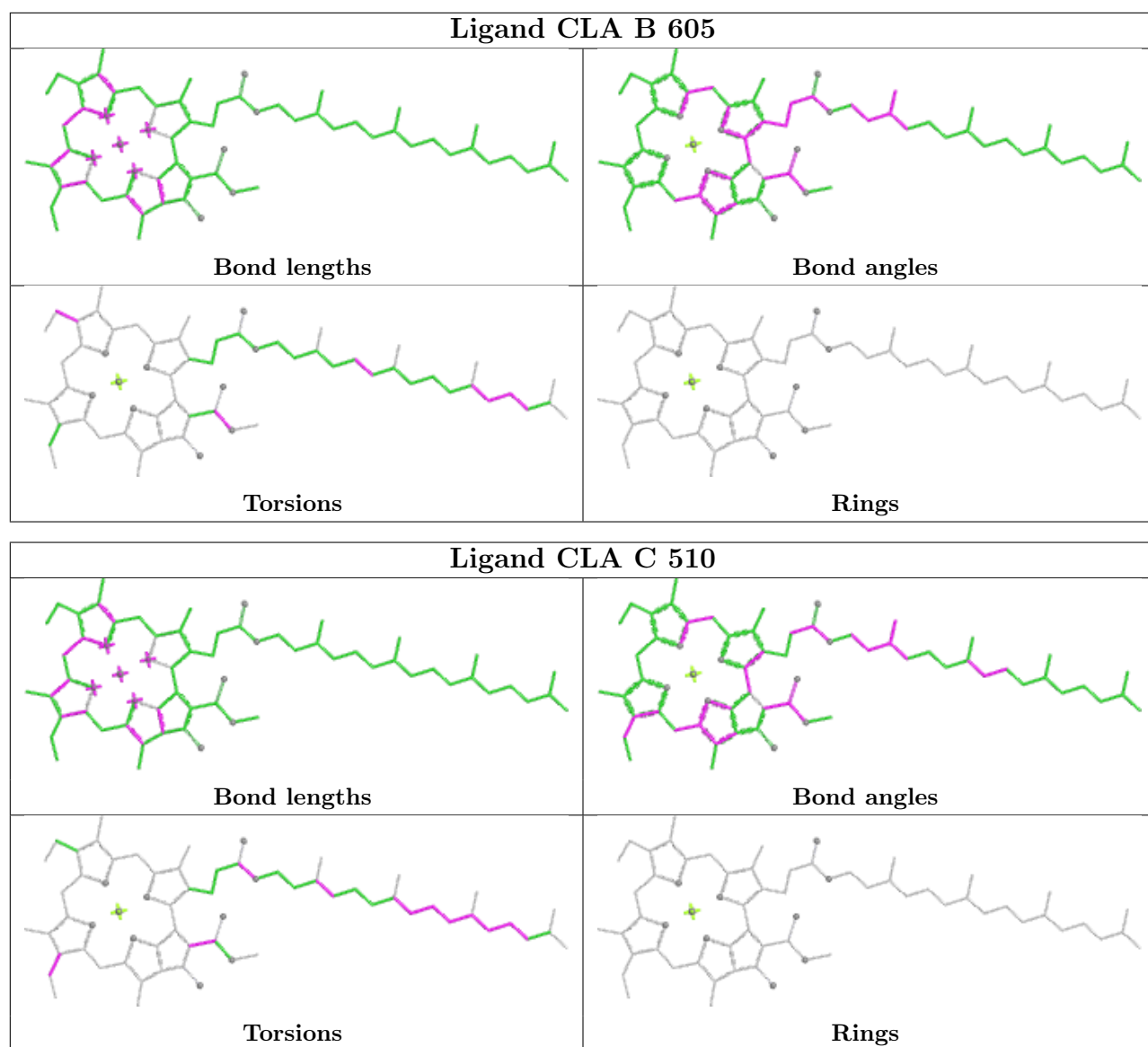




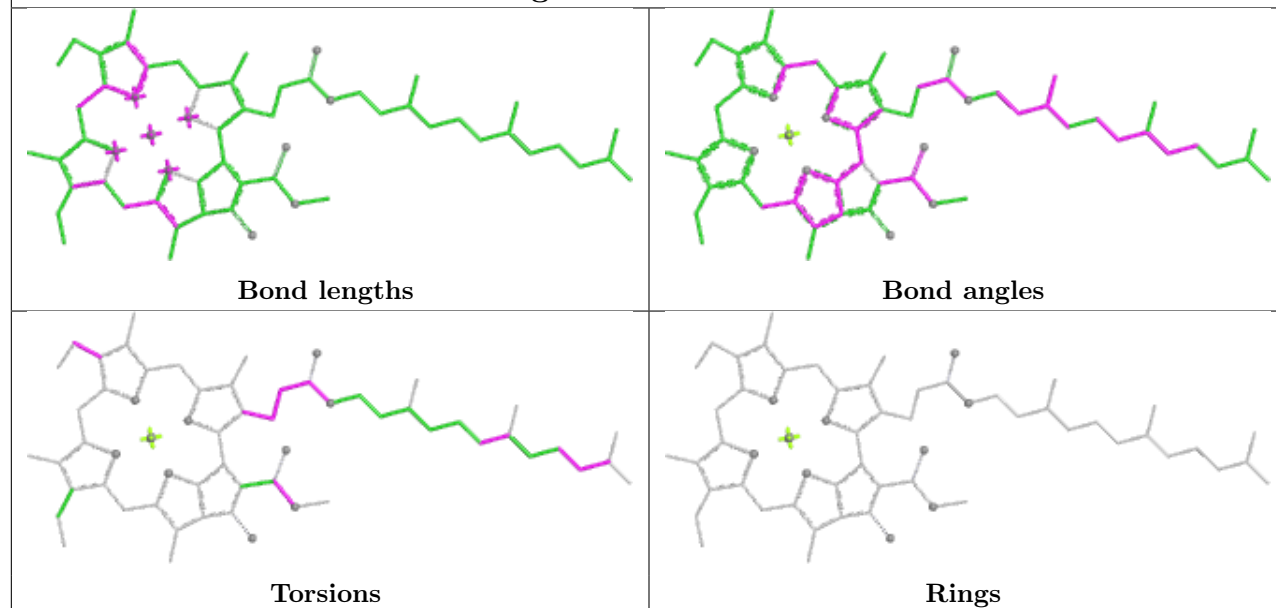




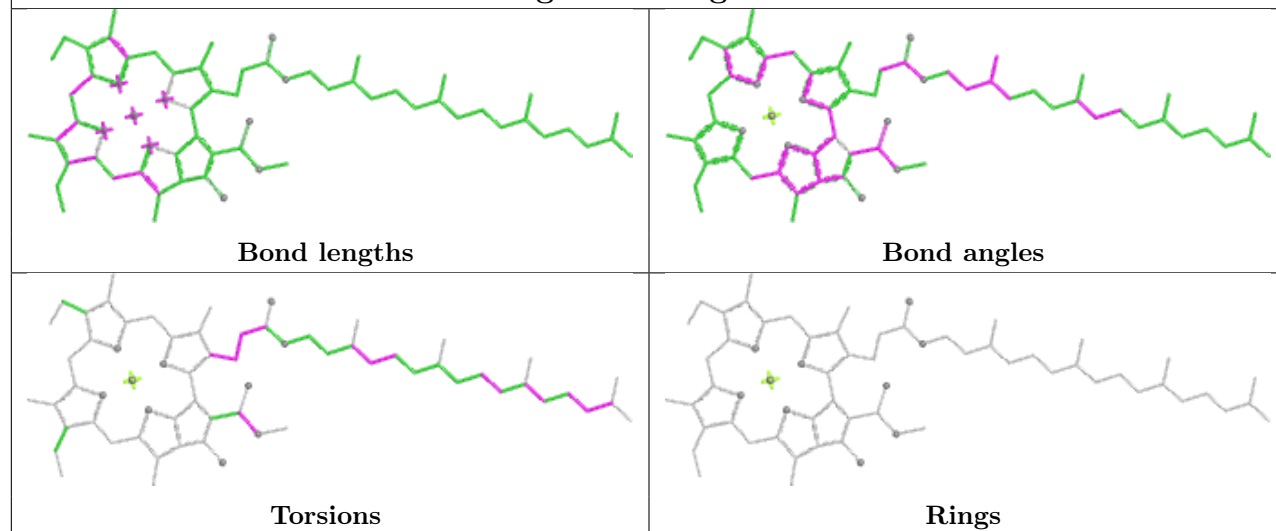


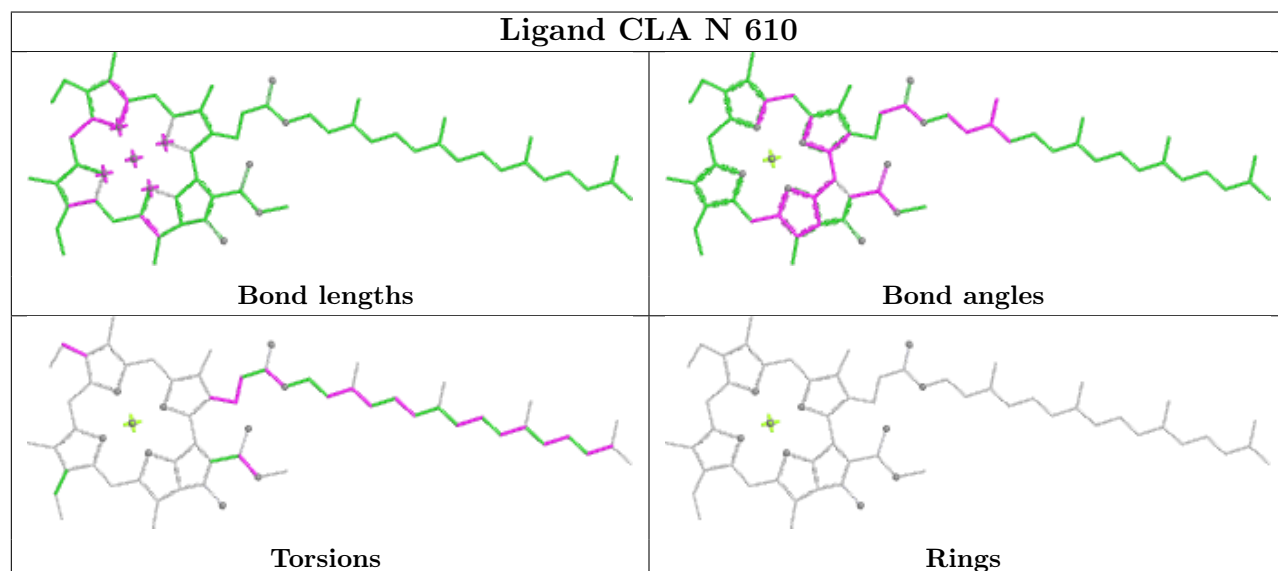
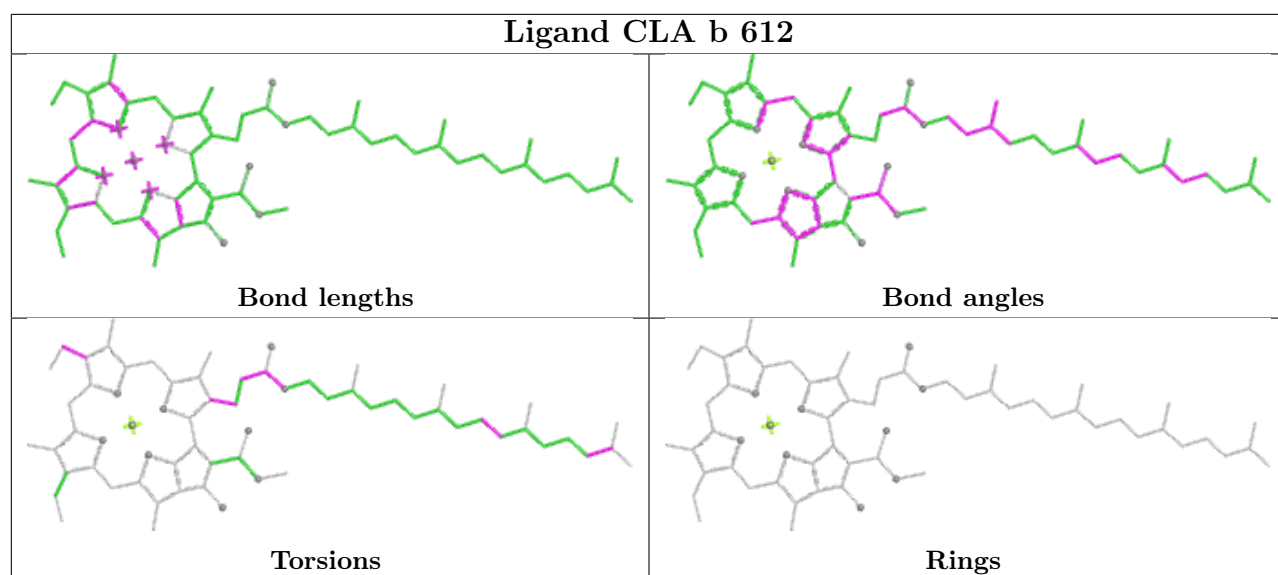


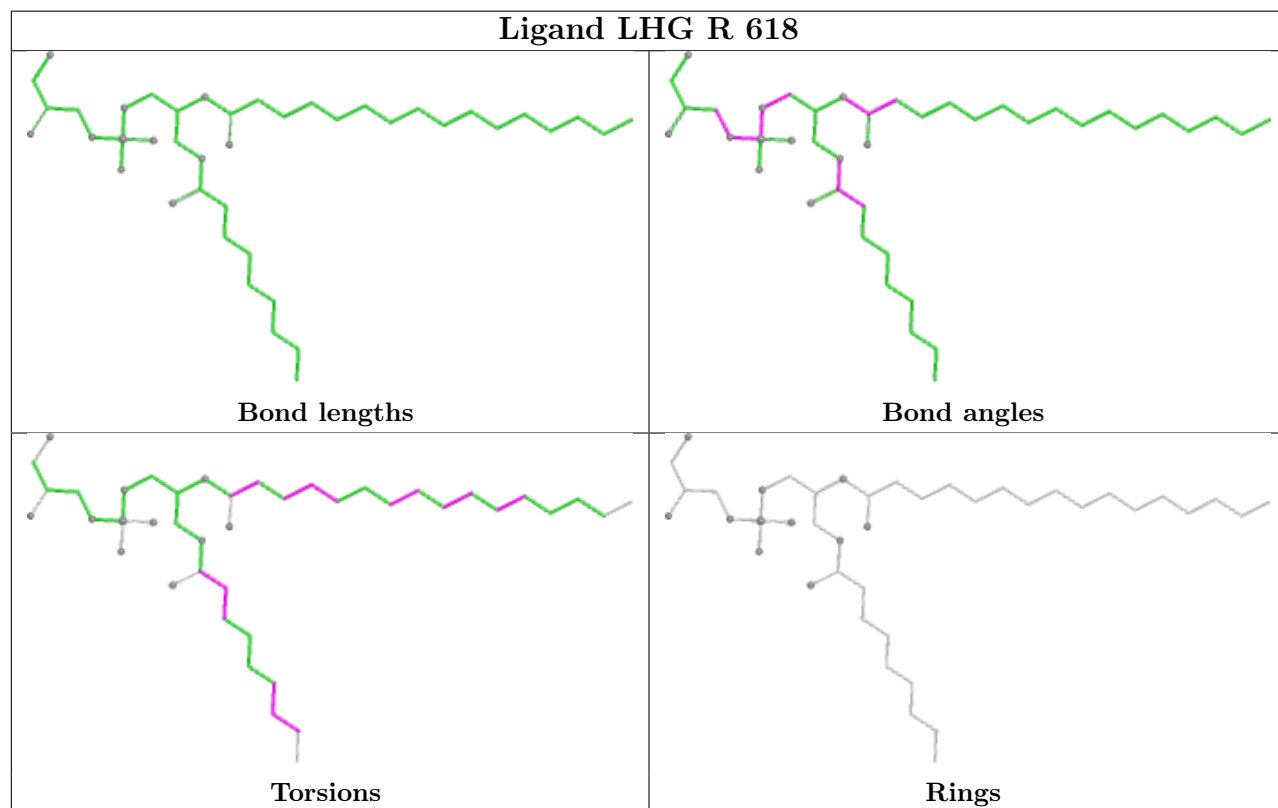
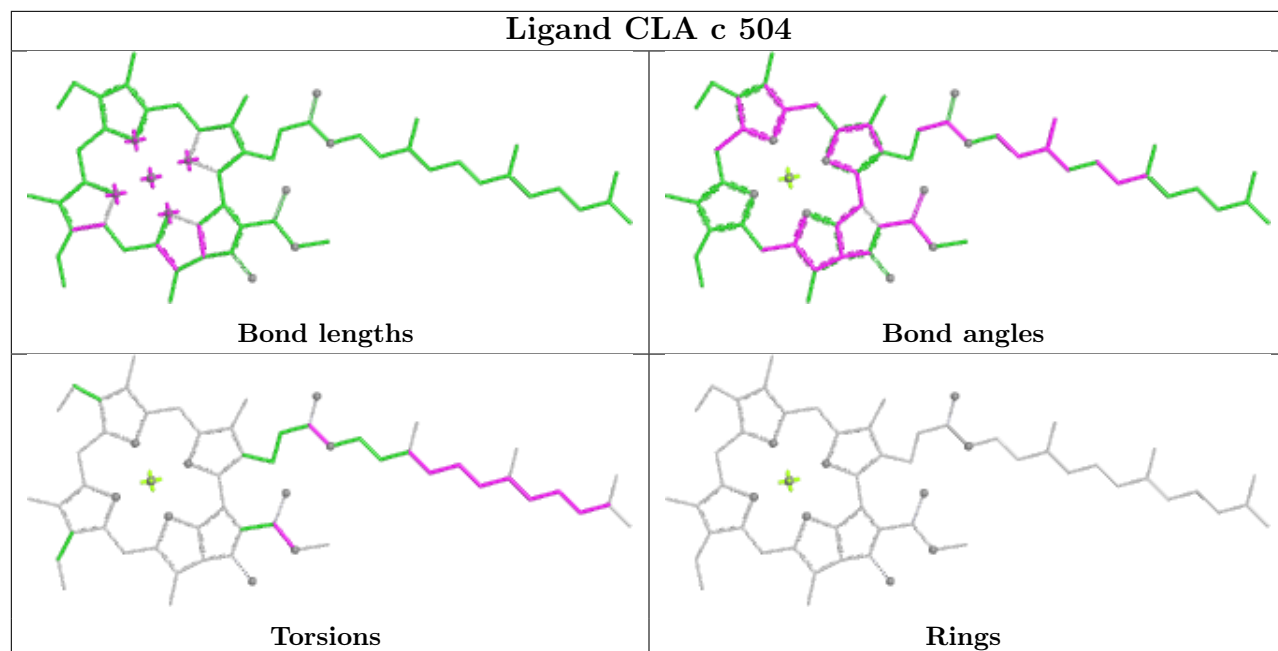
Ligand CLA N 611

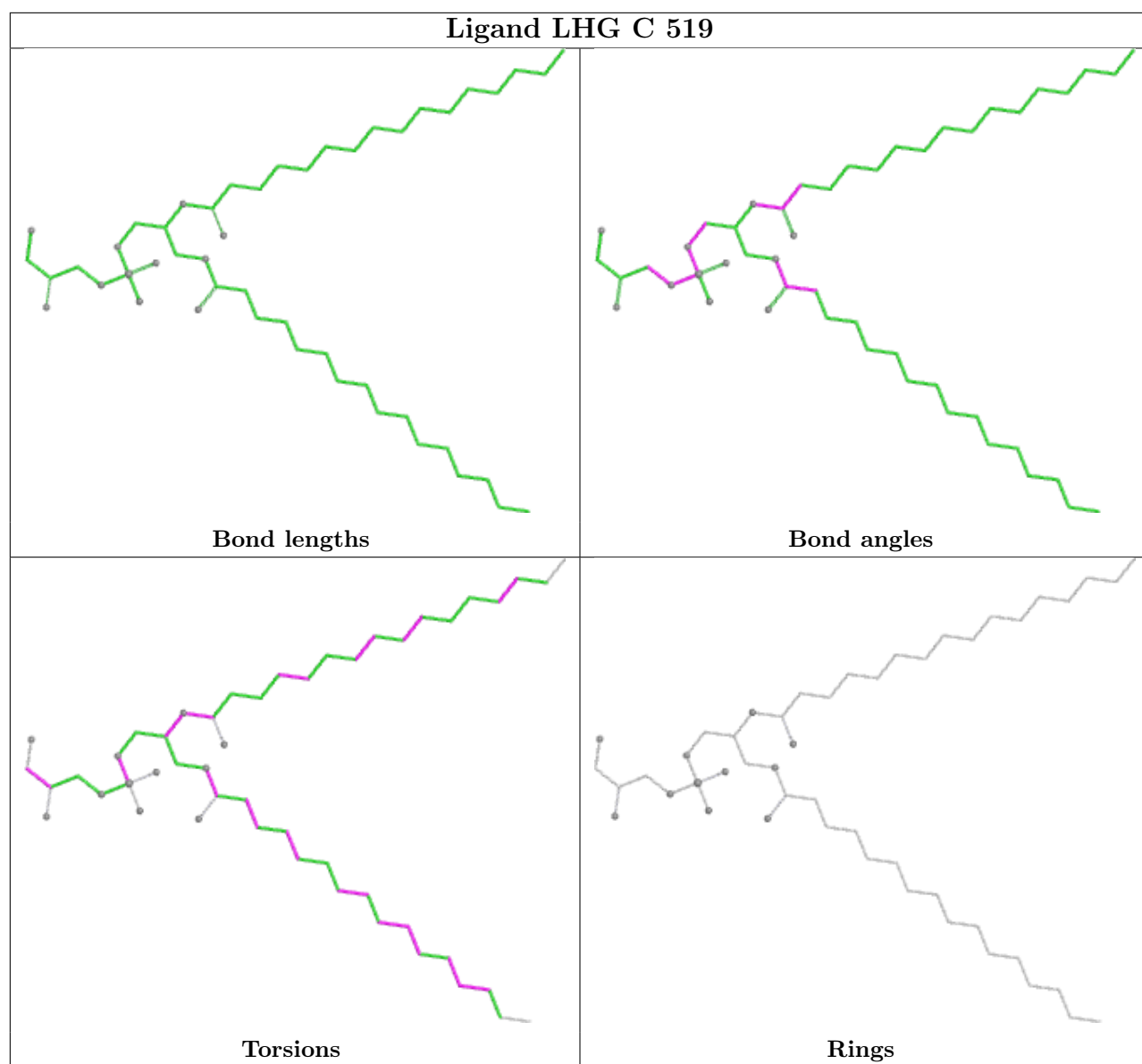


Ligand CLA g 613

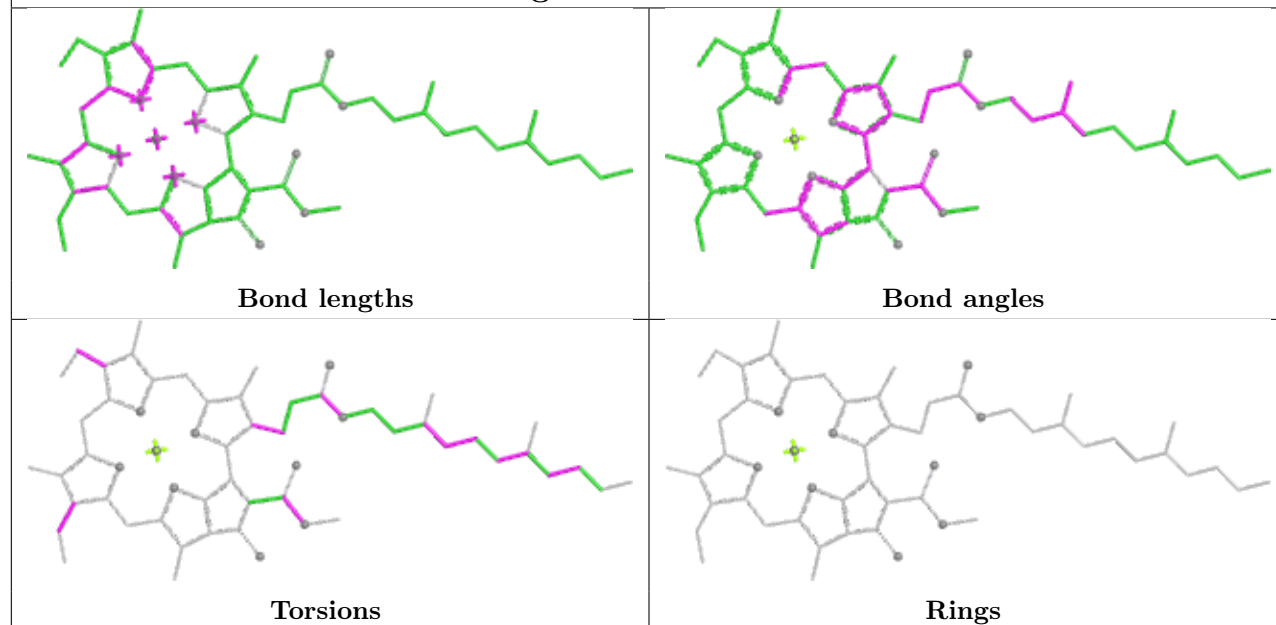




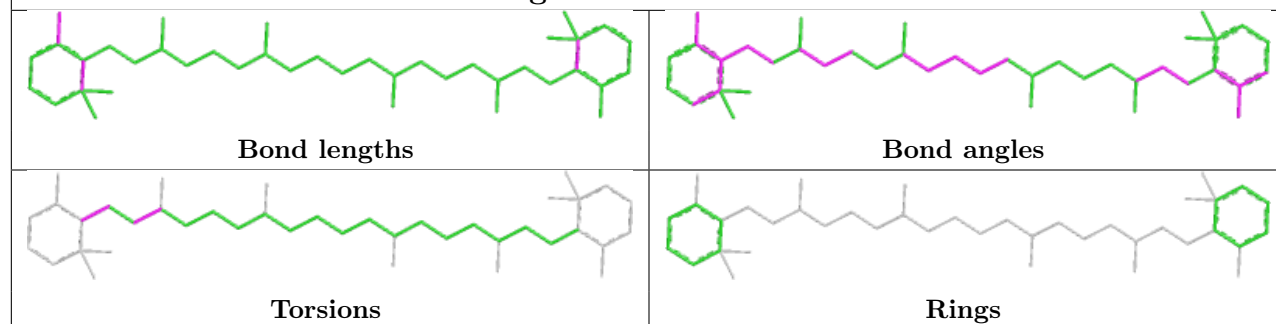




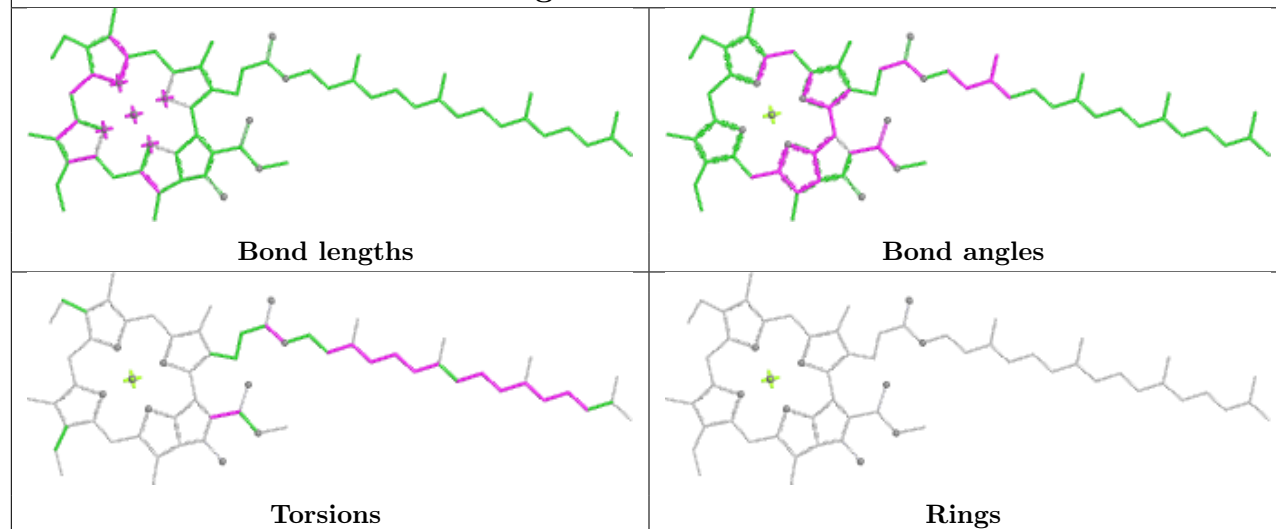
Ligand CLA R 608

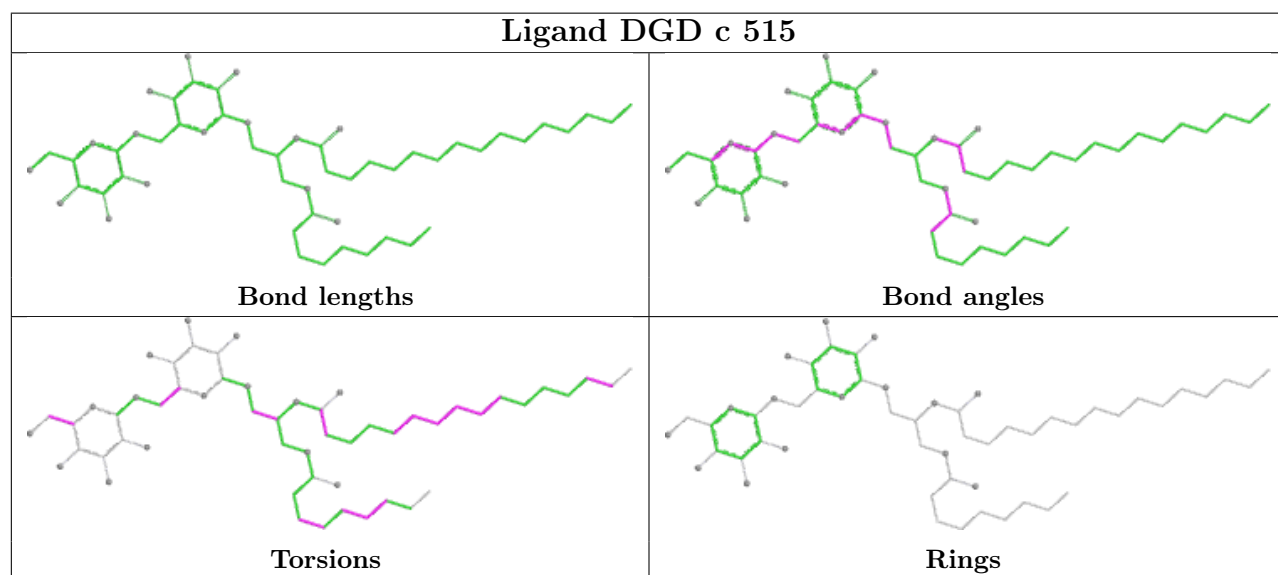
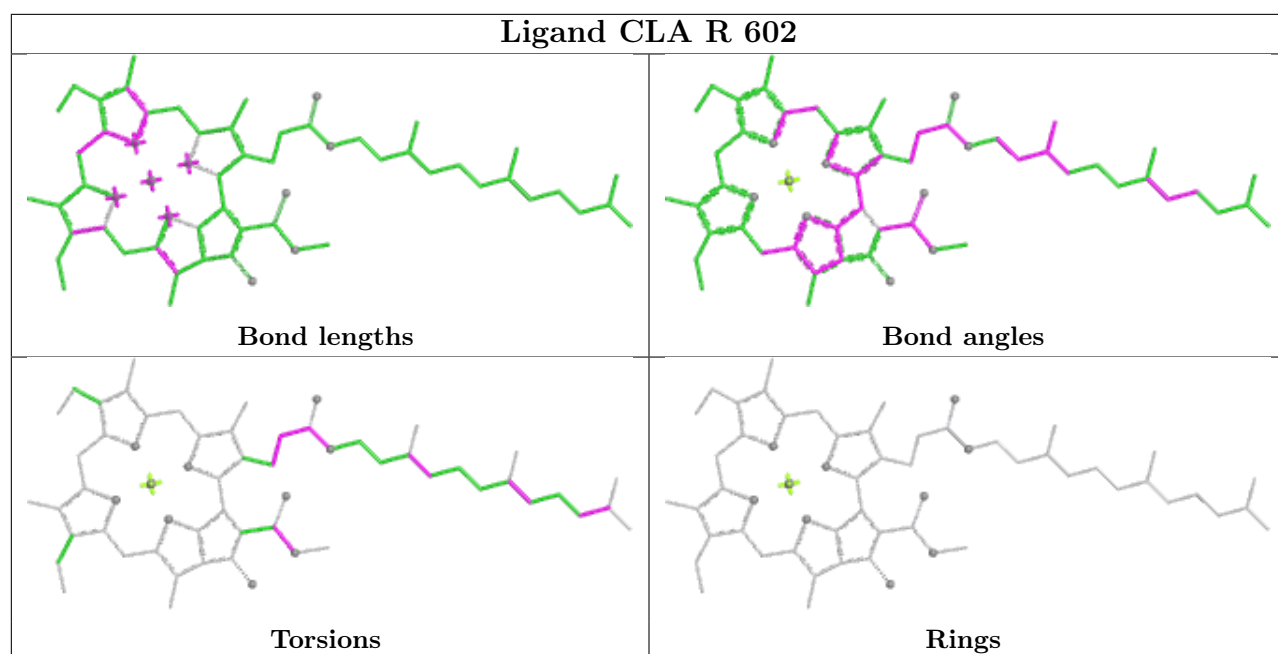


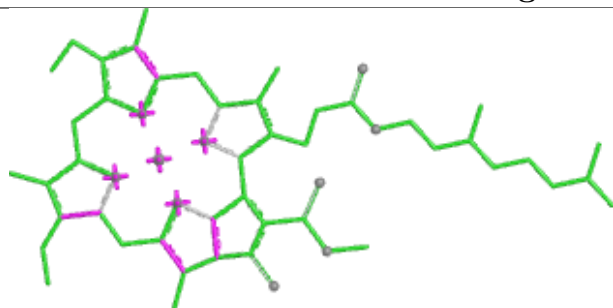
Ligand BCR K 101



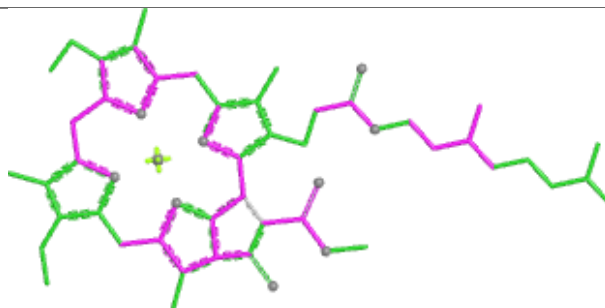
Ligand CLA b 607



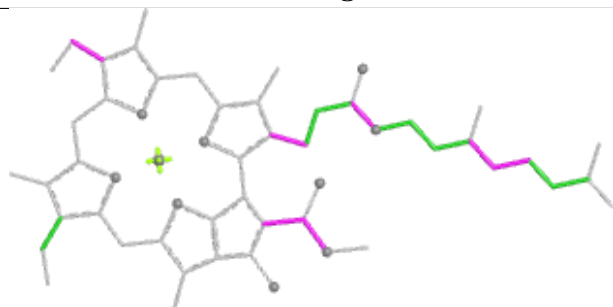


Ligand CLA 2 604

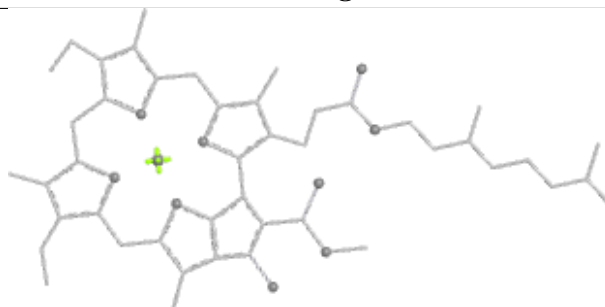
Bond lengths



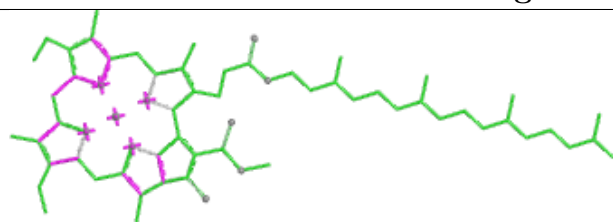
Bond angles



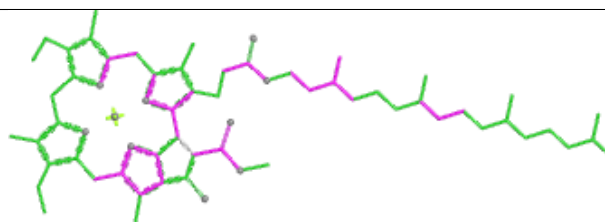
Torsions



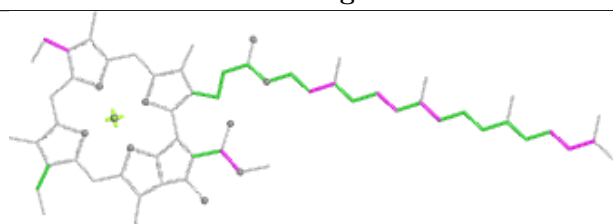
Rings

Ligand CLA C 503

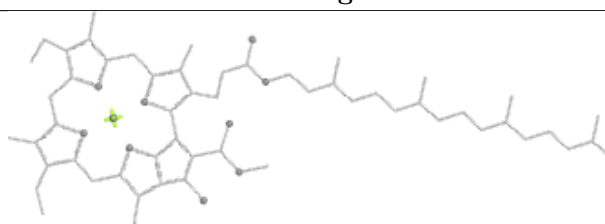
Bond lengths



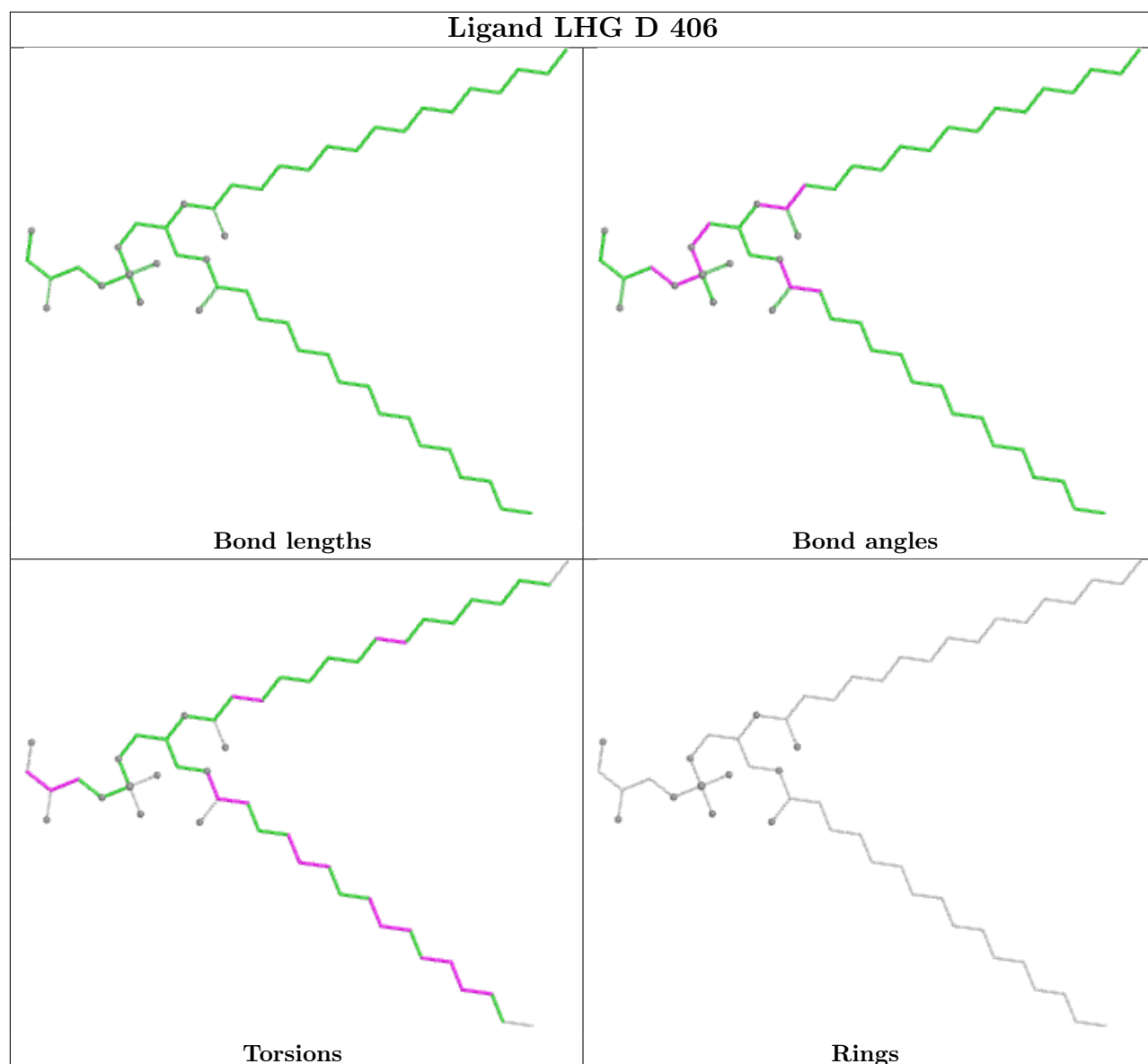
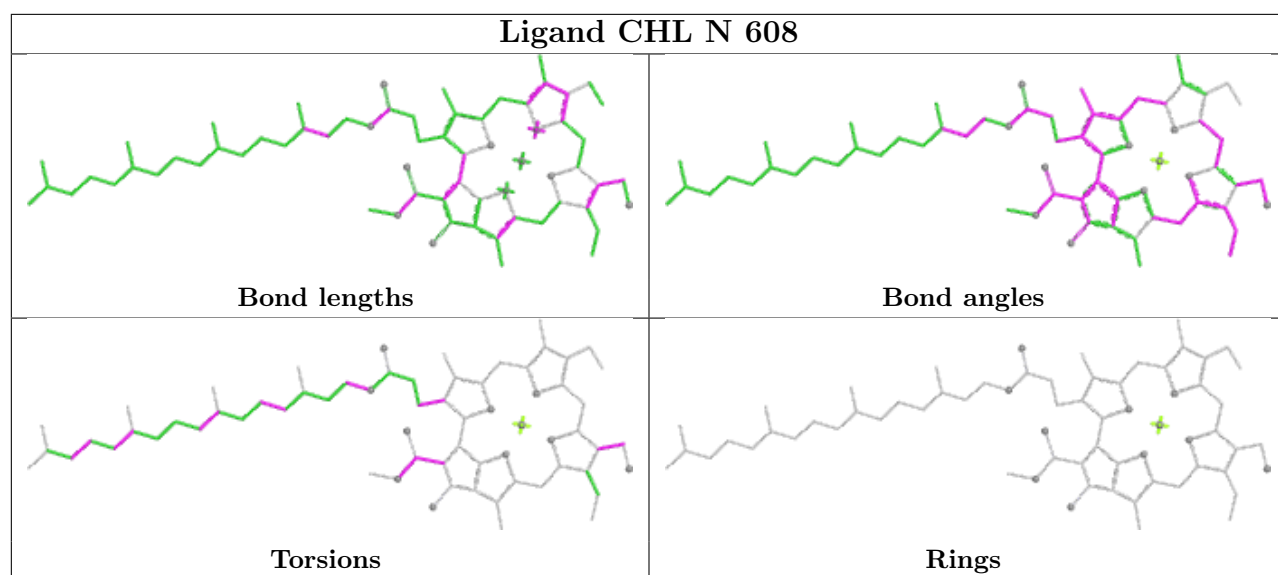
Bond angles

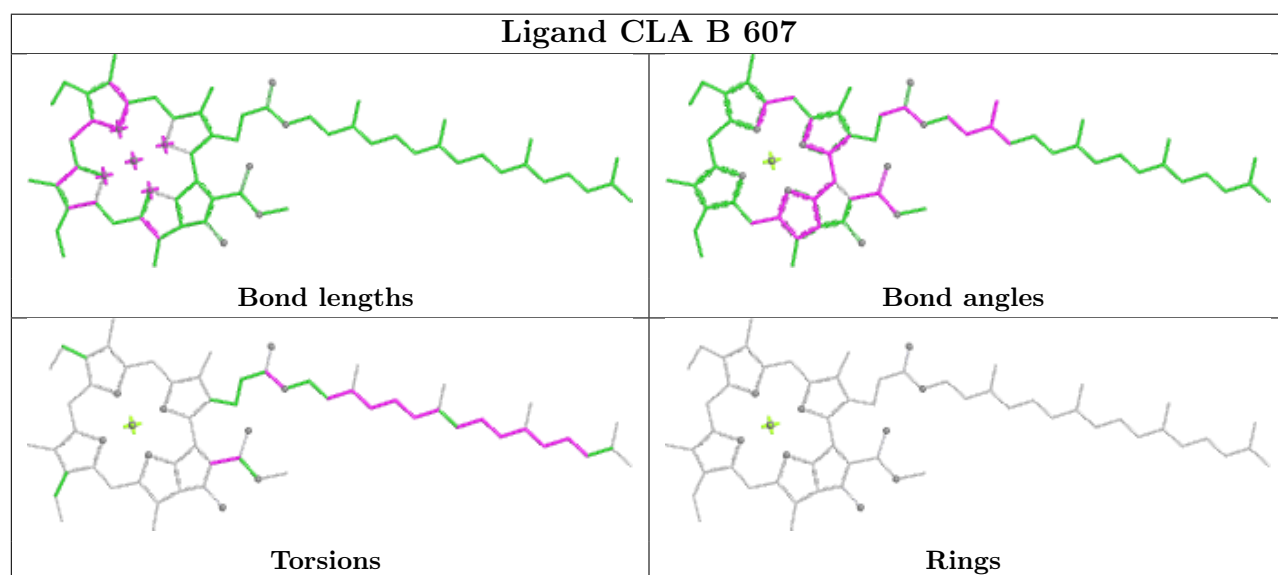
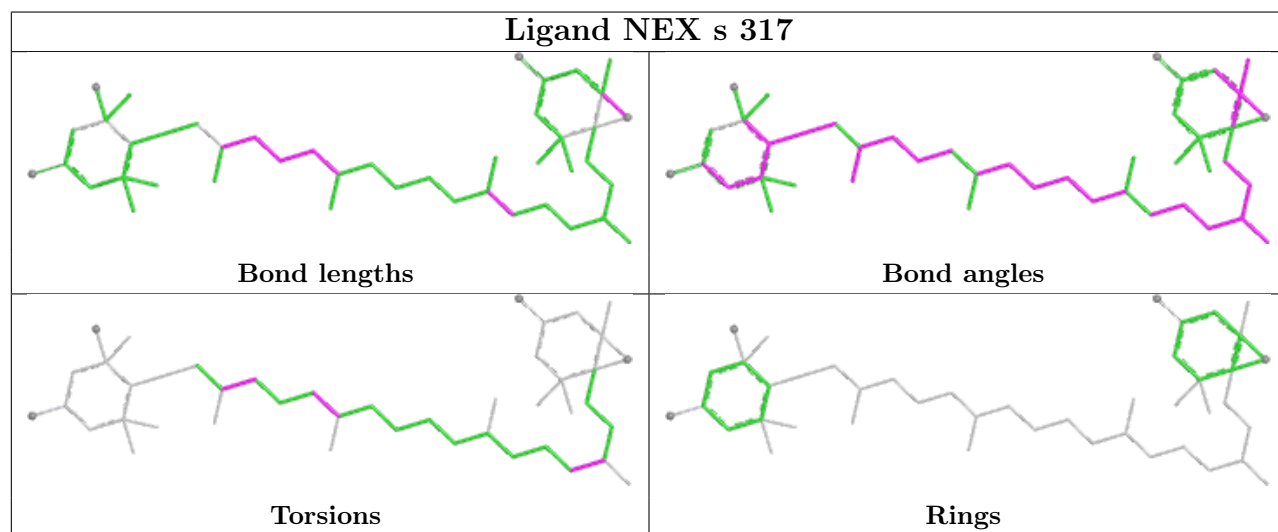
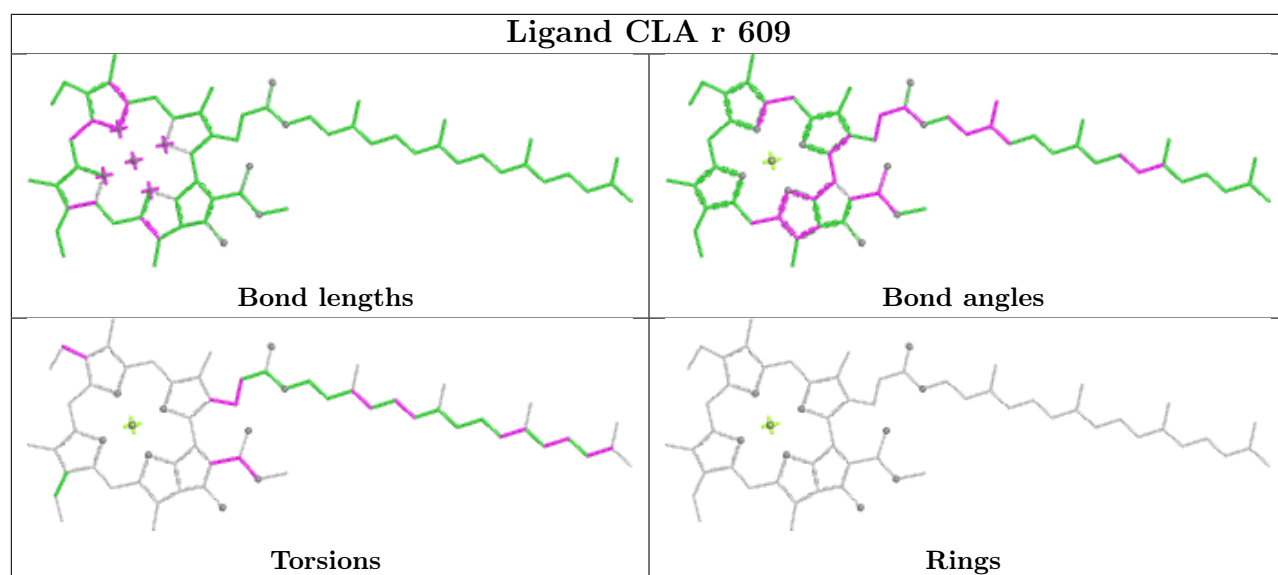


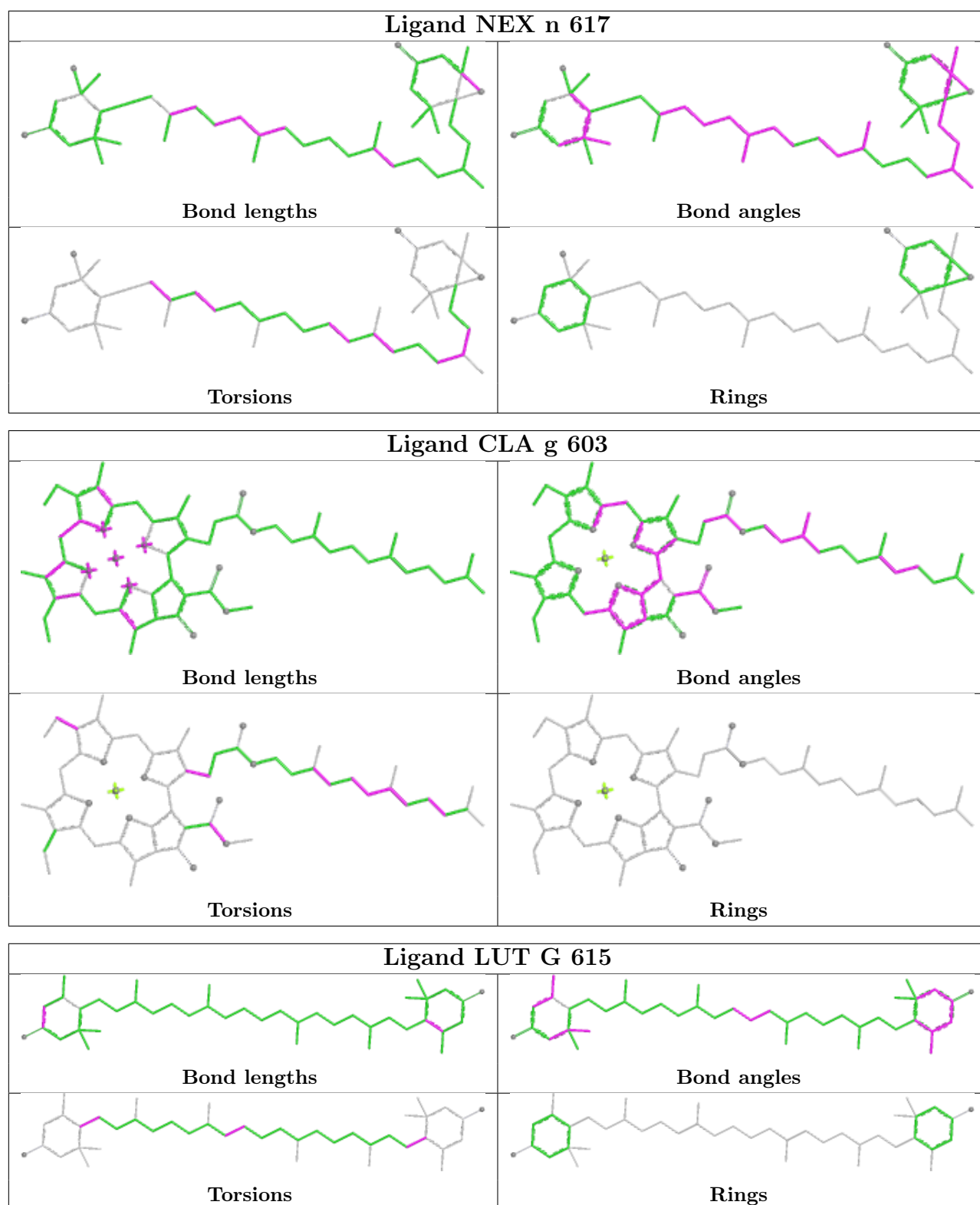
Torsions

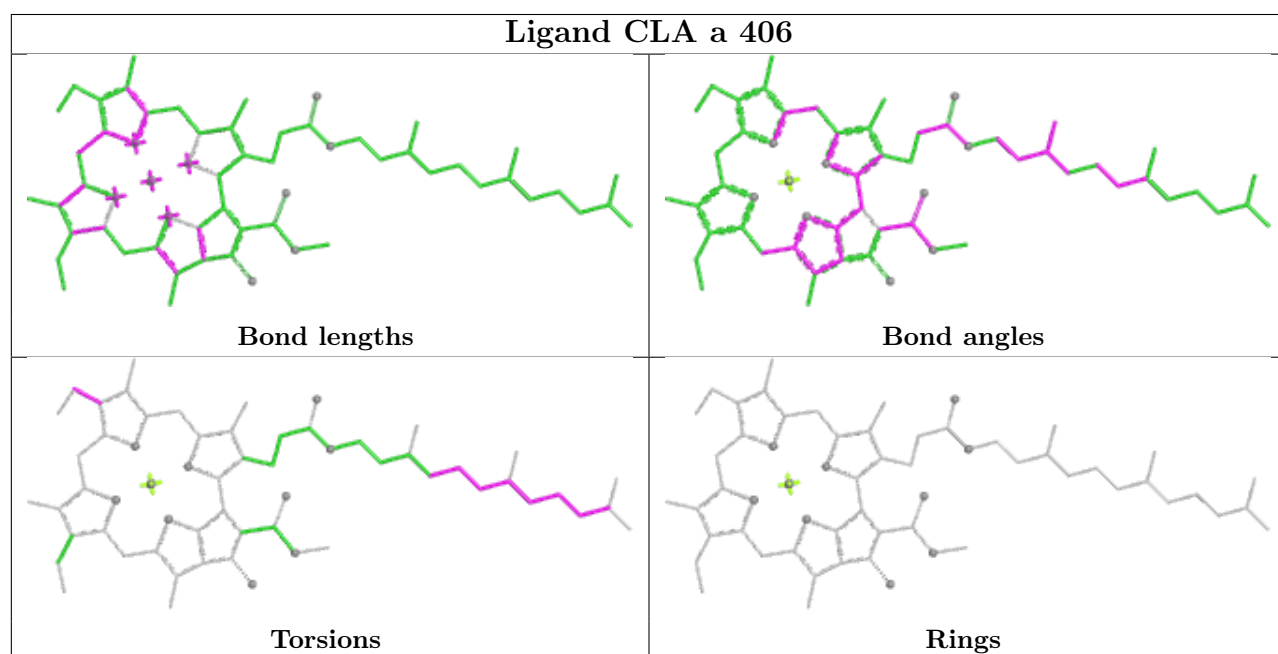
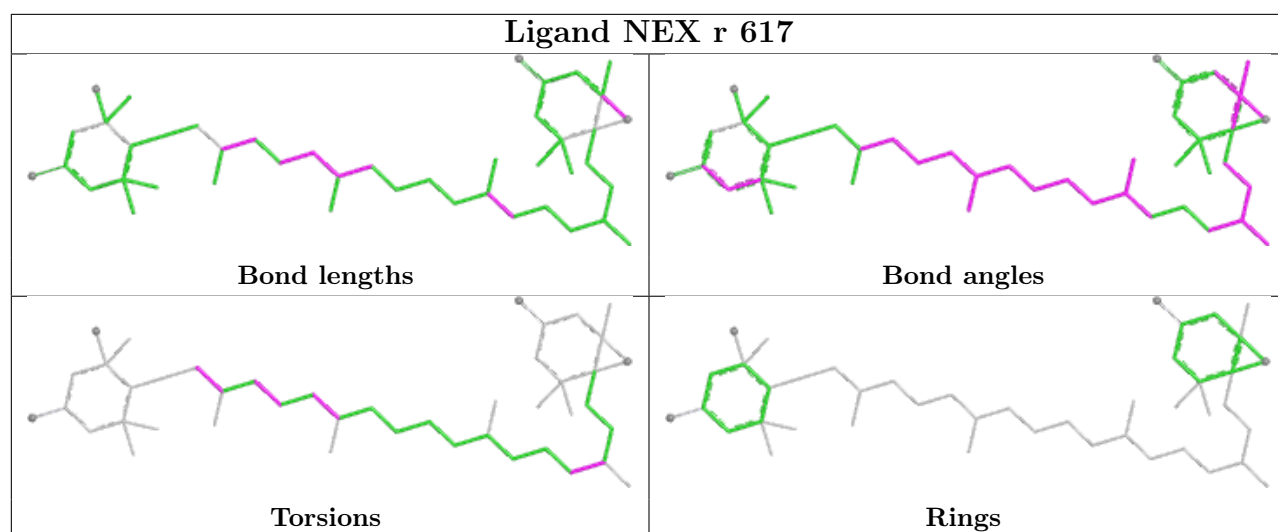


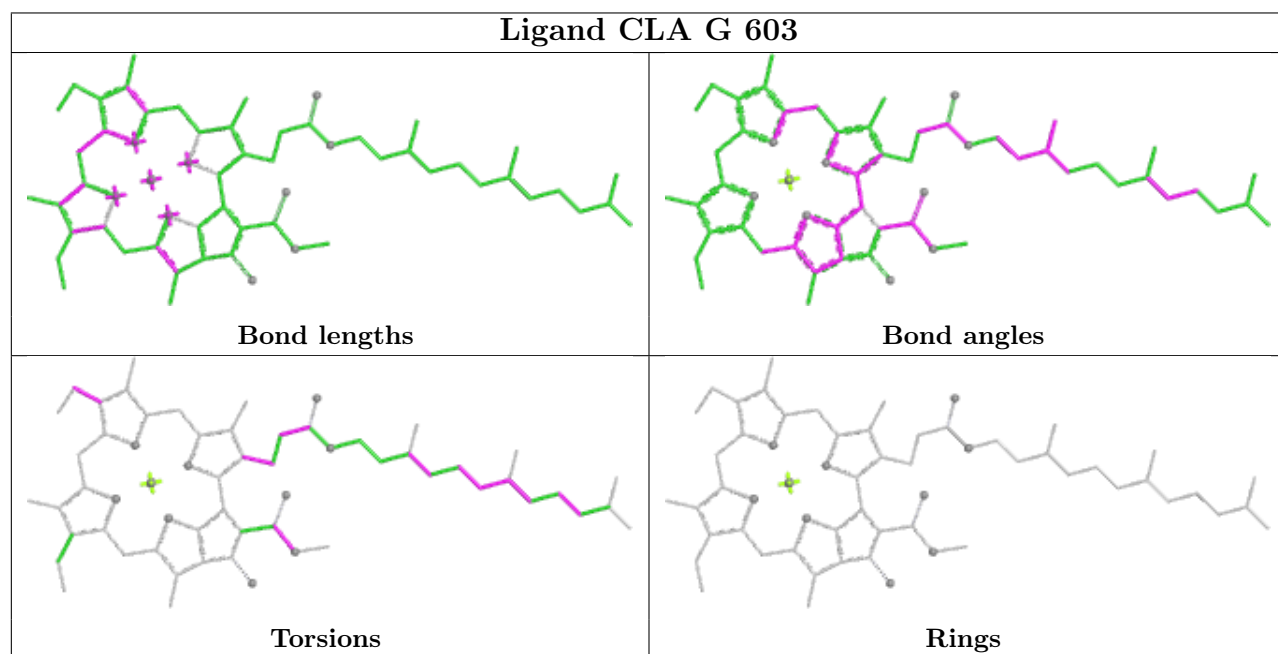
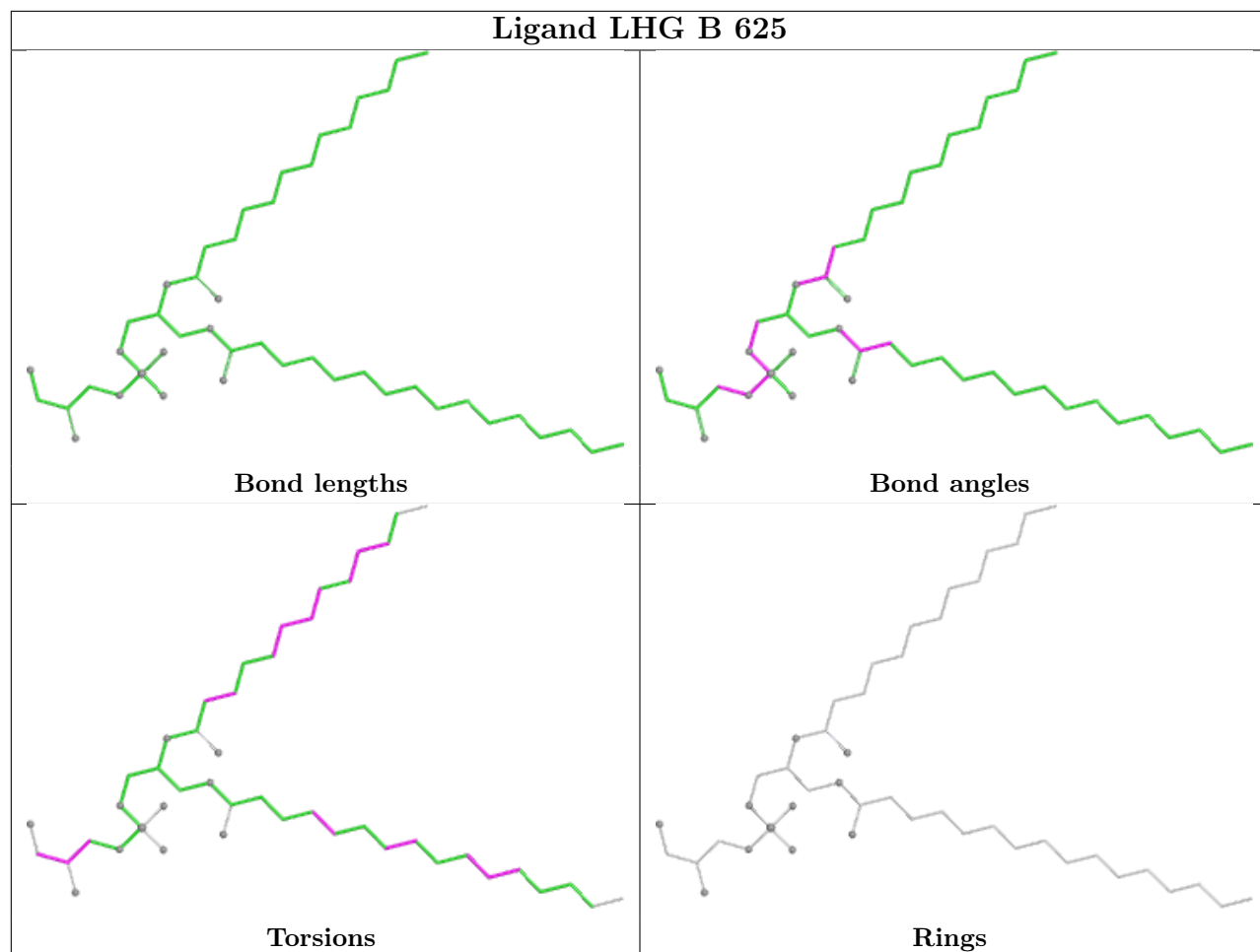
Rings

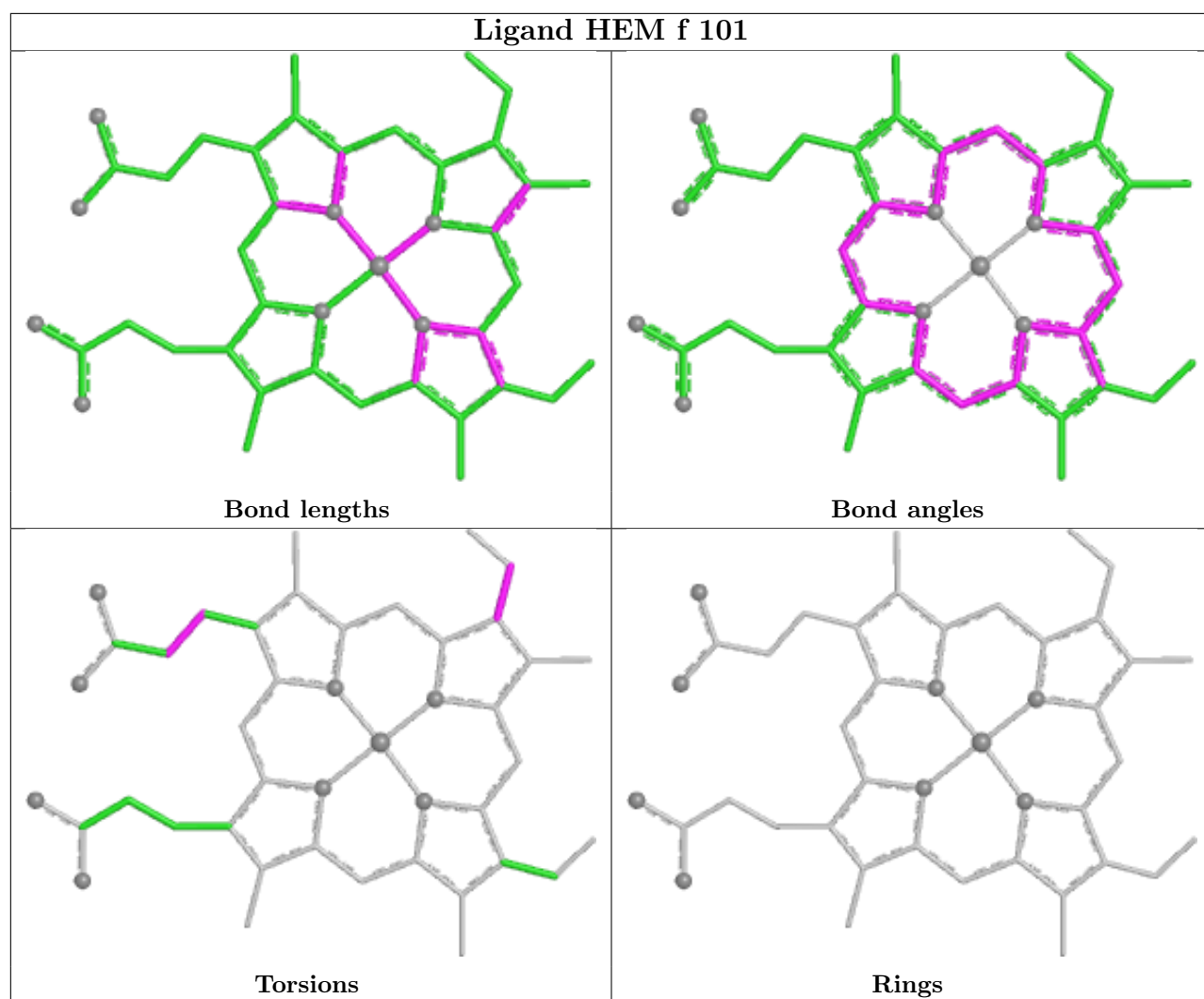


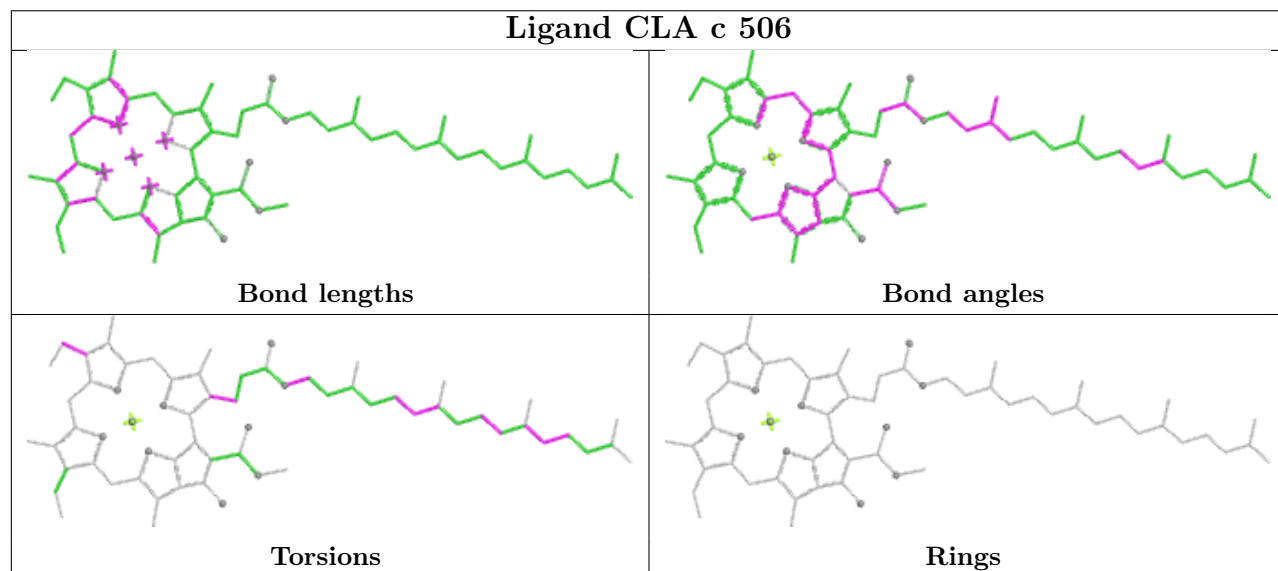
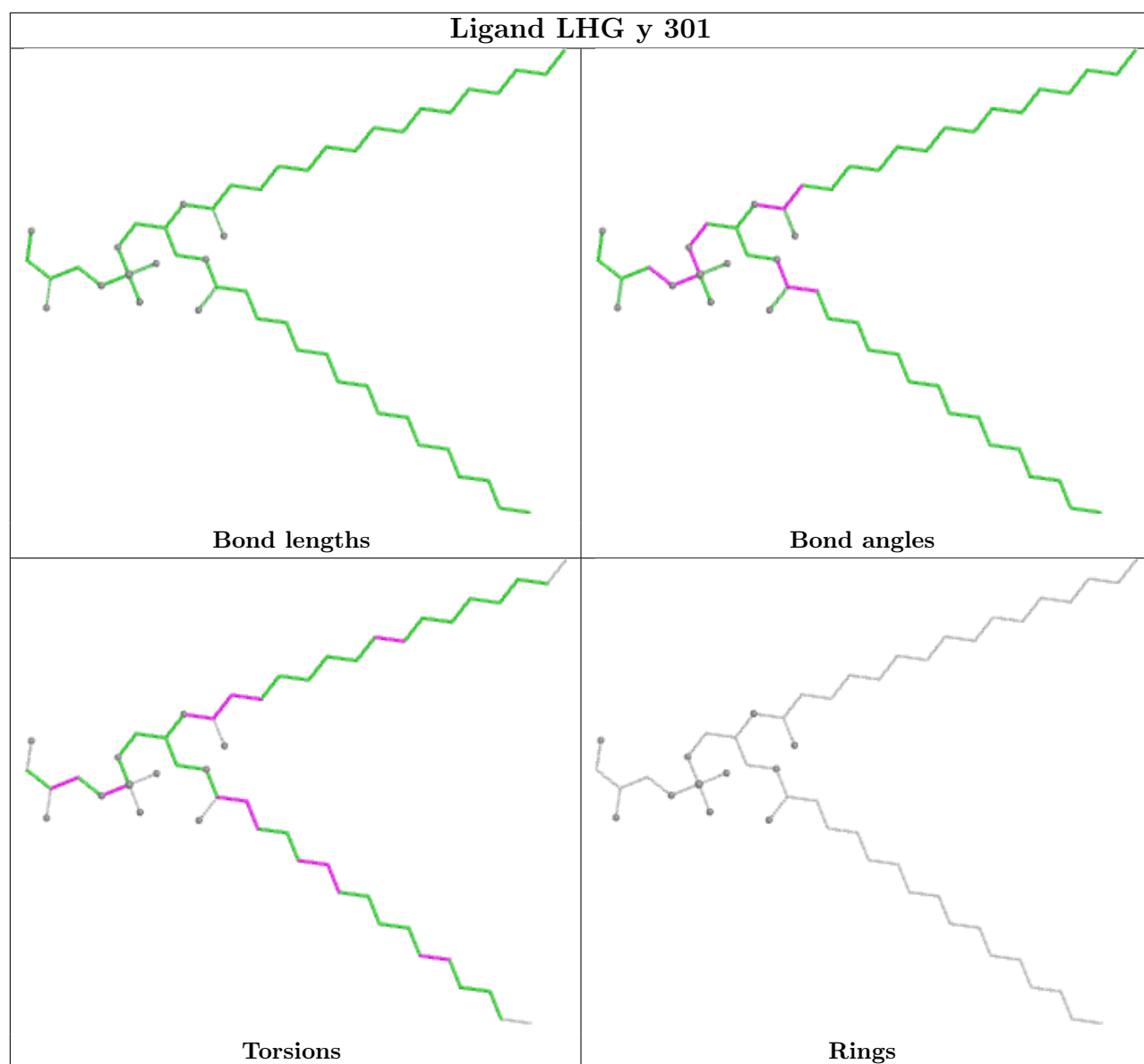


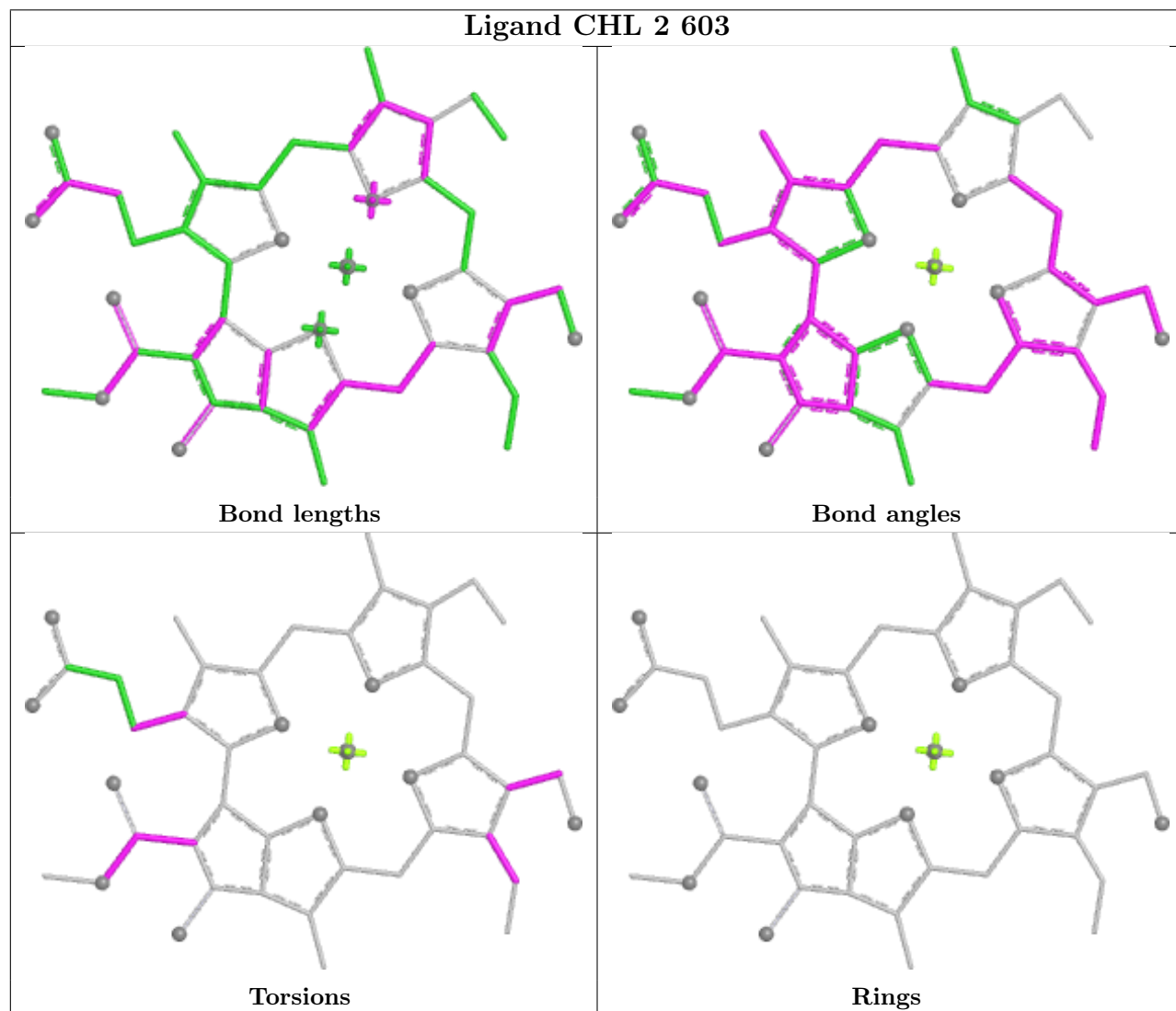
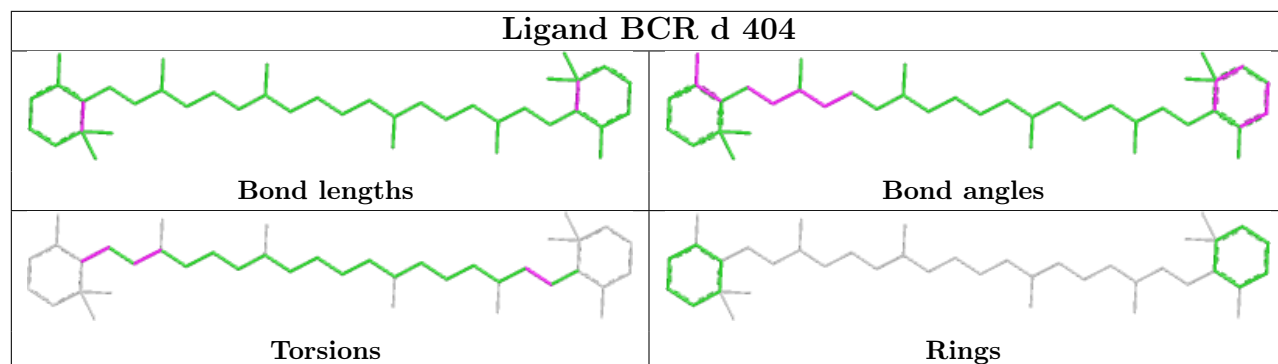


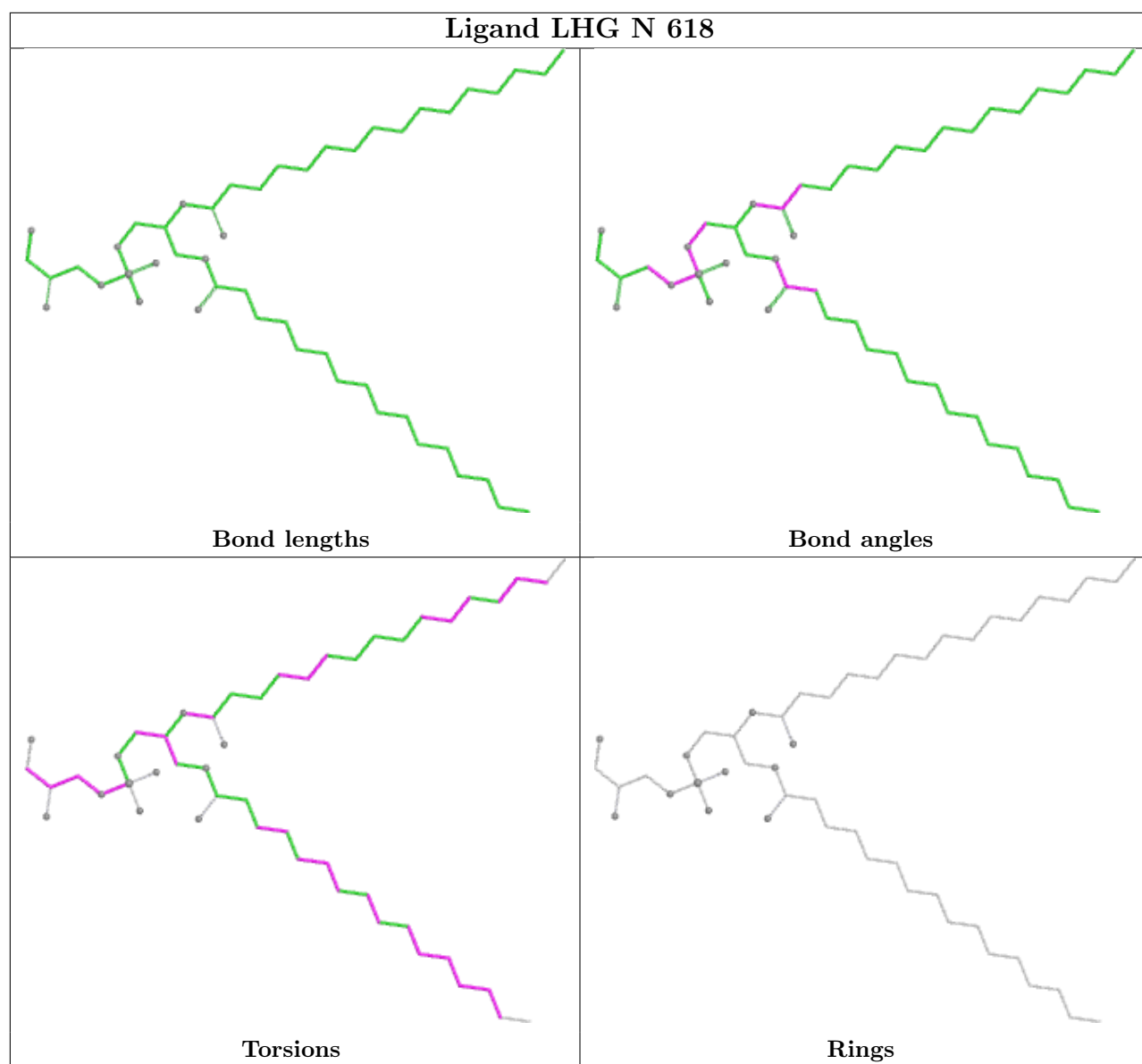


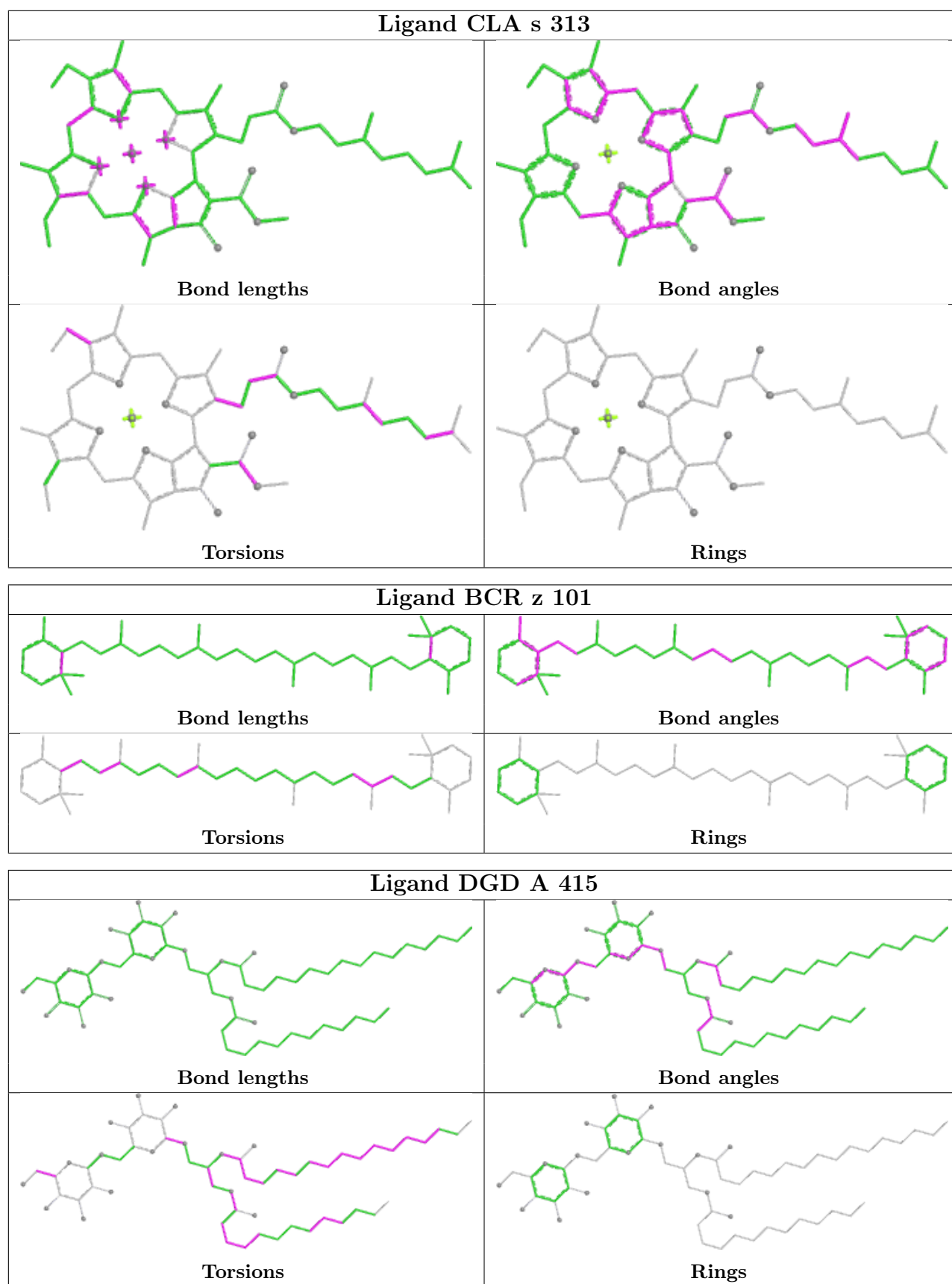


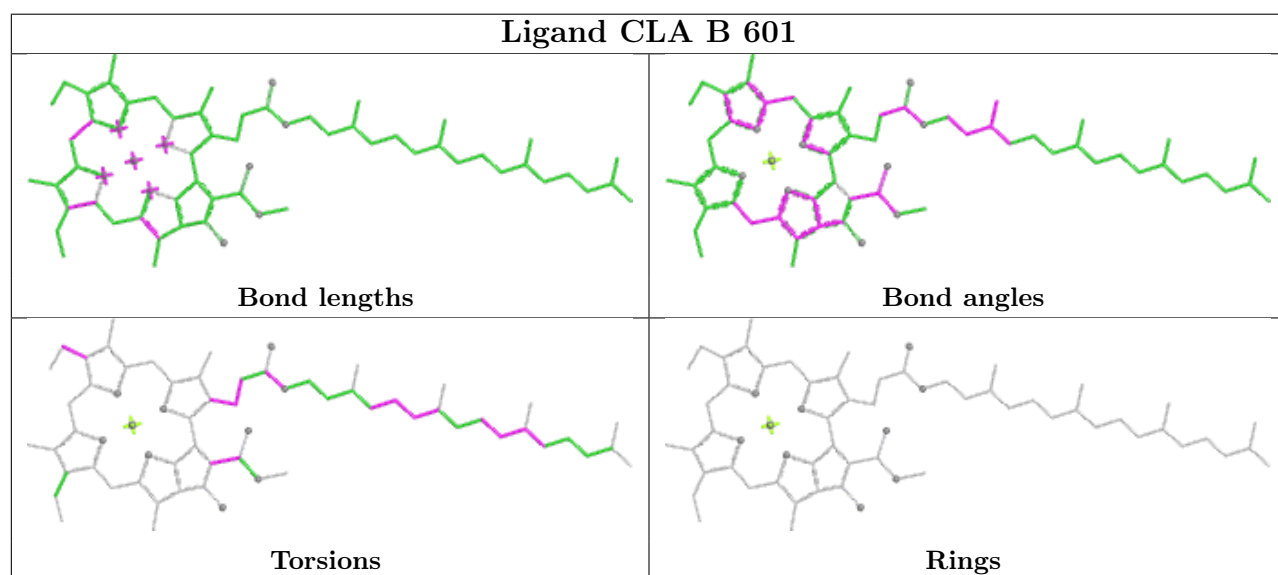
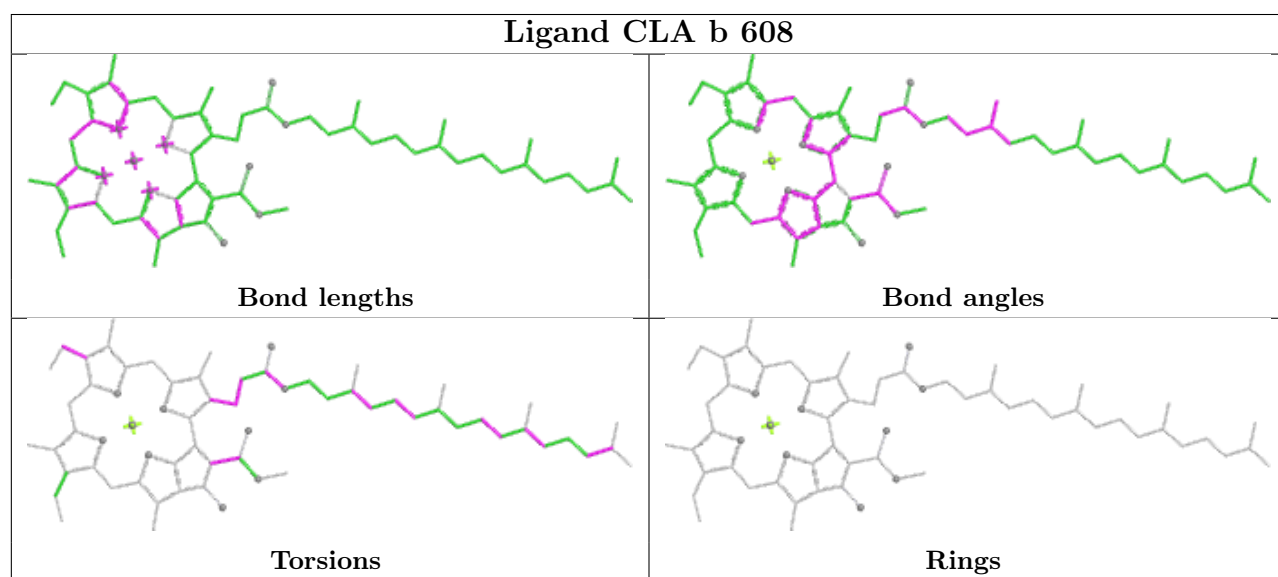
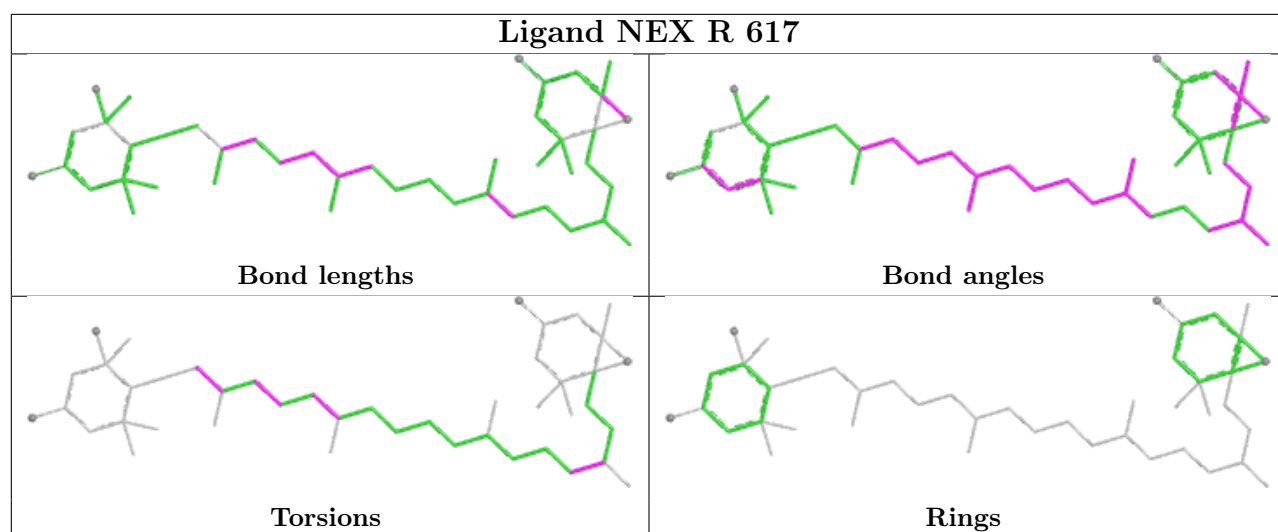


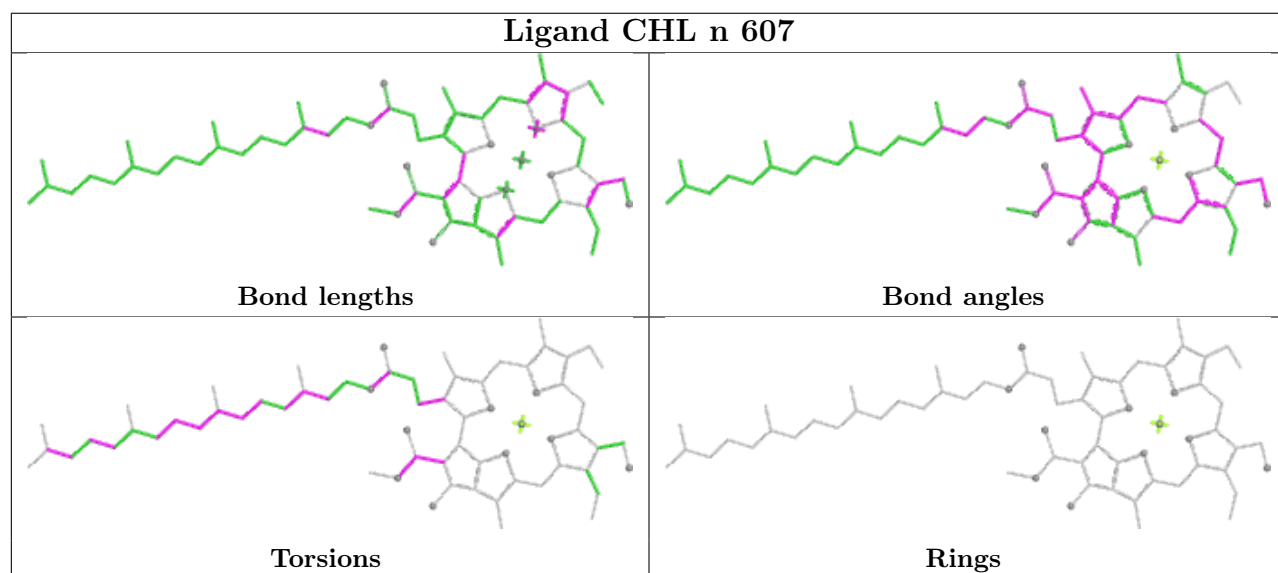
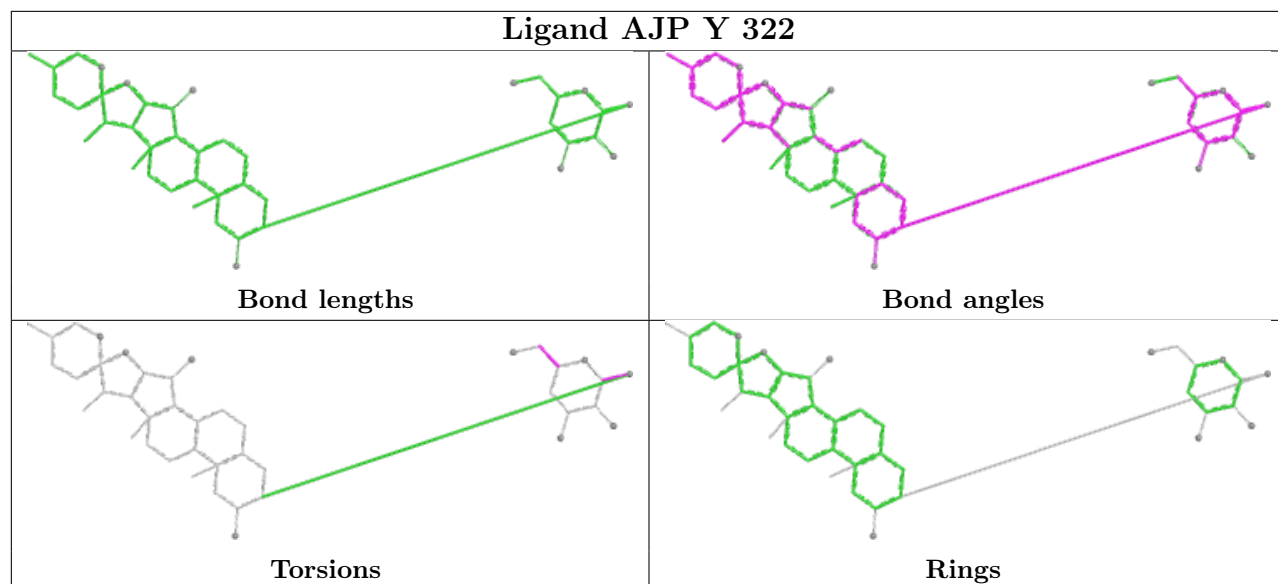




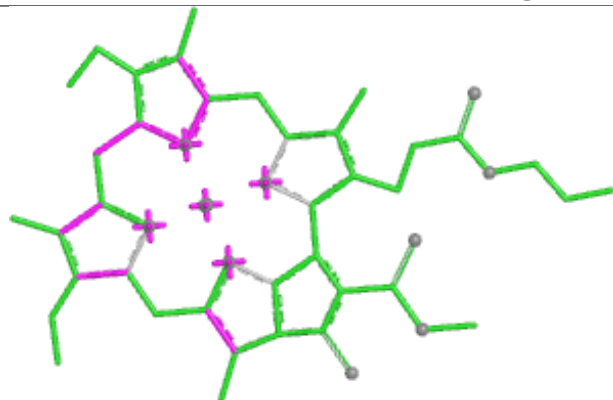




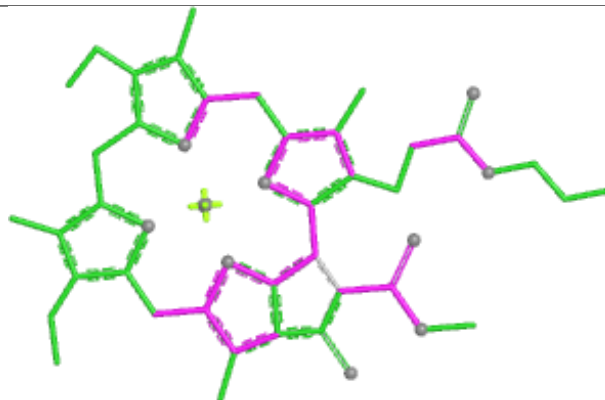




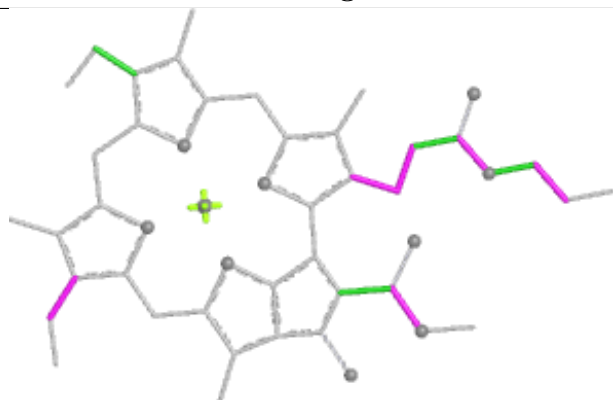
Ligand CLA 2 605



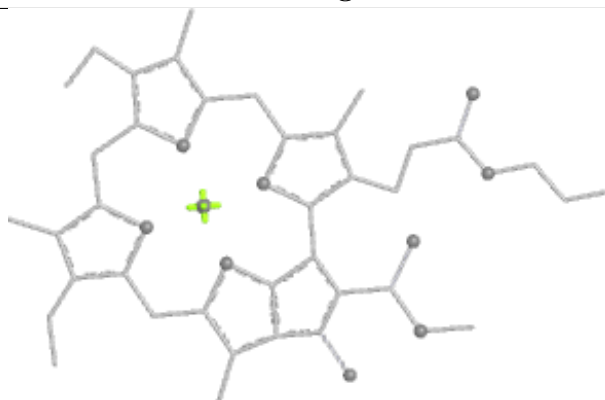
Bond lengths



Bond angles

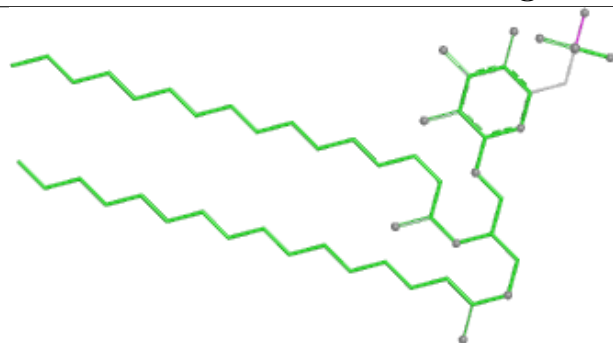


Torsions

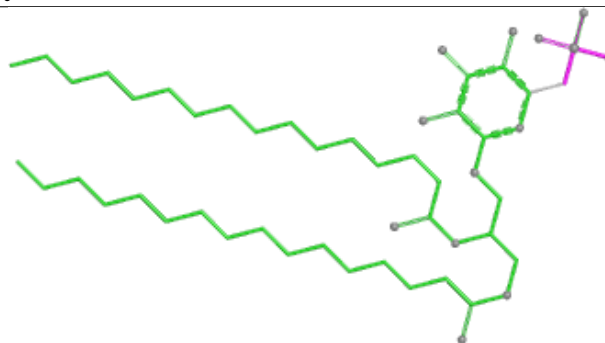


Rings

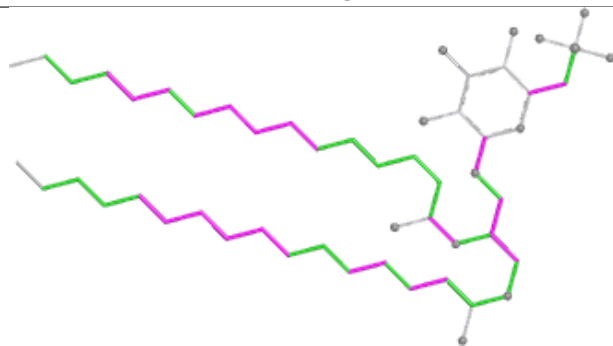
Ligand SQD a 412



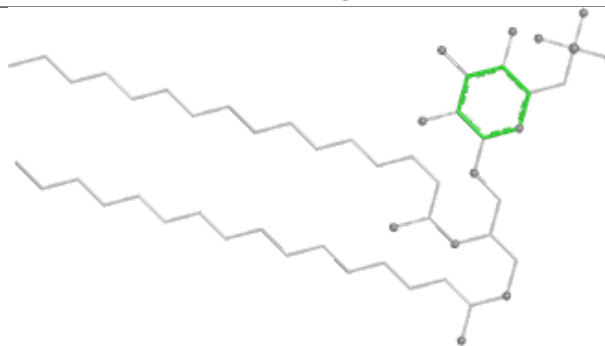
Bond lengths



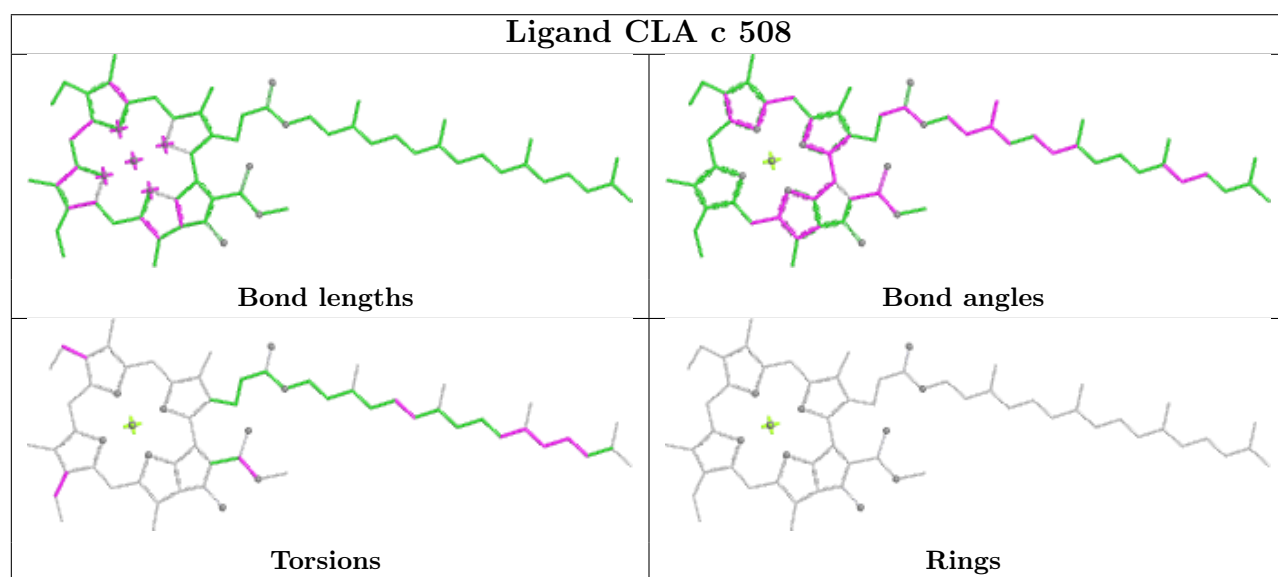
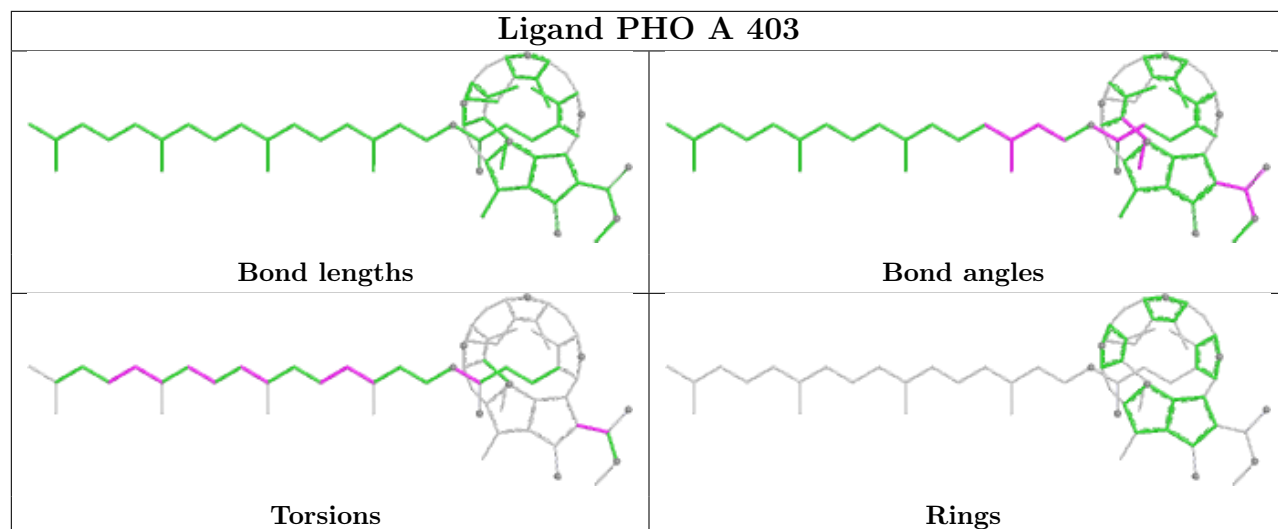
Bond angles

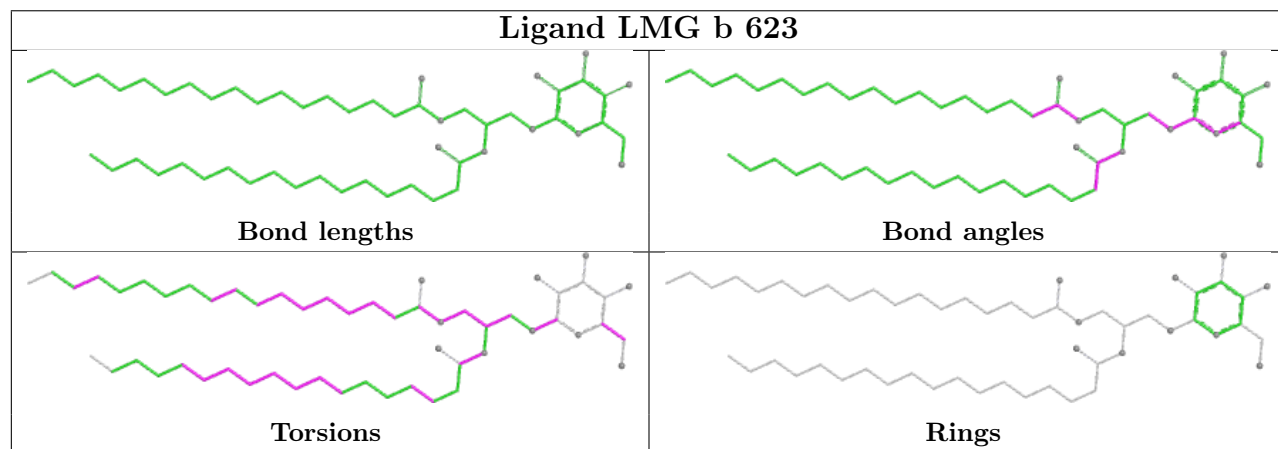
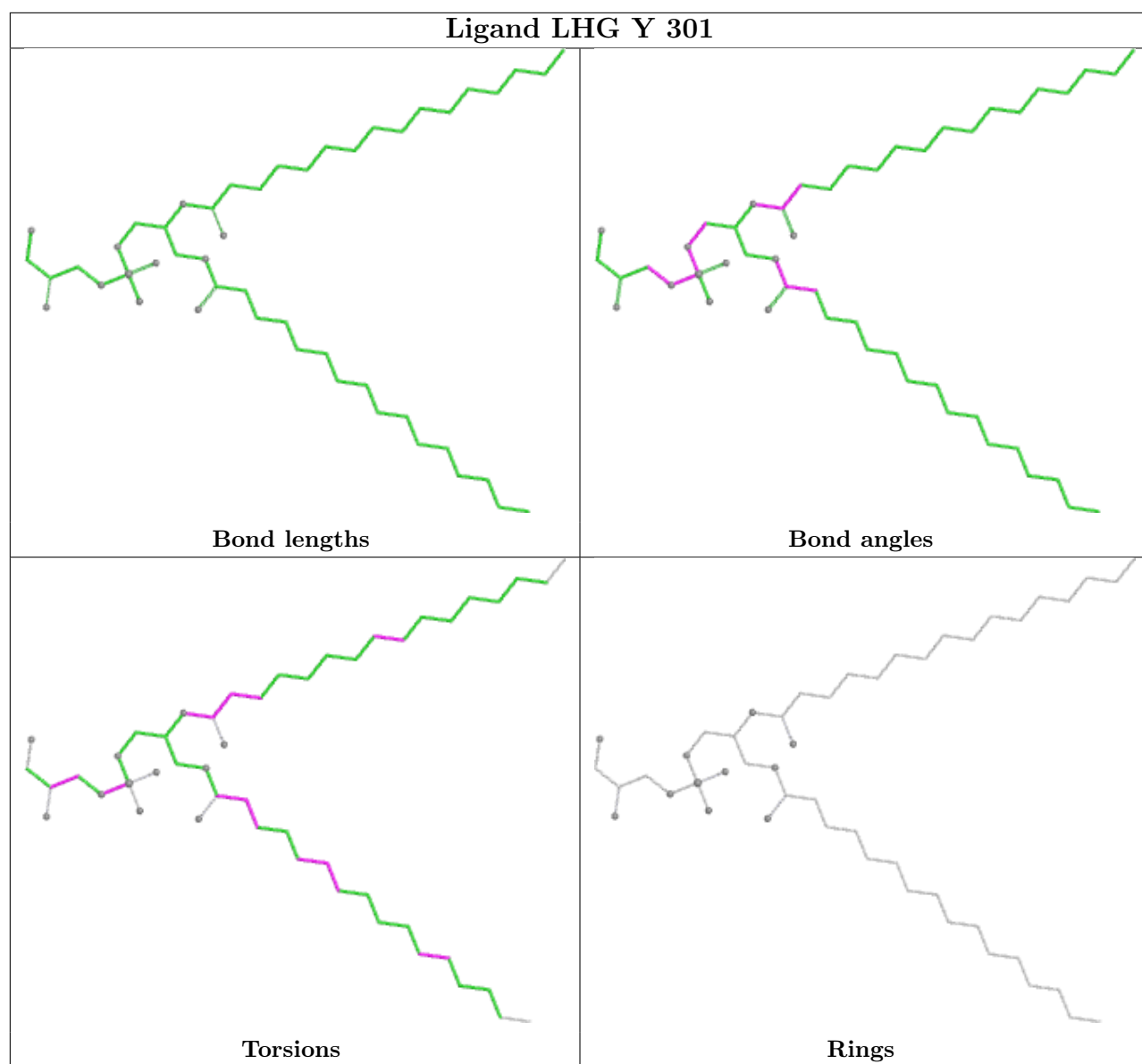


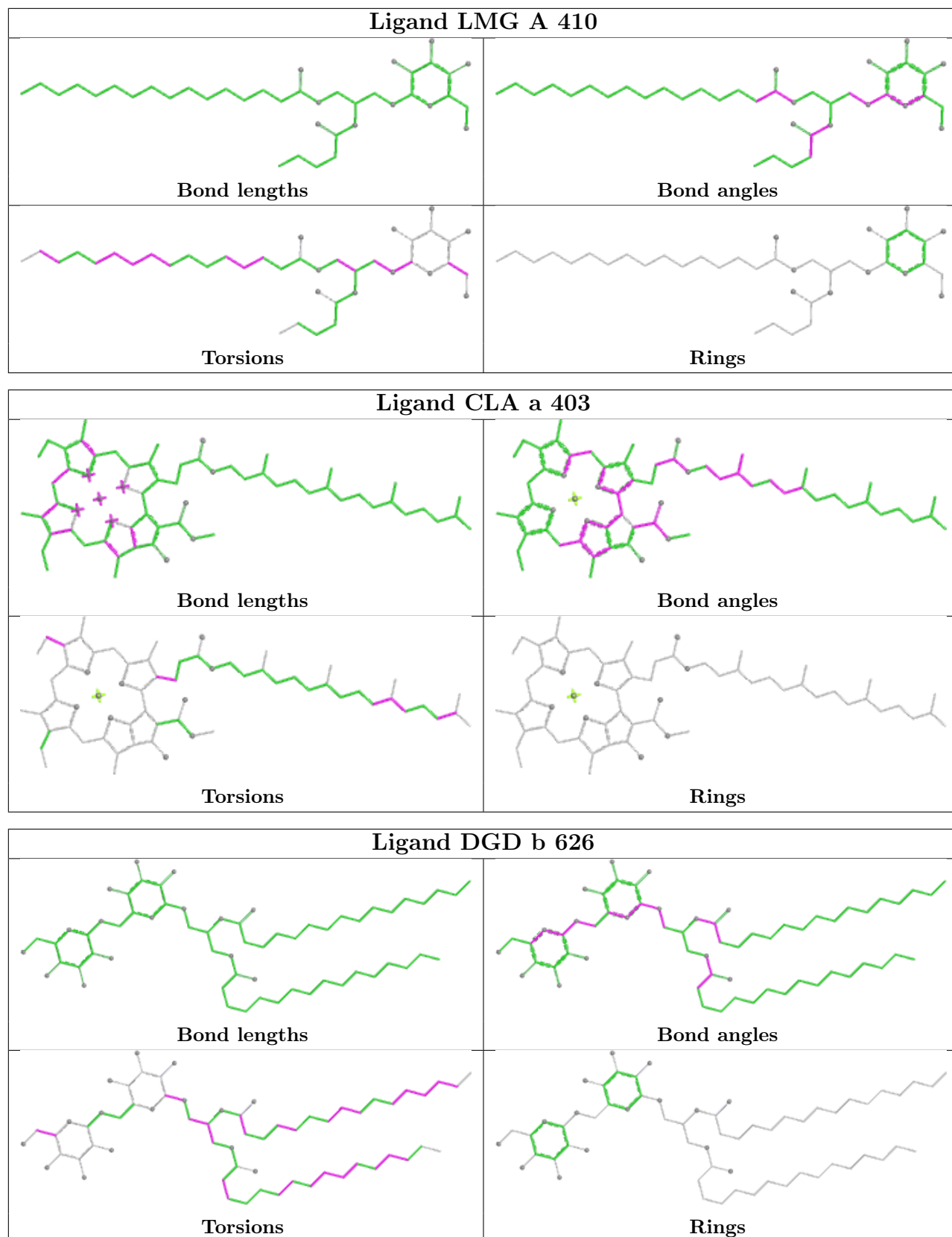
Torsions

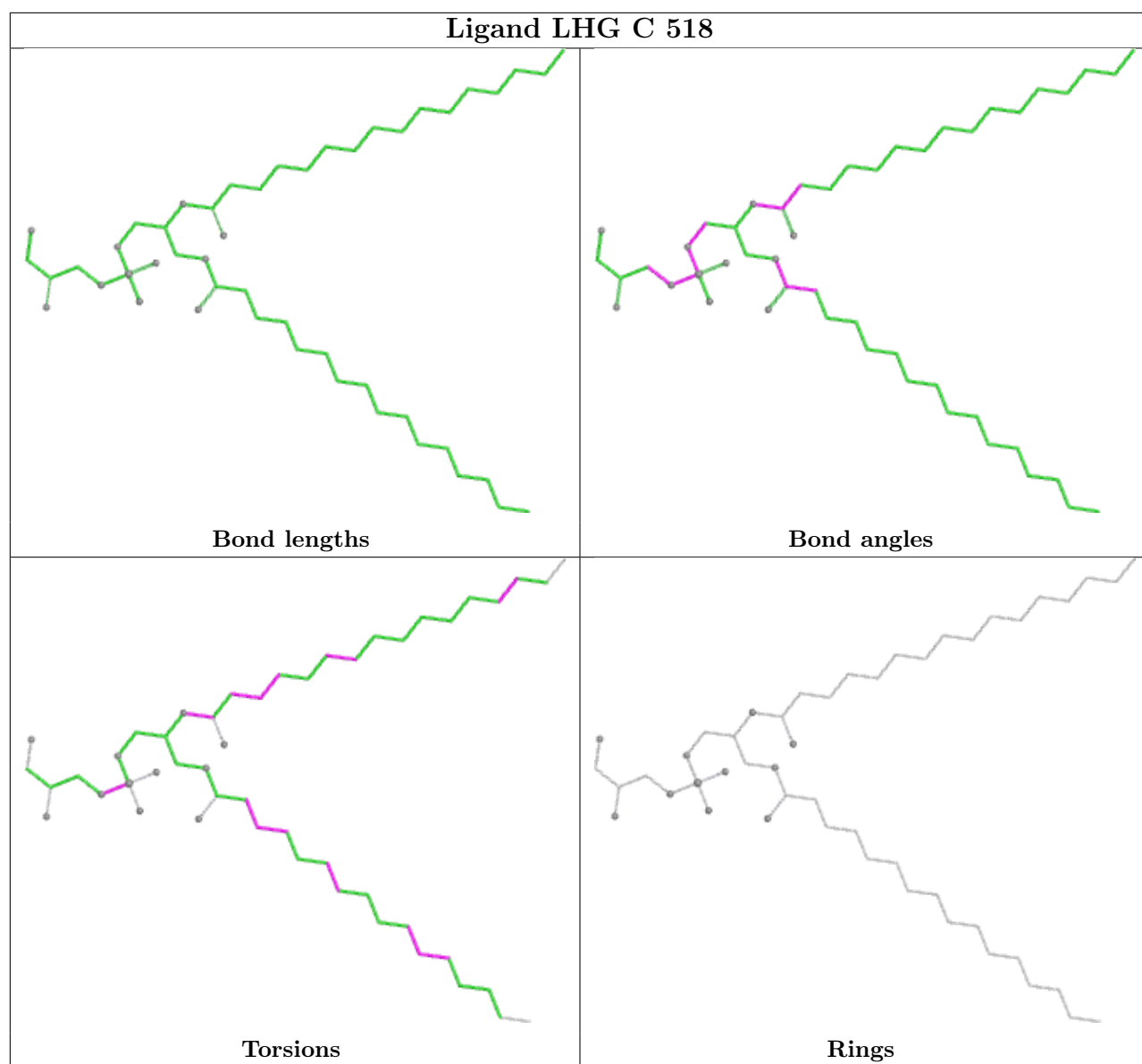


Rings

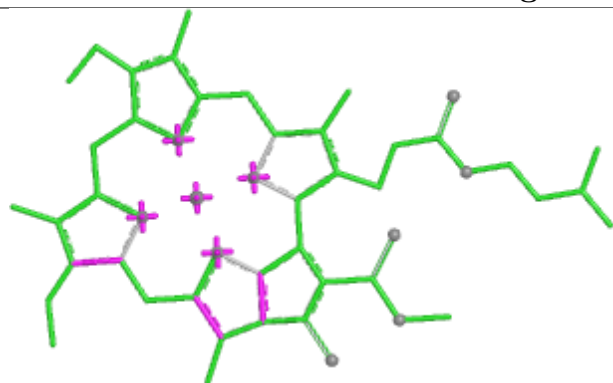




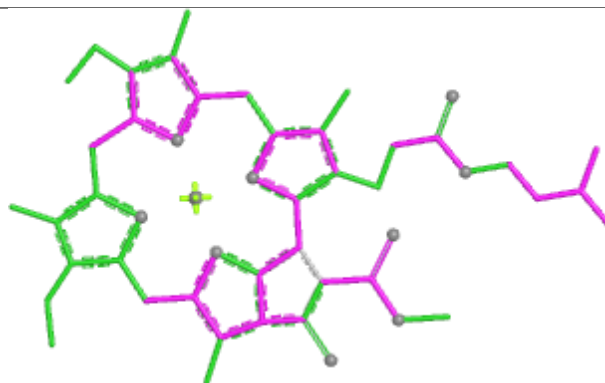




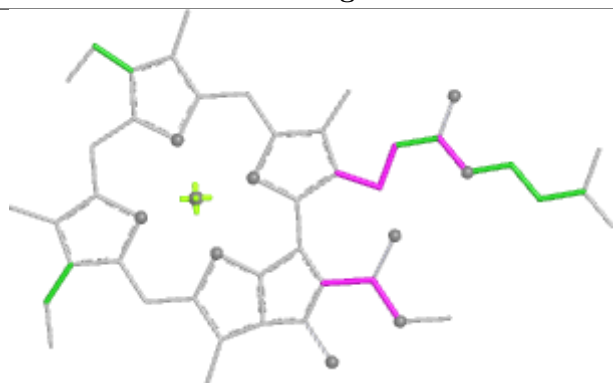
Ligand CLA s 305



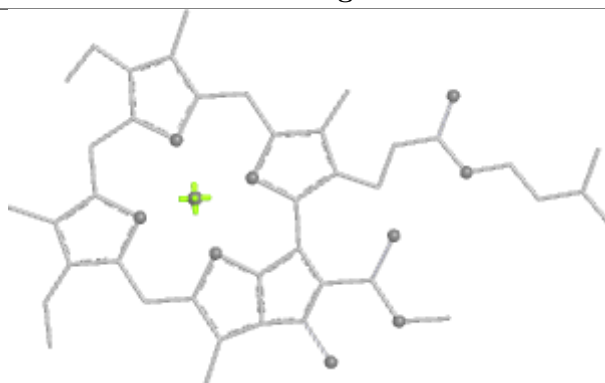
Bond lengths



Bond angles

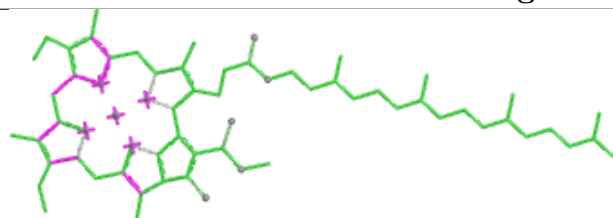


Torsions

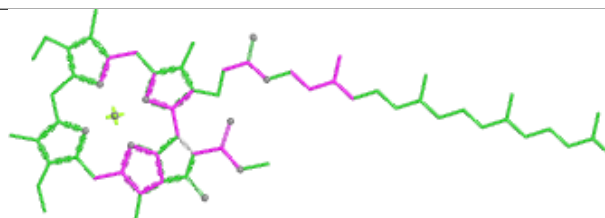


Rings

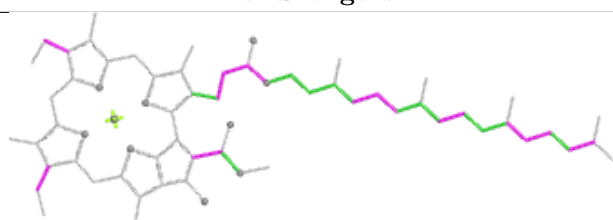
Ligand CLA b 616



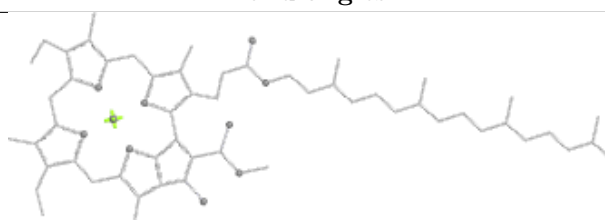
Bond lengths



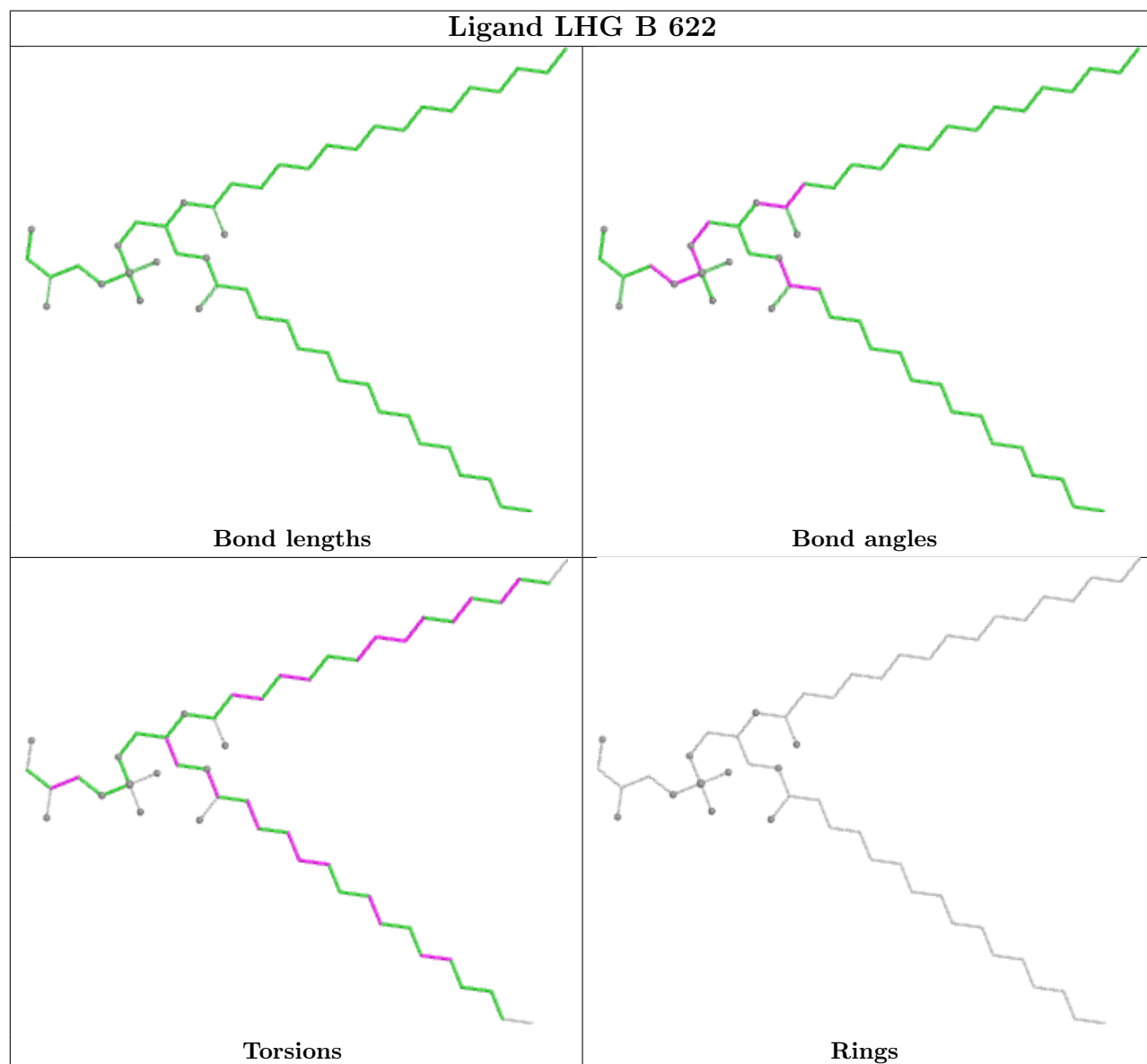
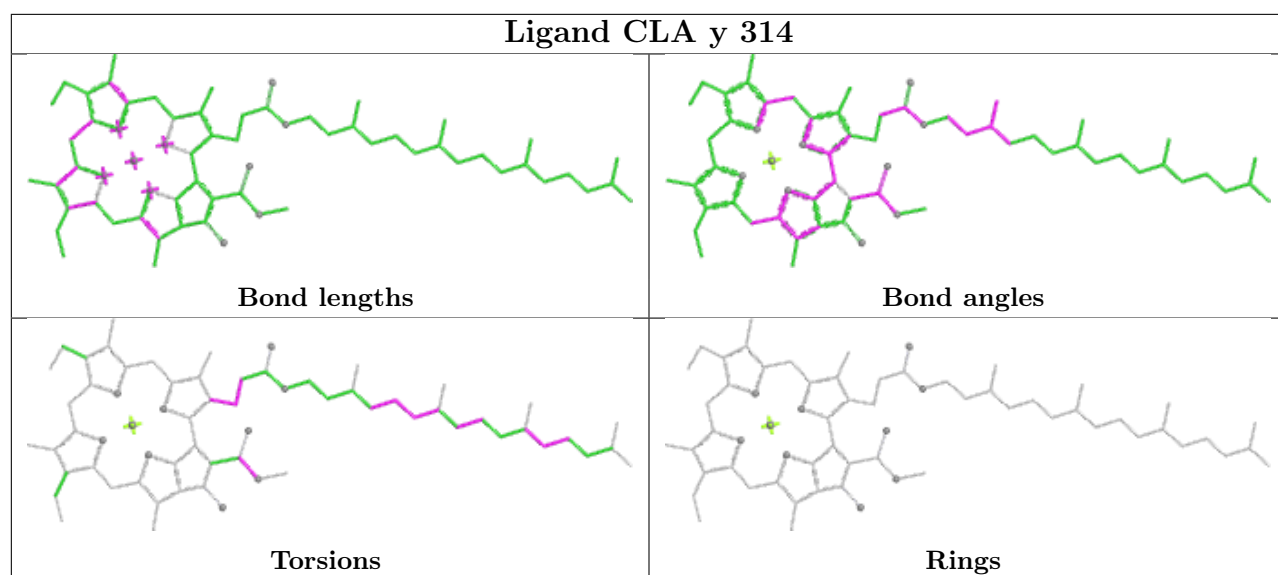
Bond angles

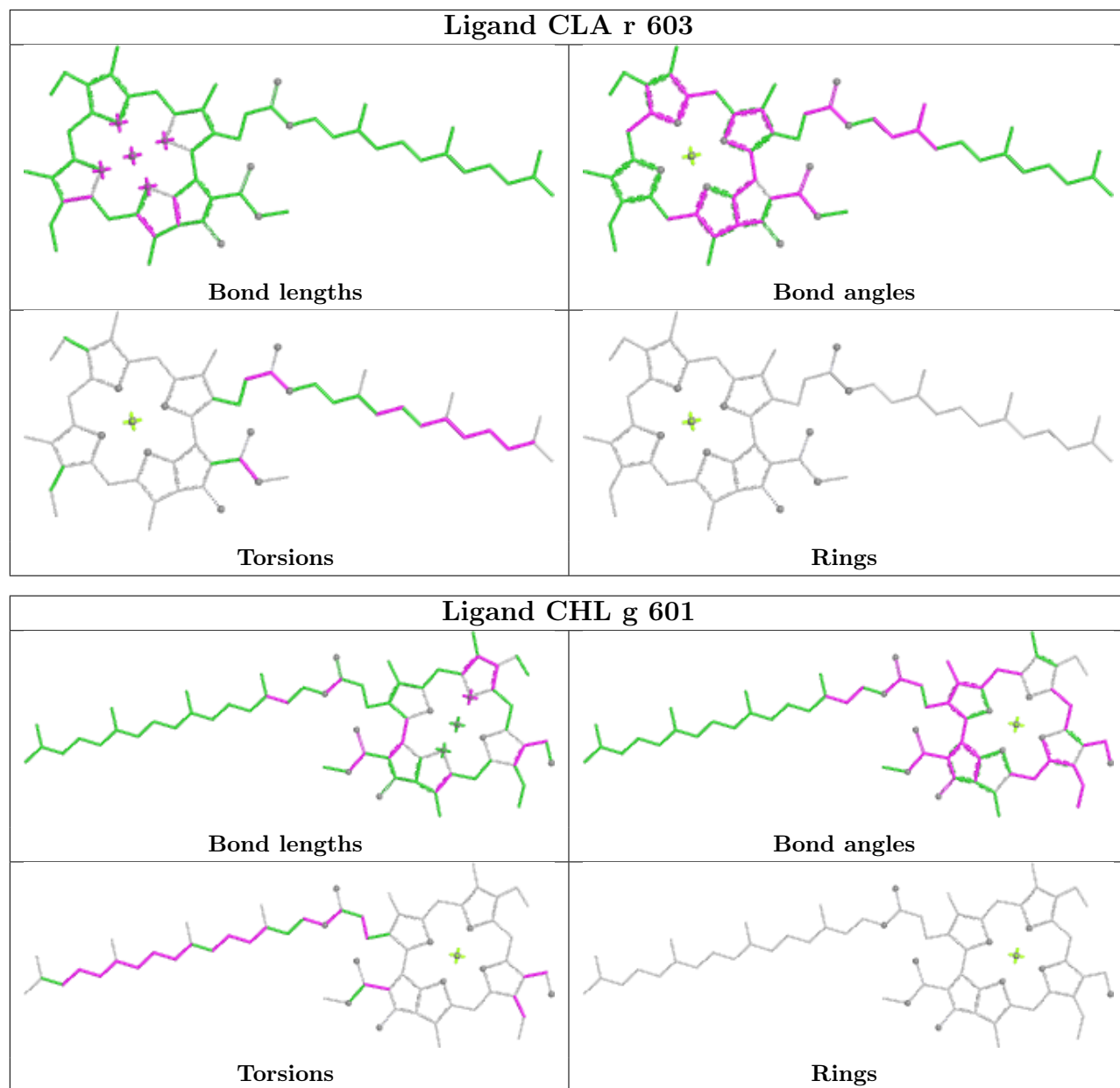


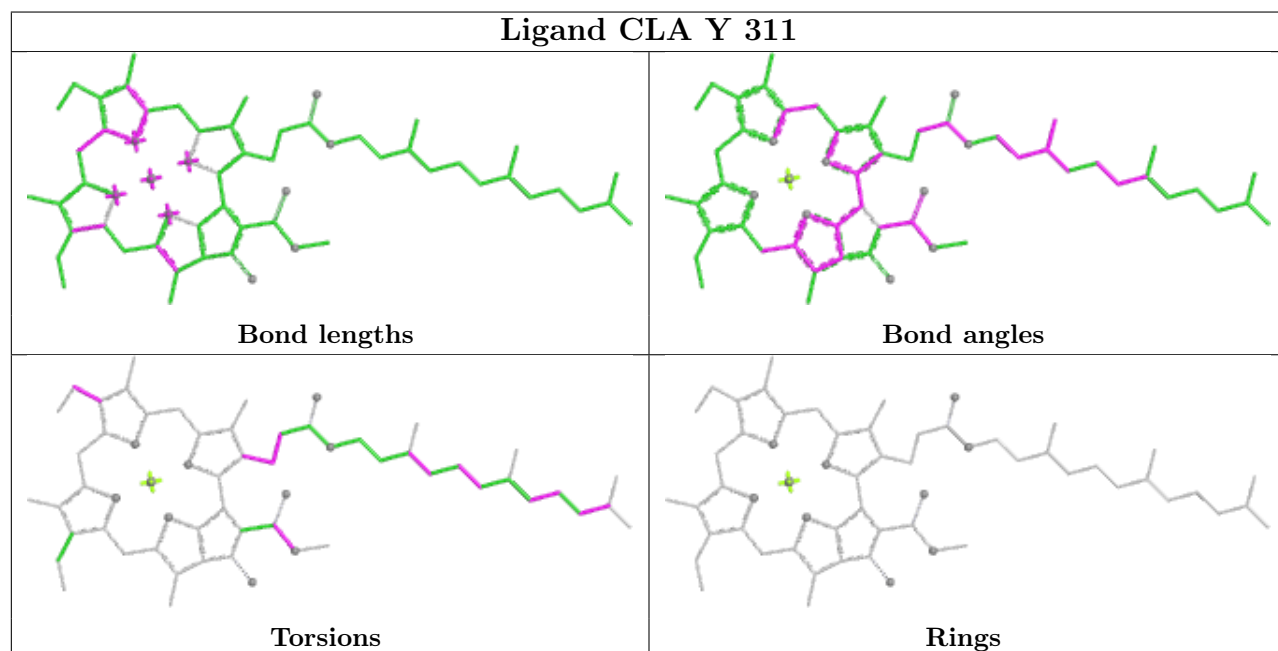
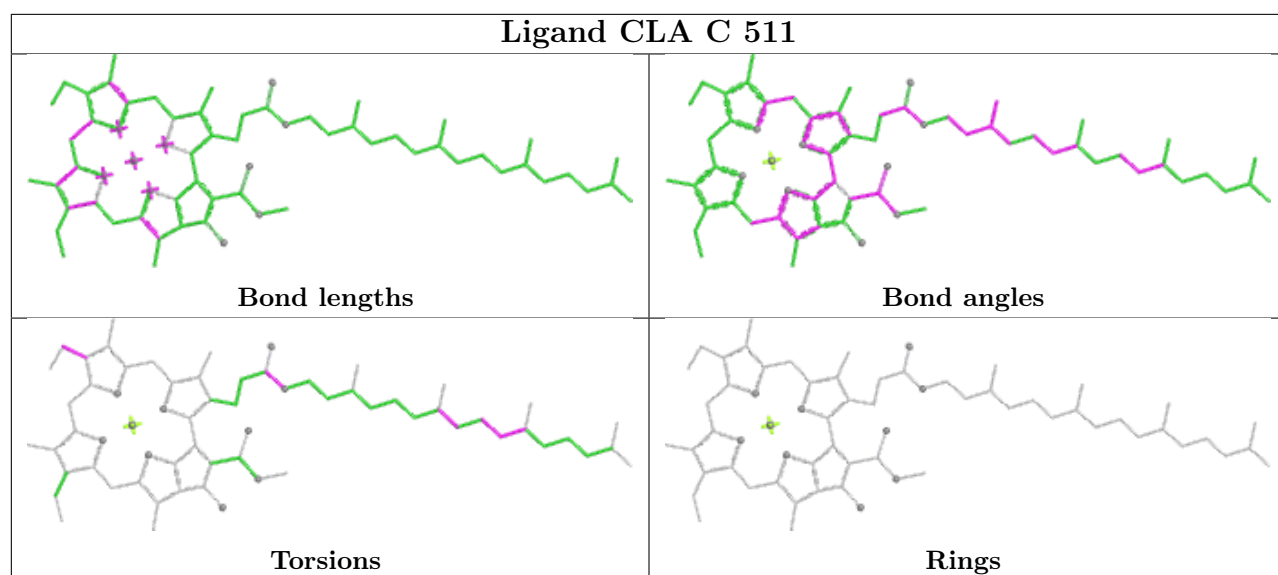
Torsions

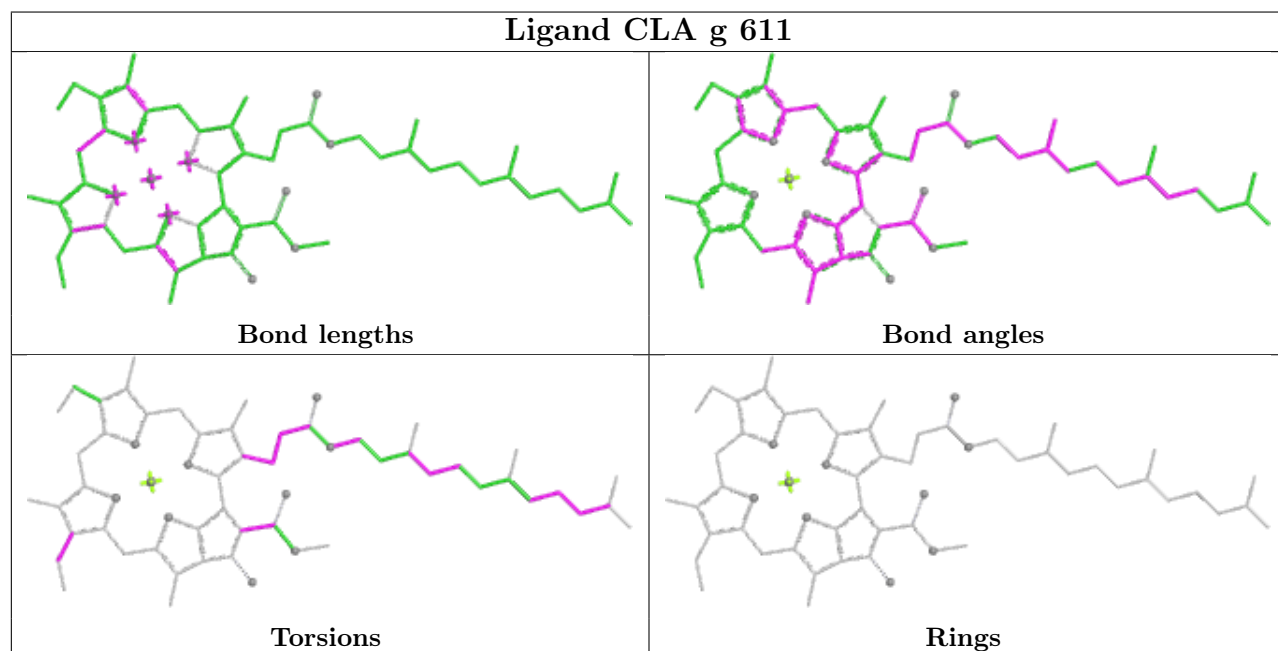
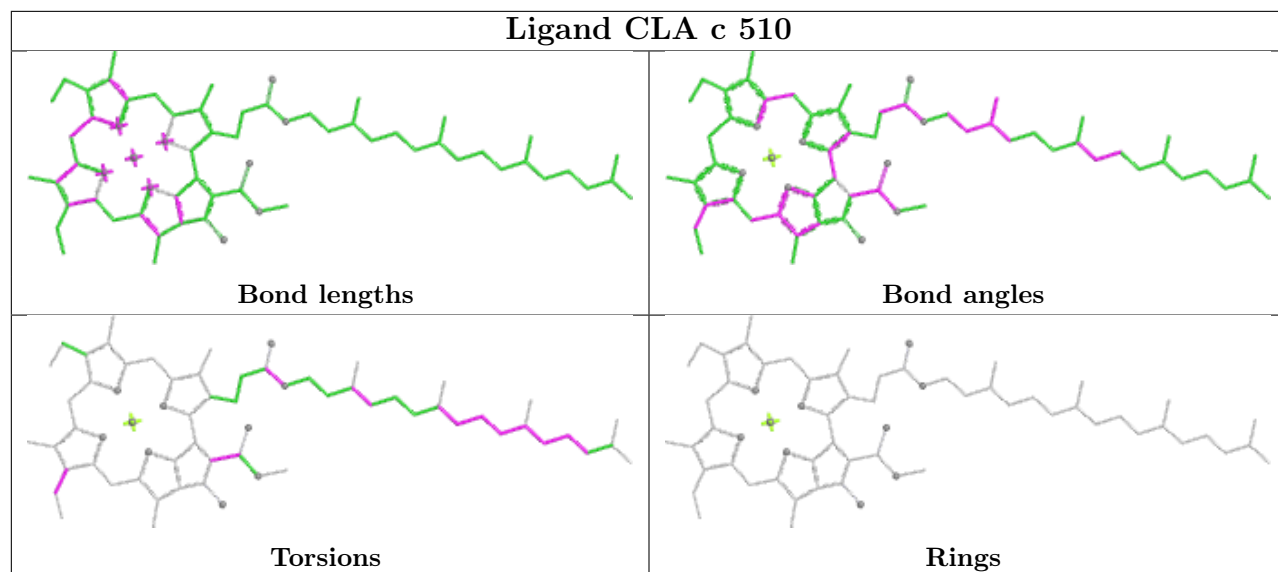


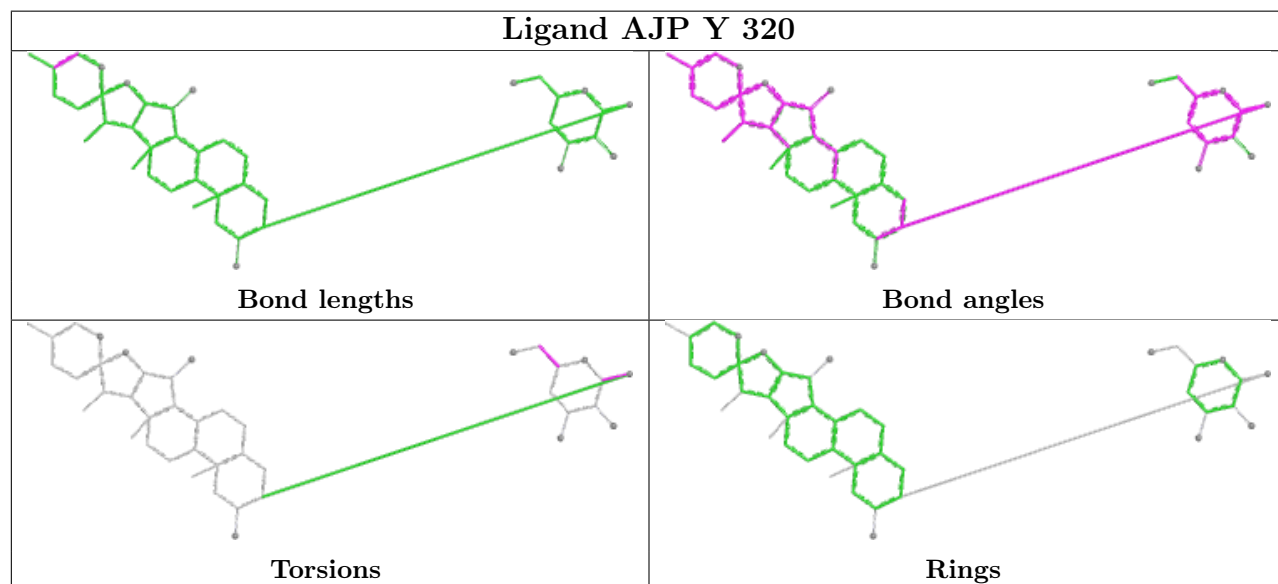
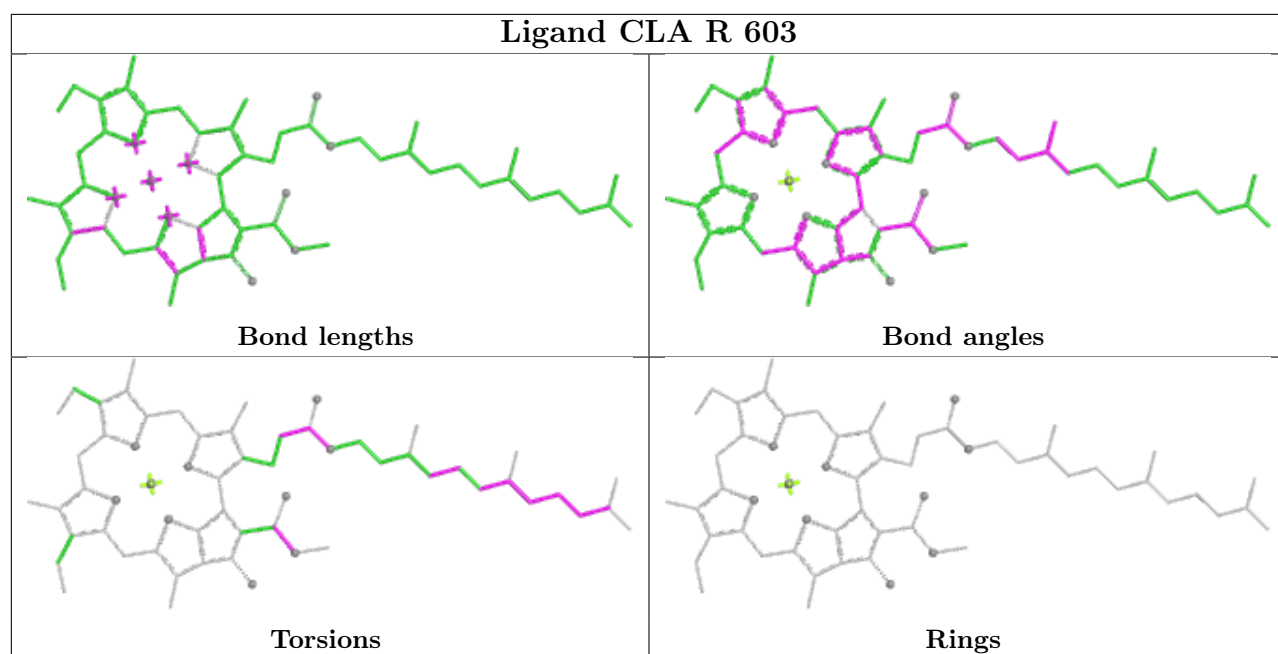
Rings

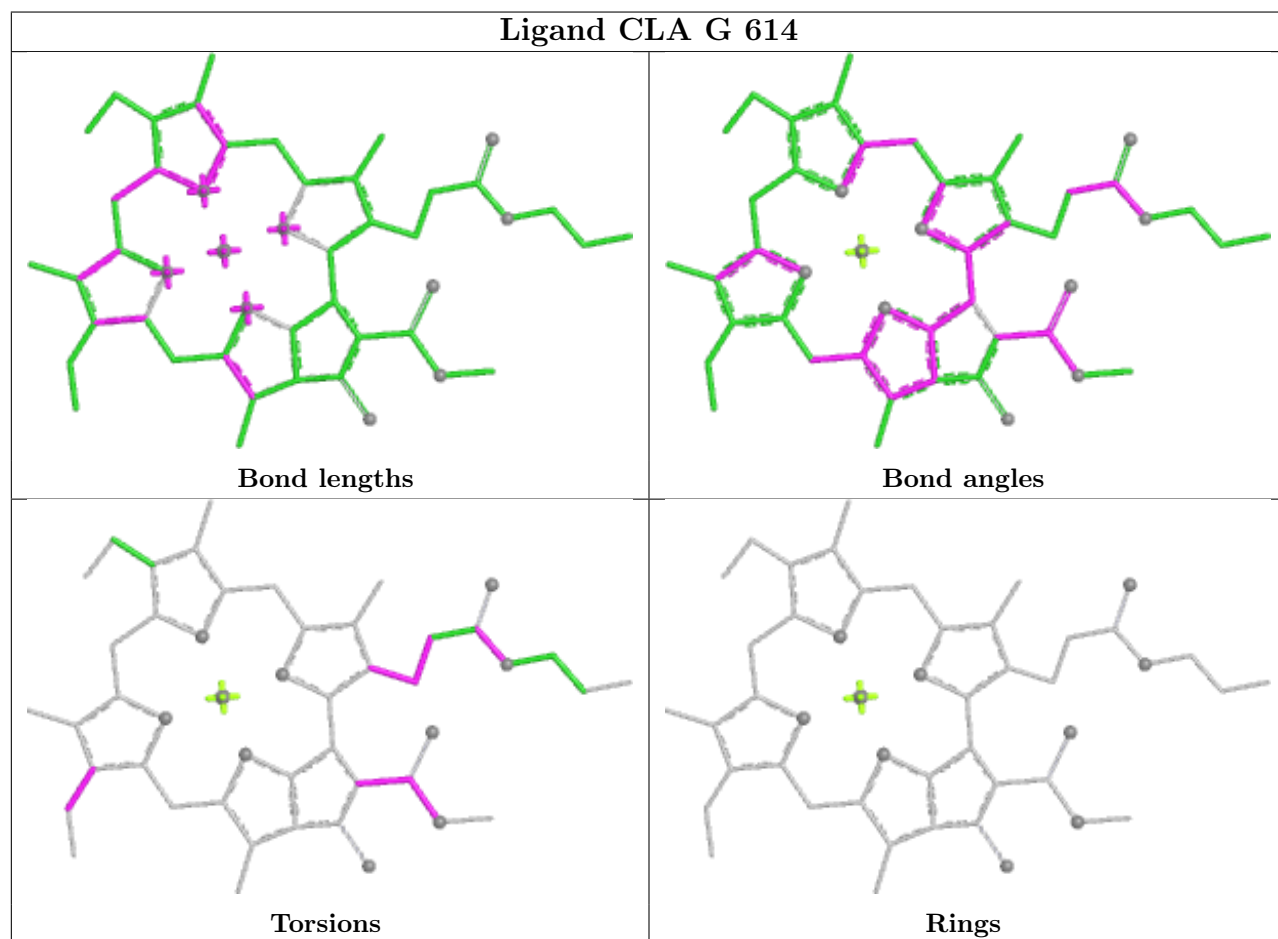
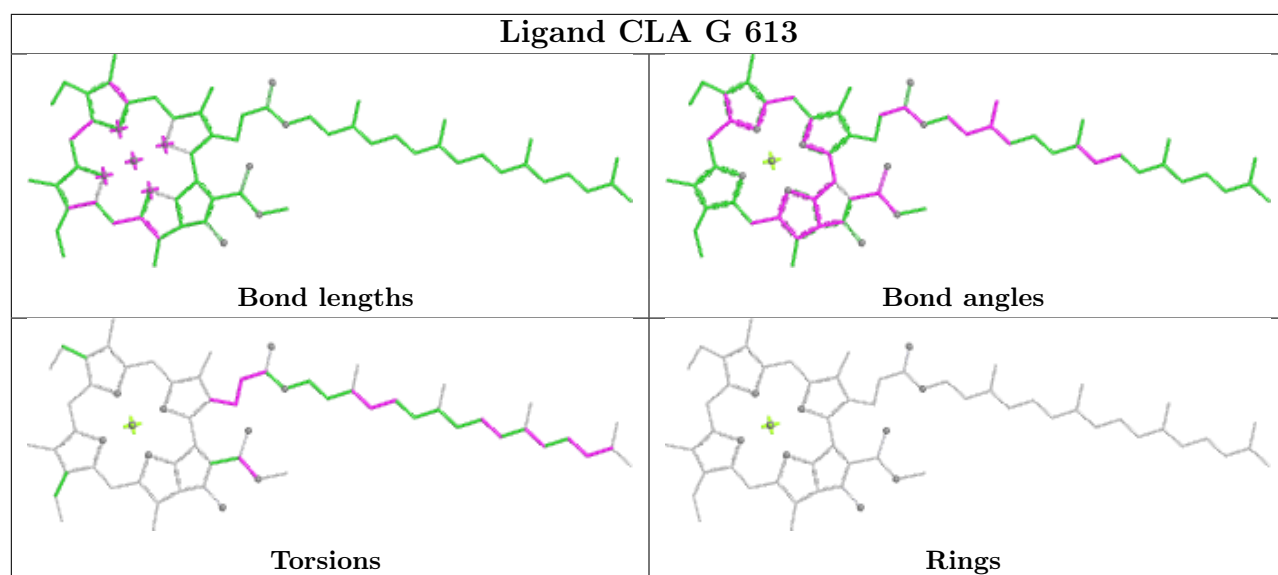


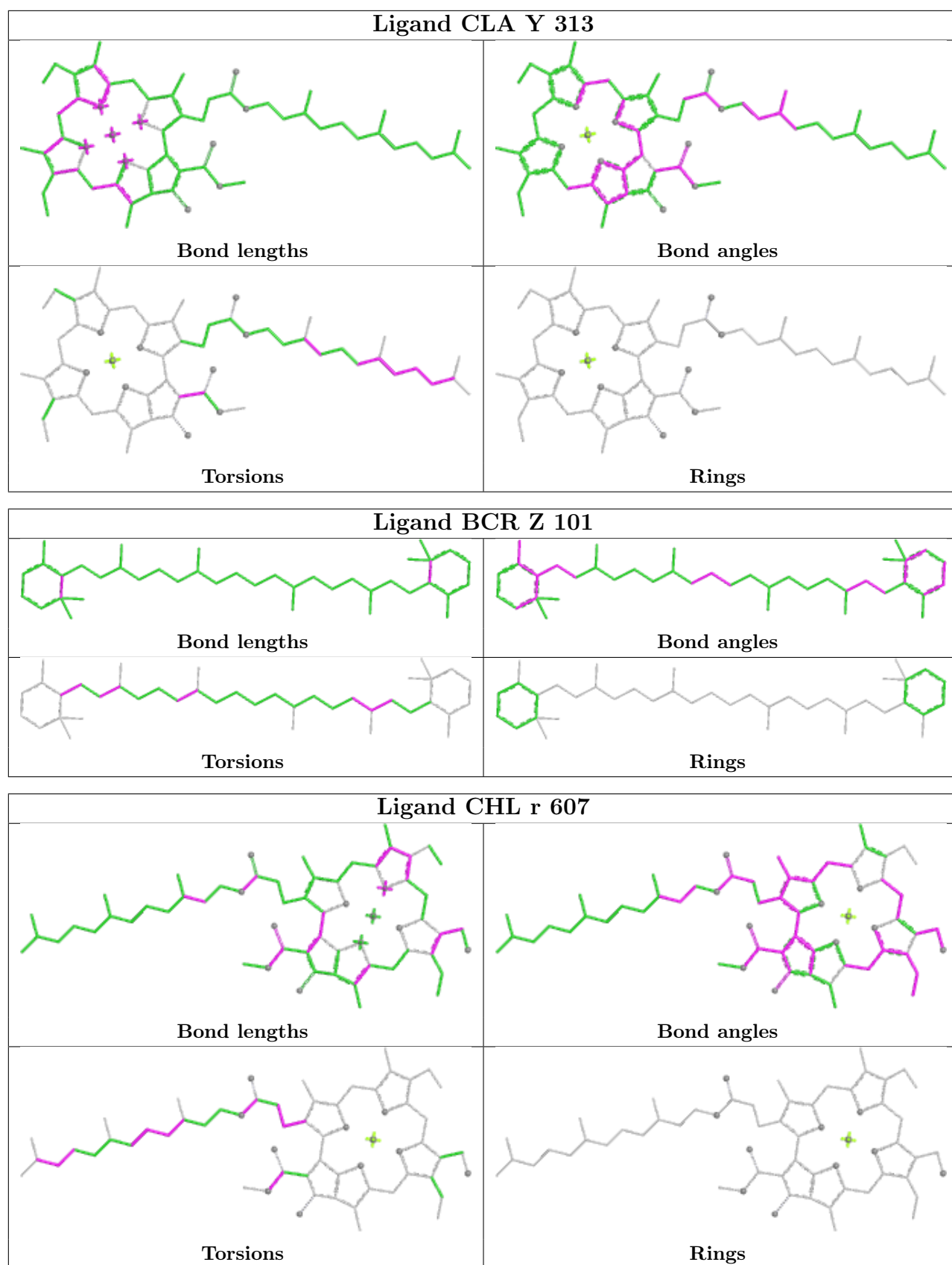


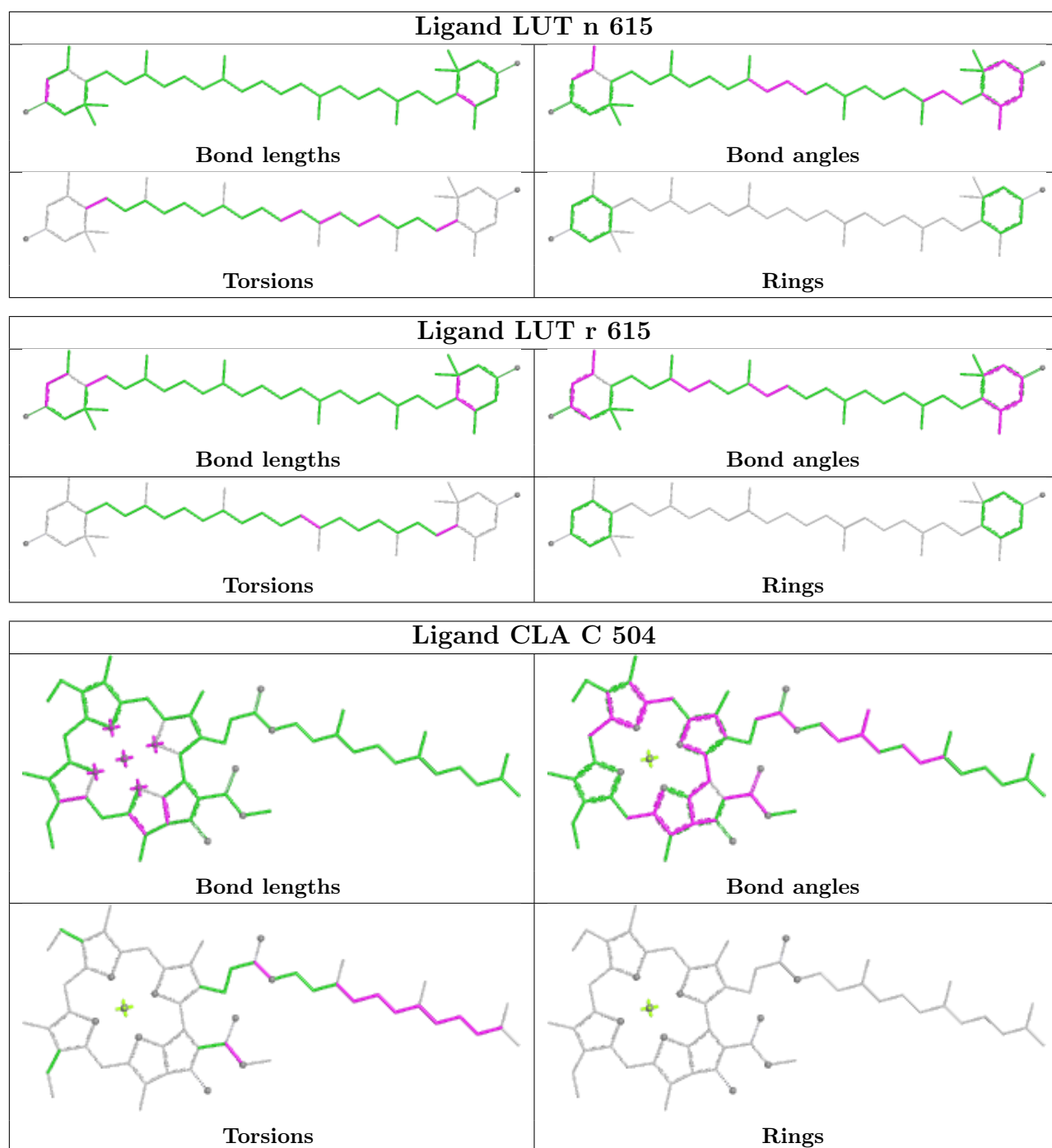


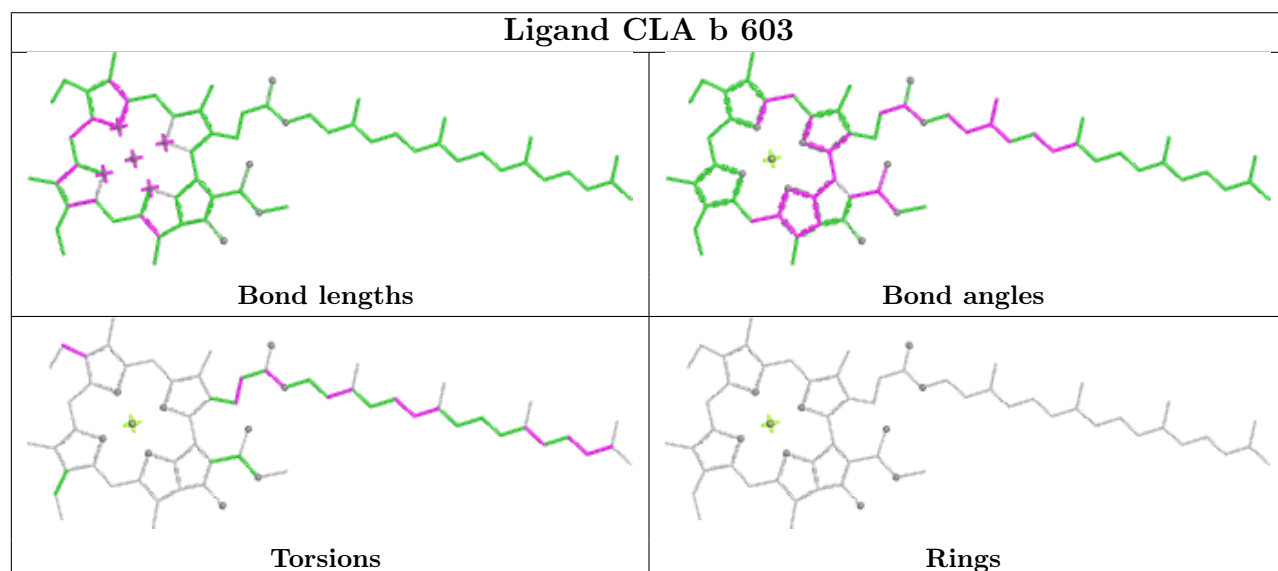
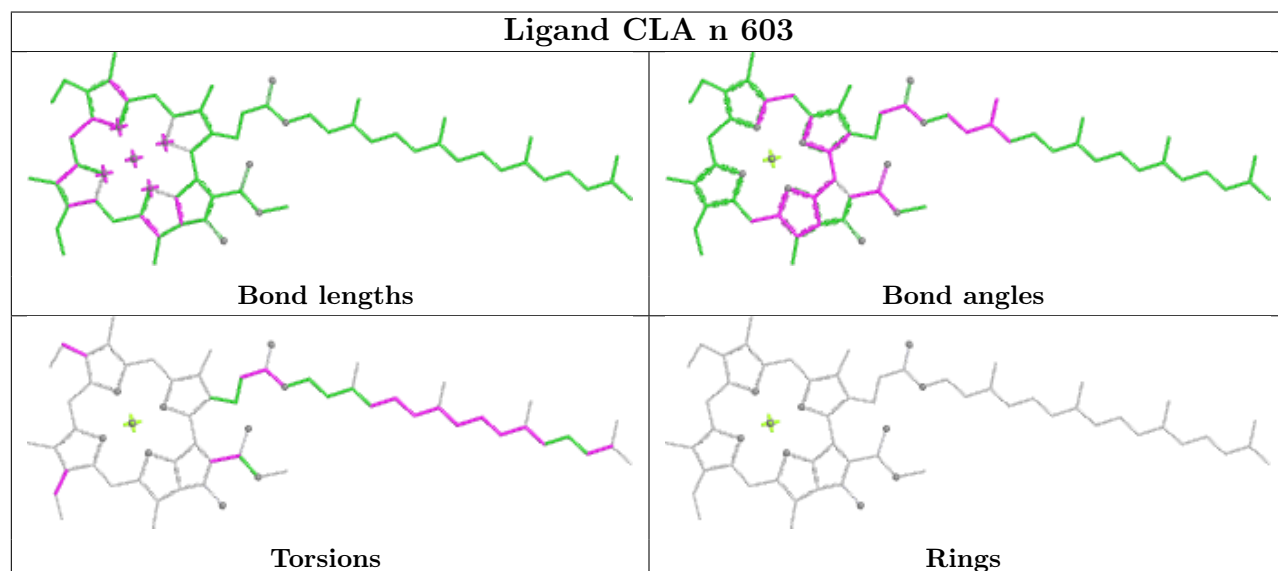
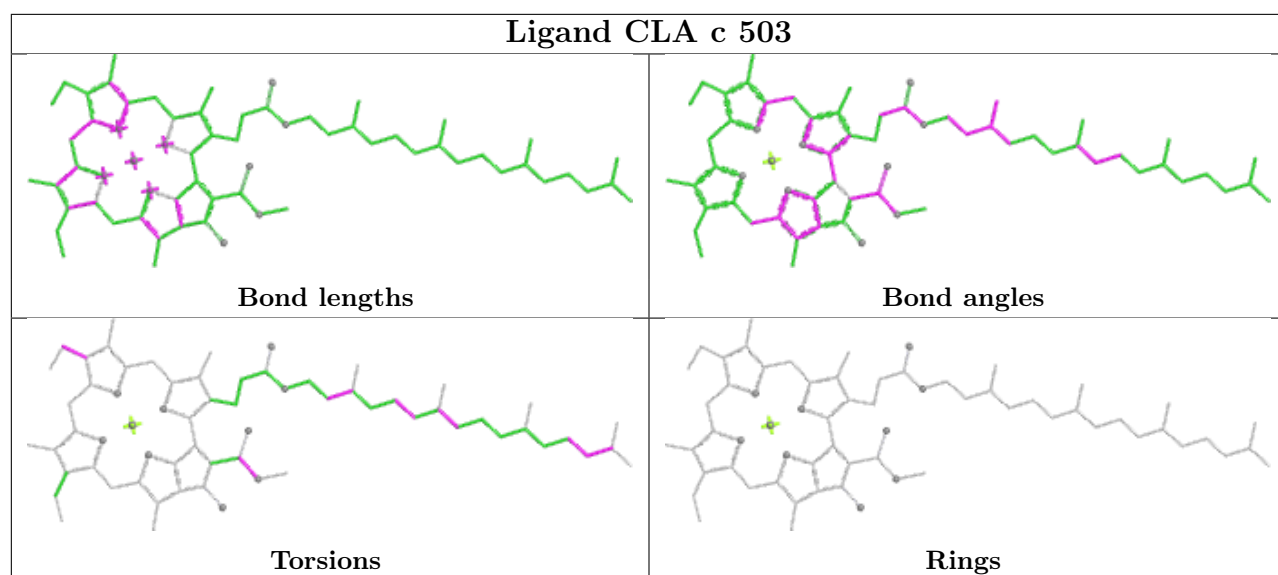


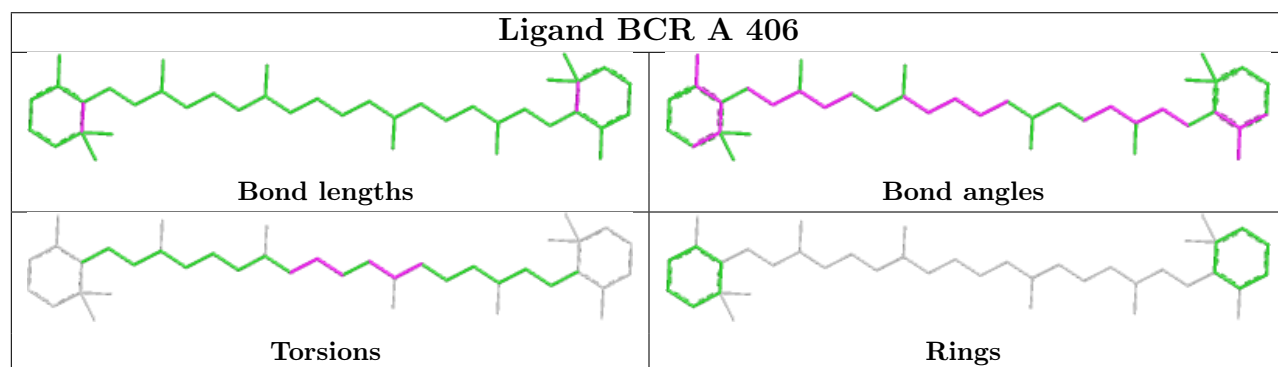
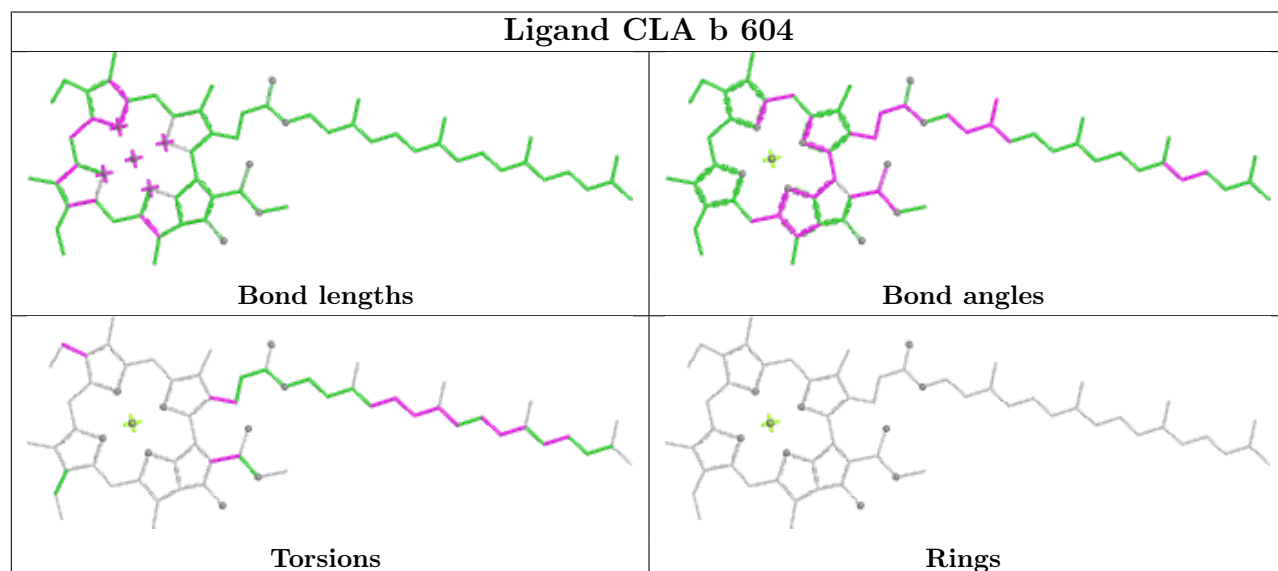
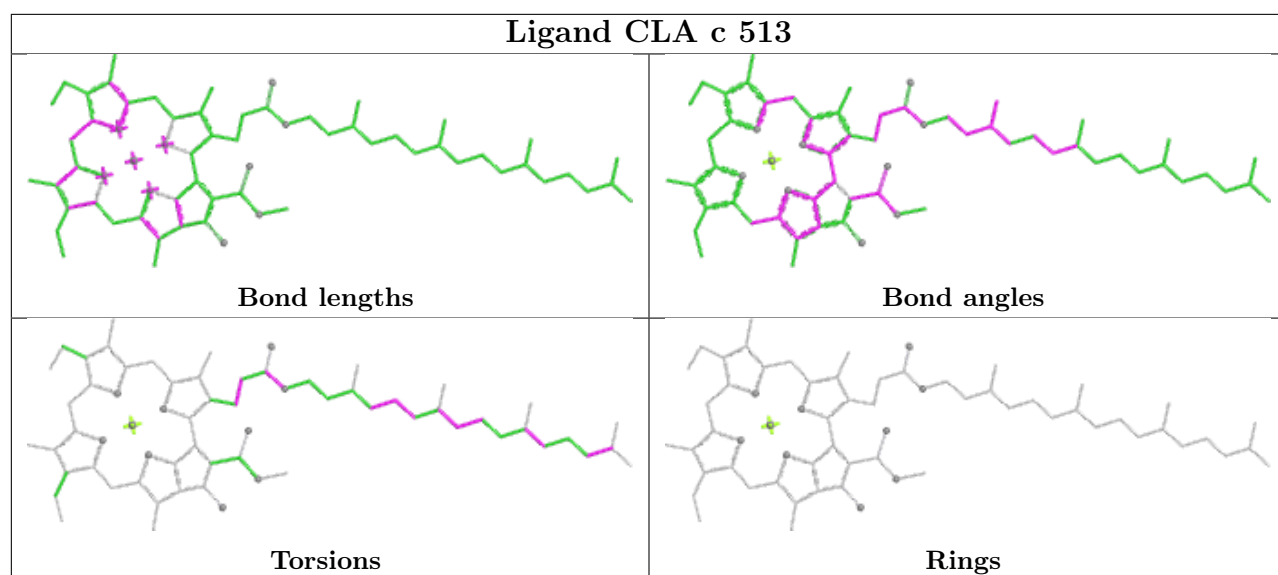


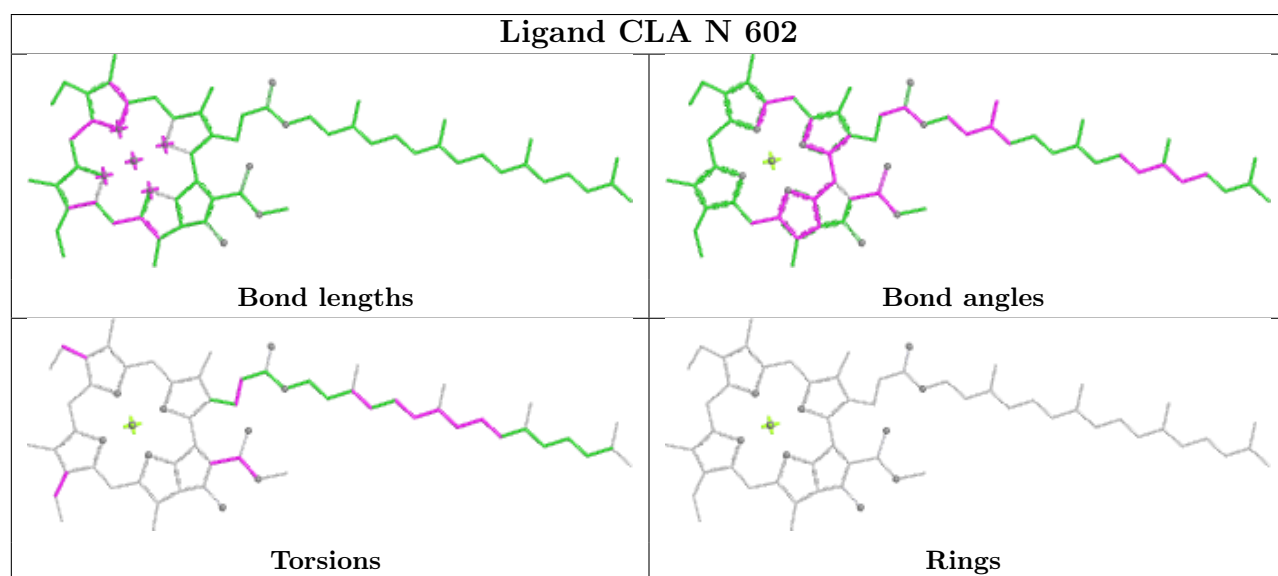
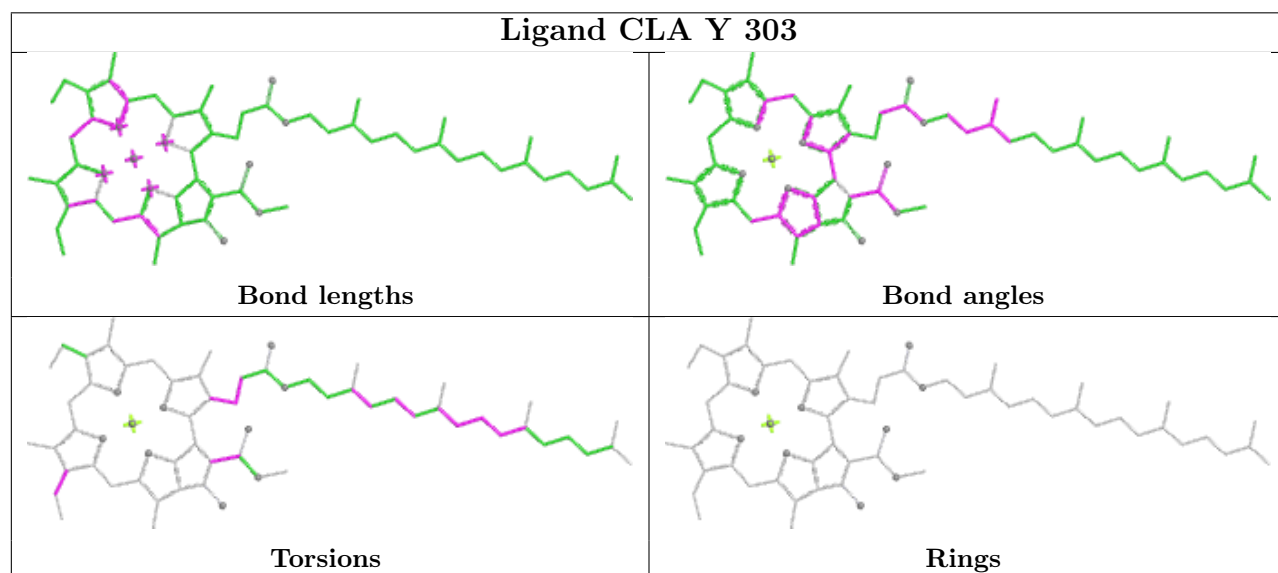
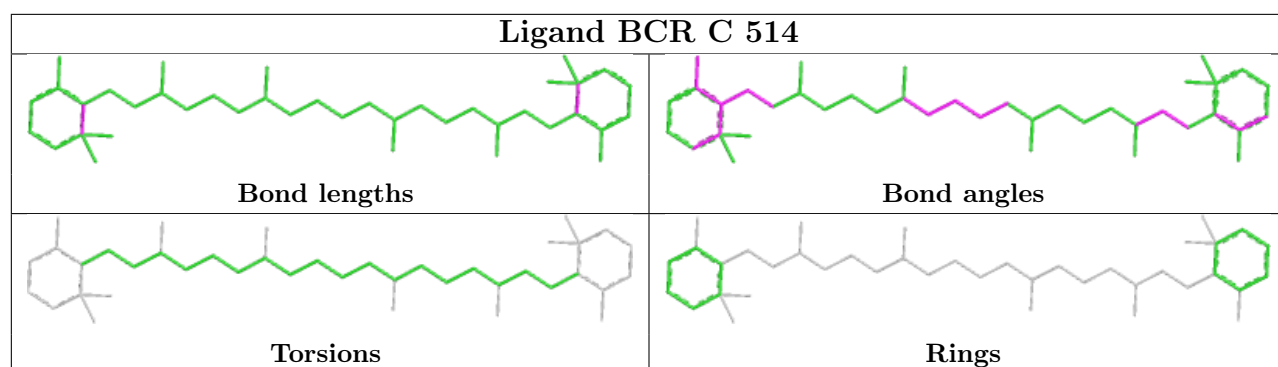


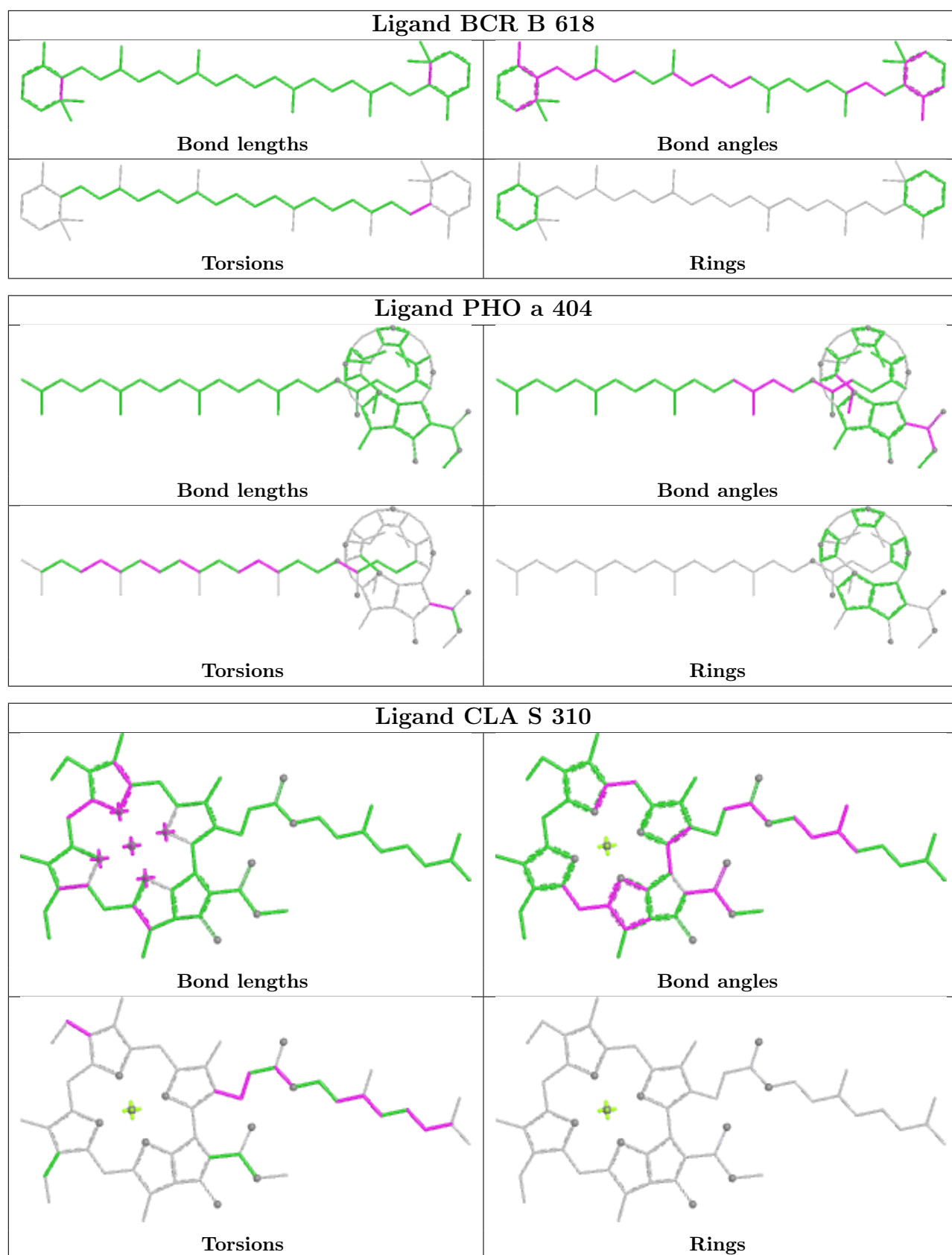


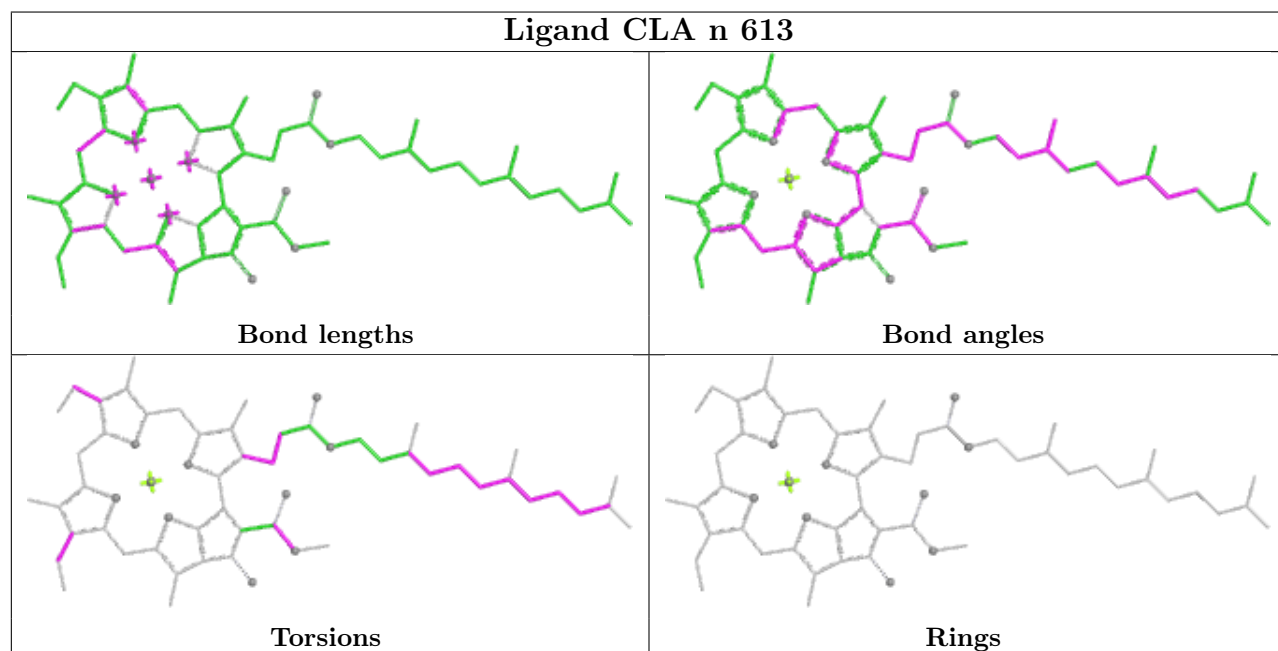
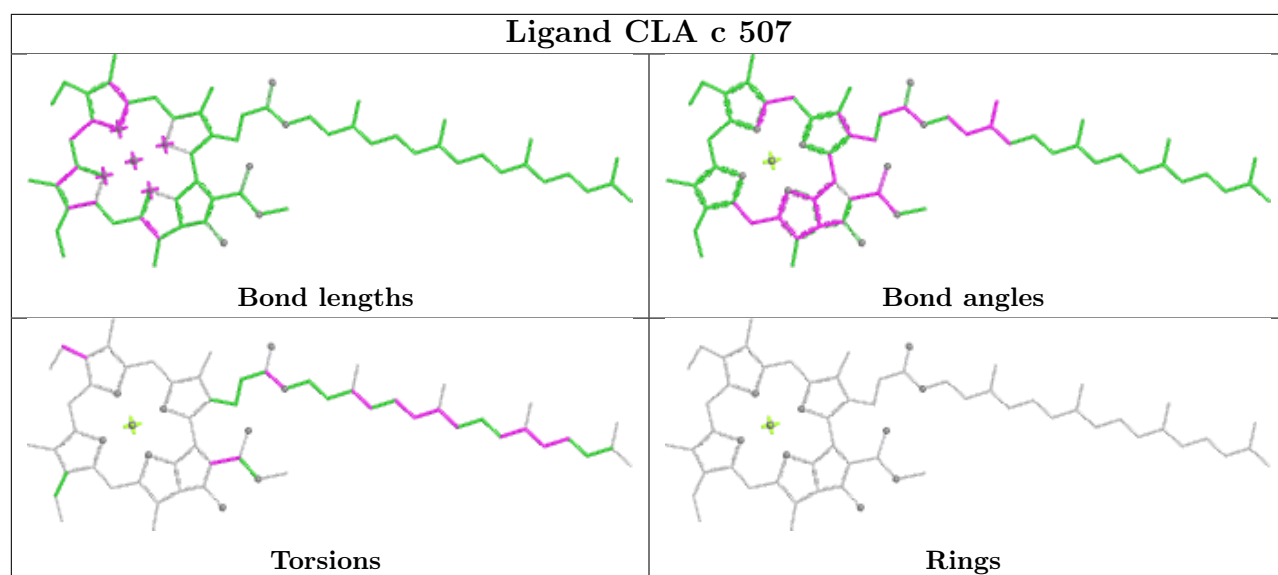




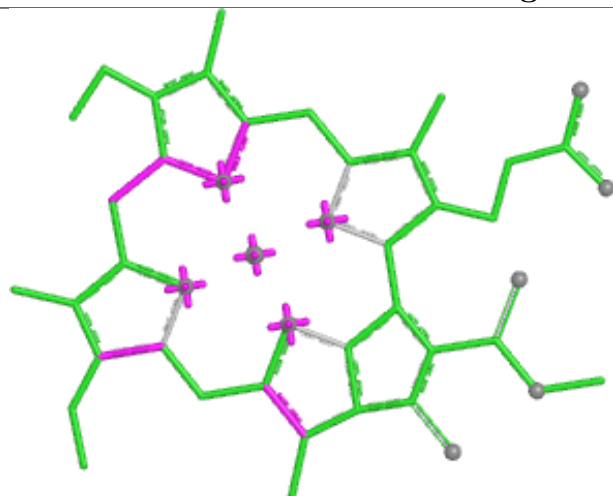




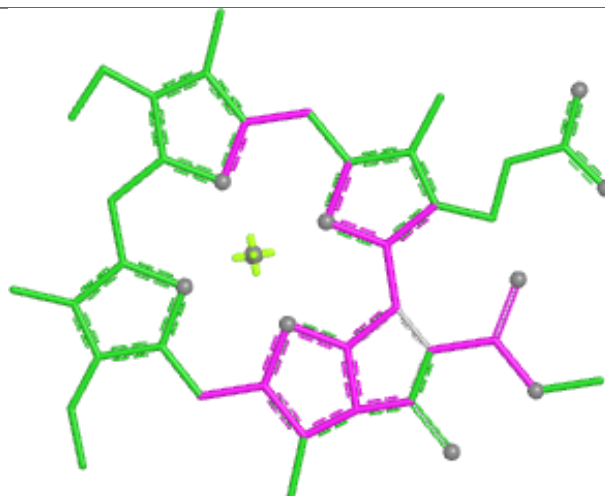




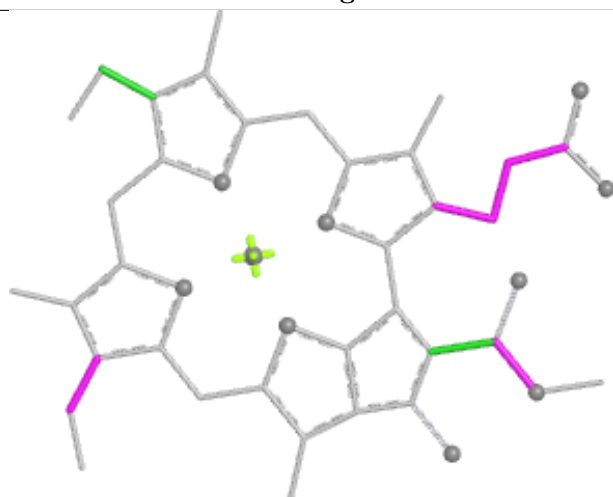
Ligand CLA r 614



Bond lengths



Bond angles

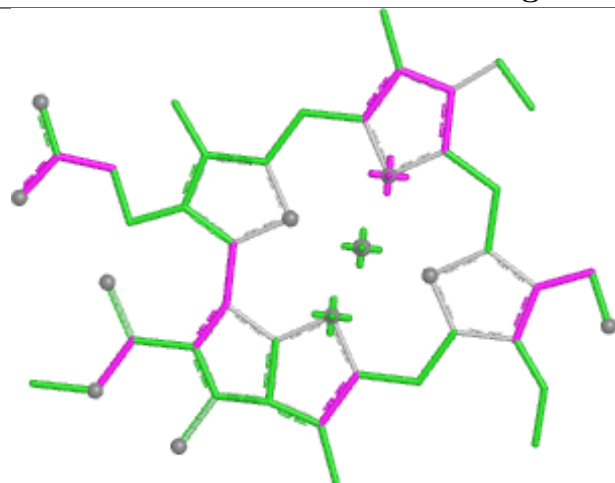


Torsions

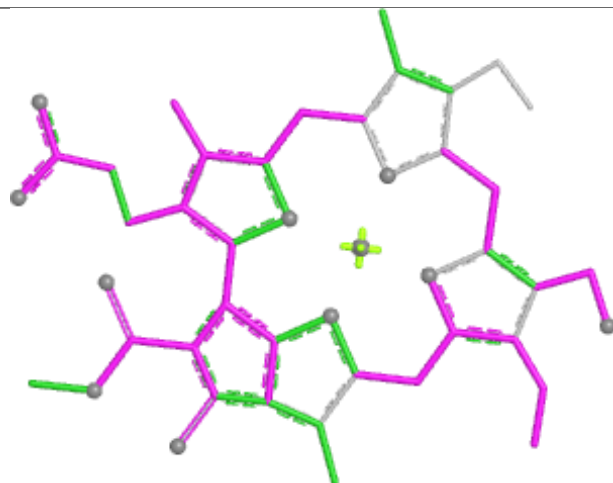


Rings

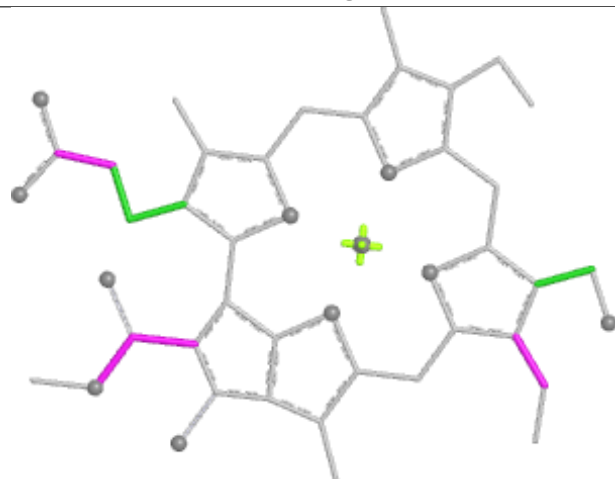
Ligand CHL s 306



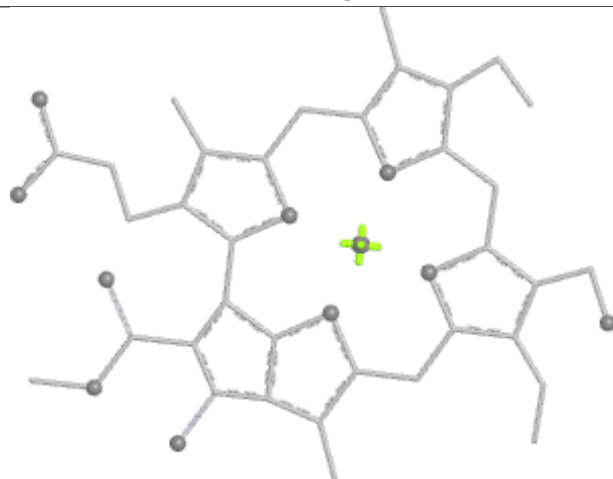
Bond lengths



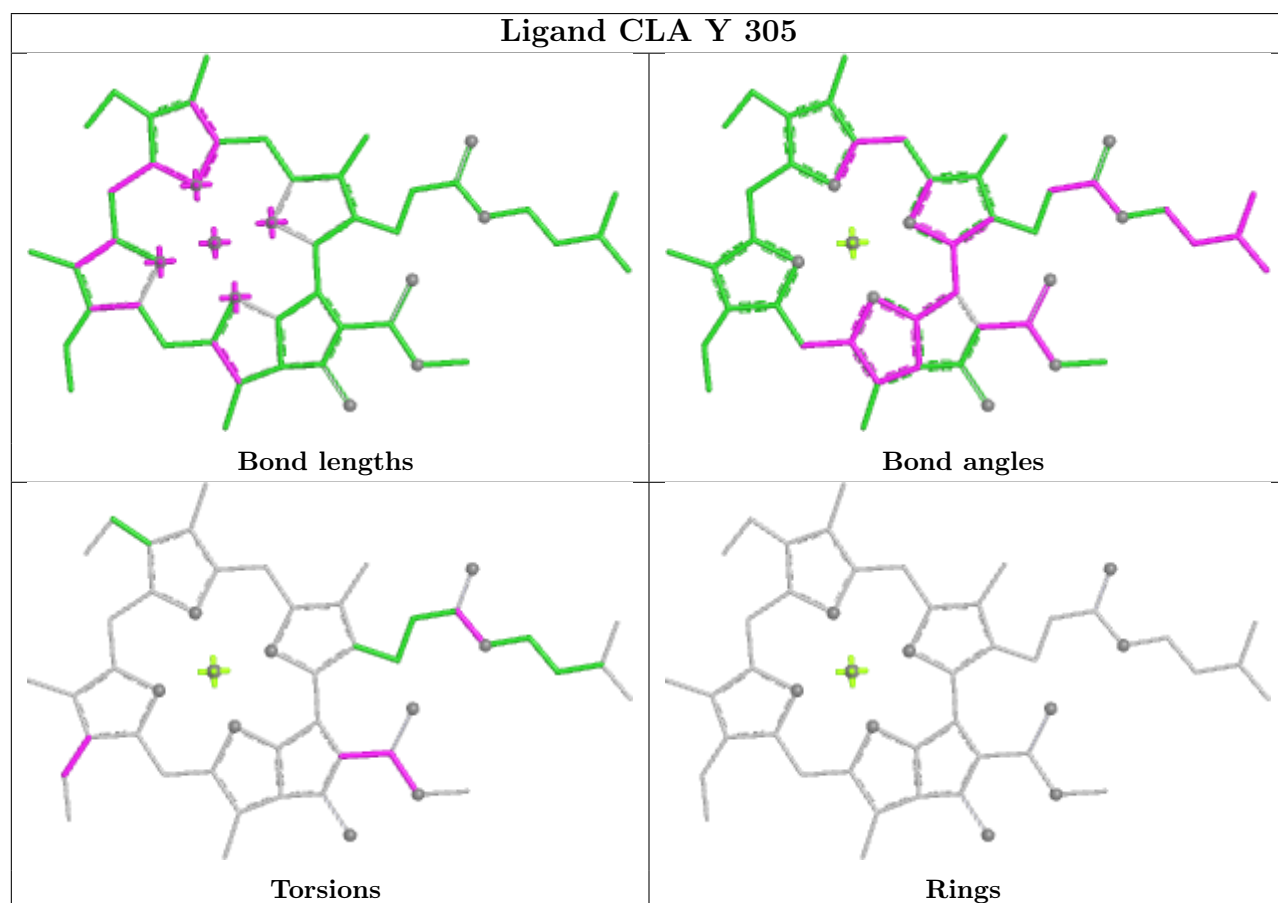
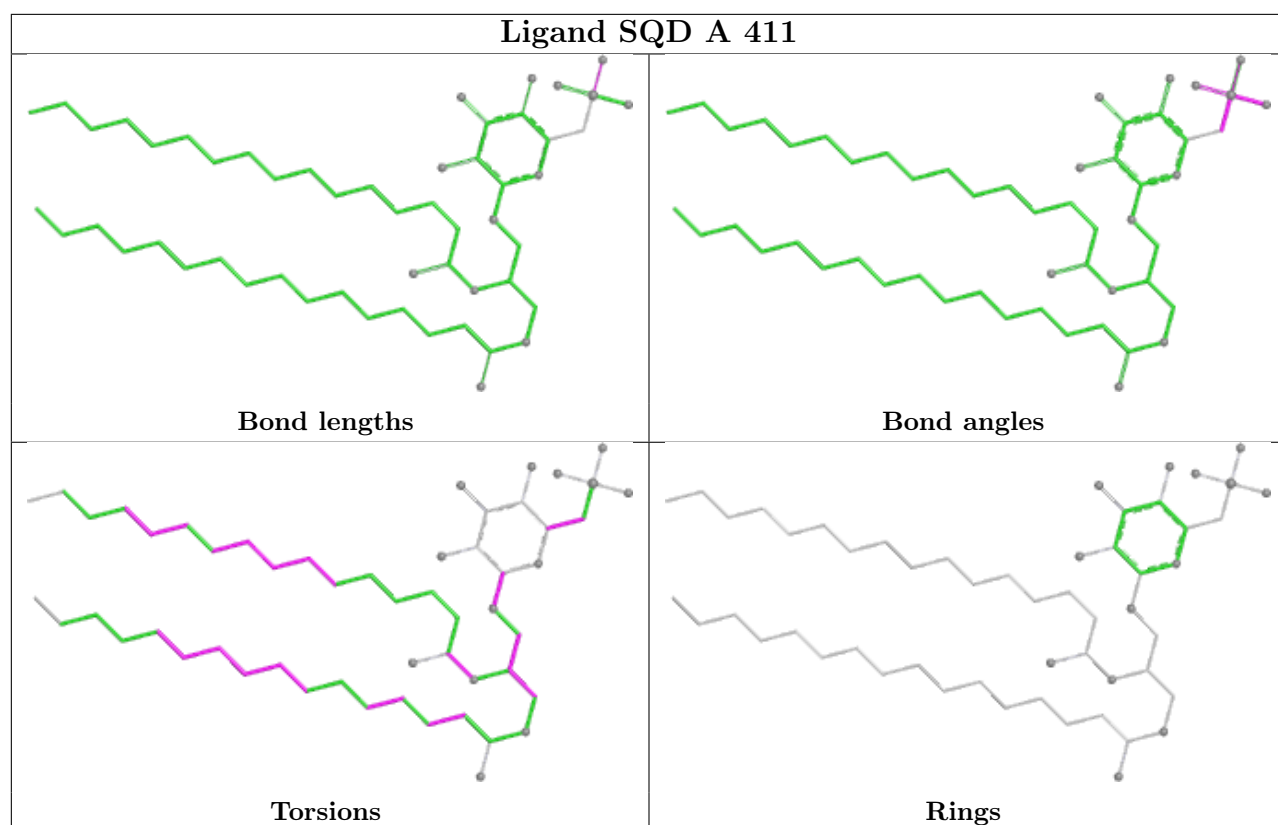
Bond angles

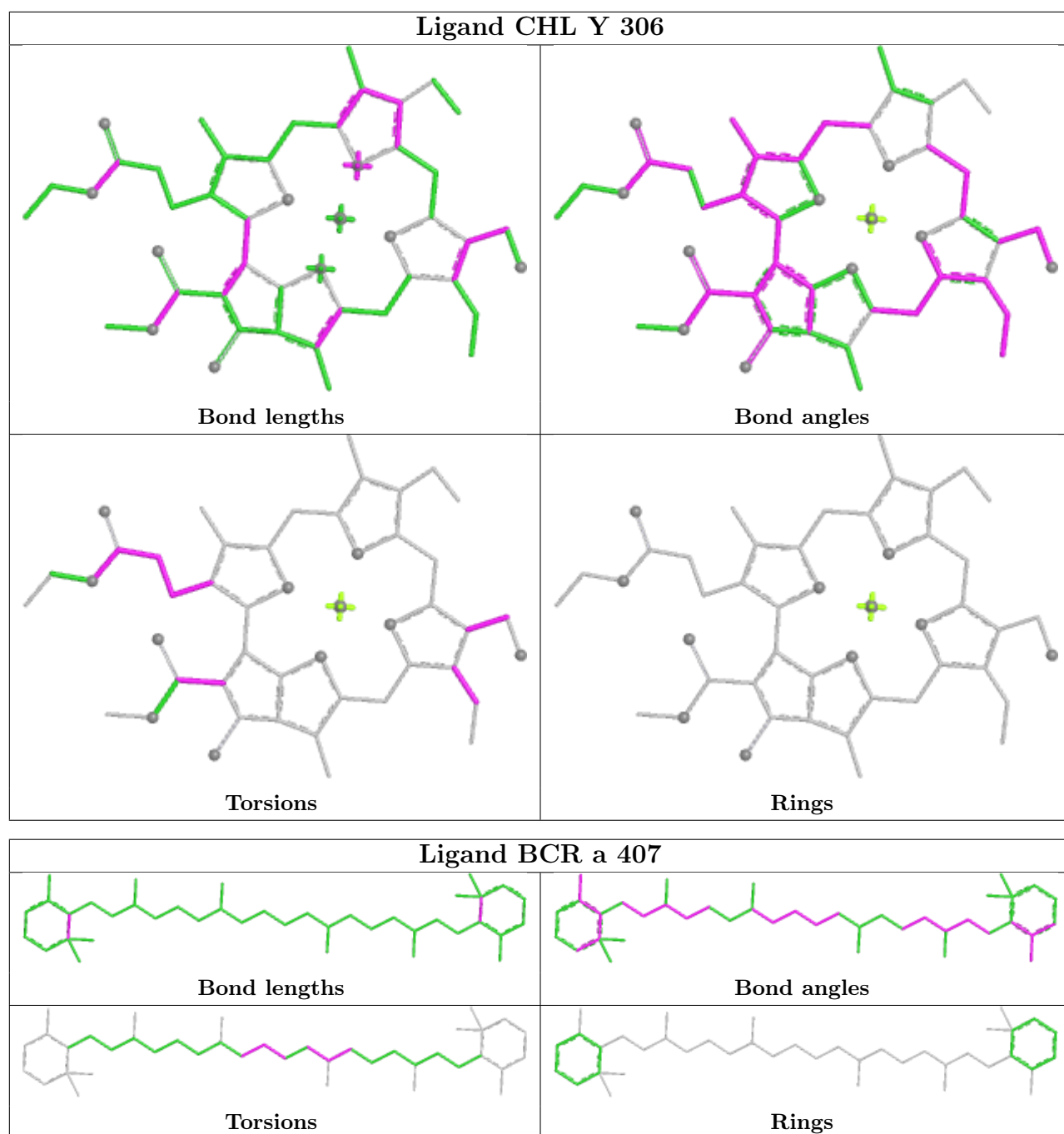


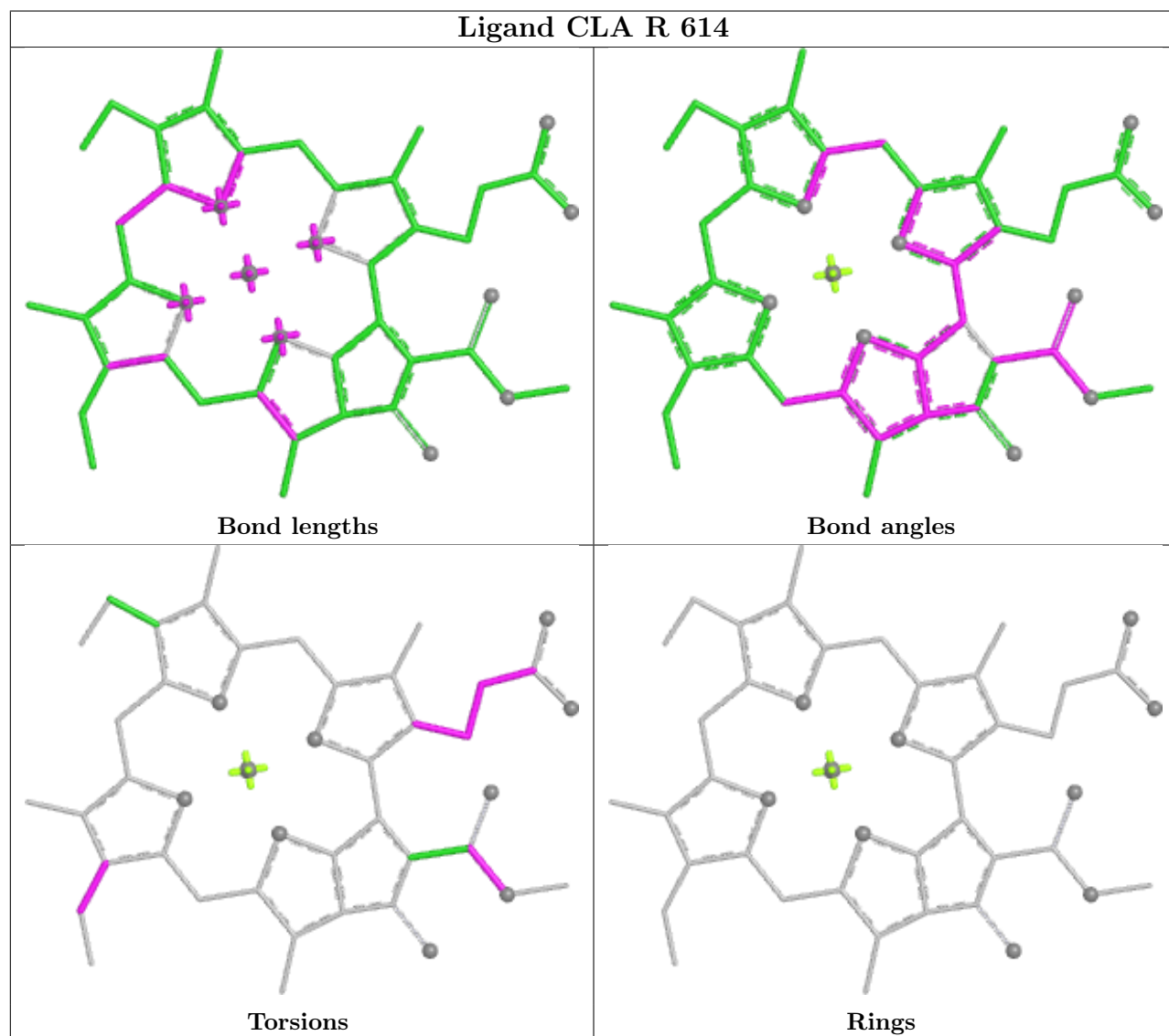
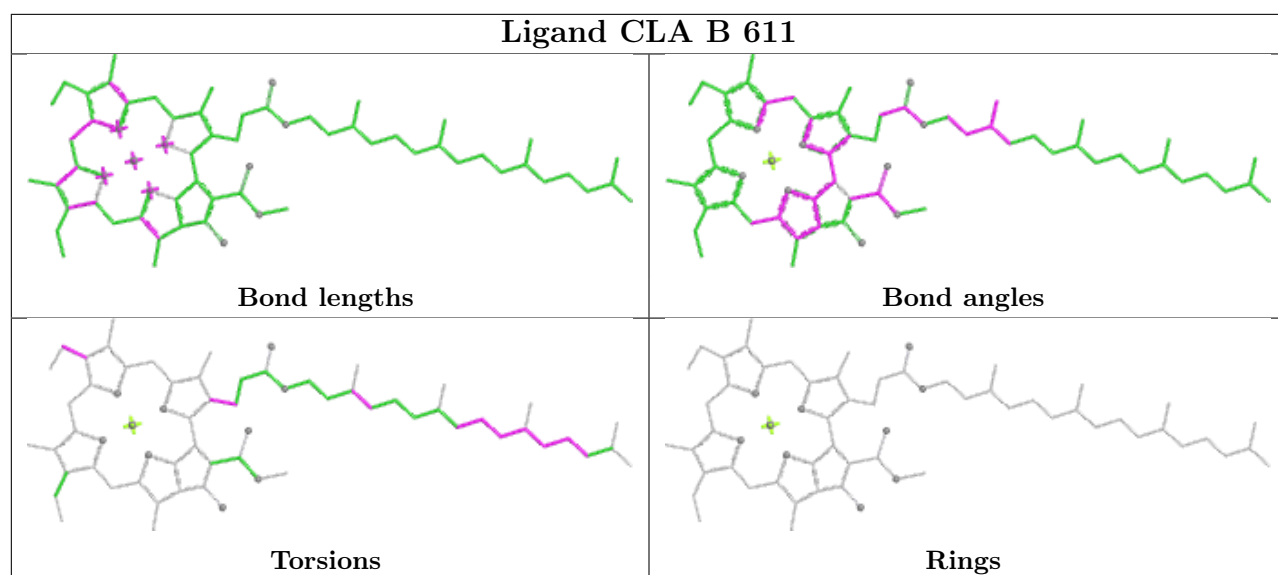
Torsions

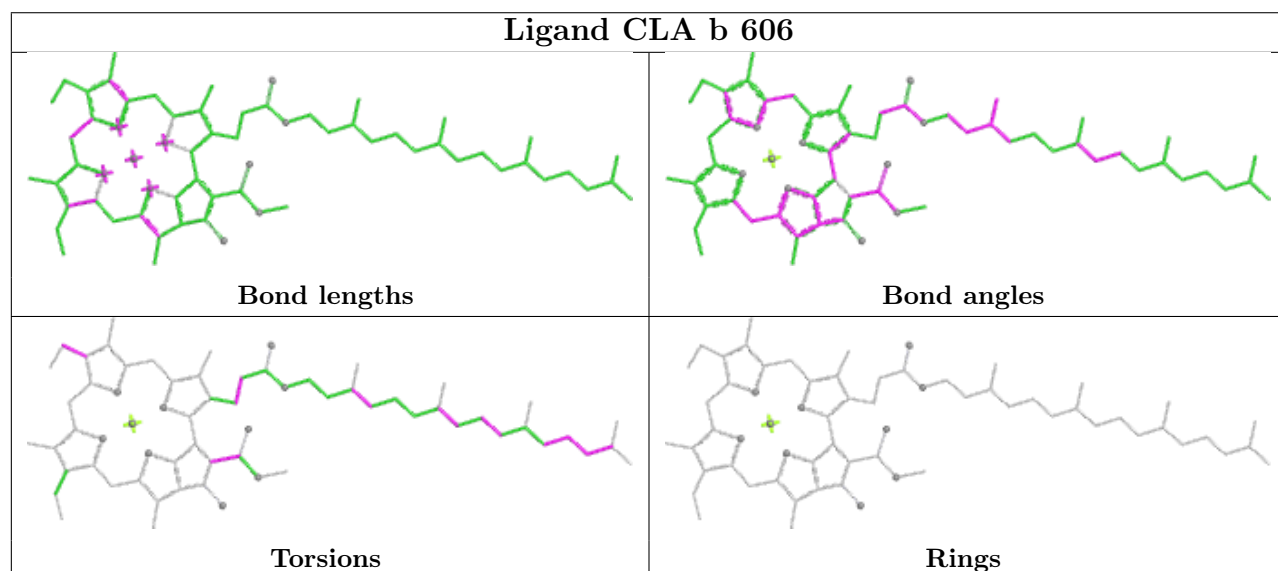
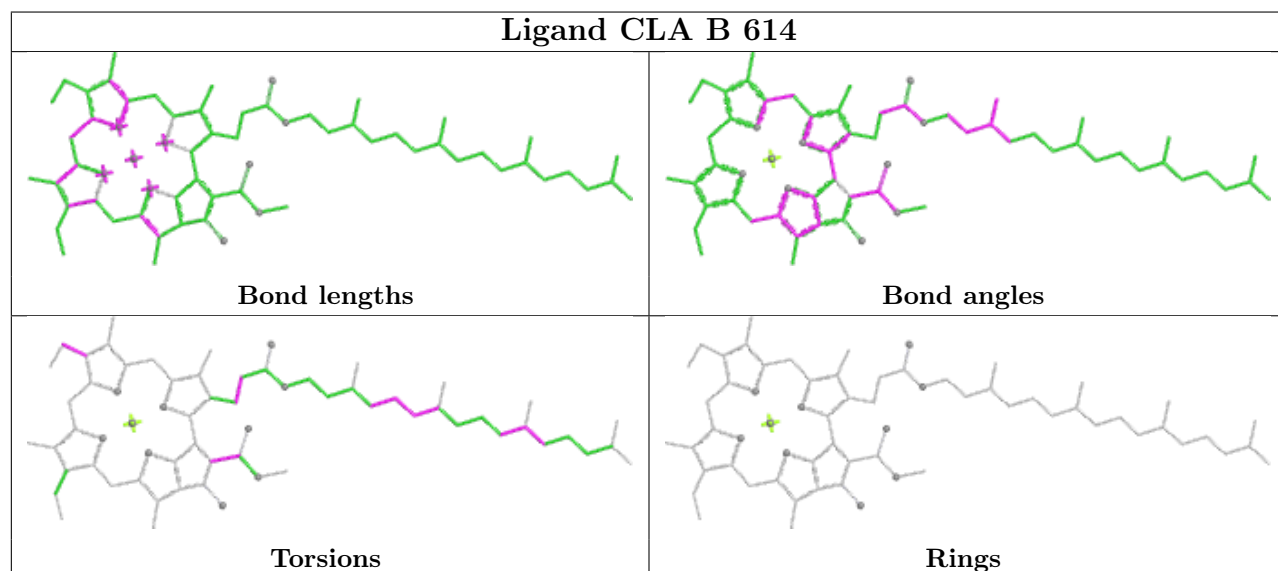
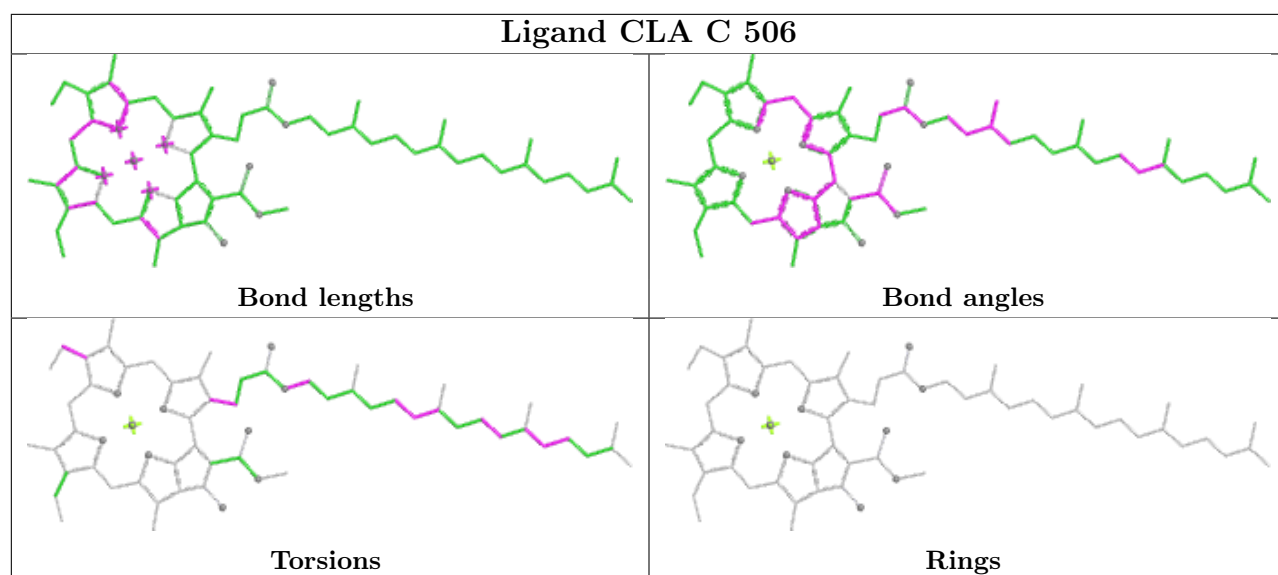


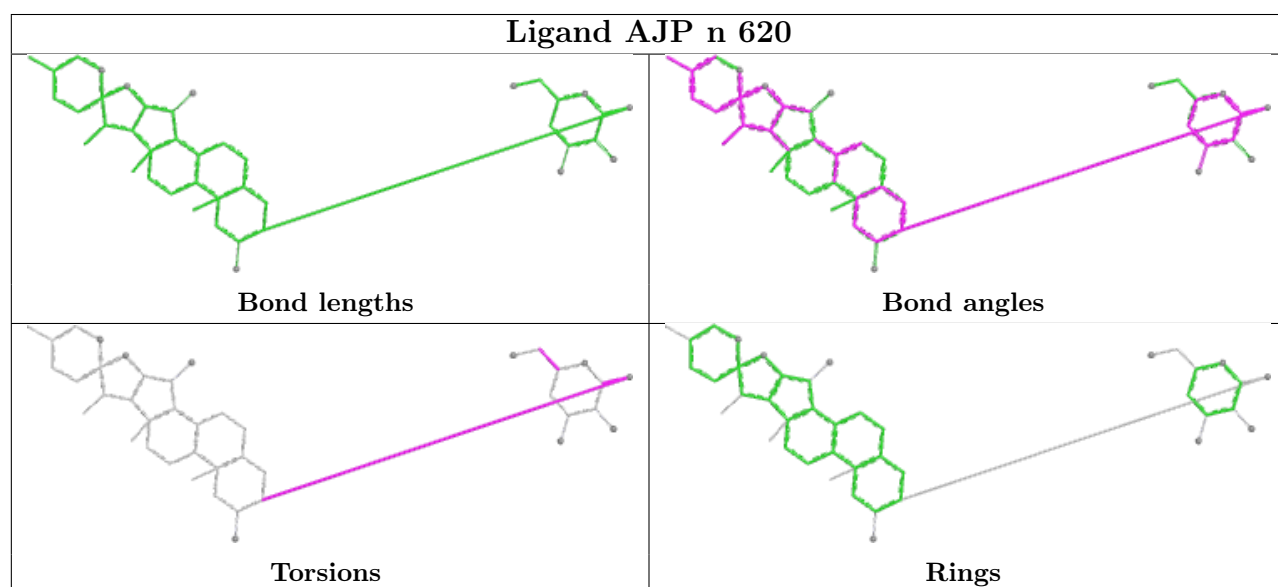
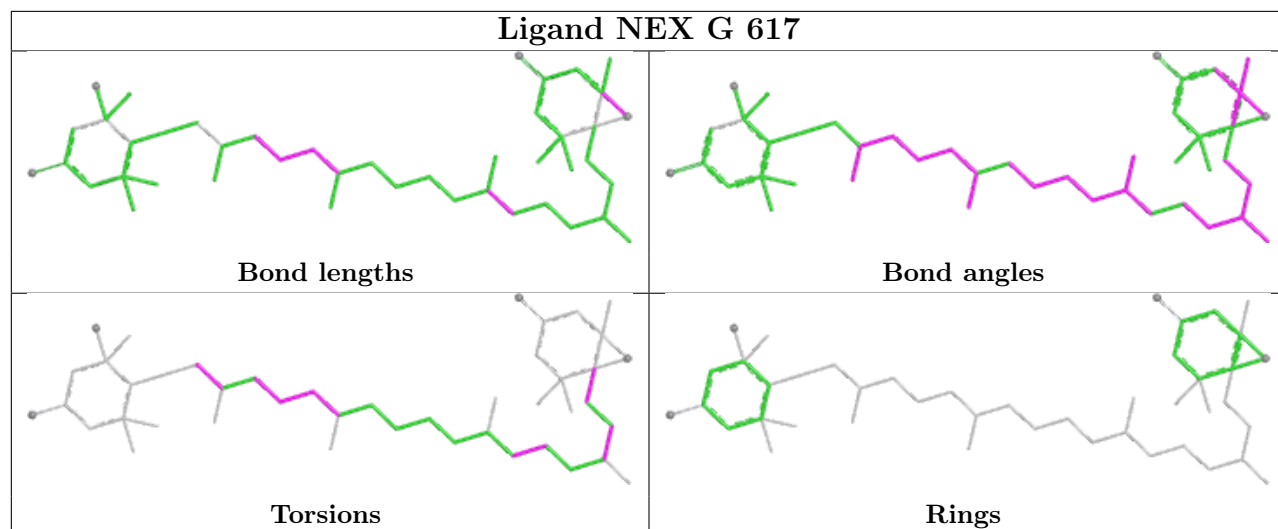
Rings

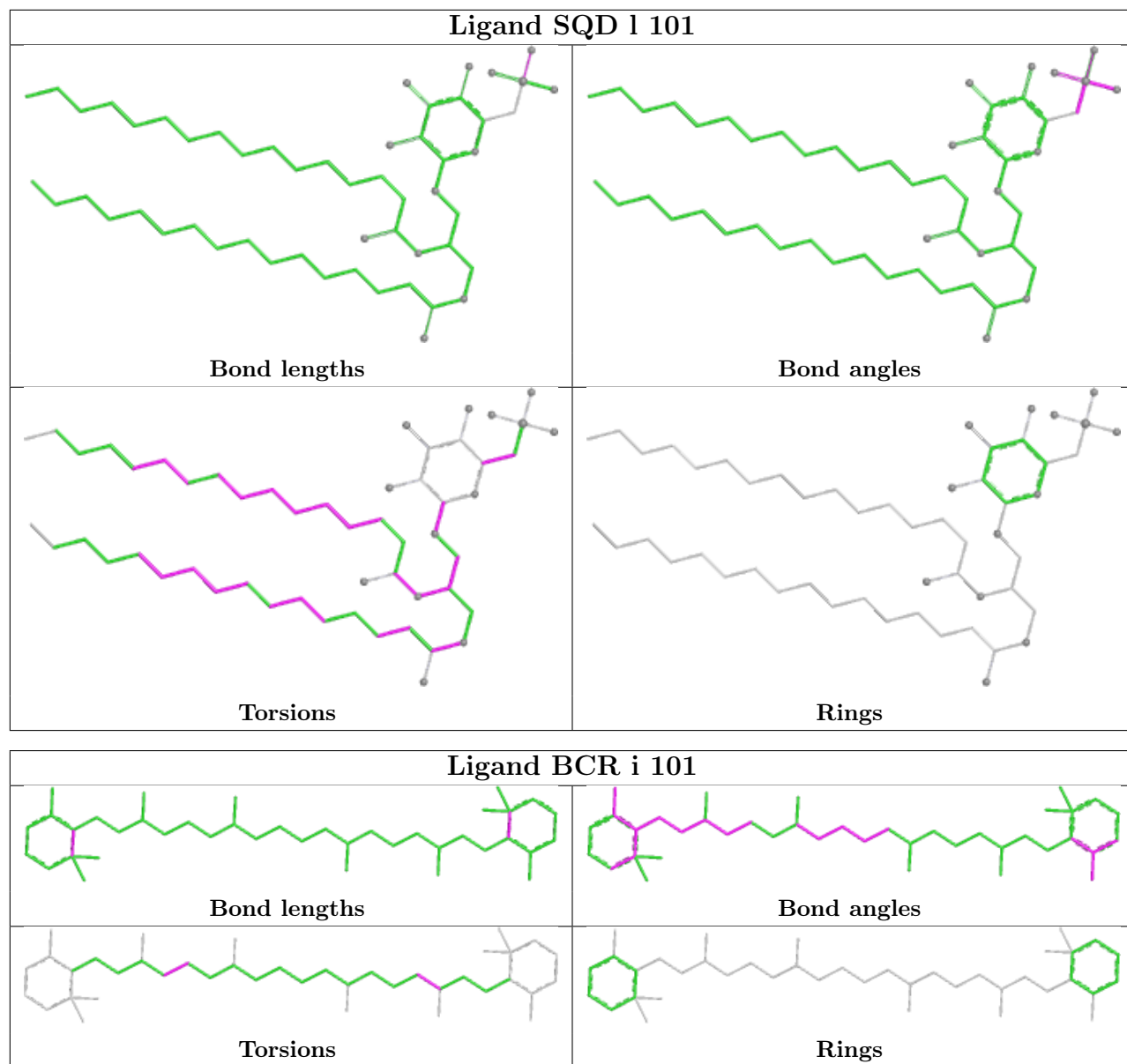




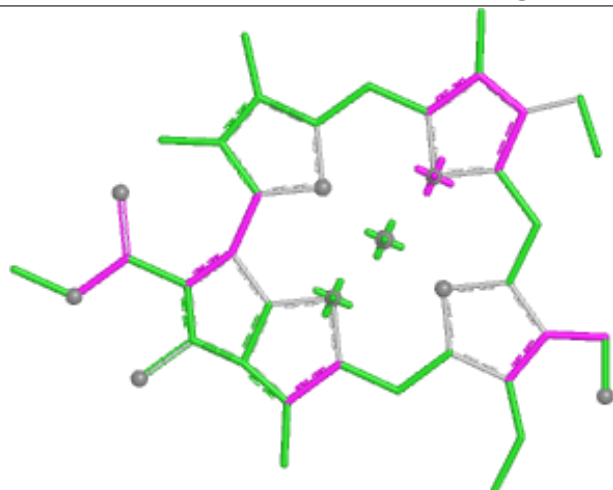




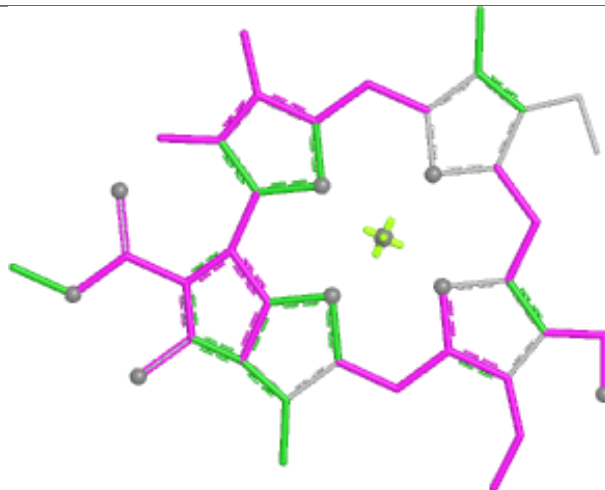




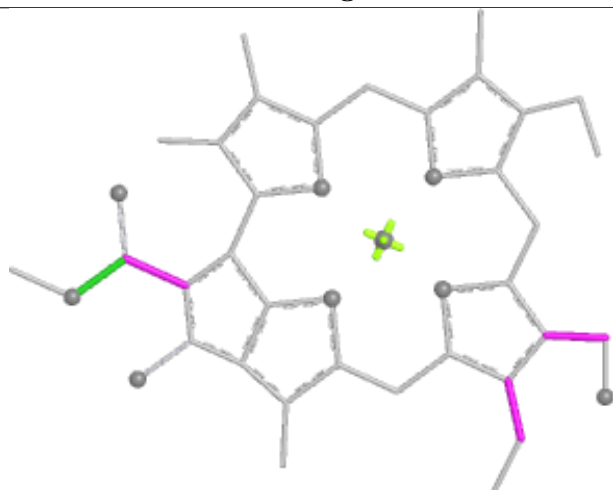
Ligand CHL R 613



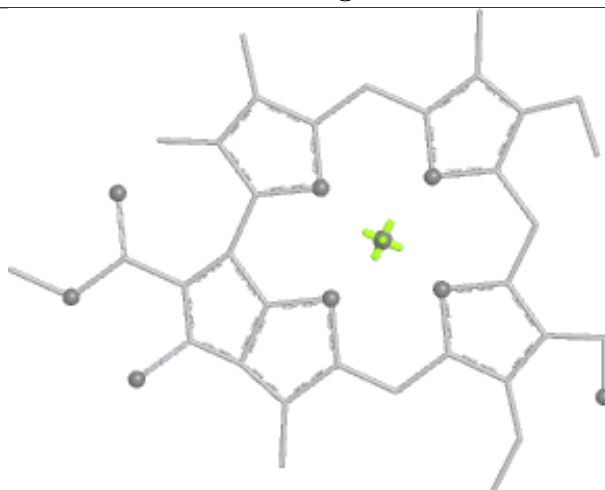
Bond lengths



Bond angles

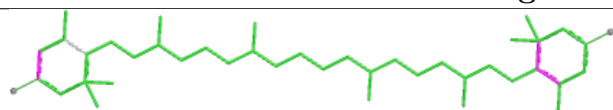


Torsions

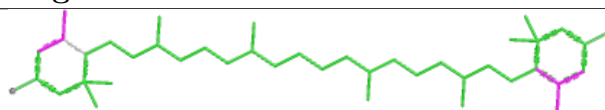


Rings

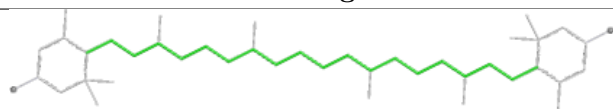
Ligand LUT g 616



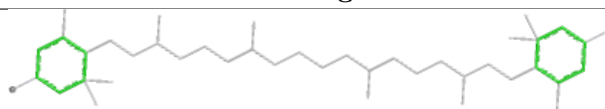
Bond lengths



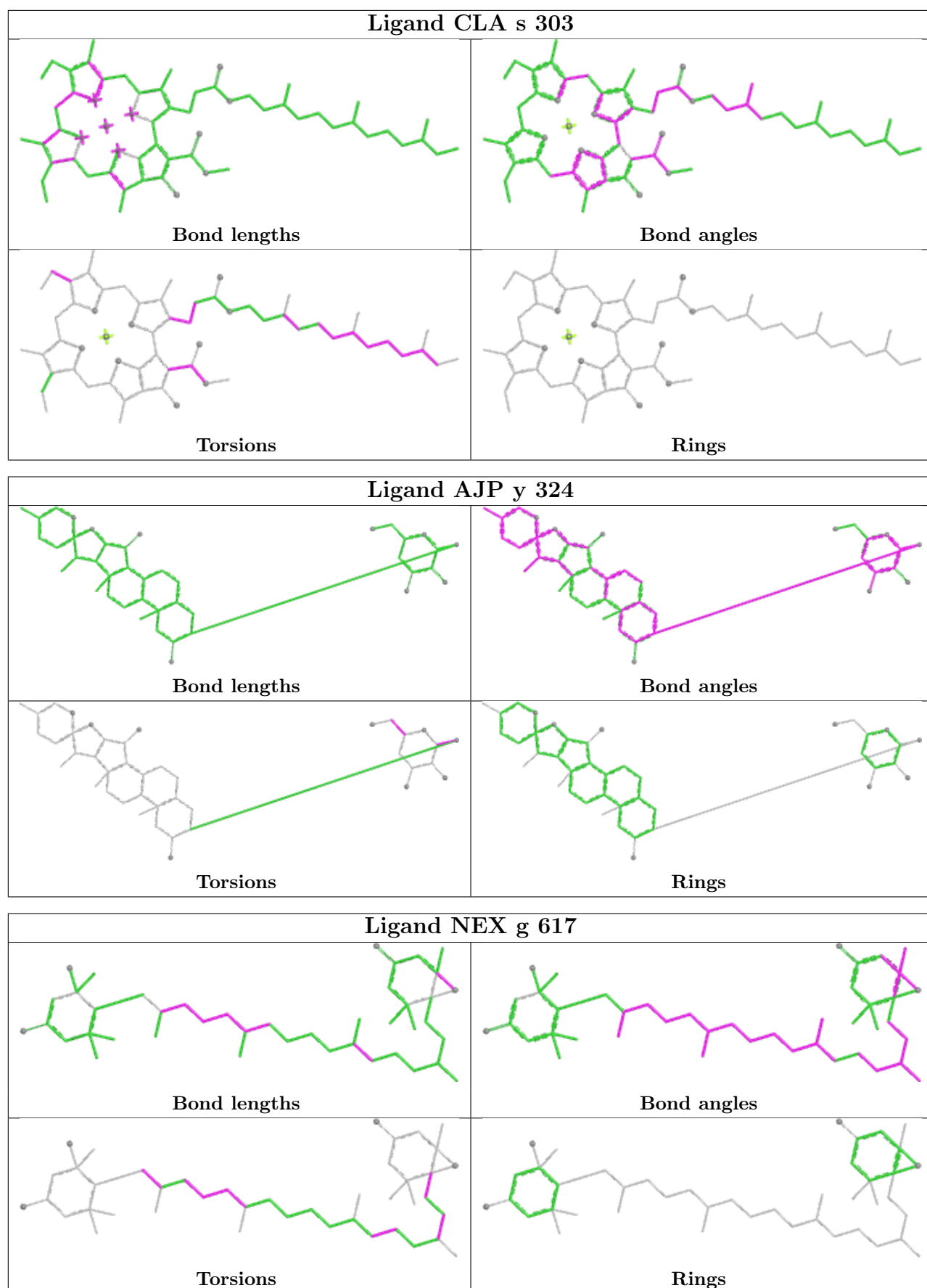
Bond angles

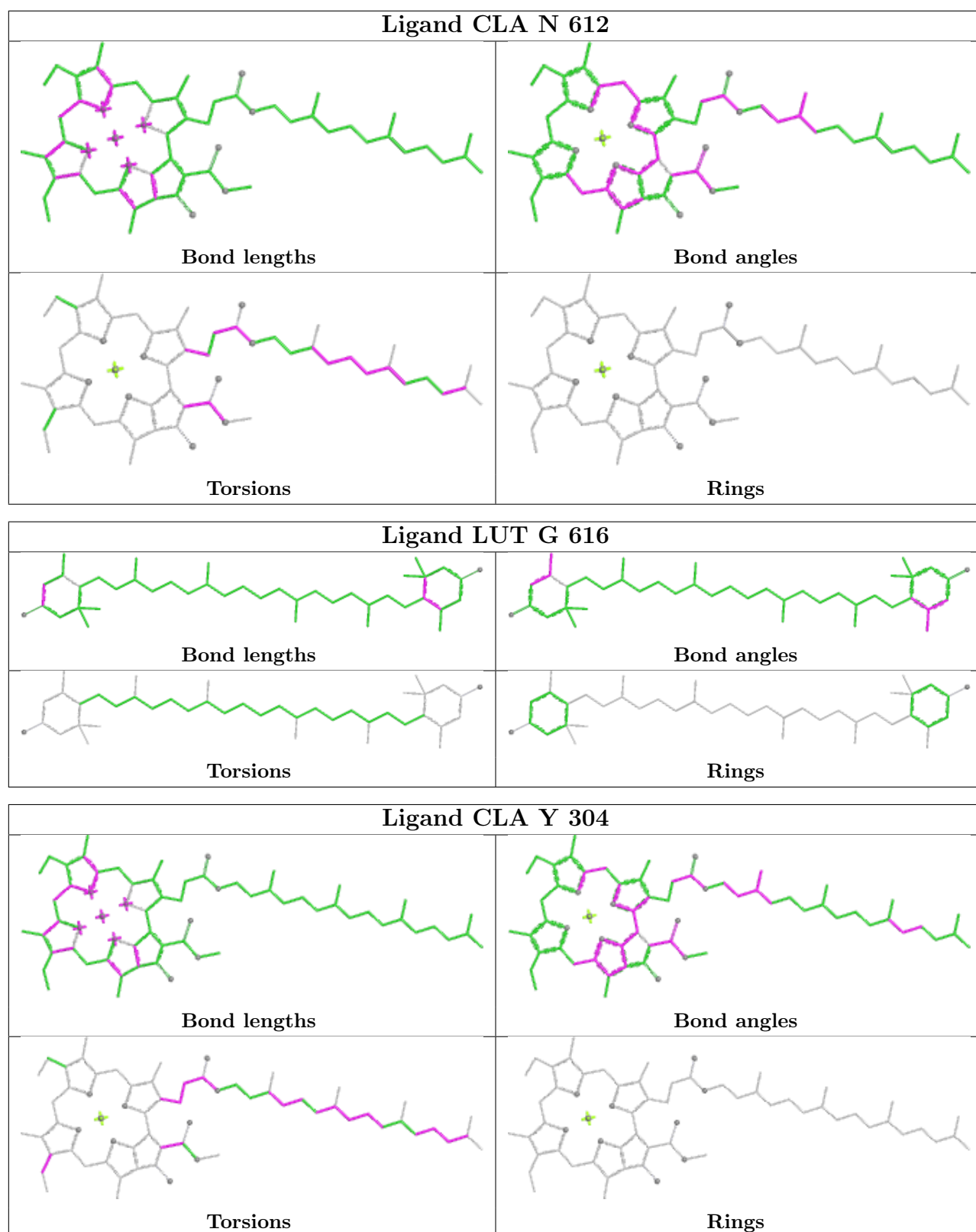


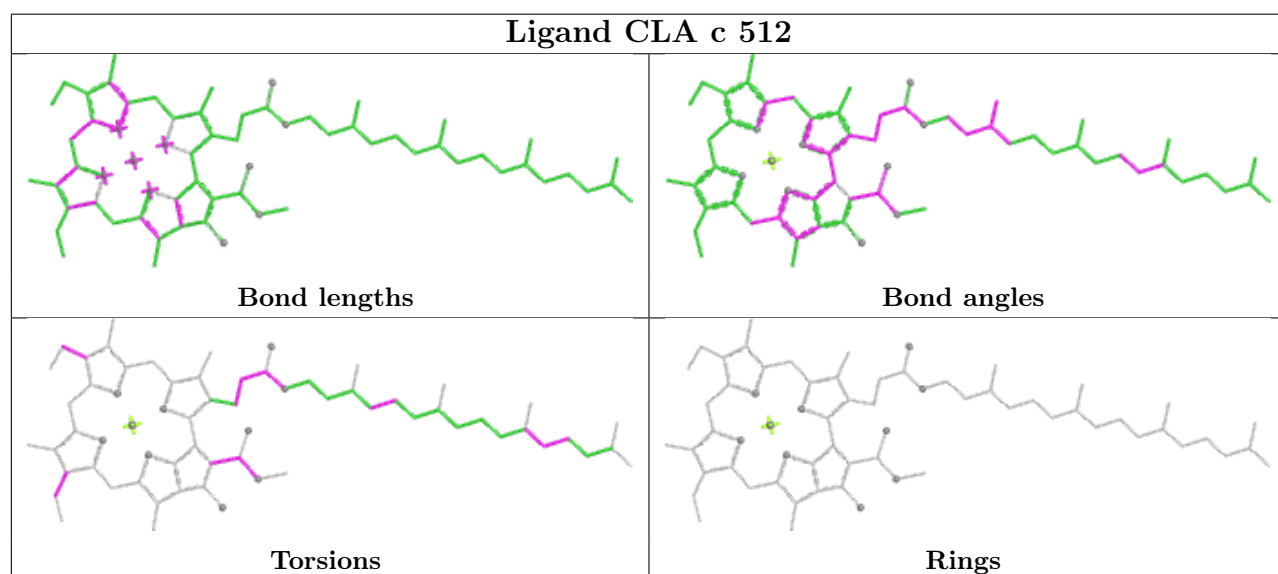
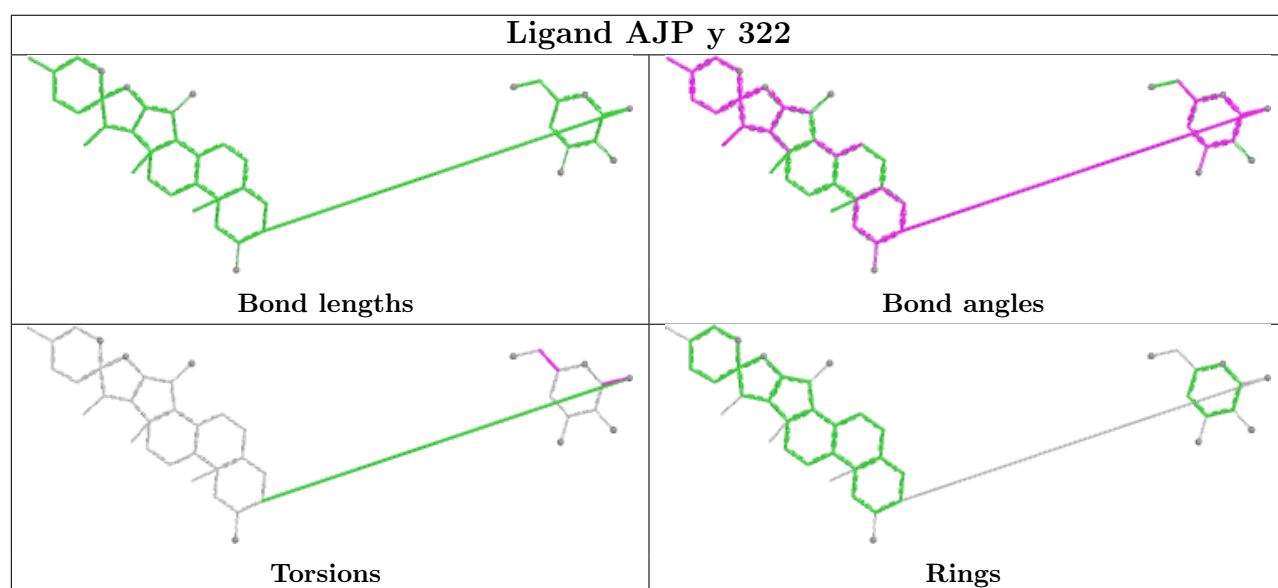
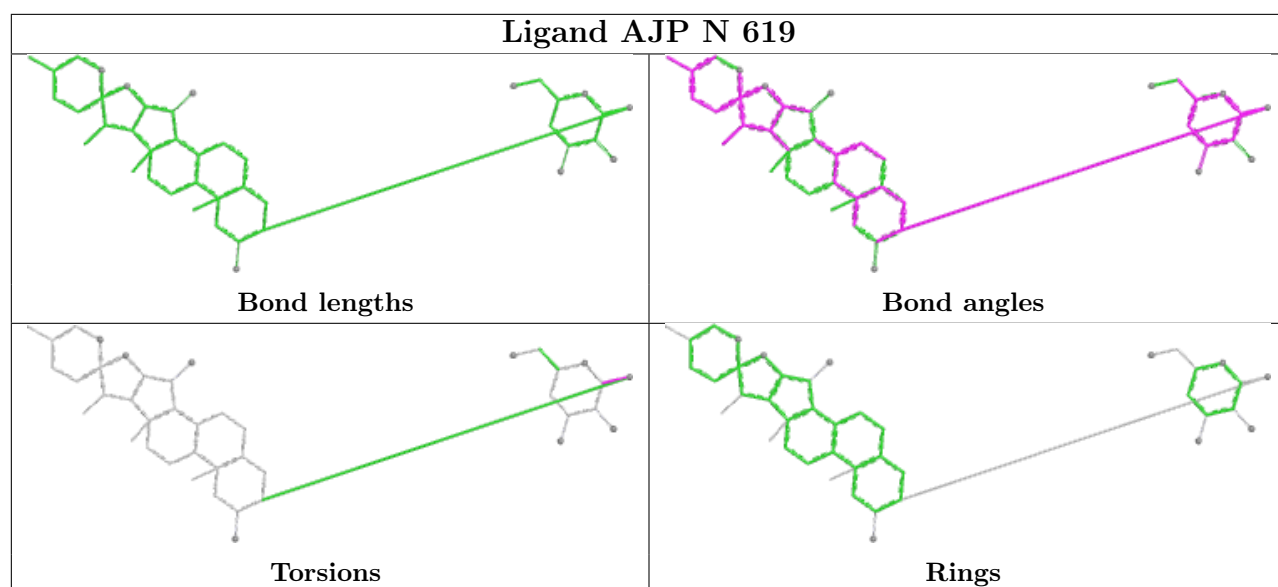
Torsions

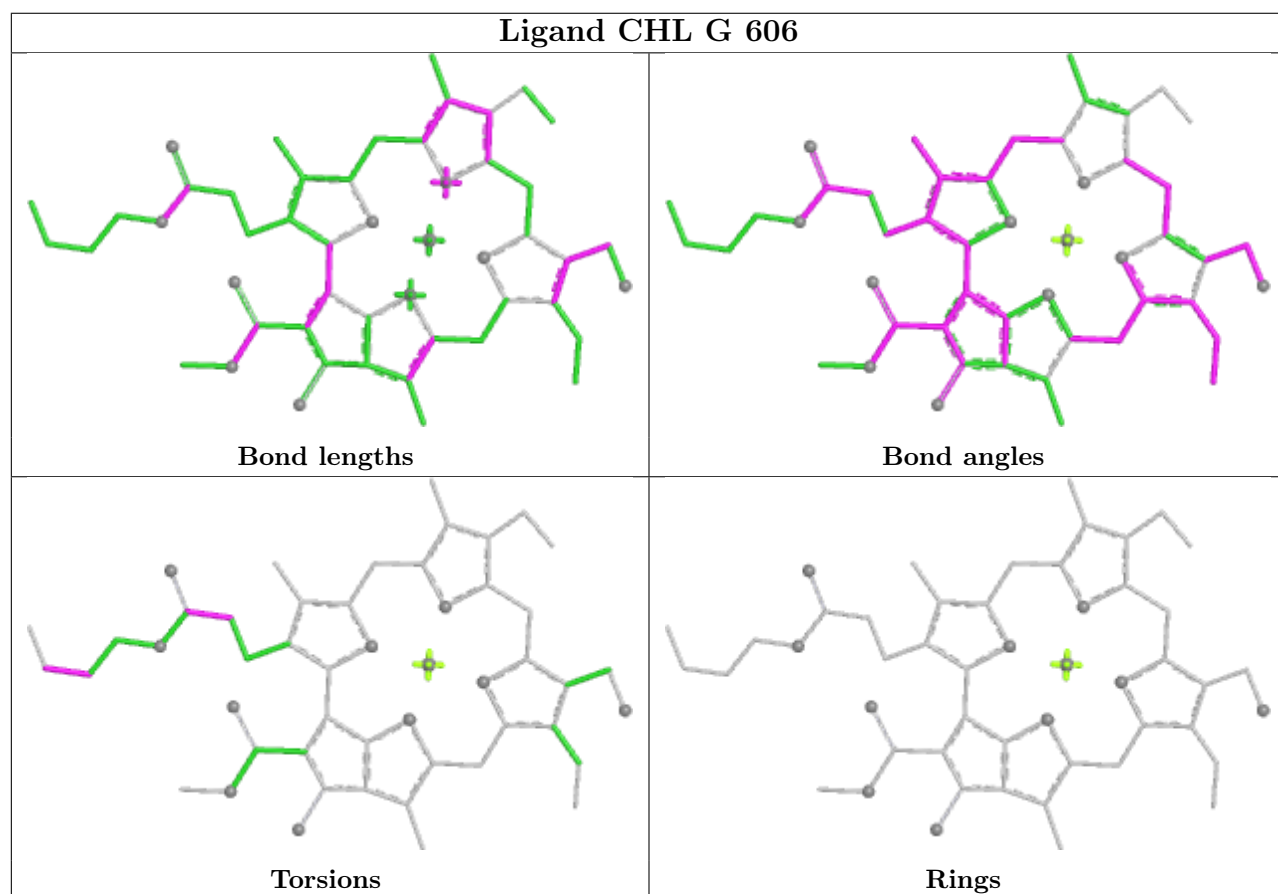
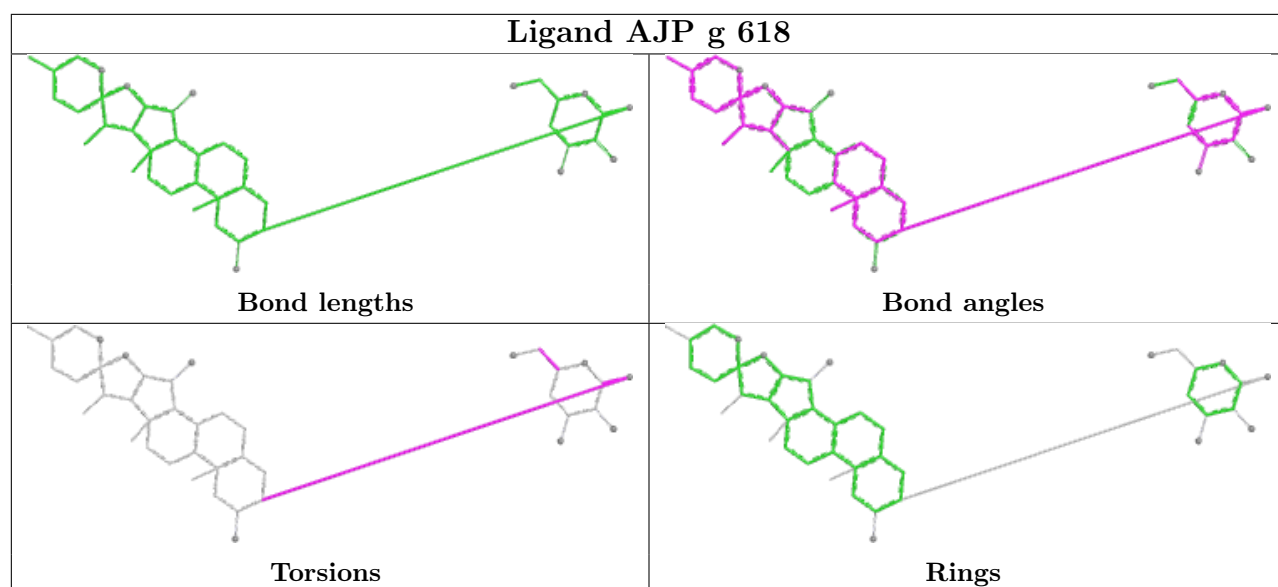


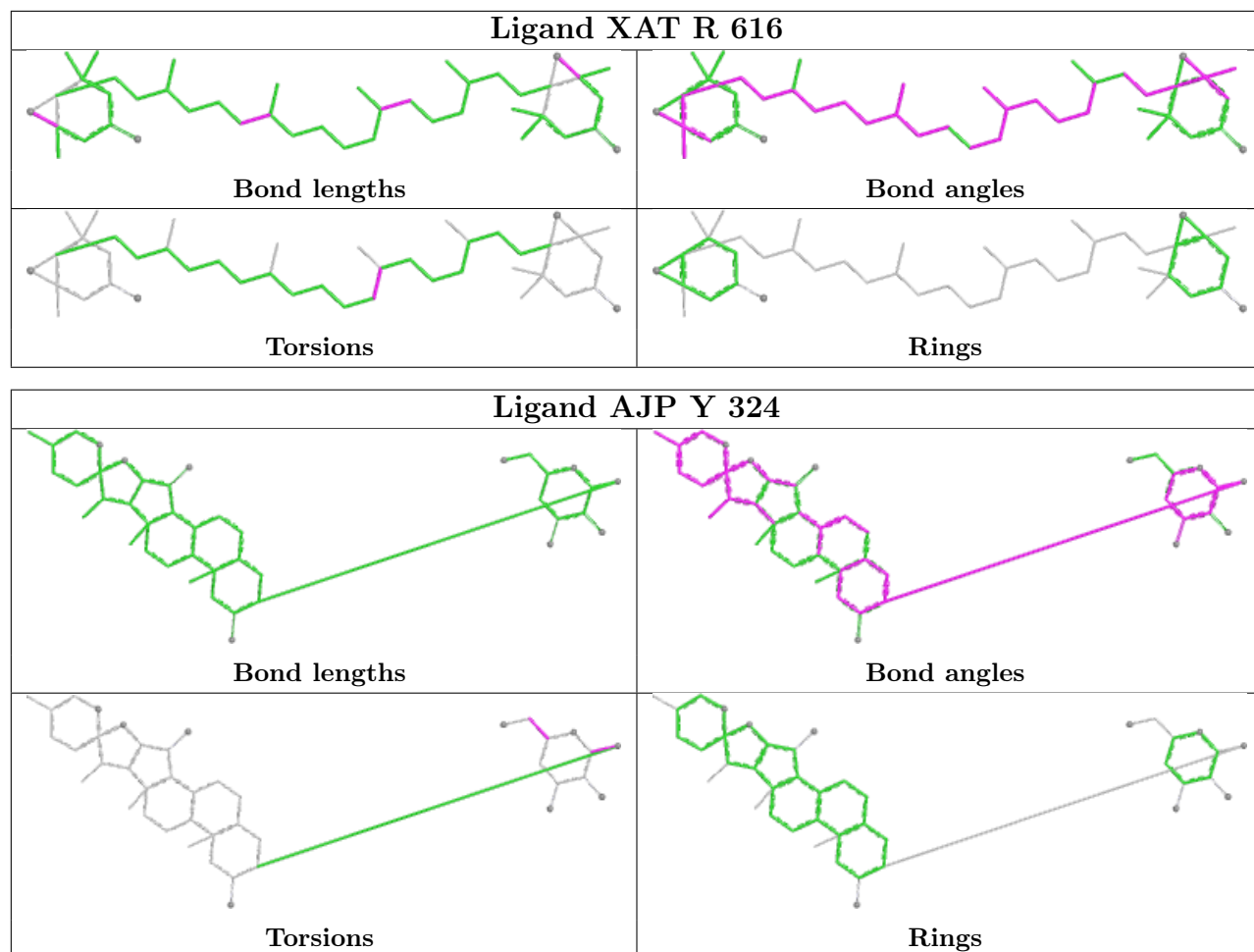
Rings



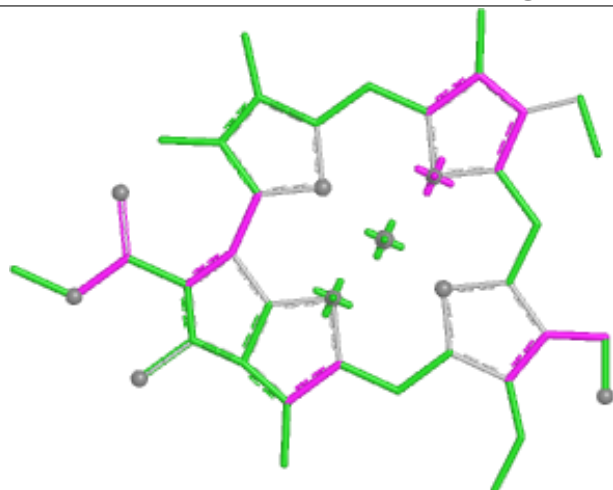




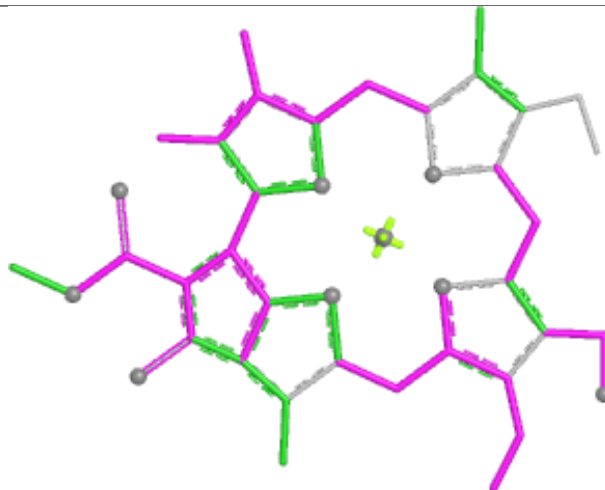




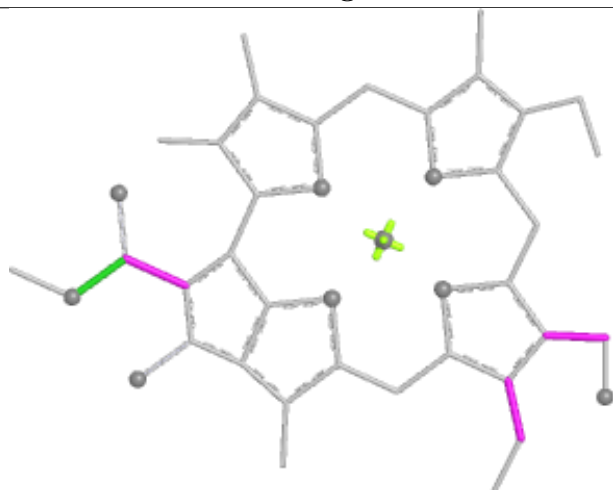
Ligand CHL r 613



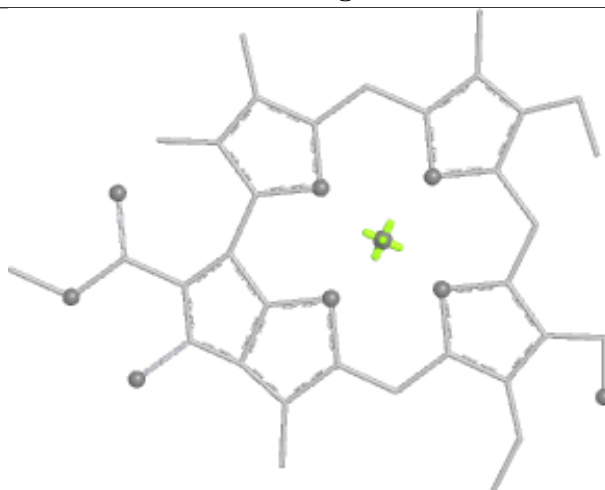
Bond lengths



Bond angles

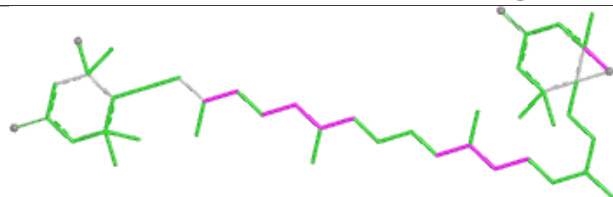


Torsions

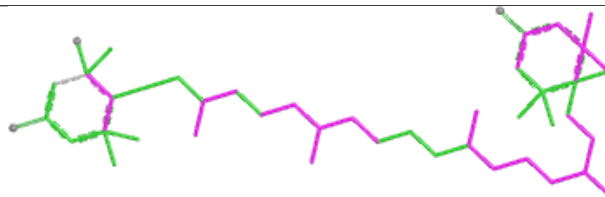


Rings

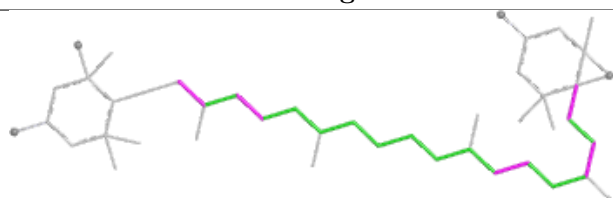
Ligand NEX Y 318



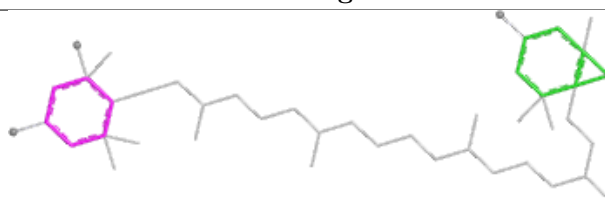
Bond lengths



Bond angles

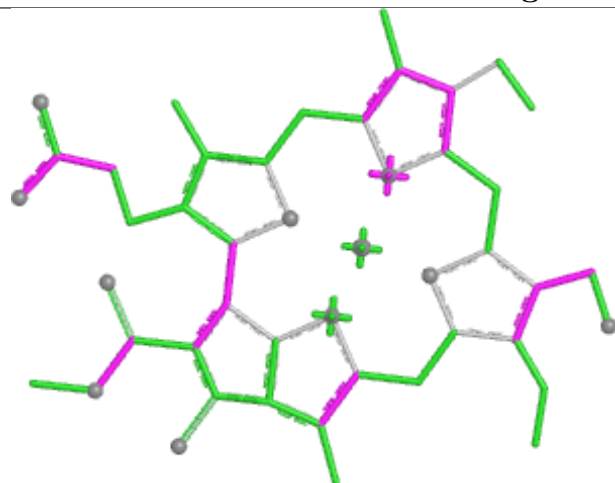


Torsions

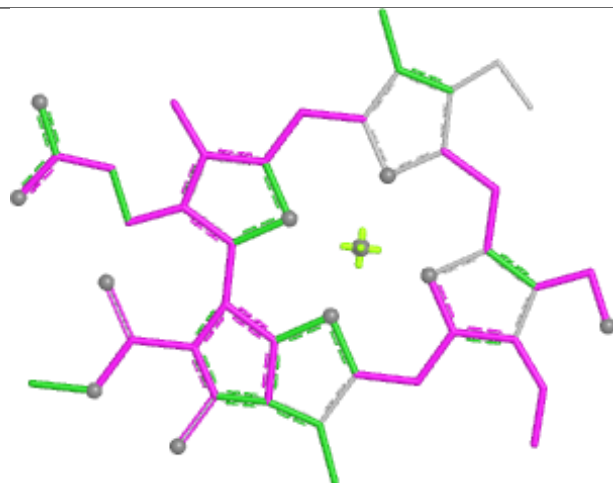


Rings

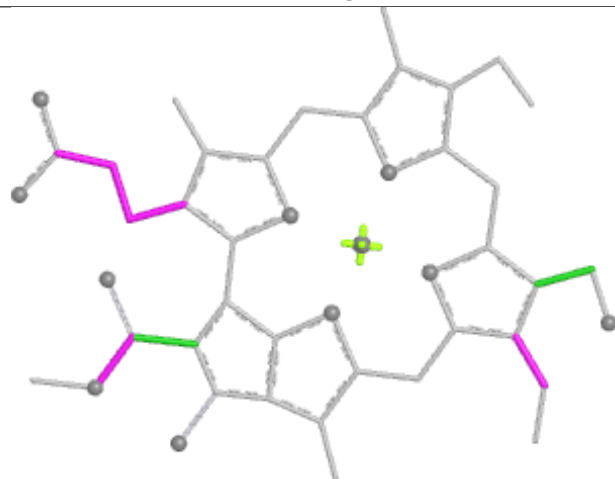
Ligand CHL r 606



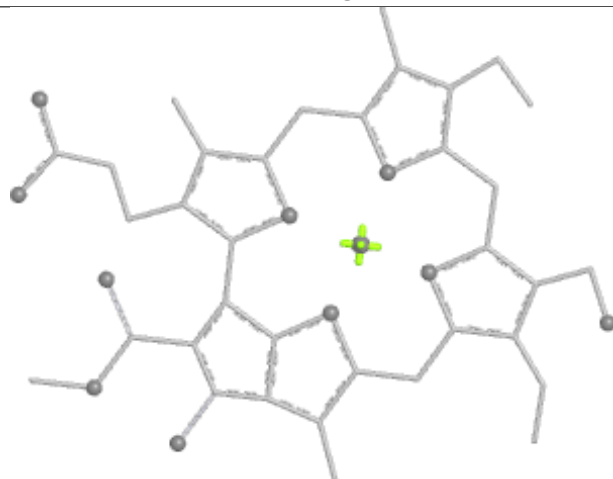
Bond lengths



Bond angles



Torsions

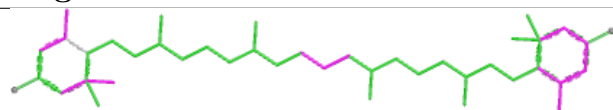


Rings

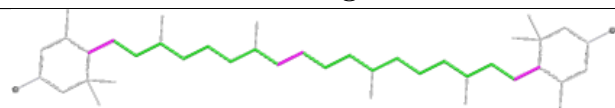
Ligand LUT g 615



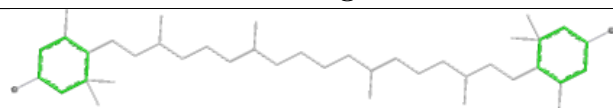
Bond lengths



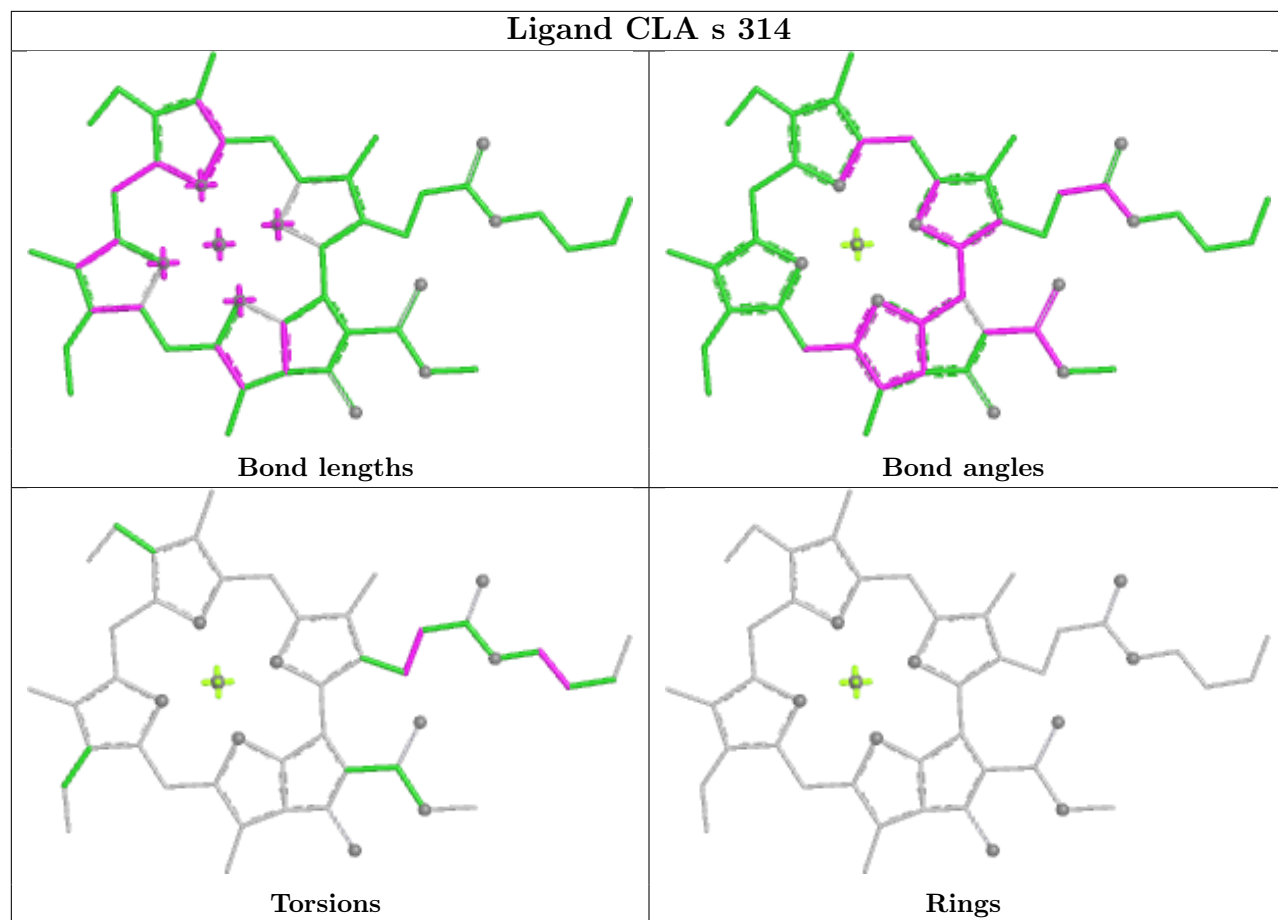
Bond angles



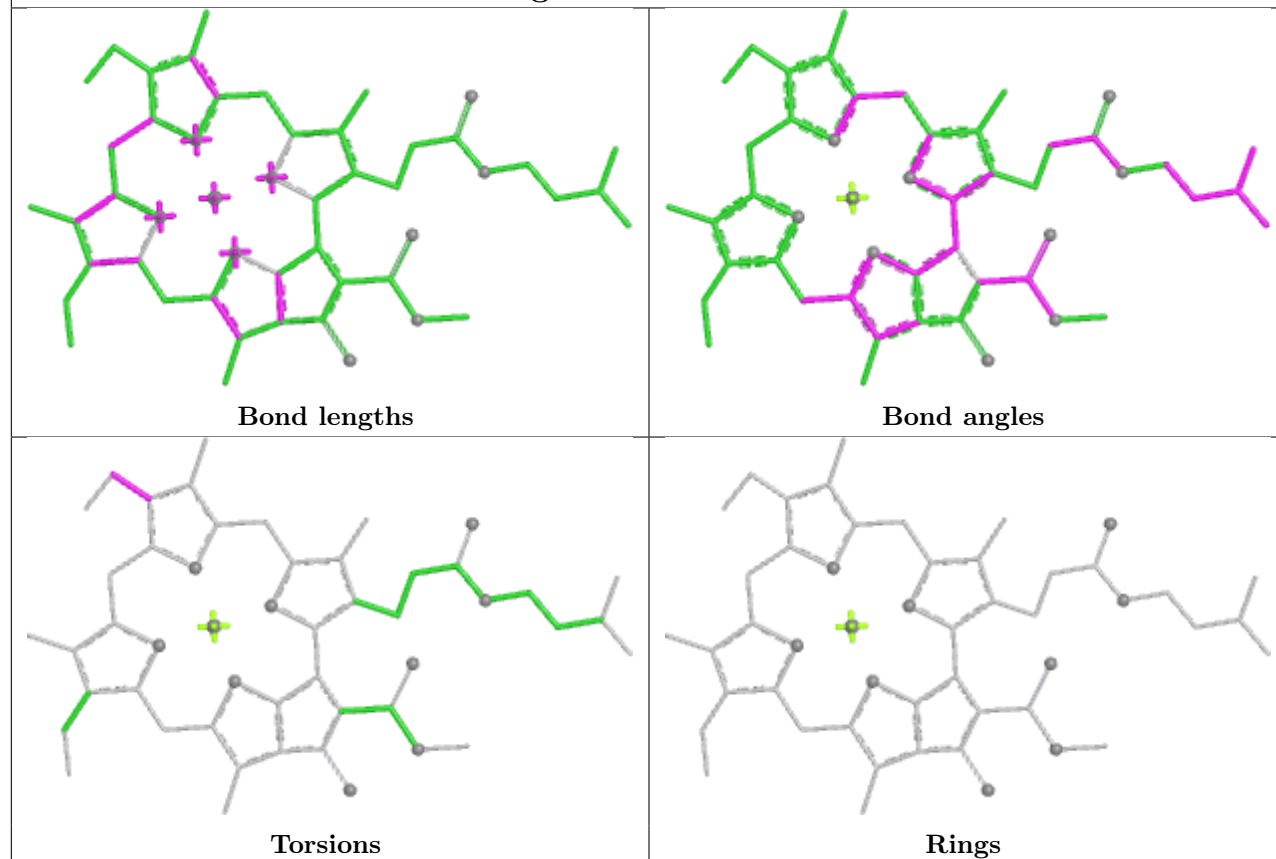
Torsions



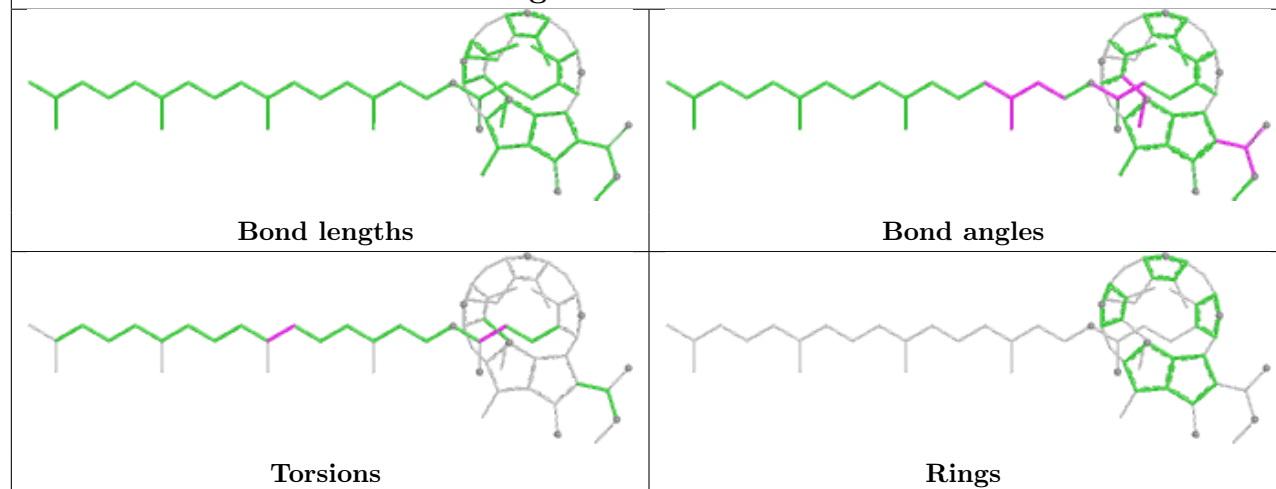
Rings

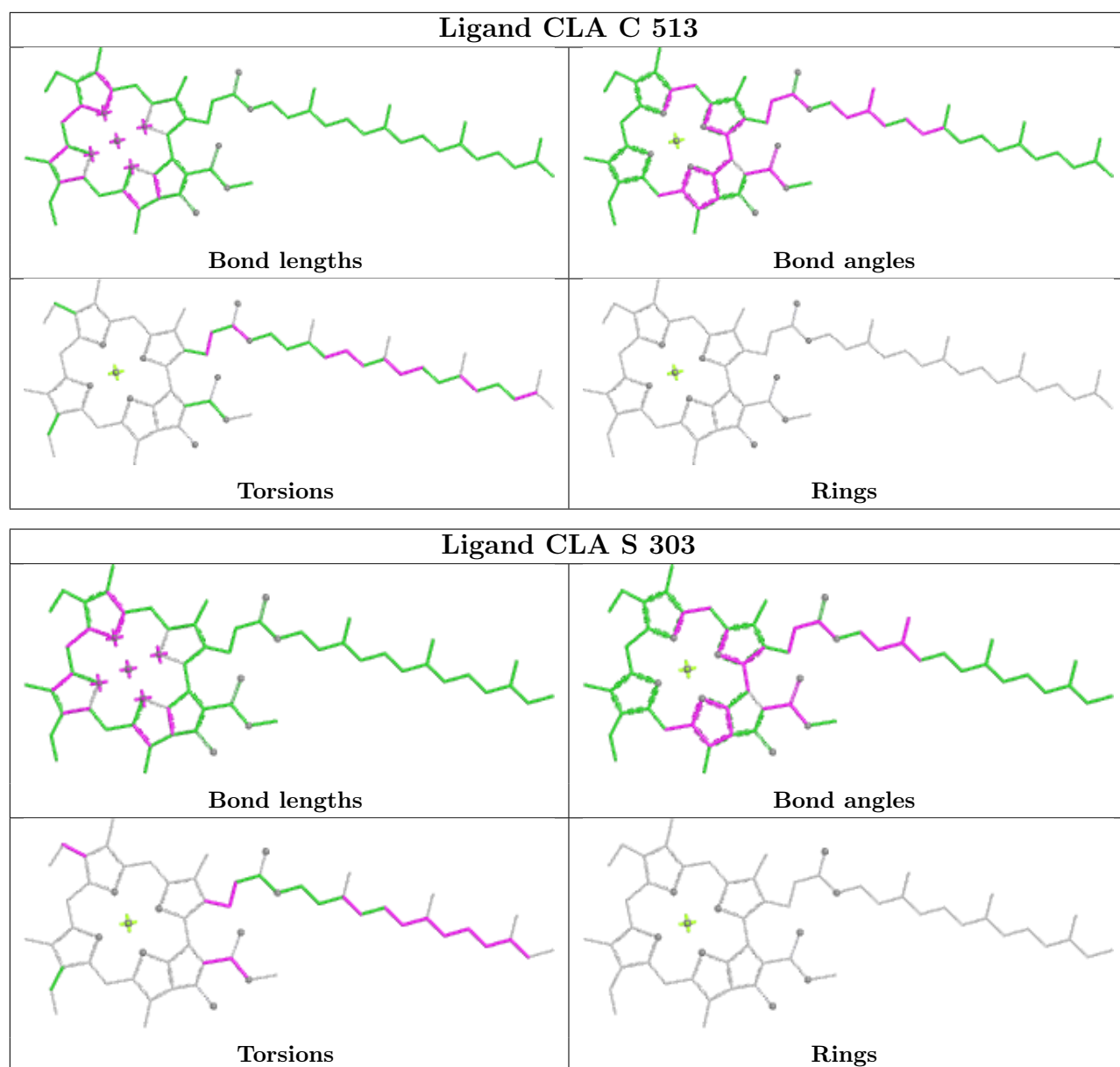


Ligand CLA D 401

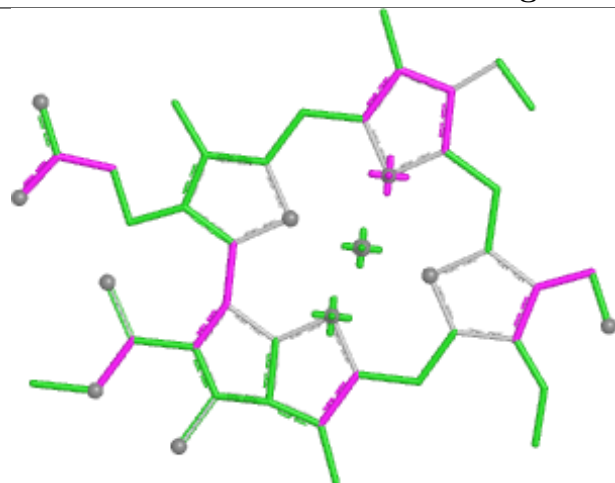


Ligand PHO A 404

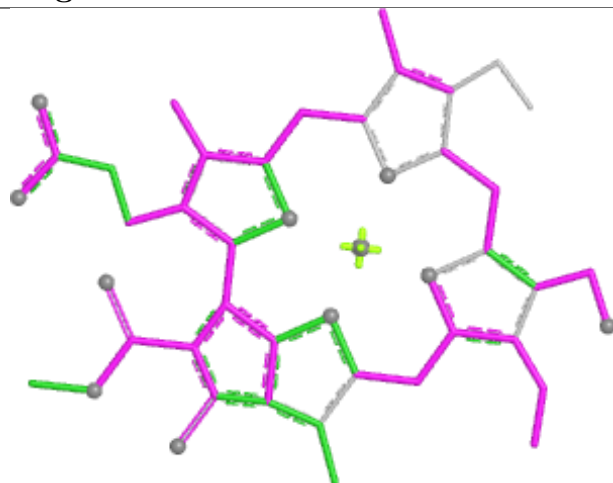




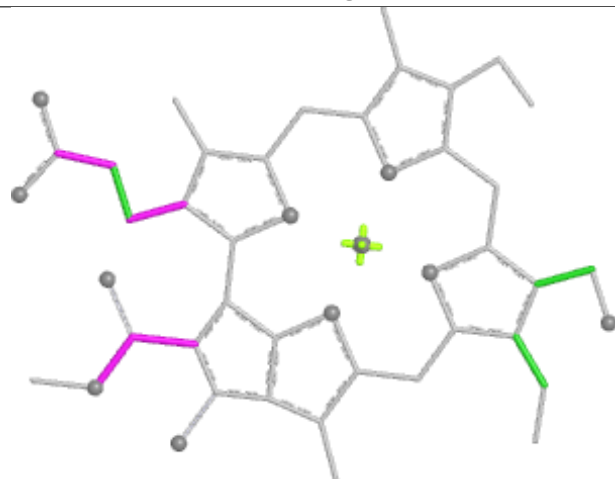
Ligand CHL g 607



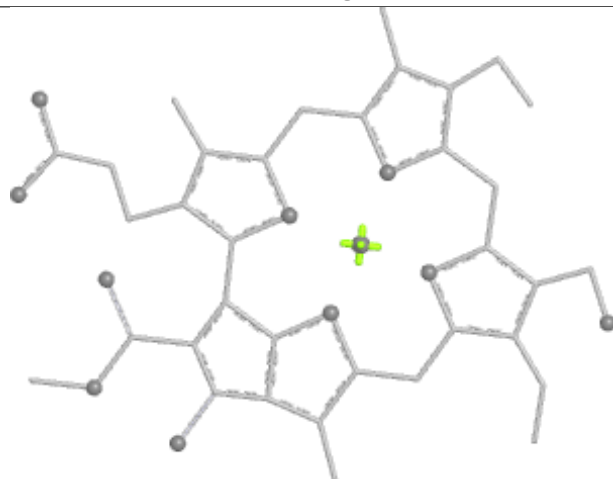
Bond lengths



Bond angles

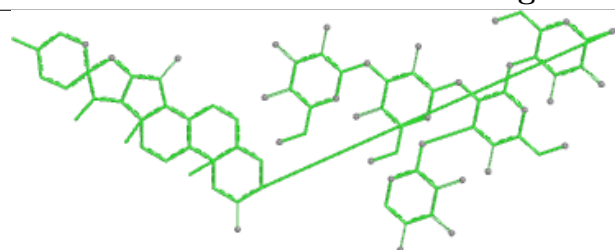


Torsions

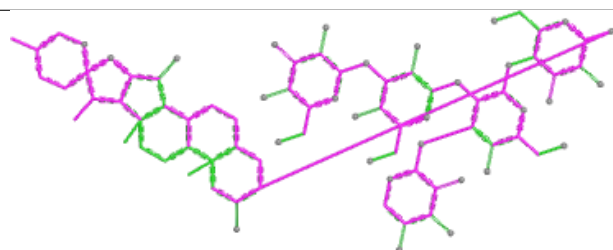


Rings

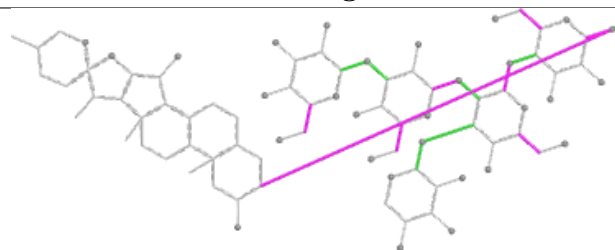
Ligand AJP A 412



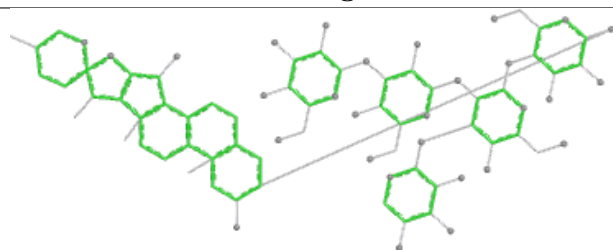
Bond lengths



Bond angles

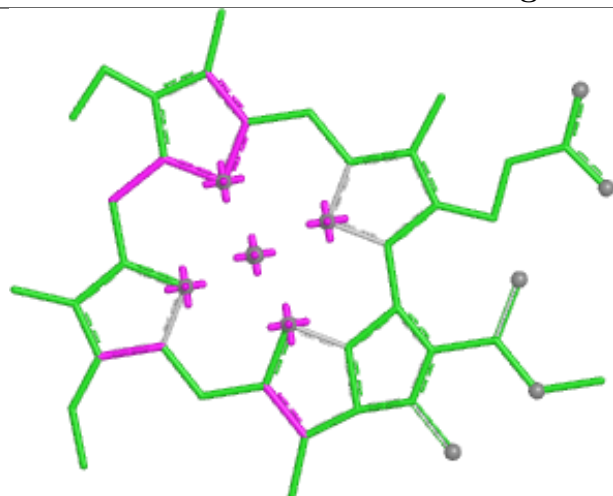


Torsions

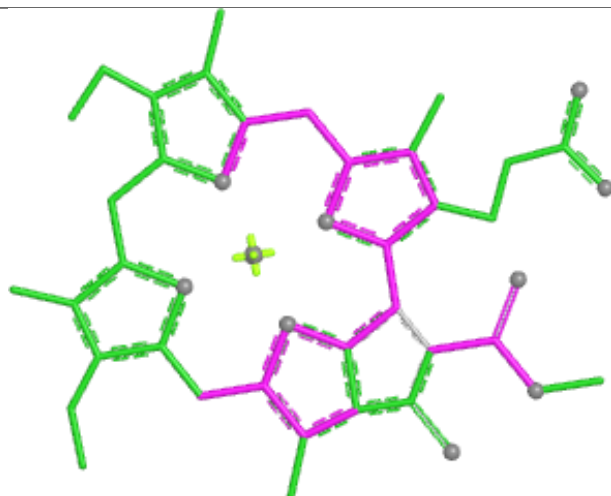


Rings

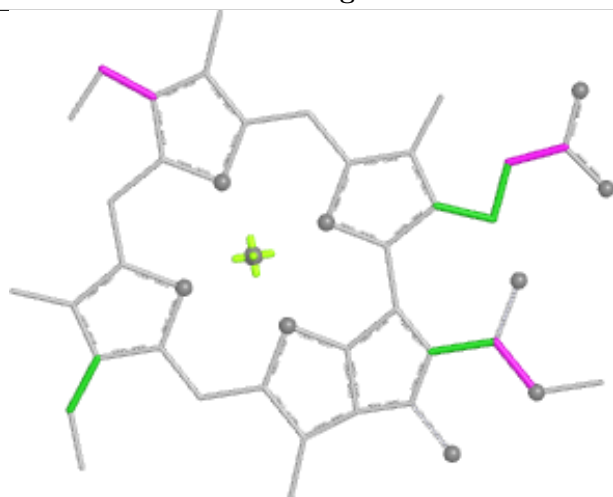
Ligand CLA s 309



Bond lengths



Bond angles

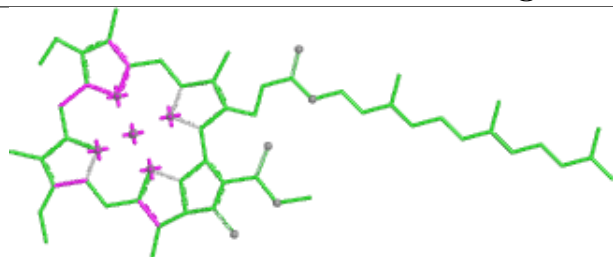


Torsions

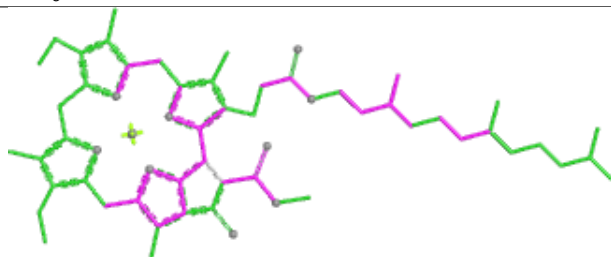


Rings

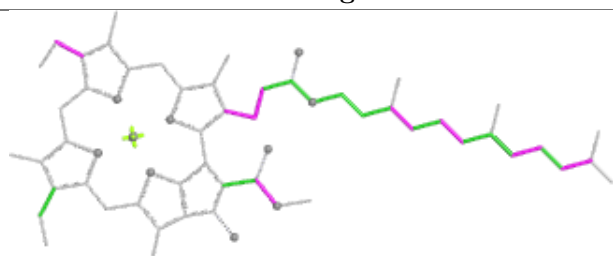
Ligand CLA y 311



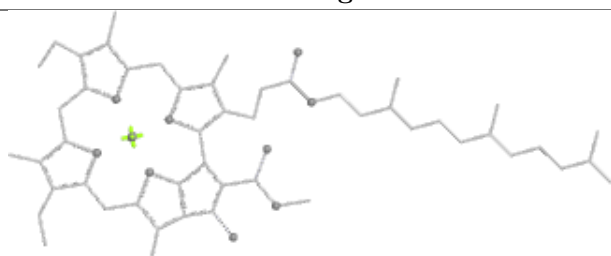
Bond lengths



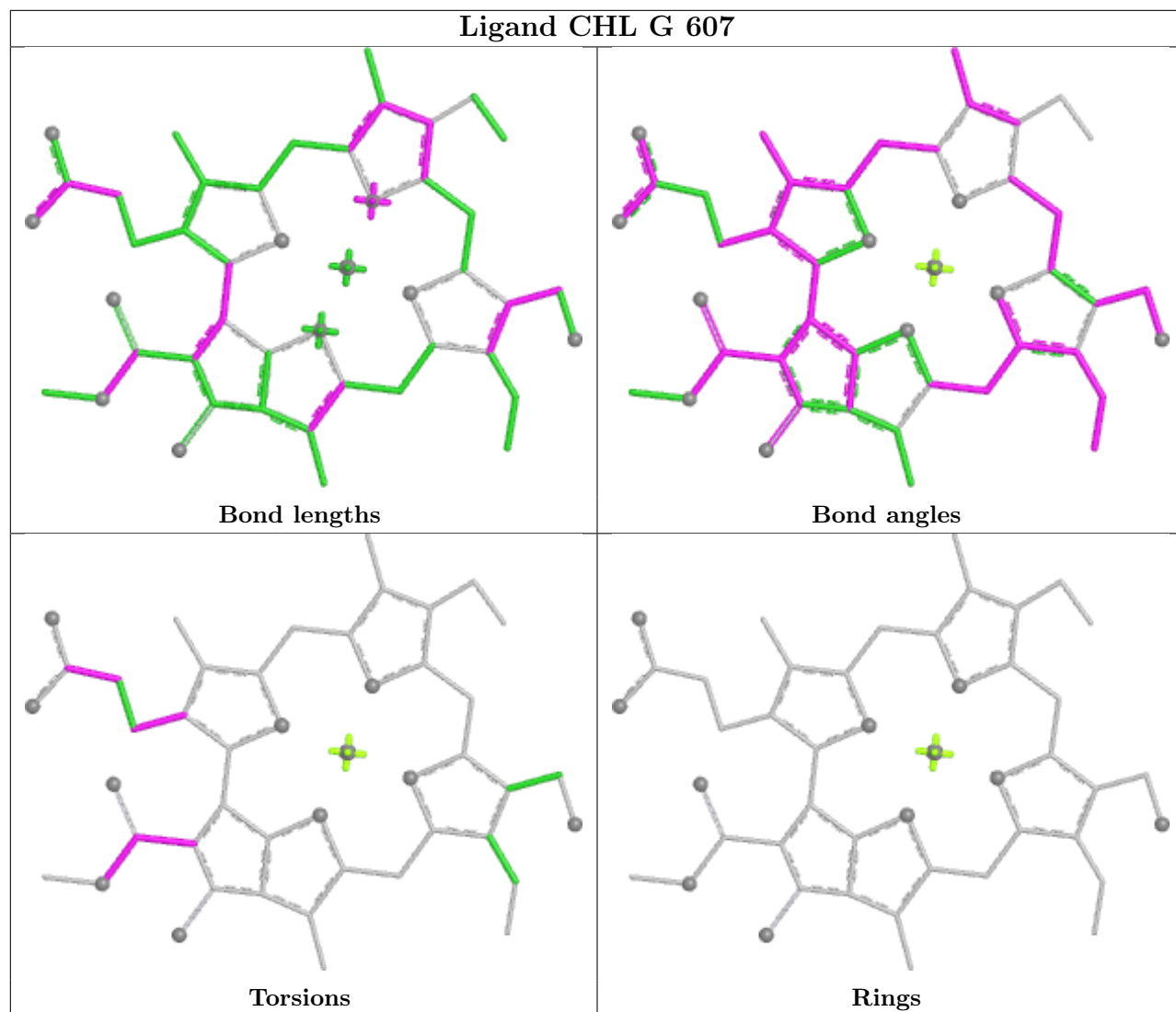
Bond angles



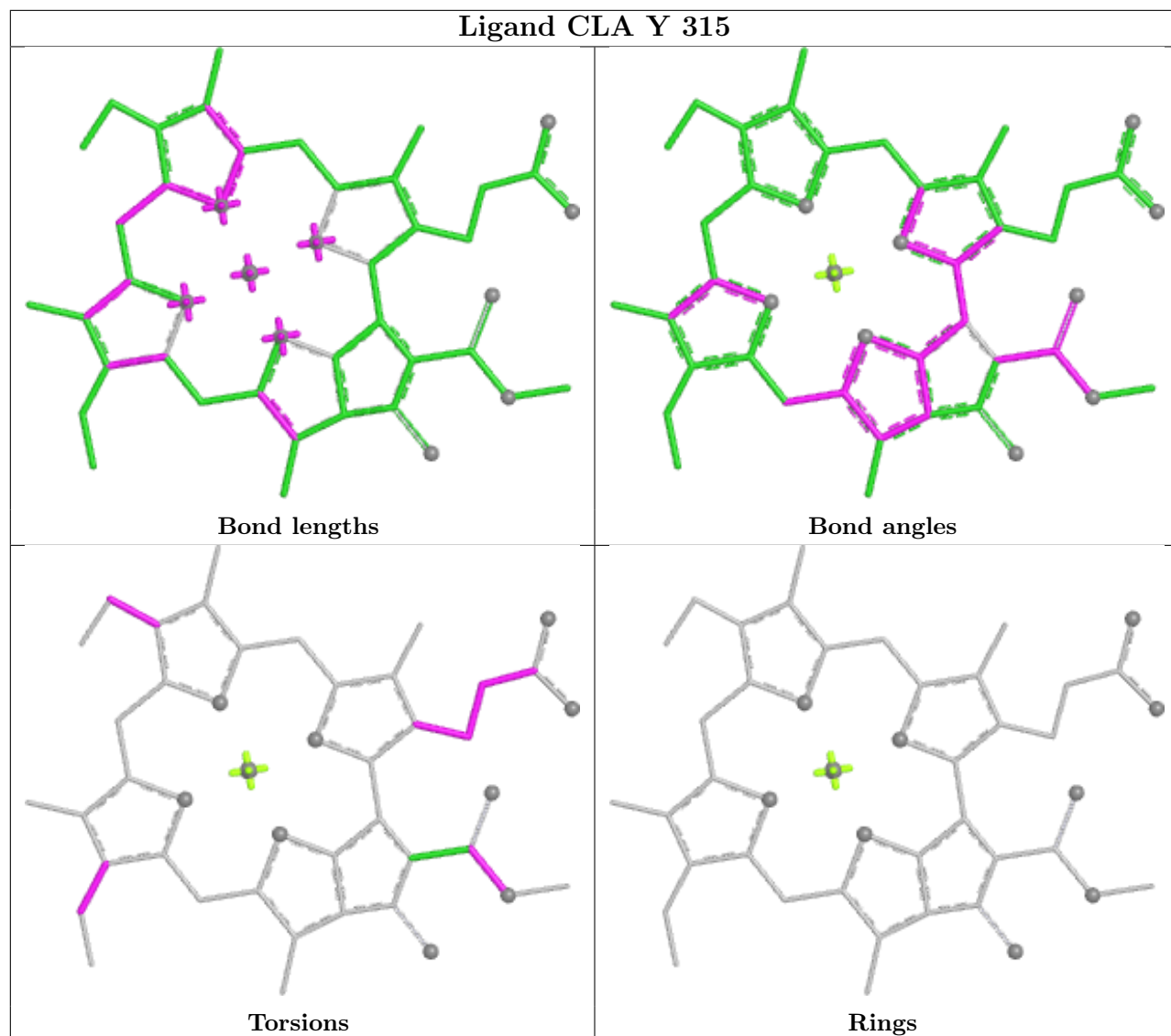
Torsions

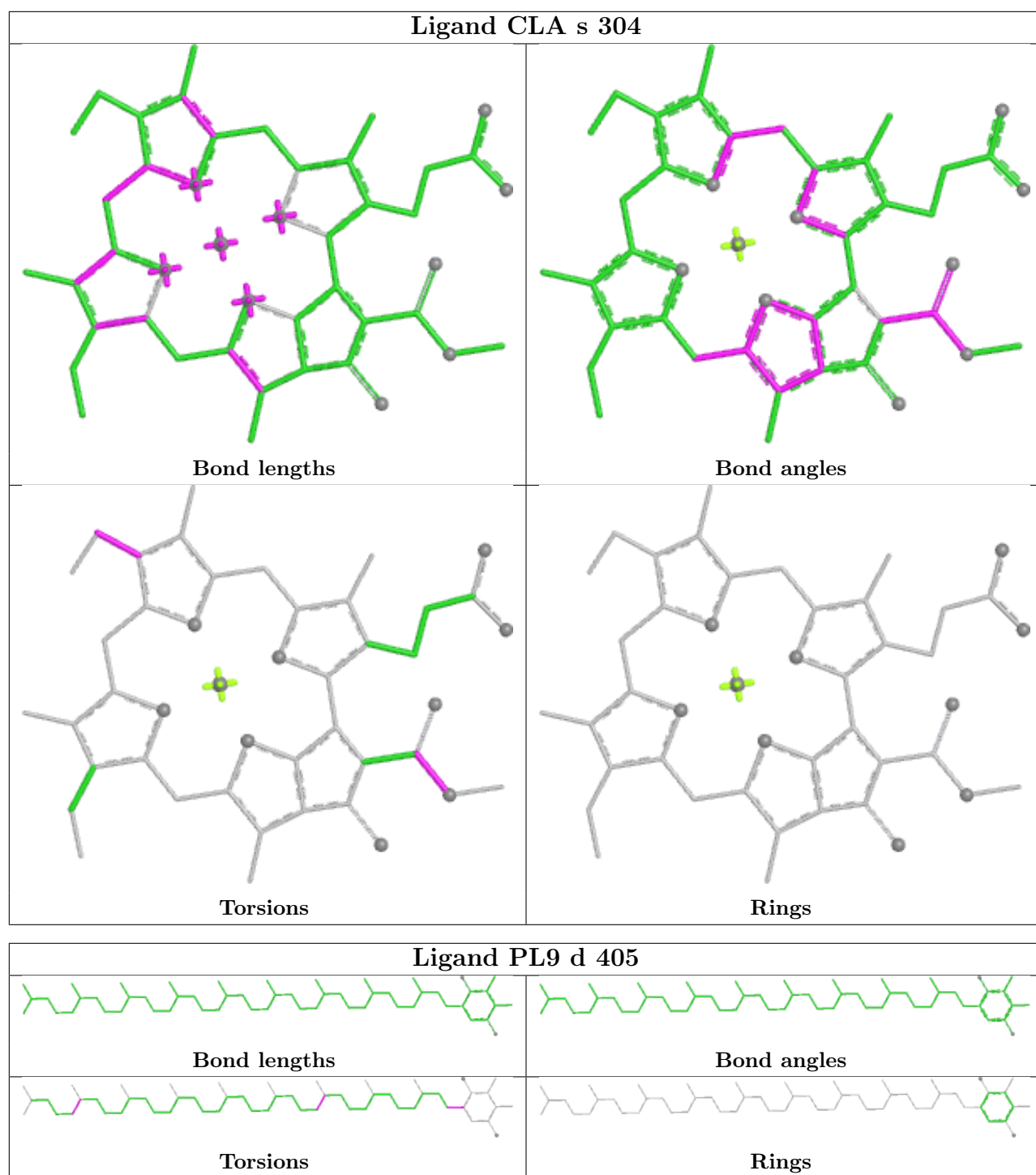


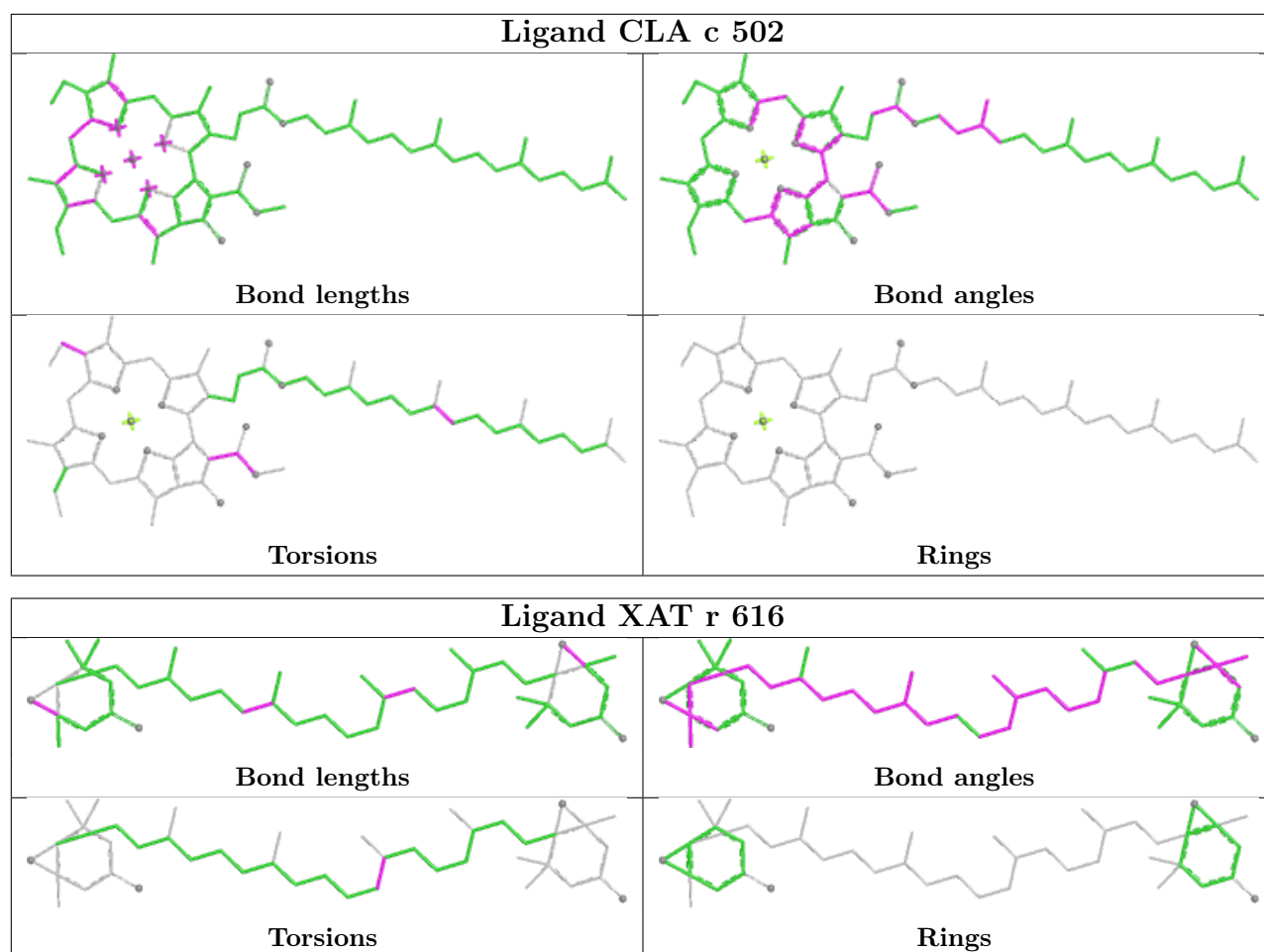
Rings



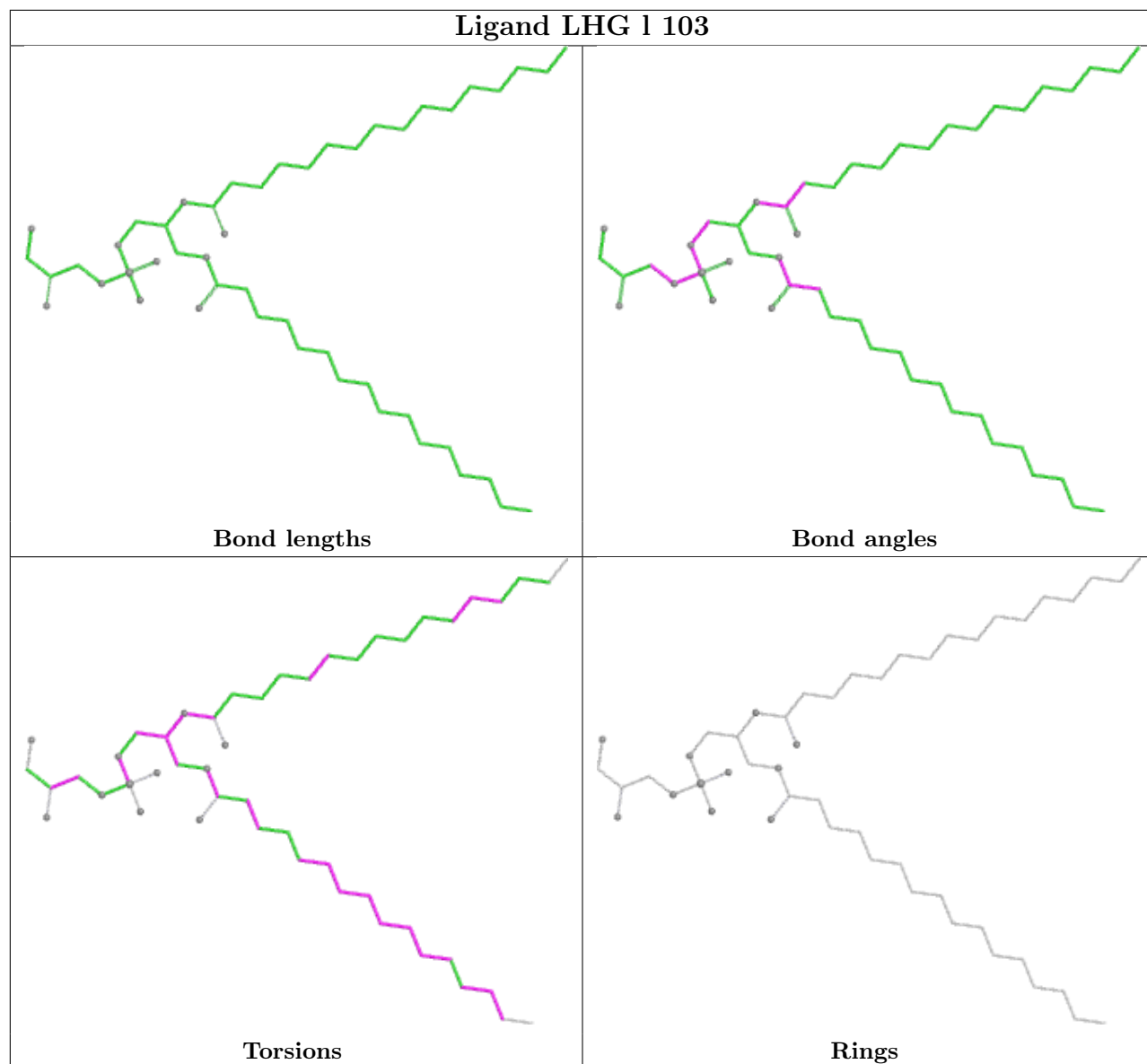
Ligand CLA Y 315



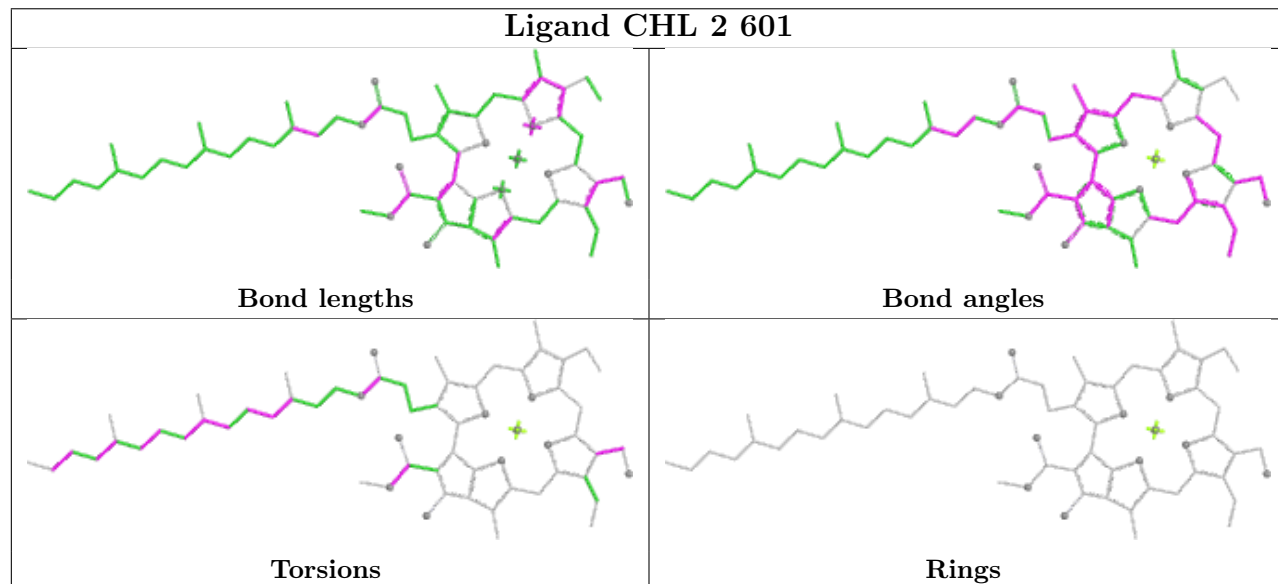


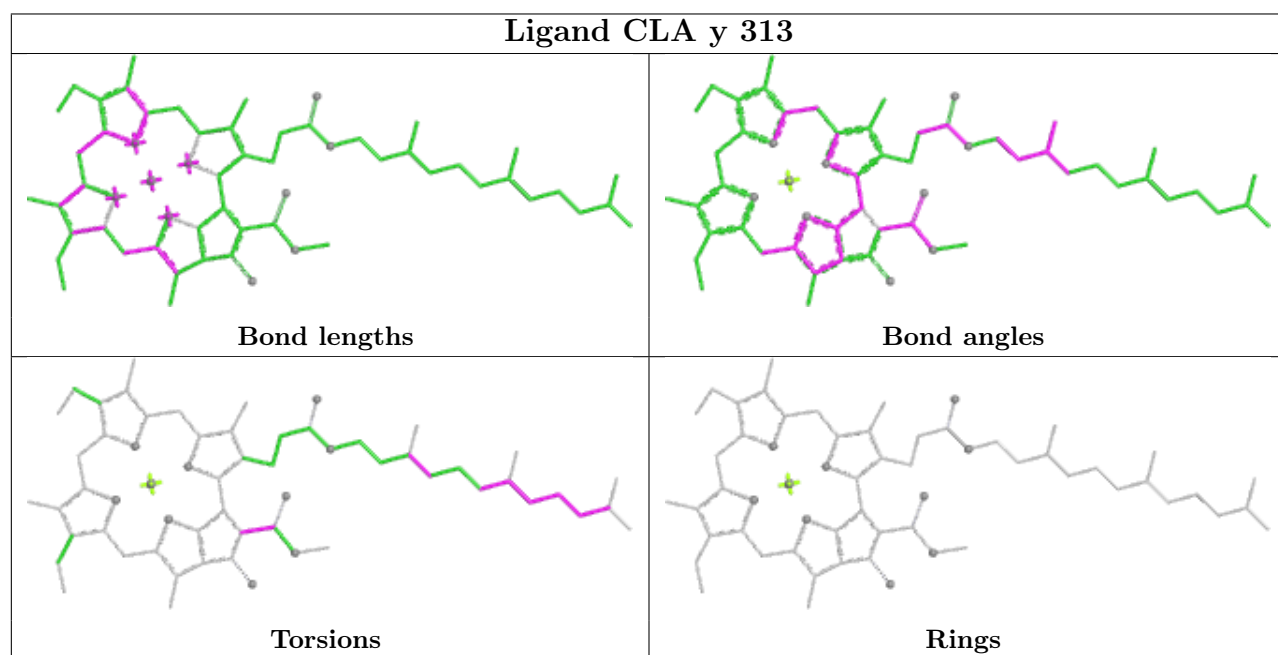
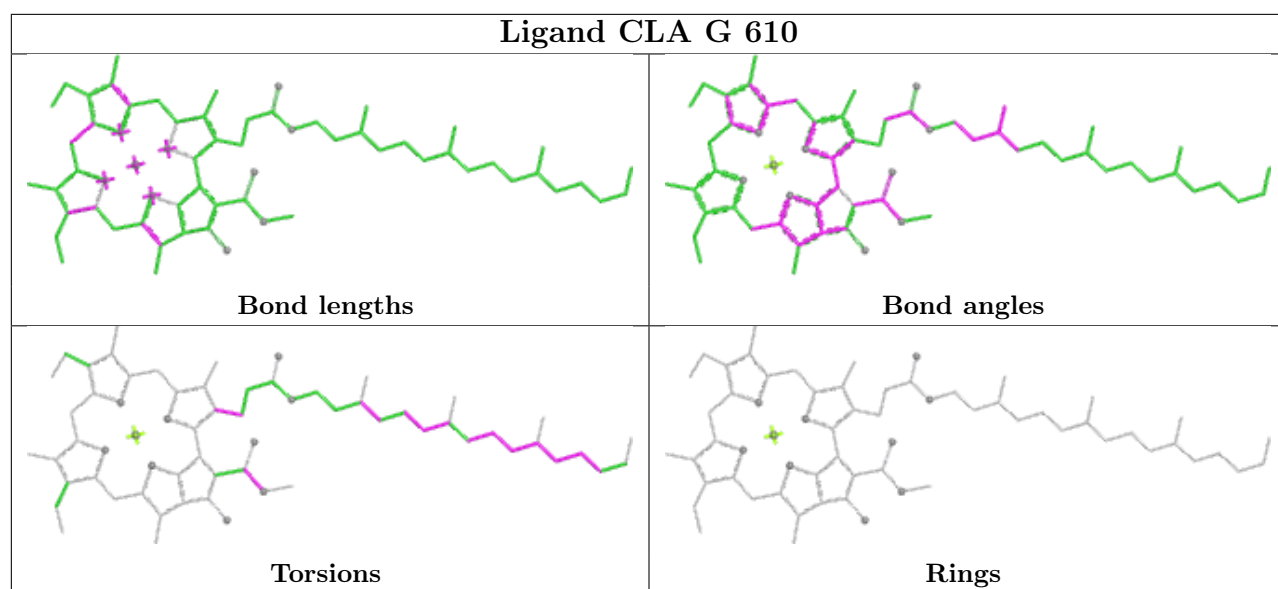


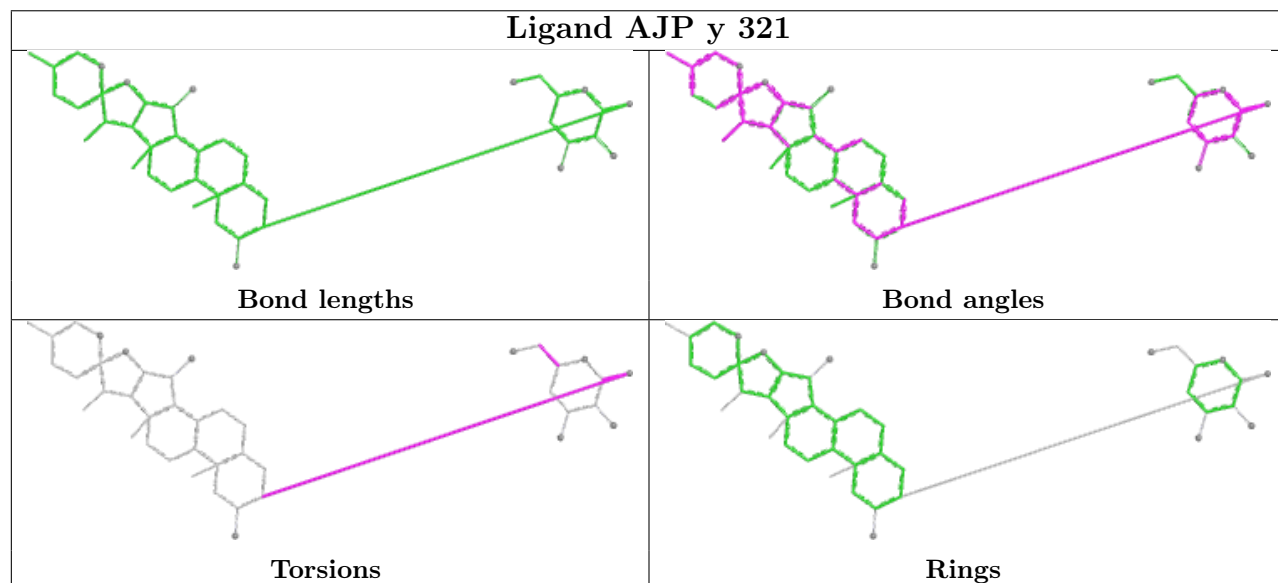
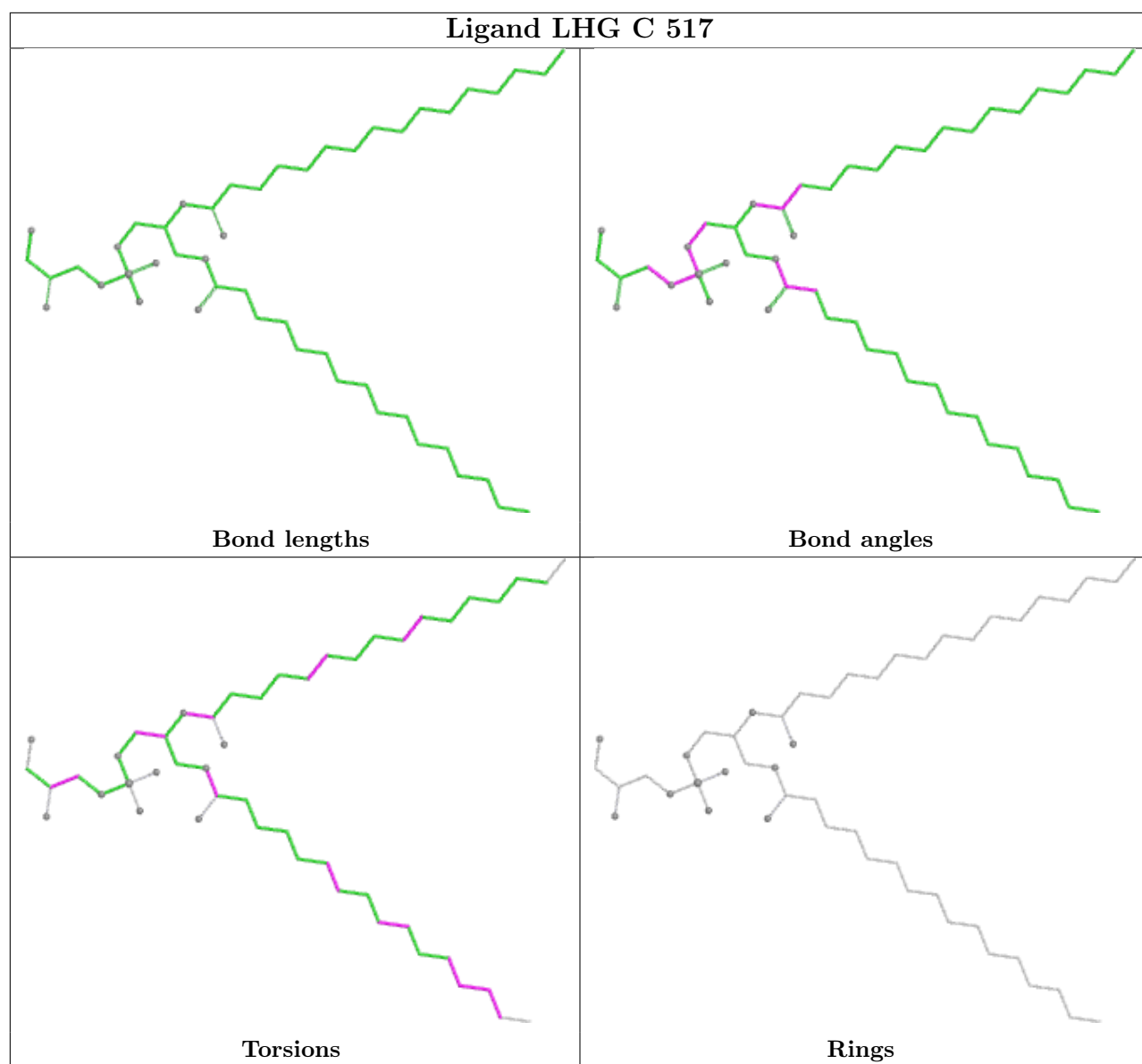
Ligand LHG 1 103

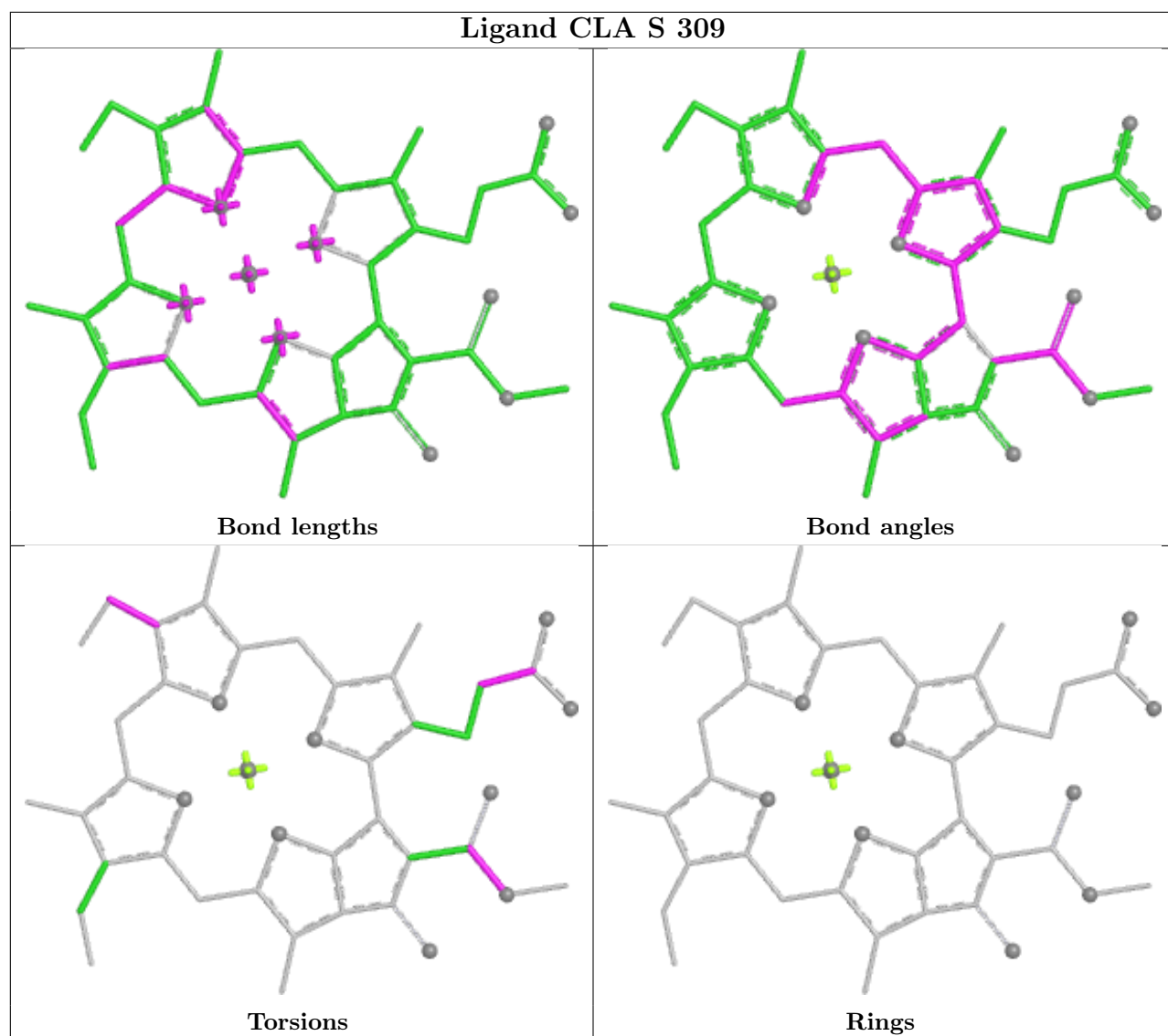
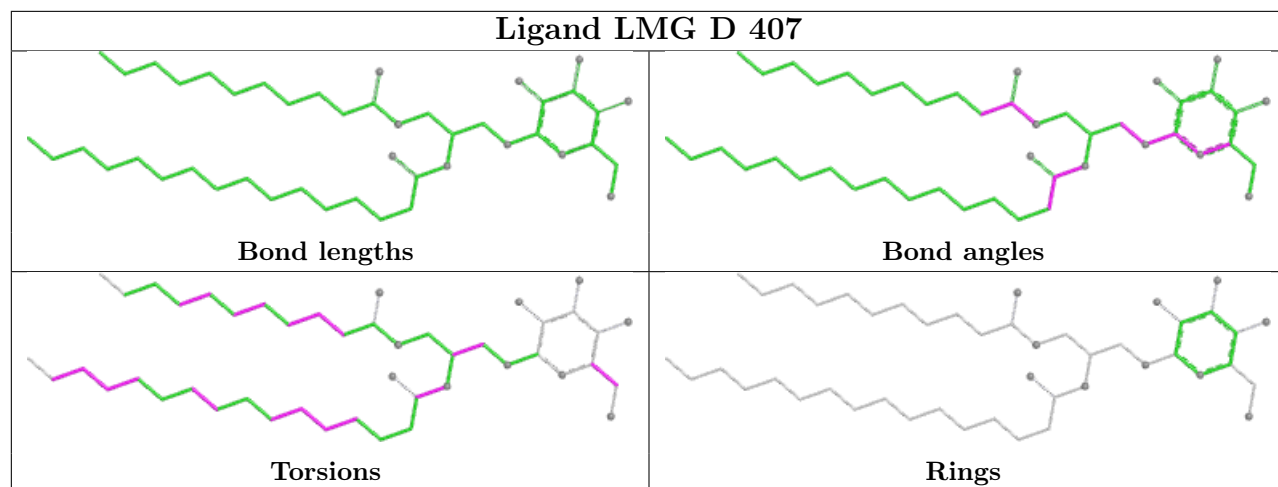


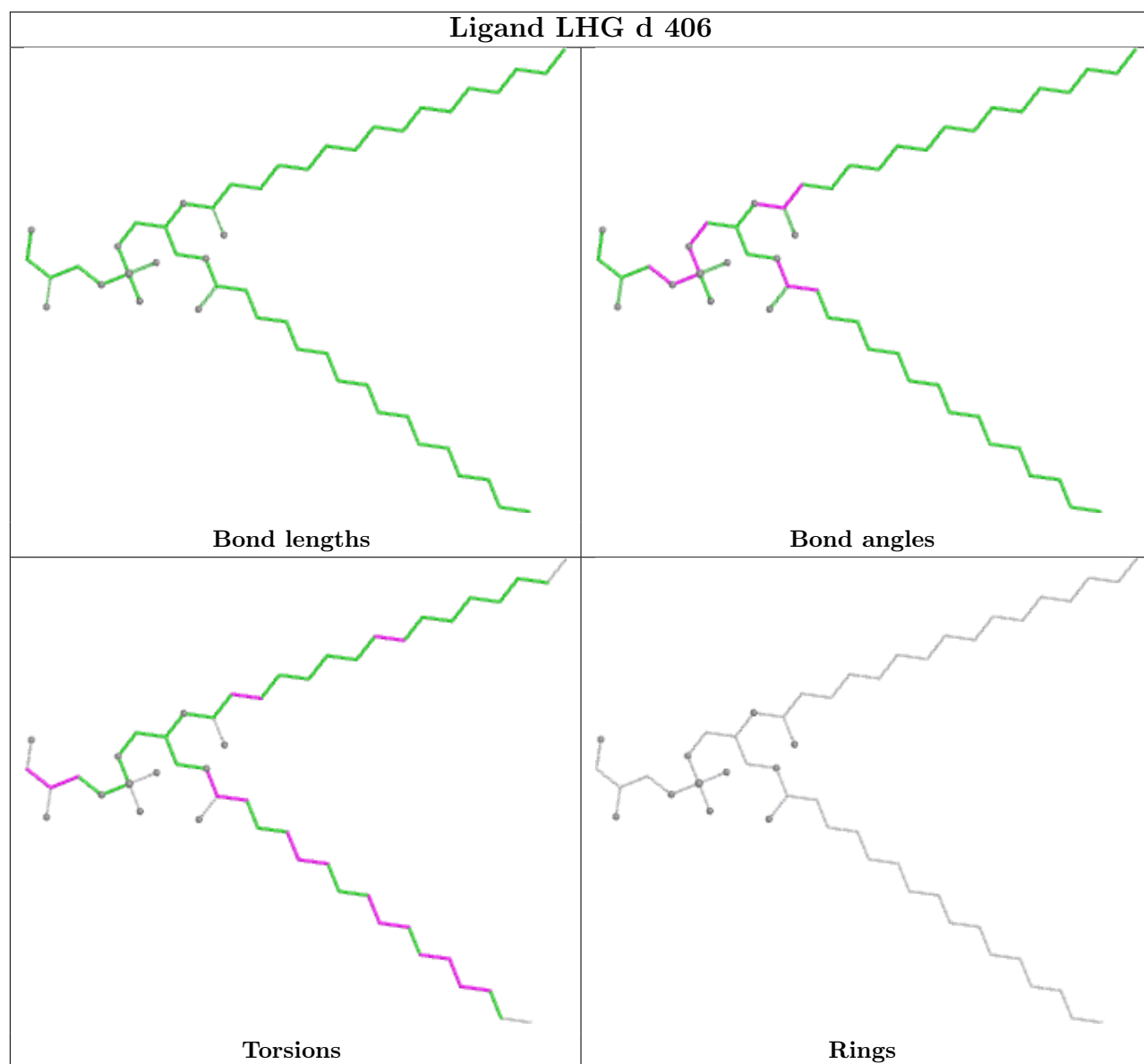
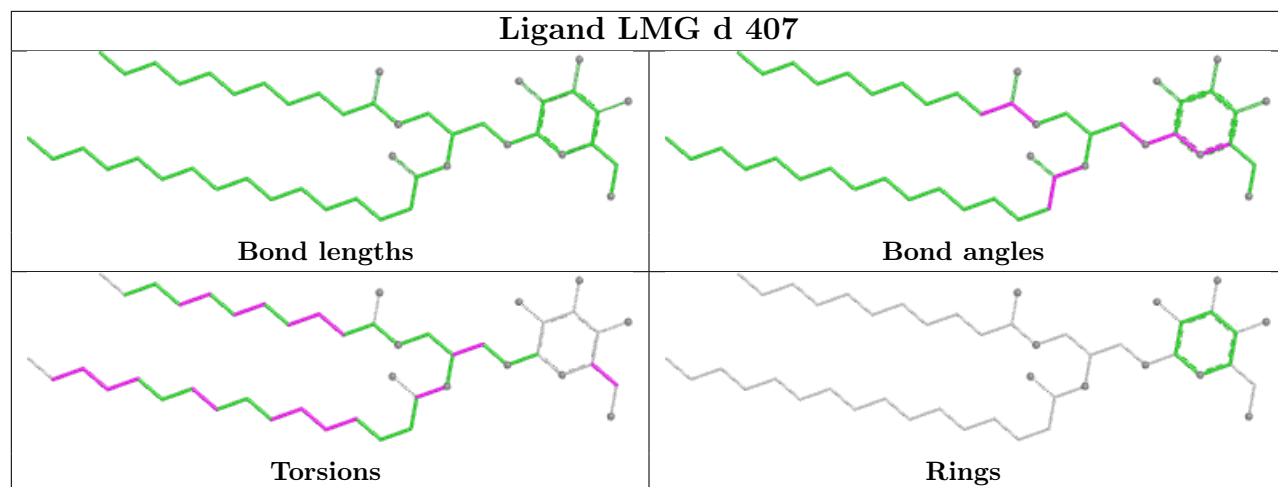
Ligand CHL 2 601



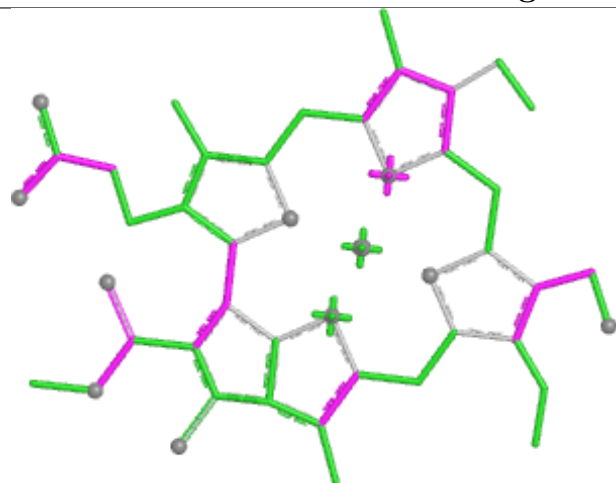




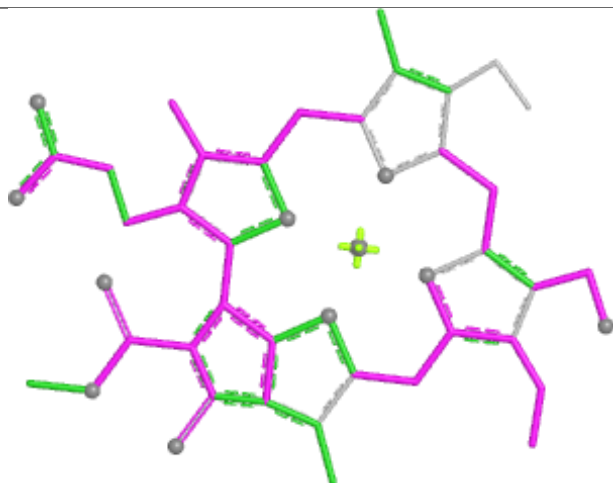




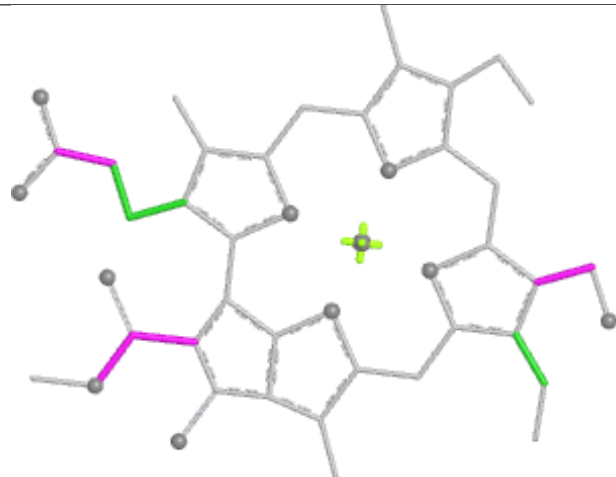
Ligand CHL n 606



Bond lengths



Bond angles

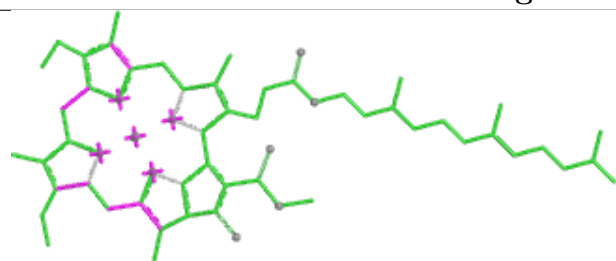


Torsions

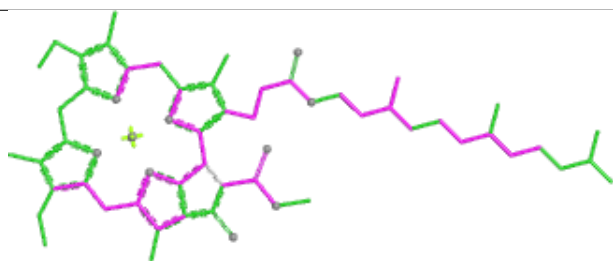


Rings

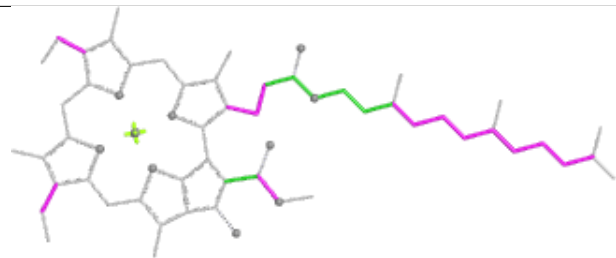
Ligand CLA N 613



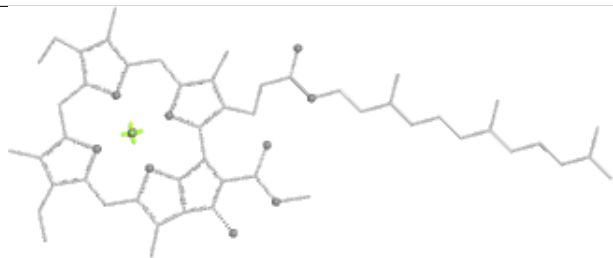
Bond lengths



Bond angles

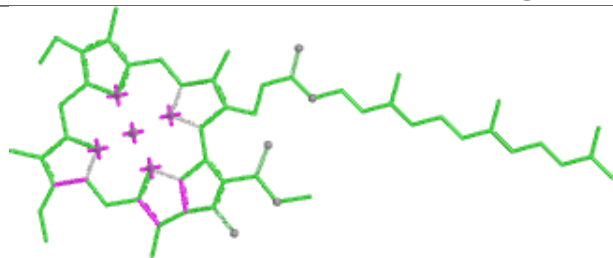


Torsions

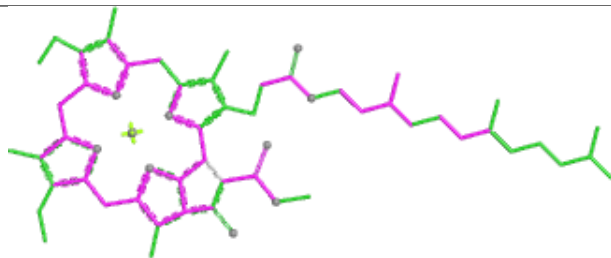


Rings

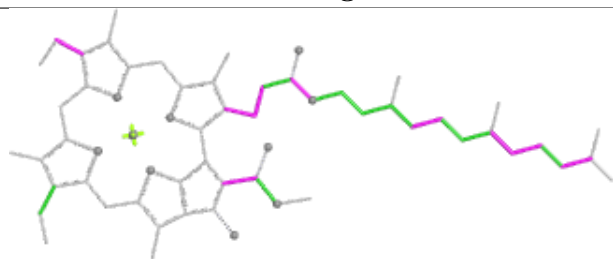
Ligand CLA 2 602



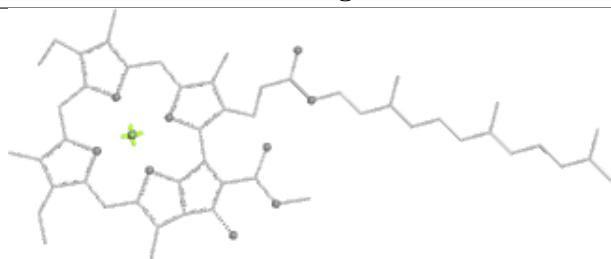
Bond lengths



Bond angles

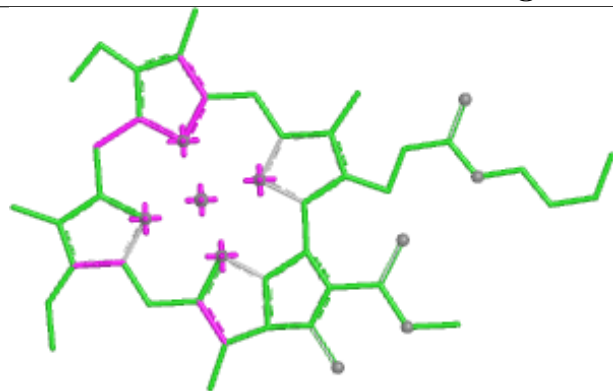


Torsions

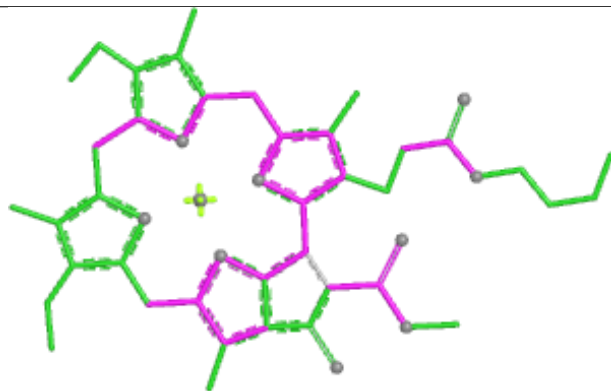


Rings

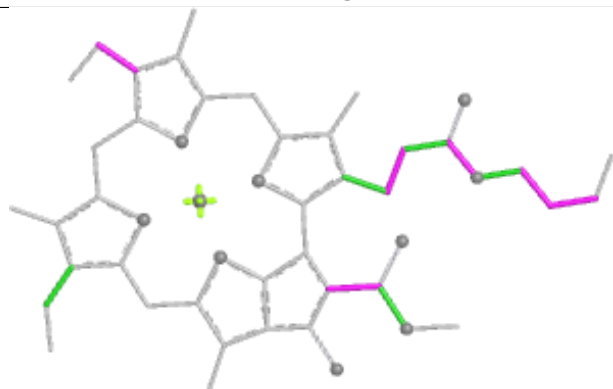
Ligand CLA S 312



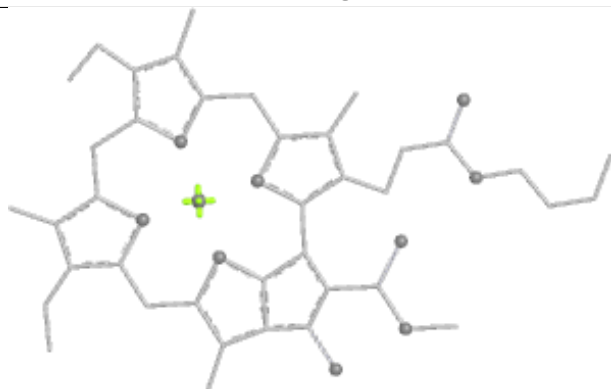
Bond lengths



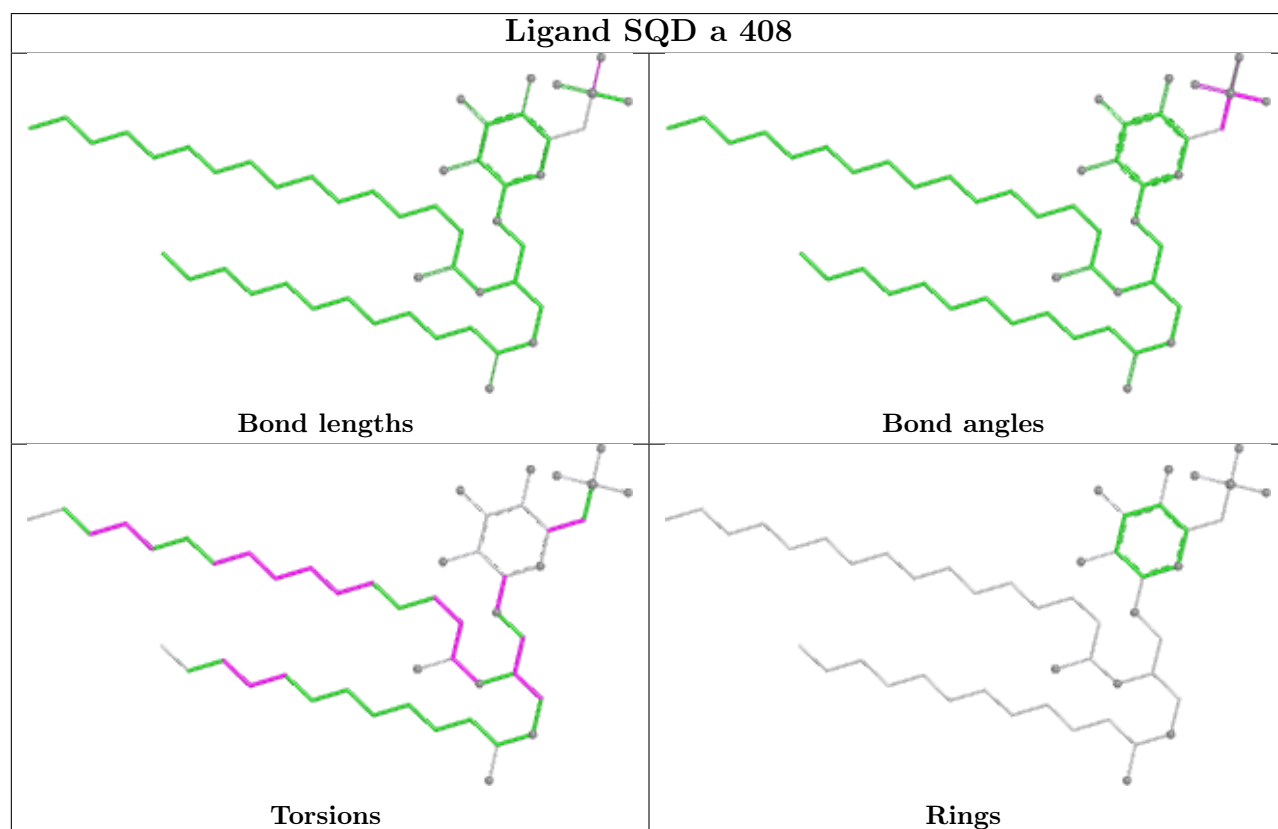
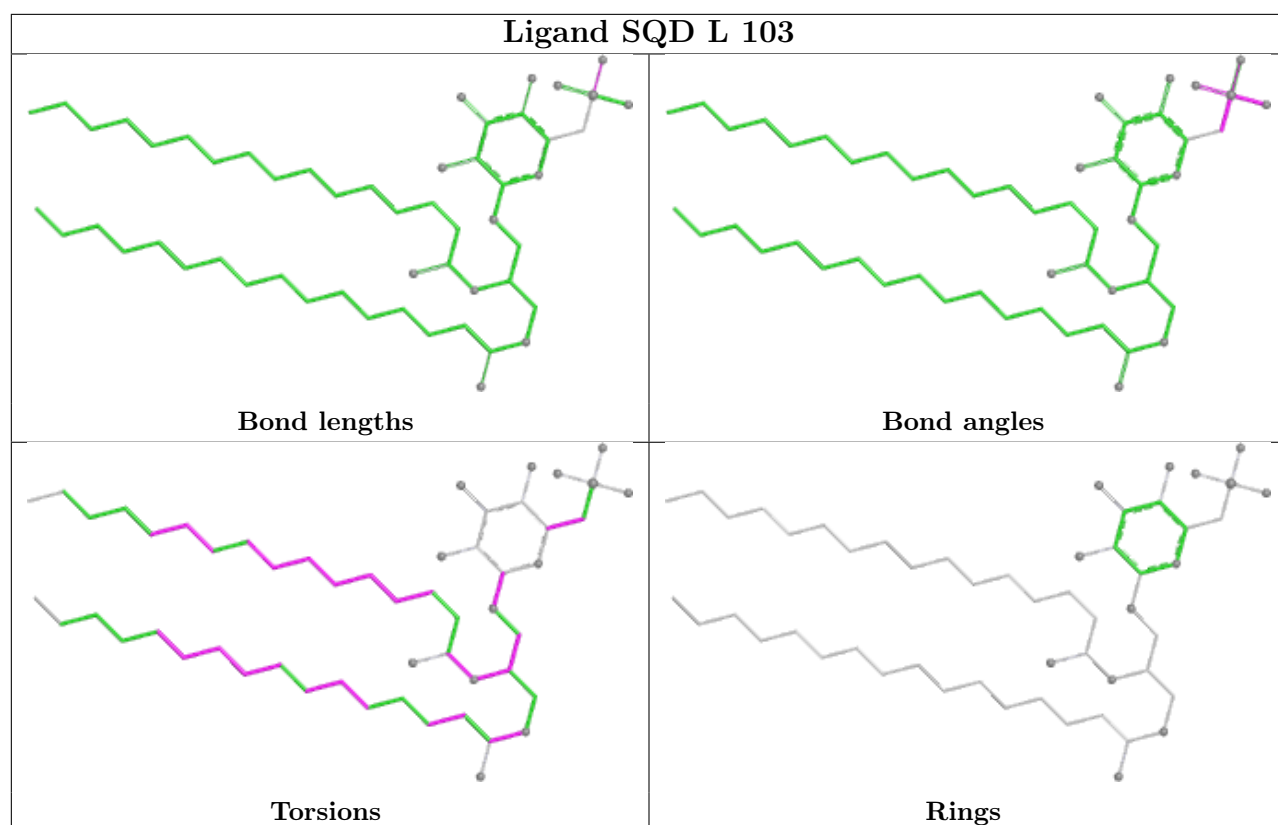
Bond angles



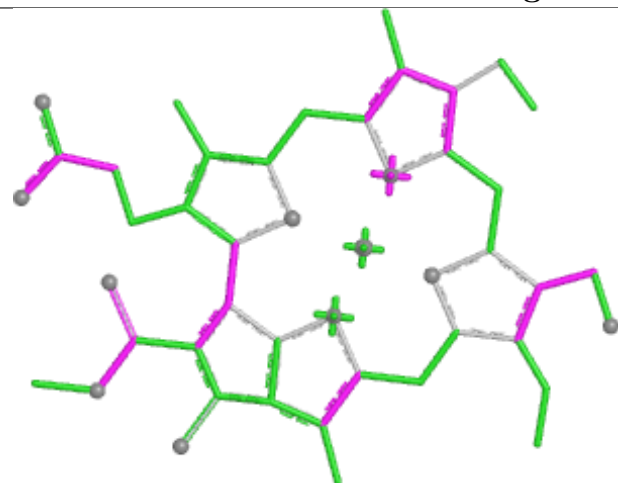
Torsions



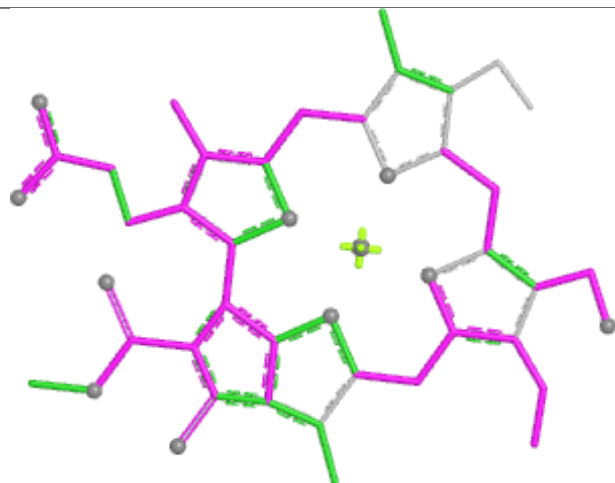
Rings



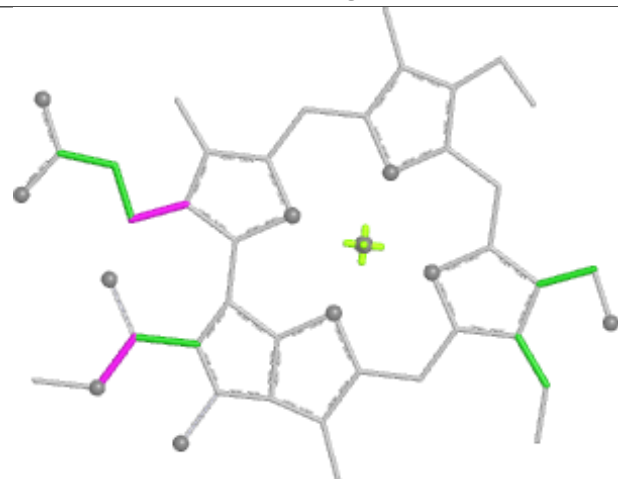
Ligand CHL r 605



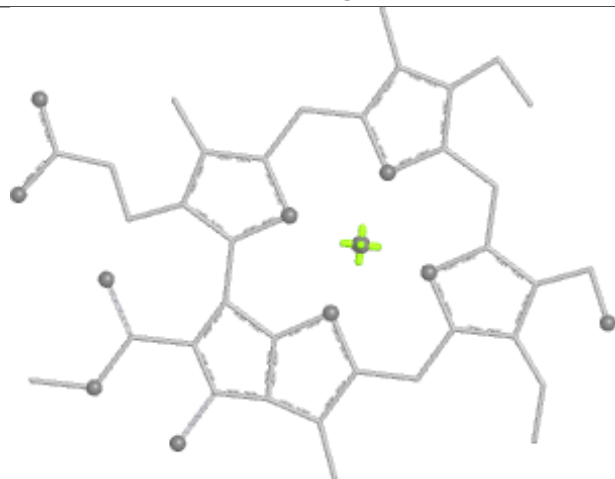
Bond lengths



Bond angles

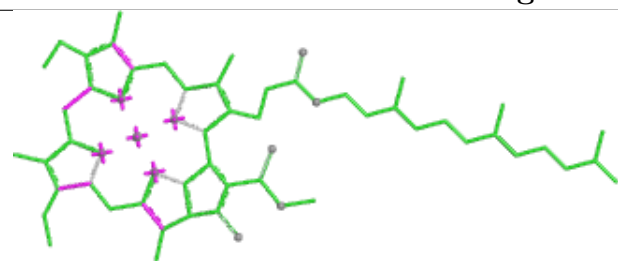


Torsions

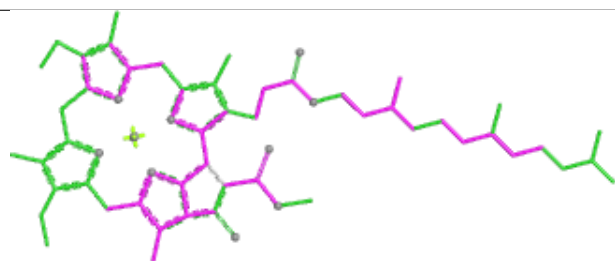


Rings

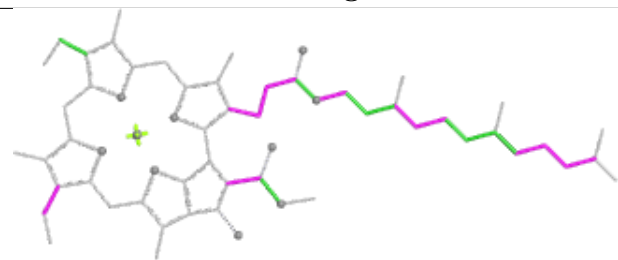
Ligand CLA G 611



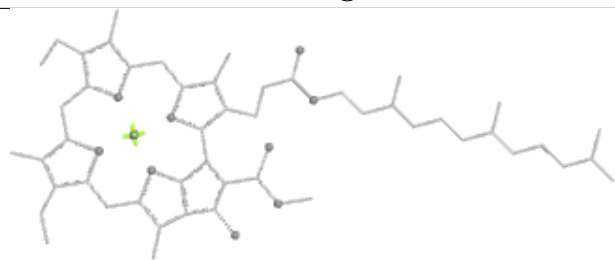
Bond lengths



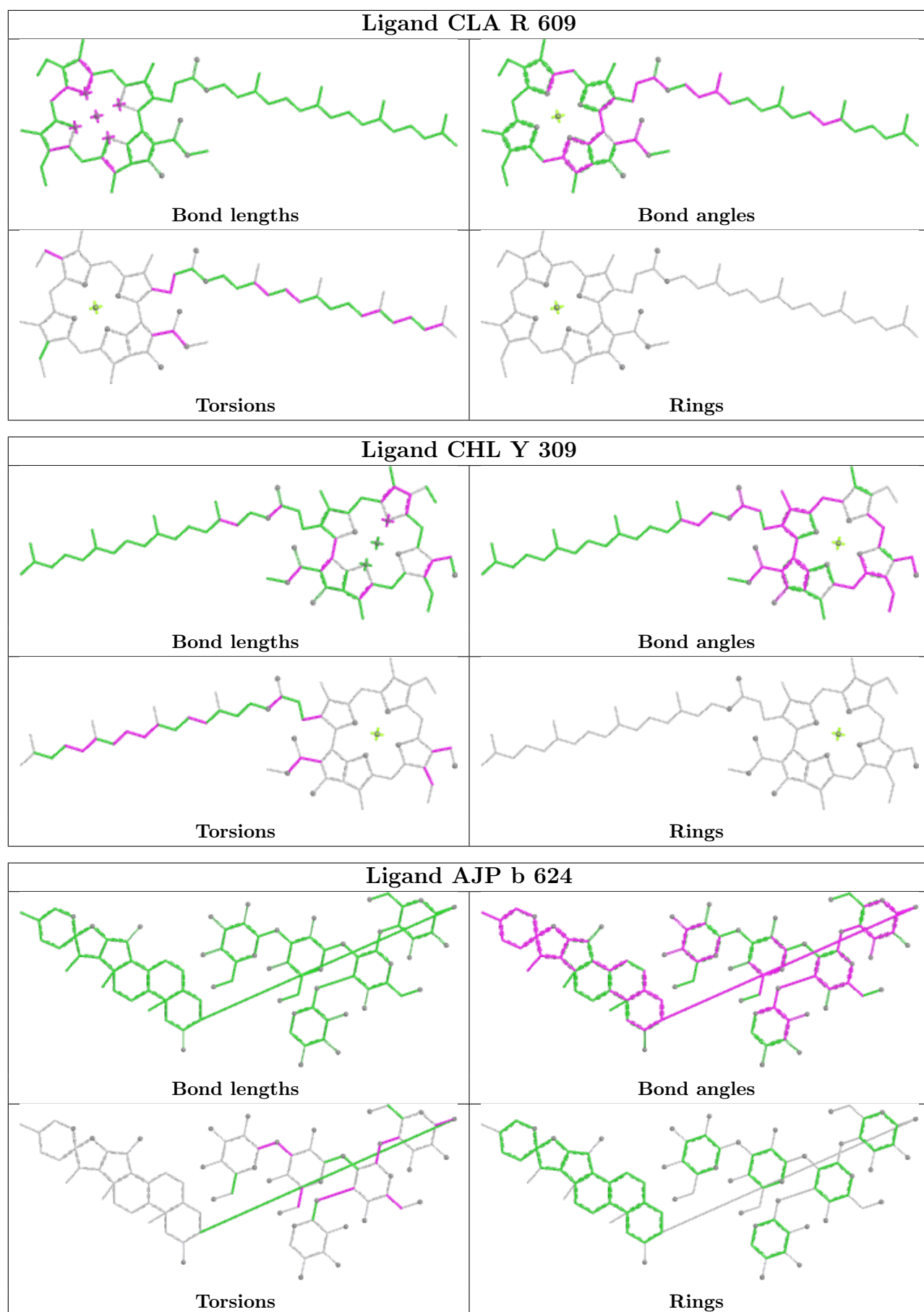
Bond angles

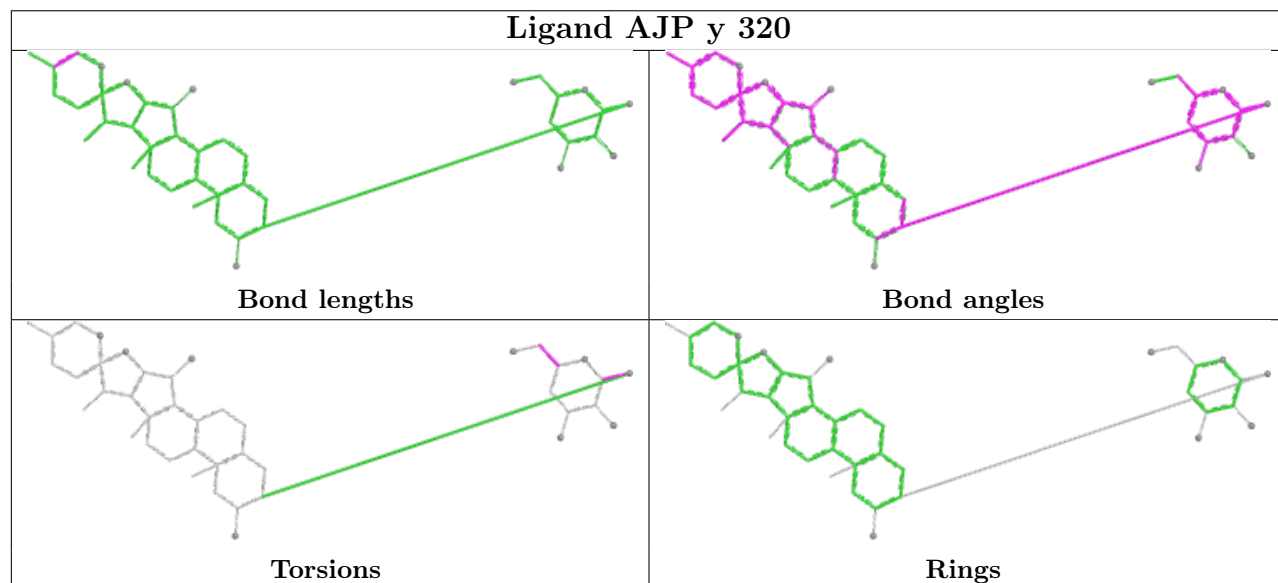
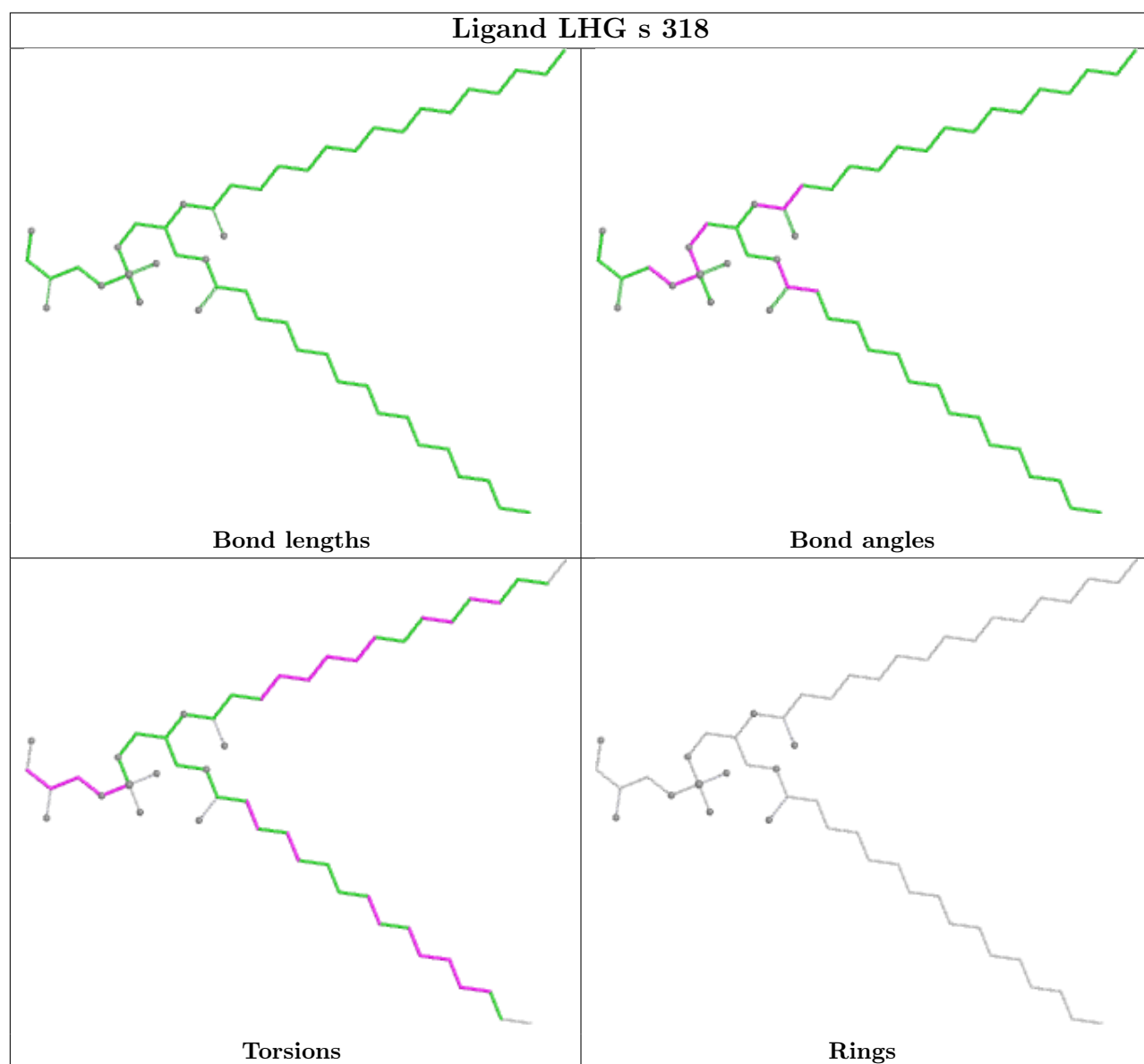


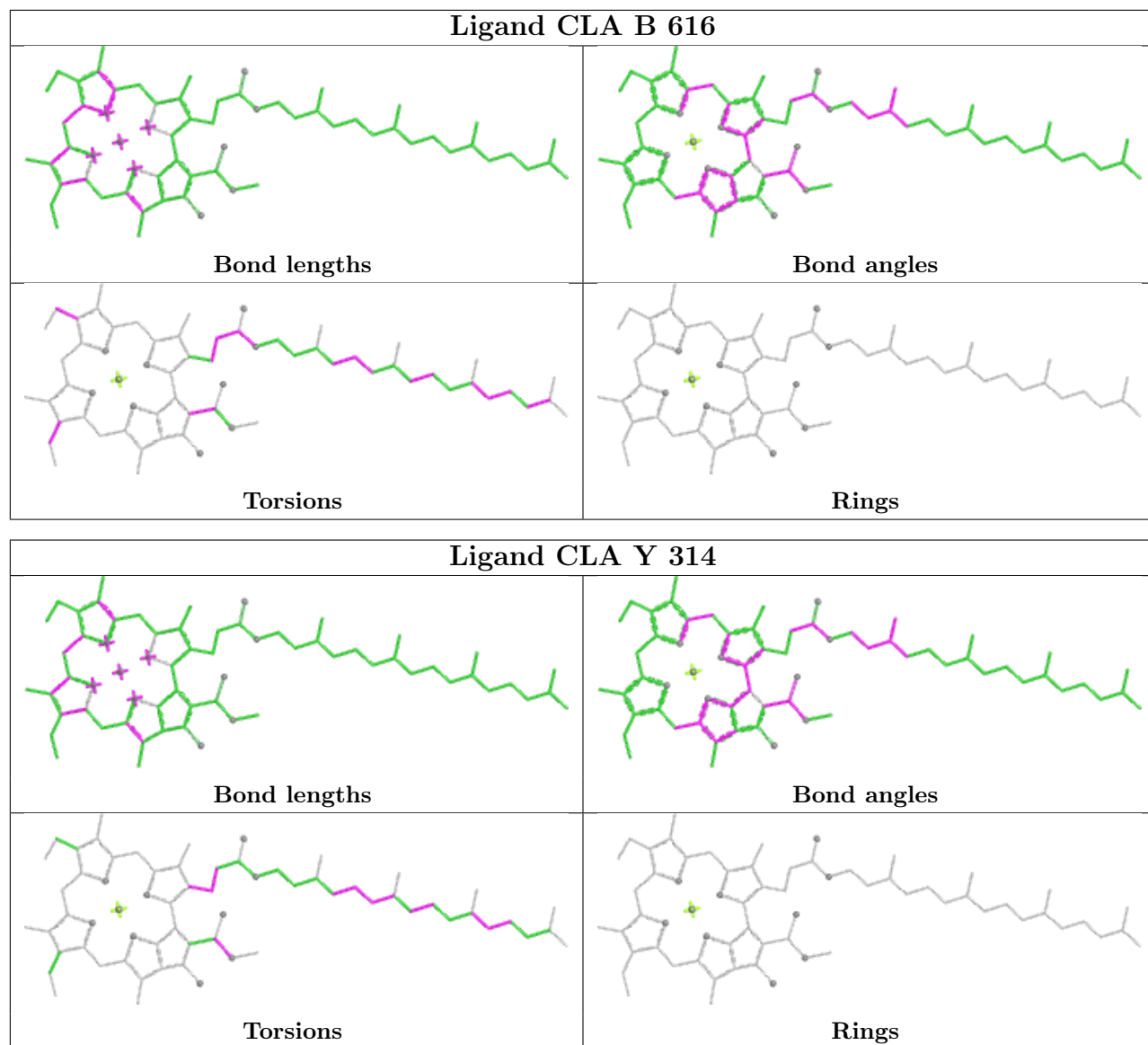
Torsions

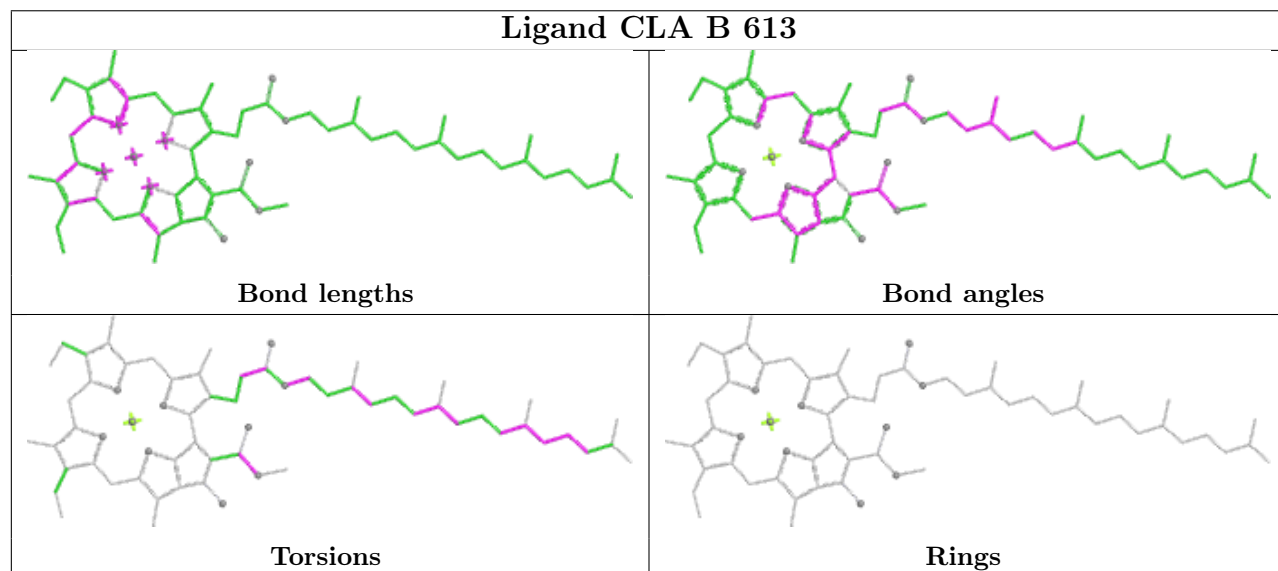
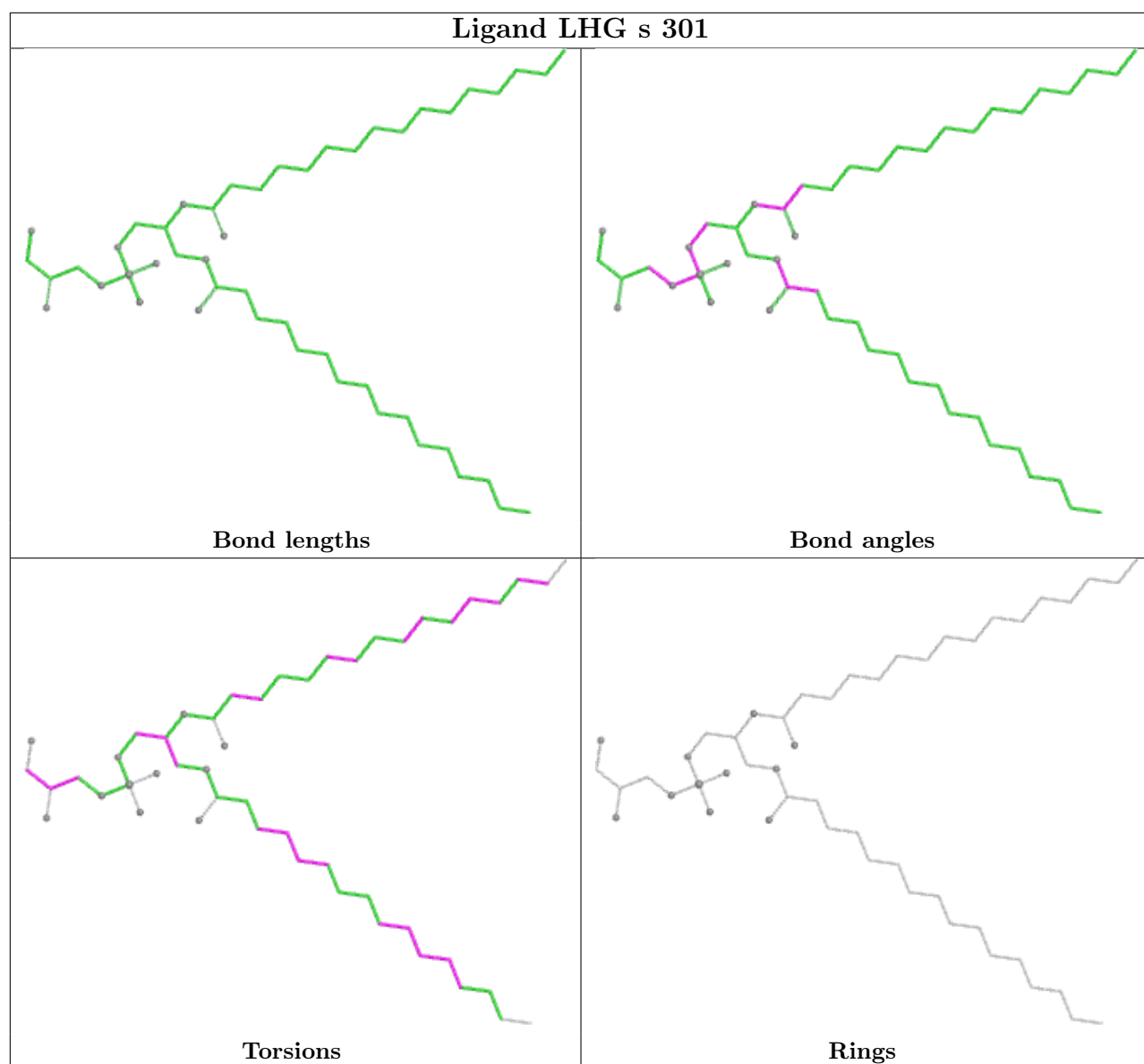


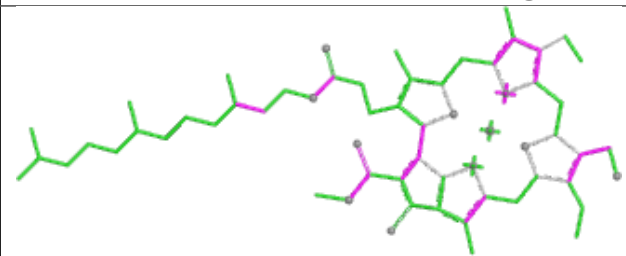
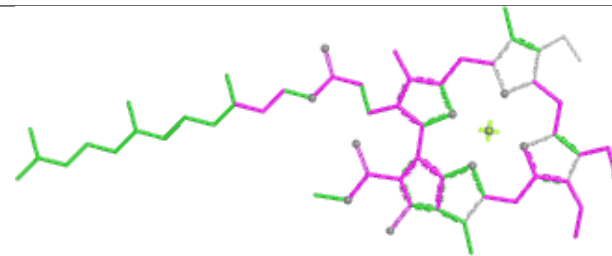
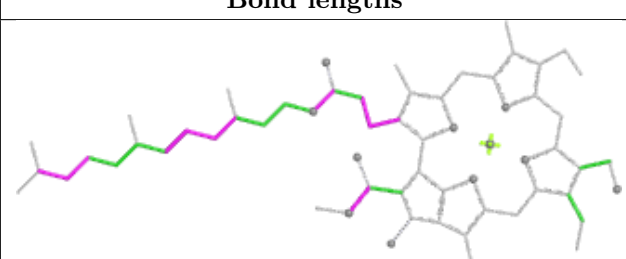
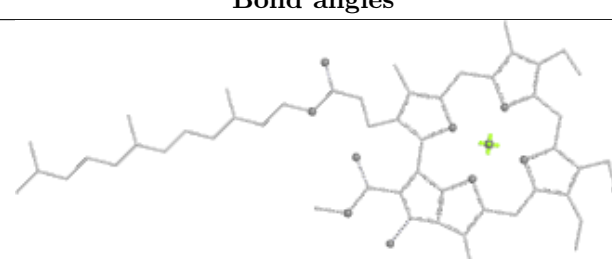
Rings

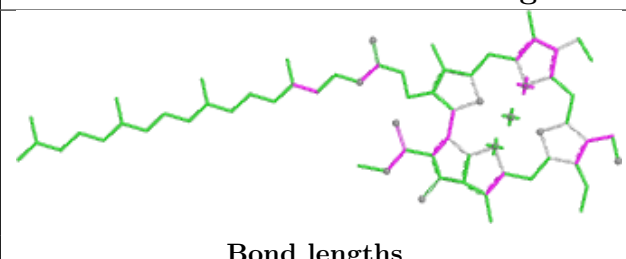
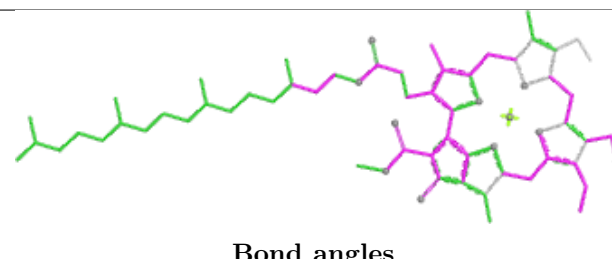
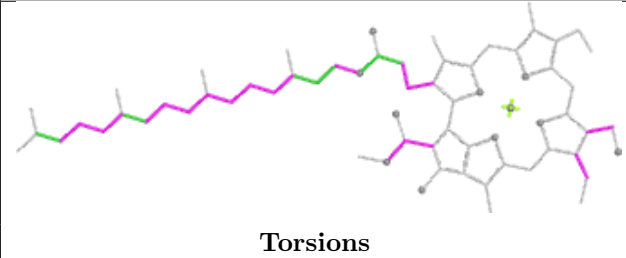
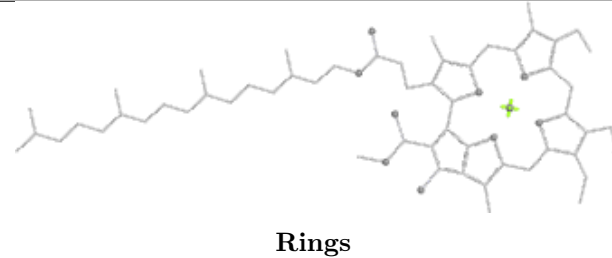


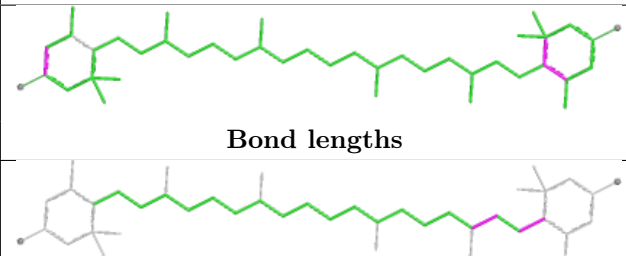
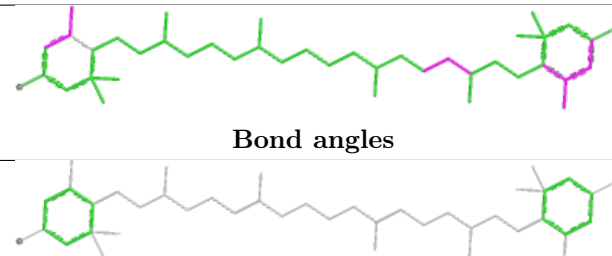
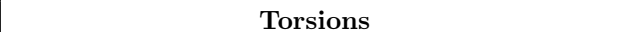


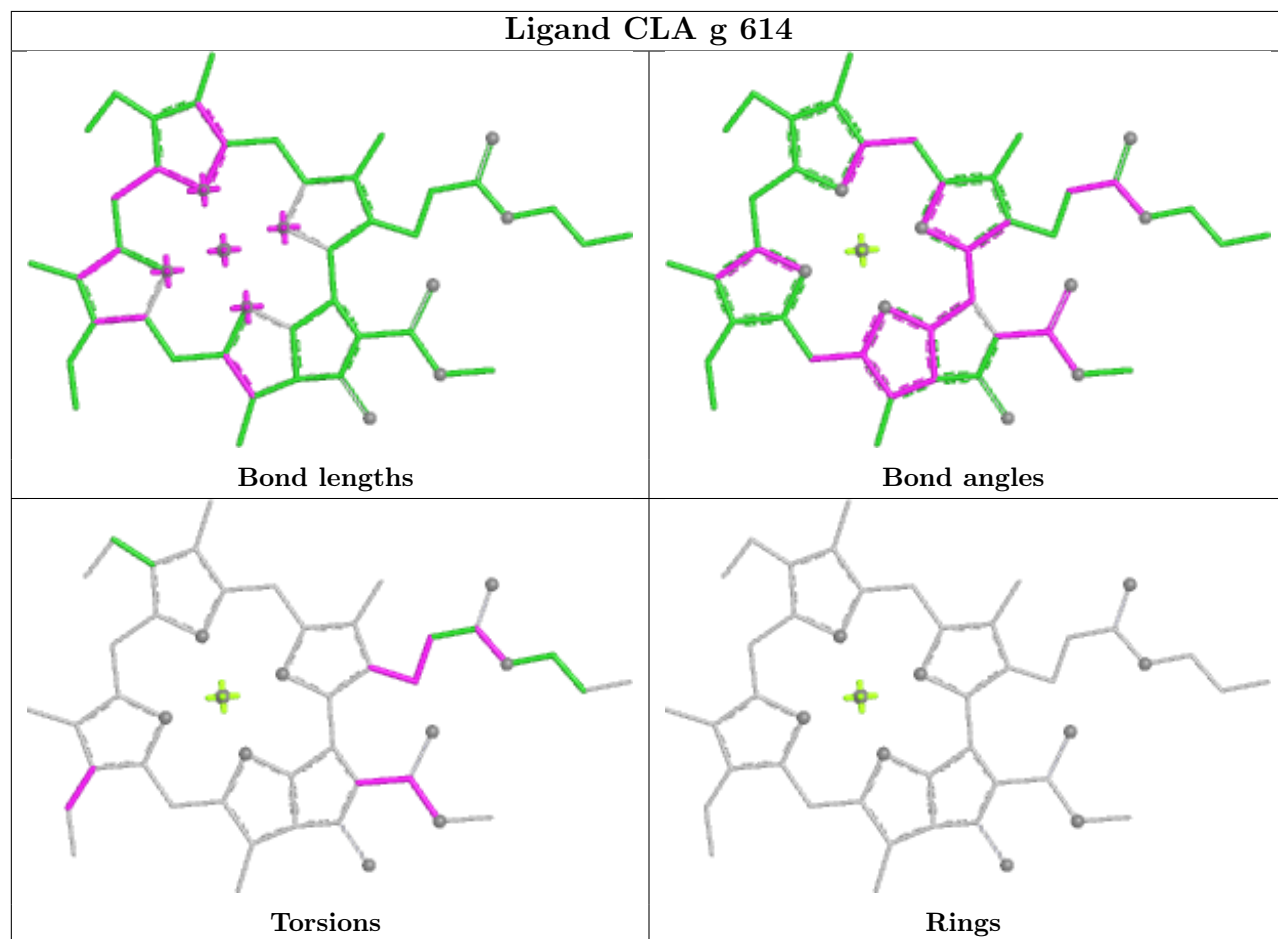
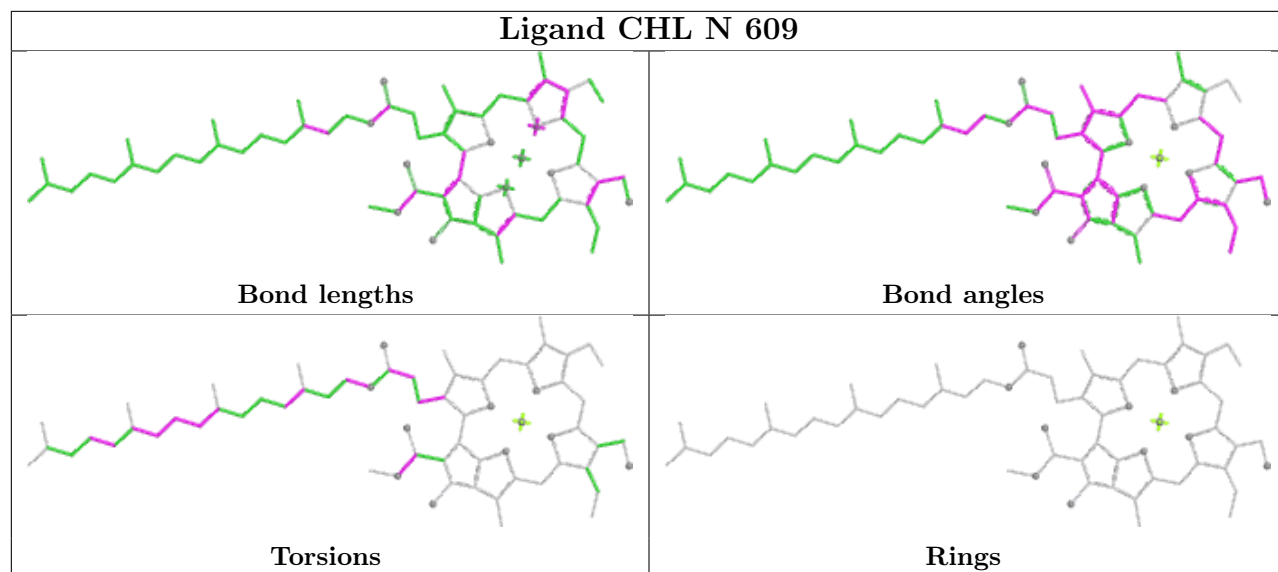


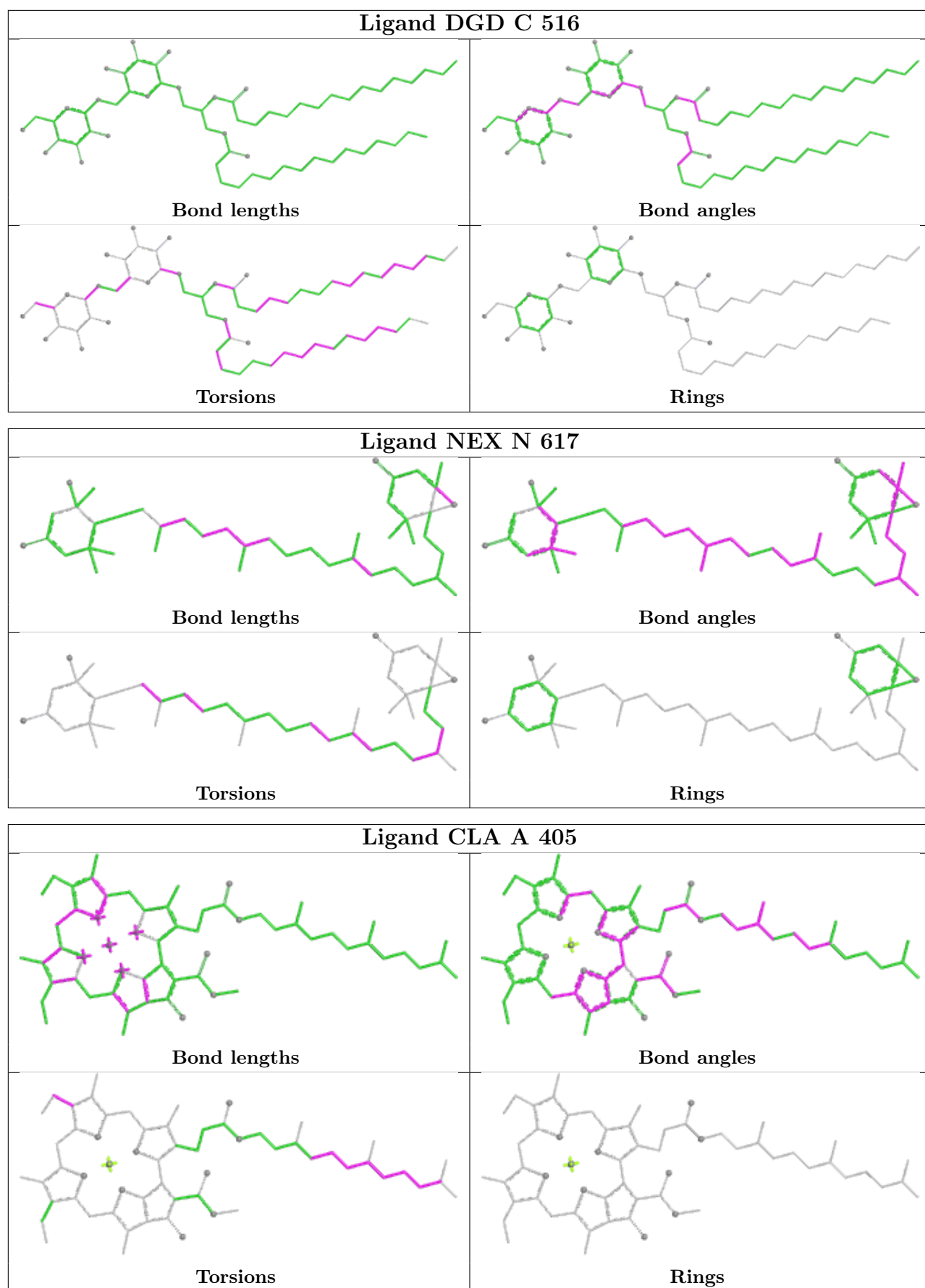


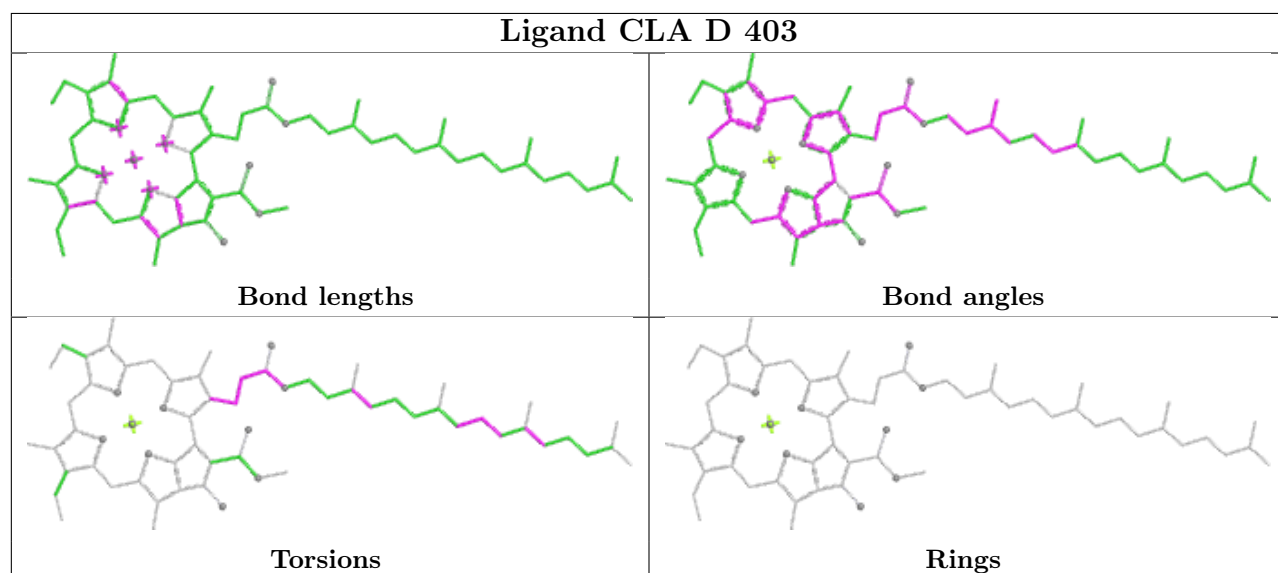
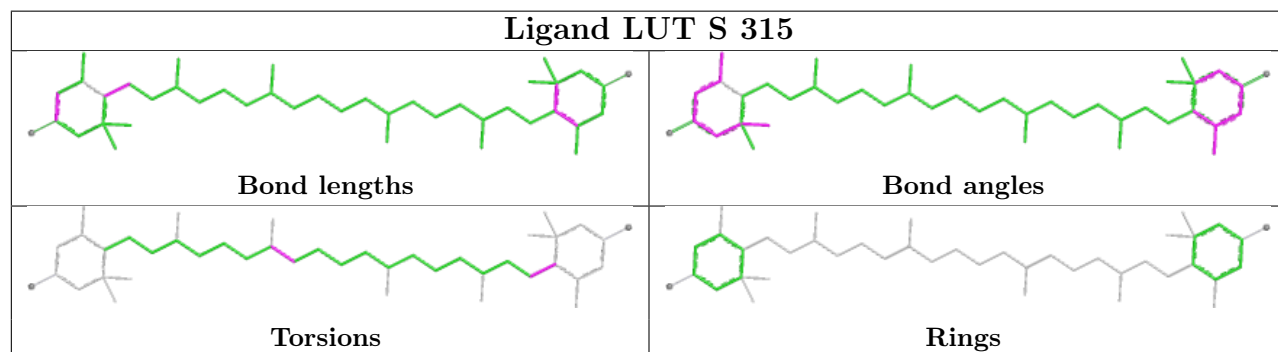
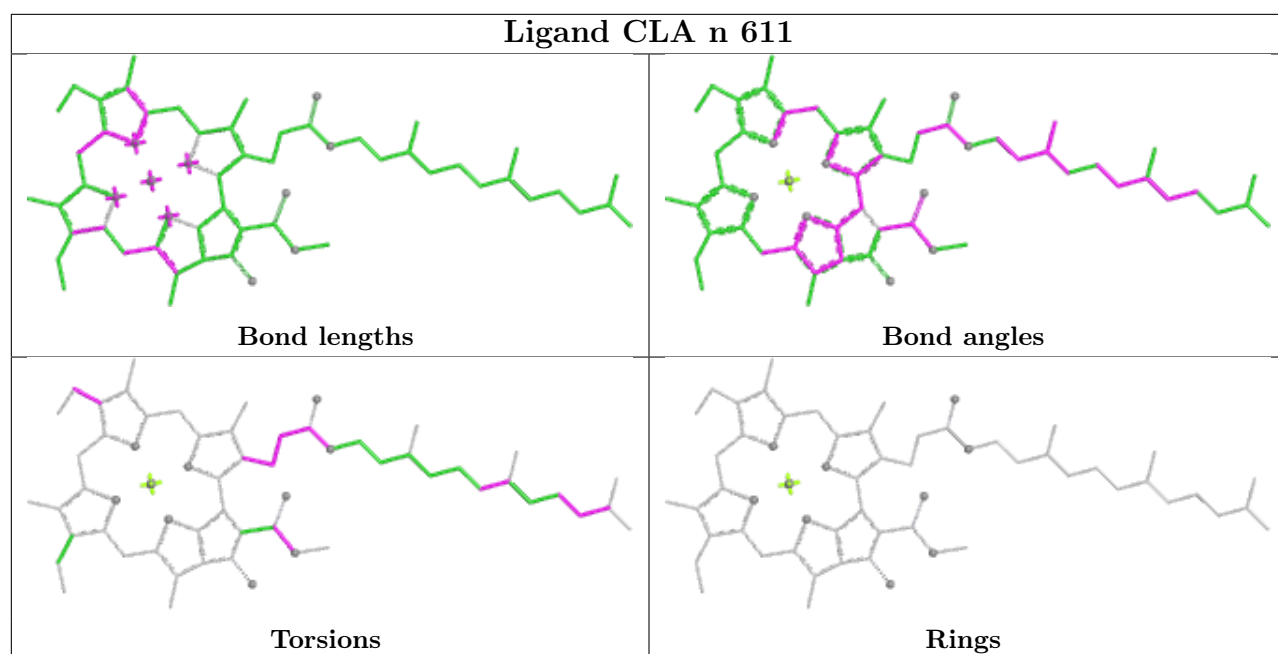
Ligand CHL R 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

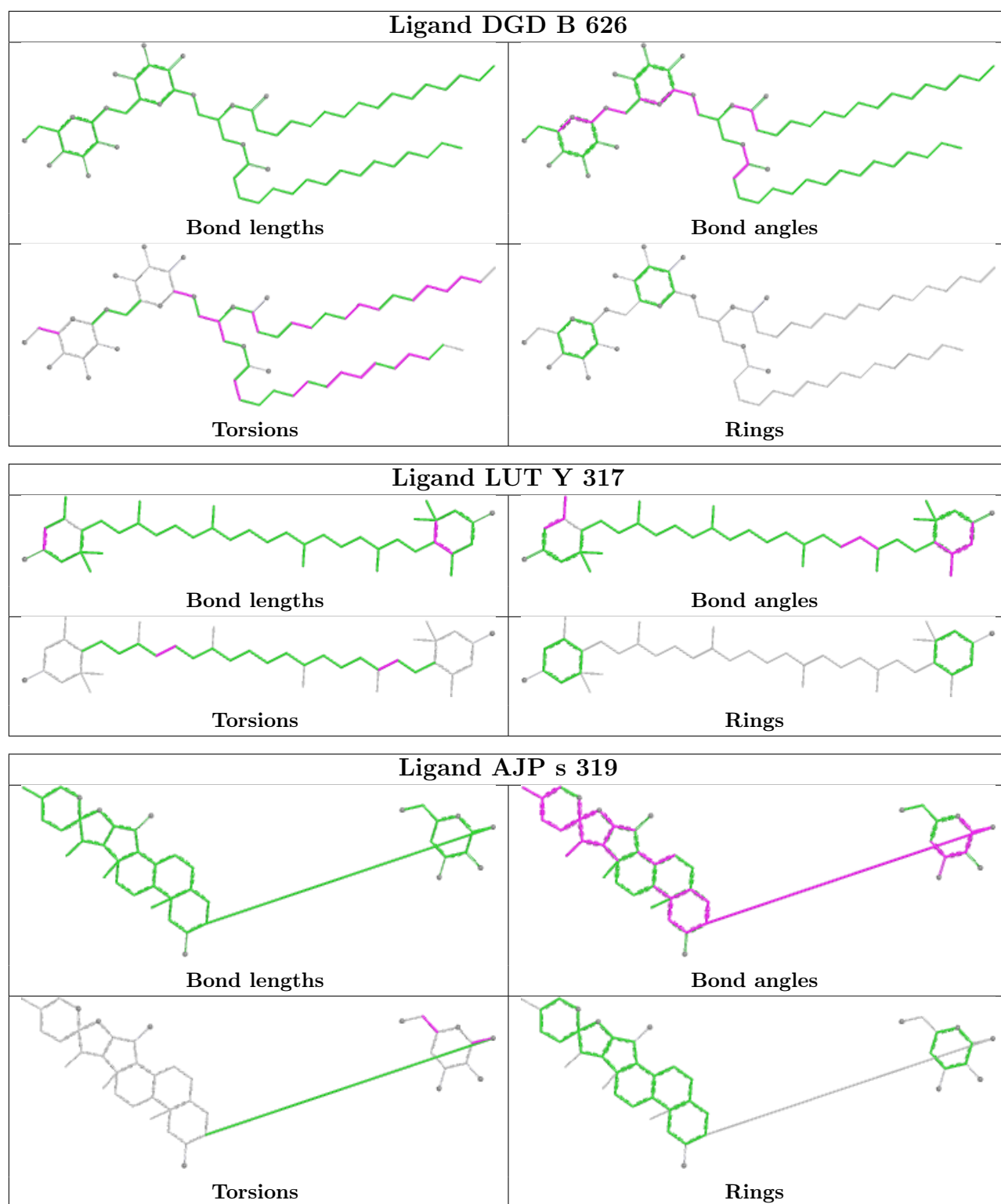
Ligand CHL G 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

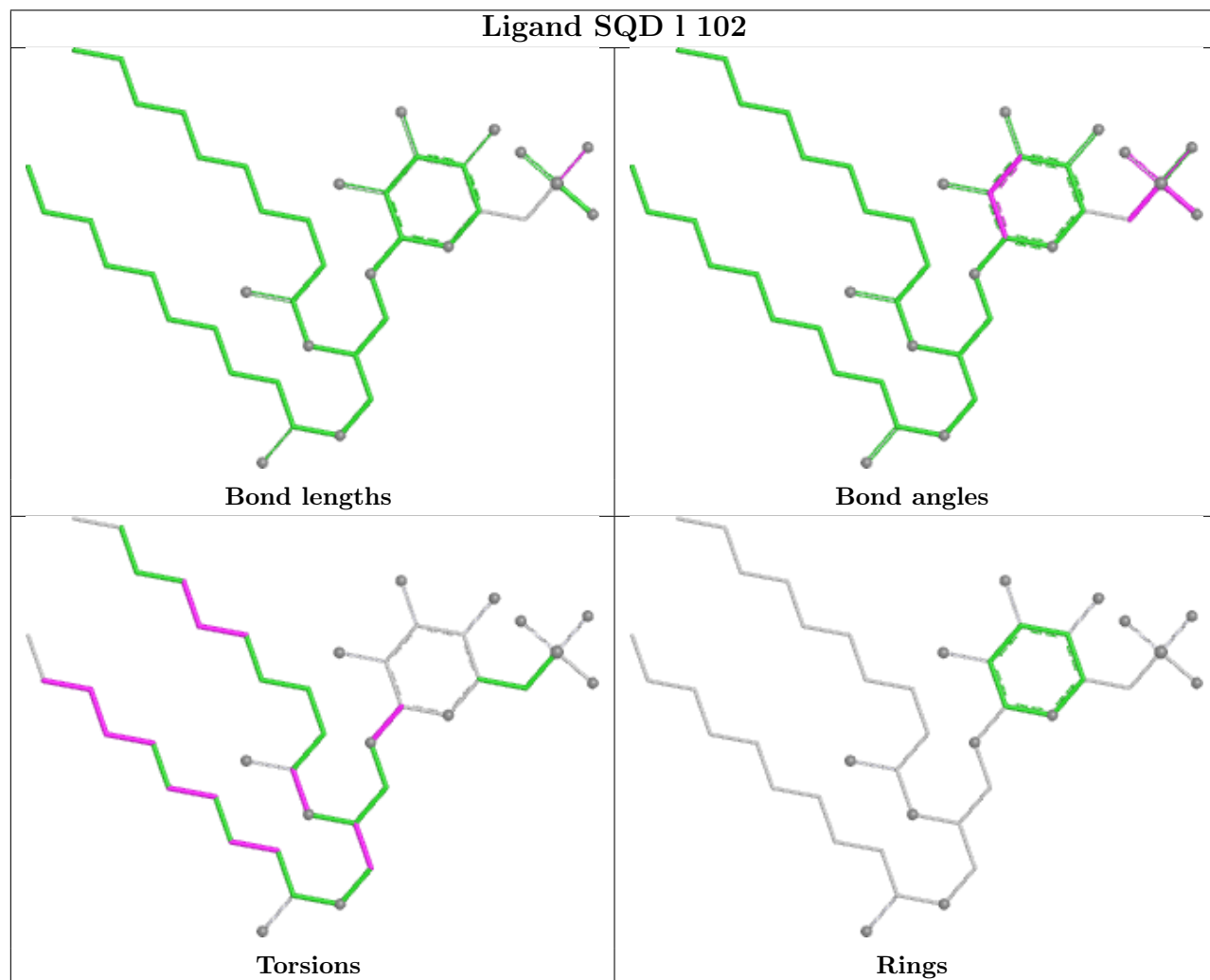
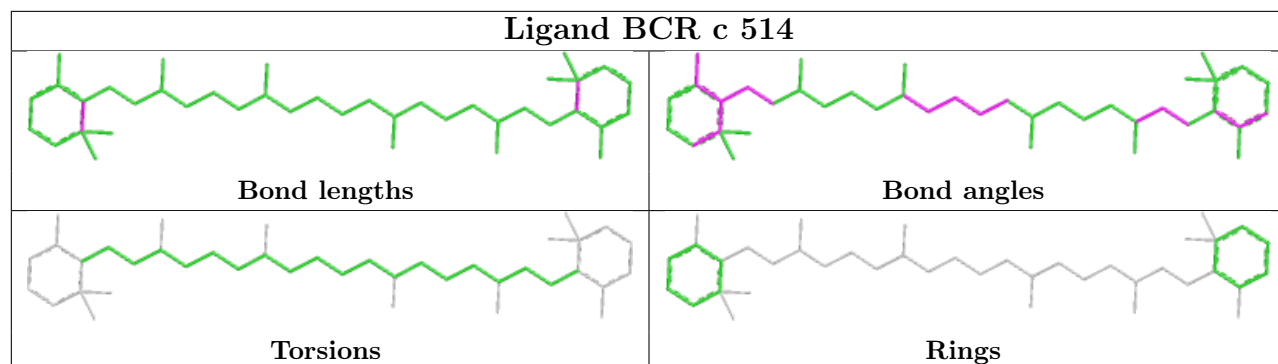
Ligand LUT N 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

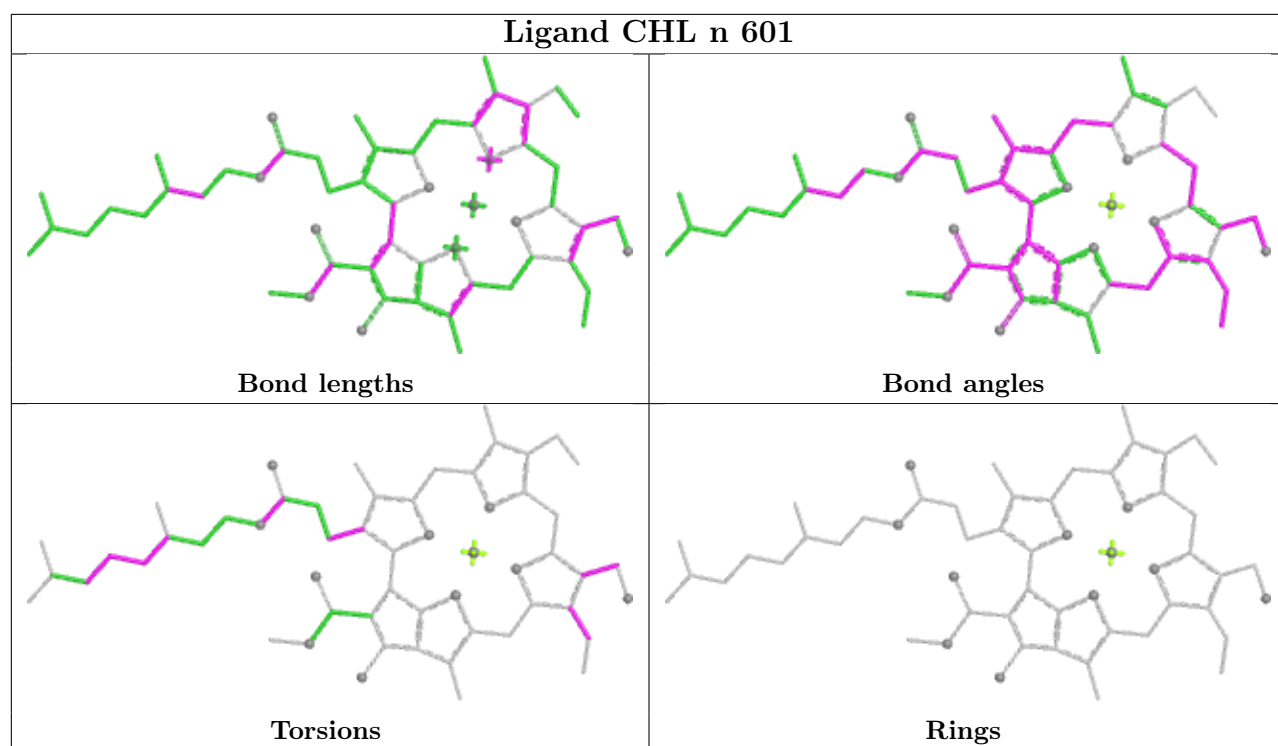




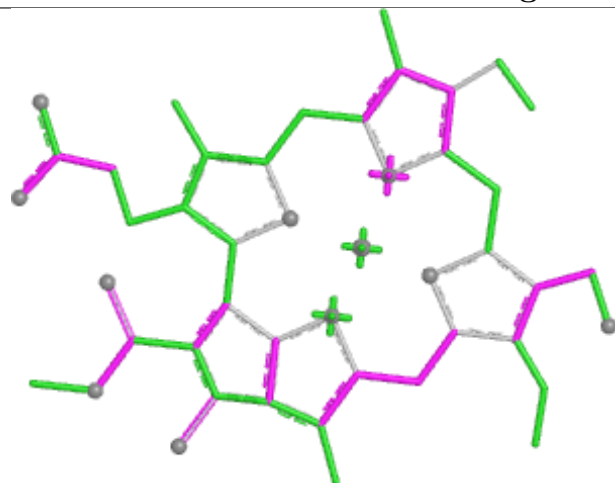




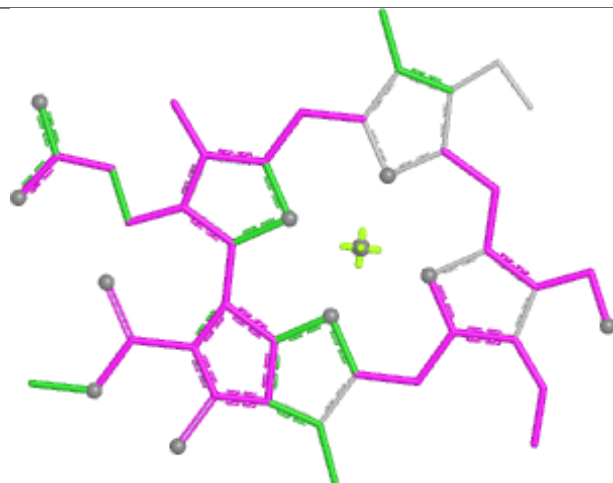




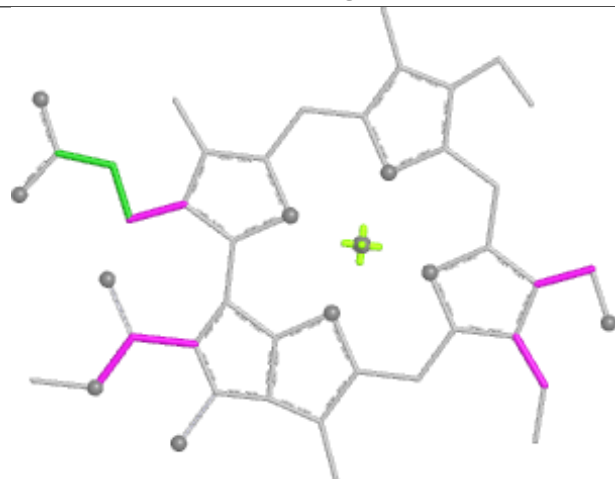
Ligand CHL 6 603



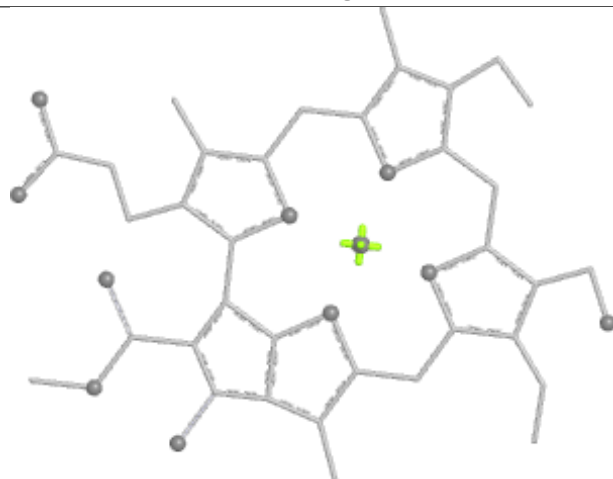
Bond lengths



Bond angles

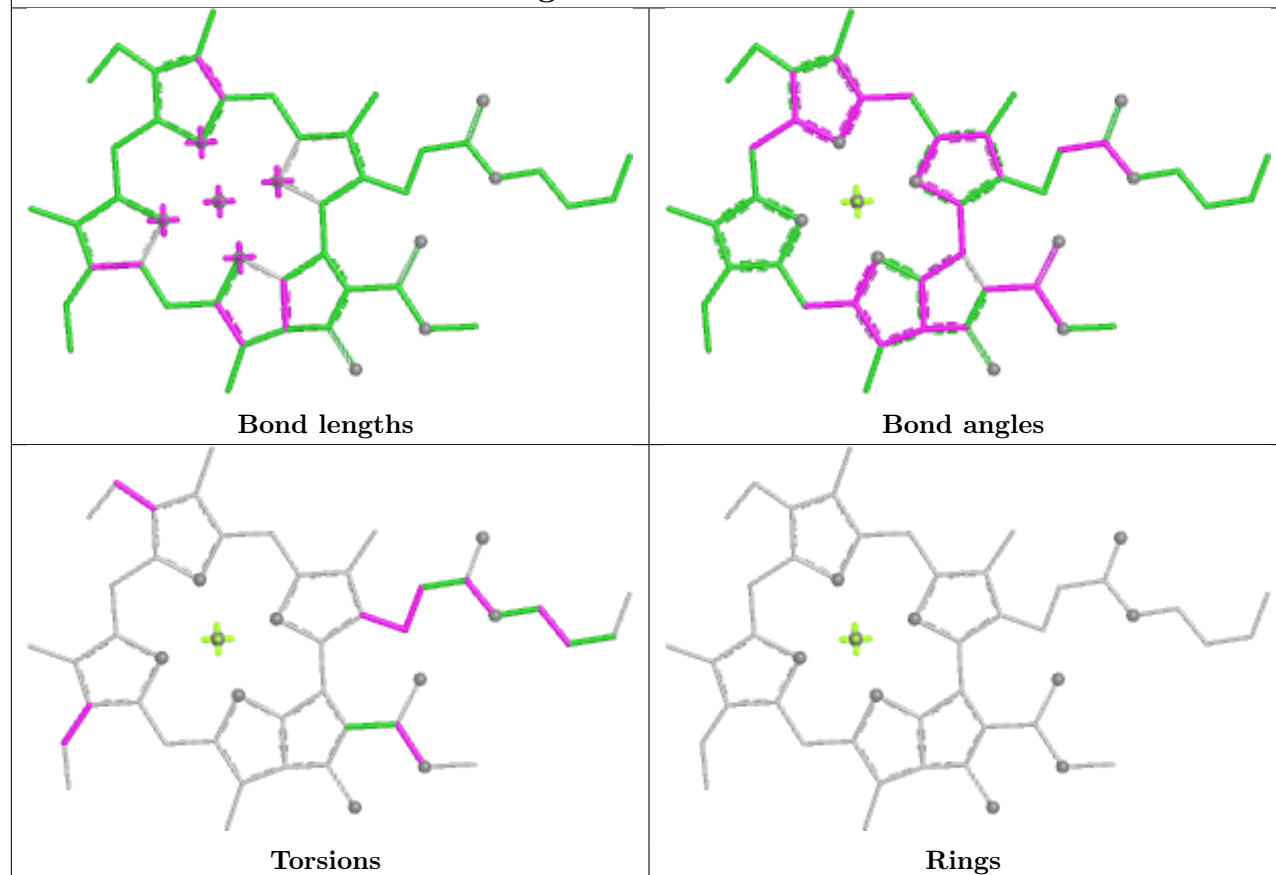


Torsions

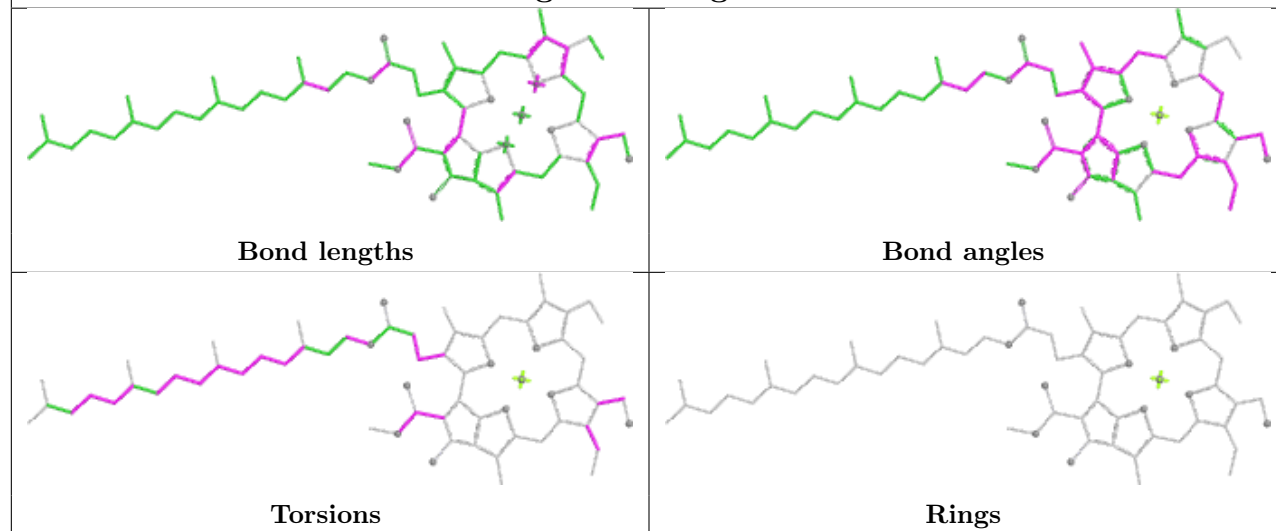


Rings

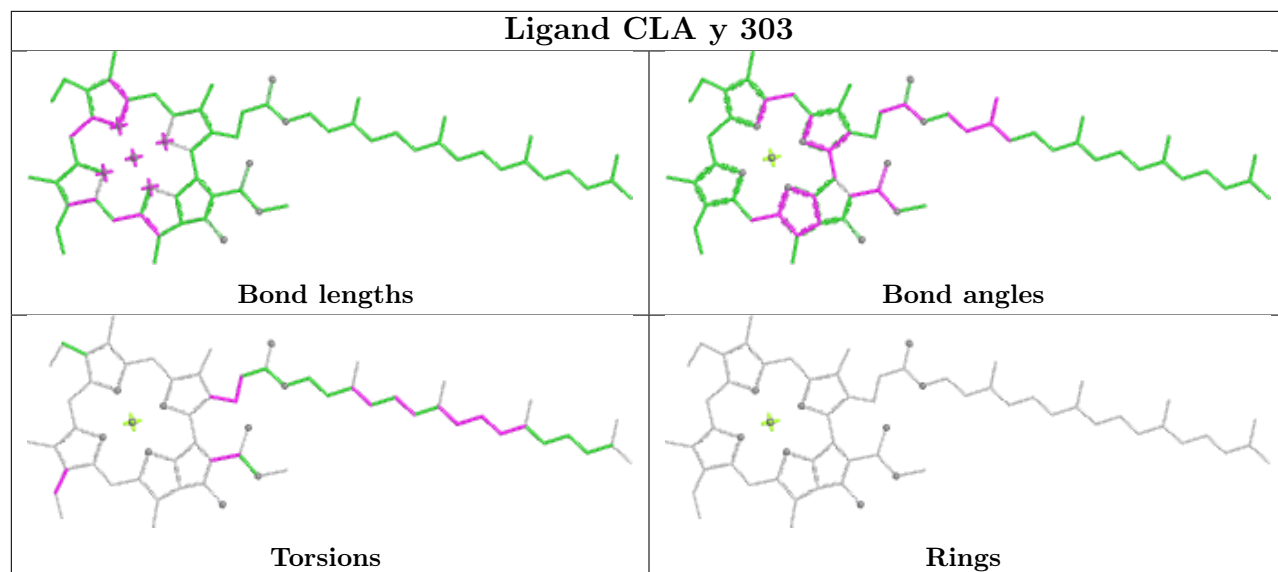
Ligand CLA r 601



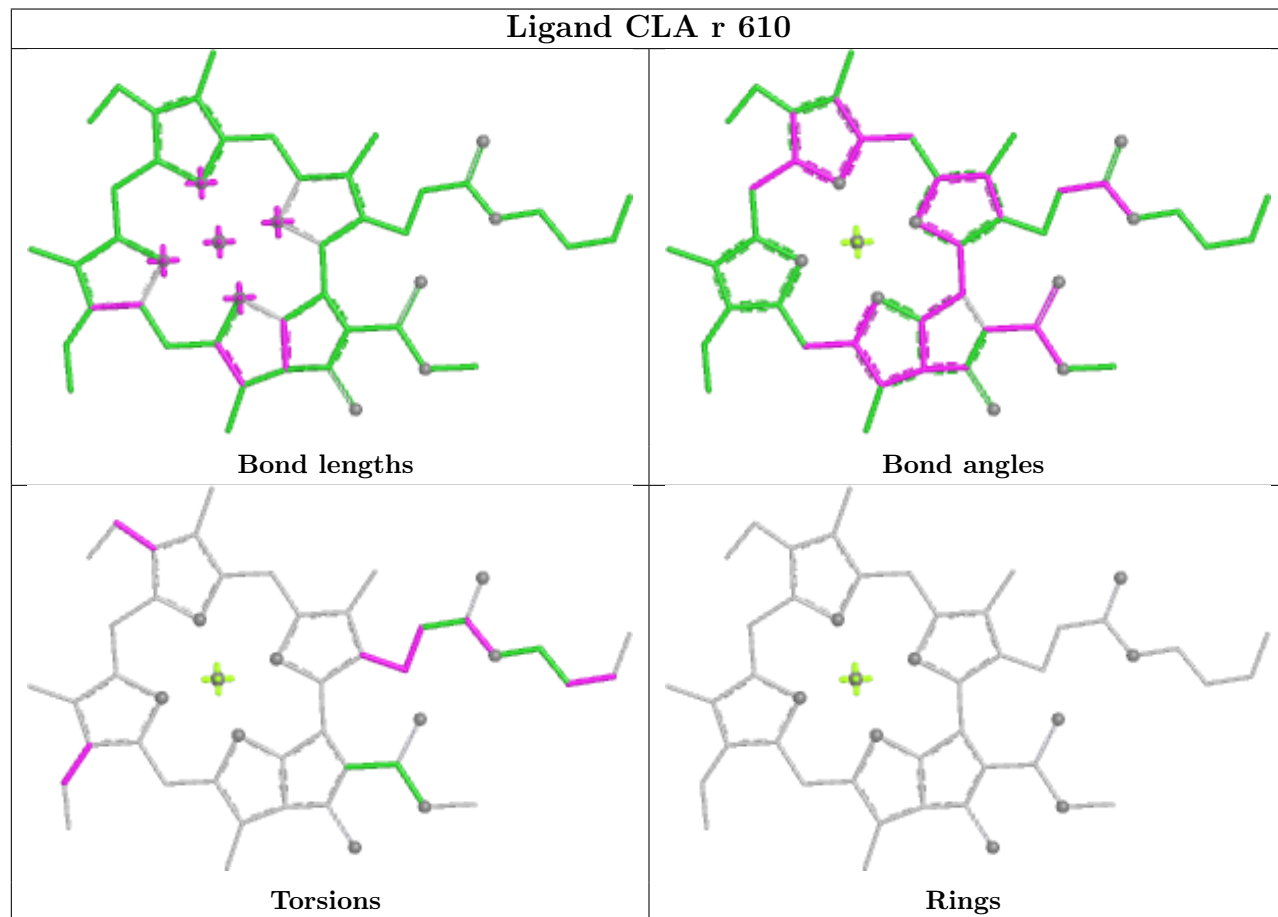
Ligand CHL g 608

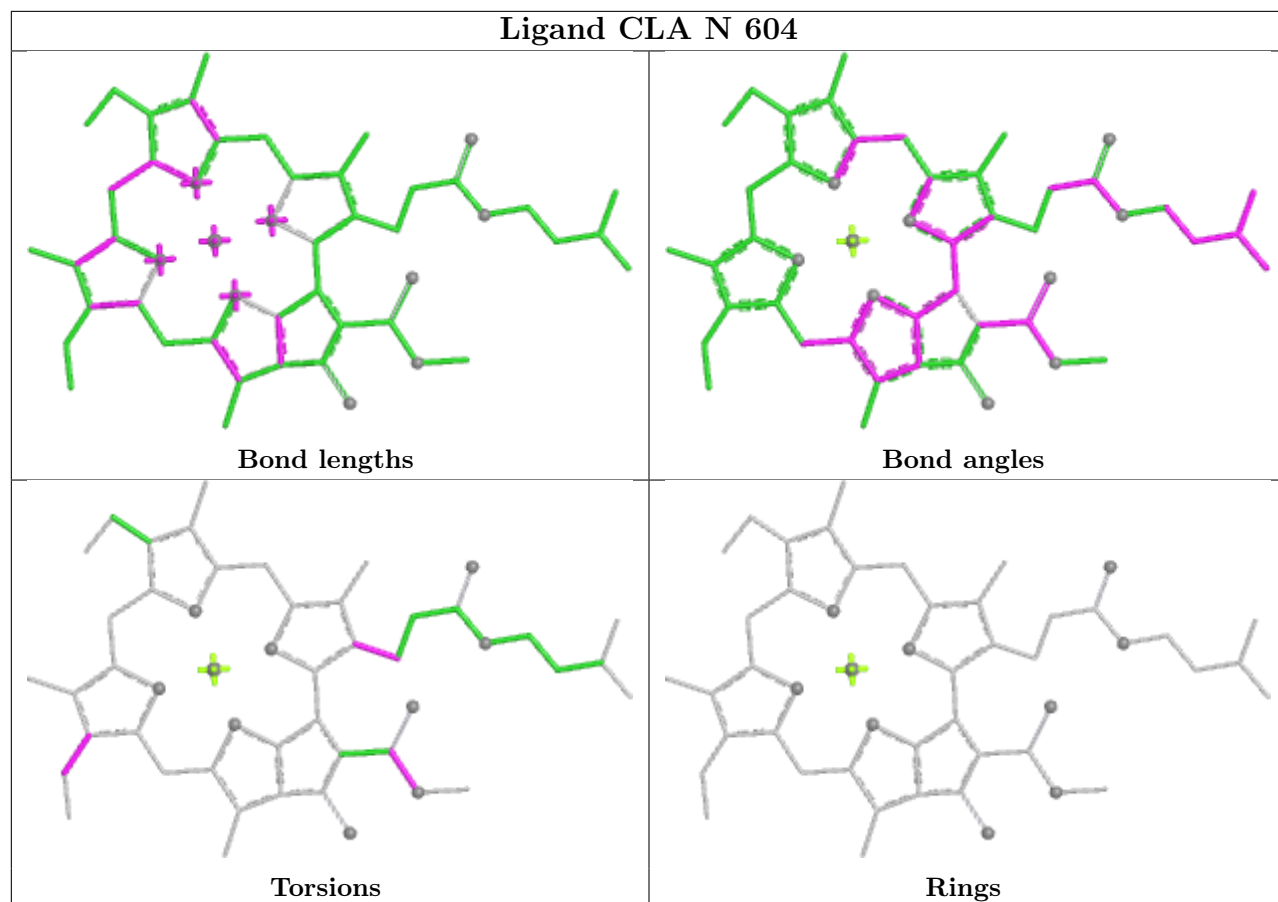


Ligand CLA y 303

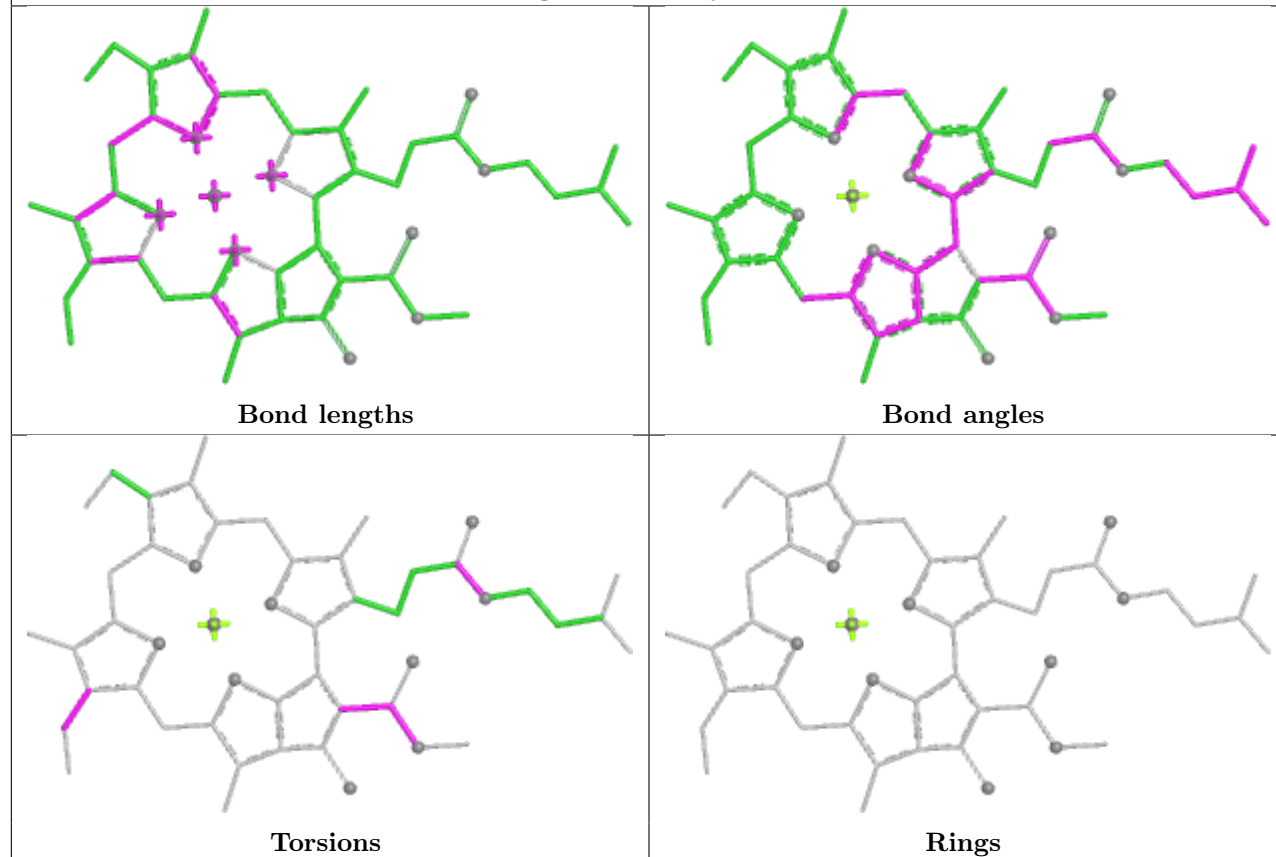


Ligand CLA r 610

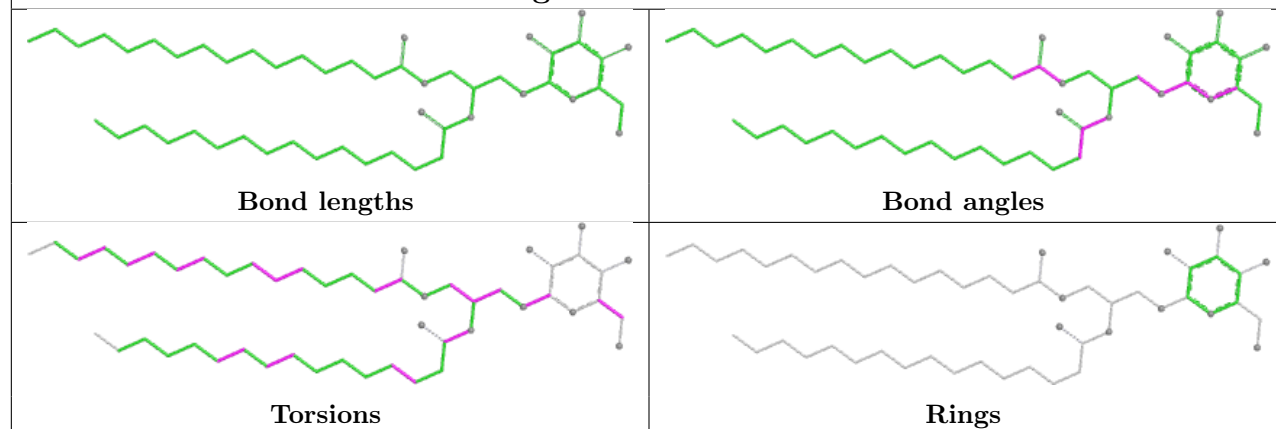




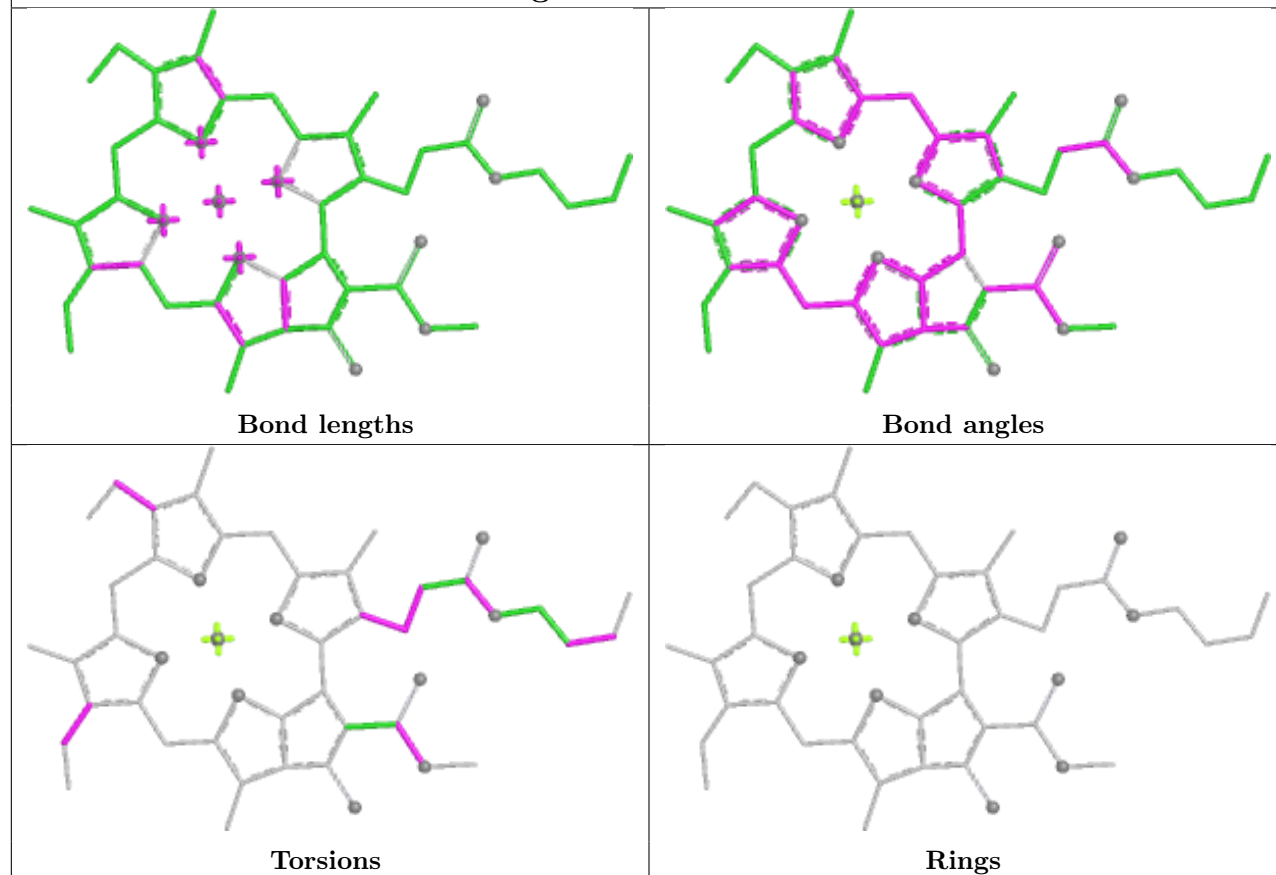
Ligand CLA y 305



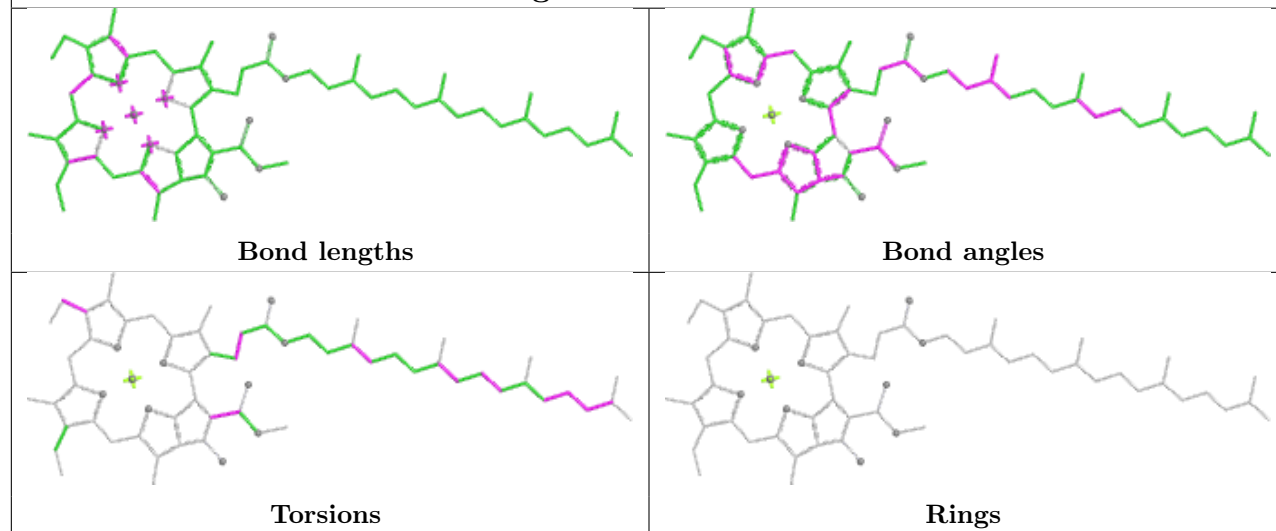
Ligand LMG c 520

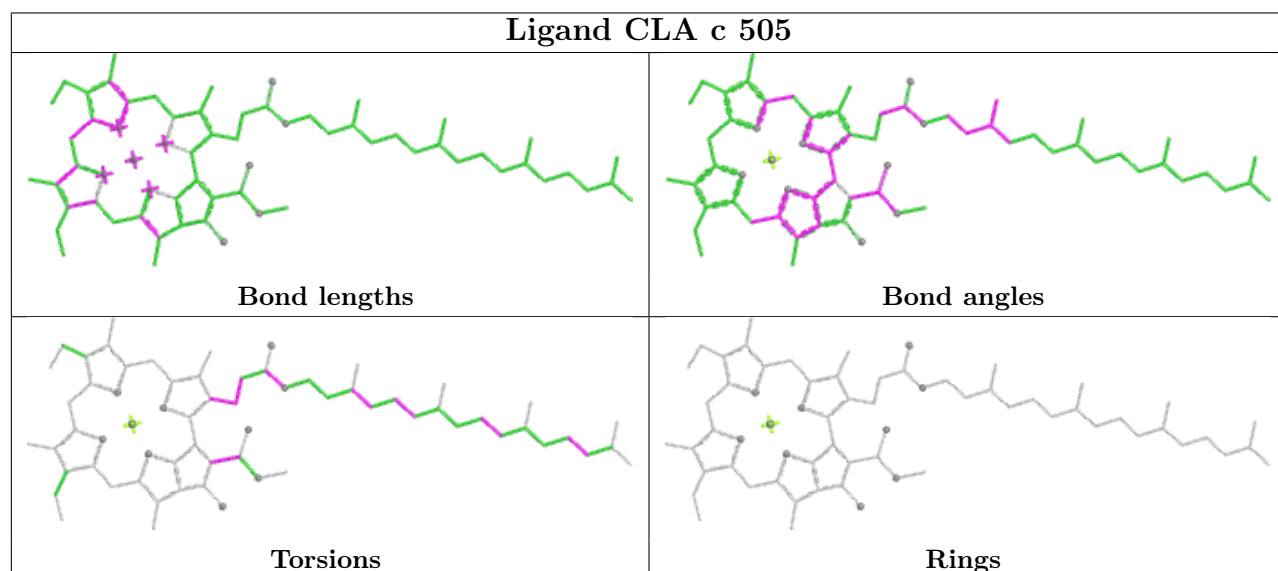
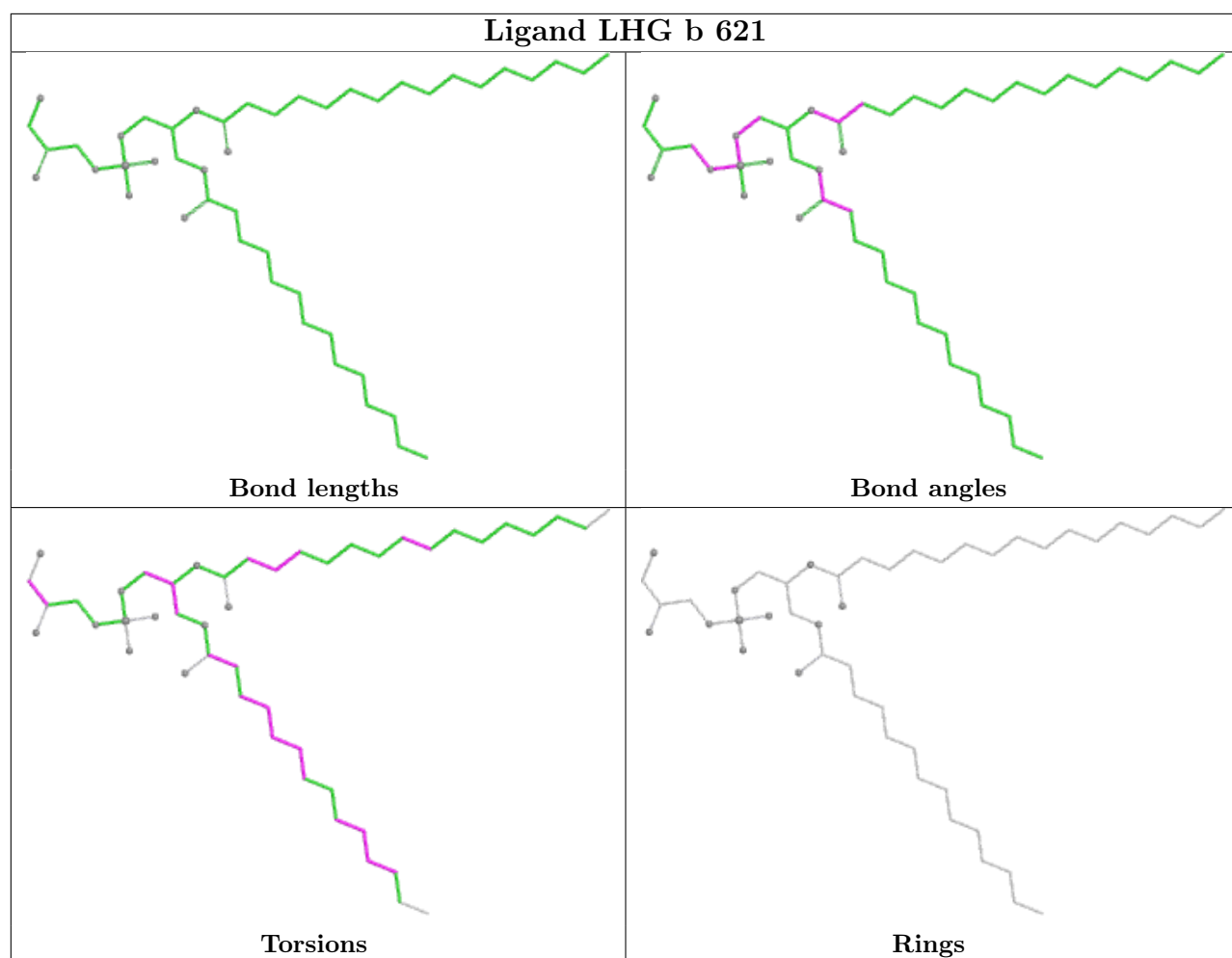


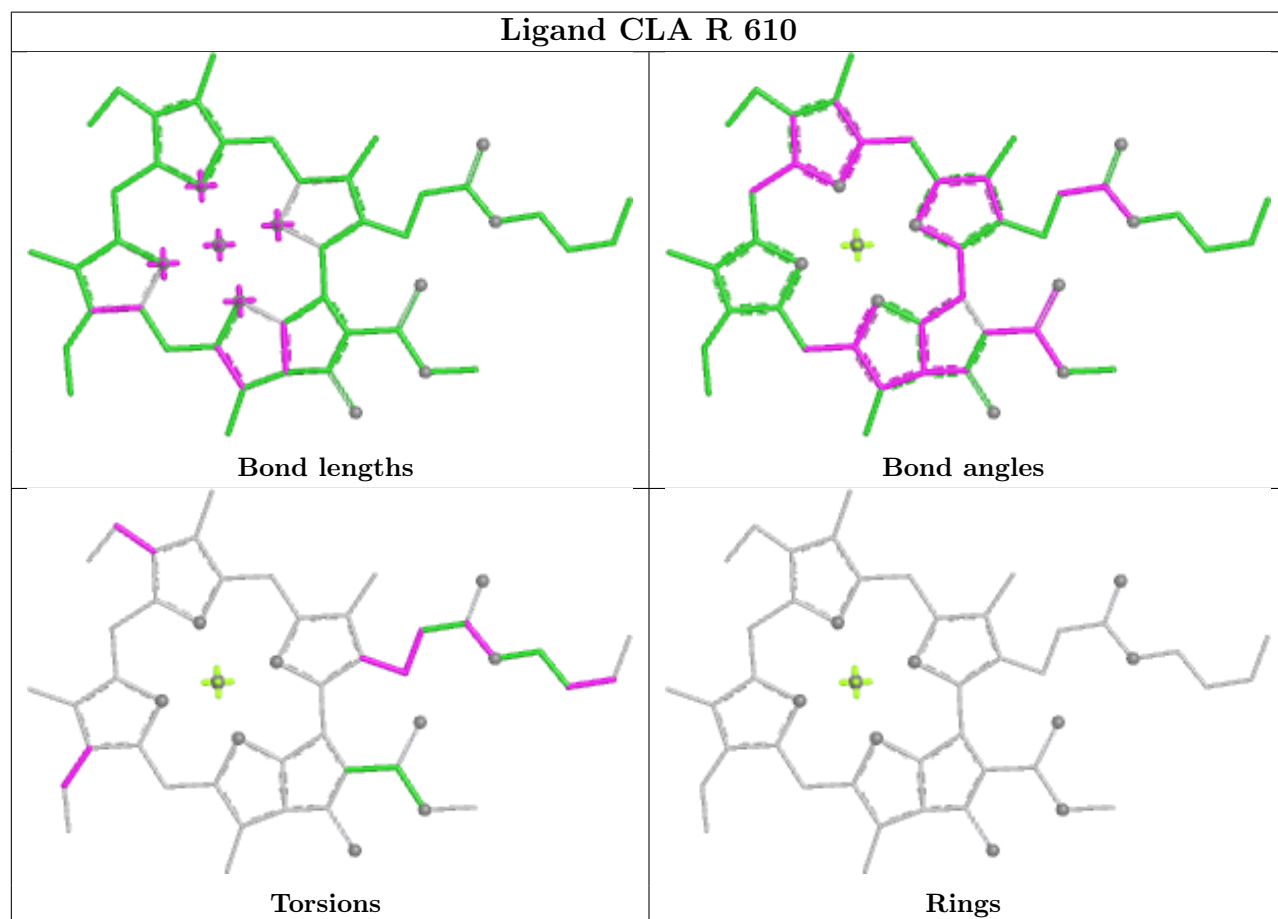
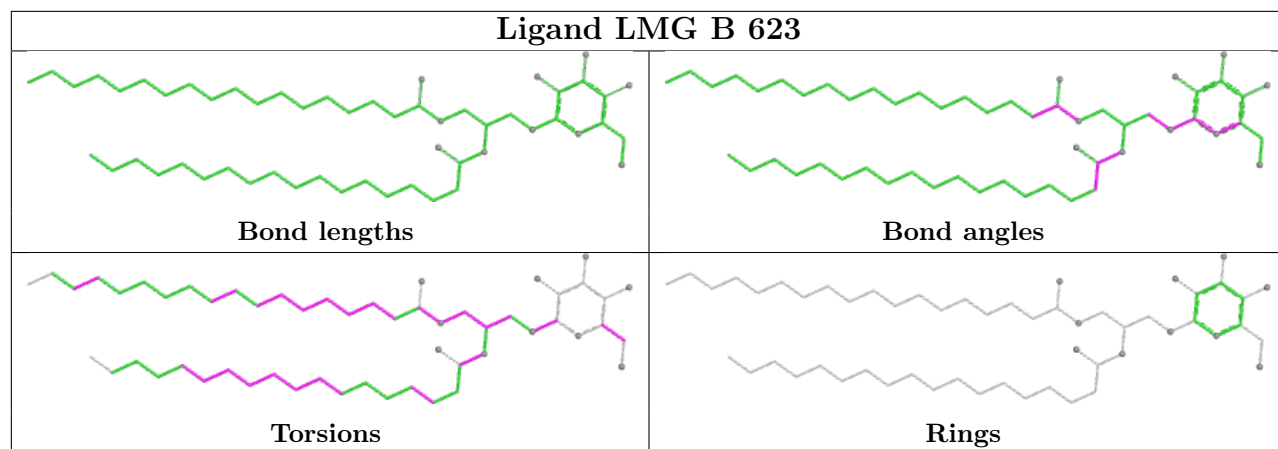
Ligand CLA R 611

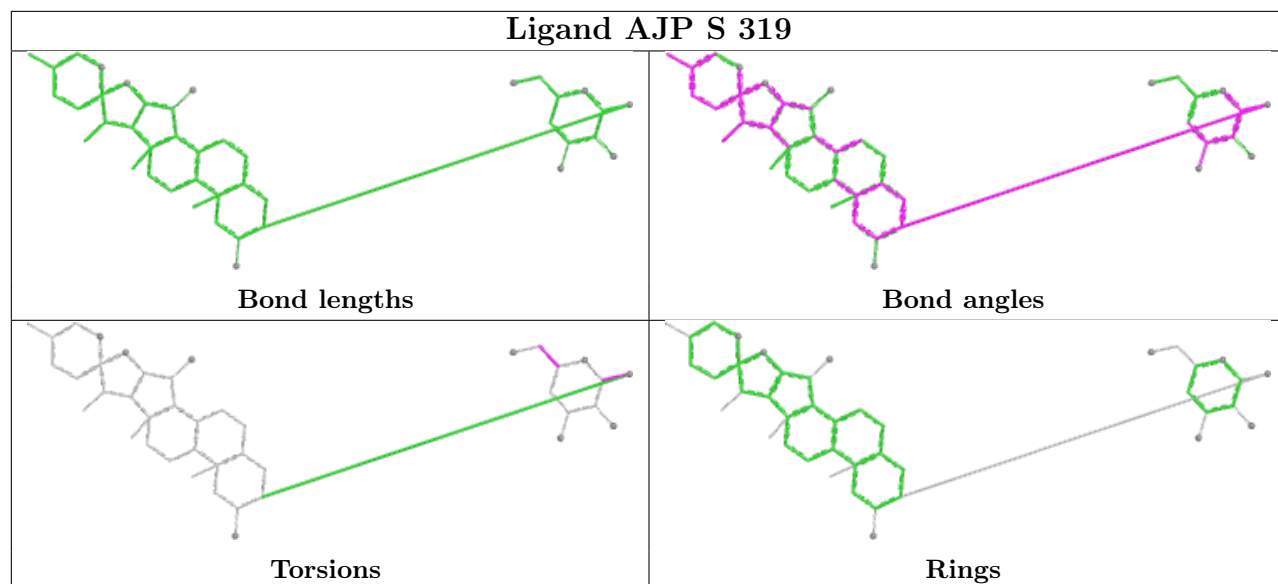
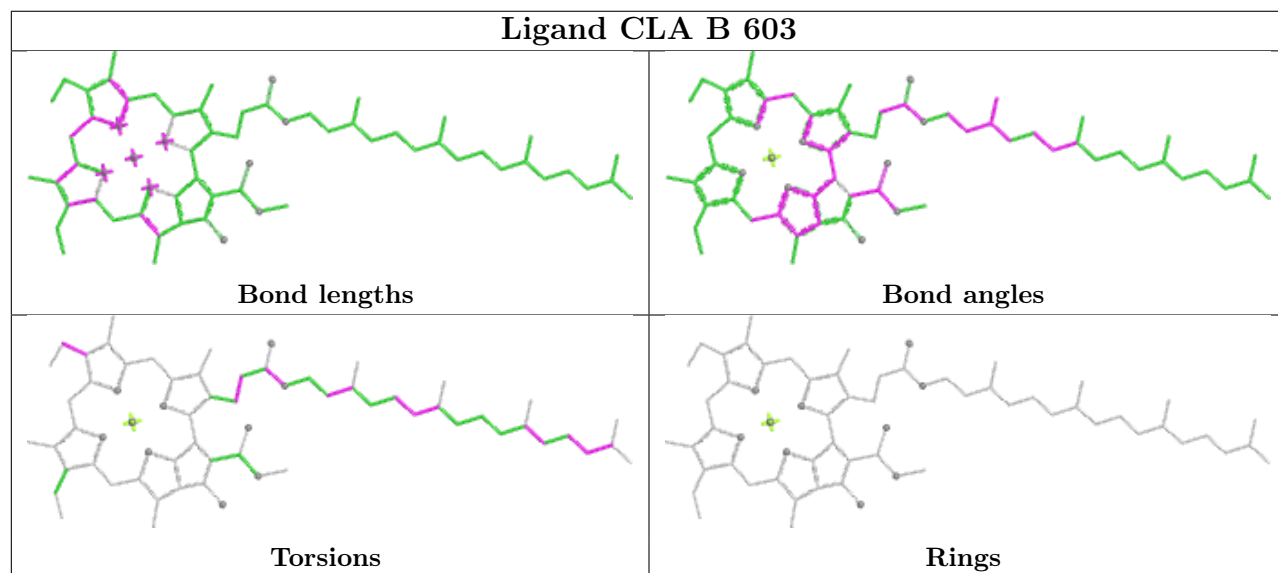


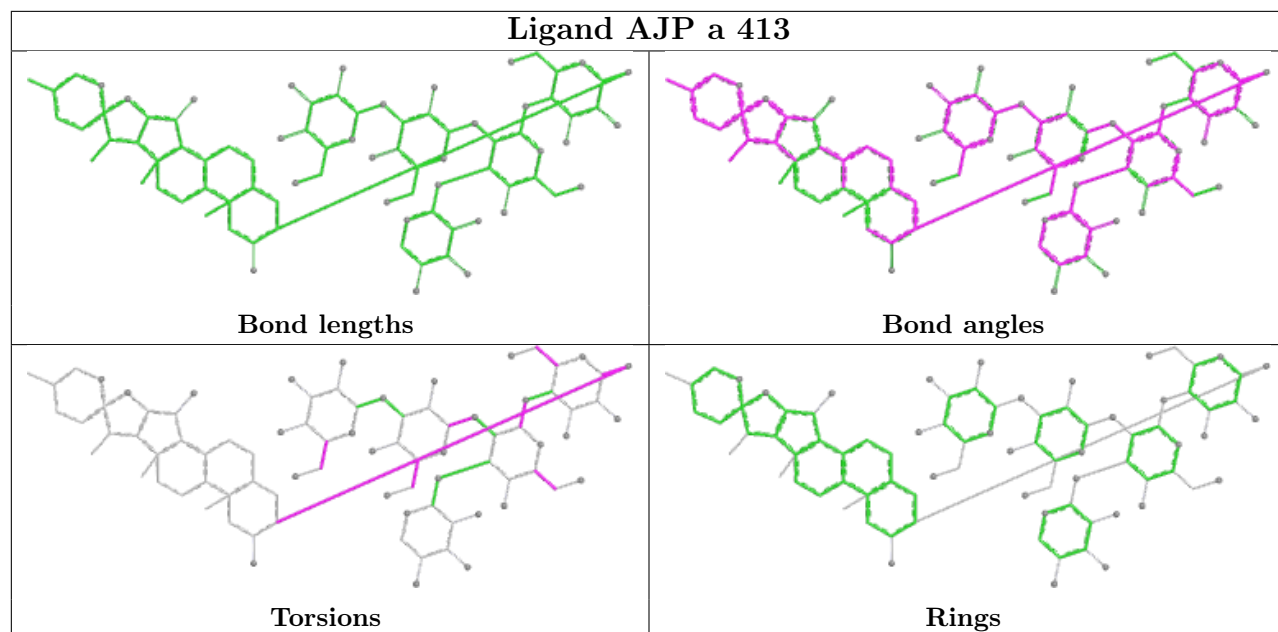
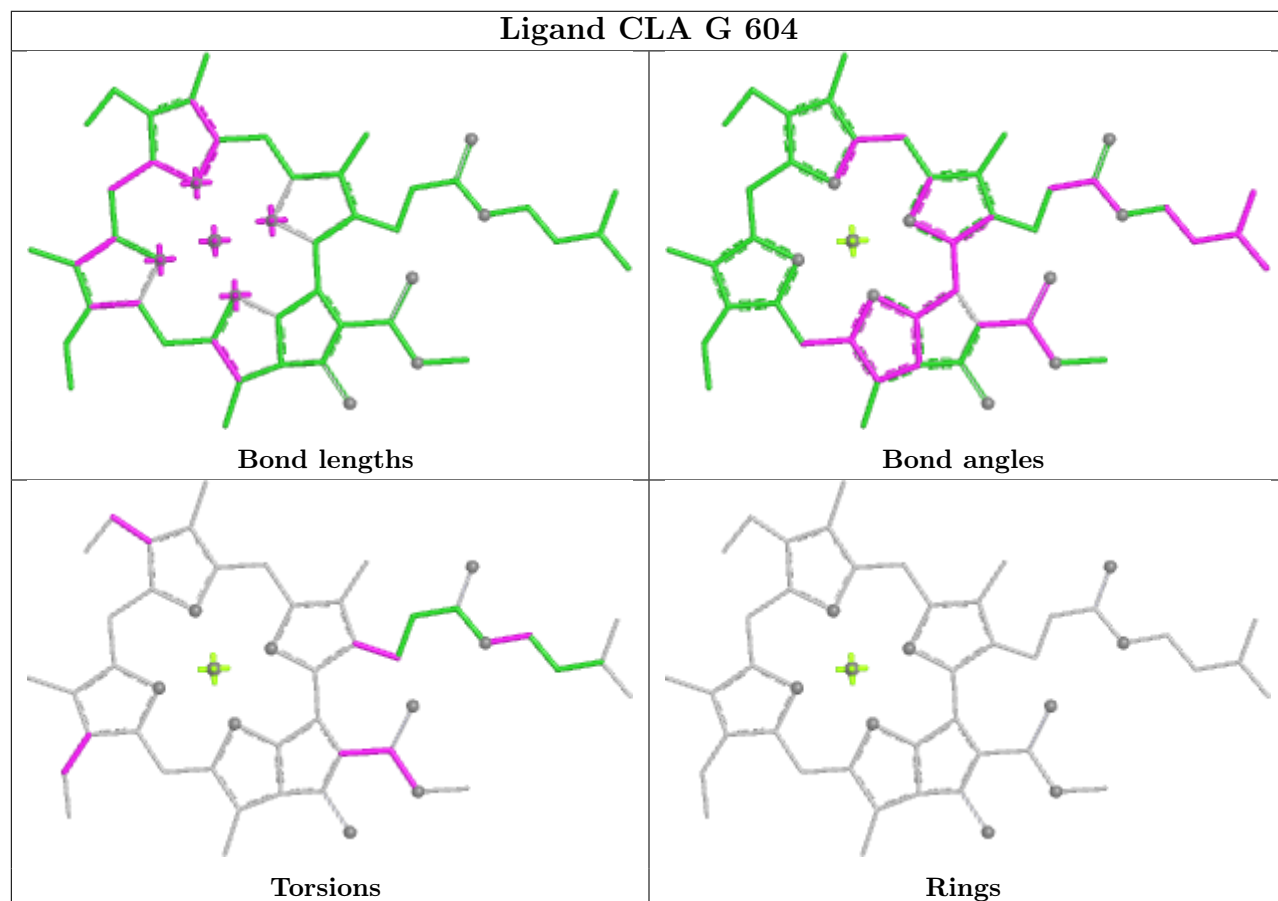
Ligand CLA B 606

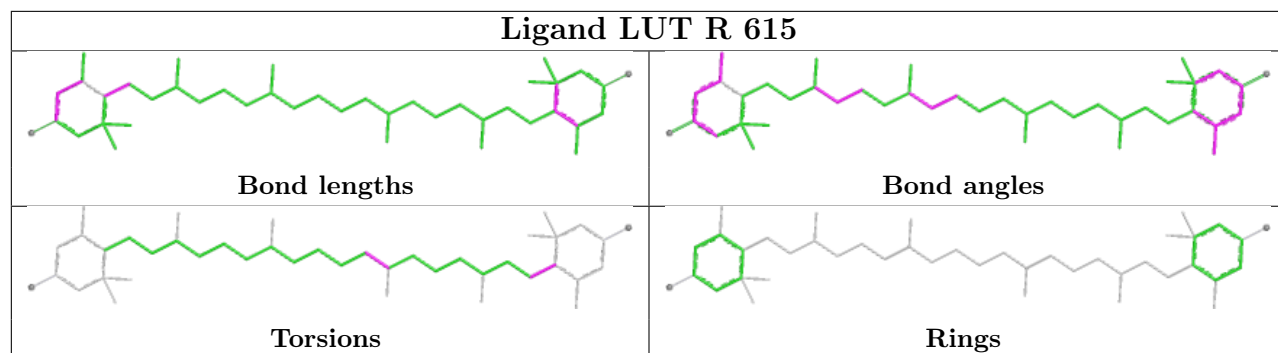
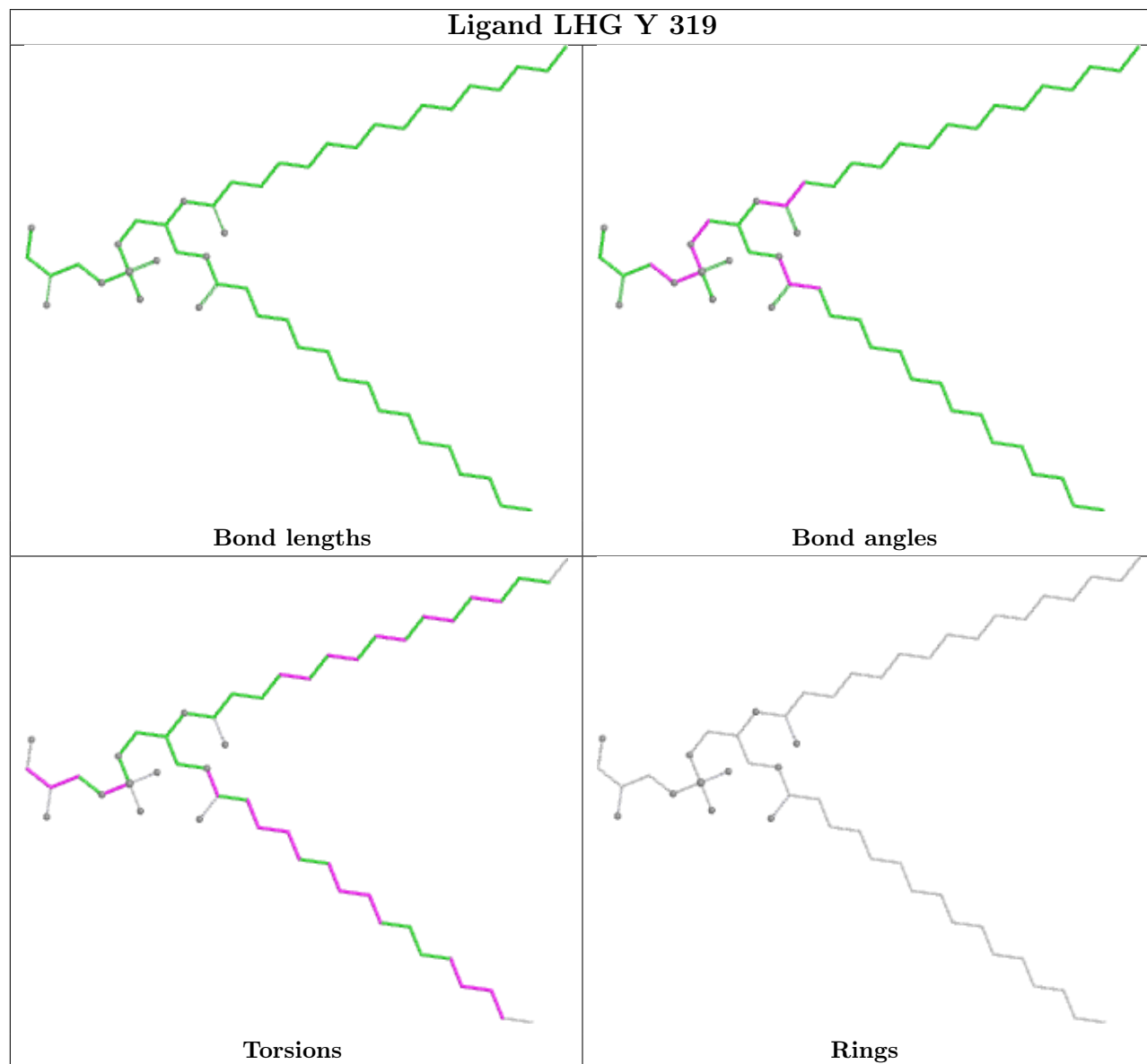


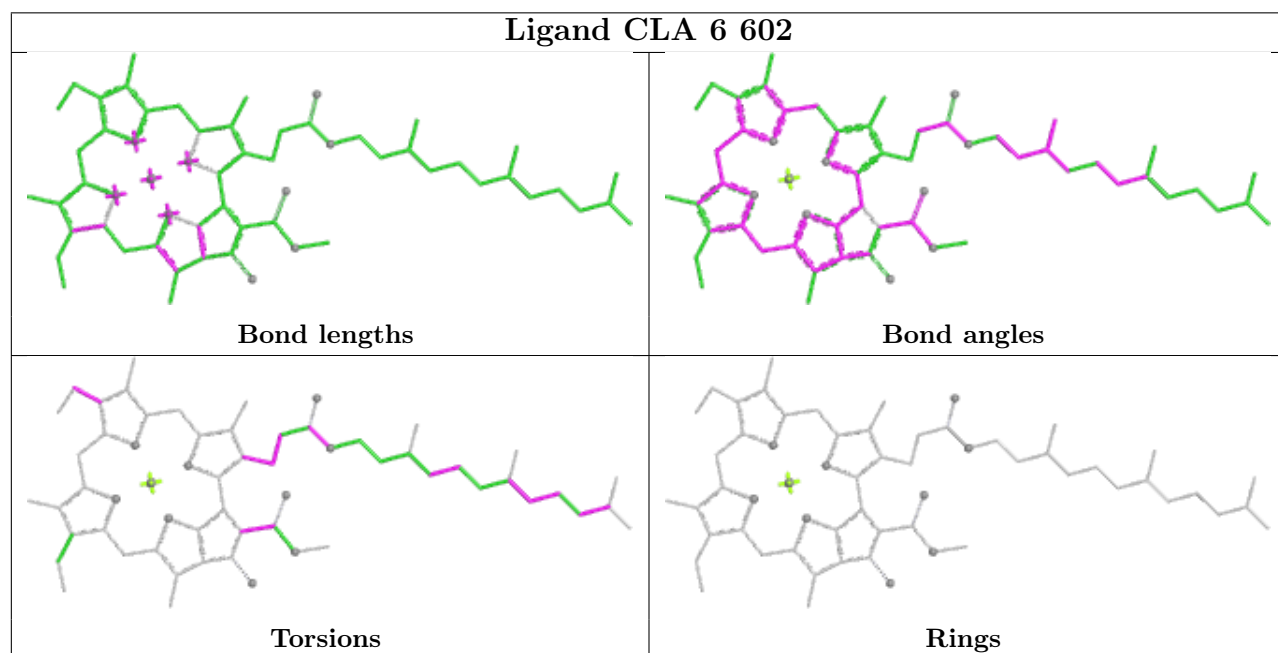
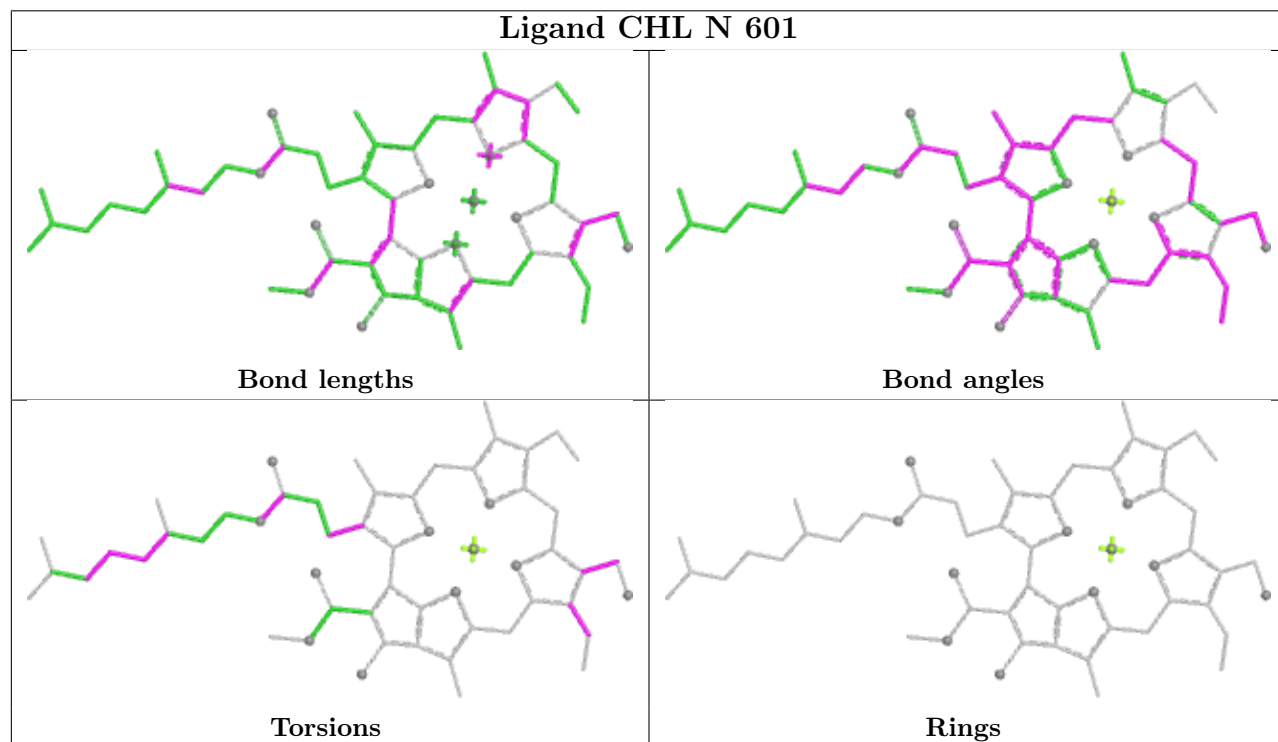
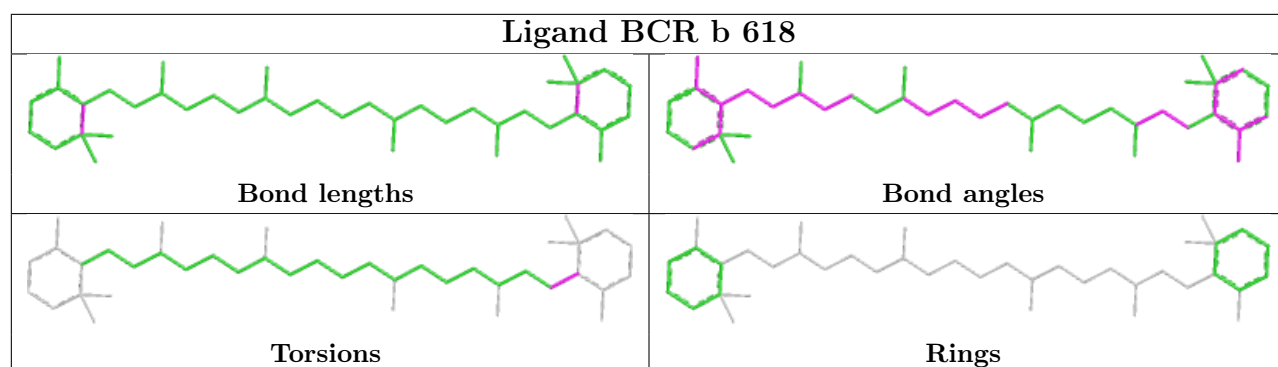


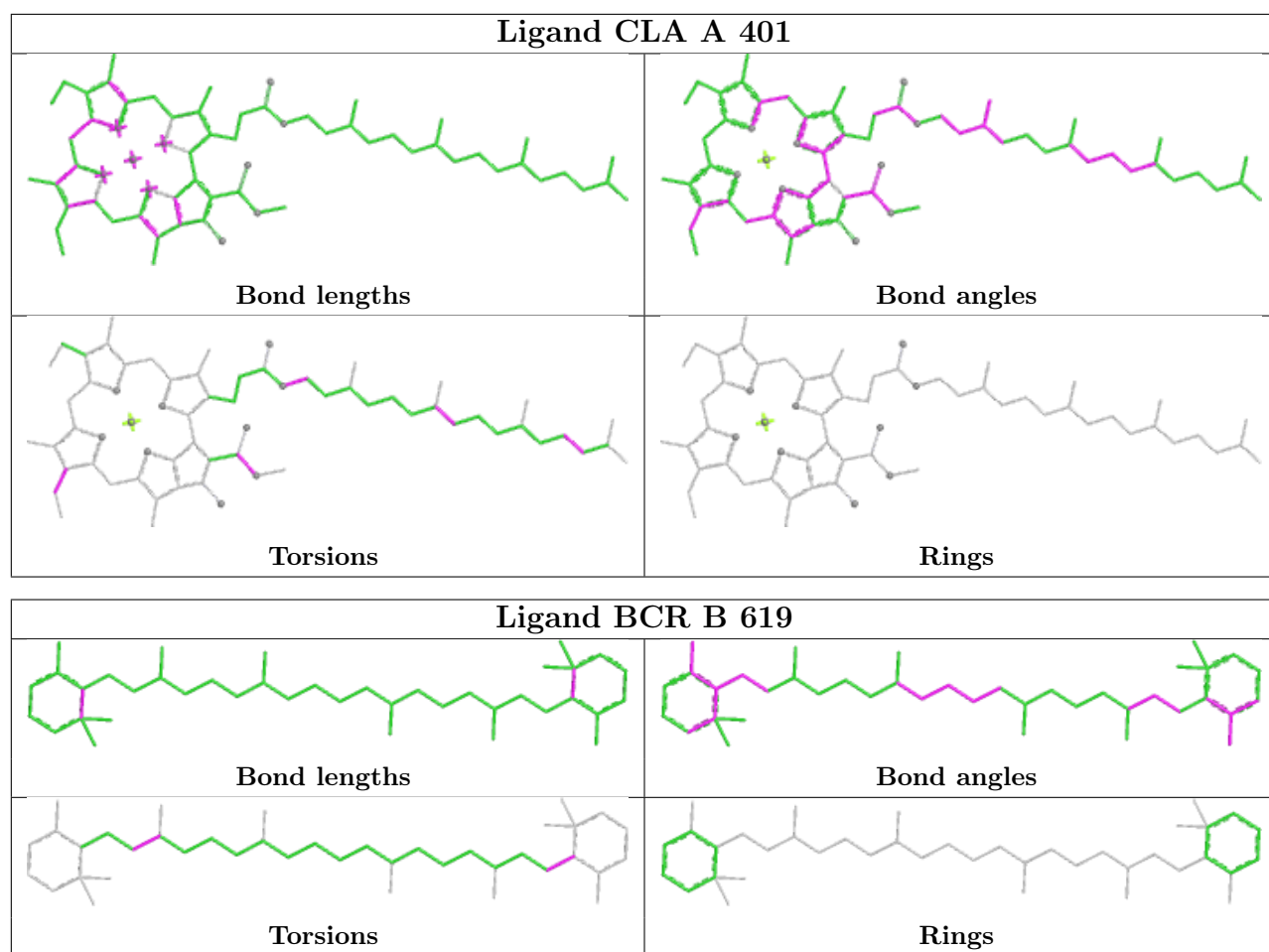


Ligand AJP S 319**Ligand CLA B 603**

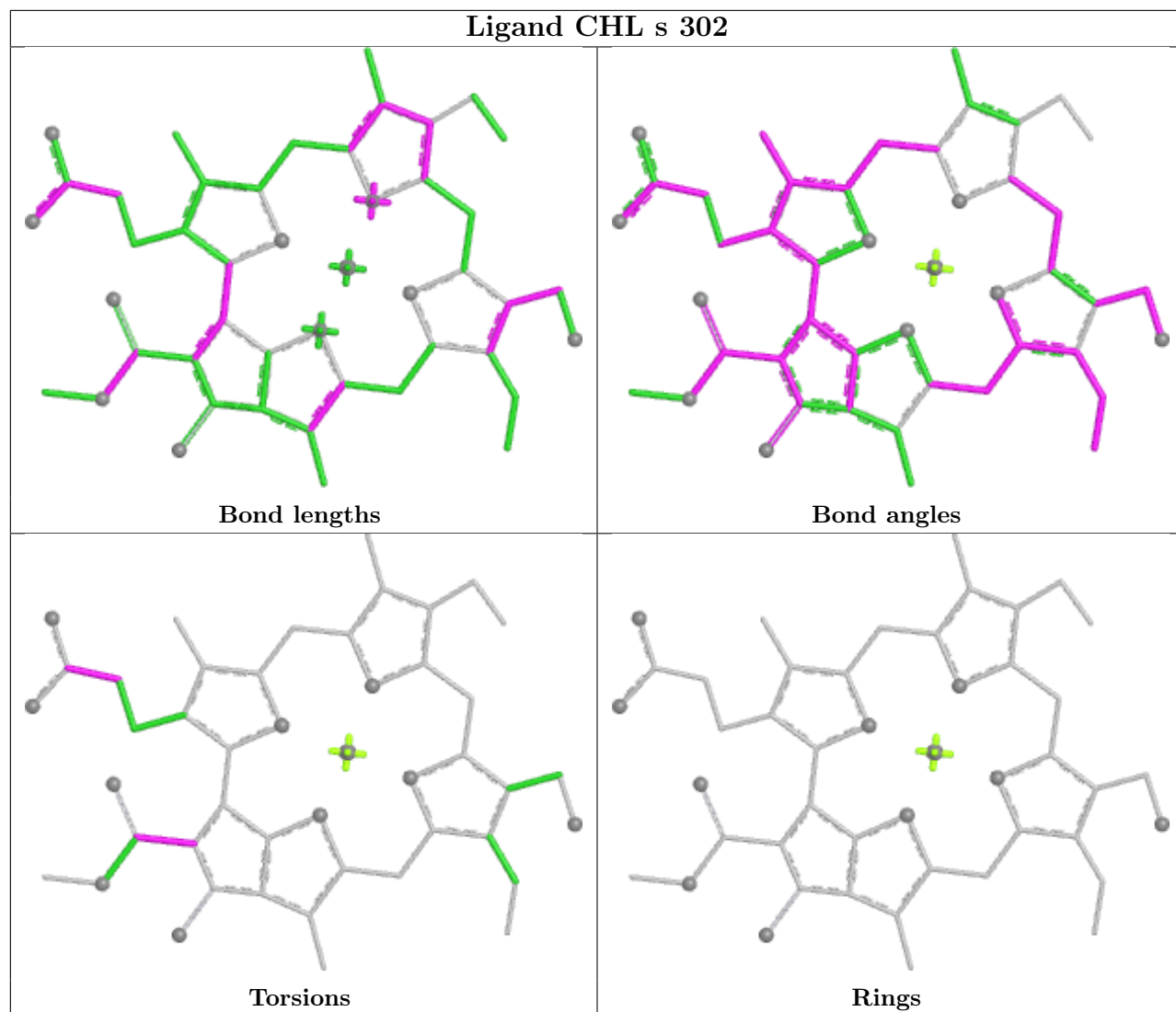
Ligand AJP a 413**Ligand CLA G 604**

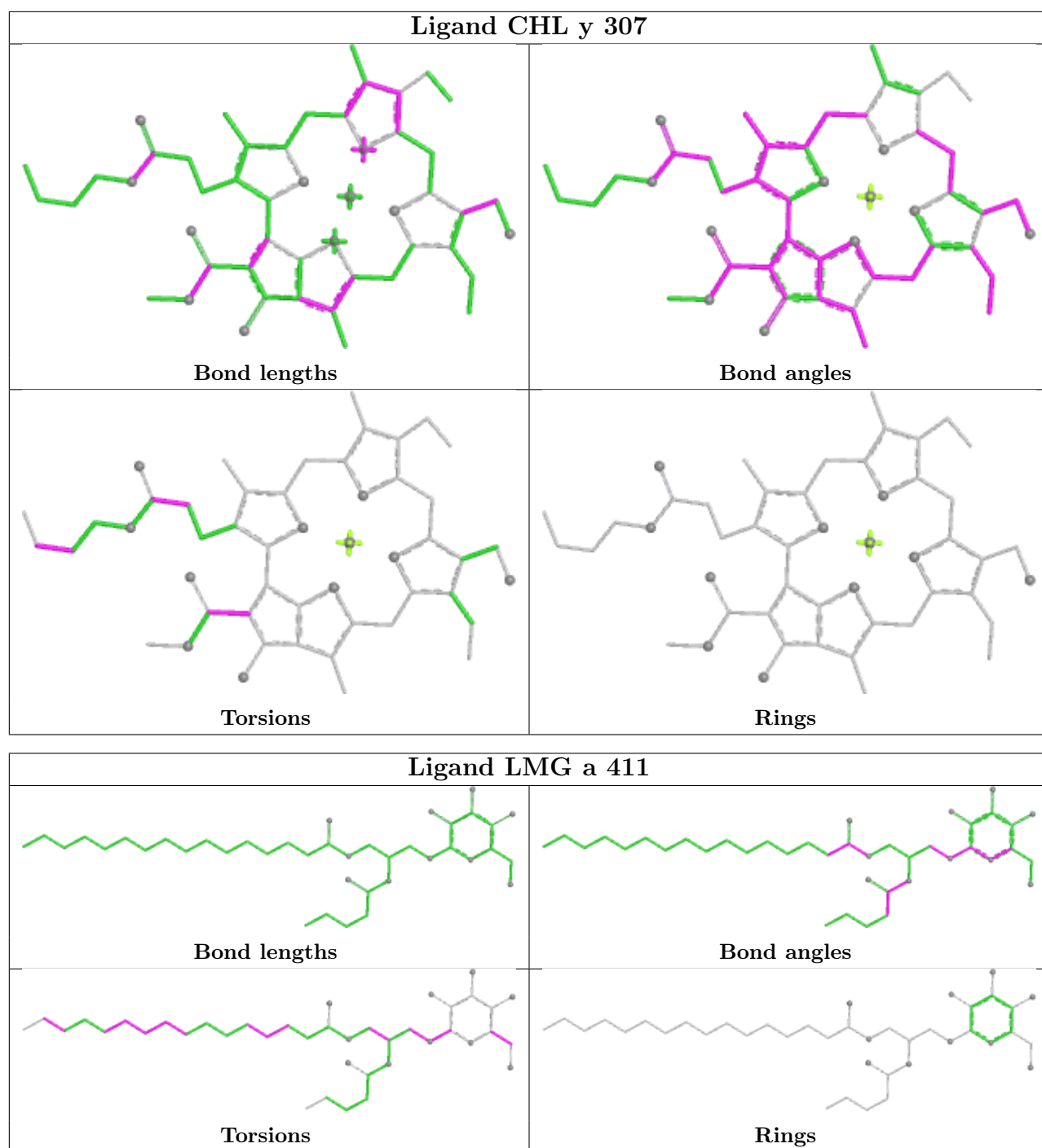
Ligand LUT R 615**Ligand LHG Y 319**



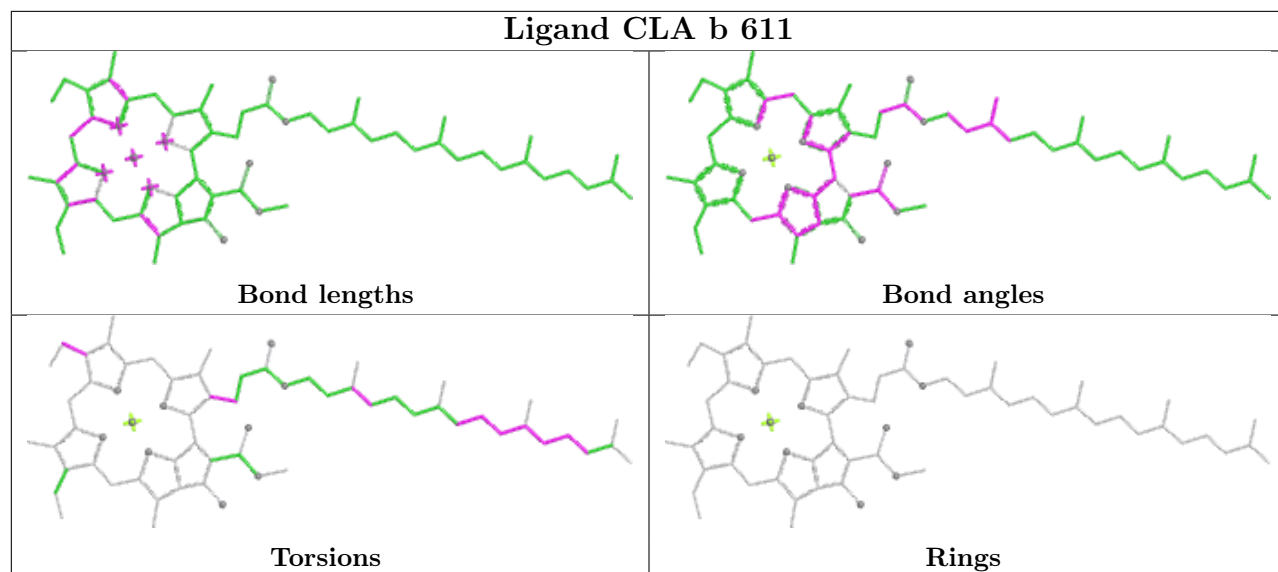


Ligand CHL s 302

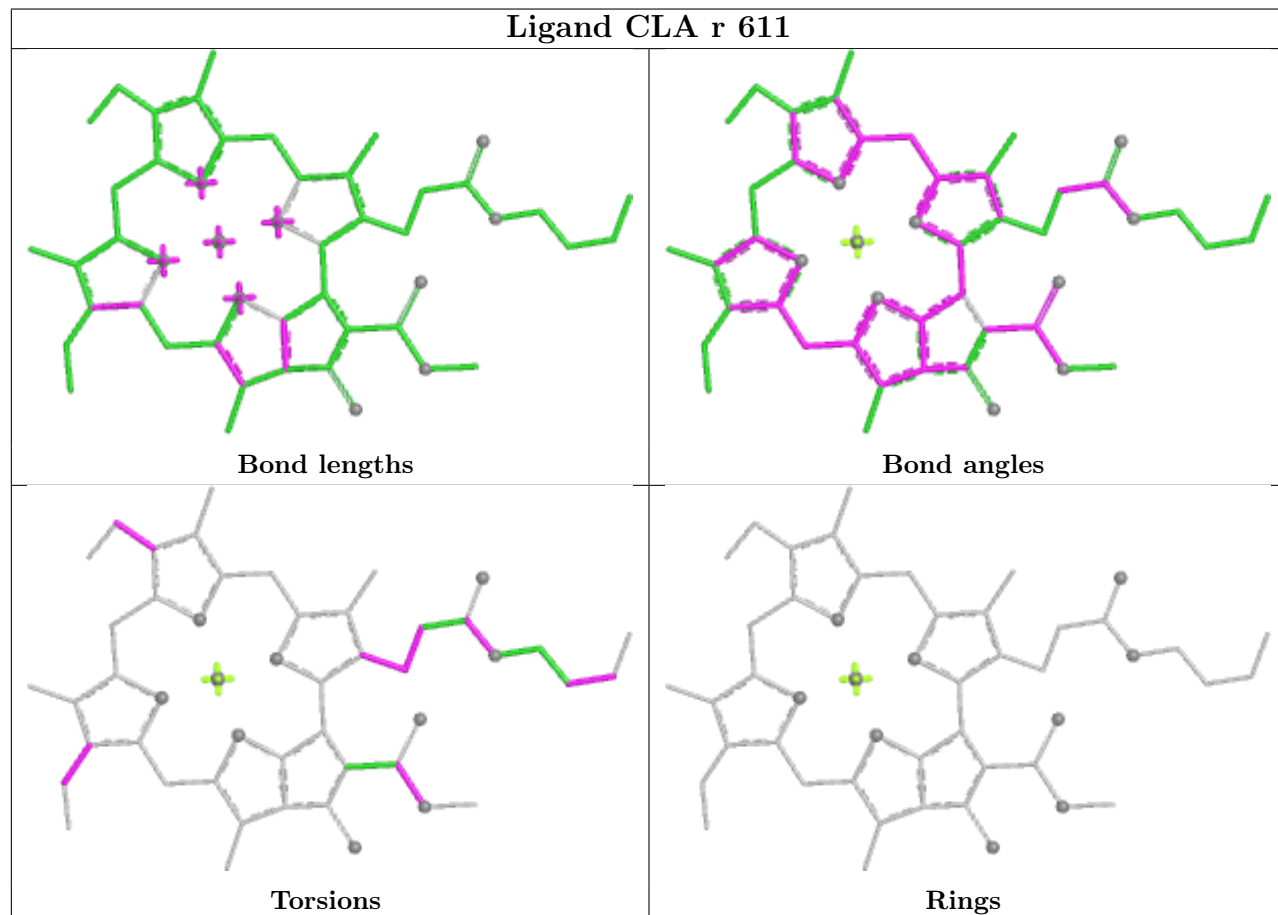


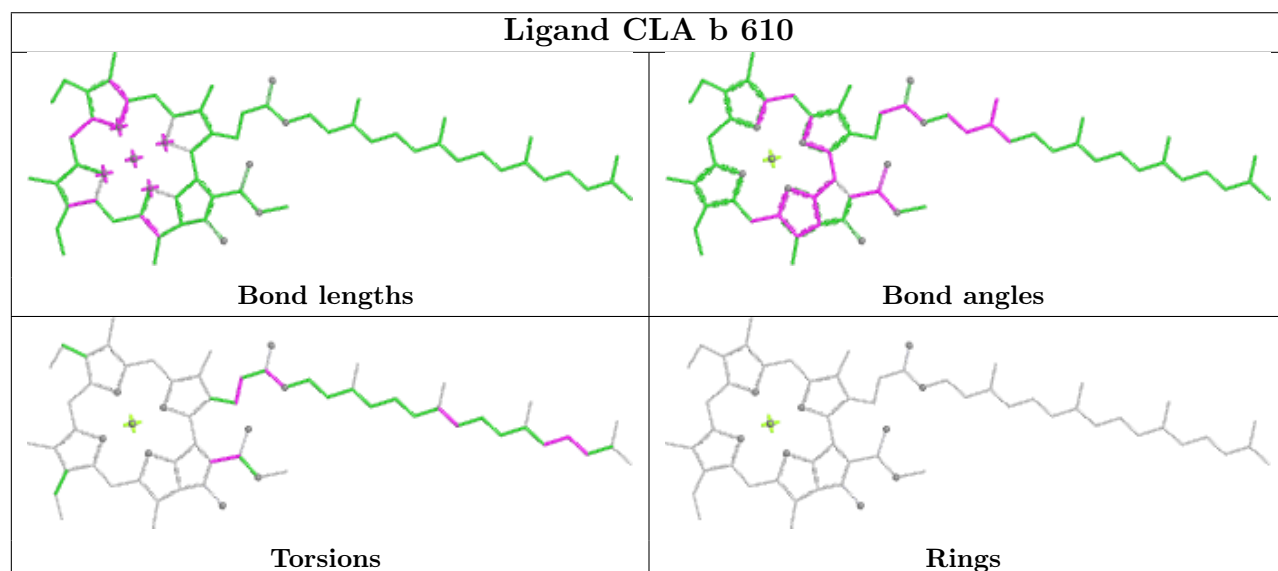
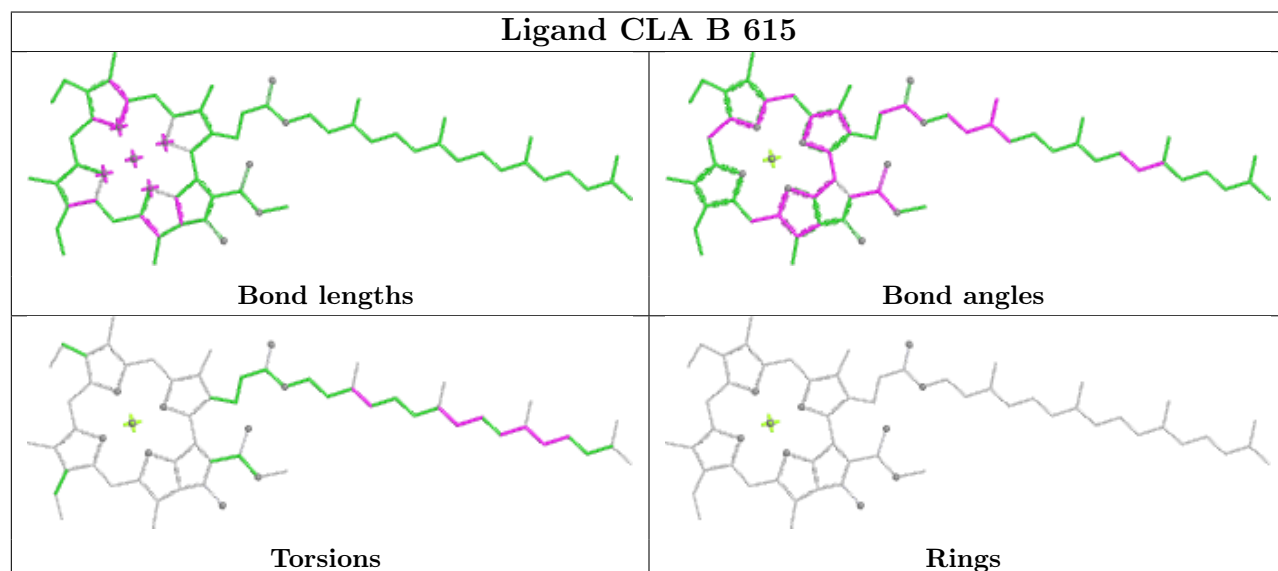
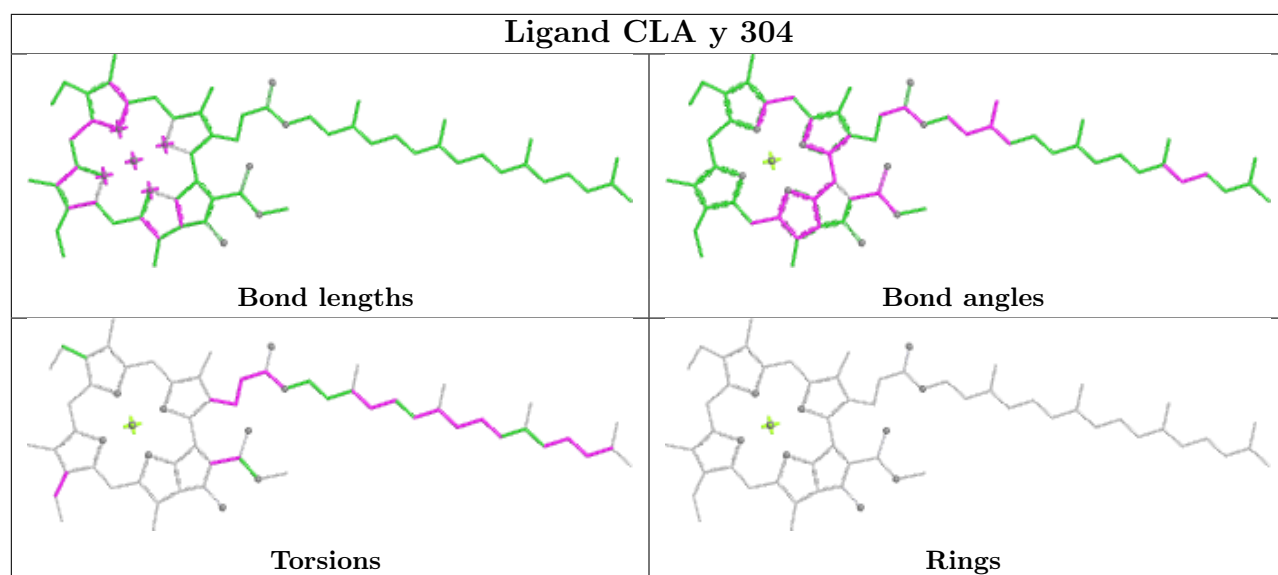


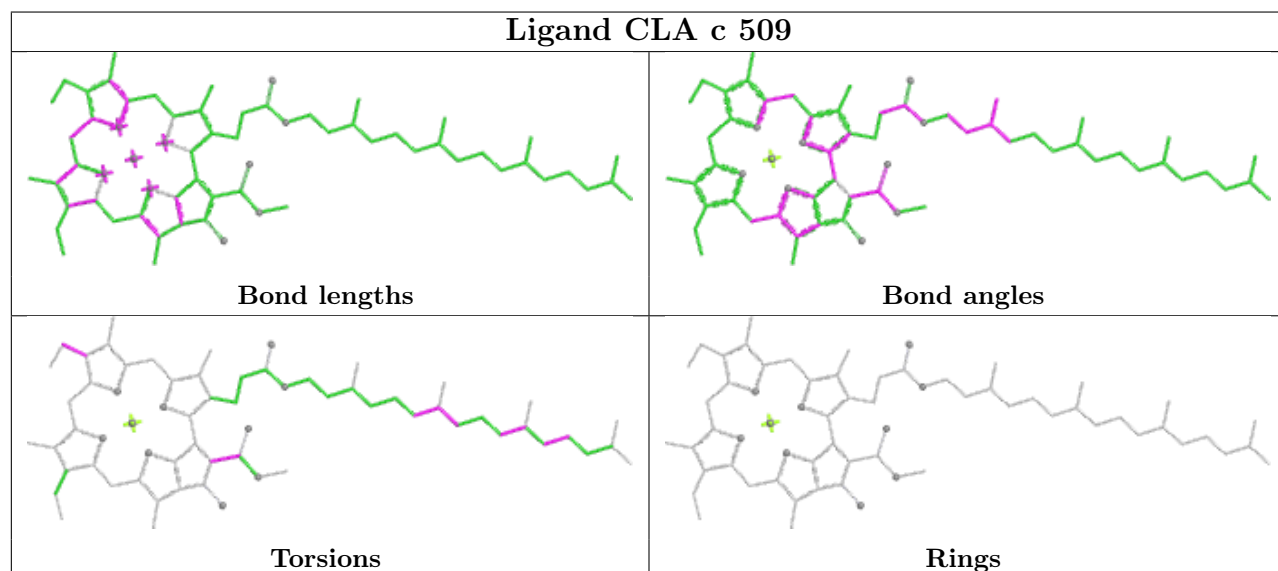
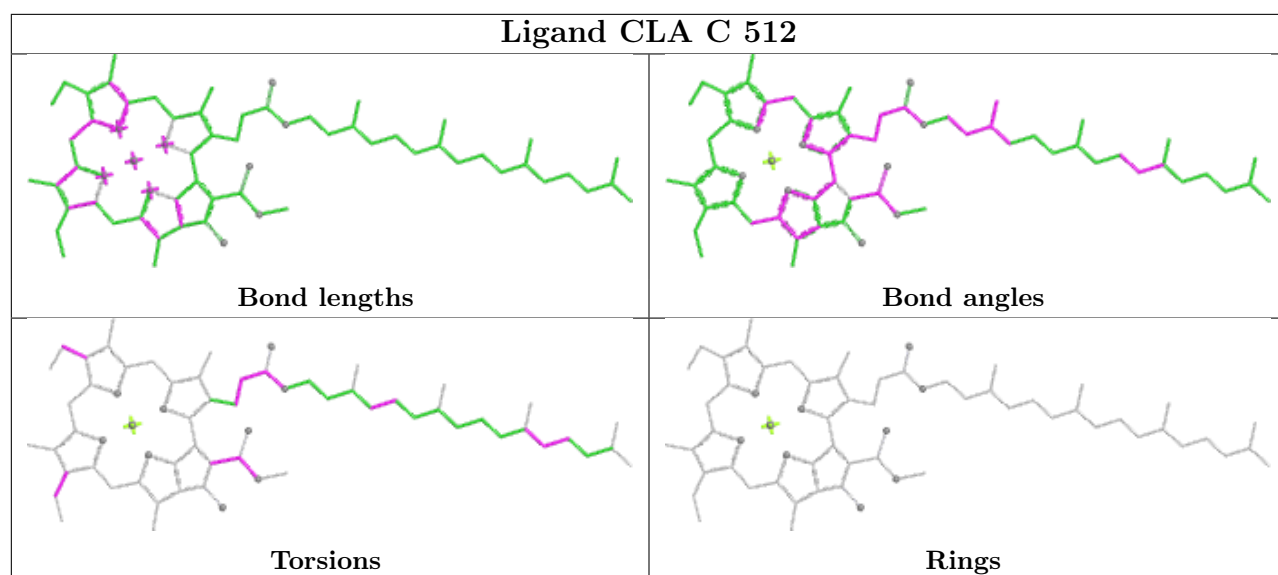
Ligand CLA b 611



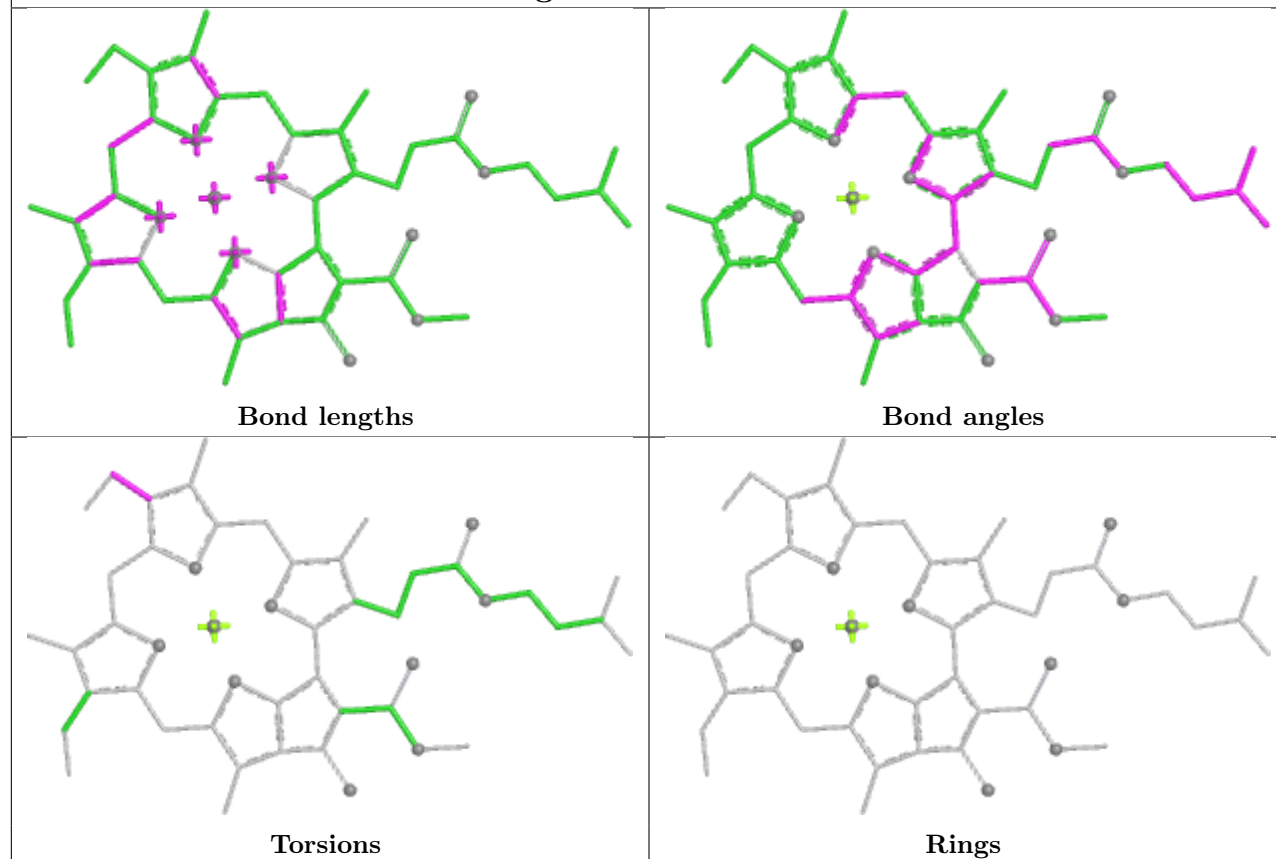
Ligand CLA r 611



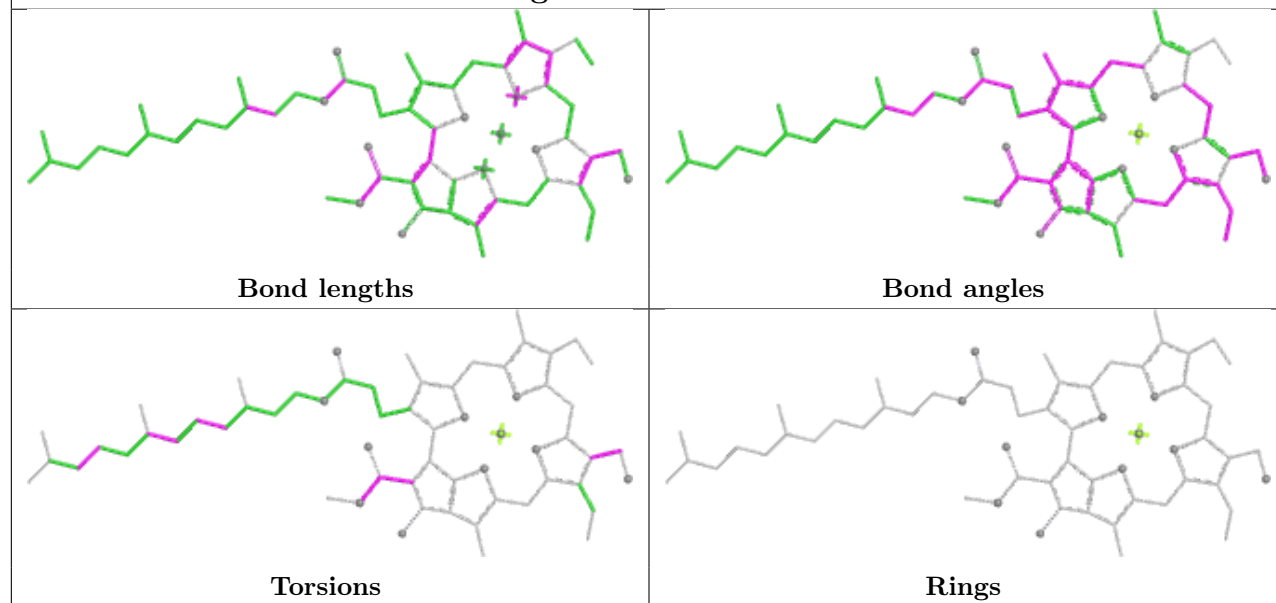




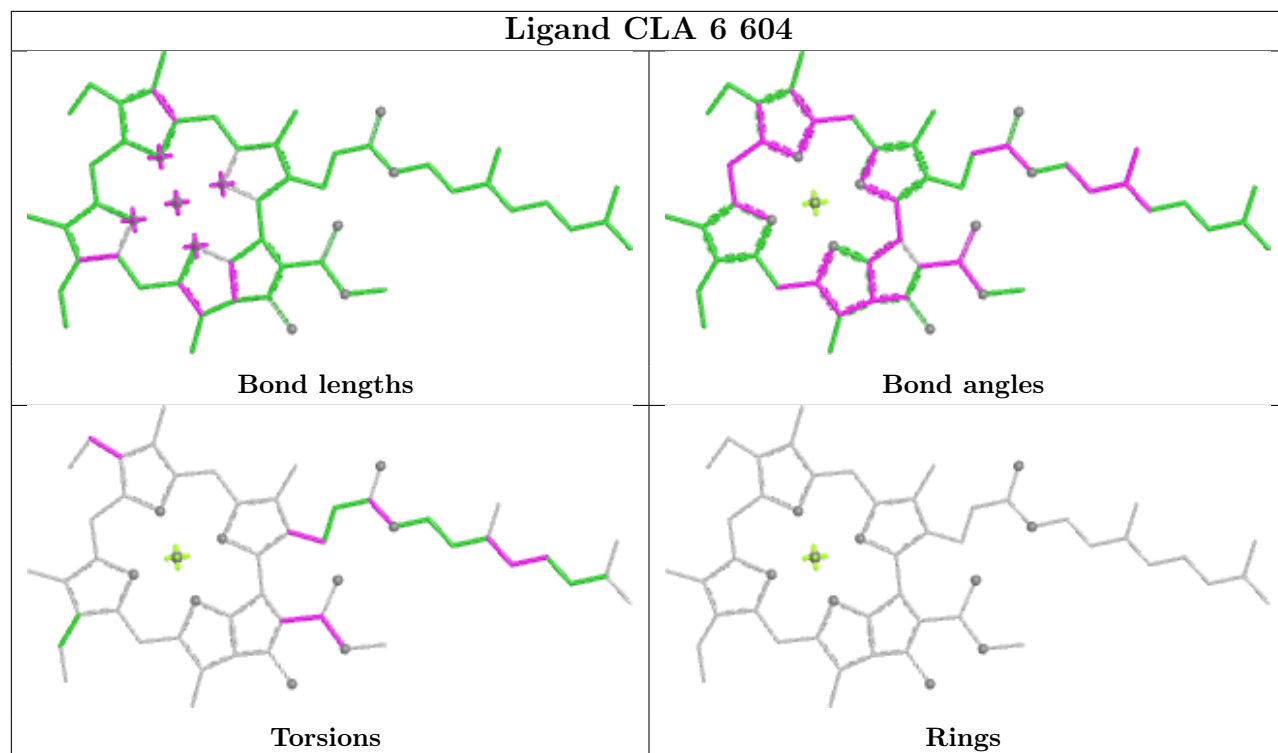
Ligand CLA d 401



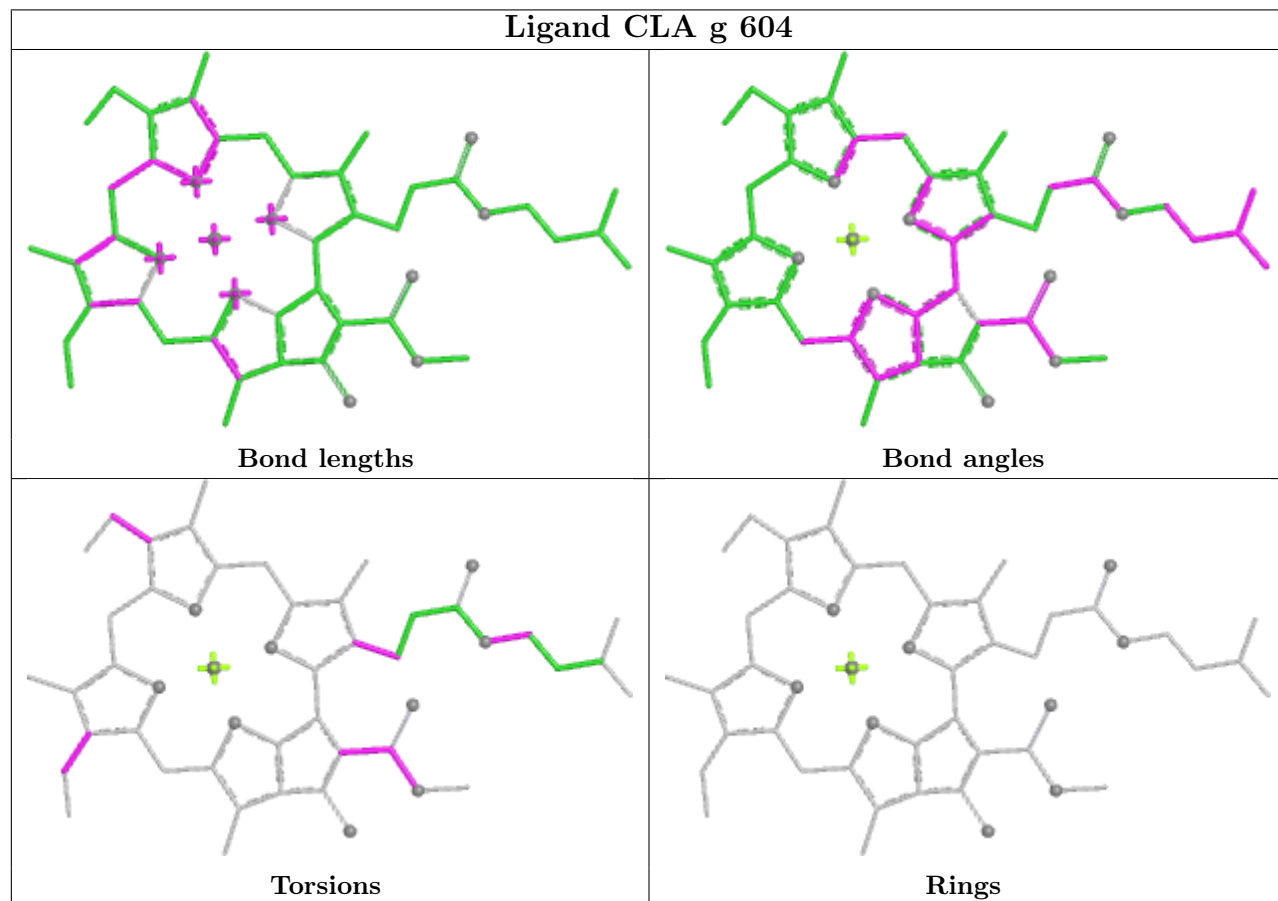
Ligand CHL G 609

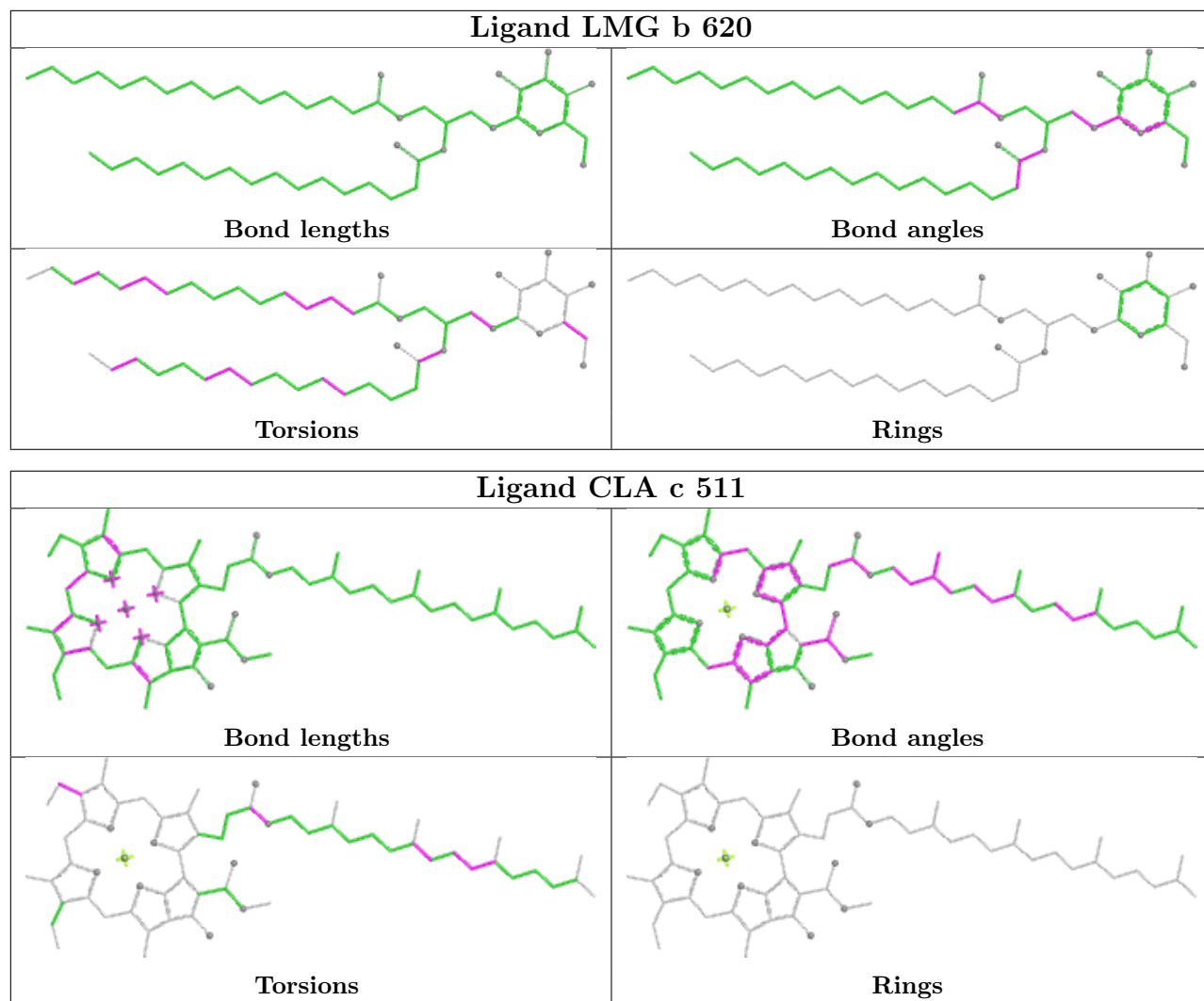


Ligand CLA 6 604

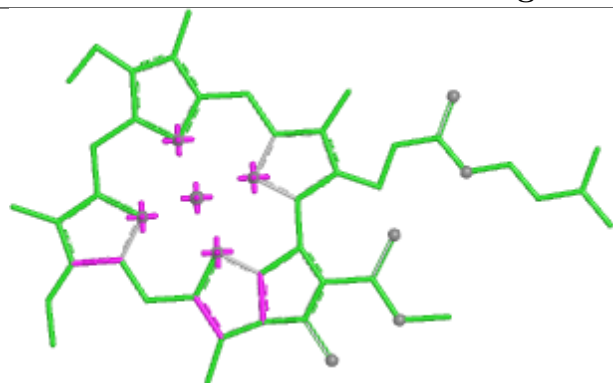


Ligand CLA g 604

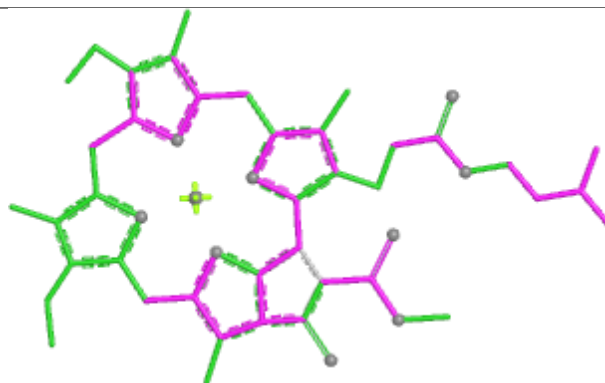




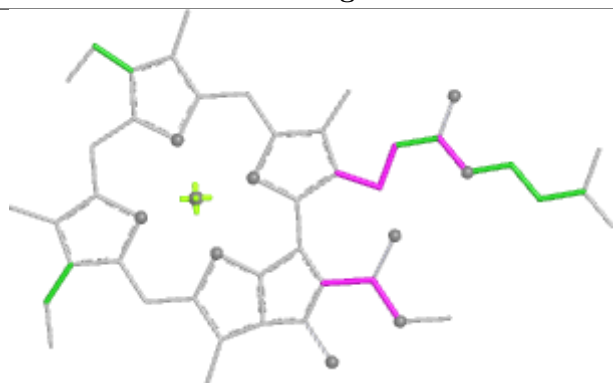
Ligand CLA S 305



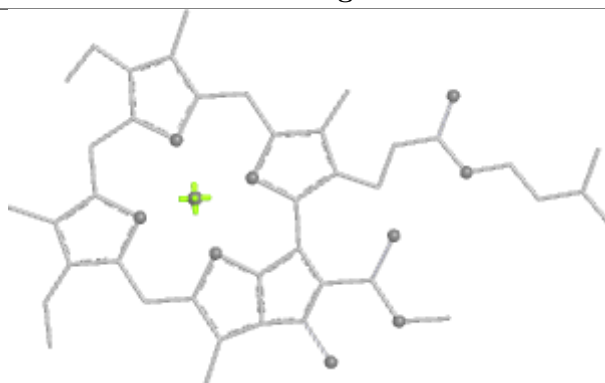
Bond lengths



Bond angles

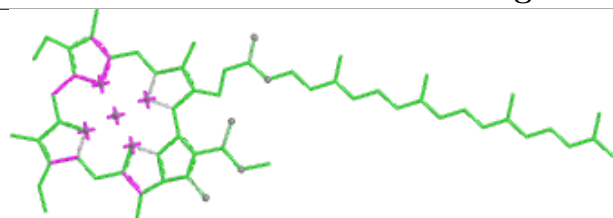


Torsions

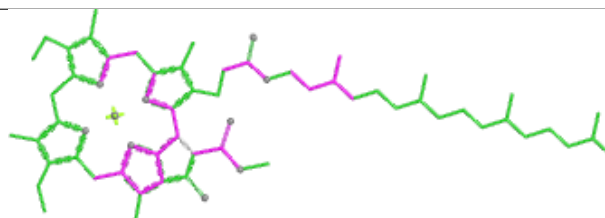


Rings

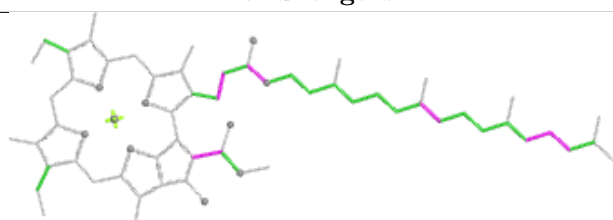
Ligand CLA B 610



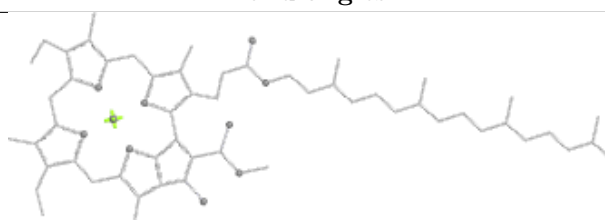
Bond lengths



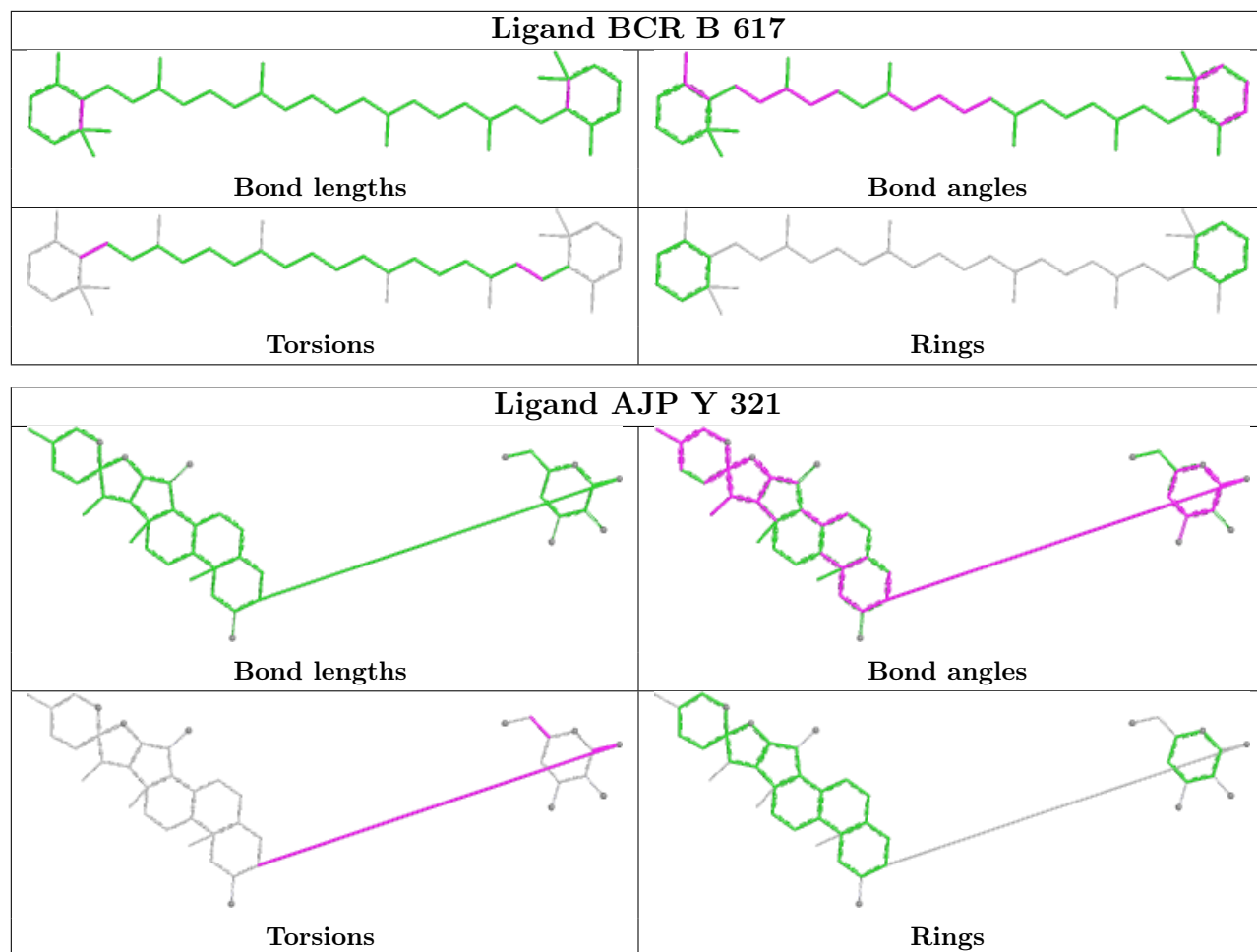
Bond angles



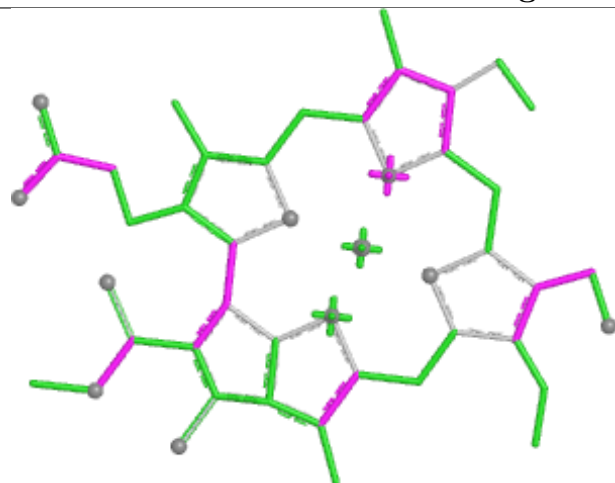
Torsions



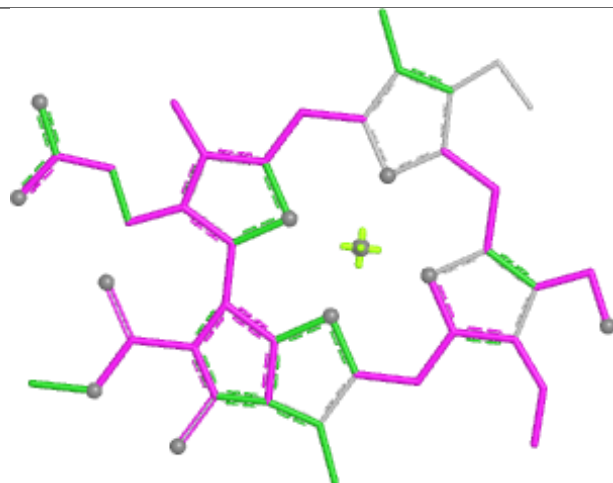
Rings



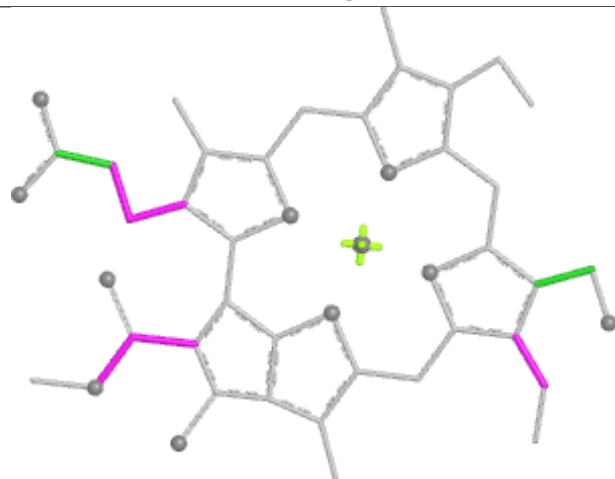
Ligand CHL S 307



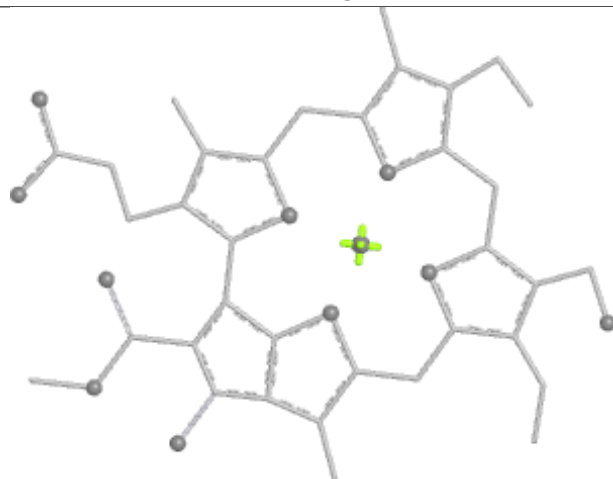
Bond lengths



Bond angles



Torsions

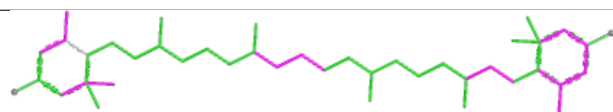


Rings

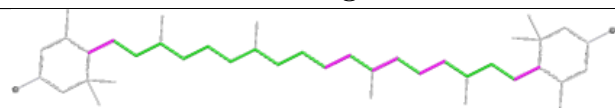
Ligand LUT N 615



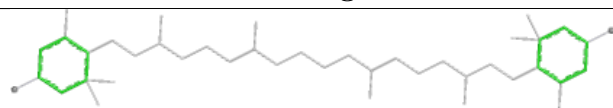
Bond lengths



Bond angles

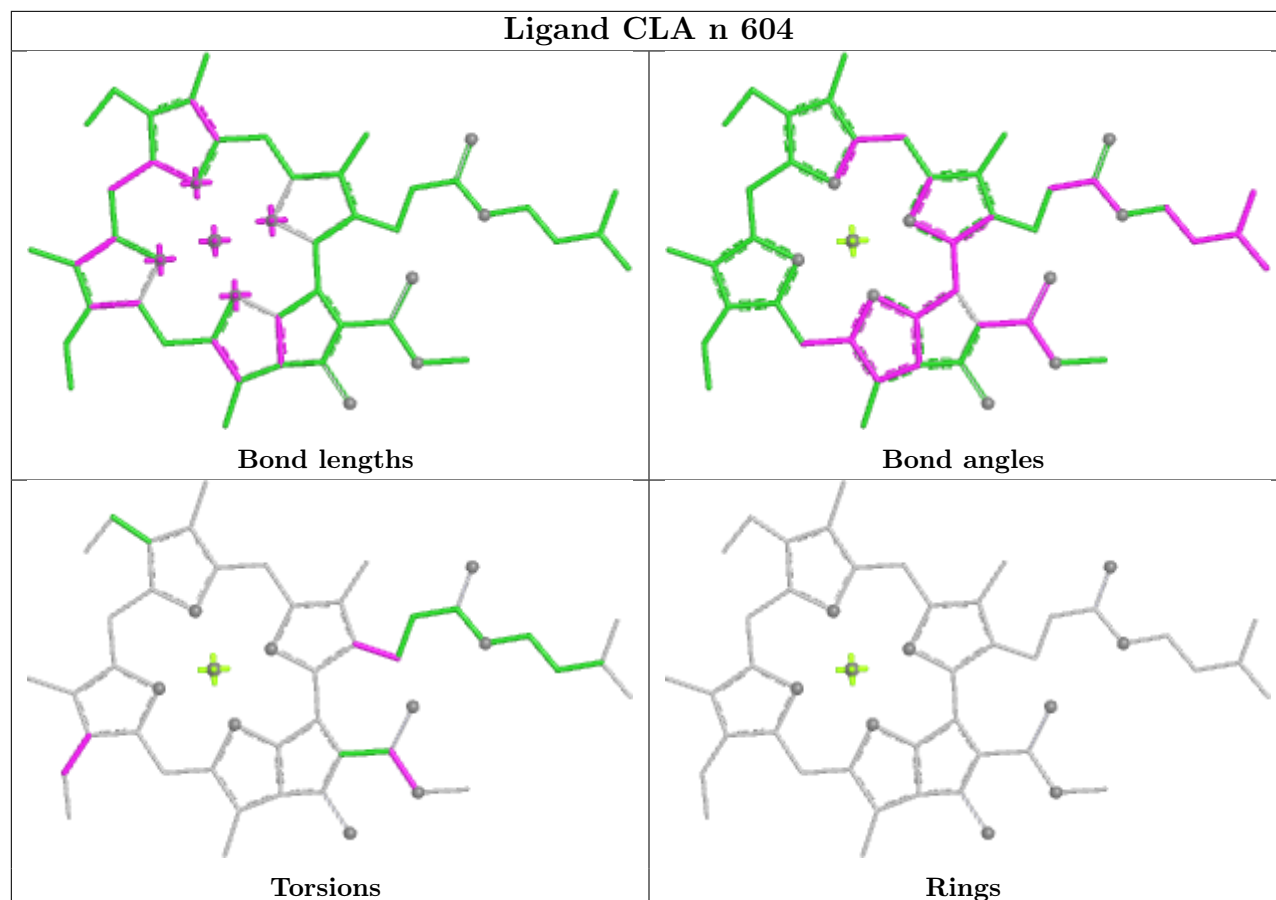


Torsions

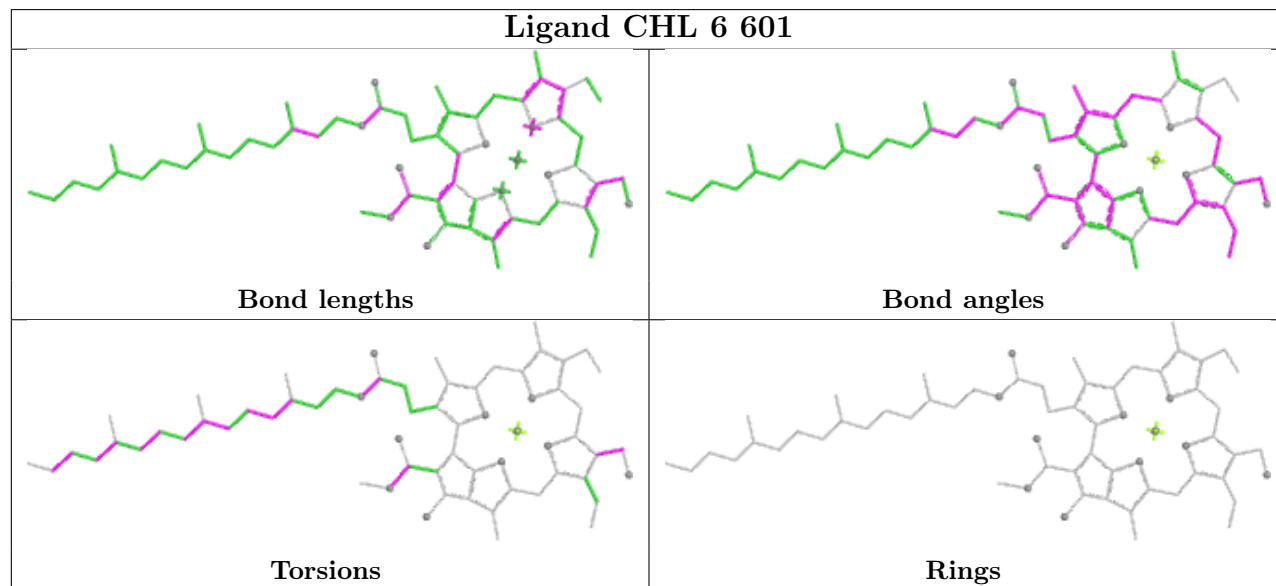


Rings

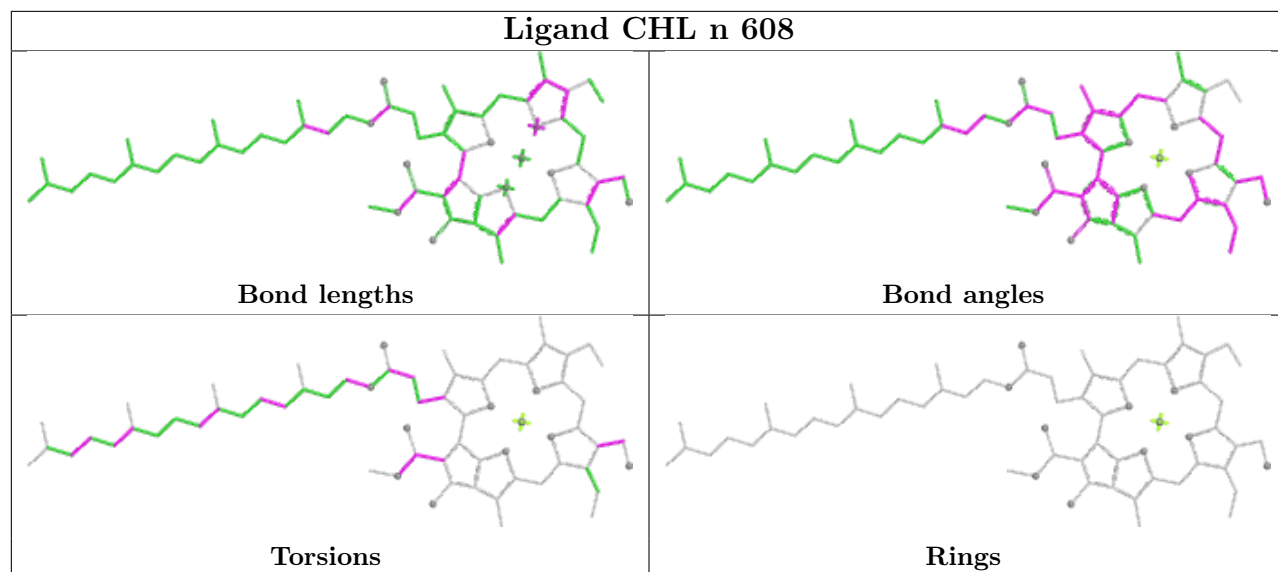
Ligand CLA n 604



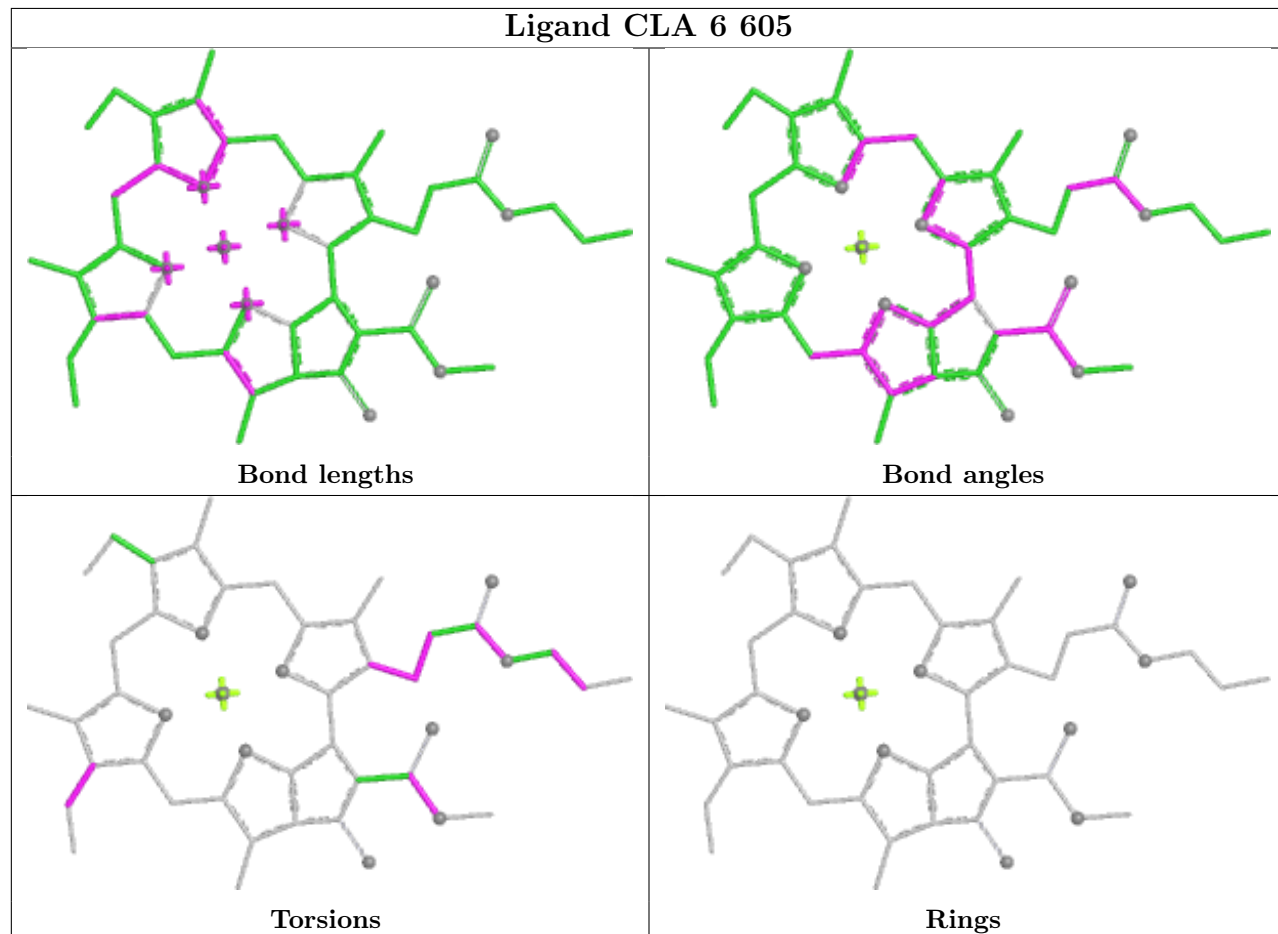
Ligand CHL 6 601



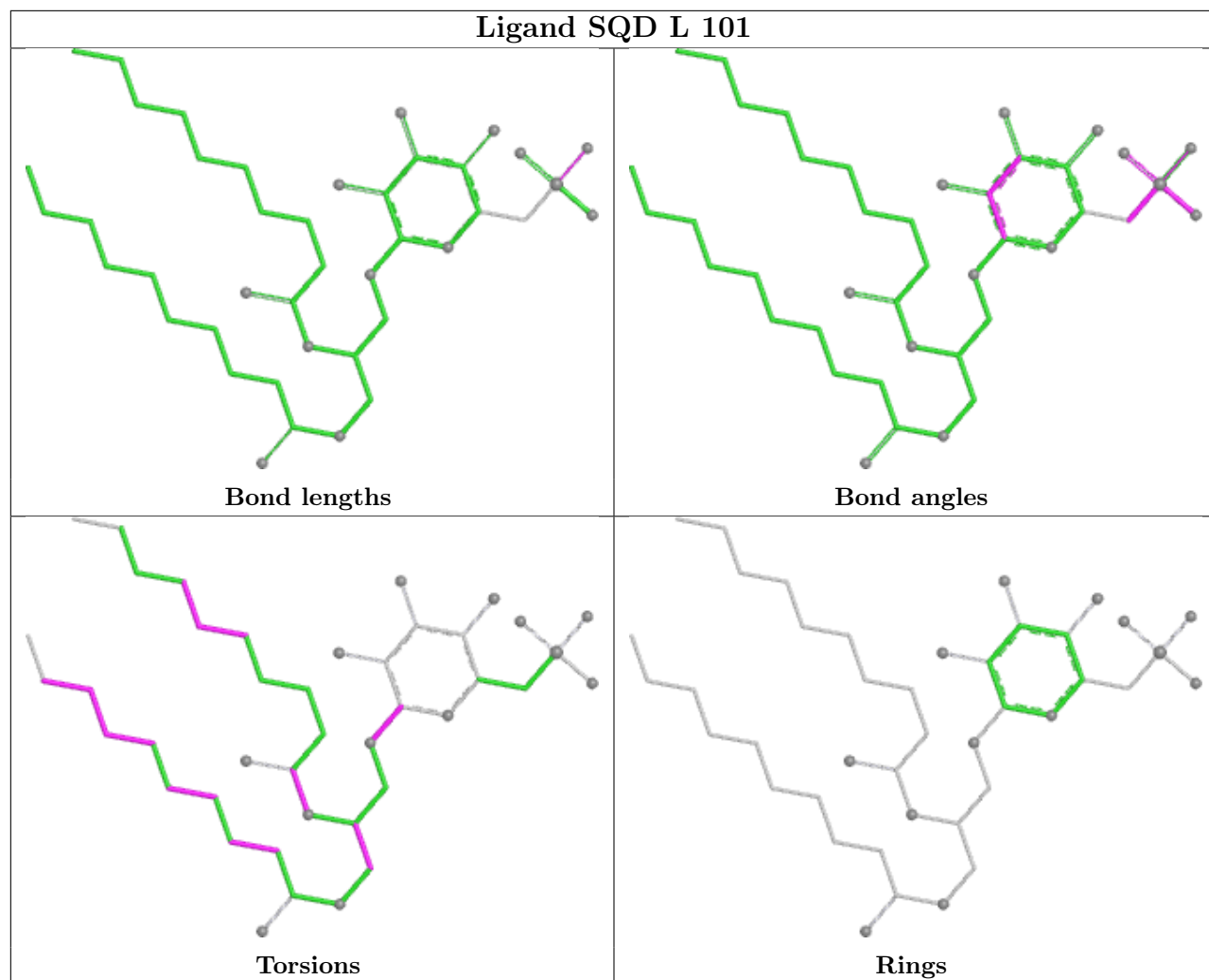
Ligand CHL n 608



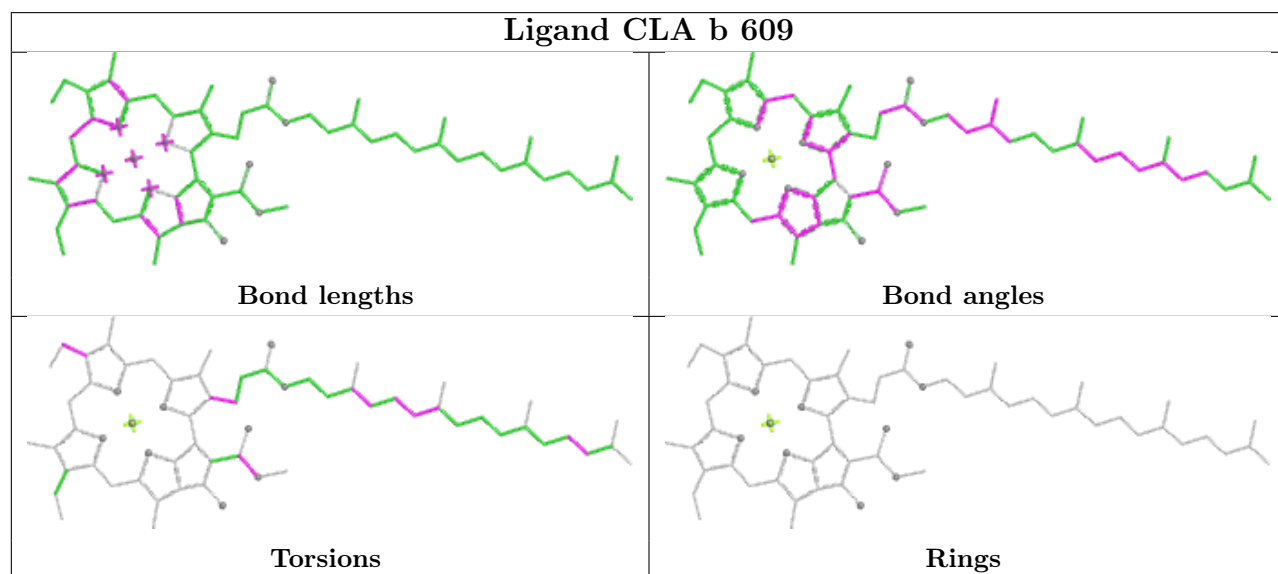
Ligand CLA 6 605



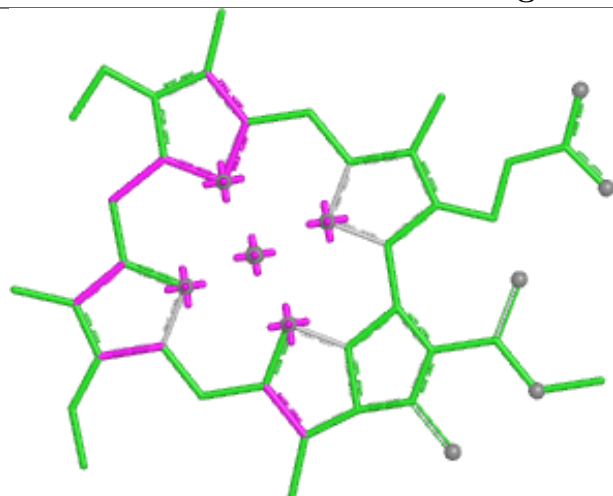
Ligand SQD L 101



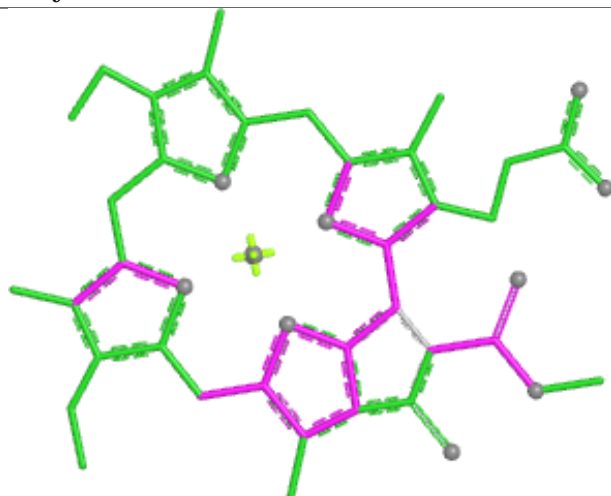
Ligand CLA b 609



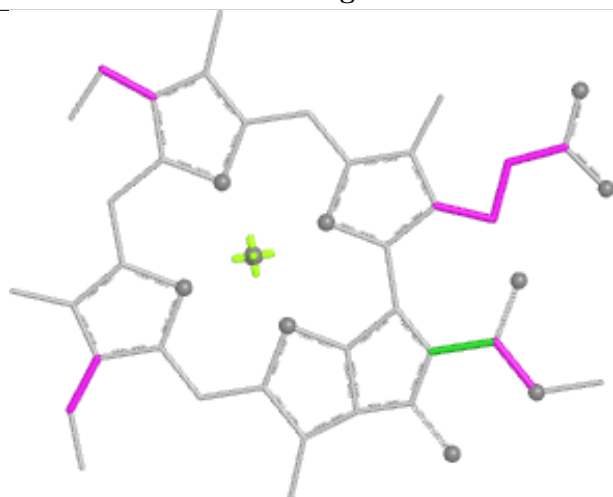
Ligand CLA y 315



Bond lengths



Bond angles

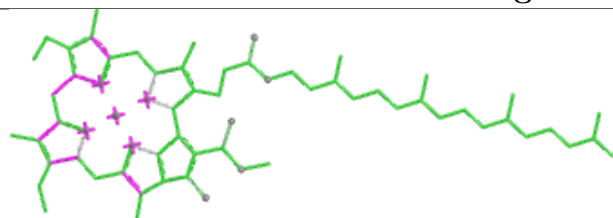


Torsions

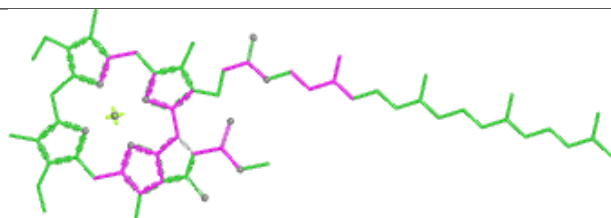


Rings

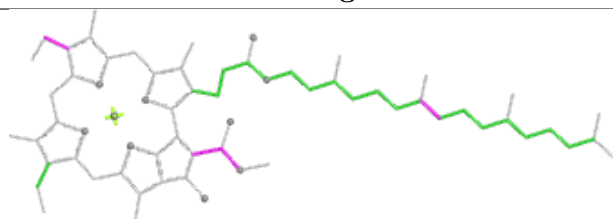
Ligand CLA C 502



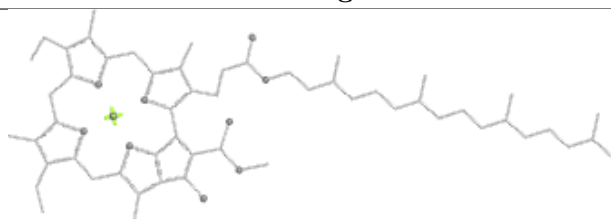
Bond lengths



Bond angles

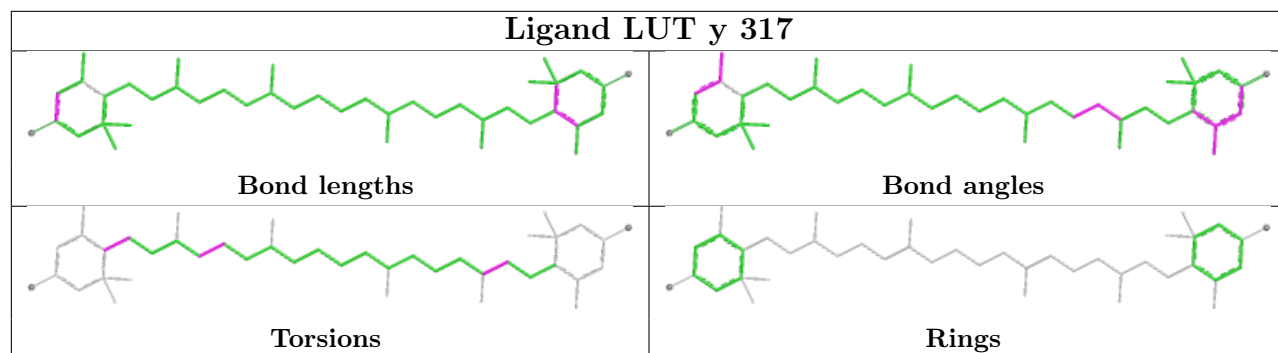


Torsions

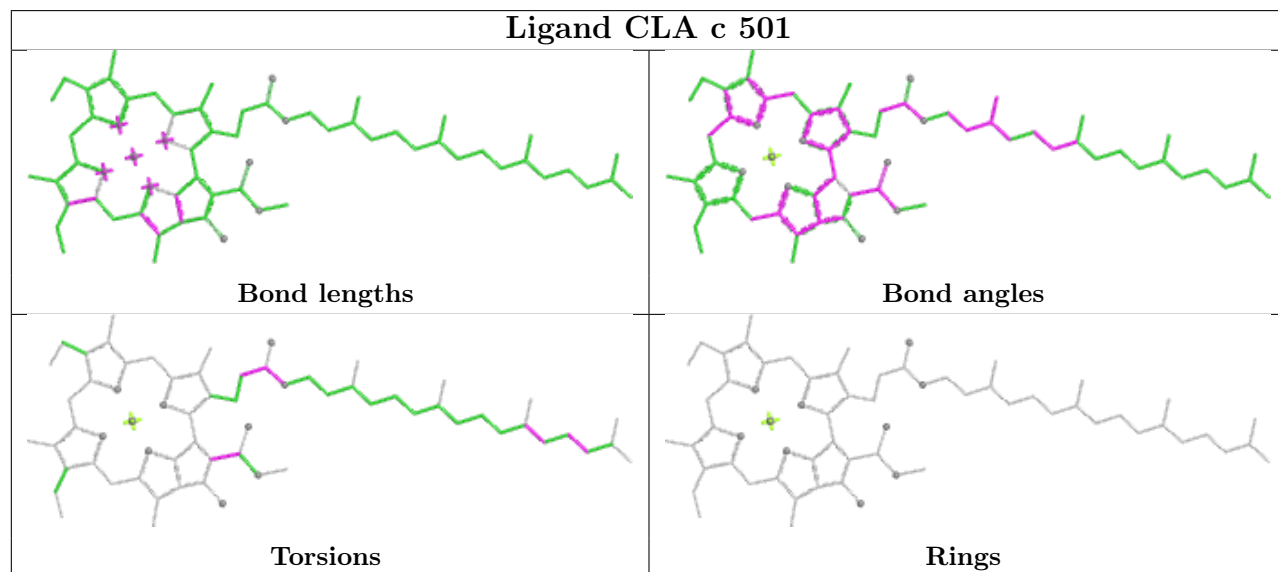


Rings

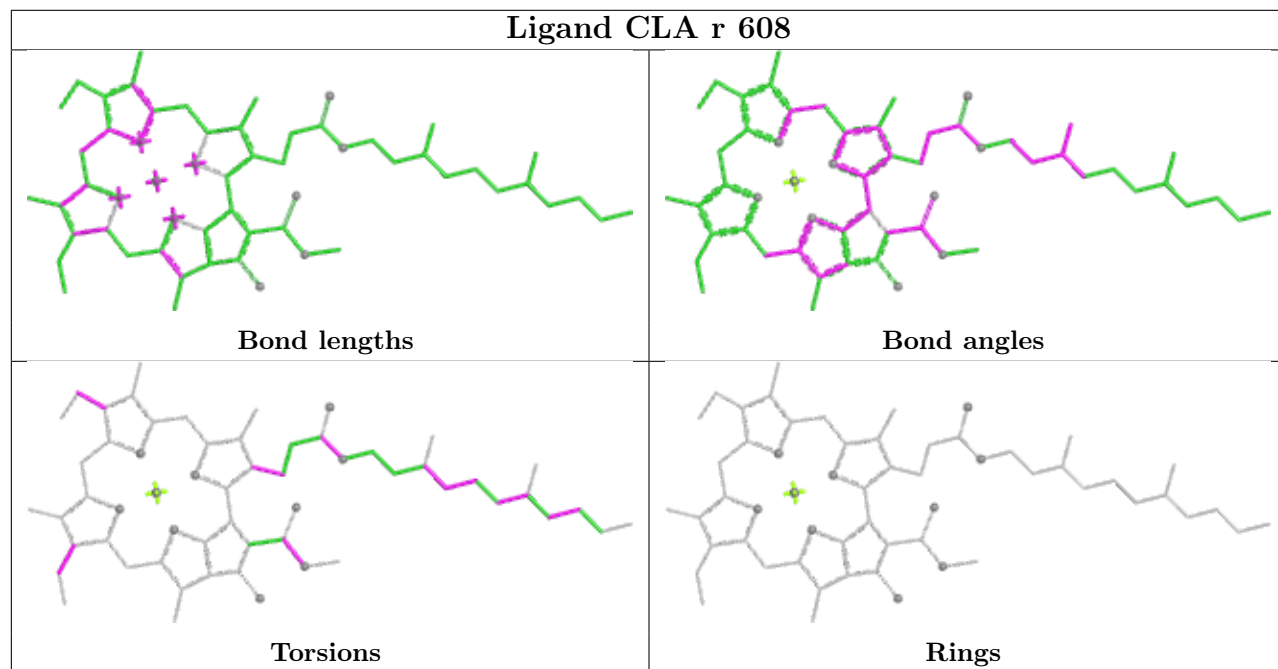
Ligand LUT y 317



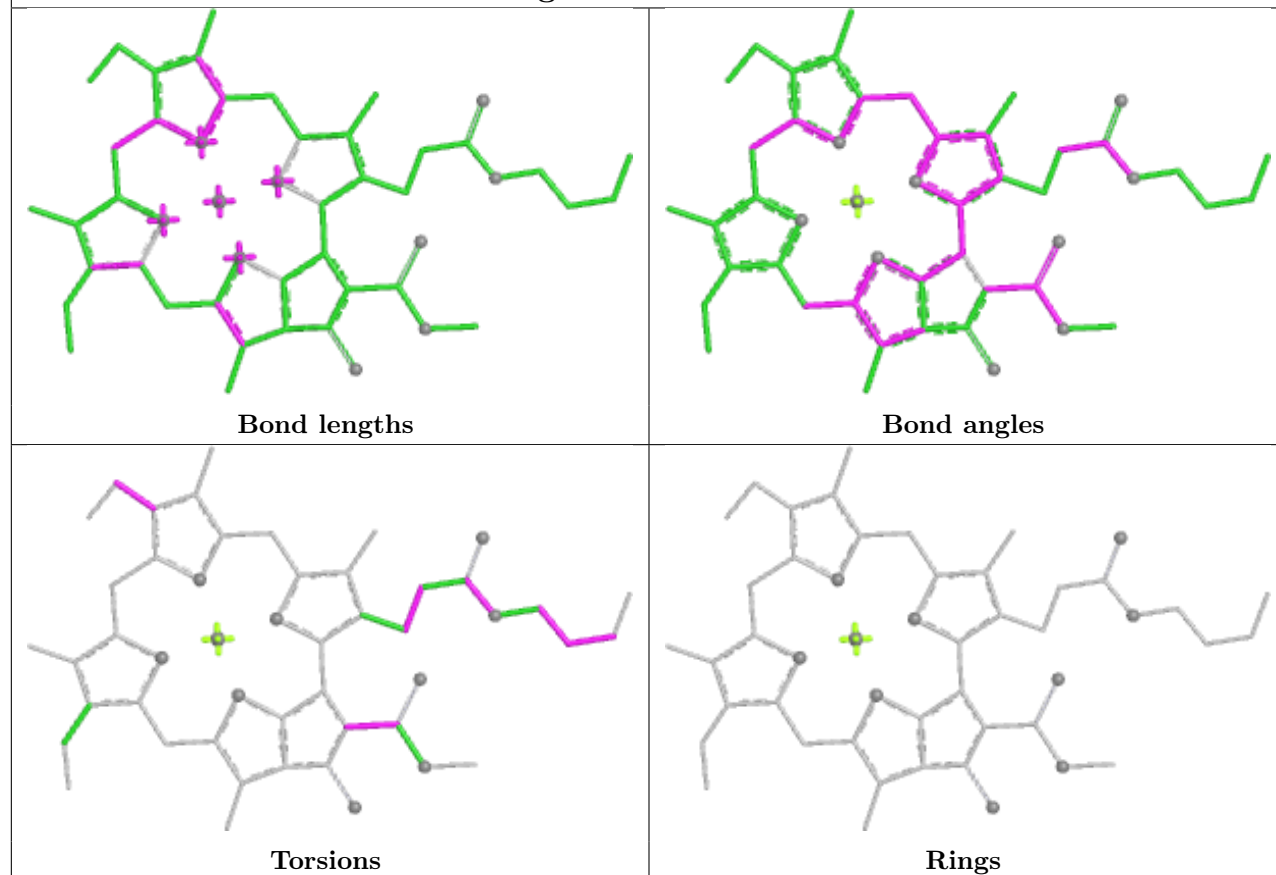
Ligand CLA c 501



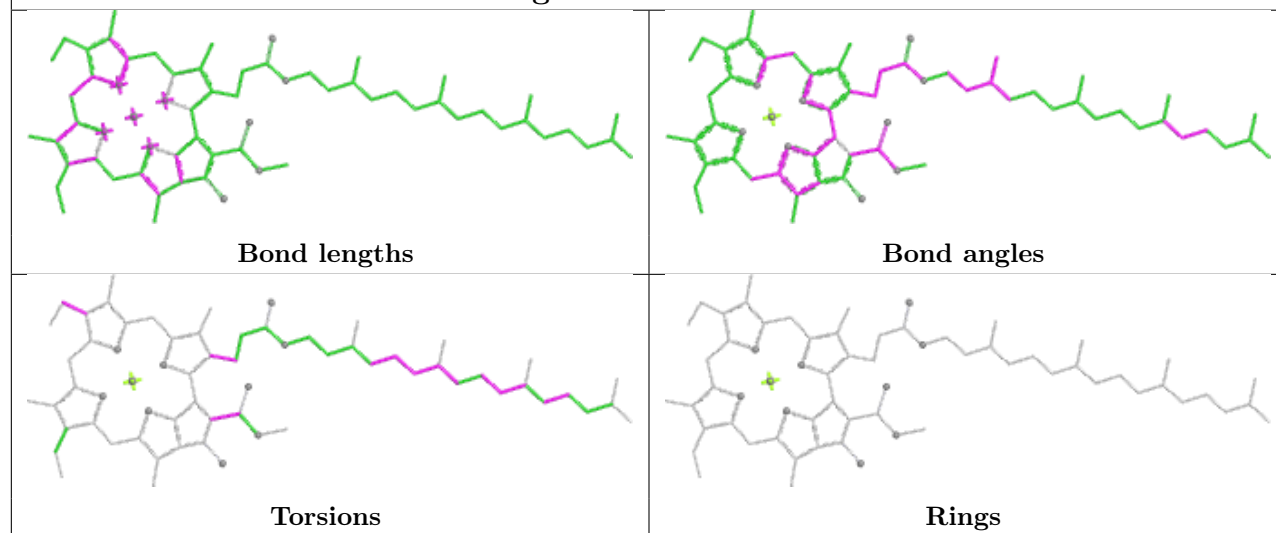
Ligand CLA r 608

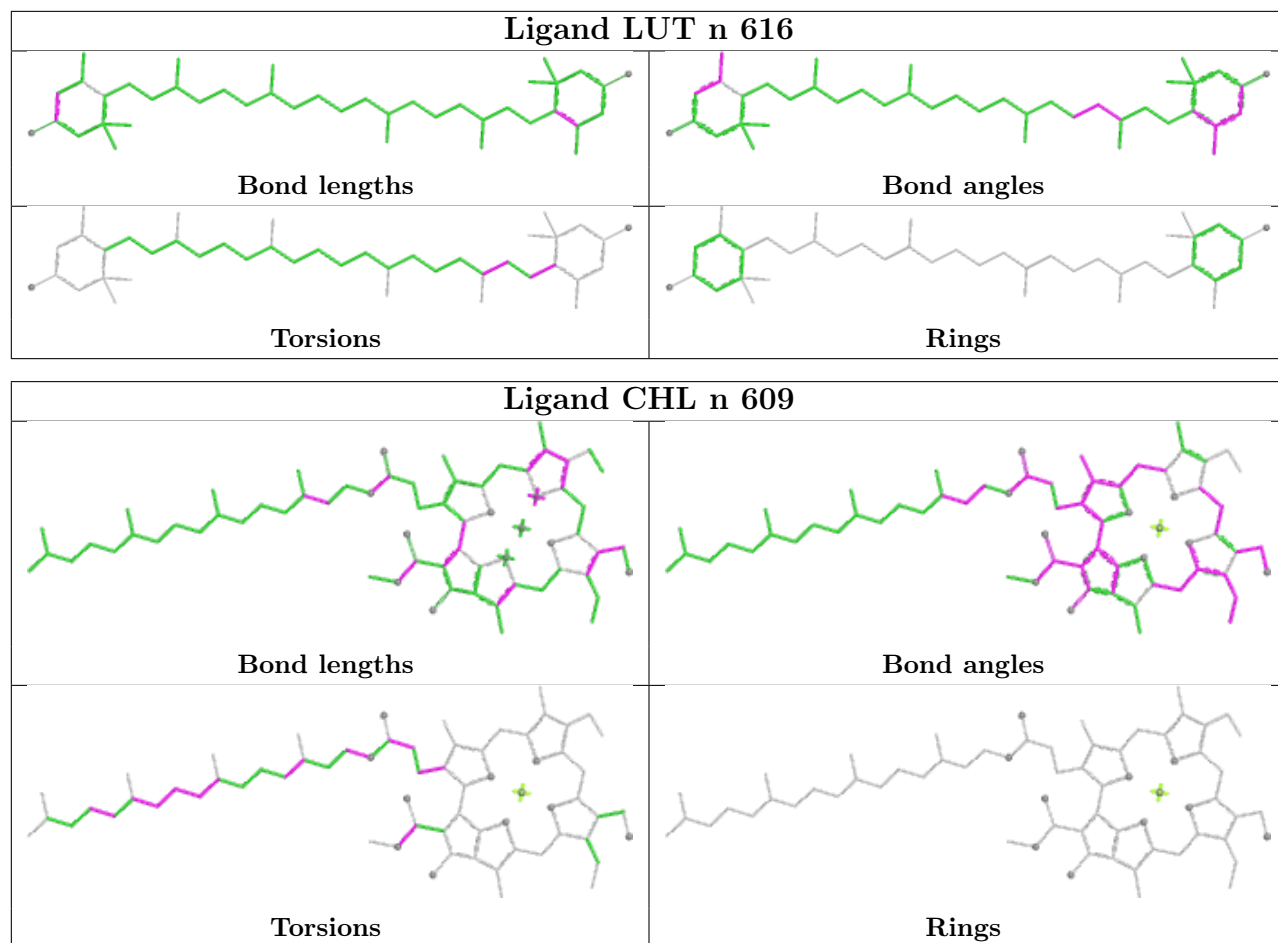


Ligand CLA s 312

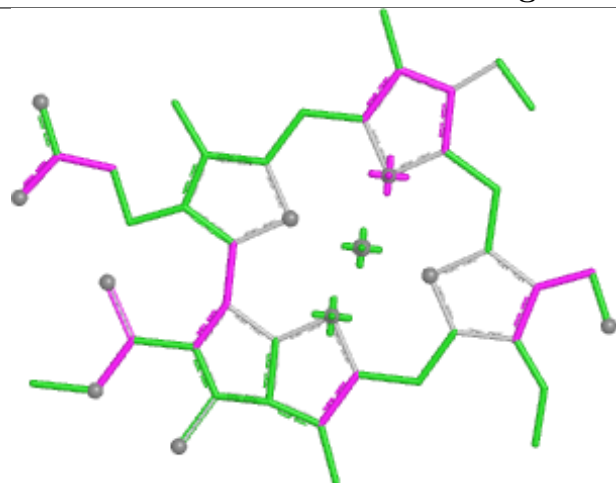


Ligand CLA B 604

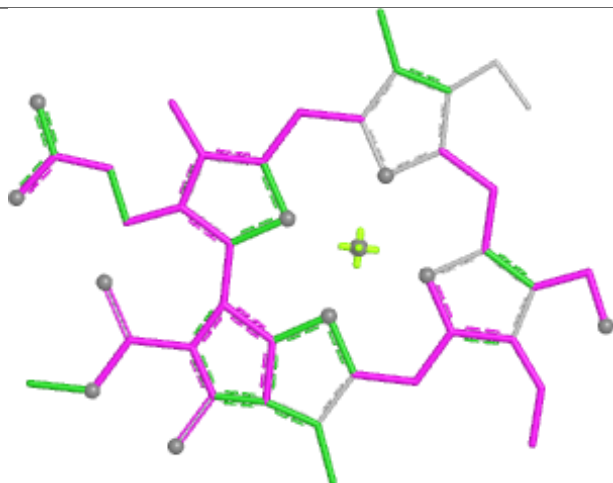




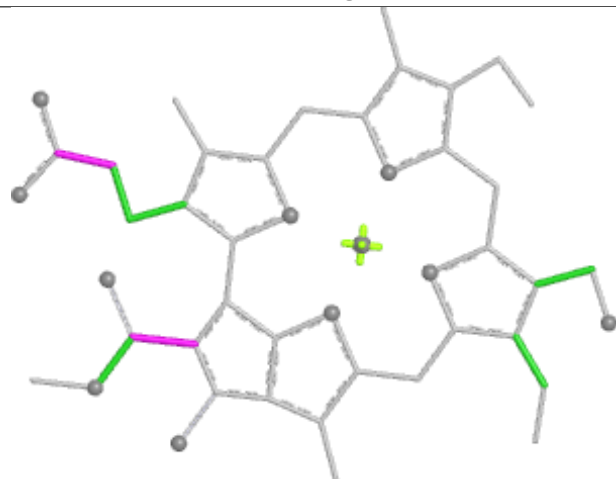
Ligand CHL S 308



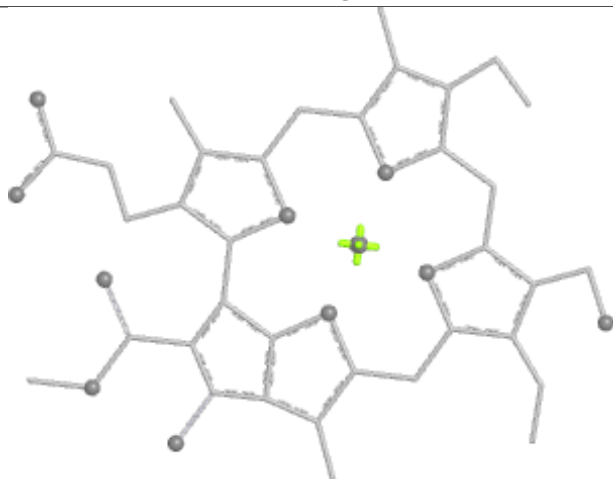
Bond lengths



Bond angles

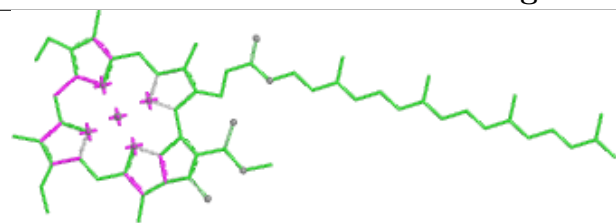


Torsions

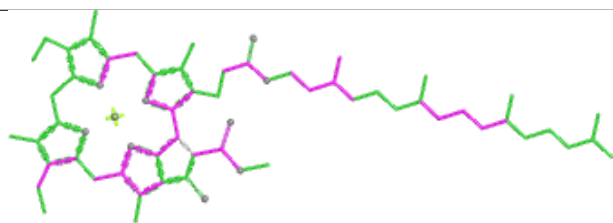


Rings

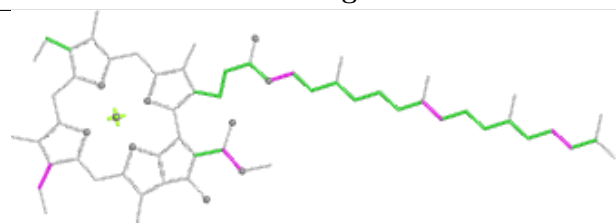
Ligand CLA a 402



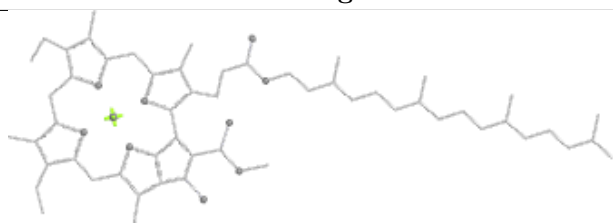
Bond lengths



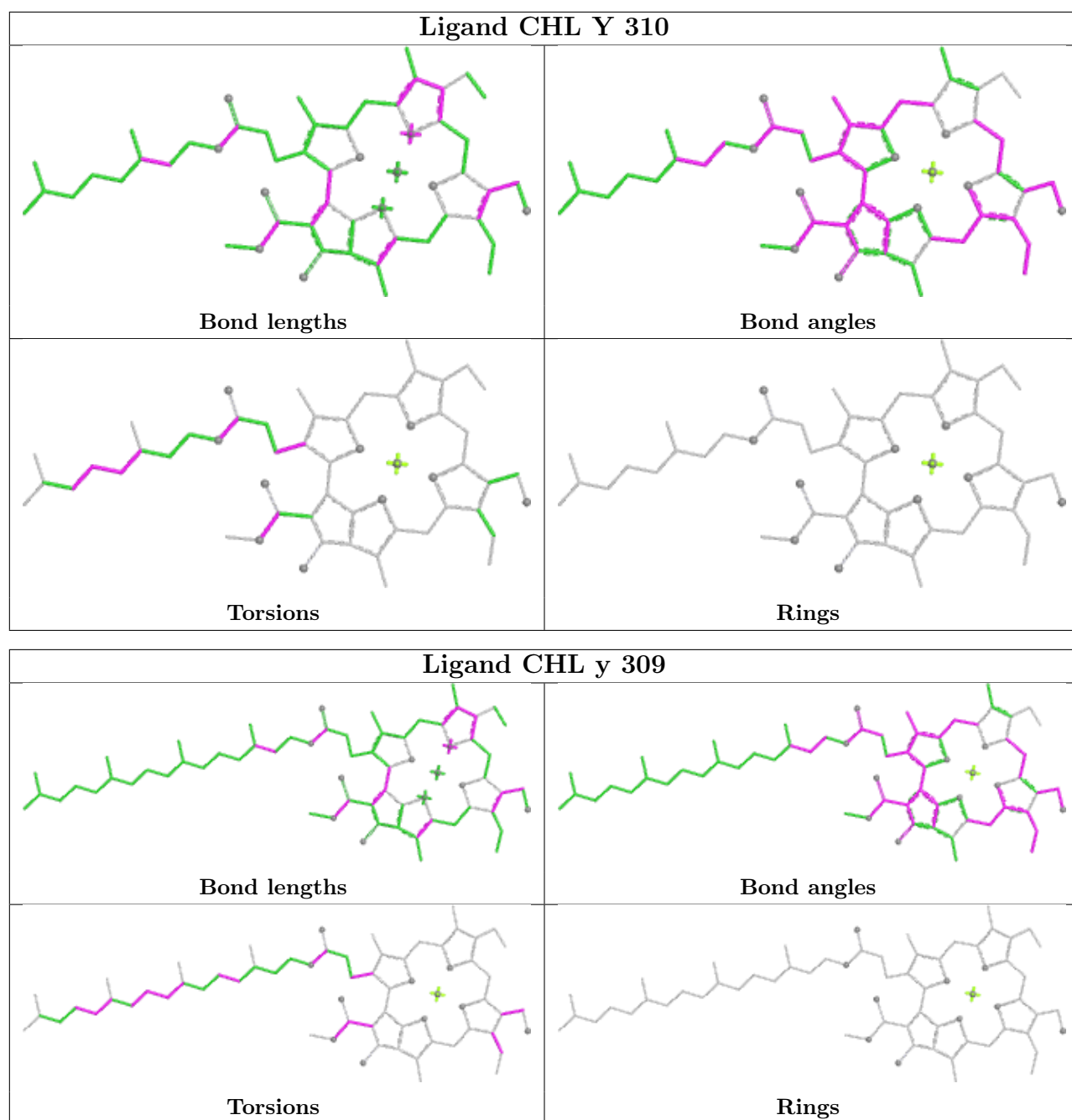
Bond angles

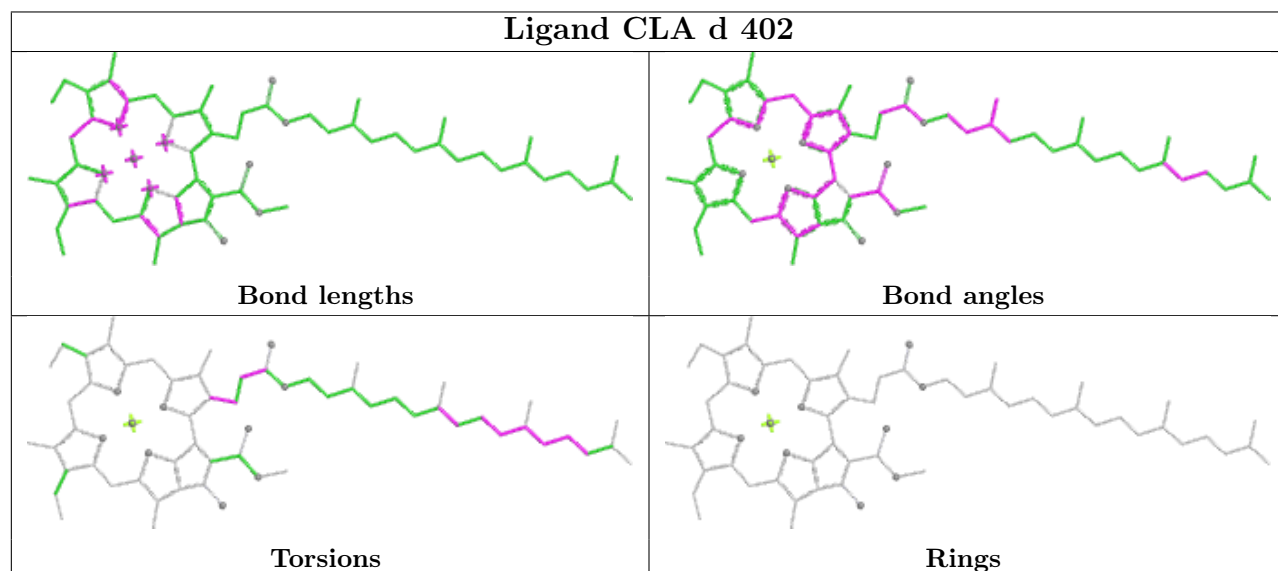
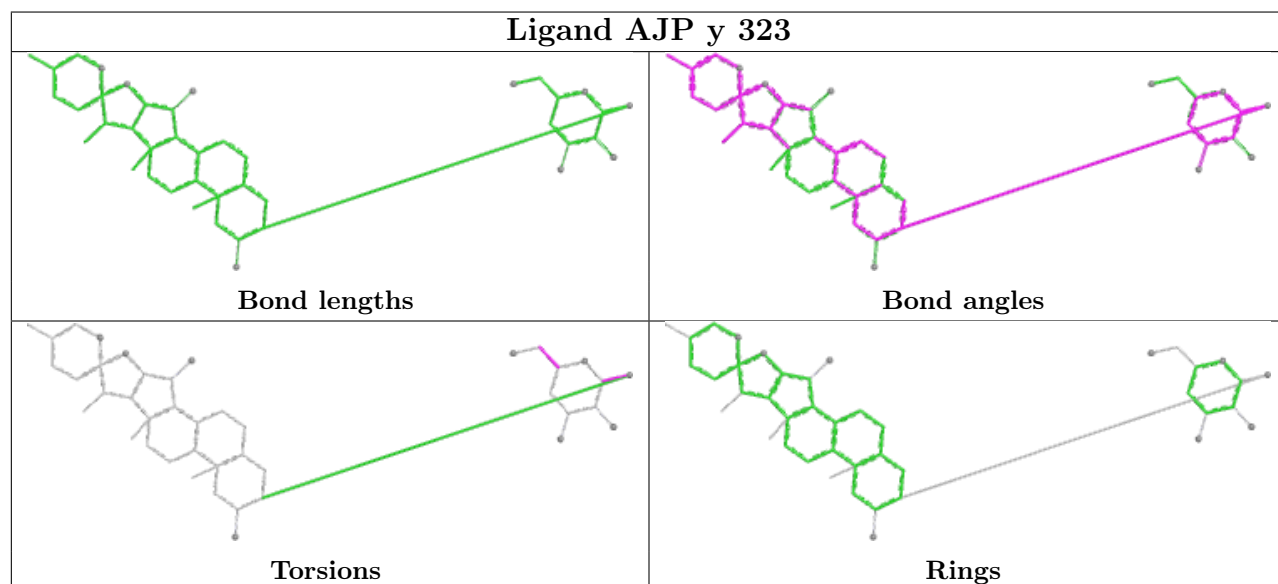
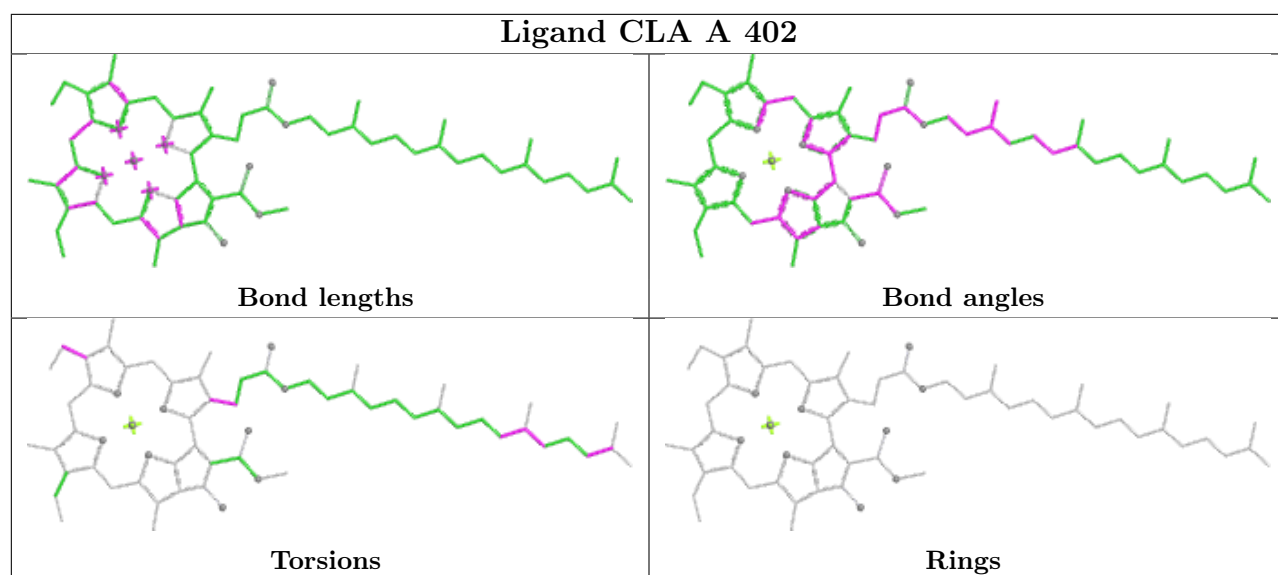


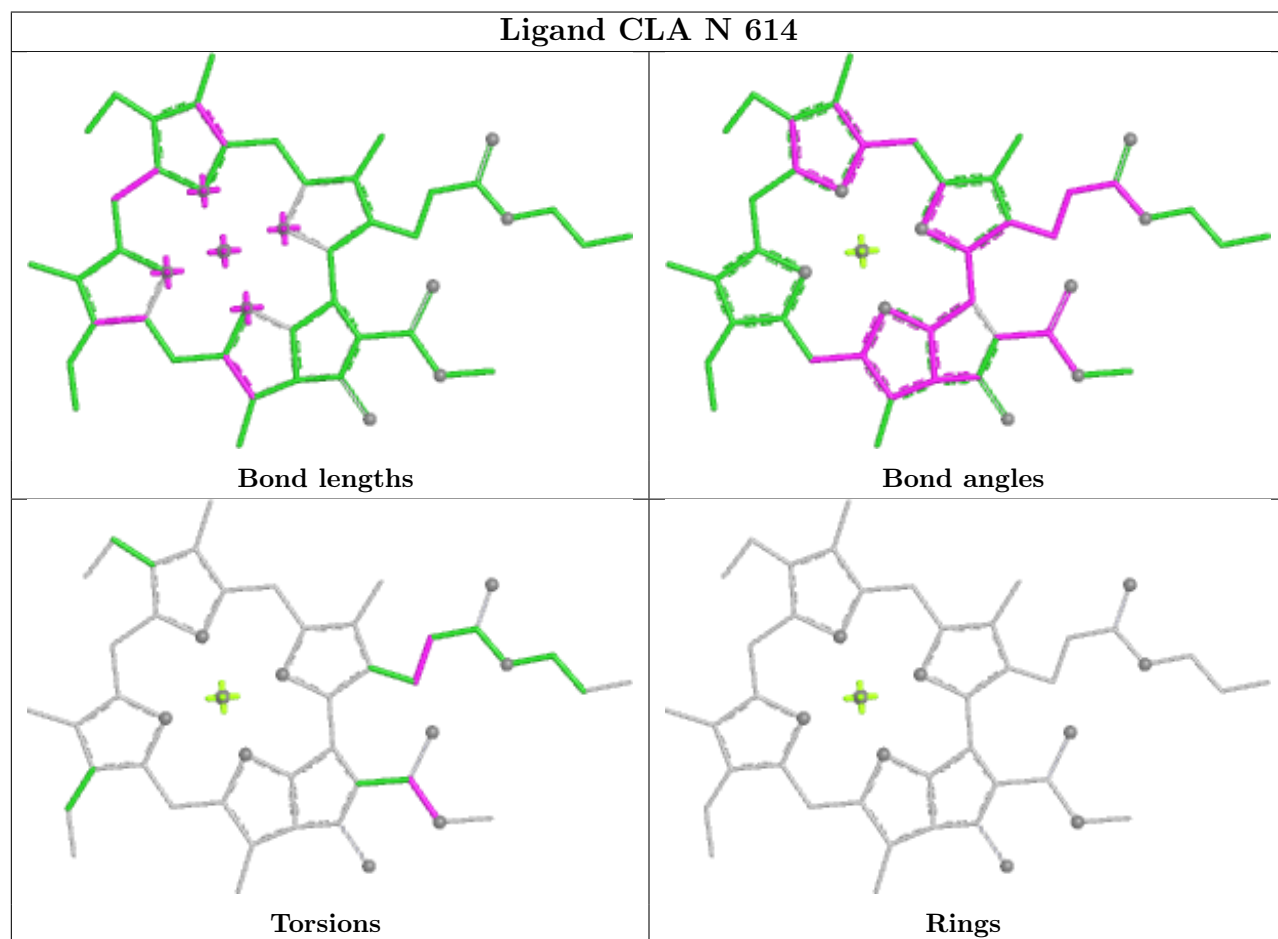
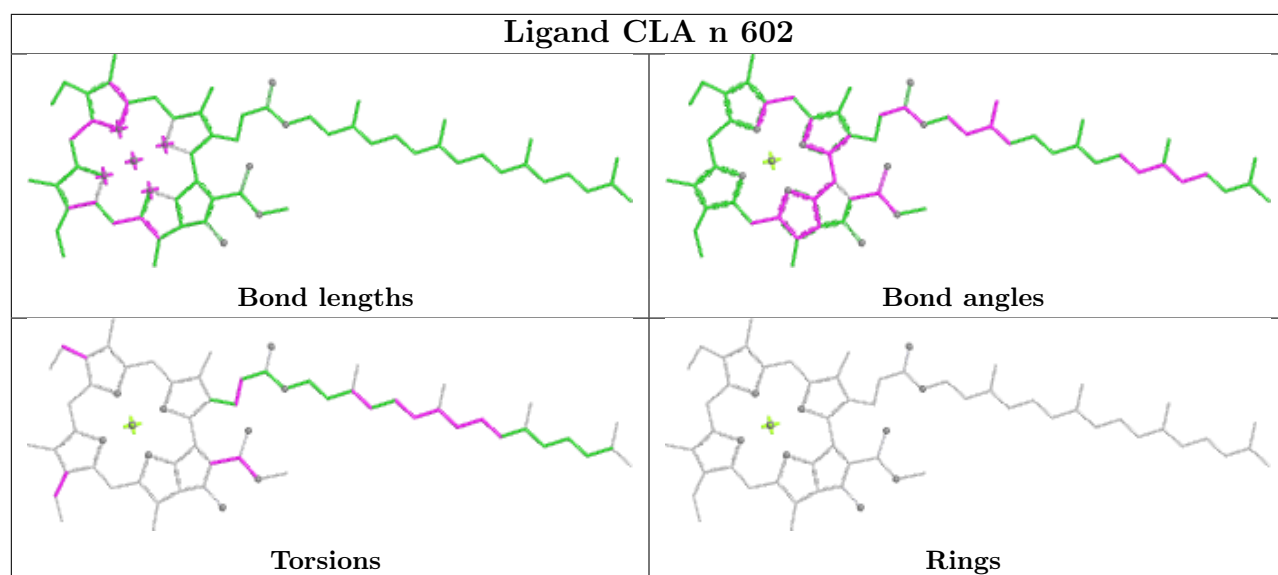
Torsions

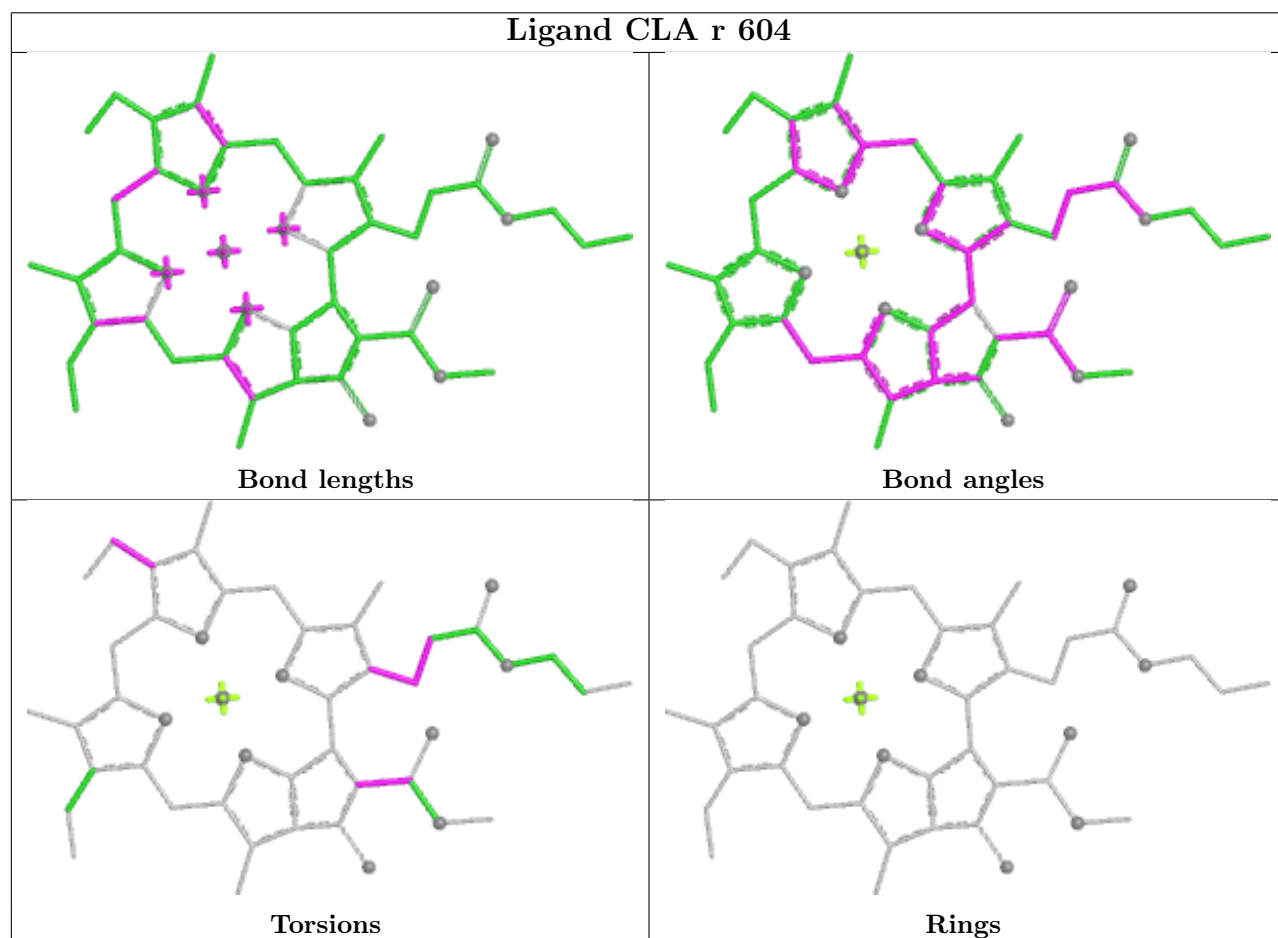
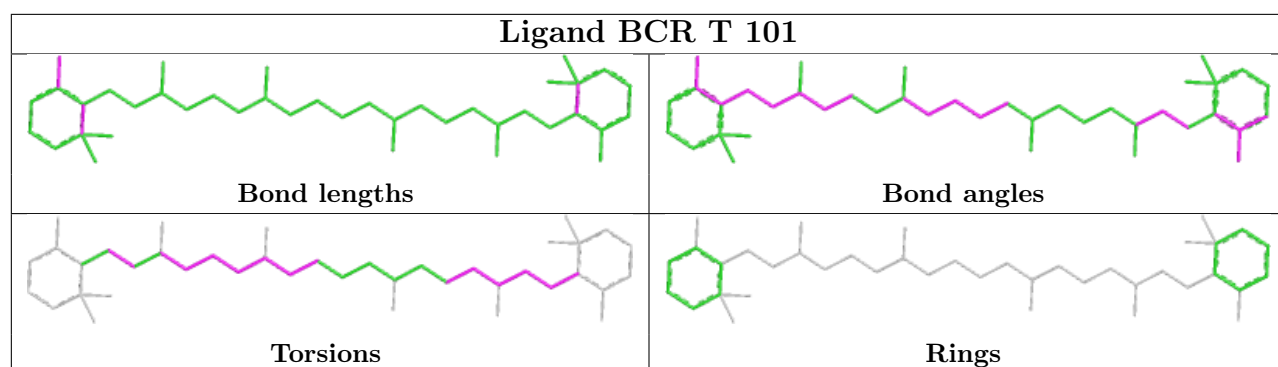


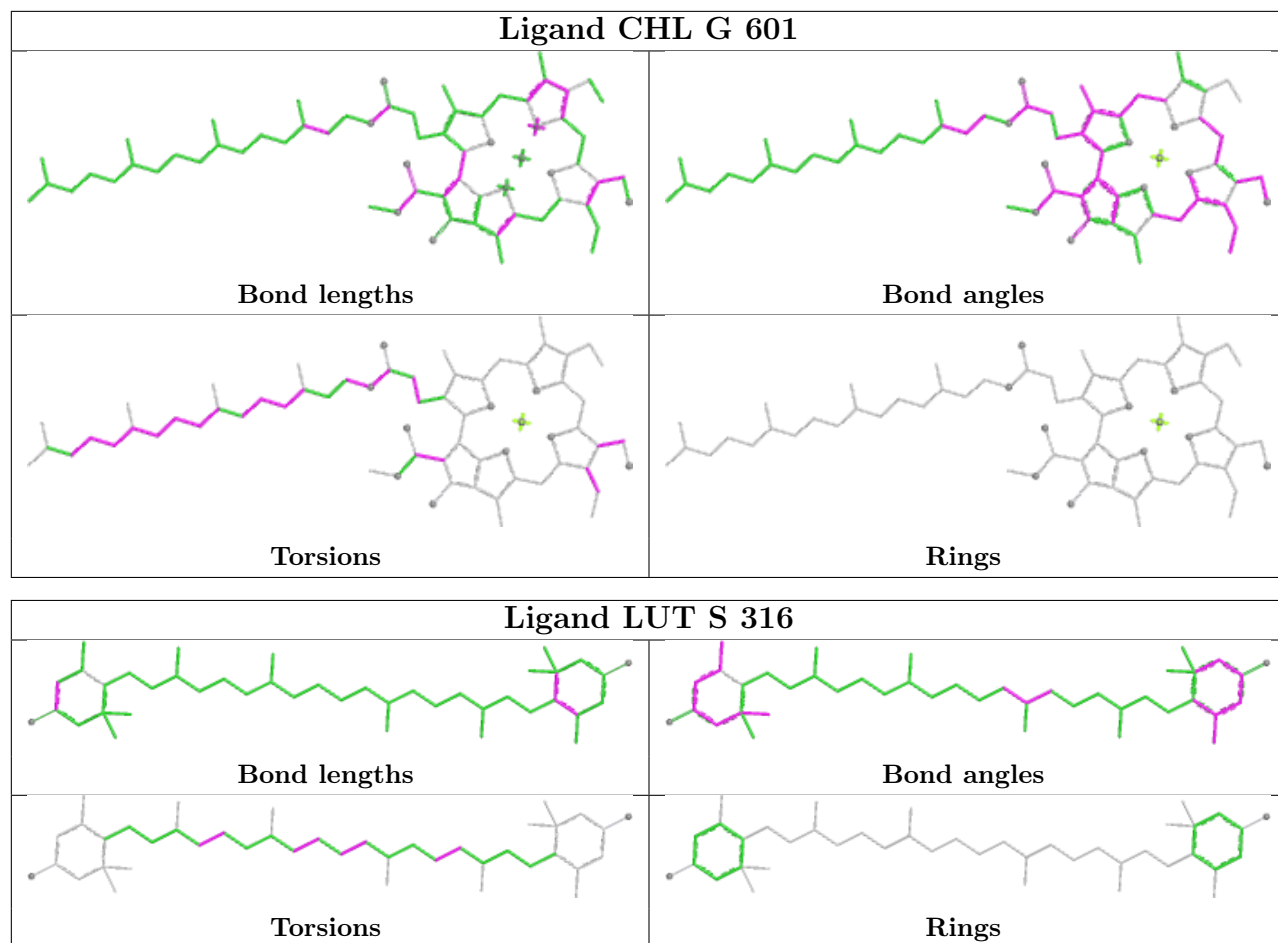
Rings

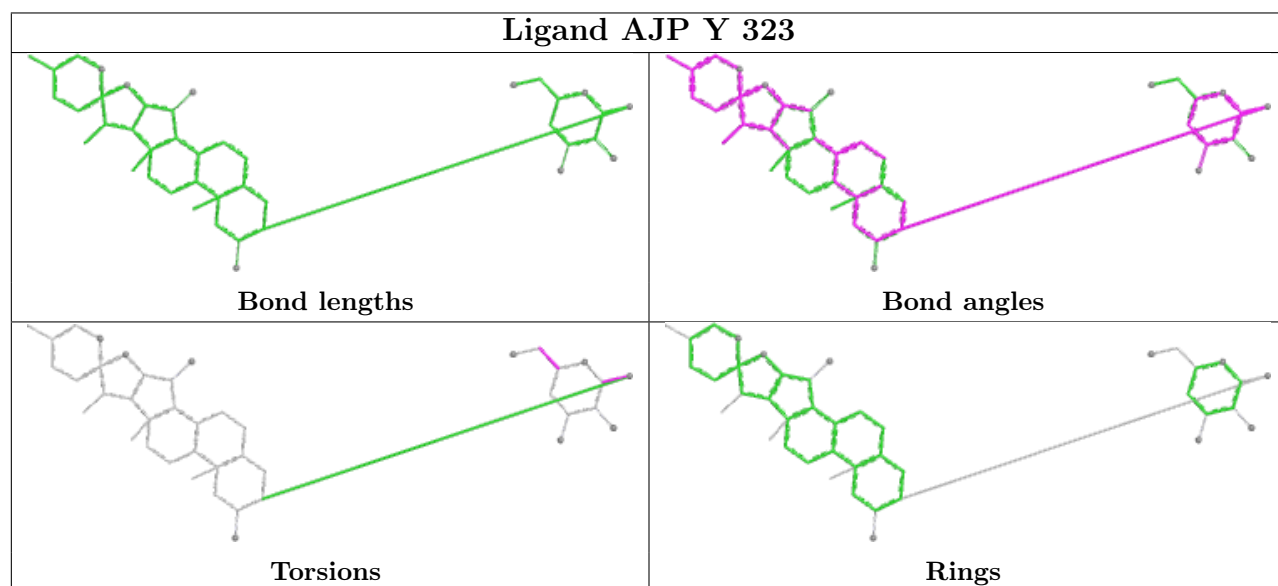
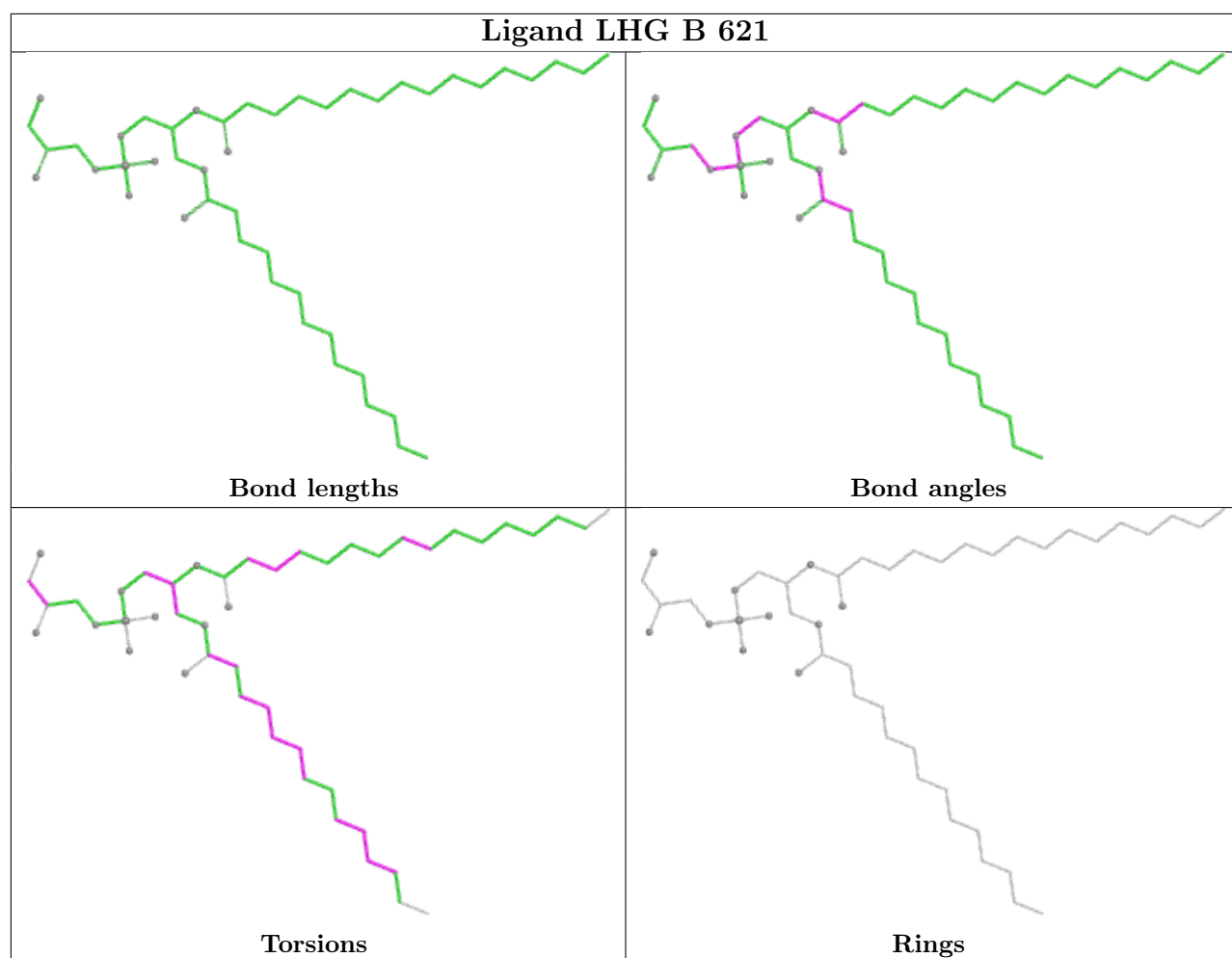


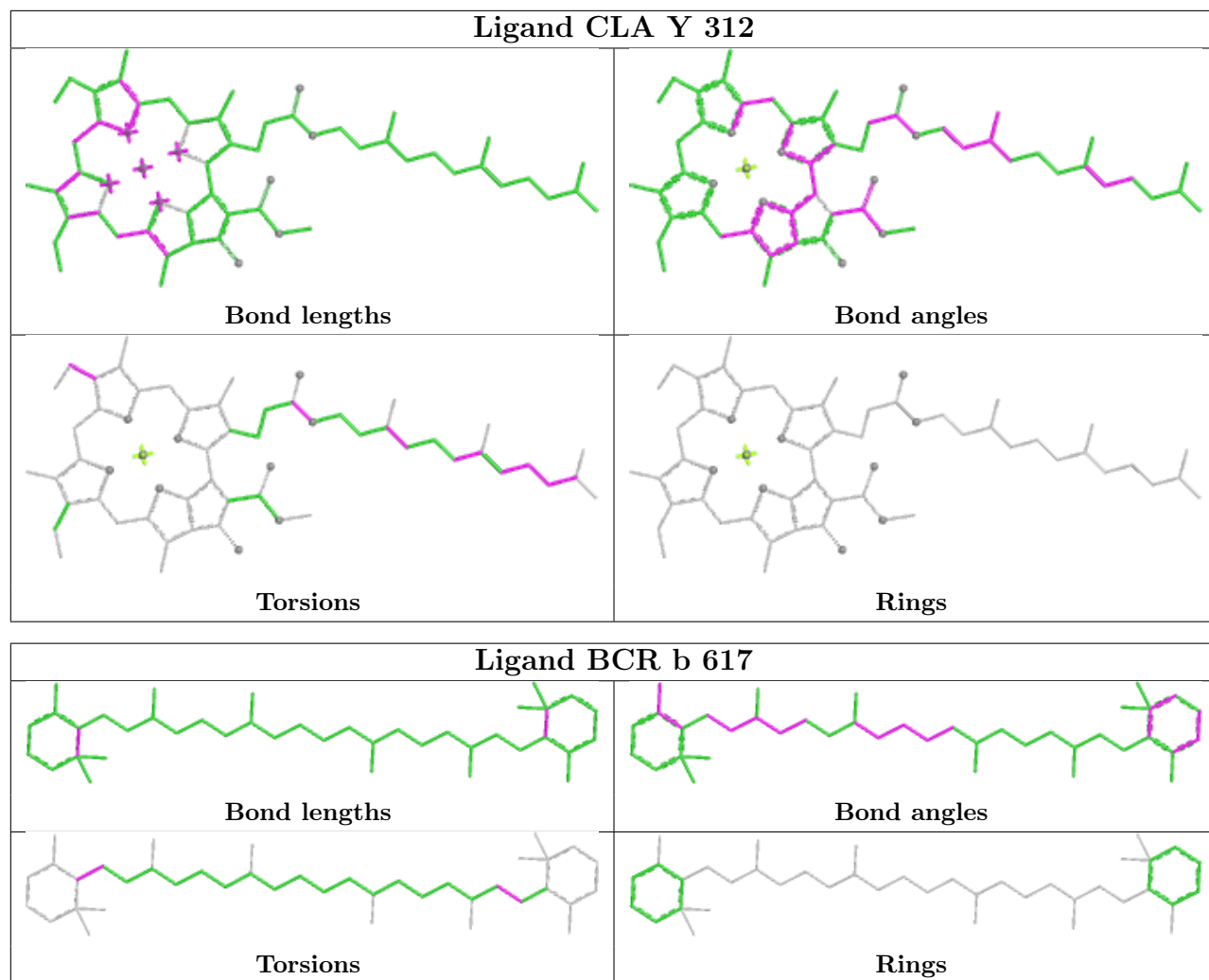


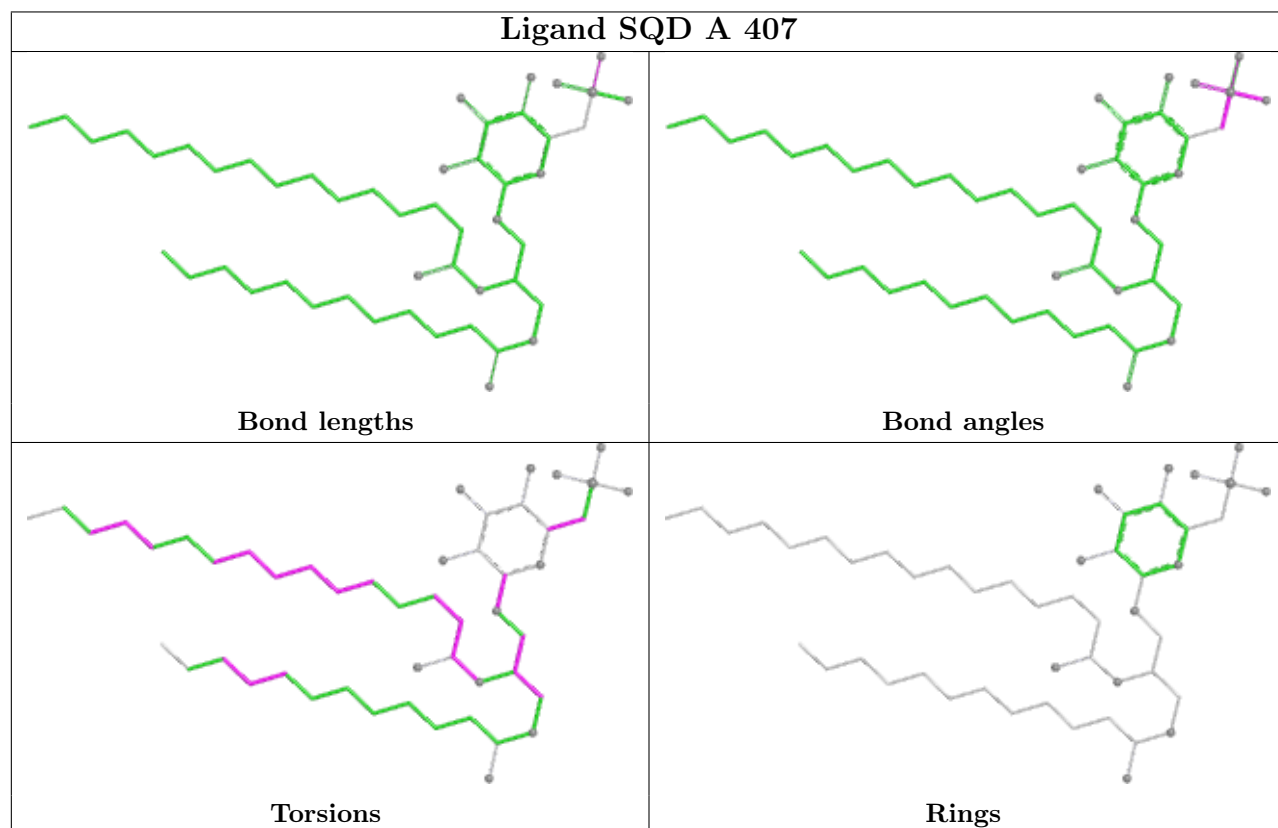
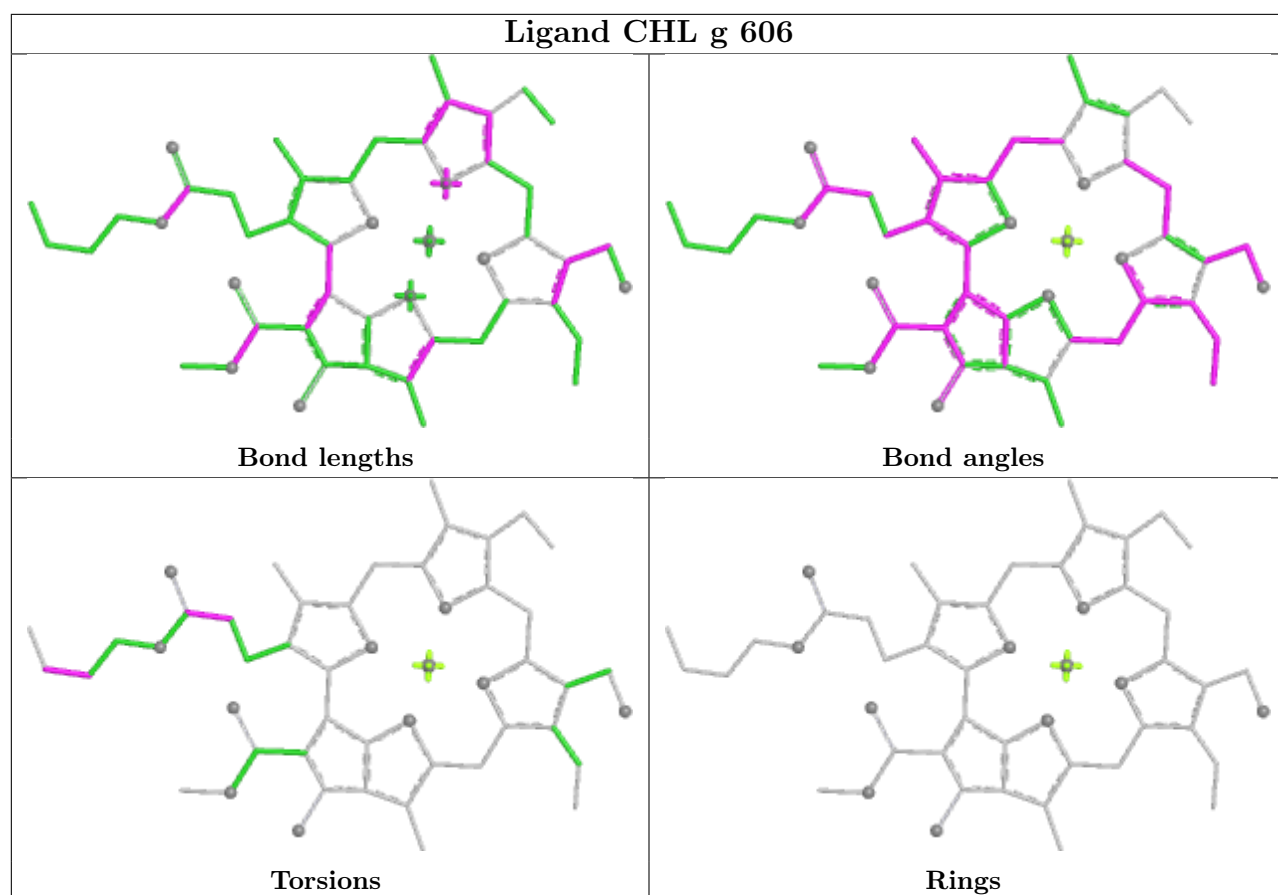


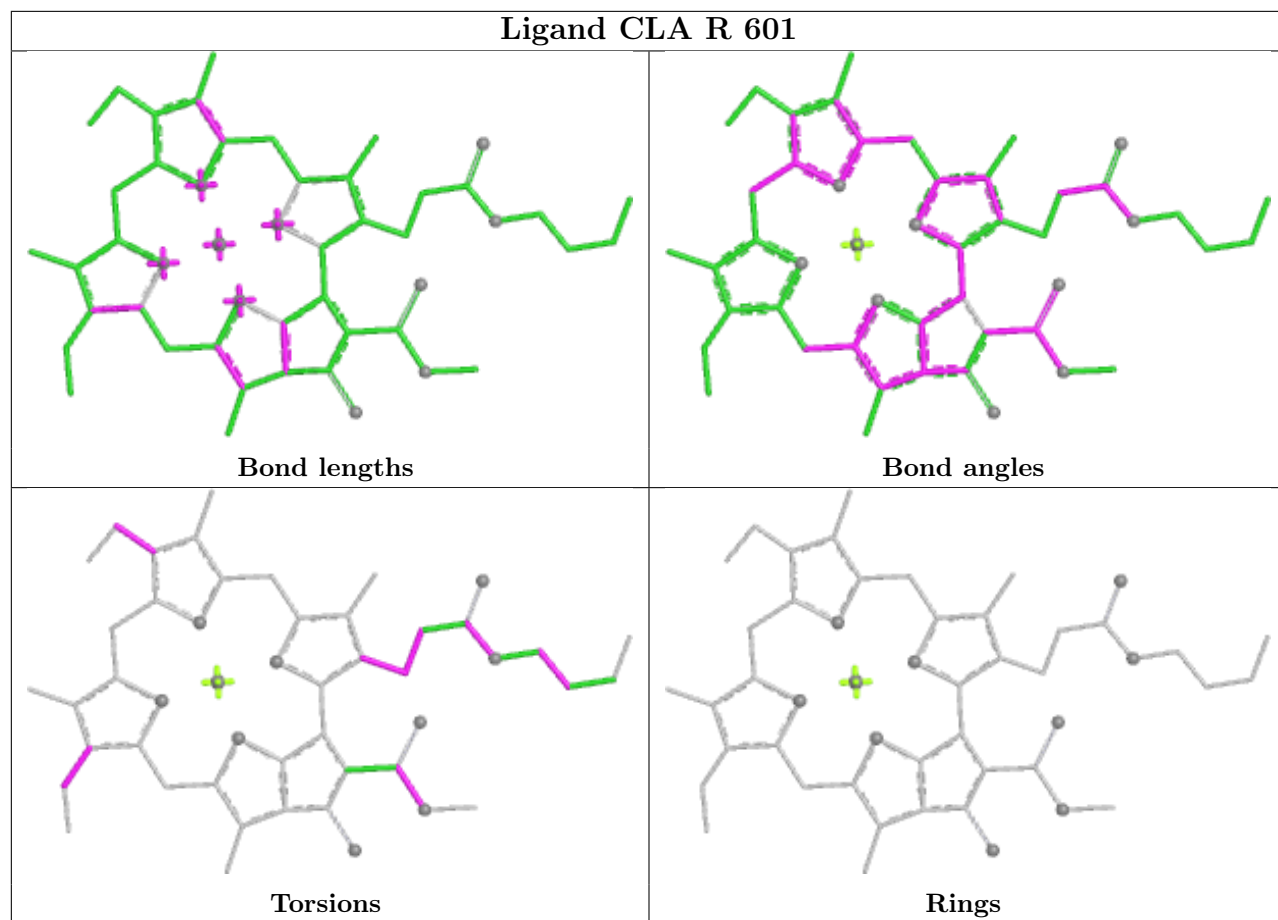




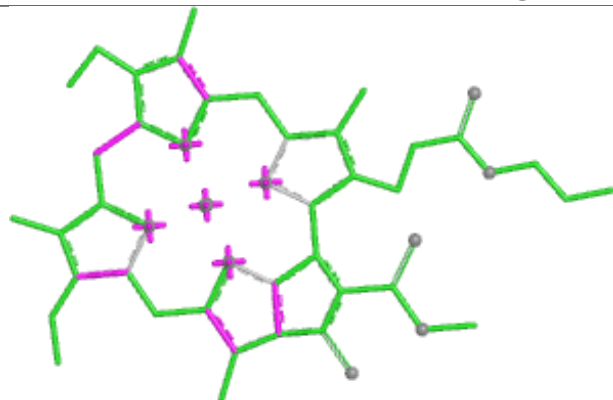




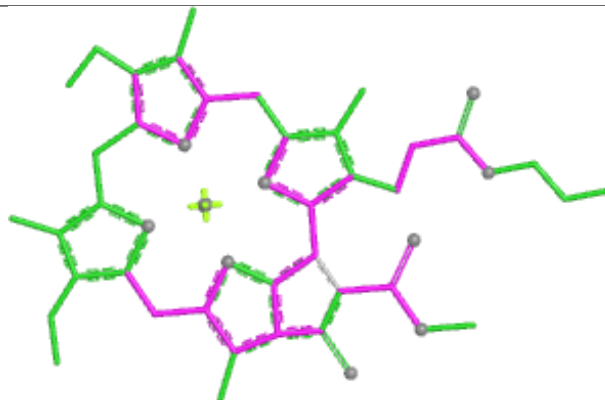




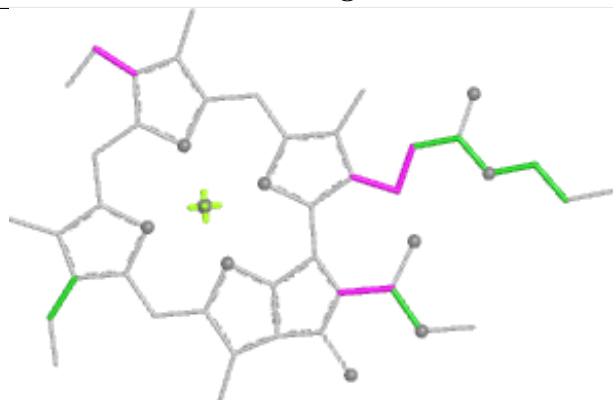
Ligand CLA R 604



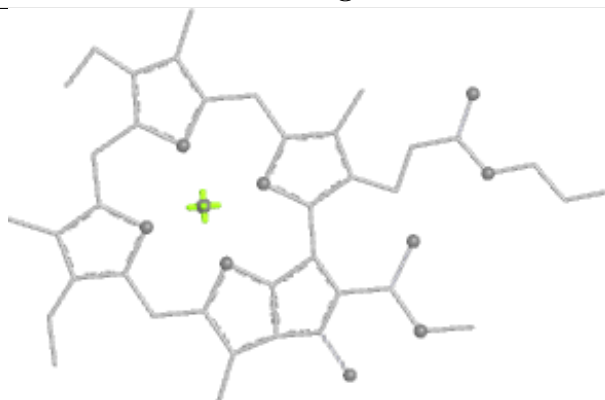
Bond lengths



Bond angles

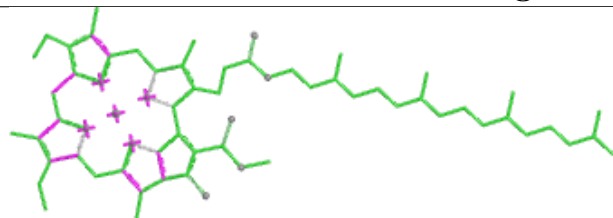


Torsions

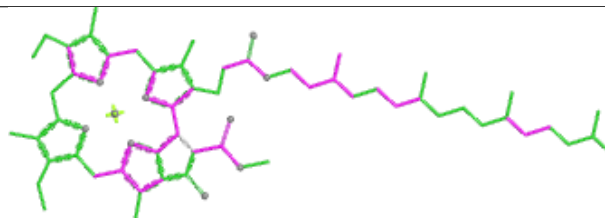


Rings

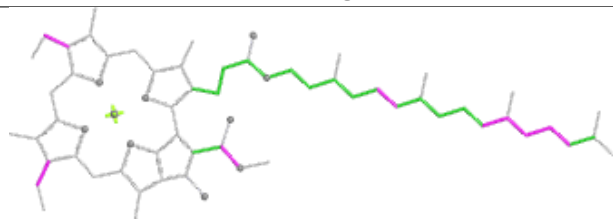
Ligand CLA C 508



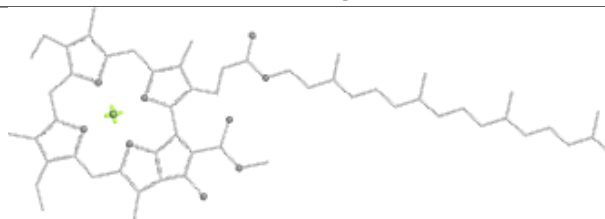
Bond lengths



Bond angles

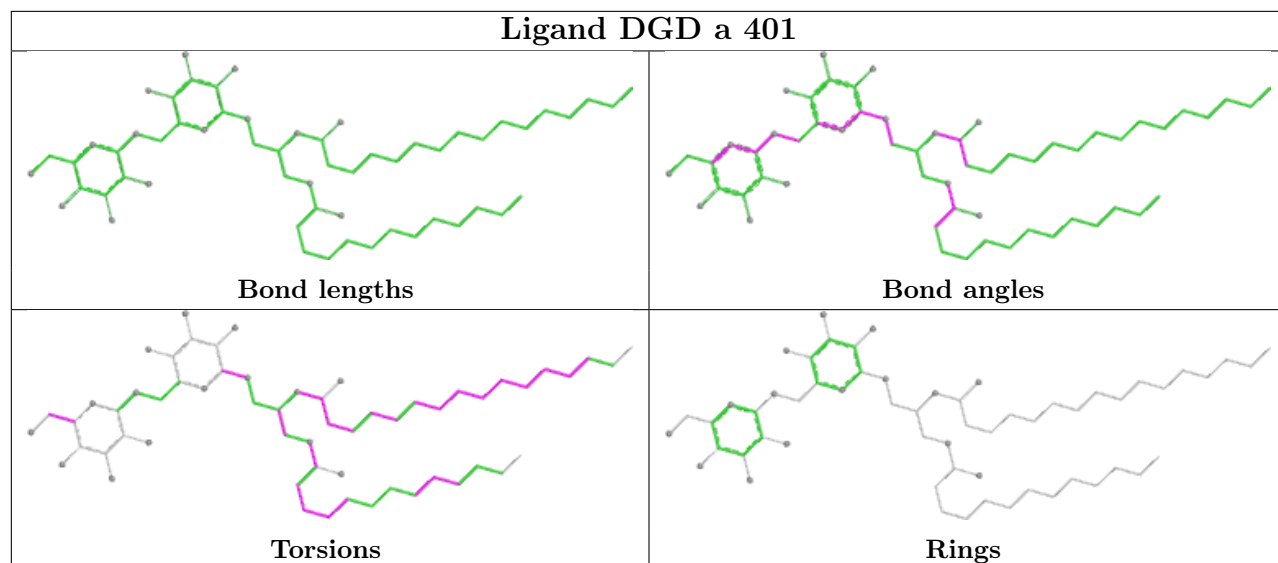


Torsions

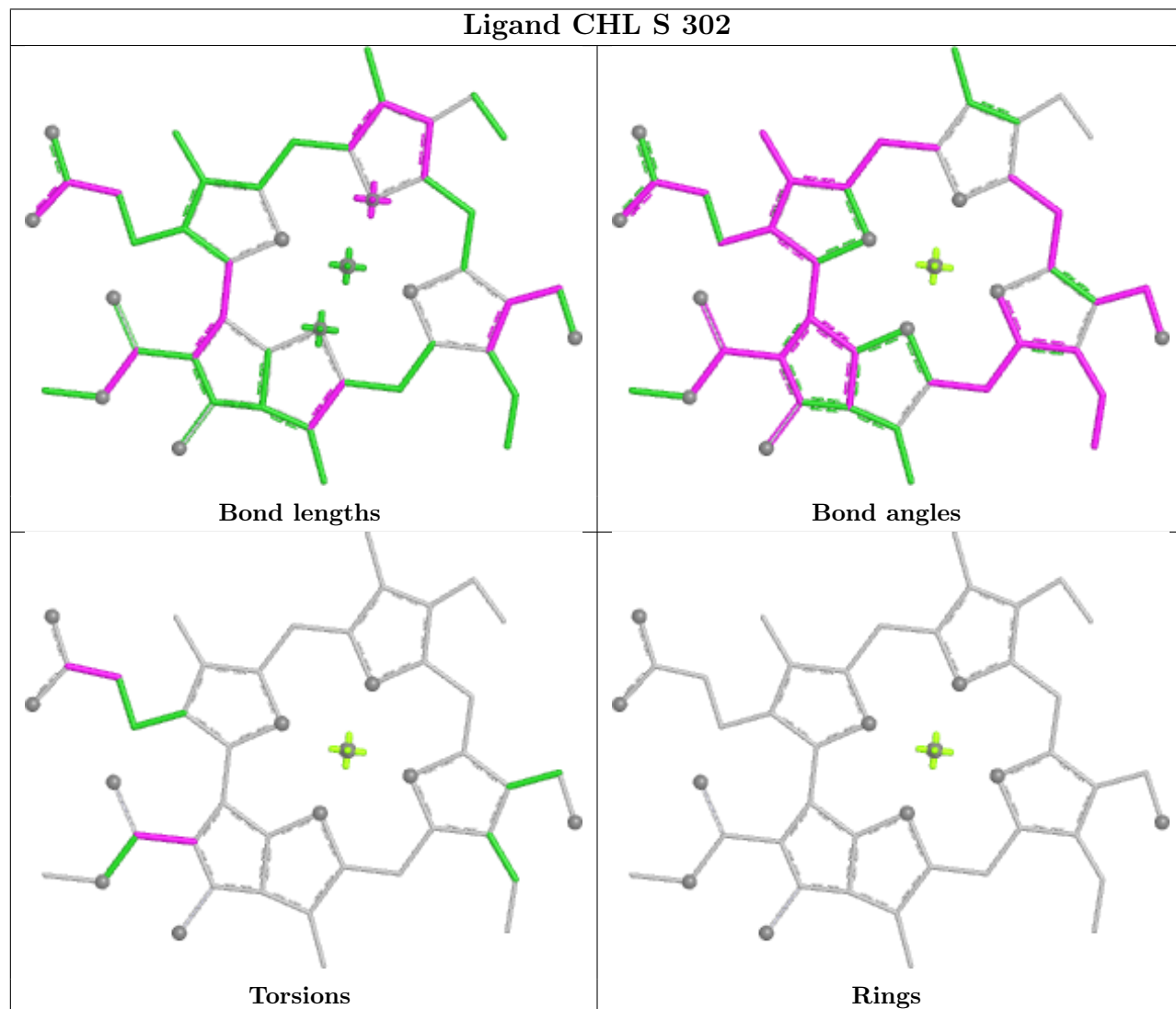


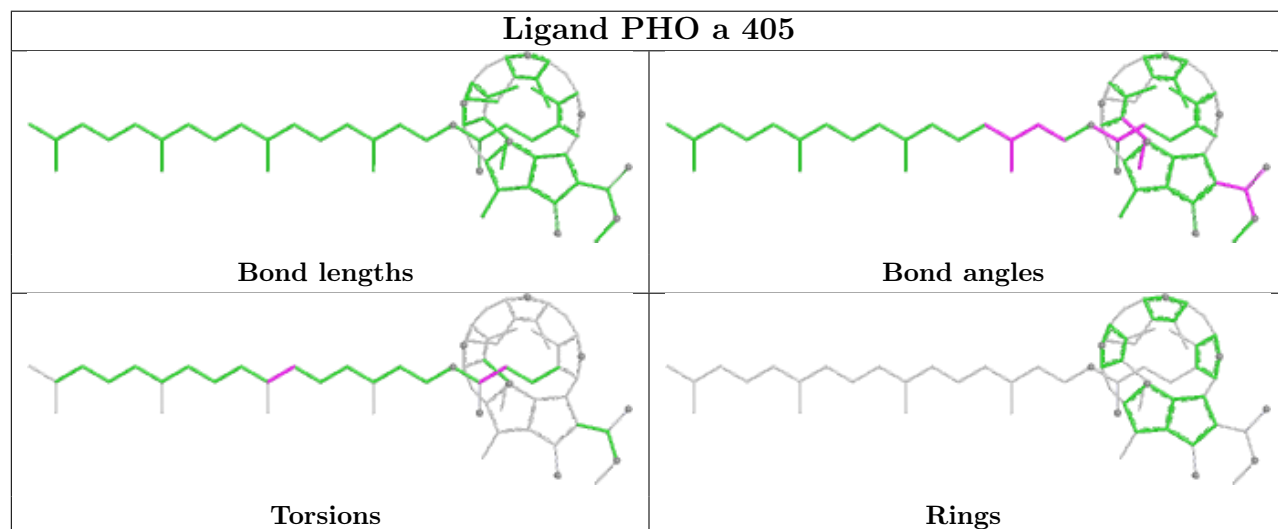
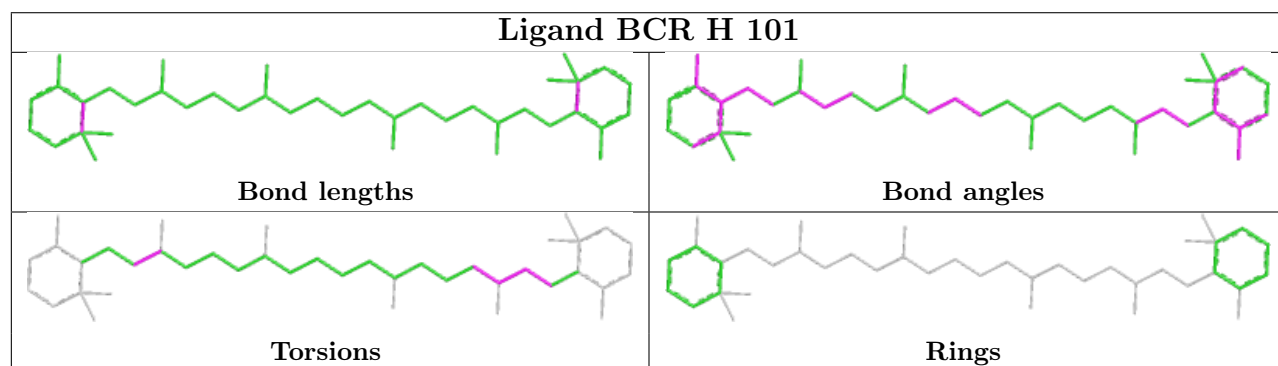
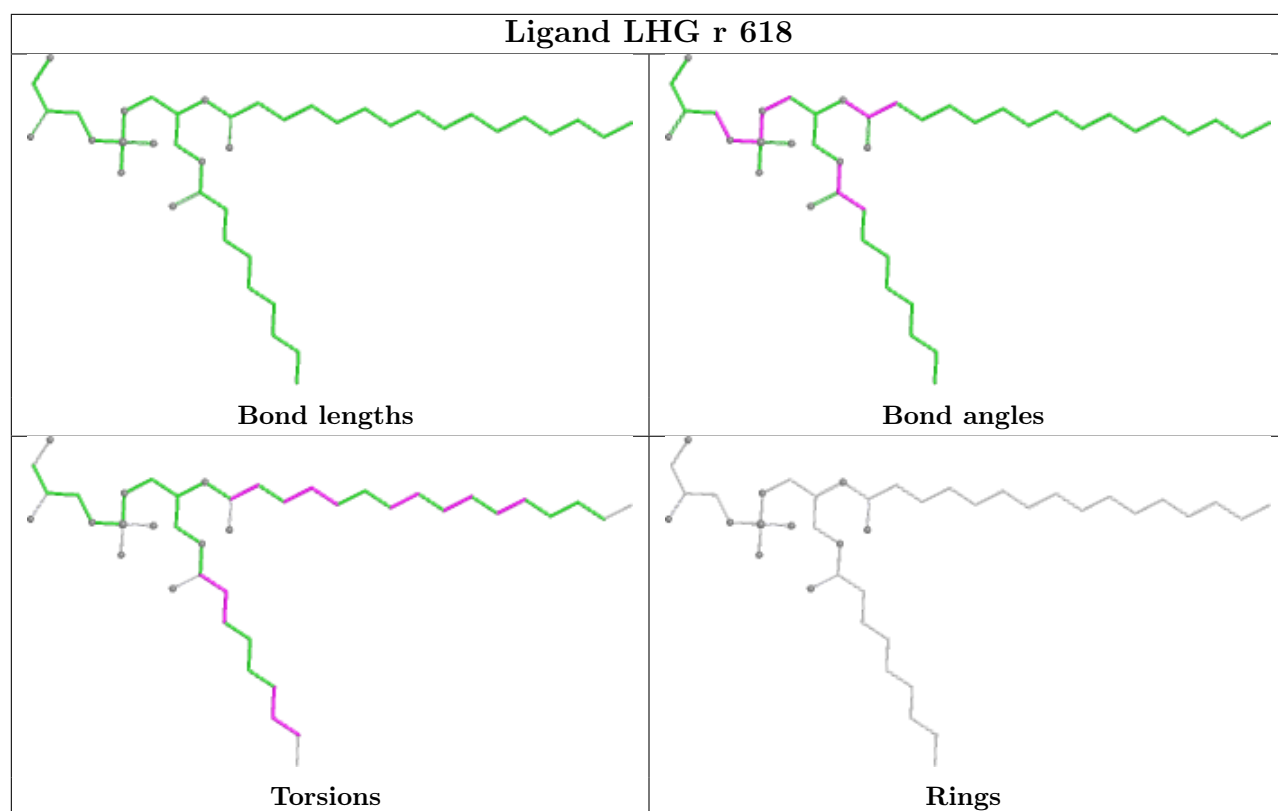
Rings

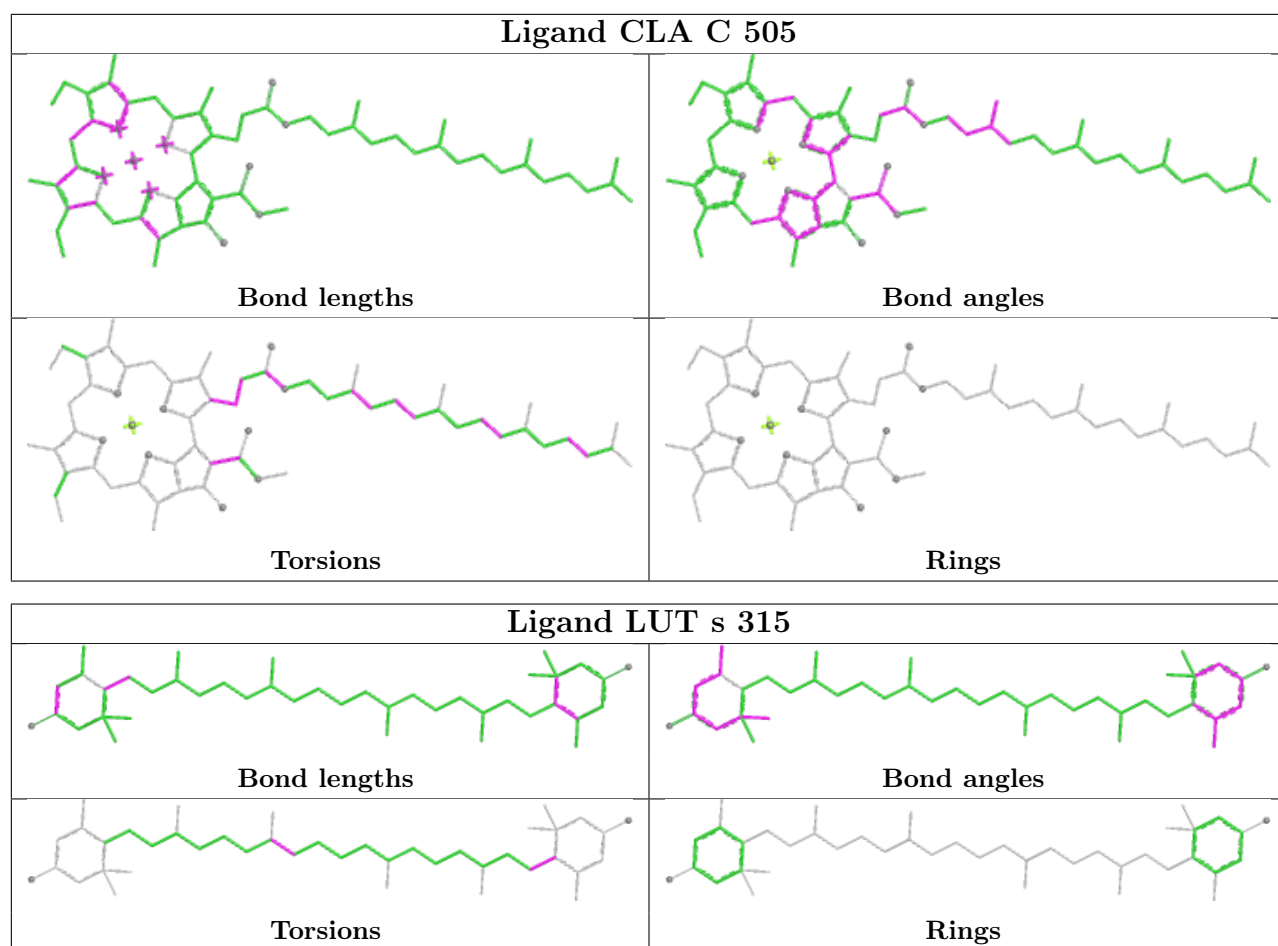
Ligand DGD a 401

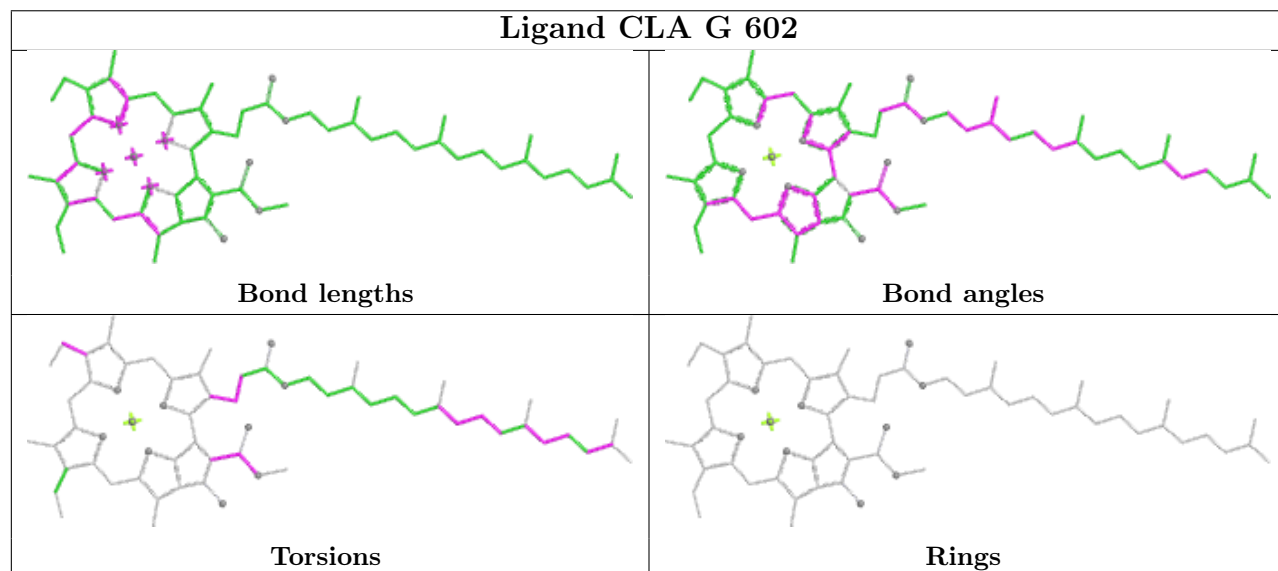
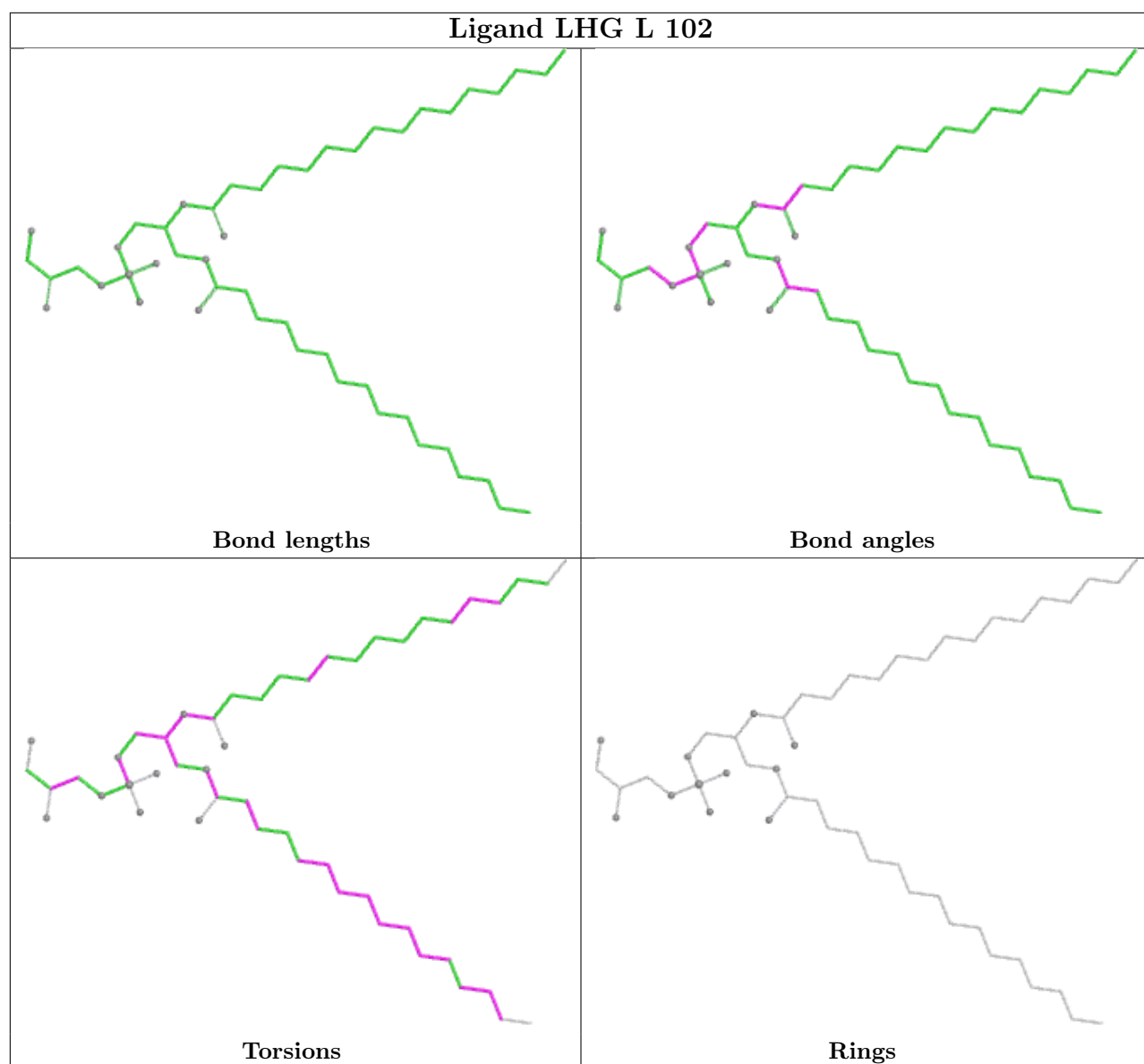


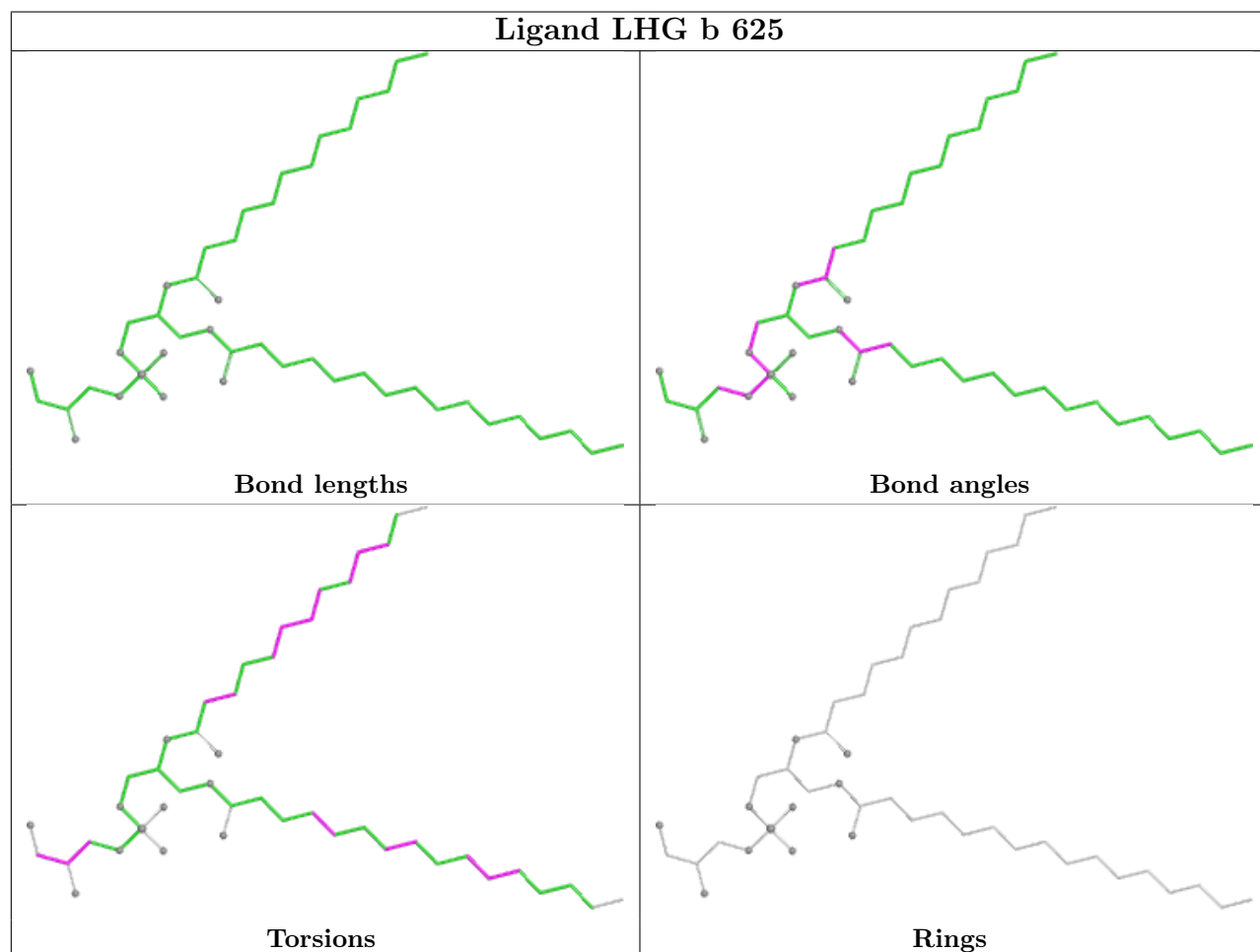
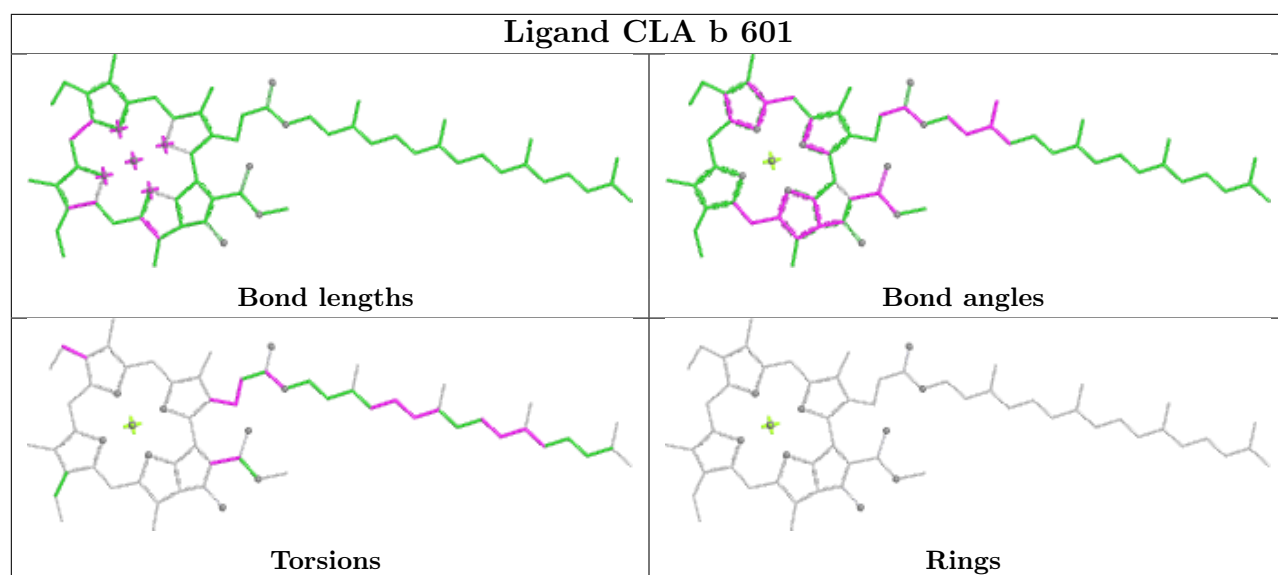
Ligand CHL S 302

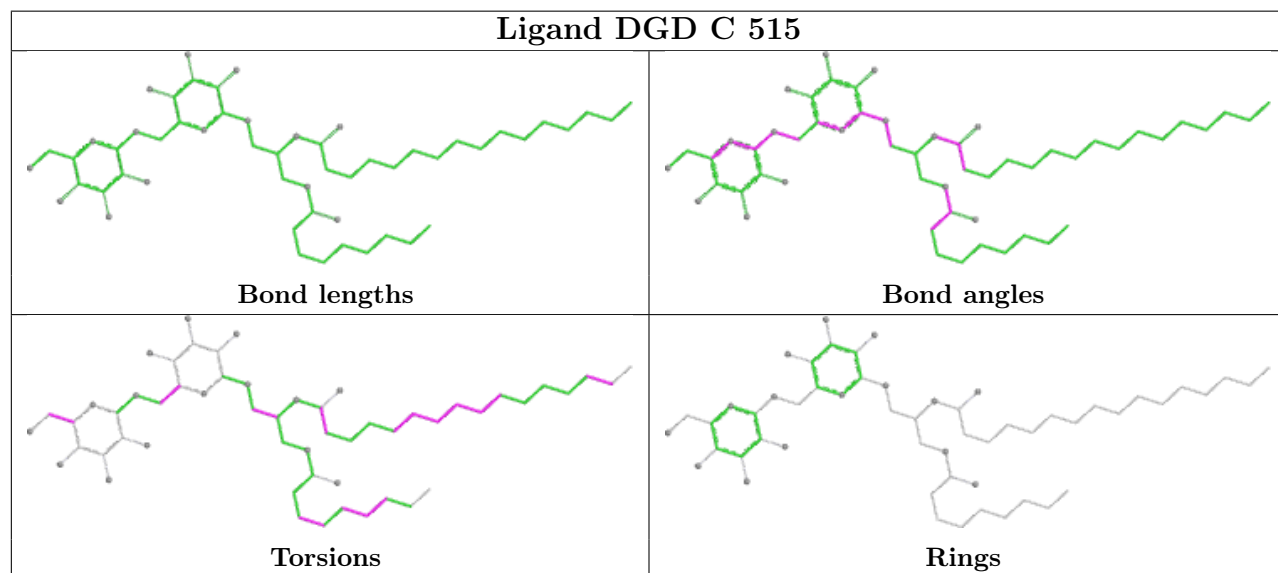
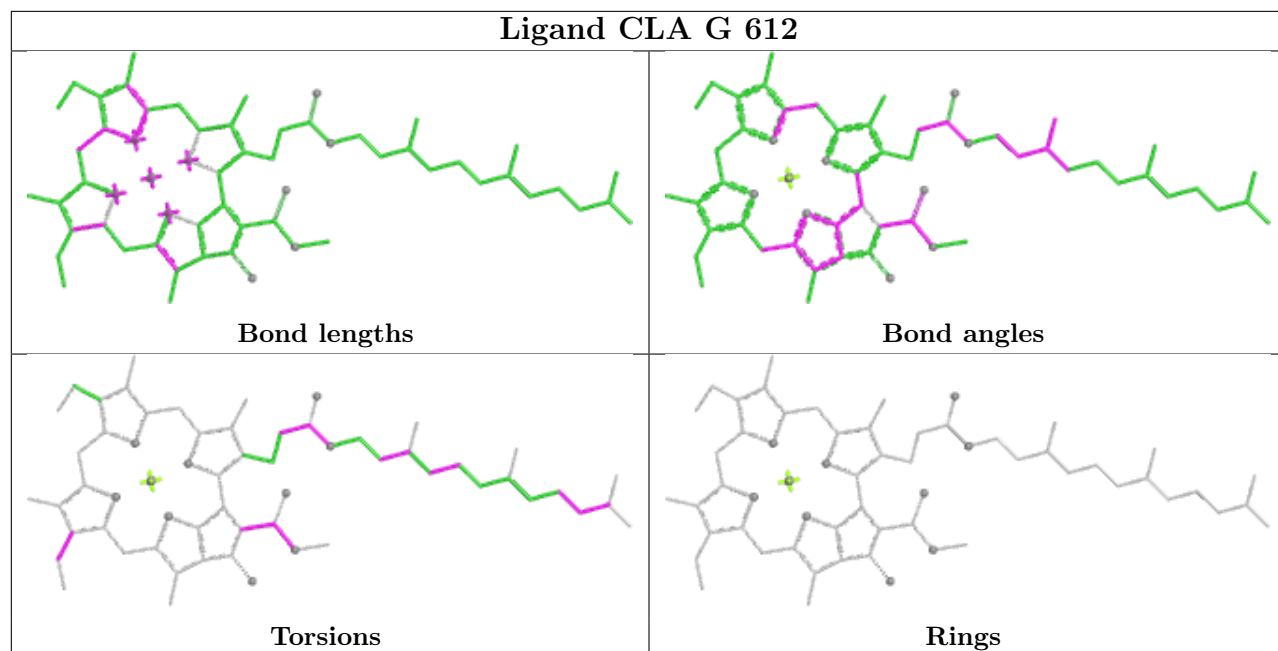


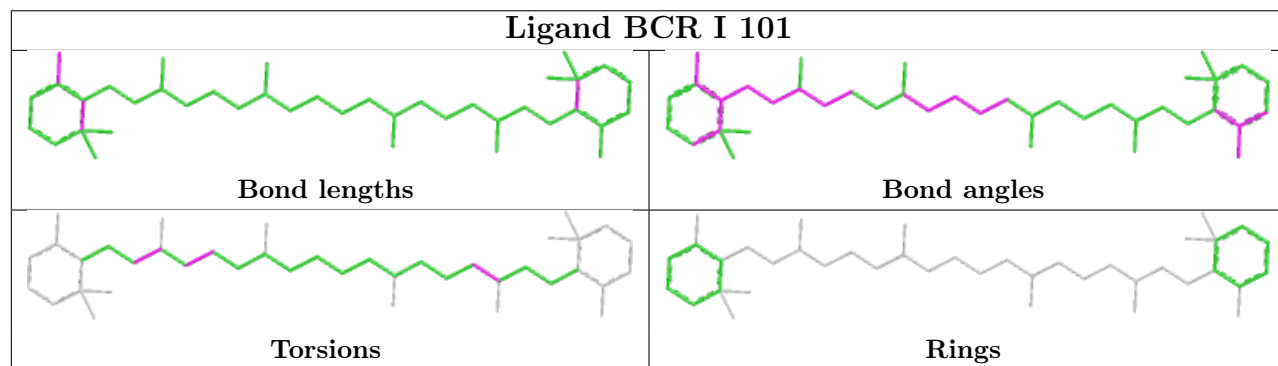
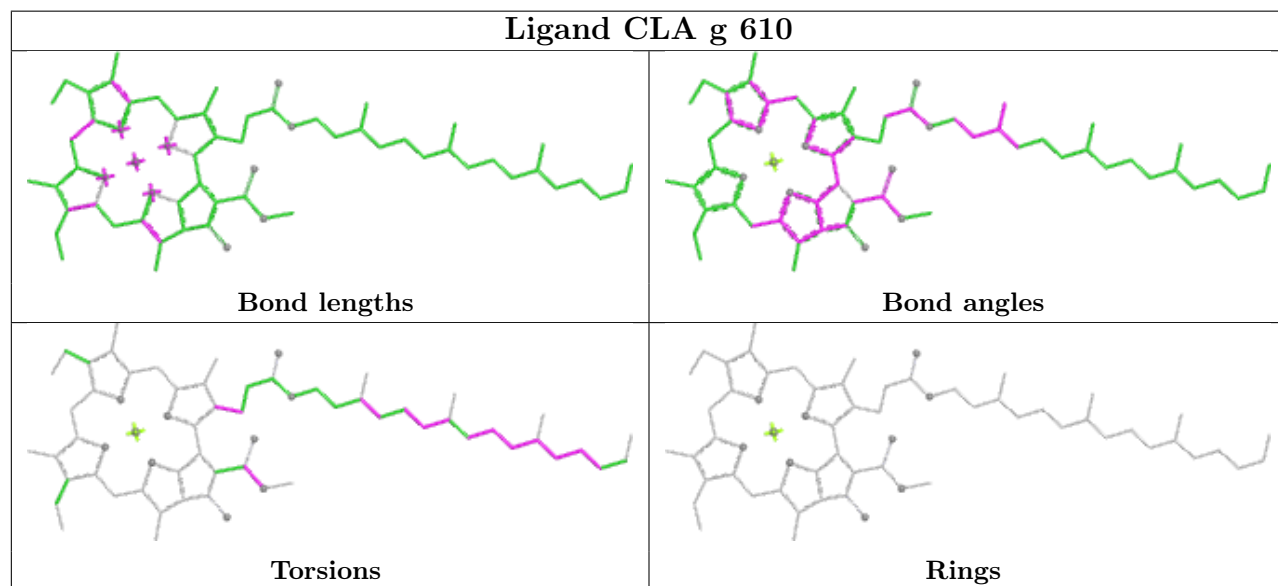
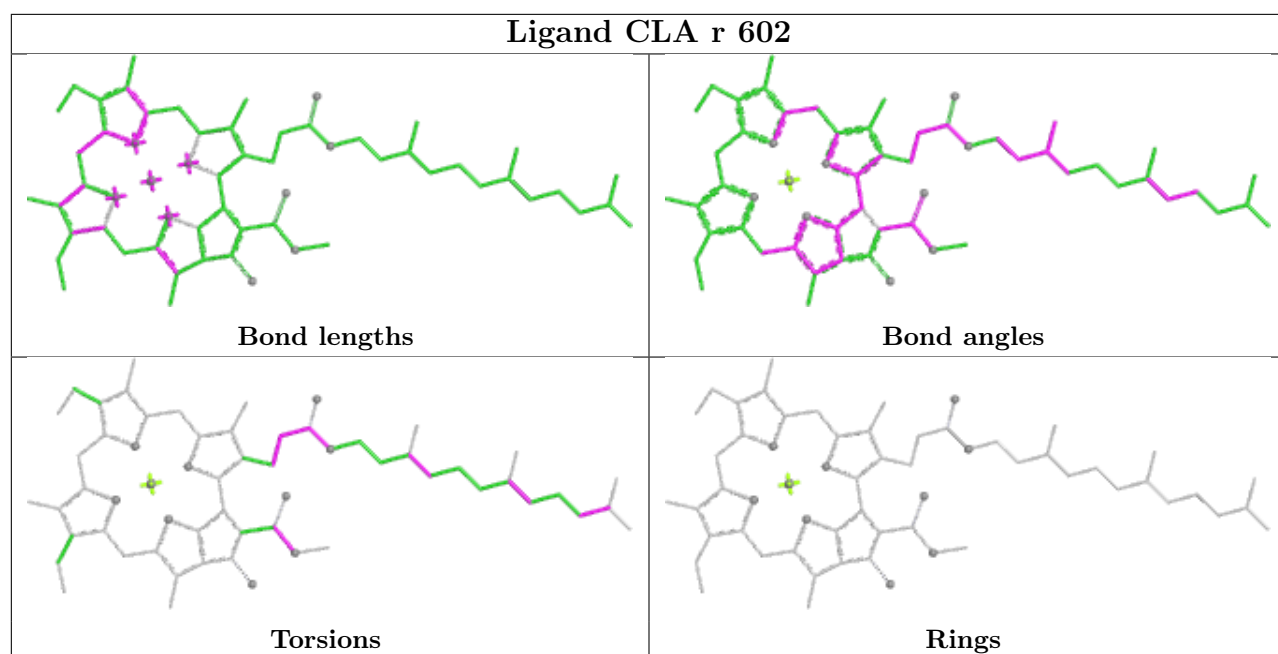


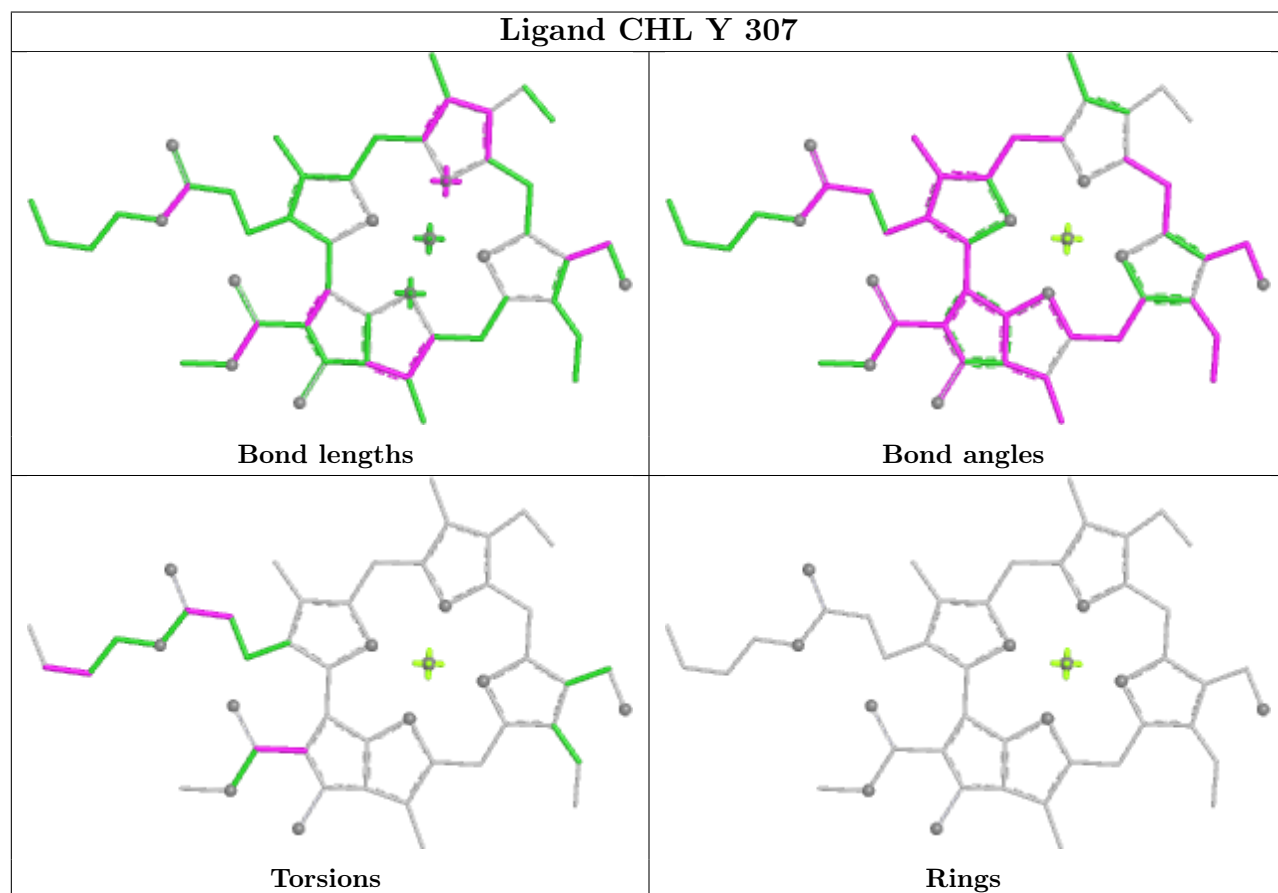
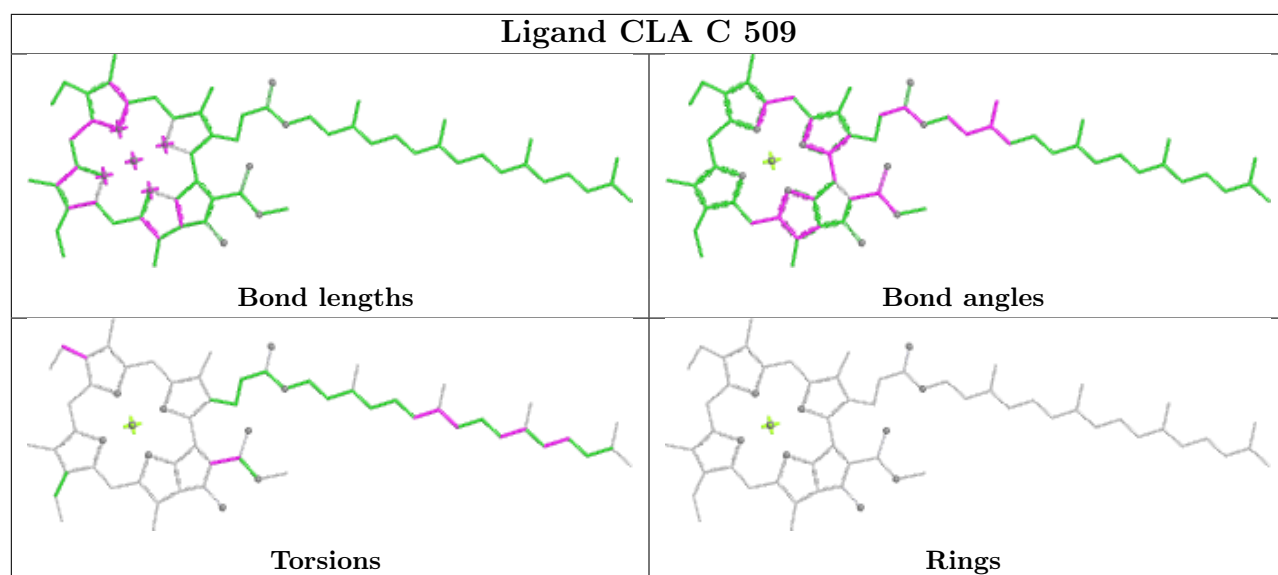


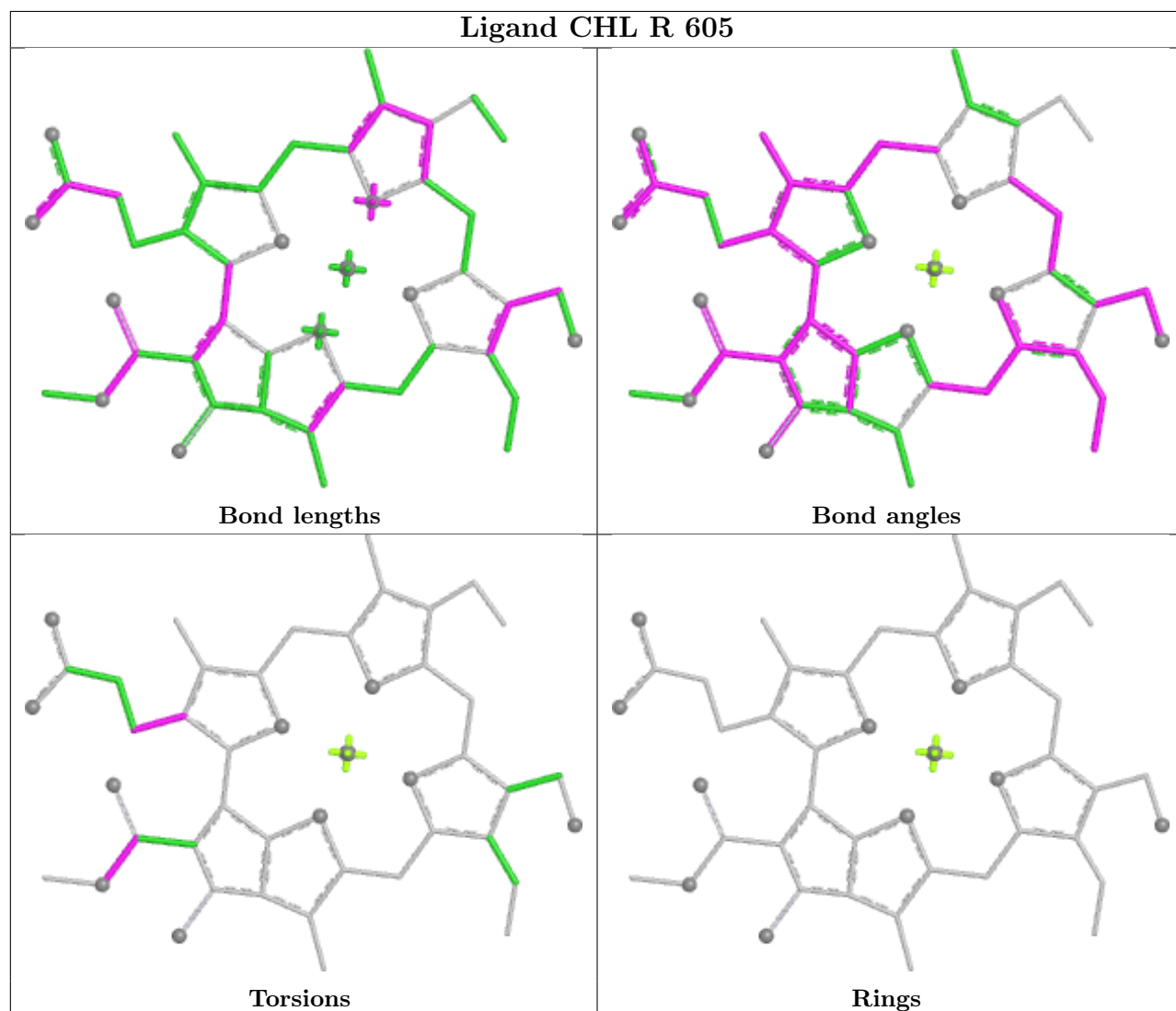
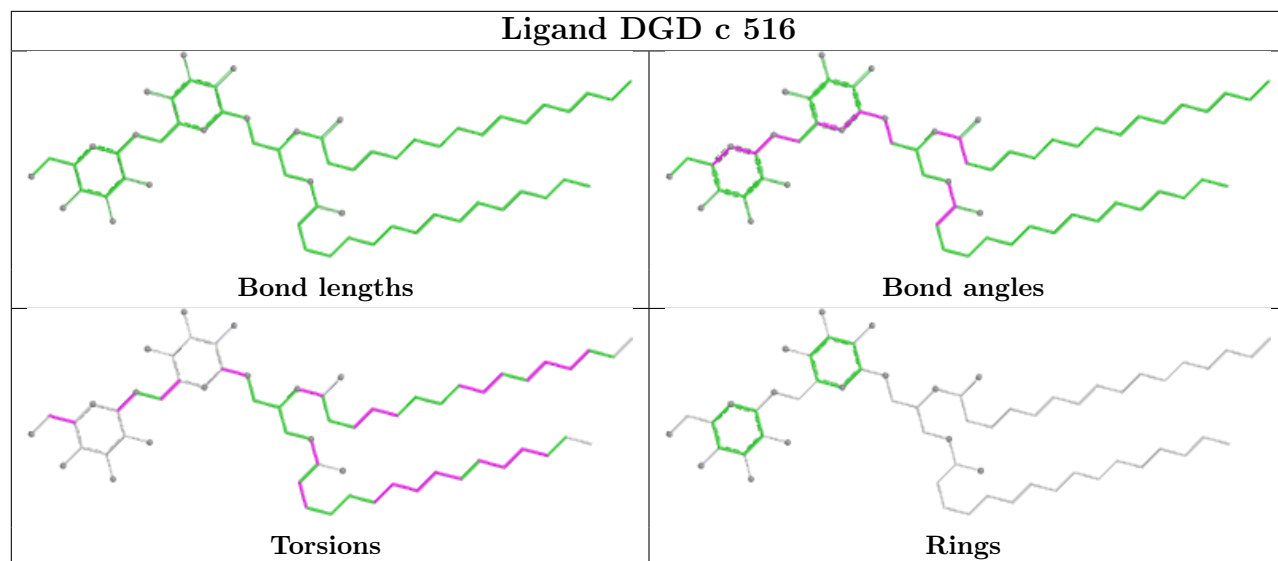


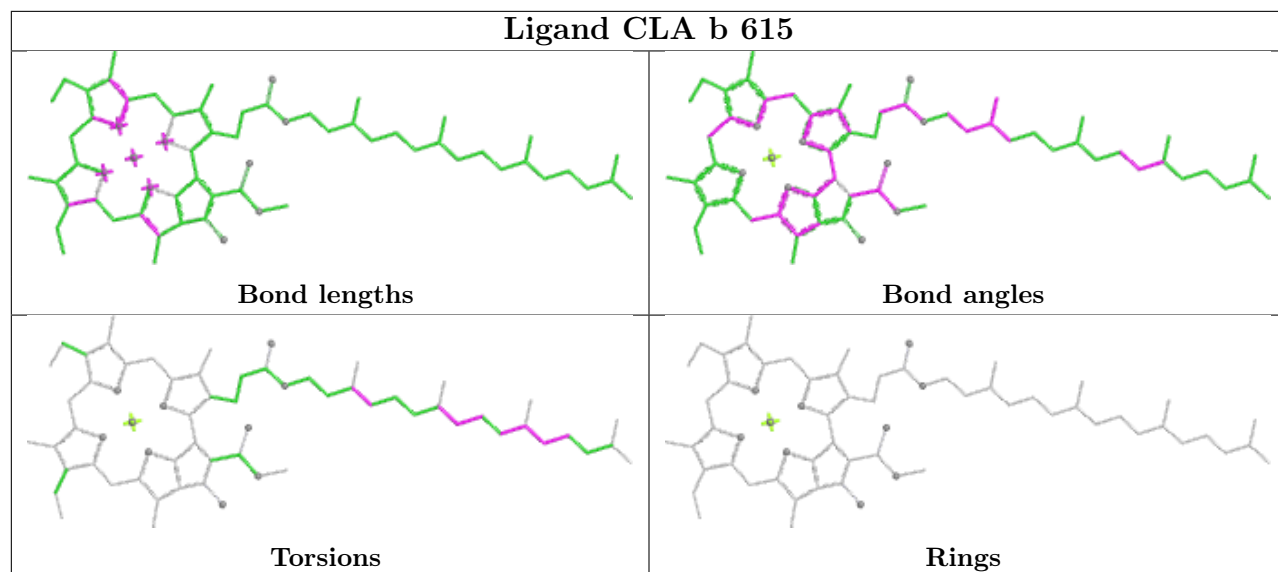
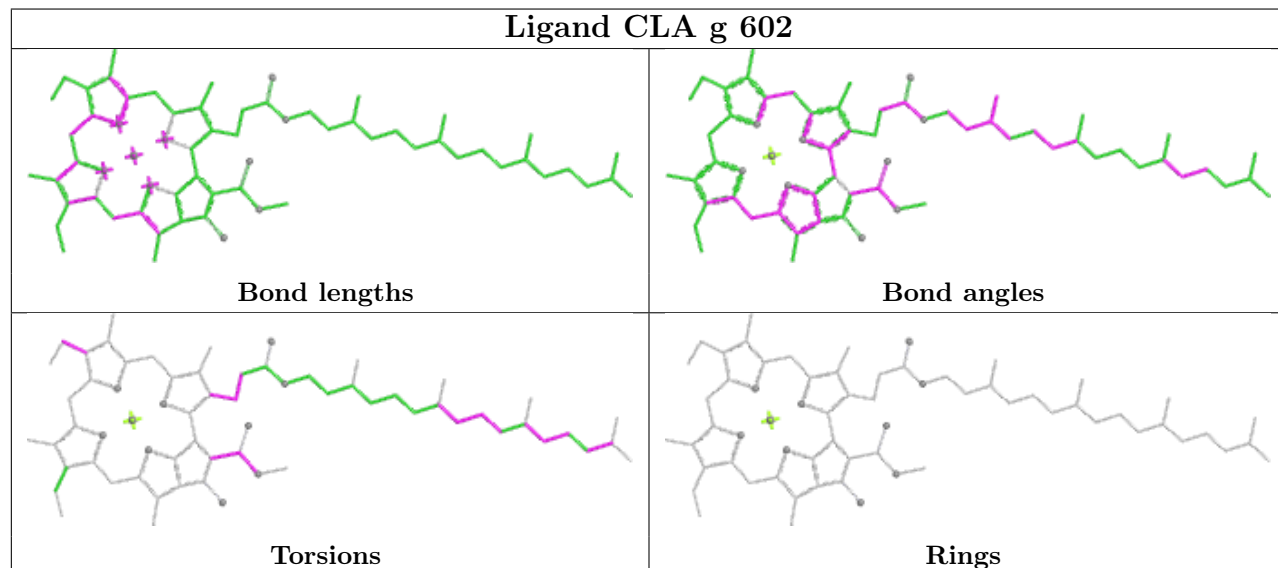




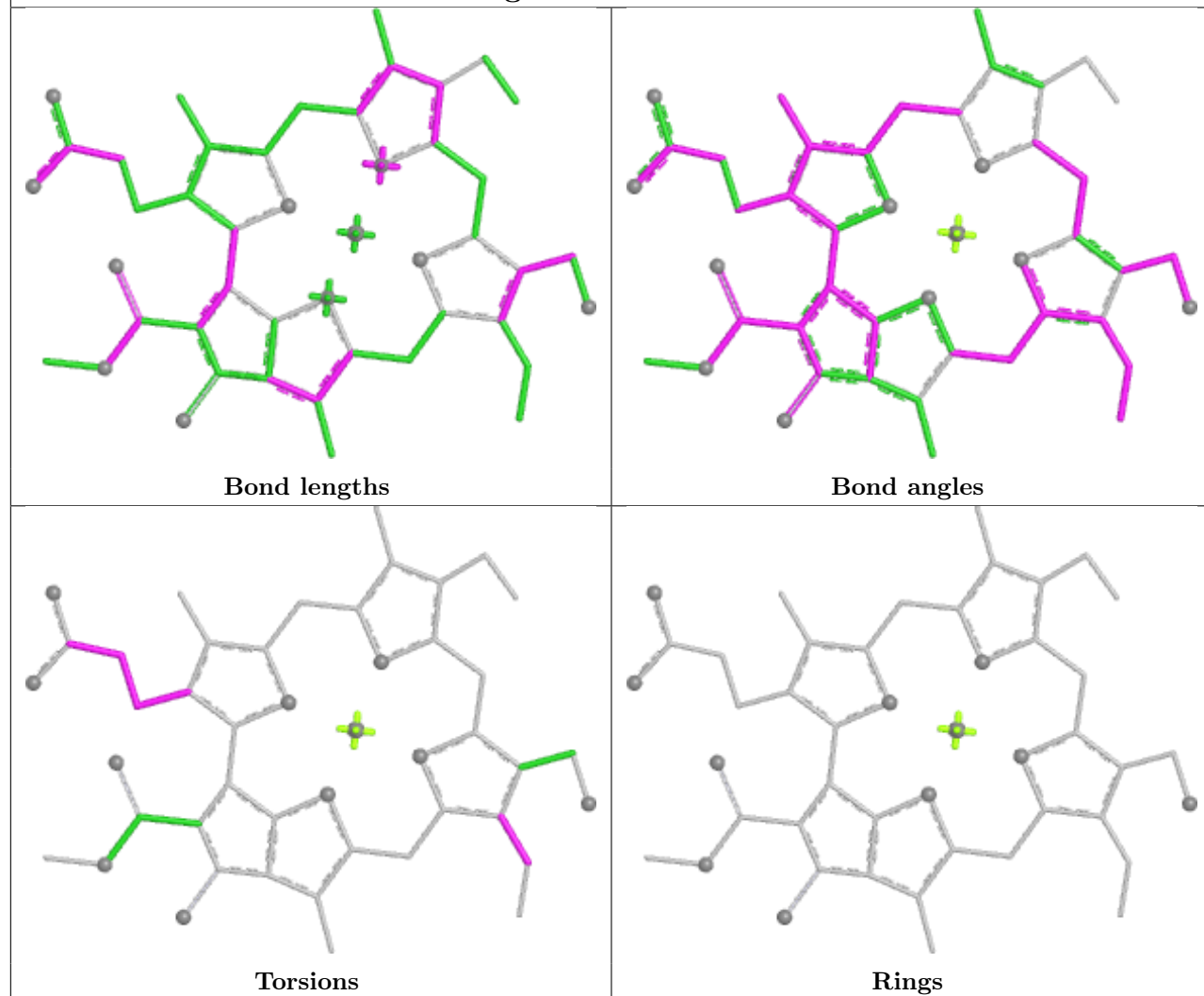




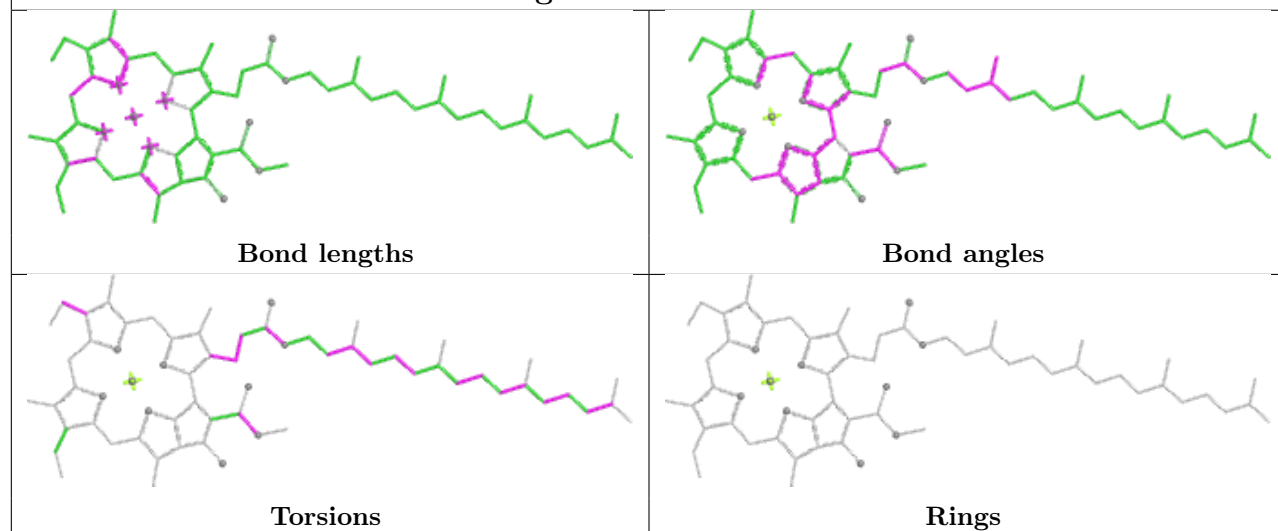


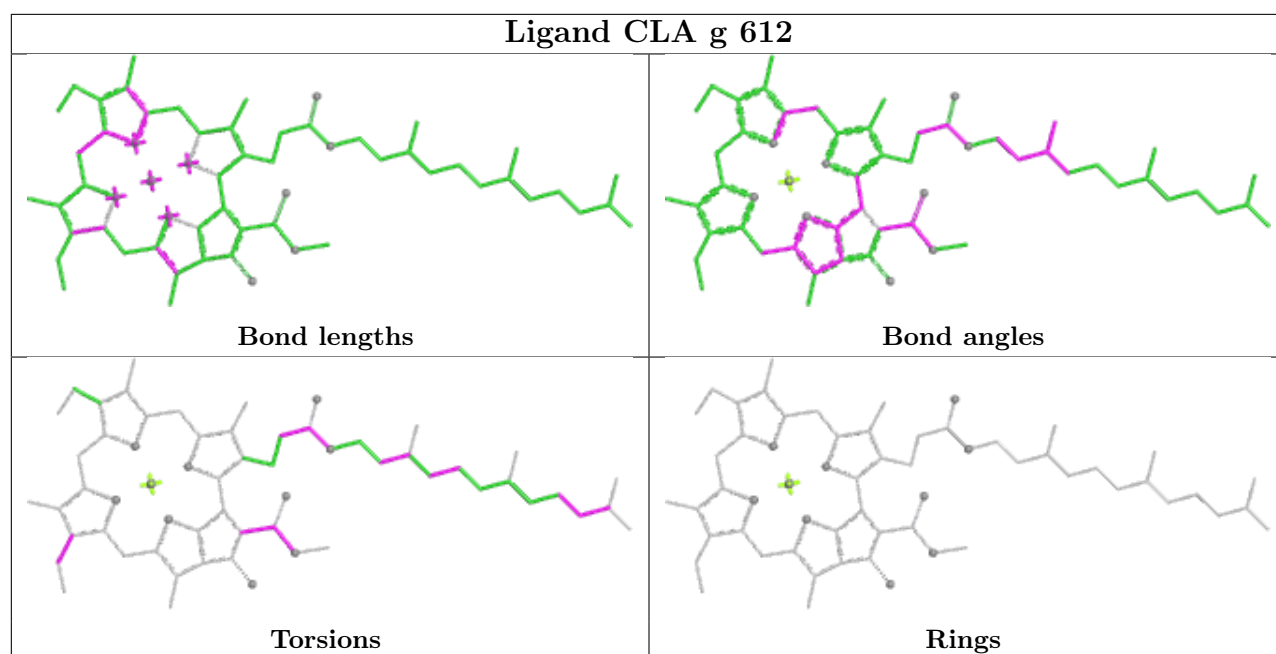
Ligand CLA b 615**Ligand CLA g 602**

Ligand CHL 5 302



Ligand CLA n 610





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

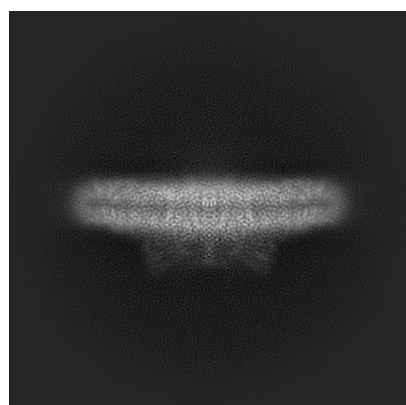
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13078. These allow visual inspection of the internal detail of the map and identification of artifacts.

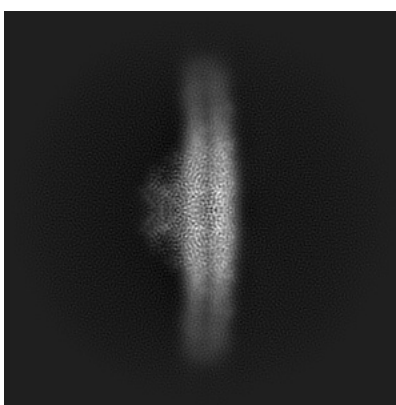
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

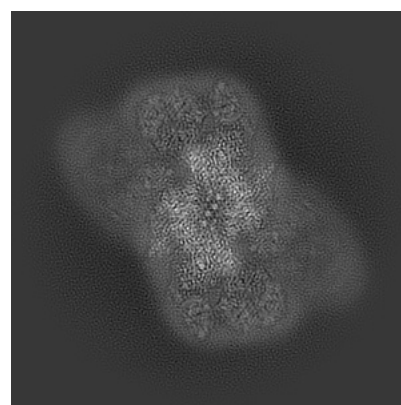
6.1.1 Primary map



X



Y

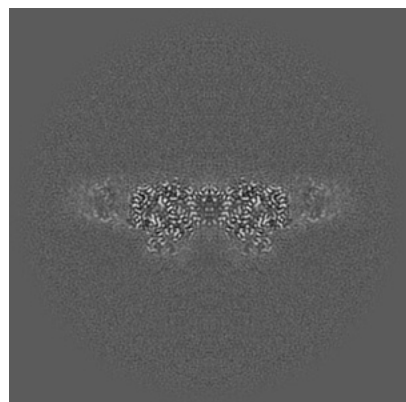


Z

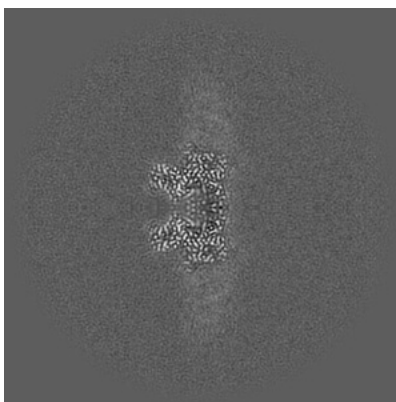
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

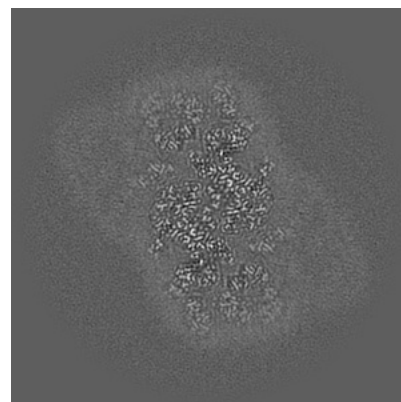
6.2.1 Primary map



X Index: 250



Y Index: 250

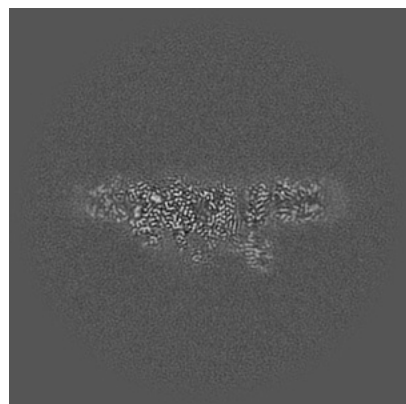


Z Index: 250

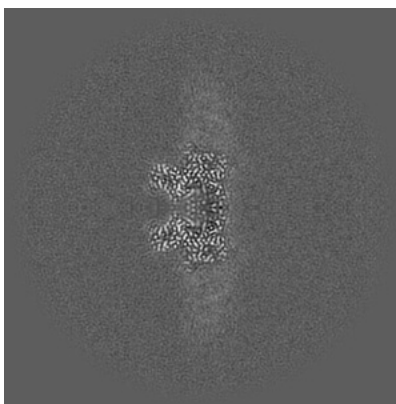
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

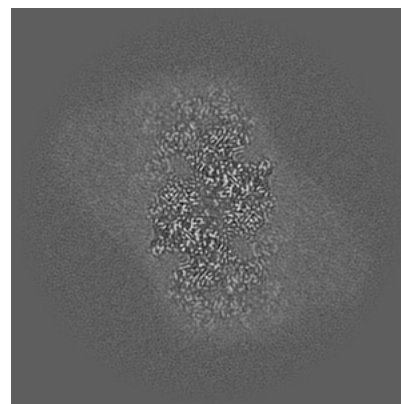
6.3.1 Primary map



X Index: 228



Y Index: 250

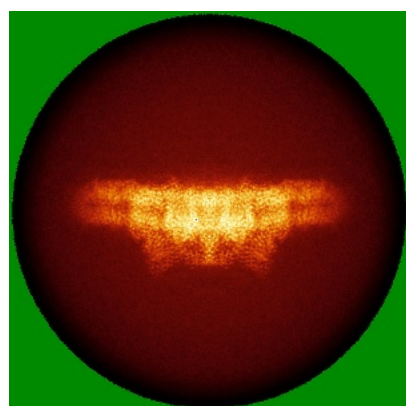


Z Index: 239

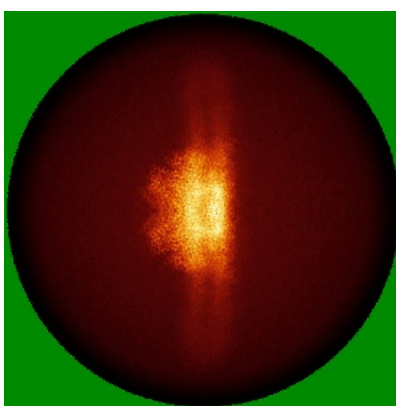
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

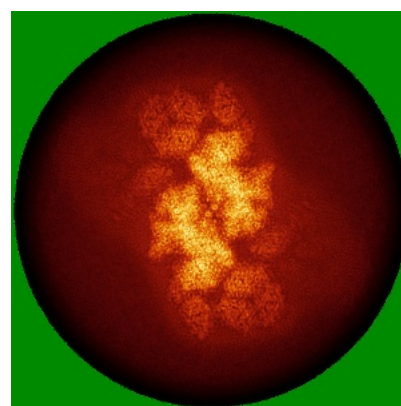
6.4.1 Primary map



X



Y

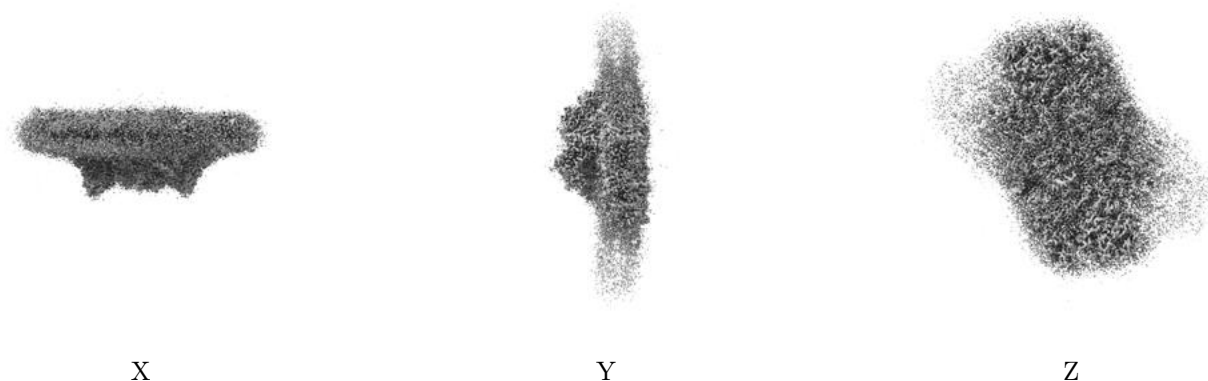


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

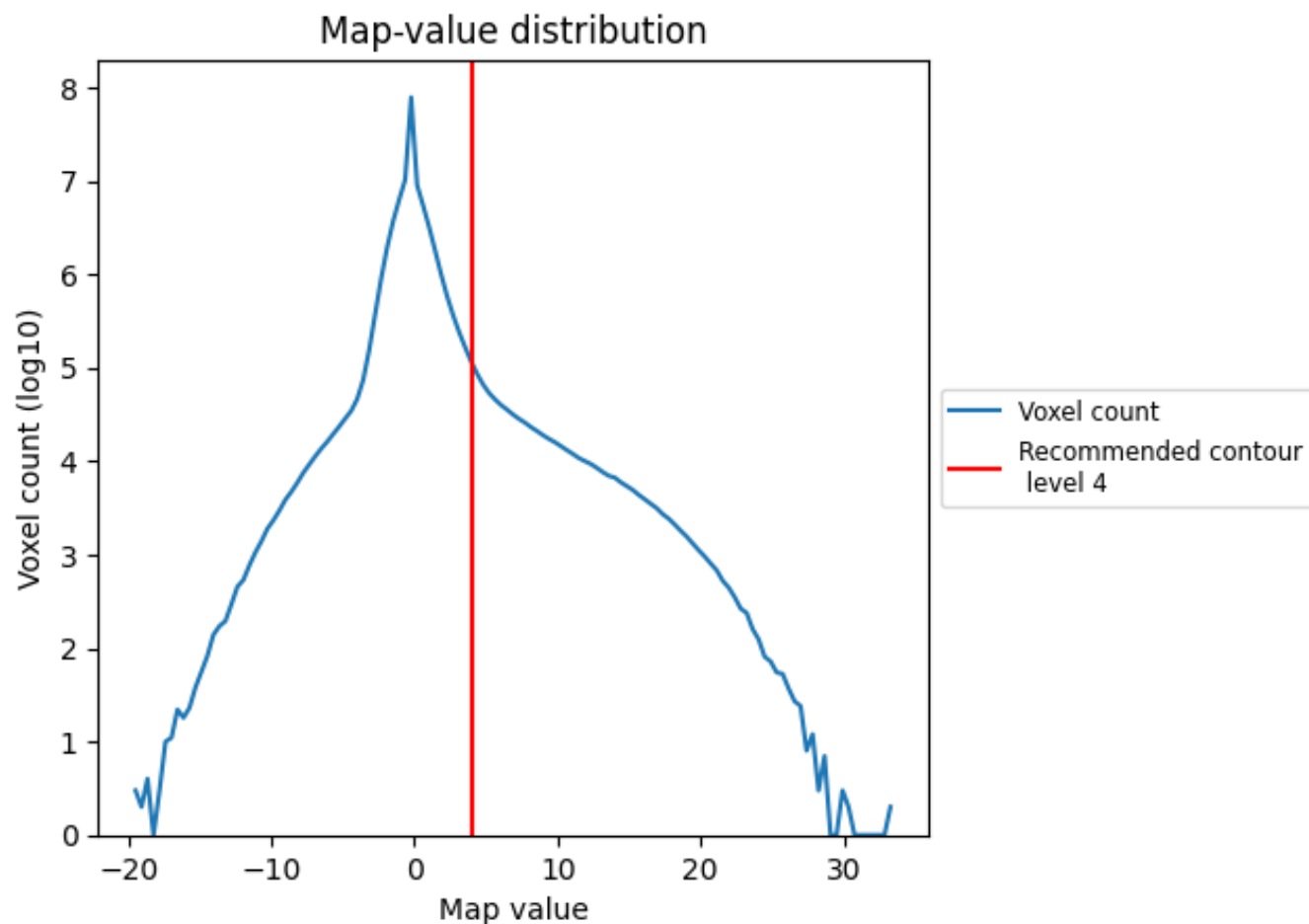
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

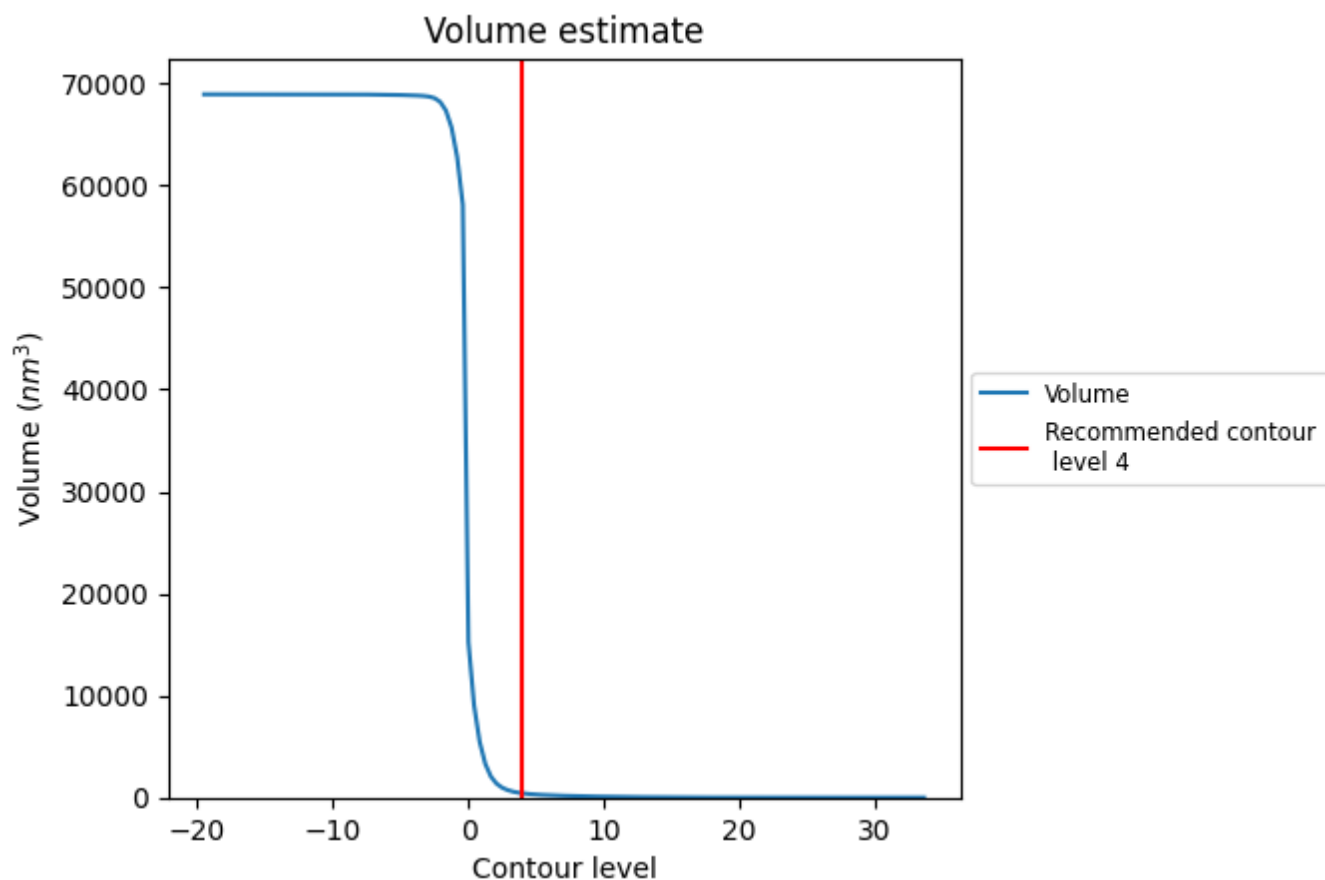
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

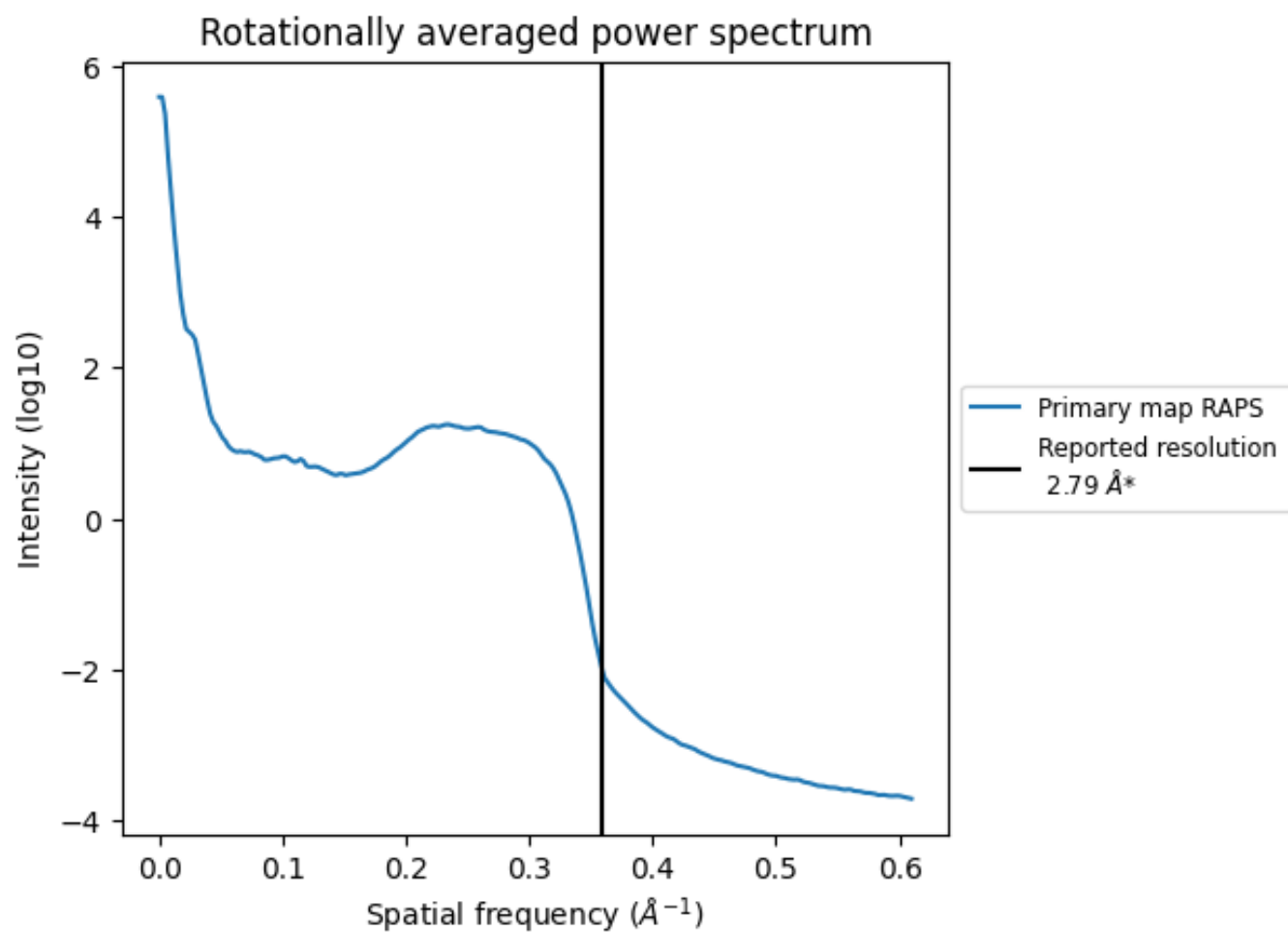
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 423 nm³; this corresponds to an approximate mass of 382 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

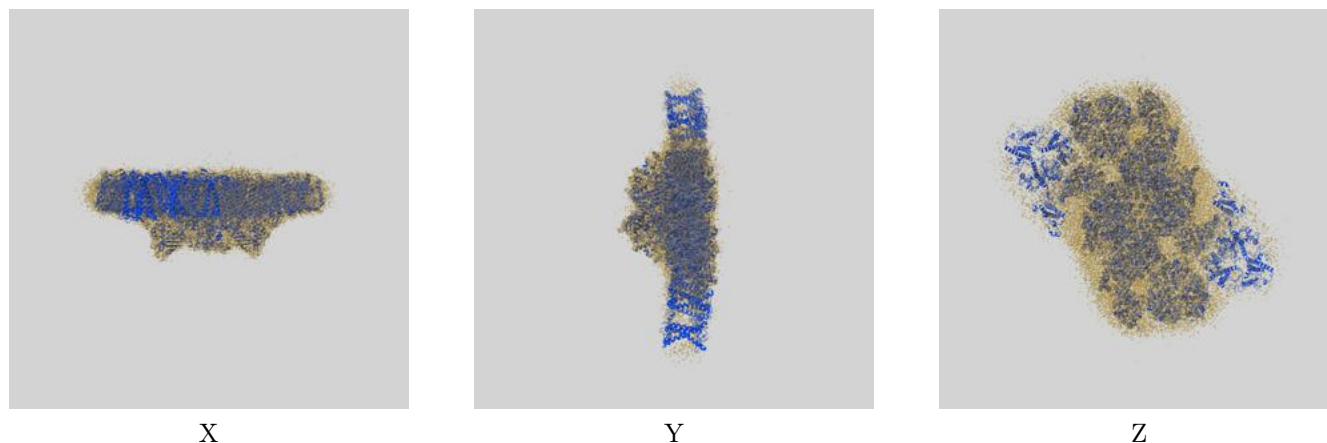
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

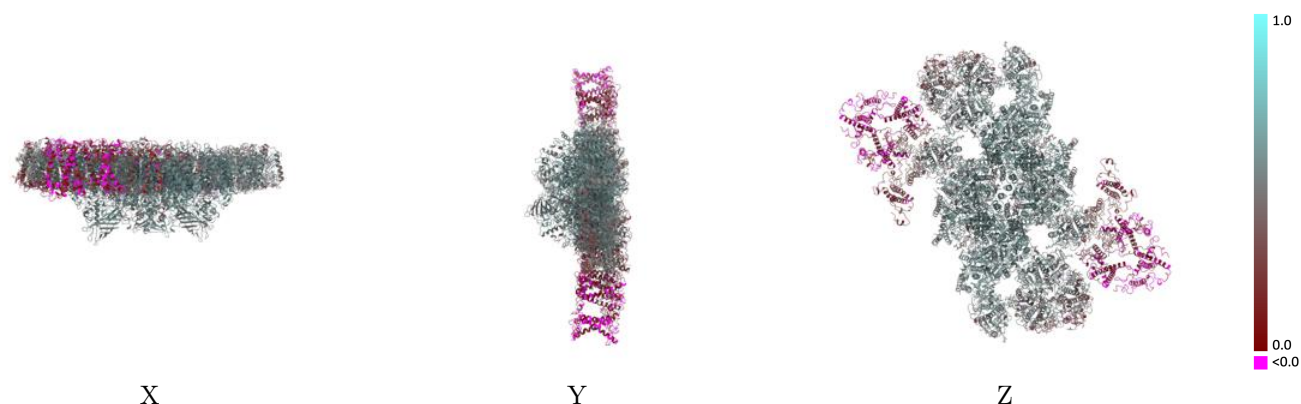
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



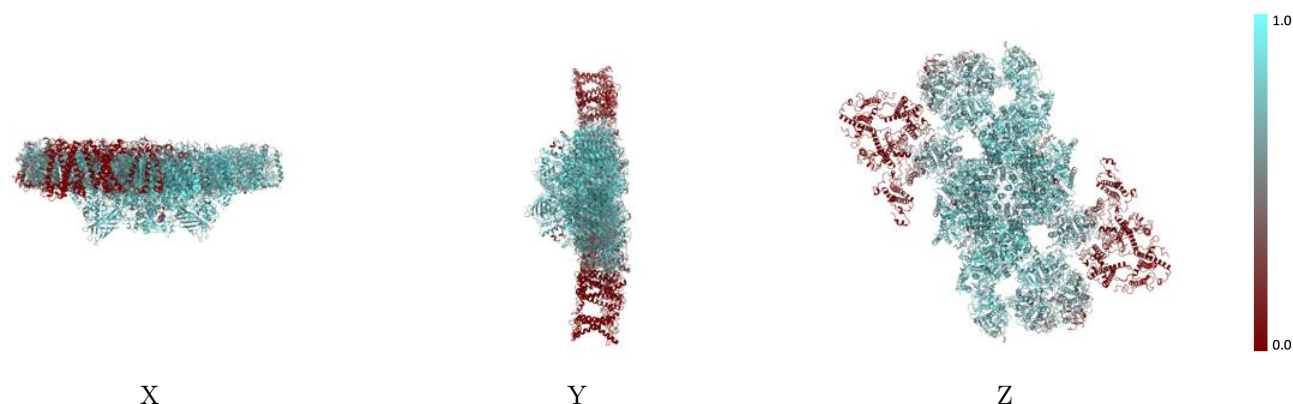
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



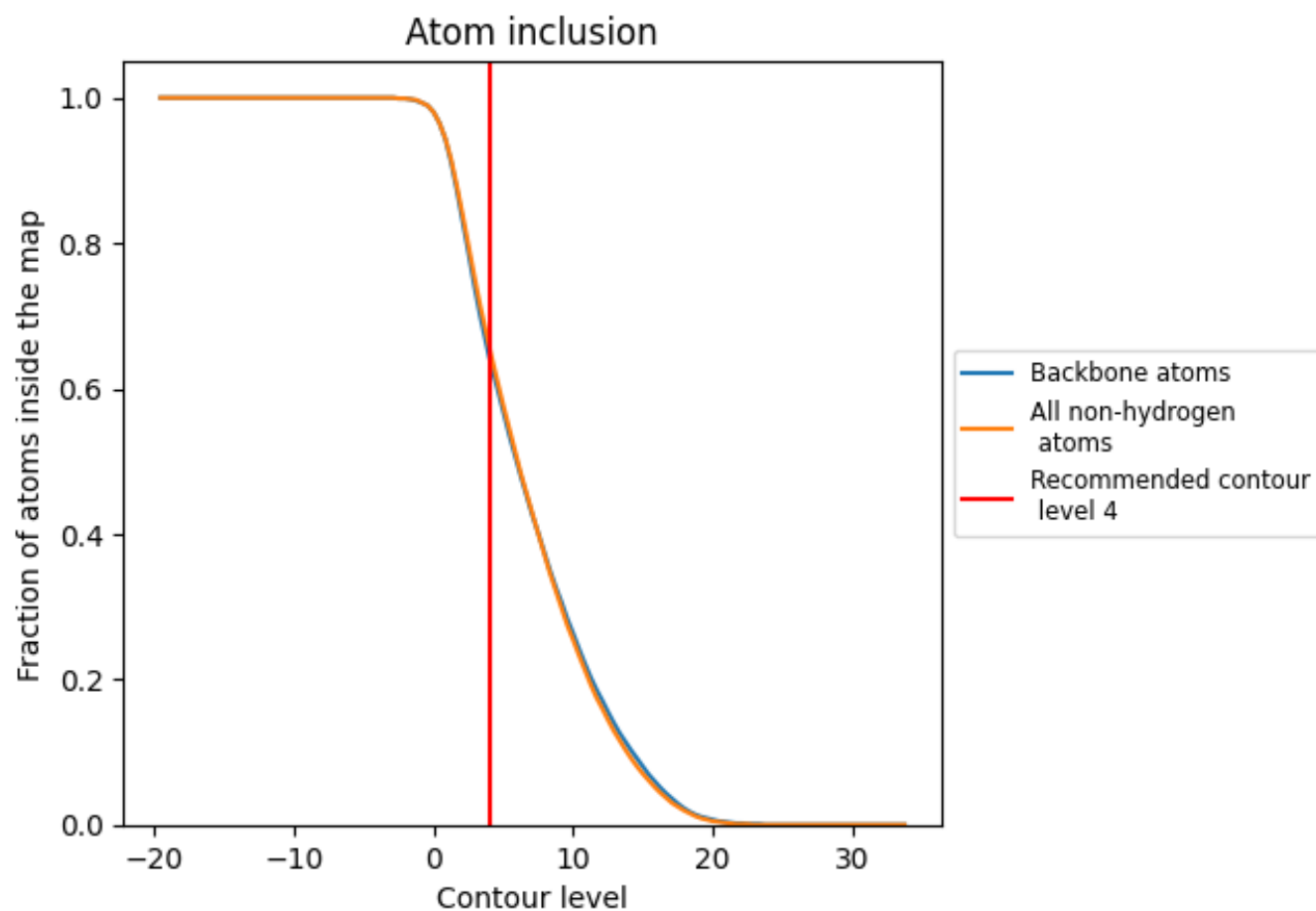
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4650
1	 0.0340	 0.0670
2	 0.0320	 0.1050
3	 0.0060	 0.0400
4	 0.0870	 0.2440
5	 0.0340	 0.0680
6	 0.0320	 0.1040
7	 0.0060	 0.0410
8	 0.0870	 0.2450
A	 0.8540	 0.5740
B	 0.8690	 0.5810
C	 0.8730	 0.5820
D	 0.8800	 0.5890
E	 0.7940	 0.5260
F	 0.7710	 0.5100
G	 0.5250	 0.3940
H	 0.7940	 0.5510
I	 0.8820	 0.6010
K	 0.8250	 0.5570
L	 0.8350	 0.5430
M	 0.8310	 0.5620
N	 0.6500	 0.4540
O	 0.7370	 0.5090
R	 0.6280	 0.4770
S	 0.7300	 0.5110
T	 0.8010	 0.5660
U	 0.2770	 0.4110
W	 0.8340	 0.5810
X	 0.6210	 0.4490
Y	 0.7790	 0.5100
Z	 0.7270	 0.5140
a	 0.8550	 0.5750
b	 0.8680	 0.5800
c	 0.8700	 0.5820
d	 0.8760	 0.5900



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Chain	Atom inclusion	Q-score
e	 0.7920	 0.5240
f	 0.7750	 0.5080
g	 0.5270	 0.3930
h	 0.7920	 0.5510
i	 0.8940	 0.5980
k	 0.8400	 0.5590
l	 0.8350	 0.5420
m	 0.8230	 0.5660
n	 0.6500	 0.4530
o	 0.7360	 0.5130
r	 0.6250	 0.4760
s	 0.7260	 0.5110
t	 0.8080	 0.5700
u	 0.2820	 0.4040
w	 0.8340	 0.5760
x	 0.6250	 0.4400
y	 0.7770	 0.5080
z	 0.7150	 0.5110