



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:23 AM UTC

PDB ID : 7CZL / pdb_00007czl
EMDB ID : EMD-30511
Title : Structural insights into a dimeric Psb27-photosystem II complex from a cyanobacterium *Thermosynechococcus vulcanus*
Authors : Pi, X.; Huang, G.; Xiao, Y.
Deposited on : 2020-09-09
Resolution : 3.78 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:

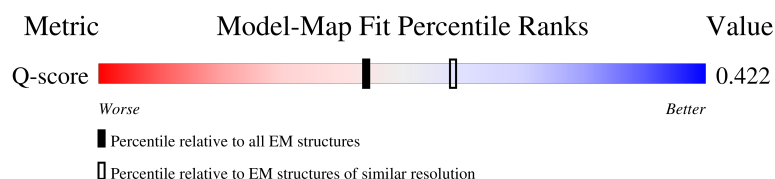
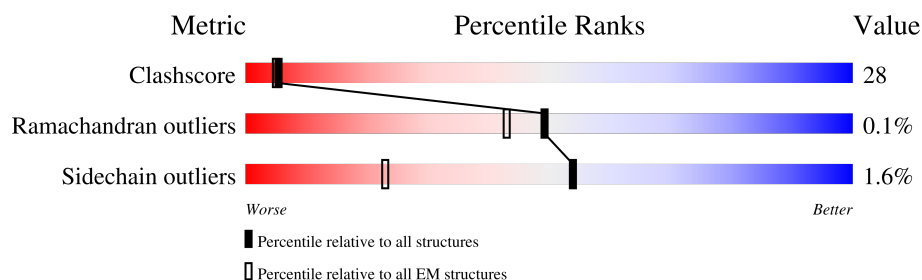
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.78 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	10074 (3.28 - 4.27)

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	A	324	 53% 46% .
1	a	324	 52% 47% ..
2	B	505	 54% 42% .
2	b	505	 53% 43% .

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Mol	Chain	Length	Quality of chain
3	C	446	
3	c	446	
4	D	339	
4	d	339	
5	E	65	
5	e	65	
6	F	31	
6	f	31	
7	H	62	
7	h	62	
8	I	34	
8	i	34	
9	K	37	
9	k	37	
10	L	37	
10	l	37	
11	M	33	
11	m	33	
12	T	30	
12	t	30	
13	Z	62	
13	z	62	
14	Y	30	
14	y	30	
15	N	108	

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Mol	Chain	Length	Quality of chain
15	n	108	
16	X	40	
16	x	40	

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
17	CLA	A	401	X	-	-	-
17	CLA	A	402	X	-	-	-
17	CLA	A	403	X	-	-	-
17	CLA	A	405	X	-	-	-
17	CLA	B	601	X	-	-	-
17	CLA	B	602	X	-	-	-
17	CLA	B	603	X	-	-	-
17	CLA	B	604	X	-	-	-
17	CLA	B	605	X	-	-	-
17	CLA	B	606	X	-	-	-
17	CLA	B	607	X	-	-	-
17	CLA	B	608	X	-	-	-
17	CLA	B	609	X	-	-	-
17	CLA	B	610	X	-	-	-
17	CLA	B	611	X	-	-	-
17	CLA	B	612	X	-	-	-
17	CLA	B	613	X	-	-	-
17	CLA	B	614	X	-	-	-
17	CLA	B	615	X	-	-	-
17	CLA	B	616	X	-	-	-
17	CLA	C	501	X	-	-	-
17	CLA	C	502	X	-	-	-
17	CLA	C	503	X	-	-	-
17	CLA	C	504	X	-	-	-
17	CLA	C	505	X	-	-	-
17	CLA	C	506	X	-	-	-
17	CLA	C	507	X	-	-	-
17	CLA	C	508	X	-	-	-
17	CLA	C	509	X	-	-	-
17	CLA	C	510	X	-	-	-
17	CLA	C	511	X	-	-	-
17	CLA	C	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	C	513	X	-	-	-
17	CLA	D	404	X	-	-	-
17	CLA	D	405	X	-	-	-
17	CLA	a	5402	X	-	-	-
17	CLA	a	5403	X	-	-	-
17	CLA	a	5404	X	-	-	-
17	CLA	a	5406	X	-	-	-
17	CLA	b	5601	X	-	-	-
17	CLA	b	5602	X	-	-	-
17	CLA	b	5603	X	-	-	-
17	CLA	b	5604	X	-	-	-
17	CLA	b	5605	X	-	-	-
17	CLA	b	5606	X	-	-	-
17	CLA	b	5607	X	-	-	-
17	CLA	b	5608	X	-	-	-
17	CLA	b	5609	X	-	-	-
17	CLA	b	5610	X	-	-	-
17	CLA	b	5611	X	-	-	-
17	CLA	b	5612	X	-	-	-
17	CLA	b	5613	X	-	-	-
17	CLA	b	5614	X	-	-	-
17	CLA	b	5615	X	-	-	-
17	CLA	b	5616	X	-	-	-
17	CLA	c	5501	X	-	-	-
17	CLA	c	5502	X	-	-	-
17	CLA	c	5503	X	-	-	-
17	CLA	c	5504	X	-	-	-
17	CLA	c	5505	X	-	-	-
17	CLA	c	5506	X	-	-	-
17	CLA	c	5507	X	-	-	-
17	CLA	c	5508	X	-	-	-
17	CLA	c	5509	X	-	-	-
17	CLA	c	5510	X	-	-	-
17	CLA	c	5511	X	-	-	-
17	CLA	c	5512	X	-	-	-
17	CLA	d	5403	X	-	-	-
17	CLA	d	5404	X	-	-	-
17	CLA	k	5501	X	-	-	-
24	BCT	A	411	-	-	X	-
24	BCT	a	5412	-	-	X	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 40859 atoms, of which 0 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	324	Total	C	N	O	S	0	0
			2533	1662	414	442	15		
1	a	322	Total	C	N	O	S	0	0
			2523	1656	412	440	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
A	286	THR	ALA	conflict	UNP P51765
a	5279	PRO	ARG	conflict	UNP P51765
a	5286	THR	ALA	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3784	2488	628	655	13		
2	b	484	Total	C	N	O	S	0	0
			3780	2486	628	653	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	ARG	LYS	conflict	UNP D0VWR1
b	5506	ARG	LYS	conflict	UNP D0VWR1

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2693	1786	438	457	12		
4	d	339	Total	C	N	O	S	0	0
			2687	1783	435	457	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total	C	N	O	0	0
			522	345	81	96		
5	e	65	Total	C	N	O	0	0
			522	345	81	96		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			482	324	75	81	2		
7	h	62	Total	C	N	O	S	0	0
			482	324	75	81	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			277	189	43	44	1		
8	i	34	Total	C	N	O	S	0	0
			277	189	43	44	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			289	201	42	46		
9	k	34	Total	C	N	O	0	0
			264	186	36	42		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	5033	LEU	PHE	conflict	UNP P19054
k	5039	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	200	48	53		
10	l	37	Total	C	N	O	0	0
			301	200	48	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	33	Total	C	N	O	S	0	0
			258	172	38	47	1		
11	m	33	Total	C	N	O	S	0	0
			258	172	38	47	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	5008	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		
13	z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		
14	y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		

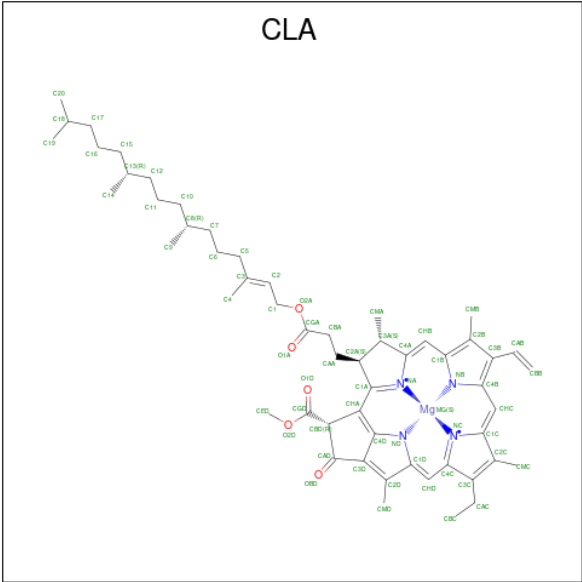
- Molecule 15 is a protein called Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	108	Total	C	N	O	S	0	0
			860	536	155	167	2		
15	N	108	Total	C	N	O	S	0	0
			860	536	155	167	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	35	Total	C	N	O	0	0
			254	173	38	43		
16	x	35	Total	C	N	O	0	0
			254	173	38	43		

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	D	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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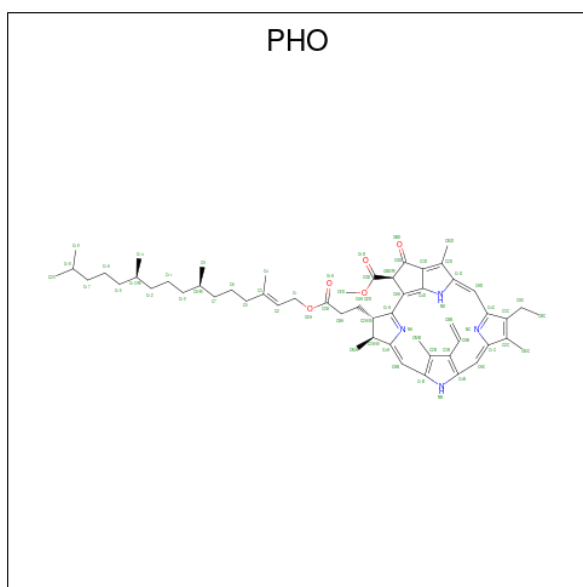
Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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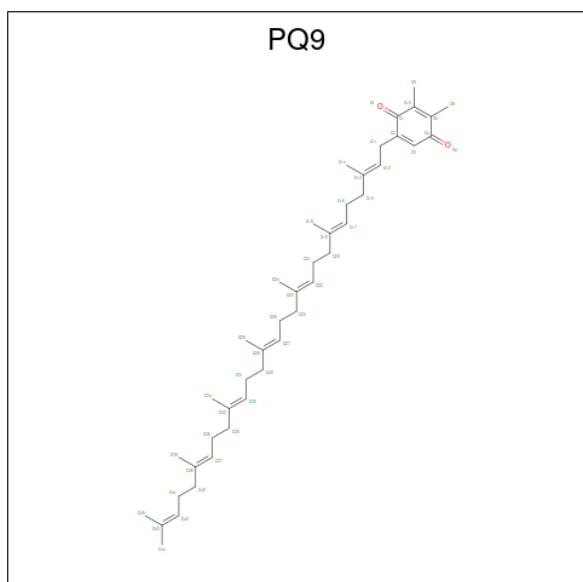
Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 18 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



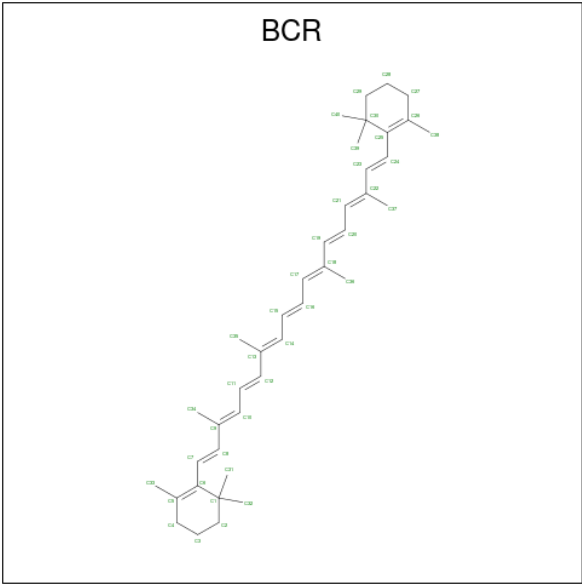
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	N	O	0
			64	55	4	5	
18	D	1	Total	C	N	O	0
			64	55	4	5	
18	a	1	Total	C	N	O	0
			64	55	4	5	
18	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 19 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: $C_{43}H_{64}O_2$).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			45	43	2	
19	D	1	Total	C	O	0
			45	43	2	
19	a	1	Total	C	O	0
			30	28	2	
19	d	1	Total	C	O	0
			45	43	2	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



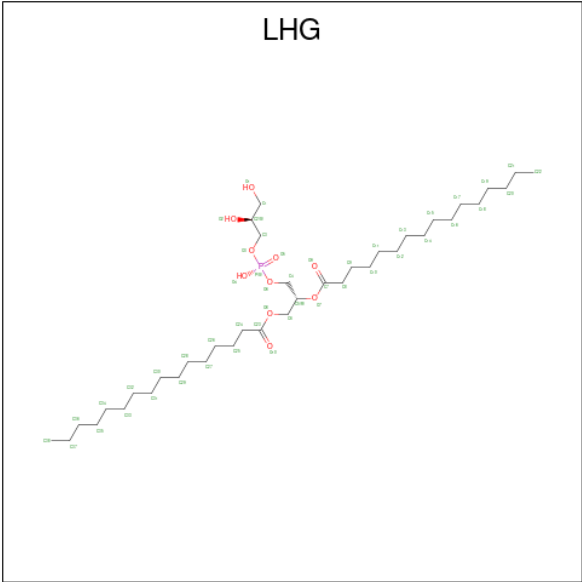
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	D	1	Total	C	0
			40	40	
20	H	1	Total	C	0
			40	40	

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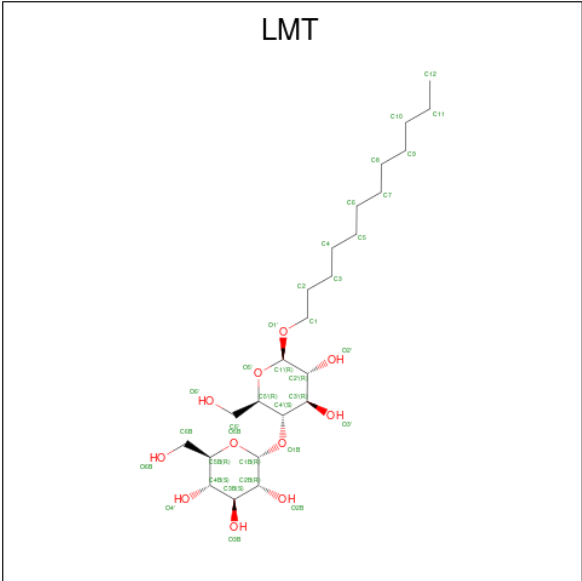
Mol	Chain	Residues	Atoms	AltConf
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	d	1	Total C 40 40	0
20	h	1	Total C 40 40	0
20	k	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	z	1	Total C 40 40	0
20	Y	1	Total C 40 40	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			39	28	10	1	
21	a	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



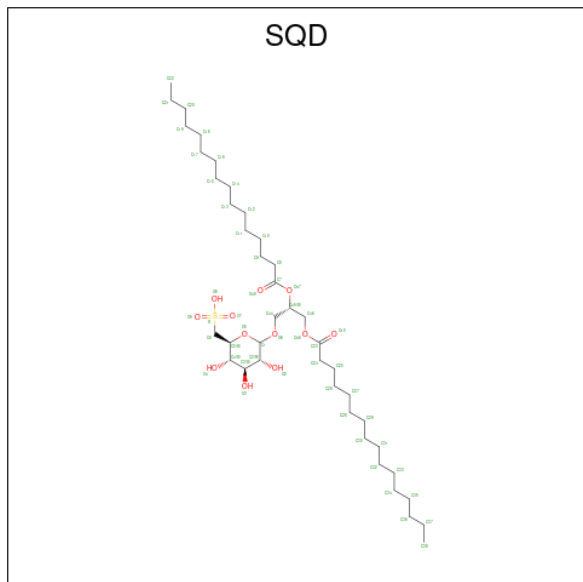
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			35	24	11	

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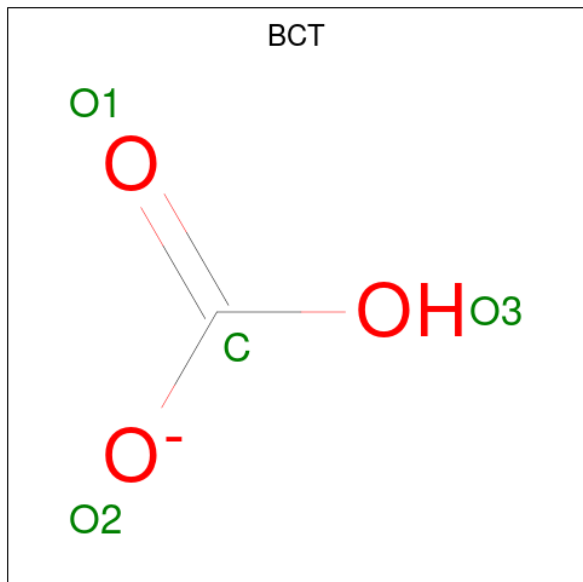
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			35	24	11	
22	M	1	Total	C	O	0
			35	24	11	
22	T	1	Total	C	O	0
			35	24	11	
22	a	1	Total	C	O	0
			35	24	11	
22	m	1	Total	C	O	0
			35	24	11	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



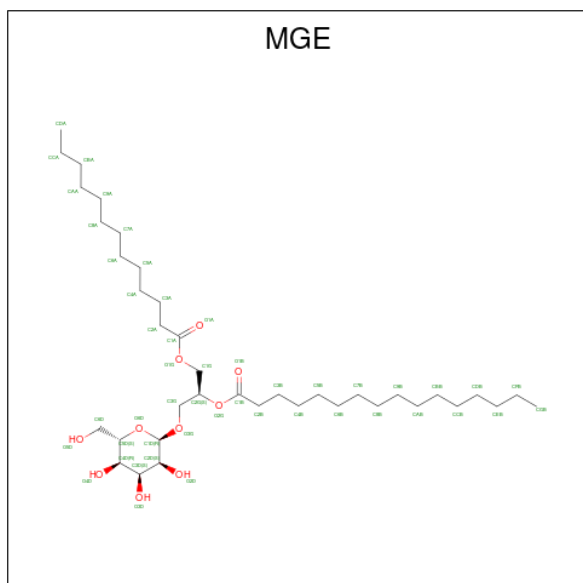
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	S	0
			26	13	12	1	
23	D	1	Total	C	O	S	0
			54	41	12	1	
23	L	1	Total	C	O	S	0
			47	34	12	1	
23	a	1	Total	C	O	S	0
			26	13	12	1	
23	d	1	Total	C	O	S	0
			54	41	12	1	
23	l	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



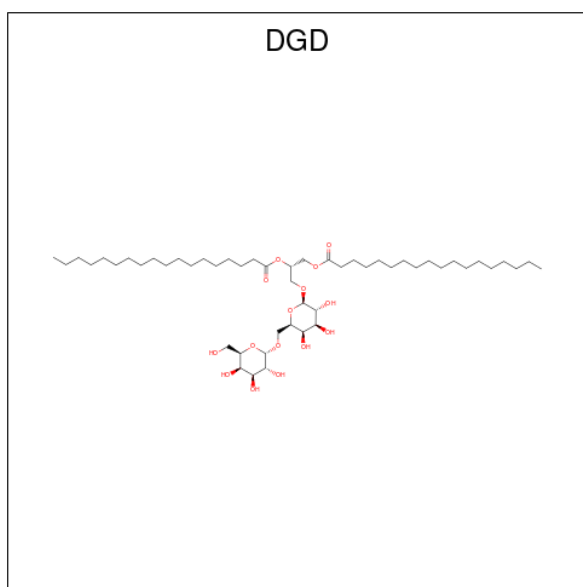
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			4	1	3	
24	a	1	Total	C	O	0
			4	1	3	

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $\text{C}_{38}\text{H}_{72}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			48	38	10	
25	B	1	Total	C	O	0
			48	38	10	
25	C	1	Total	C	O	0
			48	38	10	
25	D	1	Total	C	O	0
			47	37	10	
25	D	1	Total	C	O	0
			41	31	10	
25	D	1	Total	C	O	0
			48	38	10	
25	b	1	Total	C	O	0
			48	38	10	
25	c	1	Total	C	O	0
			48	38	10	
25	d	1	Total	C	O	0
			47	37	10	
25	d	1	Total	C	O	0
			41	31	10	
25	d	1	Total	C	O	0
			48	38	10	
25	l	1	Total	C	O	0
			48	38	10	
25	m	1	Total	C	O	0
			48	38	10	
25	m	1	Total	C	O	0
			48	38	10	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			53	38	15	
26	C	1	Total	C	O	0
			47	32	15	
26	C	1	Total	C	O	0
			57	42	15	
26	D	1	Total	C	O	0
			54	39	15	
26	a	1	Total	C	O	0
			57	42	15	
26	b	1	Total	C	O	0
			54	39	15	
26	c	1	Total	C	O	0
			53	38	15	
26	c	1	Total	C	O	0
			47	32	15	

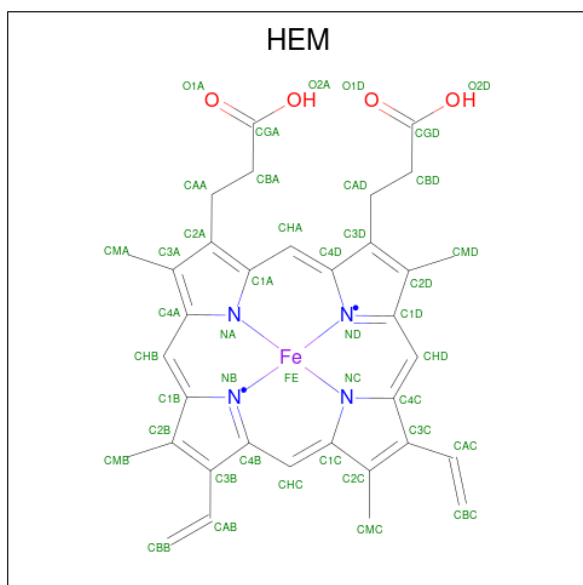
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	C	1	Total	Ca	0
			1	1	
27	c	1	Total	Ca	0
			1	1	

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
28	D	1	Total Fe 1 1	0
28	d	1	Total Fe 1 1	0

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

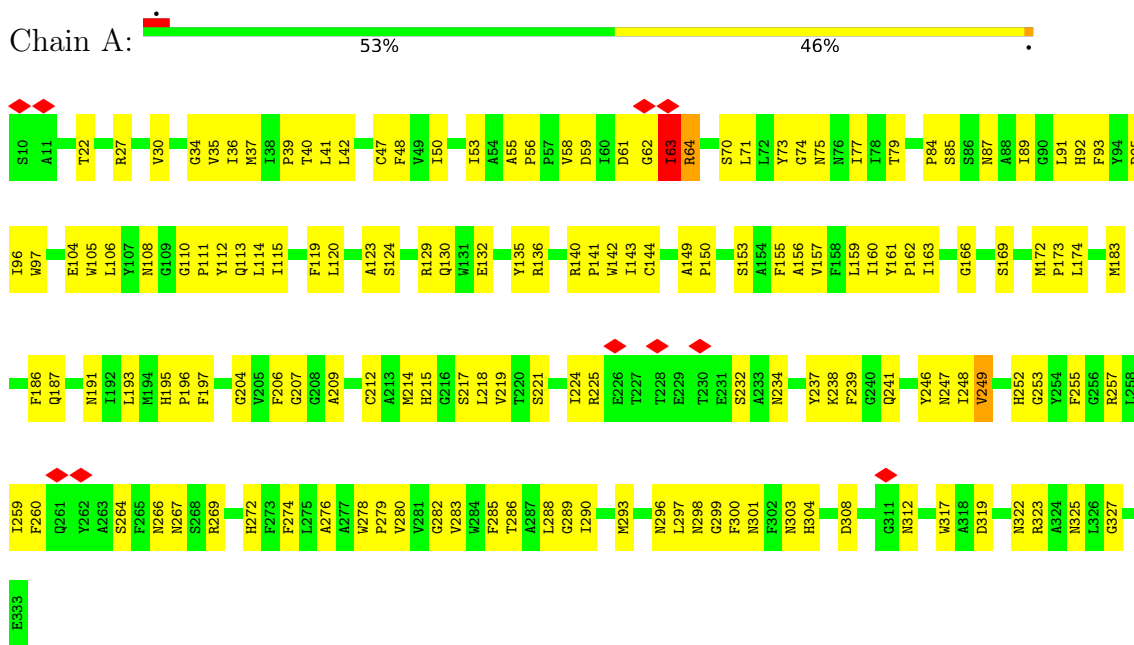
- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
30	n	1	Total Cl 1 1	0
30	N	1	Total Cl 1 1	0

3 Residue-property plots [i](#)

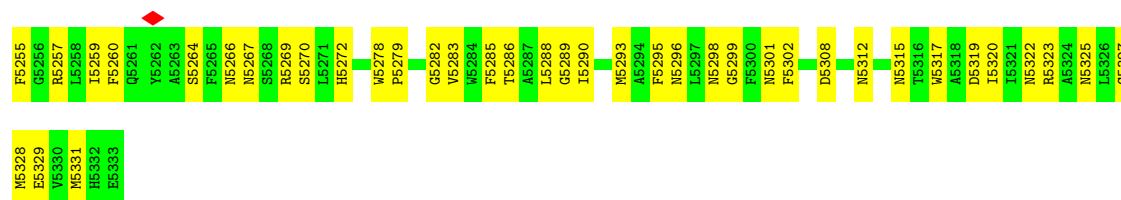
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem II protein D1

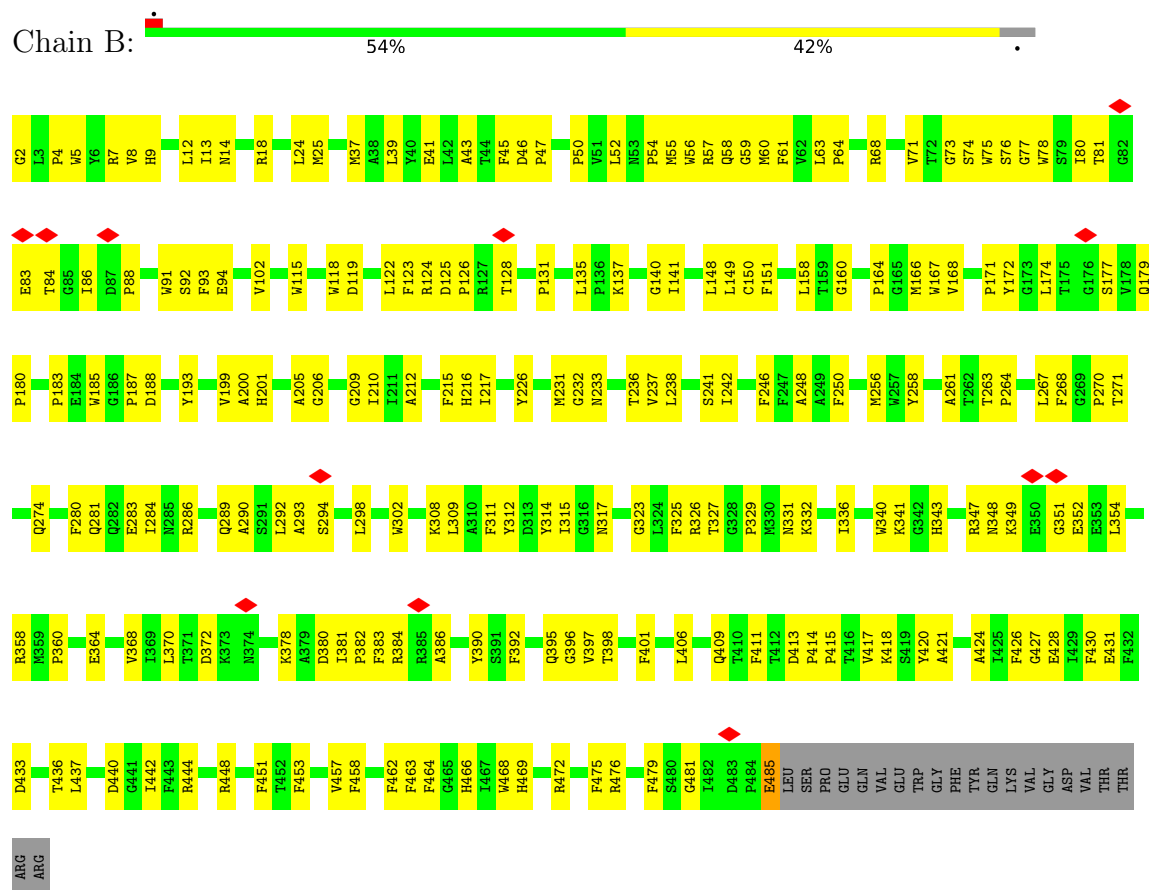


• Molecule 1: Photosystem II protein D1

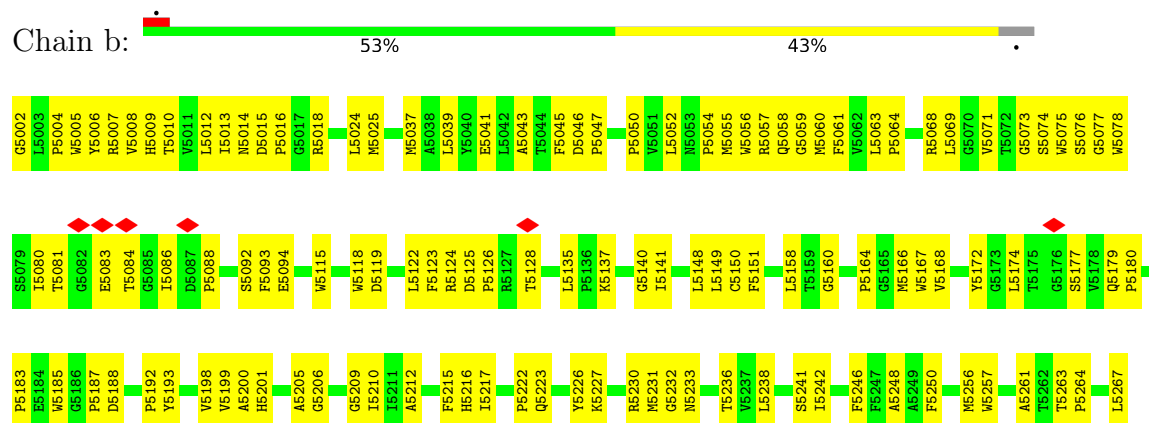


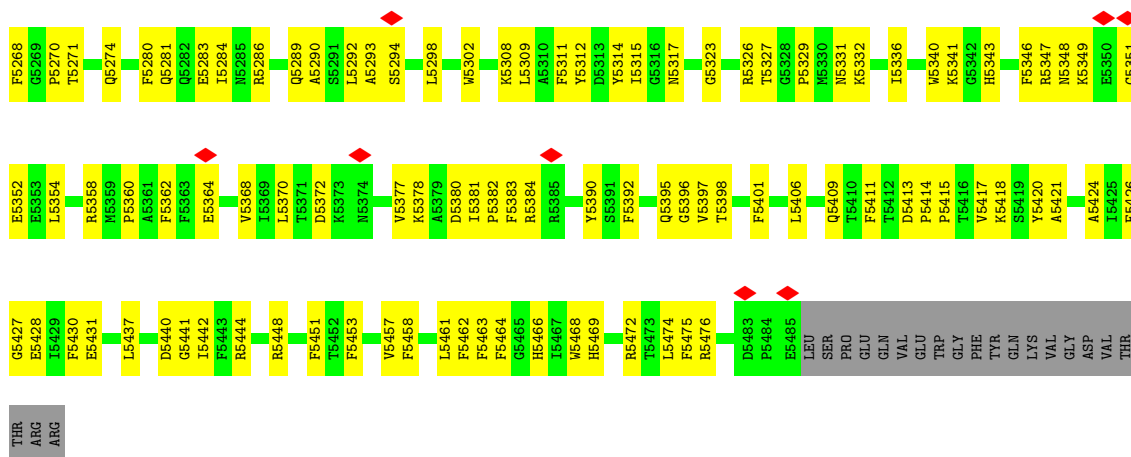


• Molecule 2: Photosystem II CP47 reaction center protein

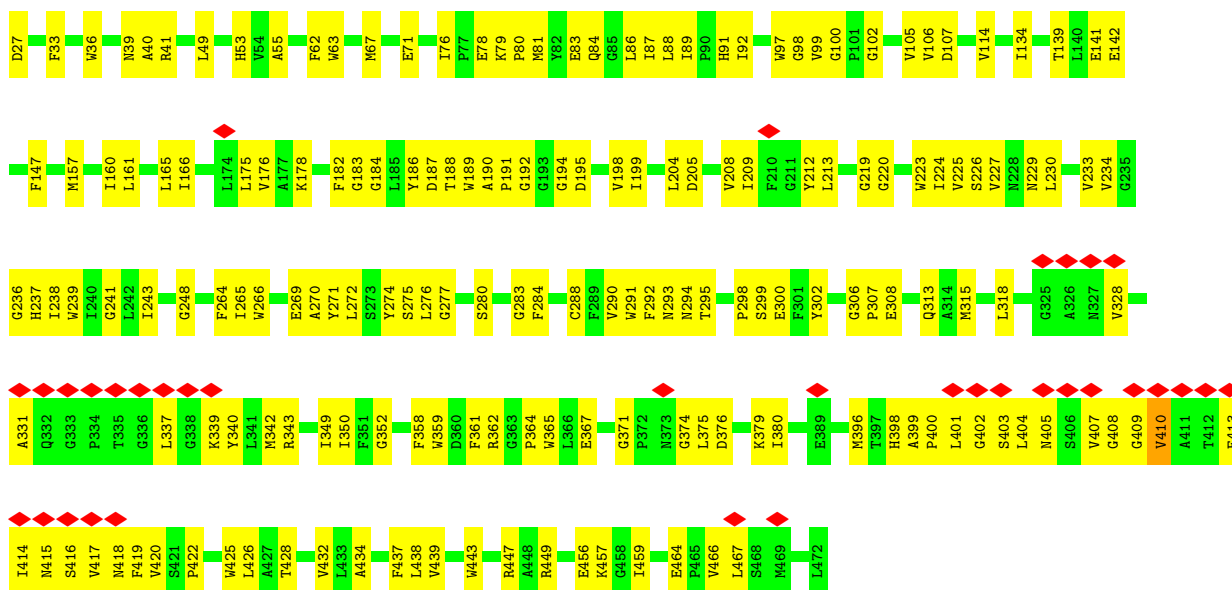


• Molecule 2: Photosystem II CP47 reaction center protein

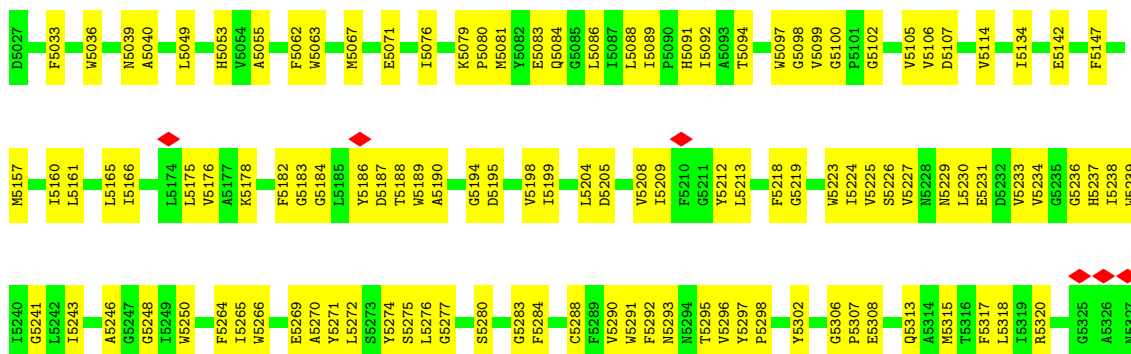


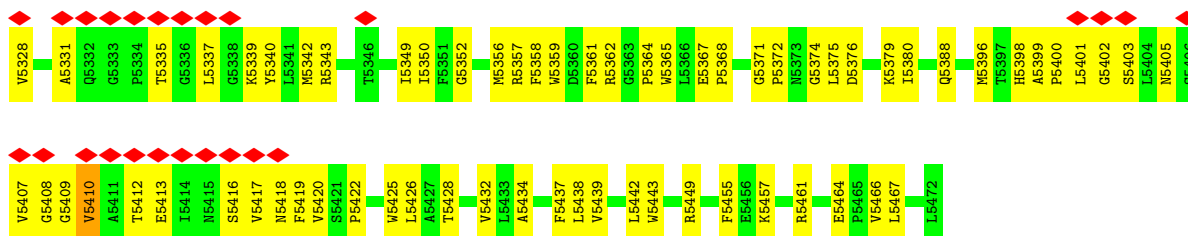


• Molecule 3: Photosystem II CP43 reaction center protein

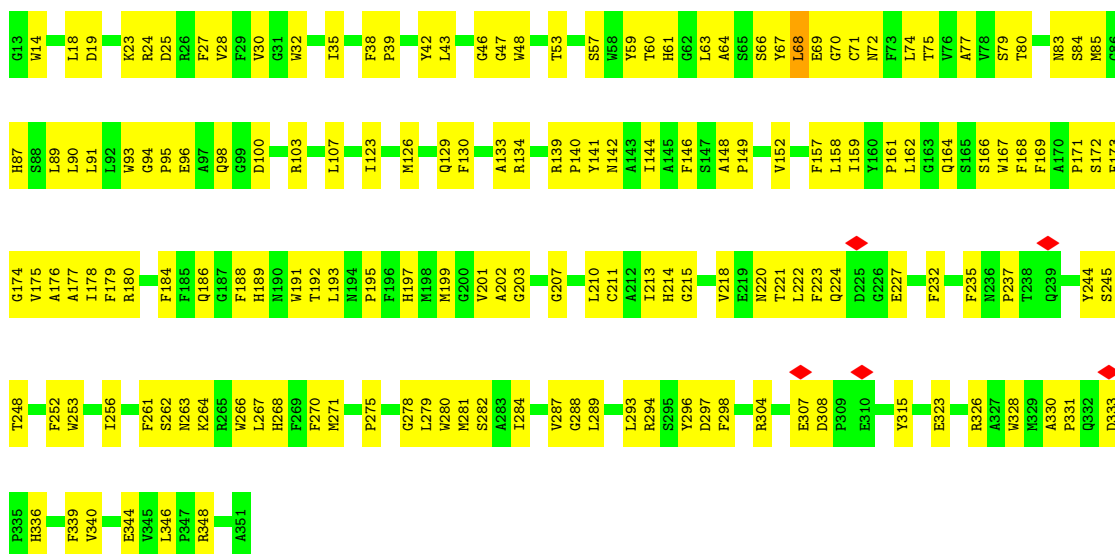


• Molecule 3: Photosystem II CP43 reaction center protein

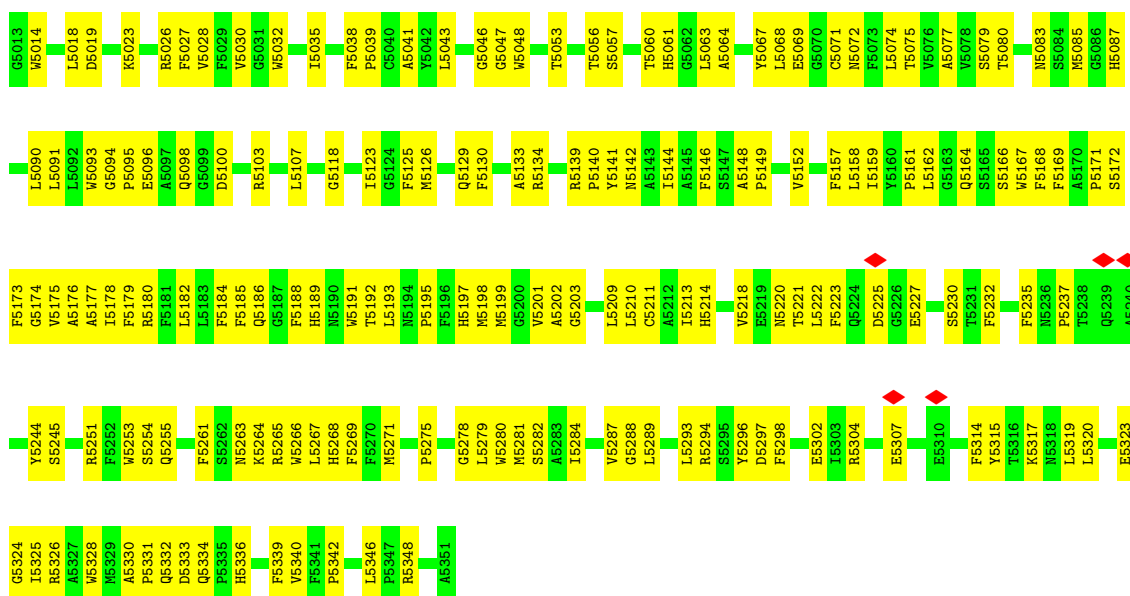




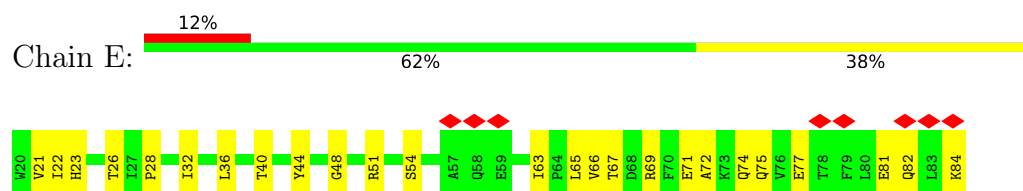
• Molecule 4: Photosystem II D2 protein



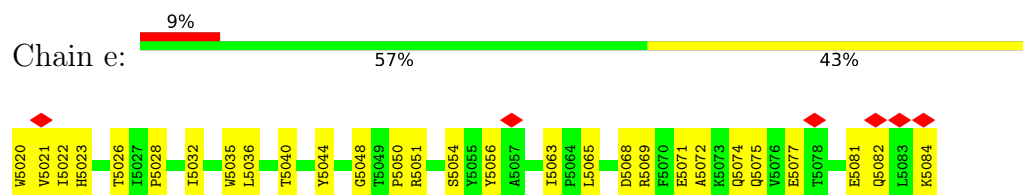
• Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



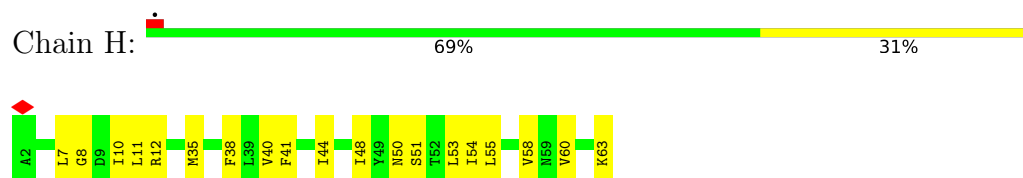
- Molecule 6: Cytochrome b559 subunit beta



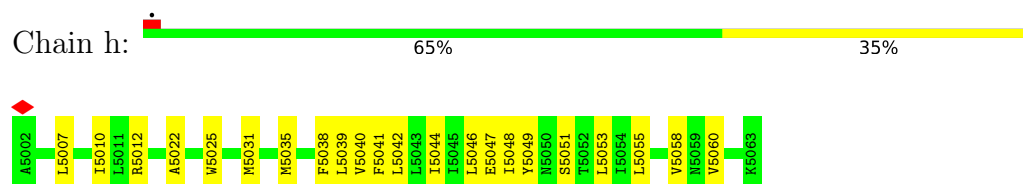
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I





- Molecule 8: Photosystem II reaction center protein I

Chain i: 76% 24%



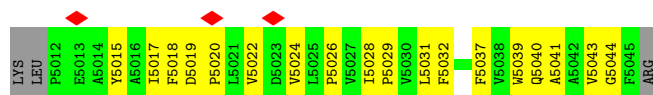
- Molecule 9: Photosystem II reaction center protein K

Chain K: 11% 51% 46%



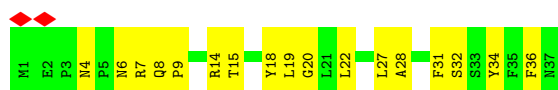
- Molecule 9: Photosystem II reaction center protein K

Chain k: 8% 43% 49% 8%



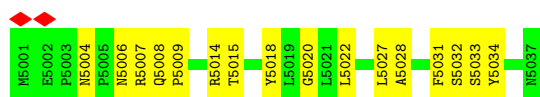
- Molecule 10: Photosystem II reaction center protein L

Chain L: 5% 54% 46%



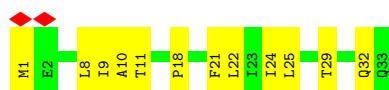
- Molecule 10: Photosystem II reaction center protein L

Chain l: 5% 57% 43%

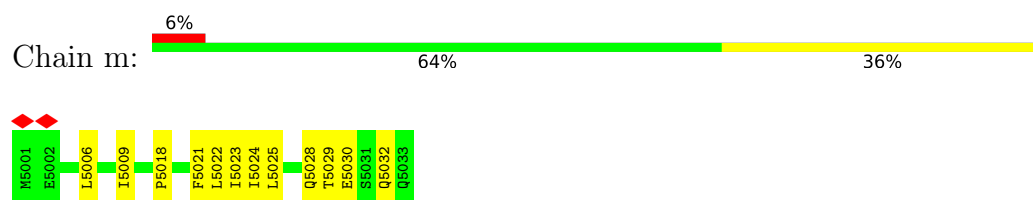


- Molecule 11: Photosystem II reaction center protein M

Chain M: 6% 64% 36%



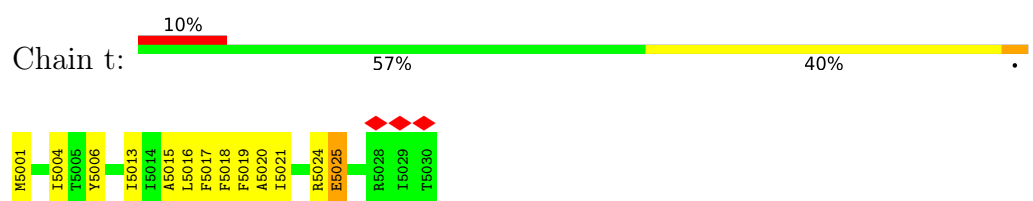
- Molecule 11: Photosystem II reaction center protein M



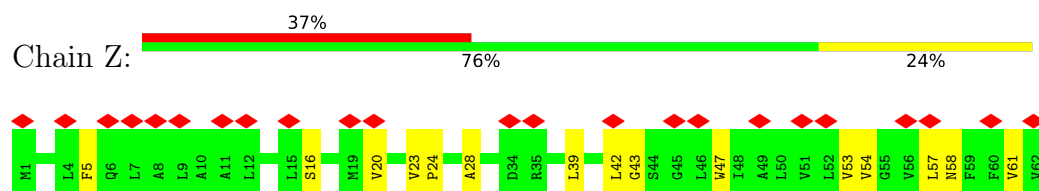
- Molecule 12: Photosystem II reaction center protein T



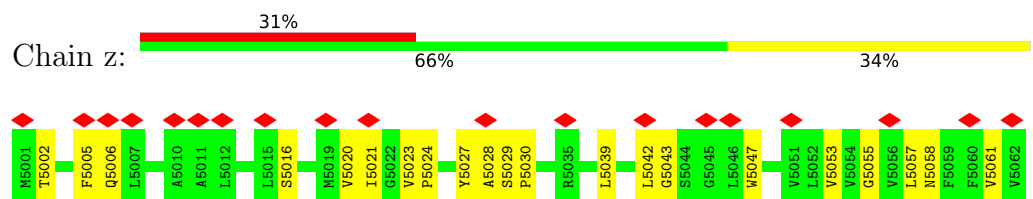
- Molecule 12: Photosystem II reaction center protein T



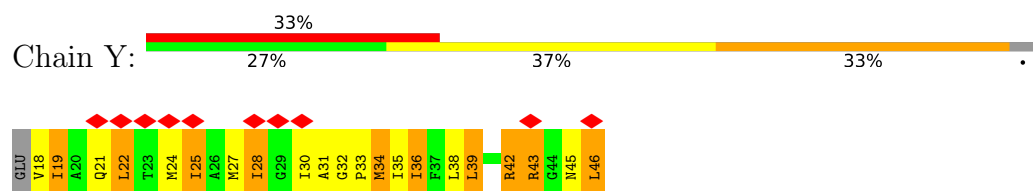
- Molecule 13: Photosystem II reaction center protein Z



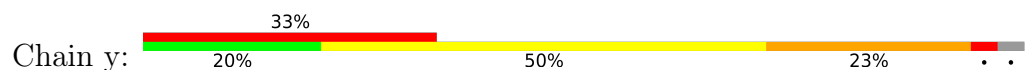
- Molecule 13: Photosystem II reaction center protein Z

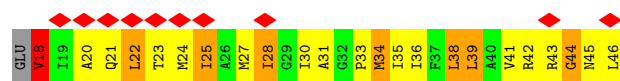


- Molecule 14: Photosystem II reaction center protein Ycf12

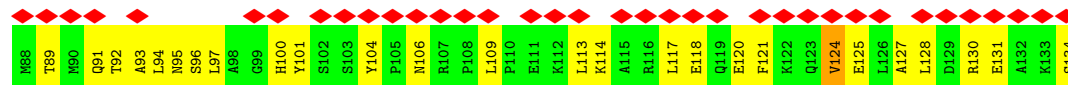
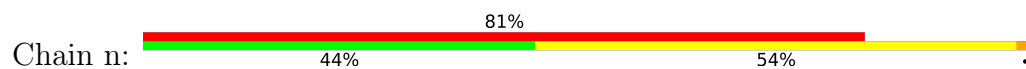


- Molecule 14: Photosystem II reaction center protein Ycf12

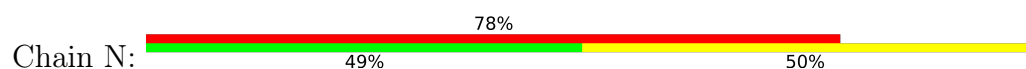




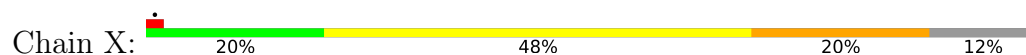
• Molecule 15: Psb27



• Molecule 15: Psb27



• Molecule 16: Photosystem II reaction center protein X



• Molecule 16: Photosystem II reaction center protein X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87473	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 ($e^-/\text{\AA}^2$)	50	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	0.227	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.038	Depositor
Map size ($\text{\AA}$)	313.5696, 313.5696, 313.5696	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PHO, BCR, LHG, SQD, BCT, PQ9, CA, CLA, FE2, MGE, DGD, HEM, CL

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	A	0.44	0/2615	0.53	4/3568 (0.1%)
1	a	0.44	0/2605	0.50	1/3554 (0.0%)
2	B	0.45	0/3919	0.51	0/5343
2	b	0.45	0/3915	0.51	0/5338
3	C	0.38	0/3524	0.48	0/4804
3	c	0.38	0/3524	0.49	1/4804 (0.0%)
4	D	0.48	1/2788 (0.0%)	0.52	2/3802 (0.1%)
4	d	0.49	1/2782 (0.0%)	0.50	0/3795
5	E	0.29	0/538	0.50	0/737
5	e	0.29	0/538	0.50	0/737
6	F	0.30	0/250	0.50	0/342
6	f	0.29	0/225	0.41	0/308
7	H	0.37	0/495	0.49	0/678
7	h	0.37	0/495	0.49	0/678
8	I	0.36	0/284	0.40	0/384
8	i	0.36	0/284	0.40	0/384
9	K	0.37	0/299	0.65	0/412
9	k	0.38	0/274	0.65	0/379
10	L	0.41	0/308	0.47	0/419
10	l	0.41	0/308	0.48	0/419
11	M	0.39	0/261	0.51	0/356
11	m	0.38	0/261	0.45	0/356
12	T	0.51	0/263	0.48	0/356
12	t	0.51	0/263	0.48	0/356
13	Z	0.19	0/451	0.31	0/620
13	z	0.19	0/451	0.32	0/620
14	Y	0.30	0/216	0.70	0/289
14	y	0.53	0/216	1.43	6/289 (2.1%)
15	N	0.28	0/873	0.46	0/1172
15	n	0.21	0/873	0.43	0/1172
16	X	0.41	0/257	0.83	1/348 (0.3%)
16	x	0.34	0/257	0.77	0/348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.42	2/34612 (0.0%)	0.51	15/47167 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	2
9	K	0	2
9	k	0	2
14	y	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	340	VAL	C-N	-5.98	1.21	1.33
4	d	5340	VAL	C-N	-5.96	1.21	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	y	28	ILE	CA-C-N	-8.76	104.23	121.41
14	y	28	ILE	C-N-CA	-8.76	104.23	121.41
1	A	249	VAL	CG1-CB-CG2	-7.19	94.98	110.80
14	y	20	ALA	N-CA-C	-7.07	103.51	111.14
1	A	64	ARG	N-CA-C	6.17	123.94	110.80
14	y	28	ILE	N-CA-C	6.17	116.91	110.62
3	c	5410	VAL	CG1-CB-CG2	-6.12	97.33	110.80
4	D	68	LEU	CA-C-N	-5.94	110.19	121.54
4	D	68	LEU	C-N-CA	-5.94	110.19	121.54
1	A	63	ILE	CA-C-N	5.87	132.75	121.54
1	A	63	ILE	C-N-CA	5.87	132.75	121.54
1	a	5249	VAL	CG1-CB-CG2	5.61	123.14	110.80
16	X	5	PRO	N-CA-C	-5.48	105.91	113.53
14	y	18	VAL	CA-C-N	5.38	128.05	120.42
14	y	18	VAL	C-N-CA	5.38	128.05	120.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ILE	Mainchain
1	A	64	ARG	Peptide
9	K	17	ILE	Peptide
9	K	24	VAL	Peptide
1	a	5063	ILE	Mainchain
1	a	5064	ARG	Peptide
9	k	5017	ILE	Peptide
9	k	5024	VAL	Peptide
14	y	18	VAL	Mainchain

5.2 Too-close contacts [i](#)

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	A	2533	0	2433	168	0
1	a	2523	0	2426	161	0
2	B	3784	0	3634	194	0
2	b	3780	0	3630	197	0
3	C	3412	0	3321	180	0
3	c	3412	0	3321	175	0
4	D	2693	0	2591	193	0
4	d	2687	0	2580	215	0
5	E	522	0	500	19	0
5	e	522	0	500	20	0
6	F	242	0	247	14	0
6	f	219	0	228	11	0
7	H	482	0	488	32	0
7	h	482	0	488	38	0
8	I	277	0	295	14	0
8	i	277	0	292	7	0
9	K	289	0	294	37	0
9	k	264	0	269	44	0
10	L	301	0	309	19	0
10	l	301	0	306	19	0
11	M	258	0	276	16	0
11	m	258	0	273	11	0
12	T	254	0	254	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	t	254	0	254	18	0
13	Z	442	0	460	18	0
13	z	442	0	457	38	0
14	Y	215	0	246	60	0
14	y	215	0	246	95	0
15	N	860	0	864	54	0
15	n	860	0	864	58	0
16	X	254	0	284	60	0
16	x	254	0	284	74	0
17	A	250	0	265	28	0
17	B	1007	0	1086	101	0
17	C	774	0	781	65	0
17	D	115	0	111	12	0
17	a	250	0	265	28	0
17	b	985	0	1045	96	0
17	c	709	0	709	54	0
17	d	115	0	111	9	0
17	k	65	0	72	7	0
18	A	64	0	74	7	0
18	D	64	0	74	7	0
18	a	64	0	74	9	0
18	d	64	0	74	14	0
19	A	45	0	64	7	0
19	D	45	0	64	7	0
19	a	30	0	37	2	0
19	d	45	0	64	8	0
20	A	40	0	56	3	0
20	B	80	0	112	7	0
20	C	120	0	168	12	0
20	D	40	0	56	5	0
20	H	40	0	54	6	0
20	T	40	0	56	6	0
20	Y	40	0	54	9	0
20	a	40	0	56	5	0
20	b	120	0	168	12	0
20	c	80	0	112	9	0
20	d	40	0	56	4	0
20	h	40	0	54	7	0
20	k	40	0	56	9	0
20	t	80	0	112	9	0
20	z	40	0	56	4	0
21	A	39	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	a	39	0	51	3	0
22	A	35	0	45	3	0
22	B	35	0	43	1	0
22	M	35	0	44	2	0
22	T	35	0	43	0	0
22	a	35	0	45	0	0
22	m	35	0	44	1	0
23	A	26	0	15	0	0
23	D	54	0	77	6	0
23	L	47	0	61	16	0
23	a	26	0	16	0	0
23	d	54	0	77	2	0
23	l	47	0	61	13	0
24	A	4	0	1	8	0
24	a	4	0	1	6	0
25	A	48	0	69	12	0
25	B	48	0	72	6	0
25	C	48	0	72	5	0
25	D	136	0	192	24	0
25	b	48	0	72	6	0
25	c	48	0	72	5	0
25	d	136	0	194	25	0
25	l	48	0	72	9	0
25	m	96	0	143	19	0
26	A	53	0	60	7	0
26	C	104	0	124	3	0
26	D	54	0	64	7	0
26	a	57	0	72	2	0
26	b	54	0	64	7	0
26	c	100	0	112	7	0
27	C	1	0	0	0	0
27	c	1	0	0	0	0
28	D	1	0	0	0	0
28	d	1	0	0	0	0
29	F	43	0	30	8	0
29	f	43	0	30	4	0
30	N	1	0	0	0	0
30	n	1	0	0	0	0
All	All	40859	0	41299	2300	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 28.

All (2300) 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)
9:k:5020:PRO:HG3	14:y:24:MET:CG	1.20	1.58
9:k:5020:PRO:CG	14:y:24:MET:CG	1.81	1.56
9:k:5039:TRP:NE1	14:y:46:LEU:CD2	1.68	1.56
7:H:44:ILE:CD1	16:X:10:PHE:CZ	1.86	1.53
9:k:5020:PRO:HG3	14:y:24:MET:CB	1.37	1.51
13:z:5028:ALA:CB	14:y:39:LEU:HD21	1.41	1.48
7:H:44:ILE:HD11	16:X:10:PHE:CZ	1.48	1.45
14:y:35:ILE:CA	14:y:38:LEU:HD11	1.55	1.34
16:X:27:VAL:O	16:X:31:ILE:HG12	1.26	1.34
7:H:44:ILE:HD11	16:X:10:PHE:CE1	1.62	1.34
16:x:8:LYS:O	16:x:12:ILE:CD1	1.79	1.30
7:H:44:ILE:HD13	16:X:10:PHE:CZ	1.61	1.22
16:x:9:GLY:CA	16:x:12:ILE:CD1	2.17	1.22
2:B:258:TYR:CE2	26:D:411:DGD:HG32	1.75	1.21
9:K:20:PRO:CG	14:Y:24:MET:HG3	1.72	1.20
14:y:35:ILE:C	14:y:38:LEU:CD1	2.16	1.19
13:z:5028:ALA:CB	14:y:39:LEU:CD2	2.20	1.19
9:k:5020:PRO:CG	14:y:24:MET:HG3	1.57	1.18
14:y:35:ILE:O	14:y:38:LEU:CD1	1.91	1.18
9:k:5039:TRP:HE1	14:y:46:LEU:CD2	1.35	1.17
16:x:9:GLY:HA2	16:x:12:ILE:CD1	1.73	1.16
9:k:5020:PRO:HG2	14:y:24:MET:HG3	1.20	1.16
16:X:3:ILE:HA	16:X:7:LEU:HD12	1.23	1.15
9:k:5020:PRO:HG3	14:y:24:MET:HB3	1.25	1.15
13:z:5028:ALA:HB2	14:y:39:LEU:CD2	1.75	1.14
16:x:8:LYS:O	16:x:12:ILE:HD11	1.44	1.14
7:H:44:ILE:CD1	16:X:10:PHE:CE1	2.21	1.14
4:d:5035:ILE:CD1	16:x:28:LEU:HD11	1.78	1.14
9:k:5039:TRP:NE1	14:y:46:LEU:HD21	1.38	1.14
14:y:34:MET:O	14:y:38:LEU:CD1	1.96	1.13
2:B:86:ILE:CG2	2:B:88:PRO:HD3	1.78	1.13
16:x:9:GLY:CA	16:x:12:ILE:HD13	1.74	1.13
7:h:5044:ILE:HD11	16:x:10:PHE:CZ	1.84	1.12
14:y:35:ILE:HA	14:y:38:LEU:HD11	1.28	1.12
9:k:5039:TRP:CD1	14:y:46:LEU:HD21	1.85	1.10
9:k:5039:TRP:HE1	14:y:46:LEU:HD23	1.14	1.10
7:h:5047:GLU:OE2	16:x:10:PHE:CE2	2.05	1.10
16:x:8:LYS:C	16:x:12:ILE:HD11	1.76	1.09
4:D:35:ILE:HD12	16:X:28:LEU:HD11	1.17	1.09
14:y:18:VAL:O	14:y:22:LEU:HB2	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:x:9:GLY:HA2	16:x:12:ILE:HD13	1.24	1.09
16:x:9:GLY:C	16:x:12:ILE:CD1	2.26	1.08
16:x:8:LYS:O	16:x:12:ILE:HD12	1.52	1.08
9:k:5020:PRO:CG	14:y:24:MET:HG2	1.60	1.07
9:K:20:PRO:HG2	14:Y:24:MET:HG3	1.35	1.06
4:d:5035:ILE:HD12	16:x:28:LEU:HD11	1.11	1.06
16:x:9:GLY:C	16:x:12:ILE:HD13	1.81	1.06
16:x:12:ILE:HD12	16:x:12:ILE:H	1.21	1.05
14:y:35:ILE:CA	14:y:38:LEU:CD1	2.33	1.05
26:b:5621:DGD:O2D	4:d:5087:HIS:HB2	1.55	1.05
16:x:36:LYS:HD3	16:x:36:LYS:H	1.22	1.03
2:b:5086:ILE:HG22	2:b:5088:PRO:HD3	1.36	1.02
4:D:35:ILE:CD1	16:X:28:LEU:HD11	1.87	1.02
7:h:5047:GLU:CD	16:x:10:PHE:CE2	2.37	1.02
7:h:5047:GLU:OE1	16:x:10:PHE:CD2	2.12	1.02
9:K:20:PRO:HG3	14:Y:24:MET:HG3	1.43	1.01
9:k:5020:PRO:HG2	14:y:24:MET:CG	1.73	1.00
16:x:9:GLY:O	16:x:12:ILE:HD13	1.62	1.00
4:d:5035:ILE:CD1	16:x:28:LEU:CD1	2.39	0.99
7:h:5044:ILE:CD1	16:x:10:PHE:CZ	2.45	0.98
2:B:86:ILE:HG22	2:B:88:PRO:HD3	1.00	0.98
14:y:35:ILE:O	14:y:38:LEU:HD13	1.59	0.98
14:y:35:ILE:HA	14:y:38:LEU:CD1	1.93	0.97
2:B:86:ILE:HG22	2:B:88:PRO:CD	1.94	0.97
9:k:5039:TRP:NE1	14:y:46:LEU:HD22	1.79	0.97
9:k:5039:TRP:CE2	14:y:46:LEU:CD2	2.47	0.96
7:h:5047:GLU:OE2	16:x:10:PHE:HE2	1.49	0.95
7:h:5047:GLU:OE1	16:x:10:PHE:CE2	2.18	0.95
17:b:5612:CLA:H93	17:b:5612:CLA:H2	1.48	0.95
7:H:44:ILE:CD1	16:X:10:PHE:HZ	1.69	0.95
1:A:300:PHE:HA	3:C:403:SER:HB2	1.49	0.94
7:h:5047:GLU:CD	16:x:10:PHE:CD2	2.45	0.94
16:x:9:GLY:CA	16:x:12:ILE:HD11	1.97	0.94
4:d:5141:TYR:HH	25:d:5409:MGE:H2	1.12	0.94
4:d:5035:ILE:HD12	16:x:28:LEU:CD1	1.94	0.93
16:X:27:VAL:O	16:X:31:ILE:CG1	2.16	0.93
17:B:612:CLA:H93	17:B:612:CLA:H2	1.48	0.93
4:D:35:ILE:CD1	16:X:28:LEU:CD1	2.46	0.93
4:D:275:PRO:HB3	18:D:402:PHO:HBC1	1.51	0.92
16:X:3:ILE:HG23	16:X:7:LEU:CD1	2.00	0.92
16:x:9:GLY:O	16:x:12:ILE:CD1	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:y:31:ALA:O	14:y:35:ILE:HG13	1.69	0.92
7:h:5047:GLU:OE2	16:x:10:PHE:CD2	2.23	0.91
4:D:35:ILE:HD12	16:X:28:LEU:CD1	1.99	0.91
9:K:43:VAL:CG2	14:Y:46:LEU:HD13	2.00	0.91
9:K:39:TRP:NE1	14:Y:46:LEU:HD21	1.84	0.91
9:k:5020:PRO:CG	14:y:24:MET:HB3	1.98	0.90
1:a:5143:ILE:HG23	4:d:5220:ASN:HD22	1.34	0.90
14:y:34:MET:O	14:y:38:LEU:HD11	1.65	0.90
14:y:35:ILE:C	14:y:38:LEU:HD11	1.90	0.90
9:k:5020:PRO:CG	14:y:24:MET:CB	2.32	0.90
9:k:5039:TRP:CE2	14:y:46:LEU:HD22	2.05	0.90
14:Y:38:LEU:O	14:Y:42:ARG:HG3	1.72	0.90
2:B:258:TYR:CZ	26:D:411:DGD:HG32	2.07	0.89
14:y:34:MET:C	14:y:38:LEU:HD11	1.96	0.89
3:c:5229:ASN:HD22	15:n:77:ARG:HG3	1.38	0.88
9:K:43:VAL:HG23	14:Y:46:LEU:HD13	1.54	0.88
16:X:3:ILE:HG23	16:X:7:LEU:HD13	1.53	0.87
15:N:109:LEU:HB2	15:N:114:LYS:HE3	1.54	0.87
9:K:39:TRP:NE1	14:Y:46:LEU:CD2	2.38	0.87
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.57	0.86
9:K:20:PRO:HG3	14:Y:24:MET:CG	2.03	0.86
17:B:608:CLA:H201	26:D:411:DGD:HA81	1.57	0.86
22:B:620:LMT:H6'	12:t:5001:MET:N	1.73	0.86
4:d:5014:TRP:CZ2	16:x:29:ILE:HD12	2.10	0.86
13:z:5028:ALA:HB1	14:y:39:LEU:CD2	2.04	0.86
13:z:5028:ALA:HB1	14:y:39:LEU:HD21	1.58	0.86
4:D:53:THR:HA	4:D:67:TYR:HB3	1.56	0.86
9:k:5019:ASP:OD1	14:y:21:GLN:NE2	1.84	0.86
14:y:35:ILE:O	14:y:38:LEU:HD12	1.73	0.85
4:D:180:ARG:NH2	4:D:333:ASP:OD1	2.10	0.85
15:N:109:LEU:HB2	15:N:114:LYS:CE	2.06	0.85
9:K:20:PRO:CG	14:Y:24:MET:CG	2.54	0.84
4:D:123:ILE:HD11	26:D:411:DGD:HAH2	1.57	0.84
4:d:5053:THR:HA	4:d:5067:TYR:HB3	1.55	0.84
4:d:5014:TRP:CZ2	16:x:29:ILE:CD1	2.61	0.84
20:c:5513:BCR:H11C	20:k:5502:BCR:H322	1.57	0.84
4:d:5180:ARG:NH2	4:d:5333:ASP:OD1	2.10	0.84
13:z:5021:ILE:HD11	14:y:31:ALA:HB1	1.59	0.84
3:C:410:VAL:HG12	3:C:413:GLU:HB2	1.58	0.83
14:y:35:ILE:N	14:y:38:LEU:HD11	1.92	0.83
3:c:5102:GLY:N	3:c:5195:ASP:OD2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:34:MET:N	14:Y:34:MET:HE3	1.92	0.83
26:b:5621:DGD:O2D	4:d:5087:HIS:CB	2.26	0.83
4:D:89:LEU:HD11	26:D:411:DGD:HA32	1.60	0.83
3:C:102:GLY:N	3:C:195:ASP:OD2	2.11	0.83
14:y:38:LEU:HD12	14:y:38:LEU:H	1.41	0.82
2:B:77:GLY:HA2	2:B:86:ILE:CD1	2.10	0.82
7:H:44:ILE:HD11	16:X:10:PHE:HZ	1.27	0.82
7:H:44:ILE:HD13	16:X:10:PHE:CE2	2.14	0.82
4:d:5035:ILE:HD11	16:x:28:LEU:HD13	1.62	0.81
15:N:112:LYS:O	15:N:116:ARG:HG3	1.80	0.81
20:b:5617:BCR:H10C	25:b:5620:MGE:H241	1.62	0.81
17:A:405:CLA:HHC	17:A:405:CLA:HBB1	1.63	0.81
9:K:15:TYR:OH	13:Z:58:ASN:ND2	2.14	0.81
4:d:5035:ILE:HD11	16:x:28:LEU:CD1	2.08	0.81
1:a:5143:ILE:HG23	4:d:5220:ASN:ND2	1.95	0.81
1:a:5315:ASN:O	4:d:5063:LEU:HB2	1.81	0.81
15:N:34:ARG:HG3	15:N:128:LEU:HD21	1.63	0.81
4:d:5071:CYS:SG	4:d:5075:THR:OG1	2.39	0.81
14:Y:42:ARG:HG2	14:Y:42:ARG:HH11	1.45	0.81
16:X:7:LEU:O	16:X:7:LEU:HD22	1.82	0.81
9:k:5039:TRP:NE1	14:y:46:LEU:HD23	1.75	0.80
20:B:618:BCR:H382	20:t:5102:BCR:H11C	1.62	0.80
4:D:71:CYS:SG	4:D:75:THR:OG1	2.39	0.80
20:B:617:BCR:H10C	25:B:619:MGE:H241	1.62	0.80
2:b:5188:ASP:HA	7:h:5058:VAL:HG12	1.64	0.80
15:n:34:ARG:HG3	15:n:128:LEU:HD21	1.63	0.80
3:C:308:GLU:OE2	3:C:365:TRP:NE1	2.11	0.79
15:N:117:LEU:O	15:N:120:GLU:N	2.13	0.79
14:y:18:VAL:O	14:y:22:LEU:N	2.15	0.79
17:a:5406:CLA:HHC	17:a:5406:CLA:HBB1	1.63	0.79
15:N:77:ARG:HD2	15:N:77:ARG:O	1.84	0.79
1:A:143:ILE:HD13	4:D:252:PHE:HZ	1.47	0.78
3:c:5308:GLU:OE2	3:c:5365:TRP:NE1	2.11	0.78
9:k:5015:TYR:OH	13:z:5058:ASN:ND2	2.16	0.78
1:A:272:HIS:NE2	24:A:411:BCT:O3	2.14	0.78
16:x:36:LYS:H	16:x:36:LYS:CD	1.97	0.78
4:D:189:HIS:HB3	4:D:289:LEU:HD11	1.65	0.78
14:Y:19:ILE:HD12	14:Y:19:ILE:H	1.49	0.78
16:X:3:ILE:CG2	16:X:8:LYS:HB2	2.14	0.77
16:x:9:GLY:N	16:x:12:ILE:HD11	1.98	0.77
1:A:288:LEU:HD13	3:C:432:VAL:HG13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:406:PQ9:H37	4:D:42:TYR:HB2	1.65	0.77
3:C:189:TRP:HB2	15:N:76:ARG:CZ	2.15	0.77
2:B:168:VAL:O	2:B:177:SER:OG	2.03	0.77
1:a:5027:ARG:NH1	4:d:5254:SER:O	2.18	0.77
17:B:606:CLA:H51	20:t:5101:BCR:H322	1.65	0.77
4:d:5189:HIS:HB3	4:d:5289:LEU:HD11	1.65	0.77
9:k:5020:PRO:HG3	14:y:24:MET:HG2	1.26	0.77
13:z:5028:ALA:HB2	14:y:39:LEU:HD21	0.78	0.77
9:K:39:TRP:HE1	14:Y:46:LEU:CD2	1.97	0.77
4:d:5210:LEU:HD12	19:d:5405:PQ9:H17	1.67	0.77
2:B:86:ILE:CG2	2:B:88:PRO:CD	2.60	0.76
14:y:18:VAL:O	14:y:22:LEU:CB	2.33	0.76
9:K:39:TRP:CD1	14:Y:46:LEU:HD21	2.20	0.76
2:b:5168:VAL:O	2:b:5177:SER:OG	2.03	0.76
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.66	0.76
4:D:93:TRP:CD1	4:D:94:GLY:H	2.04	0.76
17:b:5611:CLA:H41	17:b:5614:CLA:HBC3	1.67	0.76
21:a:5409:LHG:HC32	4:d:5230:SER:HA	1.68	0.76
4:D:35:ILE:HD11	16:X:28:LEU:CD1	2.16	0.76
4:D:210:LEU:HD12	19:D:406:PQ9:H17	1.67	0.76
4:d:5172:SER:HB2	4:d:5177:ALA:HB1	1.67	0.75
1:a:5269:ARG:HD2	4:d:5235:PHE:HB2	1.66	0.75
14:y:34:MET:O	14:y:38:LEU:CG	2.33	0.75
16:x:36:LYS:HD3	16:x:36:LYS:N	2.00	0.75
12:T:25:GLU:OE1	12:T:25:GLU:N	2.19	0.75
4:D:35:ILE:HD11	16:X:28:LEU:HD13	1.67	0.75
16:X:3:ILE:CA	16:X:7:LEU:HD12	2.11	0.75
3:C:342:MET:HE2	3:C:352:GLY:HA2	1.69	0.75
7:h:5044:ILE:HD11	16:x:10:PHE:CE1	2.21	0.75
1:a:5331:MET:HG3	4:d:5324:GLY:HA3	1.69	0.74
3:c:5342:MET:HE2	3:c:5352:GLY:HA2	1.69	0.74
14:Y:43:ARG:HB3	14:Y:43:ARG:NH1	2.02	0.74
4:d:5093:TRP:CD1	4:d:5094:GLY:H	2.04	0.74
17:B:611:CLA:H41	17:B:614:CLA:HBC3	1.67	0.74
14:y:25:ILE:O	14:y:25:ILE:HD13	1.87	0.74
4:D:69:GLU:HG2	4:D:70:GLY:H	1.50	0.74
23:L:101:SQD:O7	10:l:5007:ARG:NH1	2.19	0.74
16:x:8:LYS:C	16:x:12:ILE:CD1	2.48	0.74
17:A:402:CLA:H13	19:D:406:PQ9:H452	1.70	0.73
4:d:5297:ASP:HB3	4:d:5302:GLU:HG3	1.69	0.73
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:x:9:GLY:HA2	16:x:12:ILE:HD11	1.58	0.73
20:k:5502:BCR:C33	14:y:28:ILE:O	2.36	0.73
2:b:5086:ILE:HG22	2:b:5088:PRO:CD	2.15	0.73
16:x:9:GLY:C	16:x:12:ILE:HD12	2.11	0.73
1:a:5073:TYR:O	1:a:5075:ASN:ND2	2.21	0.73
12:t:5025:GLU:OE1	12:t:5025:GLU:N	2.19	0.73
25:D:410:MGE:H8A1	12:T:21:ILE:HD11	1.70	0.73
14:y:35:ILE:C	14:y:38:LEU:HD12	2.05	0.73
14:Y:43:ARG:HB3	14:Y:43:ARG:HH11	1.52	0.73
16:x:15:LEU:C	16:x:15:LEU:HD22	2.14	0.73
1:A:73:TYR:O	1:A:75:ASN:ND2	2.21	0.72
16:X:27:VAL:HG13	16:X:31:ILE:HD11	1.70	0.72
20:k:5502:BCR:H332	14:y:28:ILE:O	1.90	0.72
2:B:472:ARG:NH2	17:B:611:CLA:O2D	2.21	0.72
9:k:5020:PRO:CD	14:y:24:MET:HG2	2.19	0.72
2:b:5472:ARG:NH2	17:b:5611:CLA:O2D	2.21	0.72
17:b:5603:CLA:HAB	17:b:5605:CLA:H192	1.71	0.72
14:y:38:LEU:HD12	14:y:38:LEU:N	2.05	0.72
16:X:7:LEU:HD22	16:X:7:LEU:C	2.13	0.72
16:x:21:LEU:HD23	16:x:21:LEU:C	2.14	0.72
2:b:5064:PRO:HB2	2:b:5268:PHE:HE1	1.55	0.72
7:H:40:VAL:HG13	16:X:14:LEU:CD1	2.20	0.71
4:d:5077:ALA:HB2	4:d:5174:GLY:HA3	1.70	0.71
17:B:603:CLA:HAB	17:B:605:CLA:H192	1.71	0.71
2:B:64:PRO:HB2	2:B:268:PHE:HE1	1.55	0.71
9:k:5039:TRP:CD1	14:y:46:LEU:CD2	2.57	0.71
26:a:5411:DGD:HBE2	25:d:5408:MGE:H9B1	1.71	0.71
3:C:191:PRO:O	15:N:95:ASN:HA	1.91	0.71
7:H:53:LEU:CD1	16:X:7:LEU:HA	2.21	0.71
14:Y:32:GLY:O	14:Y:35:ILE:HD12	1.89	0.71
14:Y:34:MET:HE3	14:Y:34:MET:CA	2.21	0.71
17:C:511:CLA:H72	14:Y:35:ILE:HG21	1.71	0.70
17:C:503:CLA:H171	17:C:510:CLA:HBB2	1.73	0.70
16:X:15:LEU:HD12	16:X:15:LEU:O	1.91	0.70
5:e:5071:GLU:O	5:e:5074:GLN:N	2.25	0.70
16:x:15:LEU:HD22	16:x:15:LEU:O	1.90	0.70
14:y:34:MET:O	14:y:38:LEU:HG	1.90	0.70
1:A:267:ASN:ND2	4:D:232:PHE:O	2.24	0.70
5:E:71:GLU:O	5:E:74:GLN:N	2.25	0.70
1:A:143:ILE:HG23	4:D:220:ASN:HD22	1.57	0.70
1:A:215:HIS:NE2	24:A:411:BCT:O2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5007:ARG:NH2	25:d:5409:MGE:O3D	2.23	0.70
4:d:5046:GLY:HA2	20:d:5406:BCR:H12C	1.73	0.70
16:X:15:LEU:HD12	16:X:15:LEU:C	2.16	0.69
4:D:141:TYR:HH	25:D:409:MGE:H2	1.39	0.69
9:K:43:VAL:HG22	14:Y:46:LEU:HD13	1.75	0.69
9:K:39:TRP:HD1	14:Y:36:ILE:HD11	1.57	0.69
3:C:39:ASN:HB2	17:C:508:CLA:HBA1	1.74	0.69
1:a:5076:ASN:HB3	10:l:5033:SER:HB2	1.75	0.69
17:b:5603:CLA:HBB2	17:b:5605:CLA:H203	1.75	0.69
3:c:5039:ASN:HB2	17:c:5508:CLA:HBA1	1.75	0.69
13:z:5039:LEU:O	13:z:5043:GLY:N	2.21	0.69
14:Y:46:LEU:O	14:Y:46:LEU:HD22	1.92	0.69
2:B:280:PHE:CE2	2:B:312:TYR:HB3	2.27	0.69
4:D:46:GLY:HA2	20:D:407:BCR:H12C	1.73	0.69
4:d:5188:PHE:CD1	4:d:5326:ARG:HG2	2.28	0.69
1:A:143:ILE:HD13	4:D:252:PHE:CZ	2.27	0.69
2:b:5280:PHE:CE2	2:b:5312:TYR:HB3	2.27	0.69
17:b:5602:CLA:H203	26:b:5621:DGD:HA62	1.75	0.69
17:b:5616:CLA:H141	20:b:5619:BCR:HC8	1.75	0.69
3:c:5187:ASP:N	3:c:5195:ASP:O	2.20	0.69
3:c:5464:GLU:HB2	3:c:5467:LEU:HB2	1.74	0.69
14:y:31:ALA:O	14:y:35:ILE:CG1	2.41	0.69
16:X:21:LEU:HD23	16:X:21:LEU:H	1.58	0.69
4:D:103:ARG:NH2	5:E:77:GLU:OE2	2.23	0.69
17:k:5501:CLA:H42	14:y:46:LEU:HD23	1.75	0.69
1:a:5130:GLN:HB3	1:a:5143:ILE:HD12	1.75	0.68
17:c:5503:CLA:H171	17:c:5510:CLA:HBB2	1.73	0.68
9:k:5039:TRP:HE1	14:y:46:LEU:HD21	1.16	0.68
17:B:613:CLA:H51	25:D:409:MGE:H241	1.74	0.68
3:C:464:GLU:HB2	3:C:467:LEU:HB2	1.74	0.68
17:c:5505:CLA:HBD	17:c:5505:CLA:HBA1	1.75	0.68
7:h:5044:ILE:HD11	16:x:10:PHE:HZ	1.54	0.68
4:D:43:LEU:O	4:D:47:GLY:N	2.26	0.68
4:D:188:PHE:CD1	4:D:326:ARG:HG2	2.28	0.68
2:b:5323:GLY:HA3	2:b:5326:ARG:HH11	1.59	0.68
17:B:603:CLA:HBB2	17:B:605:CLA:H203	1.75	0.68
17:B:616:CLA:H141	20:t:5101:BCR:HC8	1.75	0.68
7:H:54:ILE:O	16:X:4:THR:HG21	1.93	0.68
13:Z:39:LEU:O	13:Z:43:GLY:N	2.21	0.68
3:c:5265:ILE:HG13	3:c:5449:ARG:HG2	1.76	0.68
14:Y:43:ARG:HH11	14:Y:43:ARG:CB	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:58:LYS:O	15:N:62:ALA:N	2.24	0.68
4:d:5176:ALA:HA	4:d:5179:PHE:HD2	1.59	0.68
14:y:18:VAL:C	14:y:22:LEU:H	2.01	0.68
1:A:166:GLY:HA3	3:C:358:PHE:HE1	1.58	0.68
3:C:147:PHE:CD2	17:C:513:CLA:H3A	2.29	0.68
3:C:265:ILE:HG13	3:C:449:ARG:HG2	1.76	0.68
3:c:5362:ARG:HG3	15:n:82:ARG:HH11	1.59	0.68
17:B:607:CLA:H203	4:D:281:MET:HE3	1.76	0.67
12:t:5015:ALA:HB2	20:t:5102:BCR:H14C	1.75	0.67
17:C:505:CLA:HBD	17:C:505:CLA:HBA1	1.75	0.67
3:c:5147:PHE:CD2	17:c:5512:CLA:H3A	2.29	0.67
15:N:109:LEU:HD22	15:N:113:LEU:HD23	1.76	0.67
4:D:24:ARG:NH2	16:X:37:VAL:HG21	2.10	0.67
3:C:212:TYR:OH	3:C:227:VAL:N	2.18	0.67
4:d:5043:LEU:O	4:d:5047:GLY:N	2.26	0.67
15:N:44:LEU:HD21	15:N:68:LEU:HD21	1.76	0.67
1:A:130:GLN:HB3	1:A:143:ILE:HD12	1.75	0.67
2:B:149:LEU:HG	17:B:603:CLA:HBC1	1.77	0.67
3:C:457:LYS:HE3	4:D:227:GLU:O	1.94	0.67
23:D:403:SQD:H172	25:D:408:MGE:H242	1.77	0.67
7:H:51:SER:HB2	7:H:60:VAL:HG21	1.77	0.67
15:n:58:LYS:O	15:n:62:ALA:N	2.24	0.67
4:D:14:TRP:CZ2	16:X:29:ILE:CD1	2.77	0.67
13:z:5021:ILE:HD11	14:y:31:ALA:CB	2.24	0.67
7:h:5051:SER:HB2	7:h:5060:VAL:HG21	1.77	0.67
4:D:84:SER:OG	5:E:67:THR:O	2.10	0.67
7:H:44:ILE:HD12	16:X:10:PHE:CE1	2.28	0.67
4:d:5100:ASP:OD2	4:d:5103:ARG:NH1	2.26	0.67
4:D:261:PHE:HA	25:D:410:MGE:H2D	1.76	0.67
2:b:5149:LEU:HG	17:b:5603:CLA:HBC1	1.76	0.67
20:C:515:BCR:H403	20:C:515:BCR:H371	1.77	0.67
2:b:5004:PRO:HD2	2:b:5007:ARG:HD2	1.76	0.67
16:X:3:ILE:HG22	16:X:8:LYS:HB2	1.77	0.67
11:M:24:ILE:HD12	25:m:5103:MGE:H212	1.75	0.66
13:z:5029:SER:HA	14:y:44:GLY:HA2	1.77	0.66
15:N:130:ARG:O	15:N:134:SER:OG	2.10	0.66
2:B:323:GLY:HA3	2:B:326:ARG:HH11	1.59	0.66
1:a:5317:TRP:CZ3	4:d:5077:ALA:HB3	2.31	0.66
24:a:5412:BCT:O2	4:d:5268:HIS:NE2	2.29	0.66
13:z:5028:ALA:C	14:y:44:GLY:HA3	2.21	0.66
15:n:109:LEU:HD22	15:n:113:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:SER:HB2	2:B:4:PRO:HG3	1.77	0.66
4:D:176:ALA:HA	4:D:179:PHE:HD2	1.59	0.66
10:l:5004:ASN:HD22	10:l:5007:ARG:HE	1.42	0.66
23:l:5102:SQD:H191	11:m:5023:ILE:HD11	1.78	0.66
17:b:5604:CLA:HBB1	17:b:5607:CLA:HAB	1.78	0.66
14:y:34:MET:O	14:y:38:LEU:HD12	1.90	0.66
25:A:412:MGE:H122	11:M:18:PRO:HG3	1.77	0.66
4:d:5139:ARG:NH2	4:d:5141:TYR:OH	2.29	0.66
15:n:44:LEU:HD21	15:n:68:LEU:HD21	1.77	0.66
13:z:5016:SER:OG	13:z:5047:TRP:NE1	2.22	0.66
24:A:411:BCT:O2	4:D:268:HIS:NE2	2.29	0.66
3:c:5208:VAL:O	3:c:5212:TYR:HB2	1.96	0.66
20:z:5101:BCR:H403	20:z:5101:BCR:H371	1.77	0.66
14:y:18:VAL:N	14:y:21:GLN:HB2	2.11	0.66
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.76	0.66
2:b:5192:PRO:HG3	7:h:5049:TYR:CD1	2.31	0.66
3:c:5349:ILE:H	3:c:5374:GLY:HA3	1.61	0.66
4:d:5275:PRO:HB3	18:d:5402:PHO:HBC1	1.76	0.66
13:z:5005:PHE:CD1	13:z:5057:LEU:HD23	2.31	0.66
4:D:139:ARG:NH2	4:D:141:TYR:OH	2.29	0.65
4:D:24:ARG:CZ	16:X:37:VAL:HG21	2.26	0.65
3:c:5388:GLN:NE2	15:n:95:ASN:HD21	1.95	0.65
1:A:30:VAL:HG23	1:A:34:GLY:HA3	1.78	0.65
3:C:187:ASP:N	3:C:195:ASP:O	2.20	0.65
17:a:5403:CLA:H13	19:d:5405:PQ9:H452	1.77	0.65
2:b:5187:PRO:HA	17:b:5601:CLA:HMA1	1.77	0.65
3:C:208:VAL:O	3:C:212:TYR:HB2	1.96	0.65
3:C:236:GLY:HA3	20:C:516:BCR:H393	1.79	0.65
13:Z:58:ASN:HA	13:Z:61:VAL:HB	1.78	0.65
2:b:5354:LEU:HD23	2:b:5370:LEU:HB3	1.78	0.65
1:A:187:GLN:HG3	1:A:325:ASN:HD21	1.61	0.65
2:B:354:LEU:HD23	2:B:370:LEU:HB3	1.78	0.65
17:C:505:CLA:HBC3	17:C:505:CLA:HHD	1.79	0.65
23:D:403:SQD:H381	20:Y:101:BCR:H21C	1.79	0.65
5:E:36:LEU:O	5:E:40:THR:N	2.24	0.65
9:K:20:PRO:HB2	14:Y:24:MET:HB2	1.77	0.65
17:b:5613:CLA:H51	25:d:5409:MGE:H241	1.77	0.65
17:B:604:CLA:HBB1	17:B:607:CLA:HAB	1.78	0.65
17:c:5505:CLA:HBC3	17:c:5505:CLA:HHD	1.79	0.65
5:e:5036:LEU:O	5:e:5040:THR:N	2.24	0.65
2:b:5025:MET:HE2	20:b:5617:BCR:H23C	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:5607:CLA:H203	4:d:5281:MET:HE3	1.79	0.65
17:b:5610:CLA:H141	17:b:5612:CLA:HBD	1.79	0.65
2:B:187:PRO:HA	17:B:601:CLA:HMA1	1.77	0.65
17:B:610:CLA:H141	17:B:612:CLA:HBD	1.79	0.65
4:D:263:ASN:HB2	4:D:266:TRP:HB3	1.79	0.65
1:a:5030:VAL:HG23	1:a:5034:GLY:HA3	1.78	0.65
15:n:68:LEU:HD22	15:n:94:LEU:HD22	1.79	0.65
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.79	0.65
2:B:124:ARG:O	7:H:12:ARG:NH2	2.30	0.65
2:B:258:TYR:CE2	26:D:411:DGD:C3G	2.67	0.65
2:B:68:ARG:NH2	17:B:603:CLA:O2D	2.30	0.65
2:B:77:GLY:C	2:B:86:ILE:HD11	2.20	0.65
3:c:5212:TYR:OH	3:c:5227:VAL:N	2.18	0.65
4:d:5263:ASN:HB2	4:d:5266:TRP:HB3	1.79	0.65
3:C:405:ASN:HD22	26:C:518:DGD:HD61	1.63	0.64
16:x:7:LEU:O	16:x:7:LEU:HD13	1.96	0.64
13:Z:16:SER:OG	13:Z:47:TRP:NE1	2.21	0.64
4:d:5188:PHE:HD1	4:d:5326:ARG:HG2	1.62	0.64
13:z:5058:ASN:HA	13:z:5061:VAL:HB	1.78	0.64
5:e:5077:GLU:O	5:e:5081:GLU:N	2.31	0.64
13:z:5021:ILE:CD1	14:y:31:ALA:HB1	2.26	0.64
3:c:5033:PHE:CZ	3:c:5040:ALA:HB3	2.33	0.64
2:B:25:MET:HE2	20:B:617:BCR:H23C	1.79	0.64
4:D:100:ASP:OD2	4:D:103:ARG:NH1	2.26	0.64
7:H:38:PHE:CD1	20:H:101:BCR:H10C	2.33	0.64
10:L:14:ARG:NH2	23:L:101:SQD:O49	2.30	0.64
1:a:5083:VAL:HG22	4:d:5314:PHE:CE2	2.33	0.64
1:a:5143:ILE:N	4:d:5220:ASN:HD21	1.96	0.64
1:a:5187:GLN:HG3	1:a:5325:ASN:HD21	1.61	0.64
2:b:5068:ARG:NH2	17:b:5603:CLA:O2D	2.30	0.64
1:A:297:LEU:HD23	3:C:428:THR:HG21	1.79	0.64
1:a:5156:ALA:HA	1:a:5160:ILE:HD12	1.79	0.64
15:N:68:LEU:HD22	15:N:94:LEU:HD22	1.79	0.64
2:B:440:ASP:OD1	2:B:442:ILE:N	2.30	0.64
2:B:462:PHE:O	2:B:466:HIS:N	2.30	0.64
3:C:349:ILE:H	3:C:374:GLY:HA3	1.61	0.64
4:D:202:ALA:HB2	19:D:406:PQ9:H342	1.80	0.64
26:a:5411:DGD:HD61	3:c:5405:ASN:HD22	1.62	0.64
3:c:5372:PRO:HB3	15:n:85:SER:HA	1.80	0.64
4:d:5041:ALA:HB1	18:d:5402:PHO:H42	1.80	0.64
4:d:5202:ALA:HB2	19:d:5405:PQ9:H342	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:z:5028:ALA:O	14:y:45:ASN:N	2.31	0.64
25:D:410:MGE:H2B1	10:L:19:LEU:HD21	1.78	0.63
16:x:7:LEU:HD13	16:x:7:LEU:C	2.22	0.63
3:C:33:PHE:CZ	3:C:40:ALA:HB3	2.33	0.63
1:a:5296:ASN:HB3	3:c:5401:LEU:HA	1.79	0.63
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.80	0.63
17:b:5603:CLA:H201	7:h:5035:MET:HG3	1.79	0.63
3:c:5236:GLY:HA3	20:c:5514:BCR:H393	1.79	0.63
26:b:5621:DGD:O2D	4:d:5087:HIS:CG	2.52	0.63
4:D:188:PHE:HD1	4:D:326:ARG:HG2	1.62	0.63
4:d:5060:THR:HG23	4:d:5061:HIS:H	1.64	0.63
15:n:130:ARG:O	15:n:134:SER:OG	2.10	0.63
17:B:605:CLA:HBB1	17:B:606:CLA:H43	1.80	0.63
3:C:187:ASP:HA	3:C:230:LEU:HD11	1.81	0.63
4:D:130:PHE:O	4:D:133:ALA:N	2.32	0.63
17:b:5601:CLA:H2A	17:b:5601:CLA:CED	2.29	0.63
3:c:5187:ASP:HA	3:c:5230:LEU:HD11	1.81	0.63
17:B:601:CLA:CED	17:B:601:CLA:H2A	2.29	0.63
2:b:5002:GLY:N	10:l:5009:PRO:O	2.32	0.63
20:b:5617:BCR:HC22	25:b:5620:MGE:H5B1	1.81	0.63
16:x:12:ILE:HD12	16:x:12:ILE:N	2.04	0.63
2:B:468:TRP:CE3	4:D:144:ILE:HD13	2.34	0.63
16:x:12:ILE:CD1	16:x:12:ILE:H	1.95	0.63
2:B:2:GLY:N	10:L:9:PRO:O	2.31	0.62
2:B:75:TRP:CZ3	2:B:94:GLU:HB2	2.34	0.62
4:D:91:LEU:HD23	4:D:93:TRP:CZ2	2.34	0.62
3:C:293:ASN:OD1	3:C:295:THR:N	2.32	0.62
4:D:72:ASN:HD21	4:D:74:LEU:HB2	1.63	0.62
10:L:8:GLN:NE2	10:L:9:PRO:HD2	2.15	0.62
15:n:86:SER:O	15:n:89:THR:OG1	2.17	0.62
1:A:105:TRP:HE3	1:A:106:LEU:HD12	1.64	0.62
4:D:60:THR:HG23	4:D:61:HIS:H	1.64	0.62
15:n:124:VAL:O	15:n:128:LEU:N	2.18	0.62
3:C:33:PHE:HZ	3:C:40:ALA:HB3	1.64	0.62
3:c:5293:ASN:OD1	3:c:5295:THR:N	2.32	0.62
4:d:5091:LEU:HD23	4:d:5093:TRP:CZ2	2.34	0.62
4:d:5192:THR:HG23	17:d:5403:CLA:HBC2	1.82	0.62
4:D:192:THR:HG23	17:D:404:CLA:HBC2	1.81	0.62
4:D:297:ASP:HA	4:D:315:TYR:OH	2.00	0.62
2:b:5256:MET:HG3	2:b:5451:PHE:CE1	2.34	0.62
7:H:38:PHE:HD1	20:H:101:BCR:H10C	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5329:GLU:OE1	3:c:5412:THR:OG1	2.09	0.62
4:d:5072:ASN:HD21	4:d:5074:LEU:HB2	1.63	0.62
7:h:5038:PHE:CD1	20:h:5101:BCR:H10C	2.33	0.62
2:B:122:LEU:HD12	7:H:8:GLY:HA2	1.82	0.62
17:B:608:CLA:H51	17:B:609:CLA:H112	1.82	0.62
3:C:157:MET:HE1	3:C:271:TYR:CG	2.35	0.62
4:d:5244:TYR:OH	4:d:5264:LYS:NZ	2.32	0.62
5:e:5074:GLN:NE2	5:e:5077:GLU:OE1	2.33	0.62
20:k:5502:BCR:H16C	14:y:33:PRO:HD3	1.82	0.62
10:l:5008:GLN:NE2	10:l:5009:PRO:HD2	2.14	0.62
15:N:109:LEU:CB	15:N:114:LYS:HE3	2.26	0.62
12:T:18:PHE:HB2	20:T:102:BCR:HC7	1.81	0.62
2:b:5160:GLY:HA3	2:b:5180:PRO:HB3	1.80	0.62
3:c:5402:GLY:HA3	3:c:5420:VAL:HG22	1.81	0.62
4:D:66:SER:OG	4:D:69:GLU:OE1	2.18	0.62
1:a:5105:TRP:HE3	1:a:5106:LEU:HD12	1.64	0.62
2:b:5292:LEU:HD21	2:b:5298:LEU:HA	1.81	0.62
1:A:253:GLY:O	1:A:257:ARG:N	2.31	0.61
2:B:256:MET:HG3	2:B:451:PHE:CE1	2.34	0.61
2:b:5440:ASP:OD1	2:b:5442:ILE:N	2.31	0.61
3:c:5461:ARG:NH1	4:d:5225:ASP:OD1	2.32	0.61
1:a:5024:THR:O	4:d:5255:GLN:NE2	2.32	0.61
1:a:5083:VAL:HG22	4:d:5314:PHE:HE2	1.64	0.61
1:a:5253:GLY:O	1:a:5257:ARG:N	2.31	0.61
2:b:5080:ILE:HD11	2:b:5093:PHE:CZ	2.35	0.61
2:B:80:ILE:HD11	2:B:93:PHE:CZ	2.35	0.61
17:b:5608:CLA:H51	17:b:5609:CLA:H112	1.82	0.61
5:e:5021:VAL:HG23	5:e:5022:ILE:H	1.65	0.61
20:B:617:BCR:HC22	25:B:619:MGE:H5B1	1.81	0.61
4:D:244:TYR:OH	4:D:264:LYS:NZ	2.32	0.61
17:a:5403:CLA:H161	25:d:5410:MGE:H252	1.83	0.61
4:D:189:HIS:CG	4:D:289:LEU:HD21	2.36	0.61
3:c:5033:PHE:HZ	3:c:5040:ALA:HB3	1.64	0.61
3:c:5157:MET:HE1	3:c:5271:TYR:CG	2.35	0.61
2:B:46:ASP:OD1	2:B:58:GLN:NE2	2.33	0.61
4:D:223:PHE:HE1	4:D:245:SER:HB3	1.65	0.61
2:b:5046:ASP:OD1	2:b:5058:GLN:NE2	2.33	0.61
4:d:5068:LEU:HA	6:f:5040:MET:SD	2.41	0.61
5:e:5020:TRP:N	5:e:5023:HIS:HD2	1.97	0.61
7:h:5038:PHE:HD1	20:h:5101:BCR:H10C	1.65	0.61
10:L:14:ARG:NH1	23:L:101:SQD:O10	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5075:TRP:CZ3	2:b:5094:GLU:HB2	2.34	0.61
4:d:5297:ASP:HA	4:d:5315:TYR:OH	2.00	0.61
13:z:5028:ALA:HB1	14:y:39:LEU:CD1	2.31	0.61
15:n:62:ALA:O	15:n:66:LYS:HG2	2.01	0.61
16:x:3:ILE:O	16:x:3:ILE:HG22	2.00	0.61
1:A:285:PHE:O	1:A:289:GLY:N	2.33	0.61
2:B:80:ILE:HD11	2:B:93:PHE:HZ	1.66	0.61
2:B:292:LEU:HD21	2:B:298:LEU:HA	1.81	0.61
4:D:210:LEU:HD22	4:D:271:MET:HG2	1.83	0.61
3:c:5189:TRP:HB3	15:n:76:ARG:NE	2.16	0.61
13:z:5039:LEU:HA	13:z:5042:LEU:HB2	1.83	0.61
23:L:101:SQD:H81	25:m:5101:MGE:H6B2	1.82	0.60
14:Y:18:VAL:O	14:Y:18:VAL:HG12	2.01	0.60
15:N:124:VAL:O	15:N:128:LEU:N	2.18	0.60
4:d:5189:HIS:CG	4:d:5289:LEU:HD21	2.36	0.60
4:d:5223:PHE:HE1	4:d:5245:SER:HB3	1.65	0.60
1:A:272:HIS:CD2	4:D:218:VAL:HG11	2.35	0.60
2:B:61:PHE:O	2:B:64:PRO:HD2	2.02	0.60
4:d:5130:PHE:O	4:d:5133:ALA:N	2.32	0.60
15:N:86:SER:O	15:N:89:THR:OG1	2.17	0.60
16:X:37:VAL:O	16:X:37:VAL:HG12	2.01	0.60
17:B:608:CLA:H72	17:B:609:CLA:H121	1.83	0.60
2:b:5185:TRP:HE1	17:b:5601:CLA:HBC3	1.66	0.60
9:k:5020:PRO:CB	14:y:24:MET:HB3	2.30	0.60
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.81	0.60
12:T:4:ILE:HD11	20:T:102:BCR:H272	1.81	0.60
2:b:5462:PHE:O	2:b:5466:HIS:N	2.30	0.60
13:Z:28:ALA:HB1	14:Y:39:LEU:CD1	2.31	0.60
2:b:5080:ILE:HD11	2:b:5093:PHE:HZ	1.66	0.60
15:N:62:ALA:O	15:N:66:LYS:HG2	2.01	0.60
2:B:75:TRP:HZ3	2:B:94:GLU:HB2	1.67	0.60
5:E:21:VAL:HG23	5:E:22:ILE:H	1.65	0.60
13:Z:39:LEU:HA	13:Z:42:LEU:HB2	1.83	0.60
1:a:5328:MET:HE2	4:d:5325:ILE:HD11	1.83	0.60
2:b:5420:TYR:O	2:b:5424:ALA:N	2.33	0.60
4:d:5261:PHE:HE1	25:d:5410:MGE:C1B	2.15	0.60
5:e:5063:ILE:HG22	5:e:5065:LEU:HB2	1.83	0.60
2:B:380:ASP:N	2:B:390:TYR:O	2.34	0.60
3:C:178:LYS:HD2	3:C:182:PHE:O	2.02	0.60
15:N:112:LYS:O	15:N:116:ARG:CG	2.48	0.60
1:a:5104:GLU:OE2	1:a:5108:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5256:MET:SD	2:b:5263:THR:HG21	2.42	0.60
4:d:5074:LEU:HD22	4:d:5175:VAL:HG11	1.84	0.60
16:X:9:GLY:HA2	16:X:12:ILE:HD12	1.82	0.60
2:b:5061:PHE:O	2:b:5064:PRO:HD2	2.02	0.60
2:b:5075:TRP:HZ3	2:b:5094:GLU:HB2	1.67	0.60
2:b:5167:TRP:CD1	2:b:5264:PRO:HG3	2.37	0.60
2:b:5340:TRP:HE1	2:b:5428:GLU:HB3	1.67	0.60
2:B:167:TRP:CD1	2:B:264:PRO:HG3	2.37	0.59
2:B:185:TRP:HE1	17:B:601:CLA:HBC3	1.66	0.59
4:D:261:PHE:HE1	25:D:410:MGE:C1B	2.15	0.59
1:a:5288:LEU:HD22	3:c:5432:VAL:HG22	1.84	0.59
1:A:104:GLU:OE2	1:A:108:ASN:ND2	2.34	0.59
2:B:420:TYR:O	2:B:424:ALA:N	2.33	0.59
24:A:411:BCT:O2	4:D:214:HIS:NE2	2.35	0.59
18:D:402:PHO:H152	17:D:404:CLA:H172	1.83	0.59
2:B:256:MET:SD	2:B:263:THR:HG21	2.42	0.59
1:a:5084:PRO:HA	1:a:5112:TYR:CG	2.38	0.59
3:c:5466:VAL:HG13	4:d:5251:ARG:HD3	1.84	0.59
4:D:103:ARG:HH21	5:E:77:GLU:CD	2.09	0.59
1:a:5283:VAL:O	1:a:5286:THR:OG1	2.19	0.59
2:b:5271:THR:HG22	2:b:5274:GLN:HG2	1.84	0.59
23:l:5102:SQD:H101	25:m:5103:MGE:H6A2	1.84	0.59
5:E:63:ILE:HG22	5:E:65:LEU:HB2	1.83	0.59
3:c:5367:GLU:HG3	15:n:91:GLN:HE22	1.66	0.59
17:c:5512:CLA:C4B	20:z:5101:BCR:H383	2.33	0.59
17:b:5608:CLA:H72	17:b:5609:CLA:H121	1.83	0.59
16:X:36:LYS:N	16:X:36:LYS:HD2	2.18	0.59
1:A:35:VAL:HG11	8:I:18:LEU:HD22	1.85	0.59
1:A:259:ILE:HG22	1:A:260:PHE:H	1.68	0.59
20:C:514:BCR:H11C	20:Y:101:BCR:H322	1.84	0.59
1:a:5195:HIS:ND1	1:a:5196:PRO:HD2	2.18	0.59
2:b:5341:LYS:HD3	2:b:5431:GLU:HG3	1.84	0.59
2:B:39:LEU:O	2:B:43:ALA:N	2.35	0.59
2:B:135:LEU:HD22	2:B:232:GLY:H	1.68	0.59
2:B:340:TRP:HE1	2:B:428:GLU:HB3	1.67	0.59
2:B:341:LYS:HD3	2:B:431:GLU:HG3	1.84	0.59
4:D:74:LEU:HD22	4:D:175:VAL:HG11	1.84	0.59
29:F:101:HEM:HBC2	29:F:101:HEM:HHD	1.84	0.59
1:a:5218:LEU:O	1:a:5221:SER:OG	2.18	0.59
2:b:5055:MET:HE1	2:b:5080:ILE:HA	1.85	0.59
29:f:5101:HEM:HBC2	29:f:5101:HEM:HHD	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:x:4:THR:HB	16:x:5:PRO:HD2	1.83	0.59
1:A:53:ILE:HA	1:A:71:LEU:HB3	1.85	0.58
2:B:150:CYS:HA	17:B:603:CLA:HBC2	1.85	0.58
2:B:271:THR:HG22	2:B:274:GLN:HG2	1.84	0.58
2:B:464:PHE:HB2	4:D:280:TRP:CH2	2.38	0.58
3:C:225:VAL:HG21	3:C:288:CYS:SG	2.43	0.58
3:C:239:TRP:O	3:C:243:ILE:N	2.32	0.58
29:F:101:HEM:HBB2	29:F:101:HEM:HMB2	1.85	0.58
2:b:5135:LEU:HD22	2:b:5232:GLY:H	1.68	0.58
2:b:5283:GLU:HA	2:b:5286:ARG:HG2	1.85	0.58
4:d:5210:LEU:HD22	4:d:5271:MET:HG2	1.83	0.58
7:h:5044:ILE:HD13	16:x:10:PHE:CZ	2.36	0.58
14:y:25:ILE:HA	14:y:28:ILE:HG12	1.85	0.58
2:b:5349:LYS:HD3	2:b:5396:GLY:HA3	1.85	0.58
29:f:5101:HEM:HMB2	29:f:5101:HEM:HBB2	1.85	0.58
9:K:39:TRP:CD1	14:Y:36:ILE:HD11	2.38	0.58
1:a:5136:ARG:NH2	8:i:5027:ASP:OD1	2.37	0.58
2:b:5418:LYS:HA	2:b:5421:ALA:HB3	1.85	0.58
4:d:5018:LEU:CD1	16:x:29:ILE:HG12	2.33	0.58
17:B:602:CLA:H112	17:B:602:CLA:H171	1.85	0.58
4:D:218:VAL:HG23	4:D:244:TYR:CG	2.38	0.58
6:F:24:HIS:NE2	29:F:101:HEM:ND	2.51	0.58
2:b:5012:LEU:HB2	17:b:5612:CLA:HMC2	1.84	0.58
3:c:5106:VAL:HG23	3:c:5107:ASP:H	1.69	0.58
26:A:413:DGD:HB71	25:C:519:MGE:H7A1	1.84	0.58
17:C:513:CLA:C4B	20:C:515:BCR:H383	2.33	0.58
5:E:22:ILE:HG22	5:E:26:THR:HG23	1.85	0.58
2:b:5222:PRO:HB3	7:h:5025:TRP:C	2.29	0.58
2:b:5290:ALA:O	2:b:5294:SER:N	2.33	0.58
17:b:5611:CLA:H172	17:b:5613:CLA:H8	1.85	0.58
2:B:205:ALA:O	2:B:209:GLY:N	2.34	0.58
2:B:280:PHE:O	2:B:284:ILE:N	2.37	0.58
2:B:349:LYS:HD3	2:B:396:GLY:HA3	1.85	0.58
3:C:331:ALA:HB1	3:C:339:LYS:HE3	1.86	0.58
1:a:5159:LEU:HD23	26:c:5515:DGD:HAT1	1.85	0.58
2:b:5360:PRO:HG2	4:d:5339:PHE:HZ	1.69	0.58
3:c:5225:VAL:HG21	3:c:5288:CYS:SG	2.43	0.58
16:X:21:LEU:HD23	16:X:21:LEU:N	2.19	0.58
3:c:5331:ALA:HB1	3:c:5339:LYS:HE3	1.86	0.58
4:d:5018:LEU:HD12	16:x:29:ILE:HG12	1.85	0.58
4:d:5146:PHE:HD1	18:d:5402:PHO:C3D	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:MET:HE1	2:B:80:ILE:HA	1.85	0.58
3:C:290:VAL:HG11	3:C:426:LEU:HB2	1.86	0.58
11:M:9:ILE:HG13	11:m:5009:ILE:HG13	1.86	0.58
24:a:5412:BCT:O2	4:d:5214:HIS:NE2	2.36	0.58
3:c:5178:LYS:HD2	3:c:5182:PHE:O	2.02	0.58
4:d:5129:GLN:HE21	4:d:5142:ASN:CG	2.12	0.58
6:f:5017:THR:OG1	6:f:5018:VAL:N	2.37	0.58
16:X:29:ILE:O	16:X:32:SER:OG	2.18	0.58
1:A:84:PRO:HA	1:A:112:TYR:CG	2.38	0.58
1:A:218:LEU:O	1:A:221:SER:OG	2.18	0.58
25:A:412:MGE:H3A2	11:M:22:LEU:HD11	1.86	0.58
2:B:418:LYS:HA	2:B:421:ALA:HB3	1.85	0.58
3:C:212:TYR:HH	3:C:227:VAL:H	1.50	0.58
4:D:195:PRO:HB2	10:L:31:PHE:HE1	1.69	0.58
1:a:5259:ILE:HG22	1:a:5260:PHE:H	1.68	0.58
2:b:5150:CYS:HA	17:b:5603:CLA:HBC2	1.86	0.58
17:b:5602:CLA:H171	17:b:5602:CLA:H112	1.85	0.58
19:d:5405:PQ9:H301	25:l:5101:MGE:H241	1.86	0.58
14:Y:42:ARG:HH11	14:Y:42:ARG:CG	2.14	0.58
1:A:195:HIS:ND1	1:A:196:PRO:HD2	2.18	0.58
2:B:12:LEU:HB2	17:B:612:CLA:HMC2	1.85	0.58
2:B:413:ASP:HB2	2:B:415:PRO:HD2	1.86	0.58
3:C:229:ASN:HD22	15:N:77:ARG:HB2	1.68	0.58
1:a:5053:ILE:HA	1:a:5071:LEU:HB3	1.85	0.58
25:d:5410:MGE:H6A2	12:t:5017:PHE:CD1	2.39	0.58
1:A:272:HIS:CD2	24:A:411:BCT:HO3	2.18	0.57
3:C:106:VAL:HG23	3:C:107:ASP:H	1.69	0.57
3:C:459:ILE:HG22	4:D:222:LEU:O	2.04	0.57
3:c:5376:ASP:O	3:c:5380:ILE:HG12	2.04	0.57
2:B:283:GLU:HA	2:B:286:ARG:HG2	1.85	0.57
23:L:101:SQD:H101	25:m:5101:MGE:H4B2	1.86	0.57
15:N:54:ASP:HB2	15:N:55:PRO:HD2	1.87	0.57
26:A:413:DGD:HA51	3:C:284:PHE:HB3	1.86	0.57
26:C:518:DGD:HBE2	25:D:408:MGE:H9B1	1.86	0.57
3:C:99:VAL:O	3:C:105:VAL:N	2.36	0.57
2:b:5380:ASP:N	2:b:5390:TYR:O	2.34	0.57
4:d:5218:VAL:HG23	4:d:5244:TYR:CG	2.38	0.57
24:A:411:BCT:C	4:D:214:HIS:HE2	2.17	0.57
2:B:13:ILE:HG23	2:B:14:ASN:H	1.70	0.57
2:B:78:TRP:HA	2:B:84:THR:HG22	1.86	0.57
3:C:376:ASP:O	3:C:380:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:TYR:OH	6:F:25:THR:O	2.14	0.57
3:c:5284:PHE:HB3	26:c:5515:DGD:HA51	1.86	0.57
19:d:5405:PQ9:H241	25:l:5101:MGE:H242	1.87	0.57
9:k:5043:VAL:HG23	14:y:46:LEU:HD13	1.86	0.57
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.40	0.57
7:H:53:LEU:HD11	16:X:7:LEU:HA	1.85	0.57
2:b:5238:LEU:O	2:b:5242:ILE:HG12	2.05	0.57
5:e:5022:ILE:HG22	5:e:5026:THR:HG23	1.85	0.57
1:A:303:ASN:ND2	3:C:414:ILE:HG13	2.20	0.57
4:D:129:GLN:HE21	4:D:142:ASN:CG	2.12	0.57
1:a:5238:LYS:O	1:a:5241:GLN:HG3	2.05	0.57
3:c:5178:LYS:HZ2	3:c:5183:GLY:HA3	1.70	0.57
4:d:5087:HIS:CE1	4:d:5162:LEU:HA	2.40	0.57
17:B:611:CLA:H172	17:B:613:CLA:H8	1.85	0.57
3:c:5097:TRP:HE1	3:c:5178:LYS:NZ	2.03	0.57
4:d:5093:TRP:CG	4:d:5094:GLY:H	2.23	0.57
9:k:5026:PRO:O	9:k:5029:PRO:HD2	2.05	0.57
15:n:51:PRO:HG2	15:n:54:ASP:HB3	1.87	0.57
1:A:238:LYS:O	1:A:241:GLN:HG3	2.05	0.57
9:K:43:VAL:HG23	14:Y:46:LEU:CD1	2.30	0.57
1:a:5144:CYS:HB2	3:c:5442:LEU:HD21	1.87	0.57
17:a:5404:CLA:HMB2	18:d:5402:PHO:H161	1.87	0.57
2:b:5005:TRP:HE1	25:l:5101:MGE:H3G2	1.68	0.57
7:h:5047:GLU:OE2	16:x:10:PHE:HD2	1.86	0.57
2:B:122:LEU:HD11	7:H:11:LEU:HB2	1.87	0.57
2:B:401:PHE:CD2	2:B:406:LEU:HD11	2.39	0.57
20:H:101:BCR:H331	20:H:101:BCR:H343	1.87	0.57
1:a:5087:ASN:ND2	1:a:5169:SER:OG	2.38	0.57
13:z:5028:ALA:O	14:y:44:GLY:CA	2.53	0.57
14:y:30:ILE:HG12	14:y:30:ILE:O	2.04	0.57
2:B:7:ARG:NH1	17:B:611:CLA:HED1	2.20	0.56
2:B:81:THR:OG1	2:B:83:GLU:OE1	2.18	0.56
3:C:97:TRP:HE1	3:C:178:LYS:NZ	2.03	0.56
9:K:26:PRO:O	9:K:29:PRO:HD2	2.05	0.56
1:a:5320:ILE:HD11	4:d:5063:LEU:HD21	1.87	0.56
24:a:5412:BCT:C	4:d:5214:HIS:HE2	2.17	0.56
14:Y:33:PRO:HD3	20:Y:101:BCR:H16C	1.87	0.56
1:A:87:ASN:ND2	1:A:169:SER:OG	2.38	0.56
20:D:407:BCR:H11C	6:F:29:PRO:CB	2.36	0.56
10:L:7:ARG:NH1	23:l:5102:SQD:O7	2.38	0.56
14:Y:34:MET:HA	14:Y:34:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:398:HIS:HA	3:C:419:PHE:CZ	2.40	0.56
4:D:93:TRP:CG	4:D:94:GLY:H	2.23	0.56
2:b:5280:PHE:O	2:b:5284:ILE:N	2.37	0.56
17:b:5609:CLA:CGA	7:h:5031:MET:HE1	2.35	0.56
3:c:5099:VAL:O	3:c:5105:VAL:N	2.36	0.56
3:c:5368:PRO:HG3	15:n:91:GLN:HE21	1.70	0.56
4:d:5195:PRO:HB2	10:l:5031:PHE:HE1	1.70	0.56
16:X:3:ILE:HG22	16:X:8:LYS:CB	2.35	0.56
17:A:401:CLA:C2	18:A:404:PHO:HBB1	2.36	0.56
2:B:314:TYR:HB3	2:B:317:ASN:HB2	1.88	0.56
2:b:5078:TRP:HA	2:b:5084:THR:HG22	1.86	0.56
2:b:5241:SER:OG	17:b:5612:CLA:O1D	2.19	0.56
2:b:5401:PHE:CD2	2:b:5406:LEU:HD11	2.39	0.56
3:c:5398:HIS:HA	3:c:5419:PHE:CZ	2.40	0.56
4:d:5093:TRP:CZ2	16:x:13:GLY:HA3	2.40	0.56
3:C:165:LEU:HD13	17:C:506:CLA:HAB	1.87	0.56
5:E:77:GLU:O	5:E:81:GLU:HB2	2.06	0.56
3:c:5230:LEU:O	3:c:5233:VAL:HG22	2.06	0.56
4:d:5189:HIS:HA	4:d:5294:ARG:HD2	1.87	0.56
1:A:187:GLN:HE21	1:A:325:ASN:HD21	1.54	0.56
1:A:283:VAL:O	1:A:286:THR:OG1	2.19	0.56
1:a:5285:PHE:O	1:a:5289:GLY:N	2.33	0.56
2:b:5071:VAL:HG22	17:b:5606:CLA:HED1	1.88	0.56
3:c:5165:LEU:HD13	17:c:5506:CLA:HAB	1.87	0.56
3:c:5290:VAL:HG11	3:c:5426:LEU:HB2	1.86	0.56
4:d:5261:PHE:HA	25:d:5410:MGE:H2D	1.88	0.56
15:n:72:PHE:O	15:n:76:ARG:HG3	2.06	0.56
2:B:71:VAL:HG22	17:B:606:CLA:HED1	1.88	0.56
2:B:241:SER:OG	17:B:612:CLA:O1D	2.19	0.56
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.87	0.56
1:A:162:PRO:O	1:A:166:GLY:N	2.39	0.56
2:B:290:ALA:HA	2:B:293:ALA:HB3	1.87	0.56
2:B:302:TRP:CE3	2:B:343:HIS:CD2	2.94	0.56
3:C:63:TRP:CZ2	3:C:67:MET:HG3	2.41	0.56
3:C:178:LYS:HZ2	3:C:183:GLY:HA3	1.70	0.56
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.41	0.56
1:a:5162:PRO:O	1:a:5166:GLY:N	2.39	0.56
1:a:5187:GLN:HE21	1:a:5325:ASN:HD21	1.54	0.56
2:b:5413:ASP:HB2	2:b:5415:PRO:HD2	1.86	0.56
17:b:5612:CLA:HBB1	17:b:5612:CLA:HMB1	1.88	0.56
17:c:5501:CLA:H93	20:c:5514:BCR:H19C	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:403:SQD:H371	20:Y:101:BCR:H23C	1.88	0.56
9:K:35:LEU:HB2	20:Y:101:BCR:H351	1.88	0.56
2:B:238:LEU:O	2:B:242:ILE:HG12	2.05	0.56
2:b:5013:ILE:HG23	2:b:5014:ASN:H	1.70	0.56
2:b:5364:GLU:HG3	4:d:5296:TYR:CE2	2.41	0.56
3:c:5147:PHE:CE2	17:c:5512:CLA:H3A	2.41	0.56
1:A:293:MET:SD	1:A:298:ASN:HA	2.47	0.55
2:b:5302:TRP:CE3	2:b:5343:HIS:CD2	2.94	0.55
20:h:5101:BCR:H331	20:h:5101:BCR:H343	1.87	0.55
3:C:230:LEU:O	3:C:233:VAL:HG22	2.06	0.55
17:C:511:CLA:H42	14:Y:46:LEU:HD23	1.87	0.55
4:D:304:ARG:HG2	11:M:1:MET:CE	2.36	0.55
17:a:5402:CLA:C2	18:a:5405:PHO:HBB1	2.36	0.55
2:b:5007:ARG:NH1	17:b:5611:CLA:HED1	2.20	0.55
2:b:5372:ASP:OD2	2:b:5378:LYS:HD3	2.07	0.55
17:b:5608:CLA:H13	7:h:5039:LEU:HD21	1.88	0.55
1:A:132:GLU:HB2	1:A:136:ARG:HH12	1.72	0.55
2:b:5290:ALA:HA	2:b:5293:ALA:HB3	1.87	0.55
3:c:5063:TRP:CZ2	3:c:5067:MET:HG3	2.41	0.55
5:e:5020:TRP:CD1	5:e:5021:VAL:HG13	2.41	0.55
13:z:5016:SER:HG	13:z:5047:TRP:HE1	1.51	0.55
15:n:54:ASP:HB2	15:n:55:PRO:HD2	1.87	0.55
16:x:9:GLY:O	16:x:12:ILE:HD12	1.98	0.55
2:B:263:THR:HB	2:B:268:PHE:CD2	2.41	0.55
2:b:5039:LEU:O	2:b:5043:ALA:N	2.35	0.55
2:b:5064:PRO:HB2	2:b:5268:PHE:CE1	2.41	0.55
2:b:5081:THR:OG1	2:b:5083:GLU:OE1	2.18	0.55
4:d:5223:PHE:CE1	4:d:5245:SER:HB3	2.41	0.55
15:N:45:ARG:HG3	15:N:118:GLU:HG2	1.89	0.55
2:B:289:GLN:O	2:B:293:ALA:N	2.27	0.55
2:B:372:ASP:OD2	2:B:378:LYS:HD3	2.06	0.55
3:C:147:PHE:CE2	17:C:513:CLA:H3A	2.41	0.55
3:C:223:TRP:NE1	25:C:519:MGE:H8B1	2.22	0.55
17:C:506:CLA:HBA1	17:C:506:CLA:CHA	2.37	0.55
1:a:5293:MET:SD	1:a:5298:ASN:HA	2.47	0.55
4:d:5271:MET:O	4:d:5275:PRO:HD2	2.06	0.55
16:X:3:ILE:HG21	16:X:8:LYS:HB2	1.88	0.55
1:A:135:TYR:CE2	8:I:31:ASN:HB3	2.41	0.55
1:A:246:TYR:HE2	1:A:248:ILE:HD11	1.71	0.55
25:A:412:MGE:H3G2	2:B:5:TRP:HE1	1.70	0.55
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5022:THR:HG21	8:i:5030:ARG:HD3	1.89	0.55
2:b:5314:TYR:HB3	2:b:5317:ASN:HB2	1.88	0.55
15:N:51:PRO:HG2	15:N:54:ASP:HB3	1.87	0.55
17:A:405:CLA:H52	8:I:9:TYR:CD1	2.42	0.55
17:B:612:CLA:HMB1	17:B:612:CLA:HBB1	1.88	0.55
17:C:501:CLA:HBB1	20:C:516:BCR:H23C	1.89	0.55
4:D:67:TYR:OH	25:D:408:MGE:H3G1	2.06	0.55
2:b:5205:ALA:O	2:b:5209:GLY:N	2.34	0.55
17:b:5614:CLA:H2	25:m:5101:MGE:H211	1.89	0.55
2:B:77:GLY:CA	2:B:86:ILE:CD1	2.85	0.55
1:a:5063:ILE:HG13	1:a:5064:ARG:N	2.22	0.55
1:a:5246:TYR:HE2	1:a:5248:ILE:HD11	1.71	0.55
2:b:5263:THR:HB	2:b:5268:PHE:CD2	2.41	0.55
3:c:5376:ASP:HB2	3:c:5379:LYS:HE2	1.89	0.55
2:B:290:ALA:O	2:B:294:SER:N	2.33	0.55
3:C:376:ASP:HB2	3:C:379:LYS:HE2	1.89	0.55
4:d:5191:TRP:CZ2	4:d:5197:HIS:HB2	2.42	0.55
17:C:501:CLA:H93	20:C:516:BCR:H19C	1.88	0.55
7:H:44:ILE:HD11	16:X:10:PHE:HE1	1.53	0.55
1:a:5056:PRO:O	1:a:5058:VAL:N	2.40	0.55
2:b:5464:PHE:HB2	4:d:5280:TRP:CH2	2.42	0.55
17:c:5501:CLA:HBB1	20:c:5514:BCR:H23C	1.89	0.55
17:c:5506:CLA:HBA1	17:c:5506:CLA:CHA	2.37	0.55
3:C:223:TRP:CE2	25:C:519:MGE:H8B1	2.42	0.54
4:D:19:ASP:OD1	4:D:23:LYS:NZ	2.39	0.54
4:D:271:MET:O	4:D:275:PRO:HD2	2.06	0.54
3:C:186:TYR:OH	3:C:300:GLU:OE1	2.26	0.54
1:a:5132:GLU:HB2	1:a:5136:ARG:HH12	1.72	0.54
17:c:5501:CLA:H161	17:c:5507:CLA:H102	1.89	0.54
23:l:5102:SQD:H91	25:m:5103:MGE:H4A1	1.89	0.54
1:a:5317:TRP:HZ3	4:d:5077:ALA:HB3	1.69	0.54
4:d:5056:THR:HG21	5:e:5050:PRO:HD3	1.89	0.54
15:n:45:ARG:HG3	15:n:118:GLU:HG2	1.89	0.54
17:A:401:CLA:C3	18:A:404:PHO:HBB1	2.37	0.54
2:B:212:ALA:HB2	17:B:609:CLA:HMC2	1.90	0.54
4:D:83:ASN:HA	4:D:166:SER:OG	2.08	0.54
2:b:5074:SER:HA	2:b:5092:SER:HB2	1.90	0.54
17:b:5613:CLA:O1D	17:b:5613:CLA:H2A	2.08	0.54
1:A:96:ILE:HD13	1:A:105:TRP:CE2	2.43	0.54
2:B:401:PHE:HD2	2:B:406:LEU:HD11	1.72	0.54
17:a:5402:CLA:C3	18:a:5405:PHO:HBB1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5239:TRP:O	3:c:5243:ILE:N	2.33	0.54
6:f:5040:MET:O	6:f:5043:ILE:HG12	2.07	0.54
1:A:56:PRO:O	1:A:58:VAL:N	2.40	0.54
2:b:5212:ALA:HB2	17:b:5609:CLA:HMC2	1.90	0.54
3:c:5277:GLY:C	17:c:5505:CLA:HBC2	2.32	0.54
3:c:5340:TYR:O	3:c:5352:GLY:N	2.41	0.54
17:A:402:CLA:H71	25:D:410:MGE:H221	1.88	0.54
2:B:74:SER:HA	2:B:92:SER:HB2	1.90	0.54
3:C:277:GLY:C	17:C:505:CLA:HBC2	2.32	0.54
17:C:501:CLA:H161	17:C:507:CLA:H102	1.89	0.54
1:a:5053:ILE:O	1:a:5070:SER:OG	2.25	0.54
1:A:53:ILE:O	1:A:70:SER:OG	2.25	0.54
1:A:119:PHE:HD2	1:A:120:LEU:HD12	1.73	0.54
1:A:142:TRP:HH2	3:C:447:ARG:HB2	1.73	0.54
2:B:77:GLY:HA2	2:B:86:ILE:HD12	1.89	0.54
6:F:43:ILE:HG13	6:F:44:GLN:HG3	1.90	0.54
7:h:5035:MET:HB2	20:h:5101:BCR:HC42	1.89	0.54
13:z:5005:PHE:CE1	13:z:5057:LEU:HD23	2.43	0.54
13:z:5028:ALA:CB	14:y:39:LEU:HD22	2.31	0.54
15:n:97:LEU:HD12	15:n:117:LEU:HD13	1.90	0.54
4:D:304:ARG:HG2	11:M:1:MET:HE2	1.90	0.54
6:F:40:MET:O	6:F:43:ILE:HG12	2.07	0.54
7:H:35:MET:HB2	20:H:101:BCR:HC42	1.89	0.54
1:a:5290:ILE:HD11	17:a:5402:CLA:OBD	2.08	0.54
1:A:143:ILE:HG13	1:A:144:CYS:H	1.73	0.53
1:a:5096:ILE:HD13	1:a:5105:TRP:CE2	2.43	0.53
4:d:5232:PHE:CE2	23:d:5407:SQD:H461	2.43	0.53
13:z:5028:ALA:O	14:y:44:GLY:C	2.50	0.53
15:N:109:LEU:CA	15:N:114:LYS:HE3	2.37	0.53
16:X:14:LEU:C	16:X:14:LEU:HD23	2.32	0.53
1:A:91:LEU:HB2	1:A:166:GLY:O	2.09	0.53
1:A:143:ILE:CD1	4:D:252:PHE:HZ	2.21	0.53
2:B:47:PRO:HB3	2:B:78:TRP:CE3	2.43	0.53
4:D:263:ASN:N	25:D:410:MGE:O3D	2.41	0.53
2:b:5406:LEU:HD13	2:b:5409:GLN:HB3	1.90	0.53
4:d:5093:TRP:O	4:d:5098:GLN:N	2.41	0.53
15:n:50:LEU:HB2	15:n:57:LYS:HE3	1.90	0.53
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.90	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CZ3	2.44	0.53
2:B:406:LEU:HD13	2:B:409:GLN:HB3	1.90	0.53
4:D:14:TRP:CZ2	16:X:29:ILE:HD12	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:101:LMT:H4O1	22:M:101:LMT:H6B	1.55	0.53
4:d:5199:MET:HE2	10:l:5027:LEU:HD22	1.90	0.53
14:Y:34:MET:CA	14:Y:34:MET:CE	2.85	0.53
1:A:142:TRP:CH2	3:C:447:ARG:HB2	2.43	0.53
11:M:21:PHE:HD1	25:m:5103:MGE:H202	1.73	0.53
23:d:5407:SQD:H371	20:k:5502:BCR:H23C	1.89	0.53
3:C:192:GLY:HA3	15:N:99:GLY:HA2	1.89	0.53
3:C:340:TYR:O	3:C:352:GLY:N	2.41	0.53
1:a:5119:PHE:HD2	1:a:5120:LEU:HD12	1.73	0.53
2:b:5047:PRO:HB3	2:b:5078:TRP:CE3	2.43	0.53
17:b:5614:CLA:C4A	17:b:5614:CLA:HBA2	2.39	0.53
3:c:5134:ILE:HD11	17:k:5501:CLA:H12	1.91	0.53
3:c:5189:TRP:CD1	3:c:5364:PRO:HA	2.44	0.53
6:f:5043:ILE:HG13	6:f:5044:GLN:HG3	1.90	0.53
15:n:73:ALA:HA	15:n:76:ARG:HH21	1.72	0.53
1:A:55:ALA:HB3	1:A:70:SER:HB2	1.90	0.53
2:B:347:ARG:HB2	2:B:398:THR:OG1	2.09	0.53
3:C:79:LYS:HB3	3:C:80:PRO:HD2	1.91	0.53
4:D:24:ARG:NH1	16:X:37:VAL:HG21	2.24	0.53
4:D:328:TRP:CE2	4:D:346:LEU:HD23	2.44	0.53
17:b:5602:CLA:H172	26:b:5621:DGD:HAT1	1.90	0.53
4:d:5080:THR:HG21	4:d:5167:TRP:O	2.08	0.53
4:d:5083:ASN:HA	4:d:5166:SER:OG	2.08	0.53
6:f:5019:ARG:NH1	29:f:5101:HEM:O1D	2.41	0.53
2:B:18:ARG:HE	2:B:118:TRP:HB3	1.73	0.53
17:B:613:CLA:H2A	17:B:613:CLA:O1D	2.08	0.53
9:K:28:ILE:HA	9:K:31:LEU:HD13	1.91	0.53
17:c:5511:CLA:H2A	17:c:5511:CLA:O2D	2.09	0.53
4:d:5035:ILE:CD1	16:x:28:LEU:HD13	2.25	0.53
17:B:607:CLA:H171	4:D:199:MET:HE1	1.91	0.53
17:C:512:CLA:O2D	17:C:512:CLA:H2A	2.09	0.53
1:a:5055:ALA:HB3	1:a:5070:SER:HB2	1.90	0.53
2:b:5018:ARG:HH22	10:l:5007:ARG:HH21	1.56	0.53
2:b:5281:GLN:HE22	2:b:5358:ARG:HD3	1.74	0.53
3:c:5343:ARG:HA	3:c:5349:ILE:HG22	1.91	0.53
15:N:120:GLU:O	15:N:124:VAL:HG23	2.09	0.53
17:B:603:CLA:H172	17:B:609:CLA:H8	1.91	0.53
4:D:93:TRP:O	4:D:98:GLN:N	2.41	0.53
9:K:20:PRO:HB3	14:Y:21:GLN:HA	1.90	0.53
1:a:5091:LEU:HB2	1:a:5166:GLY:O	2.09	0.53
2:b:5401:PHE:HD2	2:b:5406:LEU:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5210:LEU:HA	4:d:5213:ILE:HG22	1.91	0.53
4:d:5328:TRP:CE2	4:d:5346:LEU:HD23	2.44	0.53
13:z:5028:ALA:HB1	14:y:39:LEU:HD11	1.91	0.53
4:D:323:GLU:HA	4:D:326:ARG:HE	1.74	0.53
1:a:5301:ASN:HB2	1:a:5322:ASN:HD21	1.74	0.53
2:b:5174:LEU:HA	2:b:5308:LYS:HE3	1.91	0.53
14:Y:31:ALA:O	14:Y:34:MET:HB2	2.09	0.53
25:A:412:MGE:H242	19:D:406:PQ9:H241	1.91	0.52
2:B:358:ARG:NH1	2:B:427:GLY:HA2	2.24	0.52
17:B:614:CLA:C4A	17:B:614:CLA:HBA2	2.39	0.52
4:D:80:THR:HG21	4:D:167:TRP:O	2.08	0.52
1:a:5093:PHE:HB2	3:c:5218:PHE:CB	2.39	0.52
3:c:5457:LYS:NZ	4:d:5227:GLU:O	2.41	0.52
15:n:50:LEU:H	15:n:57:LYS:NZ	2.07	0.52
15:N:50:LEU:H	15:N:57:LYS:NZ	2.07	0.52
2:B:392:PHE:HZ	2:B:418:LYS:HB3	1.75	0.52
2:B:475:PHE:HD2	4:D:140:PRO:HG3	1.73	0.52
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.91	0.52
1:a:5163:ILE:HD11	26:c:5515:DGD:O1B	2.10	0.52
1:a:5193:LEU:HD21	17:a:5402:CLA:C2C	2.40	0.52
4:d:5026:ARG:HD2	6:f:5018:VAL:HG21	1.91	0.52
2:B:174:LEU:HA	2:B:308:LYS:HE3	1.91	0.52
6:F:20:TRP:CD1	6:F:24:HIS:CE1	2.97	0.52
6:F:26:LEU:O	6:F:29:PRO:HD2	2.10	0.52
2:b:5018:ARG:HD2	2:b:5115:TRP:CZ3	2.44	0.52
2:b:5018:ARG:HE	2:b:5118:TRP:HB3	1.73	0.52
4:d:5221:THR:C	4:d:5222:LEU:HD12	2.35	0.52
20:k:5502:BCR:H333	14:y:28:ILE:O	2.08	0.52
15:n:120:GLU:O	15:n:124:VAL:HG23	2.09	0.52
3:C:62:PHE:CZ	9:K:28:ILE:HD11	2.44	0.52
2:b:5347:ARG:HB2	2:b:5398:THR:OG1	2.09	0.52
2:b:5358:ARG:NH1	2:b:5427:GLY:HA2	2.24	0.52
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.92	0.52
3:C:408:GLY:HA3	3:C:418:ASN:HA	1.92	0.52
4:D:199:MET:HE2	10:L:27:LEU:HD22	1.91	0.52
3:c:5403:SER:OG	3:c:5407:VAL:N	2.25	0.52
4:d:5085:MET:HE2	4:d:5090:LEU:HD21	1.91	0.52
15:N:50:LEU:HB2	15:N:57:LYS:HE3	1.90	0.52
1:A:193:LEU:HD21	17:A:401:CLA:C2C	2.40	0.52
1:A:204:GLY:HA3	1:A:282:GLY:HA3	1.91	0.52
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:MET:HE2	17:C:507:CLA:HAC1	1.92	0.52
3:C:437:PHE:CE2	17:C:502:CLA:HAC2	2.45	0.52
1:a:5039:PRO:HB3	20:a:5408:BCR:H10C	1.90	0.52
17:b:5612:CLA:H171	17:b:5613:CLA:HBB2	1.91	0.52
3:c:5157:MET:HE2	17:c:5507:CLA:HAC1	1.92	0.52
4:D:93:TRP:CZ2	16:X:13:GLY:HA3	2.45	0.52
4:D:221:THR:C	4:D:222:LEU:HD12	2.34	0.52
25:D:410:MGE:H6A1	12:T:17:PHE:CD1	2.45	0.52
1:a:5143:ILE:HG13	1:a:5144:CYS:H	1.73	0.52
1:a:5149:ALA:HB3	1:a:5150:PRO:HD3	1.92	0.52
2:b:5045:PHE:HA	2:b:5060:MET:HE3	1.91	0.52
2:b:5392:PHE:HZ	2:b:5418:LYS:HB3	1.75	0.52
4:d:5323:GLU:HA	4:d:5326:ARG:HE	1.75	0.52
7:h:5047:GLU:CD	16:x:10:PHE:HE2	2.01	0.52
9:k:5028:ILE:HA	9:k:5031:LEU:HD13	1.91	0.52
11:m:5028:GLN:NE2	25:m:5101:MGE:H1G2	2.25	0.52
15:N:27:THR:HG23	15:N:70:ASP:HB3	1.92	0.52
1:a:5217:SER:OG	4:d:5142:ASN:HA	2.10	0.52
3:c:5408:GLY:HA3	3:c:5418:ASN:HA	1.92	0.52
6:f:5026:LEU:O	6:f:5029:PRO:HD2	2.10	0.52
10:l:5004:ASN:ND2	10:l:5006:ASN:O	2.43	0.52
14:Y:28:ILE:N	14:Y:28:ILE:CD1	2.73	0.52
1:A:290:ILE:HD11	17:A:401:CLA:OBD	2.08	0.52
1:A:301:ASN:HB2	1:A:322:ASN:HD21	1.74	0.52
2:B:397:VAL:HG11	2:B:417:VAL:HG11	1.92	0.52
3:C:55:ALA:HB1	20:C:514:BCR:H373	1.91	0.52
3:C:134:ILE:HD11	17:C:511:CLA:H12	1.91	0.52
5:E:23:HIS:HE1	29:F:101:HEM:ND	2.07	0.52
3:c:5055:ALA:HB1	20:c:5513:BCR:H373	1.91	0.52
3:c:5264:PHE:HE1	20:c:5514:BCR:H313	1.75	0.52
10:l:5014:ARG:NH1	23:l:5102:SQD:O48	2.43	0.52
15:n:27:THR:HG23	15:n:70:ASP:HB3	1.92	0.52
16:X:21:LEU:N	16:X:21:LEU:CD2	2.73	0.52
1:A:39:PRO:HB3	20:A:407:BCR:H10C	1.90	0.52
2:B:64:PRO:HB2	2:B:268:PHE:CE1	2.41	0.52
17:B:614:CLA:H2	25:m:5103:MGE:H8A1	1.91	0.52
10:L:4:ASN:ND2	10:L:6:ASN:O	2.43	0.52
2:b:5289:GLN:O	2:b:5293:ALA:N	2.27	0.52
17:b:5603:CLA:H172	17:b:5609:CLA:H8	1.91	0.52
3:c:5079:LYS:HB3	3:c:5080:PRO:HD2	1.91	0.52
4:d:5186:GLN:HB2	17:d:5403:CLA:HBC1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:n:75:TYR:HB3	15:n:87:PHE:CE1	2.45	0.52
1:A:27:ARG:NH2	12:T:21:ILE:O	2.42	0.51
1:A:269:ARG:HD3	4:D:222:LEU:HD23	1.92	0.51
2:B:45:PHE:HA	2:B:60:MET:HE3	1.91	0.51
1:a:5204:GLY:HA3	1:a:5282:GLY:HA3	1.91	0.51
3:c:5188:THR:OG1	3:c:5295:THR:O	2.28	0.51
1:A:274:PHE:HD1	23:D:403:SQD:H82	1.75	0.51
1:A:304:HIS:CD2	3:C:415:ASN:OD1	2.64	0.51
3:C:204:LEU:HA	3:C:209:ILE:HD11	1.93	0.51
10:L:14:ARG:HH22	23:L:101:SQD:C7	2.23	0.51
13:Z:5:PHE:CZ	13:Z:54:VAL:HA	2.46	0.51
17:b:5607:CLA:H171	4:d:5199:MET:HE1	1.90	0.51
4:D:48:TRP:CG	18:D:402:PHO:H13	2.46	0.51
1:a:5093:PHE:HB2	3:c:5218:PHE:CG	2.45	0.51
2:b:5222:PRO:HA	7:h:5022:ALA:HB3	1.93	0.51
17:B:612:CLA:H171	17:B:613:CLA:HBB2	1.91	0.51
4:D:69:GLU:HG2	4:D:70:GLY:N	2.22	0.51
4:d:5019:ASP:OD1	4:d:5023:LYS:NZ	2.39	0.51
1:A:195:HIS:CD2	1:A:197:PHE:HB2	2.46	0.51
12:T:18:PHE:HB2	20:T:102:BCR:C7	2.40	0.51
1:a:5195:HIS:CD2	1:a:5197:PHE:HB2	2.46	0.51
17:a:5402:CLA:H201	25:d:5410:MGE:H232	1.92	0.51
4:d:5014:TRP:CZ2	16:x:29:ILE:HD11	2.44	0.51
1:A:219:VAL:HG11	4:D:268:HIS:CE1	2.45	0.51
3:C:188:THR:OG1	3:C:295:THR:O	2.28	0.51
4:D:186:GLN:HB2	17:D:404:CLA:HBC1	1.91	0.51
1:a:5293:MET:HE1	1:a:5299:GLY:N	2.26	0.51
17:a:5403:CLA:H91	17:a:5403:CLA:H3A	1.93	0.51
1:A:97:TRP:NE1	25:C:519:MGE:O5D	2.39	0.51
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.92	0.51
3:C:343:ARG:HA	3:C:349:ILE:HG22	1.91	0.51
25:D:410:MGE:H222	12:T:17:PHE:HZ	1.74	0.51
3:c:5437:PHE:CE2	17:c:5502:CLA:HAC2	2.45	0.51
1:A:42:LEU:HD22	20:A:407:BCR:H11C	1.93	0.51
7:H:40:VAL:CG1	16:X:14:LEU:CD1	2.87	0.51
1:a:5143:ILE:HG13	1:a:5144:CYS:N	2.26	0.51
3:c:5401:LEU:HD22	3:c:5409:GLY:O	2.11	0.51
14:Y:42:ARG:CG	14:Y:42:ARG:NH1	2.73	0.51
3:c:5204:LEU:HB2	3:c:5239:TRP:HE1	1.76	0.51
25:d:5410:MGE:H8A1	12:t:5021:ILE:HD11	1.93	0.51
5:e:5035:TRP:CE3	6:f:5039:ALA:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG13	1:A:144:CYS:N	2.26	0.51
2:B:475:PHE:HE1	4:D:134:ARG:HB2	1.76	0.51
4:D:175:VAL:O	4:D:178:ILE:HG22	2.11	0.51
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.91	0.51
1:a:5042:LEU:HD22	20:a:5408:BCR:H11C	1.93	0.51
2:b:5368:VAL:HG11	2:b:5381:ILE:HD12	1.92	0.51
4:D:164:GLN:HB3	4:D:169:PHE:HD2	1.76	0.50
7:H:55:LEU:O	7:H:58:VAL:HG22	2.10	0.50
8:I:21:PHE:HA	8:I:24:LEU:HB2	1.93	0.50
4:d:5175:VAL:O	4:d:5178:ILE:HG22	2.11	0.50
22:m:5102:LMT:H1'	12:t:5001:MET:HB2	1.92	0.50
7:h:5055:LEU:O	7:h:5058:VAL:HG22	2.10	0.50
23:l:5102:SQD:H141	25:m:5103:MGE:H7B1	1.93	0.50
15:N:75:TYR:HB3	15:N:87:PHE:CE1	2.45	0.50
2:B:281:GLN:HE22	2:B:358:ARG:HD3	1.74	0.50
3:C:243:ILE:HG22	17:C:506:CLA:HMC3	1.93	0.50
2:b:5377:VAL:HG11	4:d:5342:PRO:HG3	1.92	0.50
1:A:163:ILE:HD11	26:A:413:DGD:HB31	1.93	0.50
1:A:207:GLY:HA3	1:A:278:TRP:NE1	2.27	0.50
1:A:219:VAL:HG13	1:A:246:TYR:CG	2.46	0.50
2:B:172:TYR:HB3	2:B:174:LEU:HD13	1.93	0.50
4:D:61:HIS:CE1	4:D:79:SER:HB3	2.47	0.50
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.93	0.50
6:F:18:VAL:HG13	6:F:19:ARG:H	1.76	0.50
2:b:5397:VAL:HG11	2:b:5417:VAL:HG11	1.92	0.50
20:c:5514:BCR:H341	20:c:5514:BCR:H352	1.93	0.50
1:A:293:MET:HE1	1:A:299:GLY:N	2.26	0.50
1:a:5219:VAL:HG13	1:a:5246:TYR:CG	2.46	0.50
14:Y:34:MET:HE3	14:Y:34:MET:HA	1.93	0.50
2:B:215:PHE:HD2	2:B:216:HIS:CD2	2.29	0.50
3:C:264:PHE:HE1	20:C:516:BCR:H313	1.75	0.50
1:A:73:TYR:HE1	22:A:409:LMT:H5'	1.77	0.50
1:A:74:GLY:HA3	11:M:1:MET:SD	2.51	0.50
6:F:19:ARG:NH1	29:F:101:HEM:O1D	2.40	0.50
9:K:18:PHE:O	9:K:22:VAL:HG12	2.12	0.50
1:a:5233:ALA:O	4:d:5265:ARG:NH1	2.44	0.50
2:b:5246:PHE:CE1	2:b:5463:PHE:HB2	2.47	0.50
2:b:5475:PHE:HD2	4:d:5140:PRO:HG3	1.76	0.50
4:d:5061:HIS:CE1	4:d:5079:SER:HB3	2.47	0.50
12:t:5004:ILE:HD11	20:t:5102:BCR:H272	1.93	0.50
15:N:113:LEU:O	15:N:117:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:NE2	24:A:411:BCT:C	2.74	0.50
4:d:5085:MET:HE1	4:d:5096:GLU:HG2	1.93	0.50
4:d:5095:PRO:HG2	4:d:5096:GLU:CD	2.37	0.50
8:i:5021:PHE:HA	8:i:5024:LEU:HB2	1.93	0.50
23:l:5102:SQD:H121	23:l:5102:SQD:H242	1.94	0.50
1:A:283:VAL:HG21	18:A:404:PHO:HAC2	1.94	0.50
17:A:402:CLA:H91	17:A:402:CLA:H3A	1.93	0.50
3:C:438:LEU:HD11	17:C:505:CLA:HBB1	1.94	0.50
4:D:95:PRO:HG2	4:D:96:GLU:CD	2.37	0.50
2:b:5233:ASN:HD21	2:b:5476:ARG:HG2	1.77	0.50
3:c:5176:VAL:HG11	3:c:5238:ILE:HD11	1.93	0.50
3:c:5243:ILE:HG22	17:c:5506:CLA:HMC3	1.93	0.50
3:c:5372:PRO:HB3	15:n:85:SER:CA	2.42	0.50
1:A:63:ILE:CG2	3:C:337:LEU:HB3	2.42	0.49
1:A:130:GLN:NE2	18:A:404:PHO:O1D	2.45	0.49
17:A:401:CLA:H8	17:A:402:CLA:HBB1	1.94	0.49
2:B:52:LEU:O	2:B:54:PRO:HD3	2.12	0.49
2:B:348:ASN:O	2:B:349:LYS:HG2	2.12	0.49
17:B:608:CLA:CBB	4:D:123:ILE:HG12	2.42	0.49
1:a:5331:MET:CG	4:d:5324:GLY:HA3	2.40	0.49
2:b:5223:GLN:N	7:h:5022:ALA:O	2.45	0.49
3:c:5204:LEU:HA	3:c:5209:ILE:HD11	1.93	0.49
4:d:5203:GLY:HA3	4:d:5278:GLY:HA3	1.94	0.49
23:L:101:SQD:H162	23:L:101:SQD:H261	1.93	0.49
12:T:25:GLU:H	12:T:25:GLU:CD	2.17	0.49
1:a:5283:VAL:HG21	18:a:5405:PHO:HAC2	1.94	0.49
3:c:5175:LEU:HD12	17:c:5501:CLA:C2D	2.42	0.49
3:c:5190:ALA:H	3:c:5194:GLY:HA2	1.76	0.49
4:d:5164:GLN:HB3	4:d:5169:PHE:HD2	1.76	0.49
5:e:5069:ARG:O	5:e:5071:GLU:HG2	2.12	0.49
16:x:7:LEU:C	16:x:7:LEU:CD1	2.86	0.49
17:A:401:CLA:NB	17:D:404:CLA:HBB1	2.27	0.49
2:B:233:ASN:HD21	2:B:476:ARG:HG2	1.77	0.49
2:b:5174:LEU:HD11	2:b:5309:LEU:HB2	1.94	0.49
3:c:5189:TRP:NE1	3:c:5364:PRO:HA	2.26	0.49
3:c:5438:LEU:HD11	17:c:5505:CLA:HBB1	1.94	0.49
17:B:602:CLA:H101	17:B:609:CLA:H203	1.95	0.49
3:C:237:HIS:O	3:C:241:GLY:N	2.39	0.49
17:a:5402:CLA:H8	17:a:5403:CLA:HBB1	1.94	0.49
2:b:5172:TYR:HB3	2:b:5174:LEU:HD13	1.93	0.49
4:d:5048:TRP:CG	18:d:5402:PHO:H13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:GLU:O	2:B:485:GLU:HG3	2.11	0.49
20:C:516:BCR:H341	20:C:516:BCR:H352	1.93	0.49
4:D:157:PHE:HE1	4:D:171:PRO:HB2	1.76	0.49
5:E:69:ARG:O	5:E:71:GLU:HG2	2.12	0.49
2:b:5215:PHE:HD2	2:b:5216:HIS:CD2	2.29	0.49
25:d:5410:MGE:O2D	25:d:5410:MGE:O4D	2.28	0.49
1:A:187:GLN:HG3	1:A:325:ASN:ND2	2.28	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.94	0.49
3:C:176:VAL:HG11	3:C:238:ILE:HD11	1.93	0.49
3:C:189:TRP:HD1	15:N:76:ARG:NH2	2.10	0.49
4:D:14:TRP:CZ2	16:X:29:ILE:HD11	2.47	0.49
1:a:5130:GLN:NE2	18:a:5405:PHO:O1D	2.45	0.49
2:b:5158:LEU:HB3	2:b:5199:VAL:HG22	1.94	0.49
17:b:5602:CLA:H101	17:b:5609:CLA:H203	1.95	0.49
14:y:35:ILE:HA	14:y:38:LEU:HD13	1.91	0.49
2:B:76:SER:HB2	2:B:78:TRP:CD1	2.48	0.49
2:B:125:ASP:HB2	2:B:126:PRO:HD2	1.95	0.49
17:B:615:CLA:O1A	17:B:615:CLA:H2A	2.13	0.49
3:C:175:LEU:HD12	17:C:501:CLA:C2D	2.42	0.49
3:C:459:ILE:N	4:D:222:LEU:O	2.46	0.49
2:b:5052:LEU:O	2:b:5054:PRO:HD3	2.12	0.49
2:b:5270:PRO:HG3	2:b:5317:ASN:HD21	1.78	0.49
4:d:5157:PHE:HE1	4:d:5171:PRO:HB2	1.76	0.49
9:k:5018:PHE:O	9:k:5022:VAL:HG12	2.12	0.49
15:n:100:HIS:HE1	15:n:104:TYR:CE2	2.31	0.49
15:N:117:LEU:O	15:N:118:GLU:C	2.55	0.49
17:C:511:CLA:H41	14:Y:39:LEU:HD12	1.94	0.49
4:D:71:CYS:O	25:D:408:MGE:H3D	2.13	0.49
1:a:5077:ILE:HD11	12:t:5006:TYR:CD1	2.48	0.49
2:b:5076:SER:HB2	2:b:5078:TRP:CD1	2.48	0.49
4:d:5069:GLU:O	6:f:5040:MET:HE1	2.12	0.49
16:X:3:ILE:HD12	16:X:7:LEU:HD11	1.94	0.49
3:C:204:LEU:HB2	3:C:239:TRP:HE1	1.76	0.49
1:a:5088:ALA:HA	3:c:5356:MET:HE2	1.94	0.49
1:a:5174:LEU:O	1:a:5174:LEU:HD12	2.13	0.49
1:a:5207:GLY:HA3	1:a:5278:TRP:NE1	2.27	0.49
2:b:5468:TRP:CE3	4:d:5144:ILE:HD13	2.47	0.49
4:d:5027:PHE:CD2	4:d:5028:VAL:HG13	2.48	0.49
17:k:5501:CLA:H42	14:y:46:LEU:CD2	2.41	0.49
1:A:174:LEU:HD12	1:A:174:LEU:O	2.13	0.49
2:B:172:TYR:HE1	2:B:283:GLU:CD	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:101:SQD:H162	23:L:101:SQD:H242	1.94	0.49
1:a:5252:HIS:CE1	1:a:5264:SER:HB3	2.48	0.49
15:N:100:HIS:HE1	15:N:104:TYR:CE2	2.31	0.49
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.47	0.48
2:B:281:GLN:HE22	2:B:358:ARG:CD	2.26	0.48
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.48	0.48
21:a:5409:LHG:O3	21:a:5409:LHG:O1	2.19	0.48
2:b:5125:ASP:HB2	2:b:5126:PRO:HD2	1.95	0.48
4:d:5075:THR:HA	4:d:5176:ALA:HB3	1.95	0.48
4:d:5107:LEU:HD21	5:e:5072:ALA:CB	2.42	0.48
4:d:5269:PHE:HZ	25:d:5409:MGE:H3G2	1.78	0.48
7:h:5044:ILE:CD1	16:x:10:PHE:CE1	2.89	0.48
1:A:252:HIS:CE1	1:A:264:SER:HB3	2.48	0.48
1:A:267:ASN:ND2	4:D:235:PHE:HB3	2.27	0.48
2:B:457:VAL:HG13	4:D:284:ILE:HD12	1.94	0.48
3:C:459:ILE:HG22	4:D:222:LEU:C	2.38	0.48
2:b:5074:SER:OG	2:b:5094:GLU:OE1	2.26	0.48
26:b:5621:DGD:O2D	4:d:5087:HIS:CD2	2.65	0.48
3:c:5223:TRP:CE3	3:c:5224:ILE:HG12	2.48	0.48
3:c:5337:LEU:HB2	3:c:5342:MET:SD	2.54	0.48
20:c:5513:BCR:H272	17:k:5501:CLA:H61	1.95	0.48
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.28	0.48
2:B:174:LEU:HD11	2:B:309:LEU:HB2	1.94	0.48
3:C:190:ALA:H	3:C:194:GLY:HA2	1.78	0.48
4:D:75:THR:HA	4:D:176:ALA:HB3	1.95	0.48
5:E:28:PRO:O	5:E:32:ILE:HG12	2.14	0.48
3:c:5212:TYR:HH	3:c:5227:VAL:H	1.50	0.48
2:B:47:PRO:O	2:B:50:PRO:HD3	2.13	0.48
2:B:74:SER:OG	2:B:94:GLU:OE1	2.26	0.48
17:C:502:CLA:H12	17:C:503:CLA:C3	2.44	0.48
4:D:27:PHE:CD2	4:D:28:VAL:HG13	2.48	0.48
1:a:5187:GLN:HG3	1:a:5325:ASN:ND2	2.28	0.48
1:a:5315:ASN:ND2	4:d:5332:GLN:OE1	2.47	0.48
3:c:5237:HIS:O	3:c:5241:GLY:N	2.39	0.48
5:e:5072:ALA:HA	5:e:5075:GLN:HB3	1.95	0.48
15:n:58:LYS:NZ	15:n:106:ASN:OD1	2.29	0.48
1:A:97:TRP:CD1	8:I:5:LYS:HD2	2.48	0.48
17:B:608:CLA:H102	17:B:609:CLA:H142	1.95	0.48
3:C:275:SER:OG	17:C:509:CLA:O2D	2.26	0.48
20:D:407:BCR:H11C	6:F:29:PRO:HB3	1.95	0.48
1:a:5278:TRP:HB3	1:a:5279:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:5612:CLA:H71	17:b:5612:CLA:H162	1.95	0.48
3:c:5062:PHE:CZ	9:k:5028:ILE:HD11	2.48	0.48
3:c:5371:GLY:HA3	3:c:5376:ASP:CG	2.38	0.48
26:c:5515:DGD:HB71	25:c:5517:MGE:H7A1	1.95	0.48
4:d:5061:HIS:CD2	4:d:5168:PHE:HE1	2.31	0.48
10:l:5028:ALA:O	10:l:5032:SER:N	2.40	0.48
17:A:401:CLA:HBD	17:A:402:CLA:HAC2	1.96	0.48
2:B:77:GLY:C	2:B:86:ILE:CD1	2.87	0.48
17:B:601:CLA:H2A	17:B:601:CLA:O2D	2.13	0.48
17:B:602:CLA:H2A	17:B:602:CLA:O2D	2.14	0.48
3:C:40:ALA:HB2	17:C:508:CLA:H2A	1.96	0.48
3:C:337:LEU:HB2	3:C:342:MET:SD	2.54	0.48
3:C:371:GLY:HA3	3:C:376:ASP:CG	2.38	0.48
3:C:403:SER:OG	3:C:407:VAL:N	2.25	0.48
4:D:203:GLY:HA3	4:D:278:GLY:HA3	1.94	0.48
17:D:405:CLA:O2D	17:D:405:CLA:H2A	2.14	0.48
2:b:5008:VAL:HG23	2:b:5009:HIS:CD2	2.49	0.48
2:b:5281:GLN:HE22	2:b:5358:ARG:CD	2.26	0.48
2:b:5475:PHE:CD2	4:d:5140:PRO:HG3	2.49	0.48
17:b:5601:CLA:H2A	17:b:5601:CLA:O2D	2.13	0.48
1:A:37:MET:SD	1:A:129:ARG:NE	2.82	0.48
1:A:296:ASN:HB3	3:C:401:LEU:HD23	1.95	0.48
17:B:612:CLA:H71	17:B:612:CLA:H162	1.95	0.48
2:b:5047:PRO:O	2:b:5050:PRO:HD3	2.13	0.48
3:c:5040:ALA:HB2	17:c:5508:CLA:H2A	1.96	0.48
20:d:5406:BCR:H372	25:d:5408:MGE:H2A2	1.95	0.48
2:B:270:PRO:HG3	2:B:317:ASN:HD21	1.78	0.48
6:F:34:LEU:HD23	6:F:37:ILE:HD12	1.96	0.48
1:a:5050:ILE:HG21	20:a:5408:BCR:H393	1.96	0.48
1:a:5160:ILE:O	1:a:5163:ILE:N	2.46	0.48
1:a:5212:CYS:HB2	4:d:5211:CYS:HB2	1.96	0.48
1:a:5289:GLY:O	1:a:5293:MET:HG2	2.13	0.48
2:b:5172:TYR:HE1	2:b:5283:GLU:CD	2.21	0.48
2:b:5348:ASN:O	2:b:5349:LYS:HG2	2.12	0.48
17:b:5608:CLA:H102	17:b:5609:CLA:H142	1.95	0.48
17:b:5615:CLA:H2A	17:b:5615:CLA:O1A	2.13	0.48
3:c:5413:GLU:OE2	3:c:5416:SER:OG	2.31	0.48
13:z:5043:GLY:O	13:z:5047:TRP:N	2.47	0.48
14:Y:38:LEU:O	14:Y:42:ARG:CG	2.55	0.48
4:D:60:THR:HG23	4:D:61:HIS:N	2.28	0.48
17:a:5403:CLA:H152	17:a:5403:CLA:H111	1.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:5503:CLA:H13	17:c:5503:CLA:H101	1.47	0.48
6:f:5034:LEU:HD23	6:f:5037:ILE:HD12	1.96	0.48
13:z:5028:ALA:O	14:y:44:GLY:HA3	2.14	0.48
15:N:93:ALA:O	15:N:96:SER:OG	2.25	0.48
1:A:140:ARG:HD3	1:A:142:TRP:HE1	1.79	0.48
5:E:72:ALA:HA	5:E:75:GLN:HB3	1.95	0.48
9:K:20:PRO:HG3	14:Y:24:MET:HG2	1.93	0.48
23:L:101:SQD:O8	23:L:101:SQD:O3	2.19	0.48
11:M:24:ILE:HG12	11:m:5024:ILE:HG12	1.96	0.48
13:Z:43:GLY:O	13:Z:47:TRP:N	2.47	0.48
1:a:5037:MET:HE1	1:a:5129:ARG:HH21	1.79	0.48
1:a:5140:ARG:HD3	1:a:5142:TRP:HE1	1.79	0.48
1:a:5187:GLN:NE2	1:a:5191:ASN:HA	2.28	0.48
5:e:5028:PRO:O	5:e:5032:ILE:HG12	2.14	0.48
1:a:5063:ILE:HD12	3:c:5335:THR:HB	1.96	0.47
1:a:5138:GLY:HA2	3:c:5455:PHE:CE1	2.49	0.47
17:a:5402:CLA:HBD	17:a:5403:CLA:HAC2	1.96	0.47
17:b:5611:CLA:CBB	17:b:5613:CLA:HHB	2.44	0.47
3:c:5134:ILE:HG21	13:z:5027:TYR:HB3	1.96	0.47
17:c:5510:CLA:H122	17:c:5510:CLA:H162	1.72	0.47
4:d:5085:MET:HE2	4:d:5107:LEU:HD23	1.97	0.47
4:d:5157:PHE:CE1	4:d:5171:PRO:HB2	2.49	0.47
4:d:5263:ASN:N	25:d:5410:MGE:O3D	2.47	0.47
17:d:5404:CLA:H2A	17:d:5404:CLA:O2D	2.14	0.47
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.96	0.47
2:B:233:ASN:O	2:B:236:THR:HG22	2.14	0.47
4:D:214:HIS:O	4:D:218:VAL:HG12	2.14	0.47
13:Z:28:ALA:HB1	14:Y:39:LEU:HD13	1.95	0.47
17:a:5403:CLA:H52	19:d:5405:PQ9:H242	1.95	0.47
2:b:5326:ARG:HH22	4:d:5297:ASP:N	2.12	0.47
17:c:5502:CLA:H12	17:c:5503:CLA:C3	2.43	0.47
18:d:5402:PHO:H143	18:d:5402:PHO:H111	1.65	0.47
17:B:611:CLA:CBB	17:B:613:CLA:HHB	2.44	0.47
3:C:229:ASN:HD22	15:N:77:ARG:CB	2.28	0.47
3:C:274:TYR:HD1	17:C:505:CLA:HMD2	1.80	0.47
3:C:413:GLU:OE2	3:C:416:SER:OG	2.31	0.47
9:K:31:LEU:HB3	20:Y:101:BCR:C13	2.44	0.47
1:a:5319:ASP:O	1:a:5323:ARG:N	2.46	0.47
1:a:5323:ARG:O	1:a:5327:GLY:N	2.43	0.47
16:x:21:LEU:C	16:x:21:LEU:CD2	2.86	0.47
1:A:143:ILE:HG23	4:D:220:ASN:ND2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:C:511:CLA:H61	20:C:514:BCR:H272	1.95	0.47
4:D:85:MET:HE2	4:D:107:LEU:HD23	1.97	0.47
1:a:5084:PRO:HD3	1:a:5173:PRO:HB3	1.97	0.47
2:b:5409:GLN:HG3	2:b:5411:PHE:CE1	2.50	0.47
17:b:5602:CLA:H172	26:b:5621:DGD:HA82	1.96	0.47
17:b:5602:CLA:O2D	17:b:5602:CLA:H2A	2.14	0.47
4:d:5159:ILE:HG21	4:d:5287:VAL:HG22	1.97	0.47
4:d:5193:LEU:O	10:l:5034:TYR:OH	2.31	0.47
9:k:5020:PRO:HB3	14:y:21:GLN:O	2.15	0.47
11:m:5030:GLU:O	25:m:5103:MGE:O3D	2.32	0.47
14:y:38:LEU:CD1	14:y:38:LEU:H	2.06	0.47
4:D:157:PHE:CE1	4:D:171:PRO:HB2	2.49	0.47
4:D:261:PHE:HD2	4:D:267:LEU:HG	1.79	0.47
1:a:5165:GLN:O	3:c:5357:ARG:NH1	2.44	0.47
4:d:5297:ASP:HB3	4:d:5302:GLU:CG	2.40	0.47
16:x:36:LYS:HG2	16:x:36:LYS:O	2.14	0.47
1:A:37:MET:HE1	1:A:129:ARG:HH21	1.79	0.47
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.49	0.47
2:b:5215:PHE:HD2	2:b:5216:HIS:HD2	1.62	0.47
2:b:5233:ASN:O	2:b:5236:THR:HG22	2.15	0.47
17:b:5607:CLA:H61	17:b:5607:CLA:H41	1.52	0.47
4:d:5067:TYR:OH	25:d:5408:MGE:H3G1	2.15	0.47
9:k:5040:GLN:O	9:k:5044:GLY:N	2.38	0.47
15:N:58:LYS:NZ	15:N:106:ASN:OD1	2.29	0.47
1:A:79:THR:HG22	4:D:315:TYR:HB2	1.96	0.47
1:A:187:GLN:HE21	1:A:325:ASN:ND2	2.13	0.47
1:A:289:GLY:O	1:A:293:MET:HG2	2.13	0.47
26:A:413:DGD:HA72	3:C:284:PHE:HB3	1.97	0.47
2:B:59:GLY:HA3	2:B:329:PRO:HB3	1.97	0.47
2:B:91:TRP:CH2	17:B:606:CLA:H12	2.49	0.47
2:B:414:PRO:O	2:B:418:LYS:HG2	2.14	0.47
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.49	0.47
17:B:608:CLA:HBB2	4:D:123:ILE:HG12	1.96	0.47
17:C:505:CLA:HBA1	17:C:505:CLA:CBD	2.44	0.47
5:E:23:HIS:CE1	29:F:101:HEM:ND	2.83	0.47
2:b:5457:VAL:HG13	4:d:5284:ILE:HD12	1.97	0.47
20:b:5617:BCR:H383	25:m:5101:MGE:H202	1.97	0.47
20:b:5617:BCR:HC41	11:m:5006:LEU:HD21	1.96	0.47
3:c:5080:PRO:HG2	3:c:5083:GLU:HB2	1.97	0.47
3:c:5274:TYR:HD1	17:c:5505:CLA:HMD2	1.80	0.47
17:c:5505:CLA:HBA1	17:c:5505:CLA:CBD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:5505:CLA:H52	17:c:5505:CLA:H8	1.52	0.47
4:d:5282:SER:OG	17:d:5403:CLA:O1D	2.27	0.47
25:d:5410:MGE:H262	12:t:5013:ILE:HG21	1.96	0.47
1:A:84:PRO:HD3	1:A:173:PRO:HB3	1.97	0.47
1:A:140:ARG:NH2	3:C:456:GLU:O	2.48	0.47
1:A:183:MET:HB3	17:A:401:CLA:HBC2	1.96	0.47
17:B:604:CLA:H161	17:B:616:CLA:H192	1.97	0.47
3:C:36:TRP:O	17:C:508:CLA:H12	2.15	0.47
4:D:61:HIS:CD2	4:D:168:PHE:HE1	2.31	0.47
12:T:25:GLU:N	12:T:25:GLU:CD	2.73	0.47
17:k:5501:CLA:H112	17:k:5501:CLA:H91	1.68	0.47
12:t:5025:GLU:H	12:t:5025:GLU:CD	2.17	0.47
16:X:20:VAL:O	16:X:21:LEU:C	2.58	0.47
2:B:392:PHE:CZ	2:B:418:LYS:HB3	2.50	0.47
3:C:166:ILE:HG13	3:C:248:GLY:HA3	1.95	0.47
3:C:205:ASP:OD1	3:C:208:VAL:HG22	2.15	0.47
13:Z:28:ALA:CB	14:Y:39:LEU:HD11	2.45	0.47
2:b:5125:ASP:OD1	2:b:5128:THR:OG1	2.31	0.47
2:b:5347:ARG:HD3	2:b:5351:GLY:HA2	1.97	0.47
3:c:5184:GLY:HA3	3:c:5198:VAL:HG22	1.97	0.47
3:c:5318:LEU:HD11	3:c:5328:VAL:HG21	1.97	0.47
4:d:5214:HIS:O	4:d:5218:VAL:HG12	2.14	0.47
14:Y:28:ILE:N	14:Y:28:ILE:HD12	2.29	0.47
15:N:61:GLN:NE2	15:N:101:TYR:OH	2.46	0.47
17:B:607:CLA:H41	17:B:607:CLA:H61	1.52	0.47
3:c:5166:ILE:HG13	3:c:5248:GLY:HA3	1.95	0.47
9:k:5031:LEU:HD23	20:k:5502:BCR:C14	2.45	0.47
1:A:300:PHE:CD2	3:C:404:LEU:HD12	2.50	0.46
17:C:503:CLA:H13	17:C:503:CLA:H101	1.47	0.46
14:y:25:ILE:HA	14:y:28:ILE:CD1	2.45	0.46
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.97	0.46
1:A:50:ILE:HG21	20:A:407:BCR:H393	1.96	0.46
1:A:317:TRP:CH2	4:D:77:ALA:HB3	2.49	0.46
2:B:347:ARG:HD3	2:B:351:GLY:HA2	1.97	0.46
17:B:604:CLA:HMD1	17:B:612:CLA:H193	1.97	0.46
3:C:264:PHE:HE2	17:C:506:CLA:HAA2	1.80	0.46
4:D:83:ASN:ND2	4:D:336:HIS:CE1	2.83	0.46
4:D:159:ILE:HG21	4:D:287:VAL:HG22	1.97	0.46
4:D:221:THR:O	4:D:222:LEU:HD12	2.15	0.46
4:D:282:SER:OG	17:D:404:CLA:O1D	2.26	0.46
1:a:5218:LEU:HD21	1:a:5255:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5414:PRO:O	2:b:5418:LYS:HG2	2.14	0.46
3:c:5275:SER:OG	17:c:5509:CLA:O2D	2.26	0.46
3:c:5284:PHE:HB3	26:c:5515:DGD:HA72	1.97	0.46
3:c:5461:ARG:HH11	4:d:5223:PHE:HB2	1.80	0.46
4:d:5221:THR:O	4:d:5222:LEU:HD12	2.15	0.46
15:N:109:LEU:HB2	15:N:114:LYS:CG	2.46	0.46
1:A:142:TRP:HZ3	3:C:443:TRP:O	1.98	0.46
2:B:381:ILE:HG12	2:B:392:PHE:HE1	1.80	0.46
2:B:475:PHE:O	2:B:479:PHE:N	2.44	0.46
3:C:349:ILE:HG13	3:C:374:GLY:HA3	1.97	0.46
17:C:505:CLA:H52	17:C:505:CLA:H8	1.52	0.46
17:C:505:CLA:H152	17:C:505:CLA:H18	1.68	0.46
9:K:29:PRO:HA	9:K:32:PHE:CD2	2.51	0.46
1:a:5063:ILE:HG21	3:c:5337:LEU:HD23	1.97	0.46
17:b:5604:CLA:H161	17:b:5616:CLA:H192	1.97	0.46
17:b:5609:CLA:C3B	20:h:5101:BCR:H323	2.45	0.46
3:c:5264:PHE:HE2	17:c:5506:CLA:HAA2	1.80	0.46
4:d:5083:ASN:ND2	4:d:5336:HIS:CE1	2.83	0.46
14:y:18:VAL:O	14:y:22:LEU:CA	2.63	0.46
1:A:160:ILE:O	1:A:163:ILE:N	2.46	0.46
22:A:409:LMT:H111	2:b:5094:GLU:HG2	1.97	0.46
2:B:409:GLN:HG3	2:B:411:PHE:CE1	2.50	0.46
17:B:606:CLA:H162	17:B:606:CLA:H122	1.64	0.46
3:C:362:ARG:HD2	3:C:367:GLU:OE1	2.16	0.46
1:a:5295:PHE:HD2	3:c:5428:THR:OG1	1.98	0.46
17:b:5616:CLA:O2D	17:b:5616:CLA:H2A	2.15	0.46
3:c:5036:TRP:O	17:c:5508:CLA:H12	2.15	0.46
17:c:5510:CLA:H61	17:c:5510:CLA:H2	1.63	0.46
4:d:5279:LEU:HD11	18:d:5402:PHO:HMC3	1.97	0.46
12:t:5025:GLU:N	12:t:5025:GLU:CD	2.73	0.46
14:Y:24:MET:HA	14:Y:27:MET:SD	2.56	0.46
1:A:218:LEU:HD21	1:A:255:PHE:HB2	1.96	0.46
25:A:412:MGE:H241	19:D:406:PQ9:H301	1.97	0.46
2:B:77:GLY:HA2	2:B:86:ILE:HD13	1.91	0.46
2:B:215:PHE:HD2	2:B:216:HIS:HD2	1.62	0.46
17:B:605:CLA:H41	17:B:605:CLA:H61	1.54	0.46
3:C:161:LEU:HD13	17:C:507:CLA:C1D	2.46	0.46
3:C:439:VAL:O	3:C:443:TRP:N	2.47	0.46
9:K:24:VAL:HG11	14:Y:25:ILE:HD11	1.97	0.46
12:T:16:LEU:O	12:T:20:ALA:N	2.45	0.46
1:a:5328:MET:HE2	4:d:5325:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5392:PHE:CZ	2:b:5418:LYS:HB3	2.50	0.46
17:b:5601:CLA:H2A	17:b:5601:CLA:HED3	1.98	0.46
17:b:5602:CLA:H51	7:h:5042:LEU:HD11	1.98	0.46
9:k:5029:PRO:HA	9:k:5032:PHE:CD2	2.51	0.46
9:k:5043:VAL:HG22	14:y:46:LEU:HB3	1.98	0.46
10:l:5020:GLY:HA3	11:m:5022:LEU:HD13	1.98	0.46
3:C:318:LEU:HD11	3:C:328:VAL:HG21	1.97	0.46
4:D:139:ARG:NH2	4:D:141:TYR:HH	2.14	0.46
19:D:406:PQ9:H361	19:D:406:PQ9:H341	1.64	0.46
13:Z:53:VAL:O	13:Z:57:LEU:HB2	2.16	0.46
18:a:5405:PHO:H51	18:a:5405:PHO:H8	1.72	0.46
2:b:5381:ILE:HG12	2:b:5392:PHE:HE1	1.80	0.46
3:c:5276:LEU:O	3:c:5280:SER:N	2.39	0.46
4:d:5146:PHE:O	4:d:5149:PRO:HD2	2.16	0.46
9:k:5019:ASP:HB3	14:y:21:GLN:HG2	1.95	0.46
15:n:93:ALA:O	15:n:96:SER:OG	2.25	0.46
1:A:130:GLN:HG2	4:D:256:ILE:HG21	1.98	0.46
19:A:406:PQ9:H161	19:A:406:PQ9:H141	1.62	0.46
2:B:24:LEU:HD21	17:B:616:CLA:CAB	2.46	0.46
2:B:458:PHE:HB3	17:B:604:CLA:HMC2	1.97	0.46
4:D:193:LEU:HD21	4:D:298:PHE:CZ	2.51	0.46
9:K:39:TRP:HE1	14:Y:46:LEU:HD23	1.78	0.46
10:L:36:PHE:HE1	11:M:8:LEU:HA	1.80	0.46
2:b:5063:LEU:HB3	2:b:5064:PRO:HD3	1.98	0.46
4:d:5141:TYR:OH	25:d:5409:MGE:O2D	2.34	0.46
1:A:237:TYR:CE2	4:D:263:ASN:HA	2.50	0.46
1:A:276:ALA:HB2	4:D:215:GLY:C	2.40	0.46
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.51	0.46
17:C:501:CLA:H2A	17:C:501:CLA:O1D	2.16	0.46
17:C:508:CLA:H202	17:C:508:CLA:H161	1.84	0.46
4:D:18:LEU:HD12	16:X:29:ILE:HG12	1.96	0.46
23:D:403:SQD:H342	9:K:37:PHE:CE2	2.51	0.46
17:D:404:CLA:H201	25:D:408:MGE:H8A1	1.98	0.46
11:M:21:PHE:CZ	11:M:25:LEU:HD11	2.51	0.46
1:a:5183:MET:HB3	17:a:5402:CLA:HBC2	1.96	0.46
1:a:5207:GLY:HA3	1:a:5278:TRP:HE1	1.80	0.46
2:b:5312:TYR:O	2:b:5317:ASN:ND2	2.49	0.46
2:b:5458:PHE:HB3	17:b:5604:CLA:HMC2	1.97	0.46
3:c:5205:ASP:OD1	3:c:5208:VAL:HG22	2.15	0.46
4:d:5193:LEU:HD21	4:d:5298:PHE:CZ	2.51	0.46
23:l:5102:SQD:H262	12:t:5019:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:PHE:O	2:B:396:GLY:N	2.49	0.46
3:C:86:LEU:HD21	3:C:89:ILE:HB	1.98	0.46
4:D:146:PHE:O	4:D:149:PRO:HD2	2.16	0.46
23:L:101:SQD:H45	25:m:5101:MGE:H8B1	1.98	0.46
1:a:5140:ARG:O	4:d:5220:ASN:HB3	2.16	0.46
20:b:5617:BCR:H20C	20:b:5617:BCR:H361	1.81	0.46
3:c:5157:MET:HE1	3:c:5271:TYR:CD2	2.51	0.46
3:c:5362:ARG:HD2	3:c:5367:GLU:OE1	2.16	0.46
17:c:5501:CLA:H2A	17:c:5501:CLA:O1D	2.16	0.46
4:d:5060:THR:HG23	4:d:5061:HIS:N	2.28	0.46
5:e:5051:ARG:O	5:e:5054:SER:N	2.40	0.46
9:k:5031:LEU:HD23	20:k:5502:BCR:H14C	1.98	0.46
1:A:91:LEU:HD22	26:A:413:DGD:O2D	2.15	0.46
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.98	0.46
17:B:610:CLA:H111	17:B:610:CLA:H143	1.70	0.46
2:b:5315:ILE:HG21	2:b:5426:PHE:CD1	2.51	0.46
17:b:5604:CLA:HMD1	17:b:5612:CLA:H193	1.97	0.46
17:b:5611:CLA:H141	17:b:5611:CLA:H162	1.59	0.46
3:c:5212:TYR:OH	3:c:5226:SER:HB2	2.16	0.46
3:c:5306:GLY:N	3:c:5307:PRO:HD2	2.31	0.46
17:B:616:CLA:O2D	17:B:616:CLA:H2A	2.15	0.45
4:D:61:HIS:CD2	4:D:168:PHE:CE1	3.04	0.45
23:L:101:SQD:H82	23:L:101:SQD:H62	1.98	0.45
2:b:5024:LEU:HD21	17:b:5616:CLA:CAB	2.46	0.45
2:b:5059:GLY:HA3	2:b:5329:PRO:HB3	1.97	0.45
17:b:5604:CLA:H92	17:b:5604:CLA:H62	1.75	0.45
3:c:5229:ASN:OD1	3:c:5230:LEU:N	2.49	0.45
4:d:5118:GLY:HA3	18:d:5402:PHO:H93	1.97	0.45
15:n:61:GLN:NE2	15:n:101:TYR:OH	2.46	0.45
3:C:184:GLY:HA3	3:C:198:VAL:HG22	1.97	0.45
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.99	0.45
4:D:168:PHE:HD2	4:D:169:PHE:CE1	2.34	0.45
9:K:29:PRO:HA	9:K:32:PHE:HD2	1.81	0.45
1:a:5034:GLY:HA2	1:a:5037:MET:HB3	1.97	0.45
1:a:5048:PHE:HA	1:a:5115:ILE:HD11	1.99	0.45
1:a:5246:TYR:CE2	1:a:5248:ILE:HD11	2.51	0.45
21:a:5409:LHG:HC11	17:c:5508:CLA:O1D	2.16	0.45
3:c:5349:ILE:HG13	3:c:5374:GLY:HA3	1.97	0.45
23:l:5102:SQD:H112	23:l:5102:SQD:H82	1.56	0.45
14:y:25:ILE:HD13	14:y:25:ILE:C	2.41	0.45
21:A:408:LHG:H02	21:A:408:LHG:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:HG2	3:C:83:GLU:HB2	1.97	0.45
3:C:205:ASP:H	3:C:209:ILE:HD12	1.82	0.45
3:C:274:TYR:HE1	17:C:505:CLA:OBD	1.99	0.45
17:C:511:CLA:H91	17:C:511:CLA:H112	1.68	0.45
1:a:5120:LEU:O	1:a:5123:ALA:N	2.49	0.45
1:a:5187:GLN:HE21	1:a:5325:ASN:ND2	2.13	0.45
2:b:5226:TYR:CD1	2:b:5231:MET:HB2	2.51	0.45
3:c:5086:LEU:HD21	3:c:5089:ILE:HB	1.98	0.45
3:c:5399:ALA:O	3:c:5401:LEU:HD23	2.16	0.45
15:n:75:TYR:HB3	15:n:87:PHE:HE1	1.81	0.45
15:N:75:TYR:HB3	15:N:87:PHE:HE1	1.81	0.45
15:N:84:LEU:HD22	15:N:131:GLU:HG3	1.98	0.45
2:B:312:TYR:O	2:B:317:ASN:ND2	2.49	0.45
17:B:603:CLA:H142	17:B:603:CLA:H112	1.69	0.45
3:C:49:LEU:HD11	3:C:53:HIS:HE1	1.82	0.45
3:C:229:ASN:OD1	3:C:230:LEU:N	2.49	0.45
3:C:306:GLY:N	3:C:307:PRO:HD2	2.30	0.45
8:I:31:ASN:ND2	8:I:33:LYS:O	2.50	0.45
9:K:37:PHE:O	9:K:41:ALA:N	2.50	0.45
1:a:5091:LEU:O	1:a:5091:LEU:HD23	2.16	0.45
3:c:5307:PRO:HA	3:c:5358:PHE:CD2	2.51	0.45
4:d:5261:PHE:HD2	4:d:5267:LEU:HG	1.79	0.45
25:d:5410:MGE:H2A2	25:d:5410:MGE:H5A2	1.68	0.45
11:m:5029:THR:HA	11:m:5032:GLN:HG2	1.98	0.45
13:z:5029:SER:CA	14:y:44:GLY:HA2	2.45	0.45
1:A:234:ASN:HB2	25:A:412:MGE:O3D	2.17	0.45
17:B:613:CLA:H41	17:B:613:CLA:H61	1.70	0.45
3:C:276:LEU:O	3:C:280:SER:N	2.39	0.45
10:L:28:ALA:O	10:L:32:SER:N	2.40	0.45
1:a:5060:ILE:HD12	4:d:5317:LYS:NZ	2.31	0.45
1:a:5085:SER:HB2	1:a:5089:ILE:HG21	1.99	0.45
2:b:5124:ARG:O	7:h:5012:ARG:NH2	2.46	0.45
2:b:5392:PHE:O	2:b:5396:GLY:N	2.49	0.45
3:c:5161:LEU:HD13	17:c:5507:CLA:C1D	2.46	0.45
4:d:5014:TRP:HZ2	16:x:29:ILE:HD12	1.73	0.45
9:k:5029:PRO:HA	9:k:5032:PHE:HD2	1.81	0.45
23:l:5102:SQD:H272	23:l:5102:SQD:H151	1.98	0.45
1:A:207:GLY:HA3	1:A:278:TRP:HE1	1.80	0.45
1:A:300:PHE:HD2	3:C:404:LEU:HD12	1.81	0.45
26:C:518:DGD:HBN1	25:D:408:MGE:H211	1.97	0.45
25:D:410:MGE:H5B2	25:D:410:MGE:H8B1	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5036:ILE:O	1:a:5040:THR:HG22	2.16	0.45
2:b:5140:GLY:HA3	2:b:5217:ILE:HG13	1.99	0.45
2:b:5437:LEU:HD23	2:b:5437:LEU:O	2.17	0.45
2:b:5451:PHE:HE2	17:b:5604:CLA:HMA3	1.81	0.45
3:c:5372:PRO:HG3	15:n:85:SER:OG	2.17	0.45
4:d:5061:HIS:CD2	4:d:5168:PHE:CE1	3.04	0.45
1:A:48:PHE:HA	1:A:115:ILE:HD11	1.99	0.45
1:A:120:LEU:O	1:A:123:ALA:N	2.49	0.45
1:A:219:VAL:HG11	4:D:268:HIS:ND1	2.32	0.45
19:A:406:PQ9:H191	19:A:406:PQ9:H211	1.69	0.45
21:A:408:LHG:O3	21:A:408:LHG:O1	2.19	0.45
17:B:611:CLA:H162	17:B:611:CLA:H141	1.59	0.45
3:C:212:TYR:OH	3:C:226:SER:HB2	2.16	0.45
4:D:141:TYR:OH	25:D:409:MGE:O4D	2.19	0.45
18:D:402:PHO:H143	18:D:402:PHO:H111	1.65	0.45
1:a:5290:ILE:O	1:a:5293:MET:N	2.50	0.45
2:b:5326:ARG:NH2	4:d:5297:ASP:HB2	2.31	0.45
4:d:5168:PHE:HD2	4:d:5169:PHE:CE1	2.34	0.45
17:d:5403:CLA:H202	17:d:5403:CLA:H162	1.73	0.45
11:m:5021:PHE:CZ	11:m:5025:LEU:HD11	2.51	0.45
19:A:406:PQ9:H341	19:A:406:PQ9:H361	1.67	0.45
5:E:44:TYR:O	5:E:48:GLY:N	2.50	0.45
11:M:29:THR:HA	11:M:32:GLN:HG2	1.98	0.45
13:Z:5:PHE:HZ	13:Z:54:VAL:HA	1.80	0.45
2:b:5006:TYR:OH	25:d:5409:MGE:H6D1	2.16	0.45
2:b:5326:ARG:HH21	4:d:5297:ASP:HB2	1.81	0.45
2:b:5360:PRO:HG2	4:d:5339:PHE:CZ	2.51	0.45
3:c:5049:LEU:HD11	3:c:5053:HIS:HE1	1.82	0.45
3:c:5362:ARG:HG3	15:n:82:ARG:NH1	2.30	0.45
3:c:5379:LYS:HD2	15:n:92:THR:HG21	1.99	0.45
4:d:5148:ALA:HB3	4:d:5149:PRO:HD3	1.98	0.45
1:A:36:ILE:O	1:A:40:THR:HG22	2.16	0.45
4:D:24:ARG:HG2	4:D:25:ASP:H	1.81	0.45
2:b:5326:ARG:HB3	2:b:5444:ARG:HG2	1.99	0.45
17:b:5605:CLA:H61	17:b:5605:CLA:H41	1.54	0.45
17:c:5502:CLA:H12	17:c:5503:CLA:C2	2.47	0.45
4:d:5334:GLN:HB3	4:d:5336:HIS:CE1	2.52	0.45
17:d:5403:CLA:H201	25:d:5408:MGE:H8A2	1.98	0.45
5:e:5044:TYR:O	5:e:5048:GLY:N	2.50	0.45
1:A:91:LEU:HD23	1:A:91:LEU:O	2.16	0.45
2:B:469:HIS:O	2:B:472:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:609:CLA:H92	17:B:609:CLA:H62	1.77	0.45
3:C:308:GLU:HB2	3:C:361:PHE:CZ	2.52	0.45
4:D:141:TYR:OH	25:D:409:MGE:O2D	2.28	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.45
4:D:157:PHE:CE1	4:D:173:PHE:HE1	2.35	0.45
4:D:334:GLN:HB3	4:D:336:HIS:CE1	2.52	0.45
25:D:409:MGE:H2A1	25:D:409:MGE:H252	1.99	0.45
9:K:40:GLN:O	9:K:44:GLY:N	2.38	0.45
2:b:5122:LEU:HD22	2:b:5123:PHE:CE1	2.52	0.45
2:b:5185:TRP:HB3	2:b:5200:ALA:HB1	1.98	0.45
3:c:5283:GLY:HA3	3:c:5434:ALA:HB2	1.98	0.45
9:k:5037:PHE:O	9:k:5041:ALA:N	2.50	0.45
13:z:5028:ALA:C	14:y:44:GLY:CA	2.90	0.45
15:n:84:LEU:HD22	15:n:131:GLU:HG3	1.98	0.45
16:X:20:VAL:HG12	16:X:21:LEU:N	2.32	0.45
1:A:92:HIS:ND1	3:C:219:GLY:O	2.51	0.44
17:B:607:CLA:H122	25:B:619:MGE:H132	1.99	0.44
17:B:612:CLA:HBA1	17:B:612:CLA:H3A	1.54	0.44
17:B:615:CLA:H13	17:B:615:CLA:H172	1.73	0.44
3:C:276:LEU:HA	3:C:276:LEU:HD23	1.75	0.44
20:D:407:BCR:H371	20:D:407:BCR:H24C	1.75	0.44
2:b:5056:TRP:HB3	2:b:5267:LEU:O	2.17	0.44
3:c:5081:MET:HE3	3:c:5105:VAL:HG21	1.99	0.44
3:c:5229:ASN:OD1	3:c:5231:GLU:N	2.43	0.44
3:c:5308:GLU:HB2	3:c:5361:PHE:CZ	2.52	0.44
4:d:5297:ASP:OD1	4:d:5315:TYR:OH	2.33	0.44
9:k:5028:ILE:CG1	9:k:5029:PRO:HD3	2.48	0.44
11:m:5028:GLN:NE2	25:m:5101:MGE:H3G2	2.33	0.44
14:Y:18:VAL:HG13	14:Y:21:GLN:HE21	1.82	0.44
14:Y:32:GLY:O	14:Y:35:ILE:CD1	2.64	0.44
1:A:119:PHE:O	1:A:123:ALA:N	2.45	0.44
2:B:451:PHE:HE2	17:B:604:CLA:HMA3	1.81	0.44
4:D:93:TRP:CD1	4:D:94:GLY:N	2.81	0.44
2:b:5263:THR:HB	2:b:5268:PHE:HD2	1.82	0.44
17:b:5610:CLA:H8	17:b:5610:CLA:H51	1.66	0.44
4:d:5176:ALA:HA	4:d:5179:PHE:CD2	2.45	0.44
20:t:5101:BCR:H20C	20:t:5101:BCR:H361	1.80	0.44
13:z:5053:VAL:O	13:z:5057:LEU:HB2	2.16	0.44
1:A:85:SER:HB2	1:A:89:ILE:HG21	1.99	0.44
3:C:142:GLU:OE1	3:C:142:GLU:N	2.51	0.44
17:C:508:CLA:C4A	17:C:508:CLA:HBA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:346:LEU:O	4:D:348:ARG:N	2.48	0.44
1:a:5037:MET:SD	1:a:5129:ARG:NE	2.82	0.44
17:b:5603:CLA:C3D	17:b:5605:CLA:H43	2.48	0.44
17:b:5604:CLA:H62	17:b:5604:CLA:H41	1.59	0.44
3:c:5098:GLY:O	3:c:5106:VAL:N	2.49	0.44
3:c:5274:TYR:HE1	17:c:5505:CLA:OBD	1.99	0.44
20:h:5101:BCR:H371	20:h:5101:BCR:H24C	1.75	0.44
8:i:5015:PHE:O	8:i:5019:PHE:N	2.50	0.44
9:k:5020:PRO:HB3	14:y:24:MET:HB3	1.98	0.44
9:k:5028:ILE:HG13	9:k:5029:PRO:HD3	2.00	0.44
15:n:72:PHE:HB2	15:n:94:LEU:HD13	1.99	0.44
2:B:56:TRP:HB3	2:B:267:LEU:O	2.17	0.44
2:B:315:ILE:HG21	2:B:426:PHE:CD1	2.51	0.44
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.26	0.44
2:B:437:LEU:HD23	2:B:437:LEU:O	2.17	0.44
3:C:92:ILE:HD12	3:C:114:VAL:HG11	1.99	0.44
3:C:189:TRP:HH2	3:C:367:GLU:HB3	1.81	0.44
20:T:102:BCR:H24C	20:b:5617:BCR:H341	2.00	0.44
20:a:5408:BCR:H312	8:i:5015:PHE:CE1	2.53	0.44
3:c:5234:VAL:O	3:c:5238:ILE:HG12	2.17	0.44
3:c:5317:PHE:HD1	3:c:5320:ARG:HE	1.65	0.44
17:d:5403:CLA:H62	17:d:5403:CLA:H93	1.64	0.44
16:X:3:ILE:CG2	16:X:7:LEU:CD1	2.86	0.44
1:A:166:GLY:HA3	3:C:358:PHE:CE1	2.47	0.44
1:A:323:ARG:O	1:A:327:GLY:N	2.43	0.44
2:B:13:ILE:HG23	2:B:14:ASN:N	2.32	0.44
2:B:118:TRP:CD1	2:B:118:TRP:H	2.35	0.44
2:B:140:GLY:HA3	2:B:217:ILE:HG13	1.99	0.44
2:B:164:PRO:HG3	17:B:606:CLA:O1D	2.18	0.44
2:B:185:TRP:HB3	2:B:200:ALA:HB1	1.98	0.44
2:B:326:ARG:HB3	2:B:444:ARG:HG2	1.99	0.44
3:C:264:PHE:O	3:C:274:TYR:OH	2.33	0.44
3:C:307:PRO:HA	3:C:358:PHE:CD2	2.51	0.44
4:D:201:VAL:HG22	17:D:404:CLA:C2B	2.48	0.44
4:D:262:SER:H	25:D:410:MGE:C2D	2.30	0.44
9:K:28:ILE:HG13	9:K:29:PRO:HD3	2.00	0.44
1:a:5317:TRP:CZ3	4:d:5177:ALA:HB2	2.52	0.44
2:b:5164:PRO:HG3	17:b:5606:CLA:O1D	2.18	0.44
2:b:5390:TYR:HA	2:b:5395:GLN:OE1	2.18	0.44
17:b:5608:CLA:H202	17:b:5608:CLA:H162	1.78	0.44
17:b:5611:CLA:HBB1	17:b:5613:CLA:H3A	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5205:ASP:H	3:c:5209:ILE:HD12	1.82	0.44
4:d:5087:HIS:CD2	4:d:5166:SER:HA	2.52	0.44
4:d:5157:PHE:CE1	4:d:5173:PHE:HE1	2.35	0.44
4:d:5279:LEU:CD1	18:d:5402:PHO:HAC2	2.48	0.44
16:x:14:LEU:C	16:x:14:LEU:HD23	2.42	0.44
17:A:401:CLA:H122	18:A:404:PHO:HBA2	2.00	0.44
26:A:413:DGD:HA81	26:A:413:DGD:HAE1	1.83	0.44
17:B:601:CLA:H2A	17:B:601:CLA:HED3	1.98	0.44
17:B:613:CLA:H101	17:B:613:CLA:H62	1.68	0.44
17:B:613:CLA:H111	17:B:613:CLA:H142	1.76	0.44
3:C:234:VAL:O	3:C:238:ILE:HG12	2.17	0.44
3:C:408:GLY:CA	3:C:418:ASN:HA	2.47	0.44
18:D:402:PHO:HBA1	18:D:402:PHO:H3A	1.71	0.44
9:K:28:ILE:CG1	9:K:29:PRO:HD3	2.47	0.44
18:a:5405:PHO:H41	18:a:5405:PHO:H61	1.74	0.44
17:b:5614:CLA:HBA1	25:m:5101:MGE:H7B2	2.00	0.44
17:c:5508:CLA:C4A	17:c:5508:CLA:HBA2	2.47	0.44
4:d:5168:PHE:HD2	4:d:5169:PHE:CD1	2.36	0.44
4:d:5201:VAL:HG22	17:d:5403:CLA:C2B	2.48	0.44
20:d:5406:BCR:H15C	20:d:5406:BCR:H351	1.90	0.44
1:A:246:TYR:CE2	1:A:248:ILE:HD11	2.51	0.44
17:A:402:CLA:H18	12:T:10:PHE:HZ	1.82	0.44
17:B:603:CLA:C3D	17:B:605:CLA:H43	2.48	0.44
3:C:157:MET:HE1	3:C:271:TYR:CD2	2.51	0.44
17:b:5607:CLA:H122	25:b:5620:MGE:H132	1.99	0.44
17:b:5615:CLA:H13	17:b:5615:CLA:H172	1.73	0.44
25:d:5410:MGE:H222	25:l:5101:MGE:H262	2.00	0.44
14:Y:42:ARG:HG2	14:Y:42:ARG:NH1	2.20	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.44
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.53	0.44
2:B:122:LEU:HD22	2:B:123:PHE:CE1	2.52	0.44
2:B:141:ILE:HA	2:B:217:ILE:HD11	2.00	0.44
3:C:160:ILE:HD13	17:C:512:CLA:HAC2	2.00	0.44
17:C:508:CLA:H111	17:C:508:CLA:H91	1.73	0.44
4:D:235:PHE:CE2	4:D:237:PRO:HB3	2.53	0.44
4:D:297:ASP:OD1	4:D:315:TYR:OH	2.33	0.44
23:L:101:SQD:H271	12:T:19:PHE:CZ	2.52	0.44
13:Z:28:ALA:CB	14:Y:39:LEU:HD21	2.48	0.44
1:a:5161:TYR:CE1	1:a:5186:PHE:HE1	2.36	0.44
1:a:5193:LEU:HD22	4:d:5179:PHE:CE1	2.52	0.44
1:a:5312:ASN:HB3	5:e:5056:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5018:ARG:HD2	2:b:5115:TRP:CE3	2.53	0.44
17:b:5608:CLA:CGA	17:b:5608:CLA:C1A	2.96	0.44
17:b:5614:CLA:H71	20:b:5617:BCR:H362	1.99	0.44
3:c:5408:GLY:CA	3:c:5418:ASN:HA	2.47	0.44
26:c:5515:DGD:HAE1	26:c:5515:DGD:HA81	1.83	0.44
15:n:27:THR:HG22	15:n:67:LYS:HB3	2.00	0.44
15:N:27:THR:HG22	15:N:67:LYS:HB3	2.00	0.44
1:A:290:ILE:O	1:A:293:MET:N	2.50	0.44
1:A:303:ASN:HD21	3:C:414:ILE:HG13	1.79	0.44
2:B:226:TYR:CE1	2:B:231:MET:HB2	2.53	0.44
3:C:27:ASP:O	3:C:41:ARG:NH1	2.51	0.44
3:C:79:LYS:HE2	3:C:83:GLU:HG2	1.99	0.44
4:D:39:PRO:O	4:D:43:LEU:HD13	2.18	0.44
4:D:87:HIS:CD2	4:D:166:SER:HA	2.52	0.44
8:I:15:PHE:O	8:I:19:PHE:N	2.50	0.44
2:b:5192:PRO:HG3	7:h:5049:TYR:CE1	2.52	0.44
17:b:5603:CLA:O1D	17:b:5603:CLA:H2A	2.18	0.44
17:b:5608:CLA:CBB	4:d:5123:ILE:HG12	2.48	0.44
3:c:5175:LEU:HD11	17:c:5501:CLA:HED2	2.00	0.44
17:c:5507:CLA:H91	17:c:5507:CLA:H112	1.68	0.44
4:d:5174:GLY:N	18:d:5402:PHO:H203	2.33	0.44
8:i:5031:ASN:ND2	8:i:5033:LYS:O	2.50	0.44
13:z:5002:THR:O	13:z:5006:GLN:N	2.42	0.44
25:A:412:MGE:H121	17:B:613:CLA:H18	1.99	0.43
3:C:71:GLU:CD	3:C:86:LEU:HD12	2.43	0.43
4:D:59:TYR:O	5:E:66:VAL:HG12	2.18	0.43
6:F:18:VAL:HG13	6:F:19:ARG:N	2.33	0.43
17:a:5404:CLA:H62	17:a:5404:CLA:H101	1.81	0.43
2:b:5469:HIS:O	2:b:5472:ARG:N	2.50	0.43
17:b:5613:CLA:H142	17:b:5613:CLA:H111	1.76	0.43
25:b:5620:MGE:O2D	25:b:5620:MGE:O4D	2.36	0.43
3:c:5106:VAL:HG23	3:c:5107:ASP:N	2.33	0.43
3:c:5142:GLU:N	3:c:5142:GLU:OE1	2.50	0.43
3:c:5409:GLY:N	3:c:5417:VAL:O	2.50	0.43
18:A:404:PHO:HBA2	18:A:404:PHO:H3A	1.39	0.43
2:B:390:TYR:HA	2:B:395:GLN:OE1	2.18	0.43
17:B:611:CLA:HBB1	17:B:613:CLA:H3A	2.00	0.43
17:C:502:CLA:H12	17:C:503:CLA:C2	2.48	0.43
17:C:505:CLA:H102	17:C:505:CLA:H13	1.85	0.43
4:D:168:PHE:HD2	4:D:169:PHE:CD1	2.36	0.43
7:H:38:PHE:O	7:H:41:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:101:SQD:O9	10:l:5007:ARG:NH2	2.48	0.43
17:a:5402:CLA:H122	18:a:5405:PHO:HBA2	2.00	0.43
3:c:5071:GLU:CD	3:c:5086:LEU:HD12	2.43	0.43
3:c:5094:THR:O	3:c:5186:TYR:HB3	2.18	0.43
3:c:5401:LEU:HD22	3:c:5409:GLY:C	2.42	0.43
17:c:5506:CLA:H202	17:c:5506:CLA:H161	1.73	0.43
29:f:5101:HEM:HBC2	29:f:5101:HEM:CHD	2.48	0.43
7:h:5040:VAL:O	7:h:5044:ILE:HG12	2.18	0.43
13:z:5053:VAL:HA	13:z:5057:LEU:HD13	2.01	0.43
15:n:100:HIS:HE1	15:n:104:TYR:CZ	2.36	0.43
16:x:9:GLY:N	16:x:12:ILE:CD1	2.65	0.43
17:B:603:CLA:H61	17:B:603:CLA:H41	1.83	0.43
17:B:604:CLA:H41	17:B:604:CLA:H62	1.59	0.43
17:B:609:CLA:HBA1	17:B:609:CLA:H3A	1.60	0.43
17:B:612:CLA:H2A	17:B:612:CLA:O2D	2.18	0.43
17:B:614:CLA:H71	20:B:617:BCR:H362	1.99	0.43
3:C:81:MET:HE3	3:C:105:VAL:HG21	1.99	0.43
3:C:189:TRP:CH2	3:C:367:GLU:HB3	2.52	0.43
4:D:57:SER:O	4:D:64:ALA:HA	2.18	0.43
18:D:402:PHO:H2A	18:D:402:PHO:CED	2.48	0.43
17:a:5403:CLA:H61	17:a:5403:CLA:H93	1.74	0.43
18:a:5405:PHO:HBA2	18:a:5405:PHO:H3A	1.39	0.43
2:b:5248:ALA:HB2	17:b:5603:CLA:H52	2.01	0.43
17:b:5612:CLA:H2	17:b:5612:CLA:H62	1.32	0.43
3:c:5079:LYS:HE2	3:c:5083:GLU:HG2	1.99	0.43
3:c:5160:ILE:HD13	17:c:5511:CLA:HAC2	2.00	0.43
4:d:5235:PHE:CE2	4:d:5237:PRO:HB3	2.53	0.43
15:n:127:ALA:HA	15:n:130:ARG:HD2	2.00	0.43
2:B:201:HIS:O	2:B:205:ALA:N	2.43	0.43
17:B:602:CLA:H62	17:B:602:CLA:H41	1.71	0.43
3:C:189:TRP:CH2	3:C:364:PRO:HA	2.53	0.43
17:C:510:CLA:H122	17:C:510:CLA:H162	1.72	0.43
4:D:123:ILE:O	4:D:126:MET:N	2.52	0.43
5:E:82:GLN:C	5:E:84:LYS:H	2.27	0.43
7:H:40:VAL:O	7:H:44:ILE:HG12	2.18	0.43
1:a:5266:ASN:OD1	1:a:5267:ASN:N	2.52	0.43
2:b:5141:ILE:HA	2:b:5217:ILE:HD11	2.00	0.43
3:c:5313:GLN:HG3	3:c:5396:MET:HG3	2.00	0.43
10:l:5015:THR:O	10:l:5018:TYR:N	2.51	0.43
13:z:5055:GLY:HA3	20:z:5101:BCR:C5	2.48	0.43
15:N:72:PHE:HB2	15:N:94:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:100:HIS:HE1	15:N:104:TYR:CZ	2.36	0.43
1:A:161:TYR:CE1	1:A:186:PHE:HE1	2.36	0.43
2:B:256:MET:O	2:B:448:ARG:NH1	2.47	0.43
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.00	0.43
3:C:409:GLY:N	3:C:417:VAL:O	2.51	0.43
1:a:5089:ILE:HD12	1:a:5089:ILE:HA	1.85	0.43
2:b:5013:ILE:HG23	2:b:5014:ASN:N	2.32	0.43
17:c:5503:CLA:HBD	17:c:5503:CLA:HBA1	2.01	0.43
20:c:5513:BCR:H24C	20:c:5513:BCR:H371	1.84	0.43
12:t:5018:PHE:HB2	20:t:5102:BCR:C8	2.48	0.43
1:A:239:PHE:HE2	12:T:29:ILE:HG13	1.83	0.43
1:A:319:ASP:O	1:A:323:ARG:N	2.46	0.43
17:A:403:CLA:H2A	17:A:403:CLA:CED	2.49	0.43
17:B:604:CLA:H62	17:B:604:CLA:H92	1.75	0.43
3:C:98:GLY:O	3:C:106:VAL:N	2.49	0.43
3:C:313:GLN:HG3	3:C:396:MET:HG3	2.00	0.43
3:C:318:LEU:CD1	3:C:328:VAL:HG21	2.48	0.43
5:E:51:ARG:O	5:E:54:SER:N	2.40	0.43
1:a:5018:CYS:SG	8:i:5030:ARG:NH2	2.92	0.43
2:b:5226:TYR:CE1	2:b:5231:MET:HB2	2.53	0.43
17:b:5602:CLA:H62	17:b:5602:CLA:H41	1.71	0.43
17:b:5603:CLA:H112	17:b:5603:CLA:H142	1.69	0.43
3:c:5092:ILE:HD12	3:c:5114:VAL:HG11	1.99	0.43
3:c:5318:LEU:CD1	3:c:5328:VAL:HG21	2.48	0.43
26:c:5515:DGD:HB71	25:c:5517:MGE:H5A2	2.00	0.43
4:d:5039:PRO:O	4:d:5043:LEU:HD13	2.18	0.43
4:d:5346:LEU:O	4:d:5348:ARG:N	2.48	0.43
20:d:5406:BCR:H24C	20:d:5406:BCR:H371	1.75	0.43
15:N:127:ALA:HA	15:N:130:ARG:HD2	2.00	0.43
3:C:400:PRO:O	3:C:401:LEU:HG	2.19	0.43
1:a:5272:HIS:NE2	24:a:5412:BCT:O3	2.48	0.43
2:b:5037:MET:HE1	17:b:5607:CLA:CHD	2.49	0.43
3:c:5350:ILE:HG21	3:c:5359:TRP:HB2	2.00	0.43
14:Y:18:VAL:HG13	14:Y:21:GLN:NE2	2.34	0.43
16:x:7:LEU:HD22	16:x:7:LEU:HA	1.90	0.43
1:A:266:ASN:OD1	1:A:267:ASN:N	2.52	0.43
17:A:402:CLA:H111	17:A:402:CLA:H152	1.42	0.43
2:B:188:ASP:HA	7:H:58:VAL:HG12	2.01	0.43
3:C:147:PHE:HD2	17:C:513:CLA:H3A	1.82	0.43
3:C:187:ASP:OD1	3:C:189:TRP:N	2.52	0.43
3:C:226:SER:O	3:C:227:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:F:101:HEM:HBC2	29:F:101:HEM:CHD	2.48	0.43
10:L:15:THR:O	10:L:18:TYR:N	2.51	0.43
1:a:5093:PHE:CD2	1:a:5095:PRO:HD3	2.53	0.43
1:a:5097:TRP:NE1	25:c:5517:MGE:O5D	2.43	0.43
17:a:5403:CLA:O1A	4:d:5202:ALA:HA	2.18	0.43
17:a:5403:CLA:H12	4:d:5202:ALA:HA	2.00	0.43
2:b:5005:TRP:CZ2	25:l:5101:MGE:H2A2	2.54	0.43
2:b:5256:MET:O	2:b:5448:ARG:NH1	2.47	0.43
4:d:5057:SER:O	4:d:5064:ALA:HA	2.18	0.43
4:d:5235:PHE:HE2	4:d:5237:PRO:HB3	1.84	0.43
5:e:5082:GLN:C	5:e:5084:LYS:H	2.27	0.43
7:h:5038:PHE:O	7:h:5041:PHE:HB3	2.18	0.43
23:l:5102:SQD:H62	25:m:5103:MGE:H2A1	2.01	0.43
15:n:67:LYS:O	15:n:71:PHE:N	2.32	0.43
14:y:34:MET:HE2	14:y:34:MET:HB2	1.79	0.43
16:x:3:ILE:CD1	16:x:7:LEU:HD12	2.48	0.43
1:A:124:SER:OG	1:A:155:PHE:HZ	2.02	0.43
17:A:402:CLA:H61	17:A:402:CLA:H93	1.74	0.43
17:B:606:CLA:O2D	17:B:606:CLA:H2A	2.18	0.43
17:B:614:CLA:C2	25:m:5103:MGE:H8A1	2.49	0.43
3:C:175:LEU:HD11	17:C:501:CLA:HED2	2.00	0.43
4:D:30:VAL:HG22	4:D:38:PHE:HE2	1.84	0.43
1:a:5214:MET:O	1:a:5217:SER:N	2.52	0.43
2:b:5332:LYS:HA	2:b:5437:LEU:HD22	2.01	0.43
2:b:5347:ARG:HA	2:b:5352:GLU:O	2.19	0.43
17:b:5612:CLA:H2A	17:b:5612:CLA:O2D	2.18	0.43
3:c:5186:TYR:OH	3:c:5296:VAL:HA	2.19	0.43
18:d:5402:PHO:CED	18:d:5402:PHO:H2A	2.48	0.43
1:A:264:SER:OG	19:A:406:PQ9:O4	2.29	0.43
2:B:74:SER:OG	2:B:75:TRP:N	2.52	0.43
20:C:514:BCR:H20C	20:C:514:BCR:H361	1.84	0.43
4:D:235:PHE:HE2	4:D:237:PRO:HB3	1.84	0.43
7:H:48:ILE:HG13	7:H:53:LEU:HD23	2.01	0.43
1:a:5143:ILE:H	4:d:5220:ASN:ND2	2.17	0.43
2:b:5368:VAL:CG1	2:b:5381:ILE:HD12	2.49	0.43
17:b:5606:CLA:O2D	17:b:5606:CLA:H2A	2.18	0.43
4:d:5018:LEU:HD12	16:x:29:ILE:HA	2.01	0.43
1:A:89:ILE:HD12	1:A:89:ILE:HA	1.85	0.42
18:A:404:PHO:H51	18:A:404:PHO:H8	1.72	0.42
2:B:256:MET:HG3	2:B:451:PHE:CD1	2.54	0.42
3:C:189:TRP:HB2	15:N:76:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:TRP:CG	4:D:94:GLY:N	2.87	0.42
9:K:31:LEU:HD23	20:Y:101:BCR:H14C	2.01	0.42
11:M:11:THR:HG21	12:T:9:ILE:HD11	2.00	0.42
13:Z:23:VAL:HB	13:Z:24:PRO:HD3	2.01	0.42
1:a:5077:ILE:HD12	1:a:5077:ILE:H	1.84	0.42
1:a:5124:SER:OG	1:a:5155:PHE:HZ	2.02	0.42
1:a:5193:LEU:HD21	17:a:5402:CLA:HMC2	2.01	0.42
1:a:5317:TRP:CH2	4:d:5077:ALA:HB3	2.52	0.42
1:a:5331:MET:HE2	4:d:5320:LEU:O	2.19	0.42
2:b:5118:TRP:H	2:b:5118:TRP:CD1	2.35	0.42
2:b:5475:PHE:HE1	4:d:5134:ARG:HB3	1.84	0.42
17:b:5607:CLA:H92	17:b:5607:CLA:H62	1.61	0.42
3:c:5097:TRP:HE1	3:c:5178:LYS:HZ1	1.65	0.42
3:c:5439:VAL:O	3:c:5443:TRP:N	2.52	0.42
19:d:5405:PQ9:H212	19:d:5405:PQ9:H191	1.86	0.42
7:h:5047:GLU:CD	16:x:10:PHE:HD2	2.16	0.42
23:l:5102:SQD:H241	23:l:5102:SQD:H271	1.73	0.42
23:l:5102:SQD:C23	12:t:5019:PHE:HZ	2.31	0.42
1:A:74:GLY:HA3	11:M:1:MET:CE	2.50	0.42
25:A:412:MGE:H102	25:A:412:MGE:H7A1	1.71	0.42
2:B:7:ARG:HH11	17:B:611:CLA:HED1	1.84	0.42
2:B:37:MET:HE1	17:B:607:CLA:CHD	2.49	0.42
2:B:58:GLN:HG3	2:B:60:MET:HE2	2.01	0.42
3:C:315:MET:O	3:C:318:LEU:HB3	2.19	0.42
3:C:349:ILE:HD11	3:C:375:LEU:O	2.19	0.42
17:C:507:CLA:H91	17:C:507:CLA:H112	1.69	0.42
10:L:20:GLY:HA3	11:M:22:LEU:HD13	2.00	0.42
1:a:5047:CYS:SG	1:a:5114:LEU:HD22	2.59	0.42
1:a:5319:ASP:HA	1:a:5322:ASN:HB2	2.01	0.42
17:a:5402:CLA:H191	25:d:5410:MGE:H212	2.02	0.42
18:a:5405:PHO:NB	4:d:5209:LEU:HD12	2.34	0.42
4:d:5030:VAL:HG22	4:d:5038:PHE:HE2	1.84	0.42
4:d:5269:PHE:CZ	25:d:5409:MGE:H3G2	2.54	0.42
5:e:5068:ASP:OD1	5:e:5068:ASP:N	2.51	0.42
12:t:5016:LEU:O	12:t:5020:ALA:N	2.45	0.42
2:B:248:ALA:HB2	17:B:603:CLA:H52	2.01	0.42
2:B:332:LYS:HA	2:B:437:LEU:HD22	2.01	0.42
2:B:347:ARG:HA	2:B:352:GLU:O	2.19	0.42
17:B:610:CLA:H62	17:B:610:CLA:H41	1.81	0.42
3:C:189:TRP:CZ3	3:C:364:PRO:HA	2.54	0.42
13:Z:28:ALA:HB1	14:Y:39:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5047:PRO:HB3	2:b:5078:TRP:CD2	2.54	0.42
3:c:5223:TRP:CE2	25:c:5517:MGE:H8B1	2.55	0.42
17:c:5512:CLA:CAB	20:z:5101:BCR:H24C	2.50	0.42
4:d:5023:LYS:NZ	4:d:5032:TRP:HE1	2.17	0.42
4:d:5123:ILE:O	4:d:5126:MET:N	2.52	0.42
4:d:5304:ARG:HH11	4:d:5307:GLU:HB2	1.84	0.42
7:h:5048:ILE:HG13	7:h:5053:LEU:HD23	2.01	0.42
15:n:46:GLU:OE2	15:n:50:LEU:HD11	2.20	0.42
15:N:46:GLU:OE2	15:N:50:LEU:HD11	2.19	0.42
16:X:3:ILE:HG23	16:X:7:LEU:HD12	1.94	0.42
1:A:47:CYS:SG	1:A:114:LEU:HD22	2.59	0.42
17:A:401:CLA:H202	17:A:401:CLA:H161	1.76	0.42
2:B:381:ILE:HG22	2:B:382:PRO:O	2.20	0.42
17:C:503:CLA:H202	17:C:503:CLA:H162	1.82	0.42
17:D:404:CLA:H61	17:D:404:CLA:H41	1.62	0.42
6:F:24:HIS:NE2	29:F:101:HEM:C1D	2.87	0.42
23:L:101:SQD:O9	10:l:5007:ARG:NH1	2.52	0.42
13:Z:53:VAL:HA	13:Z:57:LEU:HD13	2.00	0.42
17:a:5404:CLA:H112	17:a:5404:CLA:H91	1.84	0.42
2:b:5256:MET:HG3	2:b:5451:PHE:CD1	2.54	0.42
3:c:5315:MET:O	3:c:5318:LEU:HB3	2.19	0.42
17:c:5503:CLA:H161	17:c:5503:CLA:H122	1.67	0.42
4:d:5026:ARG:CD	6:f:5018:VAL:HG21	2.50	0.42
25:l:5101:MGE:H263	25:l:5101:MGE:H231	1.82	0.42
13:z:5016:SER:O	13:z:5020:VAL:HG23	2.20	0.42
15:n:27:THR:N	15:n:67:LYS:HG2	2.35	0.42
15:N:56:ASN:HB3	15:N:59:ALA:HB3	2.01	0.42
1:A:153:SER:O	1:A:157:VAL:HG12	2.19	0.42
1:A:224:ILE:HD11	1:A:247:ASN:OD1	2.20	0.42
2:B:137:LYS:HE3	2:B:217:ILE:HG23	2.02	0.42
2:B:360:PRO:HG2	4:D:339:PHE:HZ	1.84	0.42
17:B:603:CLA:O1D	17:B:603:CLA:H2A	2.18	0.42
4:D:23:LYS:NZ	4:D:32:TRP:HE1	2.17	0.42
13:Z:16:SER:O	13:Z:20:VAL:HG23	2.20	0.42
3:c:5408:GLY:N	3:c:5418:ASN:HA	2.35	0.42
17:d:5403:CLA:H61	17:d:5403:CLA:H41	1.62	0.42
12:t:5018:PHE:HB2	20:t:5102:BCR:HC8	2.00	0.42
15:n:56:ASN:HB3	15:n:59:ALA:HB3	2.01	0.42
1:A:97:TRP:CG	8:I:5:LYS:HB2	2.55	0.42
1:A:159:LEU:HD23	26:A:413:DGD:HAT1	2.00	0.42
2:B:102:VAL:HG12	17:B:606:CLA:H91	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ASP:OD1	2:B:119:ASP:N	2.51	0.42
3:C:291:TRP:HD1	3:C:292:PHE:CE2	2.37	0.42
3:C:422:PRO:HA	3:C:425:TRP:HD1	1.85	0.42
17:C:513:CLA:H2A	17:C:513:CLA:HED3	2.02	0.42
17:D:404:CLA:H162	17:D:404:CLA:H202	1.73	0.42
1:a:5027:ARG:NH2	12:t:5024:ARG:HE	2.17	0.42
17:a:5404:CLA:H2A	17:a:5404:CLA:CED	2.49	0.42
2:b:5058:GLN:HG3	2:b:5060:MET:HE2	2.01	0.42
2:b:5119:ASP:N	2:b:5119:ASP:OD1	2.50	0.42
3:c:5349:ILE:HD11	3:c:5375:LEU:O	2.19	0.42
4:d:5014:TRP:CE2	16:x:29:ILE:CD1	3.03	0.42
4:d:5048:TRP:CD1	18:d:5402:PHO:H13	2.54	0.42
15:n:72:PHE:CD2	15:n:76:ARG:CZ	3.02	0.42
1:A:77:ILE:HD12	1:A:77:ILE:H	1.85	0.42
1:A:280:VAL:O	1:A:283:VAL:N	2.51	0.42
2:B:172:TYR:HE1	2:B:283:GLU:OE1	2.02	0.42
2:B:174:LEU:HD11	2:B:309:LEU:HD13	2.02	0.42
3:C:97:TRP:HE1	3:C:178:LYS:HZ1	1.68	0.42
3:C:106:VAL:HG23	3:C:107:ASP:N	2.34	0.42
3:C:157:MET:HE2	17:C:507:CLA:HHD	2.01	0.42
17:C:503:CLA:H62	17:C:503:CLA:H41	1.90	0.42
17:C:511:CLA:H61	17:C:511:CLA:H92	1.74	0.42
1:a:5061:ASP:HB3	1:a:5063:ILE:HG12	2.01	0.42
1:a:5119:PHE:O	1:a:5123:ALA:N	2.45	0.42
1:a:5125:CYS:SG	17:c:5505:CLA:H91	2.59	0.42
1:a:5161:TYR:N	1:a:5162:PRO:HD2	2.35	0.42
2:b:5010:THR:O	2:b:5013:ILE:N	2.50	0.42
2:b:5172:TYR:HE1	2:b:5283:GLU:OE1	2.02	0.42
3:c:5399:ALA:O	3:c:5400:PRO:C	2.63	0.42
17:k:5501:CLA:H61	17:k:5501:CLA:H92	1.74	0.42
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.52	0.42
2:B:148:LEU:HB2	2:B:210:ILE:HD11	2.01	0.42
2:B:368:VAL:CG1	2:B:381:ILE:HD12	2.49	0.42
17:C:510:CLA:H2	17:C:510:CLA:H61	1.63	0.42
17:C:513:CLA:CAB	20:C:515:BCR:H24C	2.50	0.42
20:D:407:BCR:H15C	20:D:407:BCR:H351	1.90	0.42
25:D:410:MGE:H5A1	25:D:410:MGE:H2A2	1.78	0.42
1:a:5093:PHE:HA	1:a:5113:GLN:NE2	2.35	0.42
2:b:5074:SER:OG	2:b:5075:TRP:N	2.52	0.42
2:b:5257:TRP:O	2:b:5271:THR:OG1	2.32	0.42
2:b:5461:LEU:HD23	2:b:5461:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:5612:CLA:HBA1	17:b:5612:CLA:H3A	1.55	0.42
3:c:5088:LEU:O	3:c:5091:HIS:N	2.52	0.42
3:c:5189:TRP:HB3	15:n:76:ARG:CZ	2.50	0.42
4:d:5195:PRO:HD3	10:l:5034:TYR:CZ	2.55	0.42
15:n:86:SER:C	15:n:89:THR:HG1	2.25	0.42
1:A:135:TYR:CZ	8:I:31:ASN:HB3	2.55	0.42
1:A:214:MET:O	1:A:217:SER:N	2.52	0.42
1:A:308:ASP:OD2	1:A:312:ASN:HB2	2.20	0.42
1:A:317:TRP:HH2	4:D:77:ALA:HB3	1.85	0.42
17:A:401:CLA:C1B	17:D:404:CLA:HBB1	2.49	0.42
17:B:606:CLA:H41	17:B:606:CLA:H62	1.44	0.42
17:B:607:CLA:O2D	17:B:607:CLA:H2A	2.20	0.42
17:B:610:CLA:H8	17:B:610:CLA:H51	1.66	0.42
17:B:614:CLA:H92	17:B:614:CLA:H62	1.85	0.42
17:C:512:CLA:H2A	17:C:512:CLA:CED	2.50	0.42
4:D:48:TRP:CD1	18:D:402:PHO:H13	2.54	0.42
4:D:279:LEU:HA	4:D:279:LEU:HD23	1.85	0.42
25:D:410:MGE:H2	25:D:410:MGE:H4	1.63	0.42
2:b:5250:PHE:CD2	17:b:5602:CLA:H152	2.55	0.42
17:b:5616:CLA:H141	17:b:5616:CLA:H161	1.84	0.42
3:c:5269:GLU:O	3:c:5272:LEU:N	2.53	0.42
25:d:5409:MGE:H6B2	25:d:5409:MGE:H9B1	1.75	0.42
7:h:5007:LEU:O	7:h:5010:ILE:N	2.53	0.42
1:A:286:THR:HB	17:A:401:CLA:O1D	2.20	0.42
1:A:300:PHE:CD2	3:C:404:LEU:HB2	2.55	0.42
25:A:412:MGE:H211	10:L:22:LEU:HG	2.02	0.42
2:B:47:PRO:HB3	2:B:78:TRP:CD2	2.54	0.42
3:C:229:ASN:ND2	15:N:77:ARG:HB2	2.34	0.42
3:C:457:LYS:HE2	4:D:224:GLN:HE21	1.85	0.42
17:C:511:CLA:H72	14:Y:35:ILE:CG2	2.46	0.42
4:D:304:ARG:HH11	4:D:307:GLU:HB2	1.84	0.42
12:T:1:MET:O	12:T:4:ILE:HG22	2.20	0.42
1:a:5140:ARG:HD3	1:a:5142:TRP:NE1	2.35	0.42
2:b:5057:ARG:HG2	2:b:5331:ASN:ND2	2.35	0.42
2:b:5174:LEU:HD11	2:b:5309:LEU:HD13	2.02	0.42
2:b:5453:PHE:HE2	25:b:5620:MGE:H102	1.85	0.42
17:b:5605:CLA:H141	17:b:5610:CLA:HMA1	2.02	0.42
3:c:5157:MET:HE2	17:c:5507:CLA:HHD	2.01	0.42
3:c:5388:GLN:NE2	15:n:95:ASN:ND2	2.66	0.42
20:h:5101:BCR:H20C	20:h:5101:BCR:H361	1.89	0.42
14:Y:22:LEU:HA	14:Y:25:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:23:LEU:HA	16:X:23:LEU:HD22	1.83	0.42
1:A:40:THR:HG23	1:A:41:LEU:N	2.35	0.41
2:B:61:PHE:HB2	17:B:607:CLA:HMA3	2.02	0.41
2:B:453:PHE:HE2	25:B:619:MGE:H102	1.85	0.41
17:B:612:CLA:H93	17:B:612:CLA:H62	1.80	0.41
17:B:612:CLA:H2	17:B:612:CLA:H62	1.32	0.41
17:B:613:CLA:H202	17:B:613:CLA:H162	1.75	0.41
17:B:615:CLA:H13	17:B:615:CLA:H101	1.92	0.41
25:B:619:MGE:H5B2	11:M:10:ALA:HB2	2.02	0.41
3:C:76:ILE:HB	3:C:84:GLN:NE2	2.35	0.41
17:C:507:CLA:HBD	17:C:507:CLA:HAA2	2.02	0.41
4:D:63:LEU:HD12	4:D:63:LEU:O	2.20	0.41
7:H:7:LEU:O	7:H:10:ILE:N	2.53	0.41
1:a:5215:HIS:NE2	24:a:5412:BCT:O2	2.52	0.41
2:b:5073:GLY:HA2	2:b:5078:TRP:O	2.19	0.41
2:b:5148:LEU:HB2	2:b:5210:ILE:HD11	2.01	0.41
2:b:5151:PHE:HB2	2:b:5206:GLY:HA3	2.02	0.41
4:d:5085:MET:CE	4:d:5090:LEU:HD21	2.50	0.41
16:x:36:LYS:HG2	16:x:36:LYS:HZ2	1.78	0.41
1:A:319:ASP:HA	1:A:322:ASN:HB2	2.01	0.41
17:A:405:CLA:C4A	17:A:405:CLA:HBA1	2.47	0.41
24:A:411:BCT:O3	4:D:214:HIS:NE2	2.53	0.41
2:B:250:PHE:CD2	17:B:602:CLA:H152	2.55	0.41
17:B:608:CLA:C1A	17:B:608:CLA:CGA	2.96	0.41
3:C:408:GLY:N	3:C:418:ASN:HA	2.35	0.41
17:C:501:CLA:C4D	17:C:503:CLA:H51	2.51	0.41
17:C:503:CLA:HBA1	17:C:503:CLA:HBD	2.01	0.41
4:D:24:ARG:HG2	4:D:25:ASP:N	2.35	0.41
4:D:193:LEU:O	10:L:34:TYR:OH	2.36	0.41
4:D:232:PHE:CE2	23:D:403:SQD:H461	2.54	0.41
20:H:101:BCR:H371	20:H:101:BCR:H24C	1.75	0.41
1:a:5059:ASP:OD2	1:a:5062:GLY:HA2	2.20	0.41
1:a:5172:MET:HE1	17:a:5403:CLA:HMC2	2.02	0.41
1:a:5308:ASP:OD2	1:a:5312:ASN:HB2	2.20	0.41
2:b:5215:PHE:CD2	2:b:5216:HIS:HD2	2.38	0.41
3:c:5291:TRP:HD1	3:c:5292:PHE:CE2	2.37	0.41
4:d:5319:LEU:HD23	4:d:5319:LEU:HA	1.88	0.41
25:d:5410:MGE:H2	25:d:5410:MGE:H4	1.63	0.41
10:l:5008:GLN:HE21	10:l:5009:PRO:HD2	1.83	0.41
15:N:27:THR:N	15:N:67:LYS:HG2	2.35	0.41
1:A:172:MET:HE1	17:A:402:CLA:HMC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLY:HA2	2:B:78:TRP:O	2.19	0.41
20:B:617:BCR:H343	20:t:5102:BCR:H382	2.01	0.41
3:C:269:GLU:O	3:C:272:LEU:N	2.53	0.41
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.45	0.41
25:D:410:MGE:O6D	10:L:15:THR:HG21	2.20	0.41
26:D:411:DGD:C1A	7:H:50:ASN:HD21	2.34	0.41
1:a:5040:THR:HG23	1:a:5041:LEU:N	2.35	0.41
1:a:5224:ILE:HD11	1:a:5247:ASN:OD1	2.20	0.41
2:b:5137:LYS:HE3	2:b:5217:ILE:HG23	2.02	0.41
17:b:5610:CLA:H101	17:b:5615:CLA:HBA2	2.02	0.41
17:b:5613:CLA:H202	17:b:5613:CLA:H162	1.75	0.41
20:b:5619:BCR:H15C	20:b:5619:BCR:H351	1.87	0.41
3:c:5099:VAL:HG23	3:c:5100:GLY:N	2.35	0.41
3:c:5218:PHE:HE2	25:c:5517:MGE:O1A	2.04	0.41
4:d:5125:PHE:CE2	18:d:5402:PHO:HBD	2.54	0.41
10:l:5022:LEU:HG	25:l:5101:MGE:H211	2.01	0.41
13:z:5023:VAL:HB	13:z:5024:PRO:HD3	2.01	0.41
15:N:33:PHE:CG	15:N:81:LEU:HD11	2.55	0.41
15:N:109:LEU:C	15:N:114:LYS:HE3	2.45	0.41
15:N:125:GLU:HA	15:N:128:LEU:HB3	2.02	0.41
16:X:4:THR:H	16:X:7:LEU:HB3	1.85	0.41
2:B:125:ASP:OD1	2:B:128:THR:OG1	2.31	0.41
2:B:215:PHE:CD2	2:B:216:HIS:HD2	2.38	0.41
2:B:386:ALA:HB1	4:D:344:GLU:HB2	2.02	0.41
17:B:607:CLA:H62	17:B:607:CLA:H92	1.61	0.41
17:B:613:CLA:H2A	17:B:613:CLA:O2A	2.19	0.41
3:C:213:LEU:HB3	3:C:224:ILE:HD11	2.02	0.41
25:C:519:MGE:H5A1	25:C:519:MGE:H8A2	1.95	0.41
4:D:203:GLY:O	4:D:207:GLY:N	2.46	0.41
20:a:5408:BCR:H371	20:a:5408:BCR:H24C	1.83	0.41
2:b:5166:MET:HG2	2:b:5167:TRP:O	2.20	0.41
2:b:5201:HIS:O	2:b:5205:ALA:N	2.43	0.41
2:b:5311:PHE:HA	2:b:5430:PHE:CZ	2.55	0.41
2:b:5474:LEU:HD13	4:d:5134:ARG:HH21	1.84	0.41
3:c:5224:ILE:HD12	3:c:5224:ILE:HG23	1.82	0.41
3:c:5226:SER:O	3:c:5227:VAL:C	2.62	0.41
3:c:5276:LEU:HD23	3:c:5276:LEU:HA	1.76	0.41
17:c:5501:CLA:H72	17:c:5501:CLA:H111	1.74	0.41
15:n:27:THR:OG1	15:n:70:ASP:OD2	2.36	0.41
15:n:33:PHE:CG	15:n:81:LEU:HD11	2.55	0.41
15:n:125:GLU:HA	15:n:128:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:y:18:VAL:N	14:y:21:GLN:CB	2.82	0.41
1:A:59:ASP:OD2	1:A:62:GLY:HA2	2.20	0.41
1:A:93:PHE:HA	1:A:113:GLN:NE2	2.34	0.41
1:A:97:TRP:HA	8:I:1:MET:HE3	2.02	0.41
25:A:412:MGE:H221	19:D:406:PQ9:H262	2.01	0.41
2:B:57:ARG:HG2	2:B:331:ASN:ND2	2.35	0.41
2:B:166:MET:HG2	2:B:167:TRP:O	2.20	0.41
4:D:158:LEU:C	4:D:161:PRO:HD2	2.46	0.41
4:D:180:ARG:O	4:D:184:PHE:HB2	2.21	0.41
9:K:31:LEU:HB3	20:Y:101:BCR:C14	2.51	0.41
22:M:101:LMT:H11	22:M:101:LMT:H42	1.77	0.41
3:c:5213:LEU:HB3	3:c:5224:ILE:HD11	2.02	0.41
17:c:5501:CLA:C4D	17:c:5503:CLA:H51	2.51	0.41
4:d:5180:ARG:O	4:d:5184:PHE:HB2	2.21	0.41
25:A:412:MGE:H2A2	2:B:5:TRP:CZ2	2.56	0.41
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.55	0.41
17:B:605:CLA:H141	17:B:610:CLA:HMA1	2.02	0.41
3:C:88:LEU:O	3:C:91:HIS:N	2.52	0.41
17:C:513:CLA:H2A	17:C:513:CLA:CED	2.50	0.41
1:a:5153:SER:O	1:a:5157:VAL:HG12	2.20	0.41
1:a:5286:THR:HB	17:a:5402:CLA:O1D	2.20	0.41
1:a:5286:THR:O	1:a:5289:GLY:N	2.54	0.41
2:b:5061:PHE:HB2	17:b:5607:CLA:HMA3	2.02	0.41
2:b:5183:PRO:HB3	2:b:5199:VAL:CG1	2.51	0.41
2:b:5362:PHE:HE2	4:d:5334:GLN:HE22	1.69	0.41
2:b:5381:ILE:HG22	2:b:5382:PRO:O	2.20	0.41
17:b:5607:CLA:O2D	17:b:5607:CLA:H2A	2.20	0.41
17:b:5608:CLA:HBB2	4:d:5123:ILE:HG12	2.02	0.41
3:c:5076:ILE:HB	3:c:5084:GLN:NE2	2.35	0.41
4:d:5063:LEU:O	4:d:5063:LEU:HD12	2.20	0.41
4:d:5152:VAL:HG21	4:d:5279:LEU:HD22	2.03	0.41
4:d:5279:LEU:HD11	18:d:5402:PHO:HAC2	2.01	0.41
9:k:5043:VAL:CG2	14:y:46:LEU:HD13	2.50	0.41
1:A:193:LEU:HD21	17:A:401:CLA:HMC2	2.01	0.41
17:B:607:CLA:H3A	17:B:607:CLA:HBA2	1.51	0.41
3:C:276:LEU:HD21	17:C:508:CLA:CBB	2.51	0.41
4:D:85:MET:CE	4:D:90:LEU:HD21	2.51	0.41
17:D:405:CLA:C4A	17:D:405:CLA:HBA2	2.50	0.41
1:a:5267:ASN:HB3	1:a:5270:SER:HB3	2.03	0.41
2:b:5077:GLY:C	2:b:5086:ILE:CD1	2.94	0.41
2:b:5198:VAL:O	2:b:5201:HIS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:5614:CLA:H43	25:m:5101:MGE:H6A2	2.02	0.41
17:c:5512:CLA:H2A	17:c:5512:CLA:CED	2.50	0.41
17:c:5512:CLA:H2A	17:c:5512:CLA:HED3	2.02	0.41
4:d:5158:LEU:C	4:d:5161:PRO:HD2	2.45	0.41
20:k:5502:BCR:H15C	20:k:5502:BCR:H351	1.91	0.41
15:n:50:LEU:H	15:n:57:LYS:HZ2	1.69	0.41
15:n:73:ALA:HA	15:n:76:ARG:NH2	2.35	0.41
1:A:161:TYR:N	1:A:162:PRO:HD2	2.35	0.41
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.55	0.41
1:A:286:THR:O	1:A:289:GLY:N	2.54	0.41
17:A:405:CLA:HBA1	17:A:405:CLA:H3A	1.64	0.41
25:A:412:MGE:H8B1	4:D:270:PHE:HE1	1.86	0.41
2:B:41:GLU:OE1	2:B:60:MET:HA	2.21	0.41
2:B:135:LEU:HD23	2:B:237:VAL:HG23	2.03	0.41
20:B:617:BCR:H20C	20:B:617:BCR:H361	1.81	0.41
3:C:399:ALA:O	3:C:400:PRO:C	2.63	0.41
17:C:501:CLA:H111	17:C:501:CLA:H72	1.74	0.41
4:D:89:LEU:HD13	7:H:50:ASN:ND2	2.35	0.41
1:a:5143:ILE:H	4:d:5220:ASN:HD21	1.67	0.41
17:a:5402:CLA:O1D	17:a:5402:CLA:H2A	2.21	0.41
2:b:5069:LEU:HA	2:b:5069:LEU:HD23	1.87	0.41
3:c:5199:ILE:HD12	3:c:5234:VAL:HG21	2.03	0.41
3:c:5276:LEU:HD21	17:c:5508:CLA:CBB	2.51	0.41
3:c:5461:ARG:HH11	4:d:5223:PHE:CB	2.33	0.41
17:c:5511:CLA:H2A	17:c:5511:CLA:CED	2.50	0.41
4:d:5072:ASN:ND2	4:d:5074:LEU:H	2.19	0.41
4:d:5330:ALA:HB3	4:d:5331:PRO:HD3	2.03	0.41
14:Y:33:PRO:O	14:Y:34:MET:C	2.63	0.41
1:A:61:ASP:HB3	1:A:63:ILE:HG12	2.01	0.41
1:A:140:ARG:HD3	1:A:142:TRP:NE1	2.35	0.41
1:A:157:VAL:HG21	1:A:172:MET:HE3	2.03	0.41
2:B:193:TYR:HA	2:B:261:ALA:HB2	2.03	0.41
2:B:383:PHE:CD2	2:B:384:ARG:HG2	2.55	0.41
17:B:610:CLA:H101	17:B:615:CLA:HBA2	2.02	0.41
3:C:99:VAL:HG23	3:C:100:GLY:N	2.35	0.41
3:C:199:ILE:HD12	3:C:234:VAL:HG21	2.03	0.41
3:C:298:PRO:HD2	3:C:302:TYR:CE2	2.56	0.41
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.56	0.41
4:D:218:VAL:HG23	4:D:244:TYR:CD1	2.56	0.41
4:D:288:GLY:O	4:D:293:LEU:HB2	2.21	0.41
5:E:63:ILE:CG2	5:E:65:LEU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:101:BCR:H20C	20:H:101:BCR:H361	1.89	0.41
9:K:20:PRO:CB	14:Y:24:MET:HB2	2.48	0.41
12:T:18:PHE:CB	20:T:102:BCR:H10C	2.50	0.41
1:a:5142:TRP:CZ3	3:c:5443:TRP:CD1	3.09	0.41
1:a:5172:MET:HE2	1:a:5179:THR:HG23	2.03	0.41
1:a:5187:GLN:HE22	1:a:5191:ASN:HA	1.84	0.41
1:a:5264:SER:OG	19:a:5407:PQ9:O4	2.29	0.41
1:a:5302:PHE:HE2	4:d:5072:ASN:HD22	1.69	0.41
17:a:5403:CLA:HED2	4:d:5198:MET:SD	2.61	0.41
17:b:5601:CLA:O1D	7:h:5041:PHE:HE1	2.04	0.41
17:b:5602:CLA:H92	7:h:5046:LEU:HD22	2.01	0.41
17:b:5611:CLA:H161	17:b:5611:CLA:H202	1.81	0.41
17:b:5613:CLA:H2A	17:b:5613:CLA:O2A	2.19	0.41
3:c:5246:ALA:O	3:c:5250:TRP:N	2.47	0.41
3:c:5270:ALA:HB1	3:c:5274:TYR:CE2	2.56	0.41
17:c:5505:CLA:H152	17:c:5505:CLA:H18	1.68	0.41
4:d:5188:PHE:CE1	4:d:5326:ARG:HG2	2.56	0.41
1:A:92:HIS:CE1	3:C:220:GLY:HA3	2.55	0.41
1:A:97:TRP:CE2	8:I:5:LYS:HG3	2.56	0.41
1:A:225:ARG:HB2	2:B:481:GLY:HA3	2.02	0.41
1:A:286:THR:HB	17:A:401:CLA:HED2	2.03	0.41
22:A:409:LMT:O6B	22:A:409:LMT:O4'	2.22	0.41
2:B:325:PHE:O	2:B:327:THR:HG23	2.21	0.41
3:C:78:GLU:OE1	3:C:78:GLU:N	2.49	0.41
3:C:139:THR:HG22	3:C:141:GLU:H	1.87	0.41
3:C:270:ALA:HB1	3:C:274:TYR:CE2	2.56	0.41
4:D:68:LEU:HA	6:F:40:MET:SD	2.61	0.41
4:D:330:ALA:HB3	4:D:331:PRO:HD3	2.03	0.41
1:a:5133:LEU:HA	1:a:5133:LEU:HD12	1.89	0.41
2:b:5041:GLU:OE1	2:b:5060:MET:HA	2.21	0.41
20:Y:101:BCR:H24C	20:Y:101:BCR:H371	1.93	0.41
16:x:31:ILE:HD12	16:x:31:ILE:HA	1.83	0.41
1:A:110:GLY:N	1:A:111:PRO:HD2	2.36	0.40
1:A:255:PHE:CD2	19:A:406:PQ9:H3	2.56	0.40
1:A:300:PHE:HD2	3:C:404:LEU:HB2	1.86	0.40
17:A:405:CLA:H52	8:I:9:TYR:HD1	1.86	0.40
2:B:183:PRO:HB3	2:B:199:VAL:CG1	2.51	0.40
3:C:408:GLY:H	3:C:418:ASN:HA	1.87	0.40
17:C:511:CLA:O2D	17:C:511:CLA:H2A	2.21	0.40
10:L:8:GLN:HE21	10:L:9:PRO:HD2	1.83	0.40
10:L:14:ARG:NH2	23:L:101:SQD:C7	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5110:GLY:N	1:a:5111:PRO:HD2	2.36	0.40
2:b:5015:ASP:O	2:b:5016:PRO:C	2.64	0.40
20:b:5618:BCR:H351	20:b:5618:BCR:H15C	1.81	0.40
20:b:5619:BCR:H11C	20:b:5619:BCR:H341	1.92	0.40
4:d:5288:GLY:O	4:d:5293:LEU:HB2	2.21	0.40
25:l:5101:MGE:H122	11:m:5018:PRO:HG3	2.04	0.40
13:z:5057:LEU:O	13:z:5061:VAL:HG23	2.20	0.40
14:Y:39:LEU:HD22	14:Y:39:LEU:HA	1.86	0.40
15:n:49:ALA:O	15:n:50:LEU:HD12	2.21	0.40
16:x:21:LEU:HD23	16:x:21:LEU:O	2.18	0.40
1:A:206:PHE:O	1:A:209:ALA:N	2.55	0.40
2:B:177:SER:HB2	2:B:179:GLN:HE22	1.86	0.40
3:C:190:ALA:HB3	3:C:194:GLY:H	1.86	0.40
3:C:307:PRO:HA	3:C:358:PHE:CE2	2.56	0.40
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.03	0.40
20:T:102:BCR:H15C	20:T:102:BCR:H351	1.85	0.40
2:b:5024:LEU:HD23	2:b:5024:LEU:HA	1.94	0.40
2:b:5331:ASN:HB3	2:b:5336:ILE:HD13	2.03	0.40
17:b:5613:CLA:H62	17:b:5613:CLA:H101	1.68	0.40
3:c:5199:ILE:HD13	3:c:5231:GLU:HG2	2.04	0.40
17:c:5505:CLA:O1D	17:c:5505:CLA:H2A	2.21	0.40
4:d:5213:ILE:HD11	4:d:5253:TRP:CH2	2.56	0.40
17:k:5501:CLA:H2A	17:k:5501:CLA:O2D	2.21	0.40
12:t:5001:MET:O	12:t:5004:ILE:HG22	2.20	0.40
14:y:39:LEU:HD22	14:y:39:LEU:HA	1.66	0.40
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.89	0.40
17:A:401:CLA:O1D	17:A:401:CLA:H2A	2.20	0.40
2:B:124:ARG:HG2	2:B:131:PRO:HA	2.04	0.40
2:B:151:PHE:HB2	2:B:206:GLY:HA3	2.02	0.40
2:B:171:PRO:HD3	7:H:63:LYS:HD3	2.02	0.40
2:B:381:ILE:HG12	2:B:392:PHE:CE1	2.56	0.40
17:B:603:CLA:H203	17:B:609:CLA:H8	2.03	0.40
3:C:294:ASN:ND2	3:C:299:SER:OG	2.54	0.40
4:D:72:ASN:ND2	4:D:74:LEU:H	2.18	0.40
13:Z:57:LEU:O	13:Z:61:VAL:HG23	2.20	0.40
1:a:5255:PHE:CZ	19:a:5407:PQ9:H152	2.57	0.40
2:b:5177:SER:HB2	2:b:5179:GLN:HE22	1.86	0.40
2:b:5193:TYR:HA	2:b:5261:ALA:HB2	2.03	0.40
2:b:5227:LYS:O	2:b:5230:ARG:NH1	2.54	0.40
2:b:5381:ILE:HG12	2:b:5392:PHE:CE1	2.56	0.40
3:c:5365:TRP:CD1	3:c:5365:TRP:H	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5368:PRO:HB2	15:n:95:ASN:HD22	1.86	0.40
3:c:5422:PRO:HA	3:c:5425:TRP:HD1	1.85	0.40
4:d:5218:VAL:HG23	4:d:5244:TYR:CD1	2.56	0.40
4:d:5279:LEU:HA	4:d:5279:LEU:HD23	1.85	0.40
15:n:41:ILE:HG12	15:n:121:PHE:CD1	2.56	0.40
15:n:109:LEU:O	15:n:114:LYS:HE3	2.21	0.40
14:y:18:VAL:CA	14:y:21:GLN:HB2	2.52	0.40
3:C:87:ILE:HG23	17:C:504:CLA:HMA3	2.04	0.40
3:C:266:TRP:H	3:C:266:TRP:CD1	2.40	0.40
7:H:40:VAL:CG2	16:X:14:LEU:HD11	2.52	0.40
1:a:5092:HIS:HA	3:c:5219:GLY:HA3	2.02	0.40
1:a:5143:ILE:N	4:d:5220:ASN:ND2	2.68	0.40
1:a:5147:TYR:O	1:a:5150:PRO:HD2	2.22	0.40
1:a:5157:VAL:HG21	1:a:5172:MET:HE3	2.03	0.40
2:b:5327:THR:HG21	25:b:5620:MGE:H2B2	2.02	0.40
2:b:5346:PHE:O	2:b:5354:LEU:N	2.48	0.40
2:b:5440:ASP:OD1	2:b:5441:GLY:N	2.55	0.40
17:b:5607:CLA:HBA2	17:b:5607:CLA:H3A	1.51	0.40
3:c:5298:PRO:HD2	3:c:5302:TYR:CE2	2.56	0.40
3:c:5408:GLY:H	3:c:5418:ASN:HA	1.87	0.40
17:c:5503:CLA:H162	17:c:5503:CLA:H202	1.82	0.40
15:N:49:ALA:O	15:N:50:LEU:HD12	2.21	0.40
1:A:77:ILE:HD11	12:T:6:TYR:CD1	2.57	0.40
1:A:187:GLN:HE22	1:A:191:ASN:HA	1.85	0.40
1:A:255:PHE:CZ	19:A:406:PQ9:H152	2.57	0.40
2:B:327:THR:HG21	25:B:619:MGE:H2B2	2.02	0.40
2:B:331:ASN:HB3	2:B:336:ILE:HD13	2.03	0.40
3:C:224:ILE:HD12	3:C:224:ILE:HG23	1.82	0.40
3:C:269:GLU:O	3:C:270:ALA:C	2.64	0.40
4:D:152:VAL:HG21	4:D:279:LEU:HD22	2.03	0.40
4:D:213:ILE:HD12	4:D:213:ILE:HA	1.86	0.40
4:D:304:ARG:NH1	4:D:308:ASP:OD1	2.54	0.40
23:L:101:SQD:H462	25:m:5101:MGE:H8B1	2.03	0.40
1:a:5137:LEU:HD23	1:a:5137:LEU:HA	1.92	0.40
1:a:5272:HIS:NE2	24:a:5412:BCT:C	2.84	0.40
2:b:5340:TRP:HH2	2:b:5343:HIS:CD2	2.40	0.40
2:b:5383:PHE:CD2	2:b:5384:ARG:HG2	2.55	0.40
3:c:5266:TRP:CD1	3:c:5266:TRP:H	2.40	0.40
3:c:5297:TYR:HD1	3:c:5302:TYR:CZ	2.39	0.40
4:d:5179:PHE:O	4:d:5182:LEU:N	2.53	0.40
4:d:5185:PHE:HB3	4:d:5191:TRP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:5405:PQ9:H262	25:l:5101:MGE:H221	2.02	0.40
13:z:5028:ALA:O	13:z:5030:PRO:HD3	2.22	0.40
14:Y:43:ARG:NH1	14:Y:43:ARG:CB	2.73	0.40
15:N:27:THR:HG21	15:N:29:LEU:HD23	2.03	0.40
16:x:23:LEU:HD22	16:x:23:LEU:HA	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	322/324 (99%)	300 (93%)	21 (6%)	1 (0%)	36	67
1	a	320/324 (99%)	299 (93%)	20 (6%)	1 (0%)	36	67
2	B	482/505 (95%)	453 (94%)	29 (6%)	0	100	100
2	b	482/505 (95%)	452 (94%)	30 (6%)	0	100	100
3	C	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
3	c	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
4	D	337/339 (99%)	292 (87%)	45 (13%)	0	100	100
4	d	337/339 (99%)	293 (87%)	44 (13%)	0	100	100
5	E	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
5	e	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
6	F	29/31 (94%)	23 (79%)	6 (21%)	0	100	100
6	f	26/31 (84%)	22 (85%)	4 (15%)	0	100	100
7	H	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	h	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
8	I	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
8	i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	k	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
10	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
11	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	T	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
12	t	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
13	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
13	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
14	Y	27/30 (90%)	23 (85%)	3 (11%)	1 (4%)	2	21
14	y	27/30 (90%)	24 (89%)	2 (7%)	1 (4%)	2	21
15	N	106/108 (98%)	92 (87%)	13 (12%)	1 (1%)	14	44
15	n	106/108 (98%)	94 (89%)	11 (10%)	1 (1%)	14	44
16	X	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
16	x	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
All	All	4240/4366 (97%)	3875 (91%)	359 (8%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	45	ASN
14	y	44	GLY
1	A	141	PRO
1	a	5141	PRO
15	n	124	VAL
15	N	124	VAL

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	A	260/262 (99%)	259 (100%)	1 (0%)	84	83
1	a	260/262 (99%)	259 (100%)	1 (0%)	84	83
2	B	379/403 (94%)	378 (100%)	1 (0%)	86	84
2	b	378/403 (94%)	378 (100%)	0	100	100
3	C	340/348 (98%)	339 (100%)	1 (0%)	86	84
3	c	340/348 (98%)	339 (100%)	1 (0%)	86	84
4	D	273/274 (100%)	273 (100%)	0	100	100
4	d	272/274 (99%)	272 (100%)	0	100	100
5	E	55/57 (96%)	55 (100%)	0	100	100
5	e	55/57 (96%)	55 (100%)	0	100	100
6	F	24/25 (96%)	24 (100%)	0	100	100
6	f	22/25 (88%)	22 (100%)	0	100	100
7	H	50/53 (94%)	50 (100%)	0	100	100
7	h	50/53 (94%)	50 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
8	i	31/31 (100%)	31 (100%)	0	100	100
9	K	29/30 (97%)	29 (100%)	0	100	100
9	k	27/30 (90%)	27 (100%)	0	100	100
10	L	34/35 (97%)	34 (100%)	0	100	100
10	l	34/35 (97%)	34 (100%)	0	100	100
11	M	30/30 (100%)	30 (100%)	0	100	100
11	m	30/30 (100%)	30 (100%)	0	100	100
12	T	26/27 (96%)	26 (100%)	0	100	100
12	t	26/27 (96%)	25 (96%)	1 (4%)	29	52
13	Z	43/52 (83%)	43 (100%)	0	100	100
13	z	43/52 (83%)	43 (100%)	0	100	100
14	Y	22/23 (96%)	11 (50%)	11 (50%)	0	0
14	y	22/23 (96%)	11 (50%)	11 (50%)	0	0
15	N	92/92 (100%)	92 (100%)	0	100	100
15	n	92/92 (100%)	91 (99%)	1 (1%)	65	73
16	X	28/33 (85%)	14 (50%)	14 (50%)	0	0
16	x	28/33 (85%)	15 (54%)	13 (46%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3426/3550 (96%)	3370 (98%)	56 (2%)	54 68

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	VAL
2	B	485	GLU
3	C	410	VAL
1	a	5249	VAL
3	c	5410	VAL
12	t	5025	GLU
14	Y	19	ILE
14	Y	22	LEU
14	Y	25	ILE
14	Y	28	ILE
14	Y	30	ILE
14	Y	34	MET
14	Y	36	ILE
14	Y	39	LEU
14	Y	42	ARG
14	Y	43	ARG
14	Y	46	LEU
15	n	77	ARG
14	y	22	LEU
14	y	23	THR
14	y	25	ILE
14	y	27	MET
14	y	34	MET
14	y	36	ILE
14	y	38	LEU
14	y	39	LEU
14	y	41	VAL
14	y	42	ARG
14	y	43	ARG
16	X	7	LEU
16	X	8	LYS
16	X	11	PHE
16	X	15	LEU
16	X	16	SER
16	X	21	LEU
16	X	23	LEU
16	X	24	THR

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Mol	Chain	Res	Type
16	X	25	PHE
16	X	29	ILE
16	X	31	ILE
16	X	33	GLN
16	X	34	ILE
16	X	36	LYS
16	x	8	LYS
16	x	11	PHE
16	x	12	ILE
16	x	15	LEU
16	x	16	SER
16	x	23	LEU
16	x	24	THR
16	x	25	PHE
16	x	29	ILE
16	x	31	ILE
16	x	34	ILE
16	x	36	LYS
16	x	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	130	GLN
1	A	181	ASN
1	A	187	GLN
1	A	304	HIS
1	A	322	ASN
1	A	325	ASN
2	B	9	HIS
2	B	58	GLN
2	B	274	GLN
2	B	281	GLN
2	B	331	ASN
2	B	338	GLN
2	B	343	HIS
2	B	469	HIS
3	C	118	HIS
3	C	311	GLN
3	C	322	GLN
3	C	385	GLN

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Mol	Chain	Res	Type
4	D	61	HIS
4	D	83	ASN
4	D	129	GLN
4	D	164	GLN
4	D	189	HIS
4	D	224	GLN
4	D	255	GLN
5	E	23	HIS
7	H	59	ASN
9	K	40	GLN
13	Z	58	ASN
1	a	5075	ASN
1	a	5087	ASN
1	a	5092	HIS
1	a	5130	GLN
1	a	5187	GLN
1	a	5322	ASN
1	a	5325	ASN
2	b	5009	HIS
2	b	5058	GLN
2	b	5281	GLN
2	b	5331	ASN
2	b	5338	GLN
2	b	5343	HIS
2	b	5469	HIS
3	c	5056	HIS
3	c	5118	HIS
3	c	5311	GLN
3	c	5382	ASN
3	c	5385	GLN
4	d	5061	HIS
4	d	5083	ASN
4	d	5129	GLN
4	d	5164	GLN
4	d	5189	HIS
4	d	5197	HIS
4	d	5220	ASN
4	d	5301	GLN
5	e	5023	HIS
5	e	5074	GLN
6	f	5024	HIS
7	h	5059	ASN

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Mol	Chain	Res	Type
9	k	5040	GLN
10	l	5004	ASN
10	l	5037	ASN
11	m	5028	GLN
11	m	5032	GLN
13	z	5058	ASN
14	Y	21	GLN
15	n	32	ASN
15	n	61	GLN
15	n	91	GLN
15	n	95	ASN
15	n	100	HIS
15	N	32	ASN
15	N	61	GLN
15	N	100	HIS
14	y	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 6 are monoatomic - leaving 140 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
17	CLA	k	5501	3	69,73,73	1.18	9 (13%)	82,113,113	1.40	6 (7%)
29	HEM	f	5101	-	50,50,50	1.35	4 (8%)	67,82,82	1.02	1 (1%)
22	LMT	a	5410	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	1 (2%)
17	CLA	d	5404	4	54,58,73	1.31	8 (14%)	64,95,113	1.39	6 (9%)
17	CLA	b	5609	2	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
17	CLA	c	5507	-	69,73,73	1.20	9 (13%)	82,113,113	1.34	6 (7%)
17	CLA	a	5403	-	69,73,73	1.20	10 (14%)	82,113,113	1.45	6 (7%)
20	BCR	c	5513	-	41,41,41	1.31	3 (7%)	56,56,56	1.41	8 (14%)
17	CLA	b	5606	-	46,50,73	1.39	9 (19%)	53,85,113	1.60	6 (11%)
18	PHO	D	402	-	58,69,69	1.95	11 (18%)	55,99,99	1.46	8 (14%)
17	CLA	b	5604	2	69,73,73	1.21	8 (11%)	82,113,113	1.40	7 (8%)
20	BCR	C	516	-	41,41,41	1.36	4 (9%)	56,56,56	1.41	9 (16%)
20	BCR	b	5617	-	41,41,41	1.43	4 (9%)	56,56,56	1.47	10 (17%)
22	LMT	A	409	-	36,36,36	1.13	5 (13%)	47,47,47	1.12	3 (6%)
23	SQD	d	5407	-	52,54,54	0.99	6 (11%)	62,65,65	1.60	11 (17%)
26	DGD	b	5621	-	55,55,67	0.99	3 (5%)	69,69,81	1.49	7 (10%)
17	CLA	C	513	3	54,58,73	1.28	10 (18%)	64,95,113	1.38	6 (9%)
17	CLA	c	5511	3	55,59,73	1.30	10 (18%)	64,96,113	1.42	5 (7%)
25	MGE	l	5101	-	48,48,48	0.92	2 (4%)	56,56,56	1.22	5 (8%)
17	CLA	A	403	-	69,73,73	1.18	8 (11%)	82,113,113	1.36	6 (7%)
17	CLA	c	5504	-	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
22	LMT	m	5102	-	36,36,36	1.16	5 (13%)	47,47,47	1.11	3 (6%)
29	HEM	F	101	6	50,50,50	1.34	5 (10%)	67,82,82	1.01	1 (1%)
19	PQ9	a	5407	-	30,30,45	0.82	1 (3%)	38,39,57	1.58	10 (26%)
17	CLA	c	5501	3	69,73,73	1.18	9 (13%)	82,113,113	1.36	6 (7%)
17	CLA	c	5503	3,17	69,73,73	1.18	9 (13%)	82,113,113	1.39	7 (8%)
17	CLA	c	5502	3,17	64,68,73	1.24	8 (12%)	76,107,113	1.47	7 (9%)
17	CLA	a	5402	1	69,73,73	1.22	8 (11%)	82,113,113	1.32	7 (8%)
17	CLA	B	603	2	69,73,73	1.19	8 (11%)	82,113,113	1.41	6 (7%)
17	CLA	C	511	3	69,73,73	1.17	9 (13%)	82,113,113	1.40	5 (6%)
26	DGD	c	5515	-	54,54,67	1.19	5 (9%)	68,68,81	1.43	8 (11%)
22	LMT	B	620	-	36,36,36	1.16	4 (11%)	47,47,47	0.97	1 (2%)
20	BCR	d	5406	-	41,41,41	1.28	3 (7%)	56,56,56	1.29	7 (12%)
20	BCR	b	5619	-	41,41,41	1.41	3 (7%)	56,56,56	1.37	9 (16%)
24	BCT	a	5412	28	3,3,3	1.23	0	2,3,3	4.10	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	MGE	c	5517	-	48,48,48	0.92	2 (4%)	56,56,56	1.11	5 (8%)
17	CLA	B	606	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	6 (7%)
17	CLA	b	5611	2	69,73,73	1.24	10 (14%)	82,113,113	1.51	8 (9%)
26	DGD	D	411	-	55,55,67	1.00	3 (5%)	69,69,81	1.49	7 (10%)
20	BCR	C	515	-	41,41,41	1.29	3 (7%)	56,56,56	1.30	7 (12%)
17	CLA	d	5403	4	69,73,73	1.23	7 (10%)	82,113,113	1.33	7 (8%)
17	CLA	b	5612	2	69,73,73	1.22	8 (11%)	82,113,113	1.41	8 (9%)
18	PHO	a	5405	-	58,69,69	1.98	12 (20%)	55,99,99	1.44	7 (12%)
21	LHG	a	5409	-	38,38,48	0.78	1 (2%)	41,44,54	1.28	5 (12%)
17	CLA	b	5602	2	69,73,73	1.20	9 (13%)	82,113,113	1.30	5 (6%)
19	PQ9	D	406	-	45,45,45	0.68	2 (4%)	56,57,57	1.84	16 (28%)
20	BCR	Y	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.28	6 (10%)
26	DGD	a	5411	-	58,58,67	0.97	3 (5%)	72,72,81	1.52	13 (18%)
20	BCR	D	407	-	41,41,41	1.29	3 (7%)	56,56,56	1.29	7 (12%)
17	CLA	a	5406	1	59,63,73	1.28	9 (15%)	70,101,113	1.40	5 (7%)
25	MGE	m	5101	-	48,48,48	0.94	2 (4%)	56,56,56	1.13	4 (7%)
20	BCR	a	5408	-	41,41,41	1.38	4 (9%)	56,56,56	1.38	9 (16%)
20	BCR	C	514	-	41,41,41	1.31	4 (9%)	56,56,56	1.41	8 (14%)
17	CLA	C	501	3	69,73,73	1.17	8 (11%)	82,113,113	1.37	6 (7%)
17	CLA	B	611	2	69,73,73	1.25	10 (14%)	82,113,113	1.50	8 (9%)
17	CLA	A	401	1	69,73,73	1.22	9 (13%)	82,113,113	1.32	7 (8%)
17	CLA	b	5614	2	60,64,73	1.26	8 (13%)	71,102,113	1.45	6 (8%)
17	CLA	b	5605	2	69,73,73	1.19	10 (14%)	82,113,113	1.38	6 (7%)
17	CLA	b	5613	2	69,73,73	1.24	9 (13%)	82,113,113	1.42	6 (7%)
20	BCR	H	101	17	41,41,41	1.38	3 (7%)	56,56,56	1.28	6 (10%)
17	CLA	B	615	2	69,73,73	1.19	7 (10%)	82,113,113	1.37	5 (6%)
20	BCR	b	5618	-	41,41,41	1.31	4 (9%)	56,56,56	1.47	10 (17%)
25	MGE	C	519	-	48,48,48	0.93	2 (4%)	56,56,56	1.11	5 (8%)
18	PHO	A	404	-	58,69,69	1.99	12 (20%)	55,99,99	1.43	7 (12%)
20	BCR	h	5101	17	41,41,41	1.38	3 (7%)	56,56,56	1.28	6 (10%)
23	SQD	a	5401	-	24,26,54	1.38	5 (20%)	34,37,65	1.82	7 (20%)
25	MGE	d	5409	-	41,41,48	1.01	2 (4%)	49,49,56	1.43	8 (16%)
17	CLA	A	402	-	69,73,73	1.20	10 (14%)	82,113,113	1.44	6 (7%)
17	CLA	c	5509	3	51,55,73	1.36	9 (17%)	60,91,113	1.36	6 (10%)
17	CLA	B	607	-	69,73,73	1.17	9 (13%)	82,113,113	1.40	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	5601	20	45,49,73	1.36	8 (17%)	54,84,113	1.41	6 (11%)
19	PQ9	d	5405	-	45,45,45	0.68	2 (4%)	56,57,57	1.84	16 (28%)
25	MGE	D	408	-	47,47,48	0.96	2 (4%)	55,55,56	1.06	3 (5%)
17	CLA	C	508	3	69,73,73	1.22	9 (13%)	82,113,113	1.45	6 (7%)
24	BCT	A	411	28	3,3,3	1.22	0	2,3,3	4.10	2 (100%)
19	PQ9	A	406	-	45,45,45	0.70	1 (2%)	56,57,57	1.61	15 (26%)
17	CLA	b	5607	-	69,73,73	1.17	9 (13%)	82,113,113	1.40	6 (7%)
17	CLA	b	5603	2	69,73,73	1.19	8 (11%)	82,113,113	1.41	6 (7%)
20	BCR	c	5514	-	41,41,41	1.36	4 (9%)	56,56,56	1.41	9 (16%)
25	MGE	d	5408	-	47,47,48	0.97	2 (4%)	55,55,56	1.14	3 (5%)
25	MGE	d	5410	-	48,48,48	0.93	2 (4%)	56,56,56	1.26	5 (8%)
17	CLA	C	505	-	69,73,73	1.15	7 (10%)	82,113,113	1.37	8 (9%)
20	BCR	t	5101	-	41,41,41	1.42	3 (7%)	56,56,56	1.38	11 (19%)
22	LMT	T	101	-	36,36,36	1.07	4 (11%)	47,47,47	1.01	1 (2%)
22	LMT	M	101	-	36,36,36	1.23	7 (19%)	47,47,47	1.10	1 (2%)
17	CLA	B	608	2	69,73,73	1.19	8 (11%)	82,113,113	1.41	8 (9%)
17	CLA	C	509	3	51,55,73	1.37	9 (17%)	60,91,113	1.37	6 (10%)
20	BCR	B	618	-	41,41,41	1.31	4 (9%)	56,56,56	1.47	10 (17%)
17	CLA	B	601	20	45,49,73	1.36	8 (17%)	54,84,113	1.41	6 (11%)
17	CLA	B	602	2	69,73,73	1.20	9 (13%)	82,113,113	1.29	5 (6%)
17	CLA	B	604	2	69,73,73	1.21	8 (11%)	82,113,113	1.40	7 (8%)
20	BCR	A	407	-	41,41,41	1.38	4 (9%)	56,56,56	1.39	10 (17%)
17	CLA	C	504	-	50,54,73	1.33	9 (18%)	59,90,113	1.42	4 (6%)
17	CLA	C	503	3,17	69,73,73	1.19	8 (11%)	82,113,113	1.40	7 (8%)
17	CLA	C	506	3	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
18	PHO	d	5402	-	58,69,69	1.94	11 (18%)	55,99,99	1.47	8 (14%)
17	CLA	a	5404	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
17	CLA	b	5608	2	69,73,73	1.18	7 (10%)	82,113,113	1.41	8 (9%)
23	SQD	A	410	-	24,26,54	1.36	4 (16%)	34,37,65	1.76	8 (23%)
20	BCR	B	617	-	41,41,41	1.43	4 (9%)	56,56,56	1.47	10 (17%)
26	DGD	C	518	-	58,58,67	0.96	3 (5%)	72,72,81	1.52	12 (16%)
26	DGD	c	5516	-	48,48,67	1.02	2 (4%)	62,62,81	1.43	7 (11%)
25	MGE	b	5620	-	48,48,48	0.95	2 (4%)	56,56,56	1.15	4 (7%)
17	CLA	b	5615	2	69,73,73	1.19	7 (10%)	82,113,113	1.37	5 (6%)
17	CLA	C	502	3,17	64,68,73	1.24	8 (12%)	76,107,113	1.48	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	5610	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	7 (8%)
17	CLA	B	610	-	69,73,73	1.19	7 (10%)	82,113,113	1.37	7 (8%)
17	CLA	D	404	4	69,73,73	1.23	7 (10%)	82,113,113	1.32	6 (7%)
17	CLA	B	613	2	69,73,73	1.24	9 (13%)	82,113,113	1.43	7 (8%)
17	CLA	B	609	2	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
17	CLA	D	405	4	54,58,73	1.31	8 (14%)	64,95,113	1.39	6 (9%)
17	CLA	c	5508	3	69,73,73	1.22	9 (13%)	82,113,113	1.45	6 (7%)
20	BCR	z	5101	-	41,41,41	1.29	3 (7%)	56,56,56	1.30	7 (12%)
17	CLA	B	614	2,25	60,64,73	1.27	8 (13%)	71,102,113	1.44	5 (7%)
17	CLA	C	510	3	69,73,73	1.20	9 (13%)	82,113,113	1.31	6 (7%)
23	SQD	L	101	-	45,47,54	1.03	5 (11%)	55,58,65	1.57	11 (20%)
17	CLA	c	5505	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
23	SQD	l	5102	-	45,47,54	1.02	3 (6%)	55,58,65	1.65	12 (21%)
17	CLA	C	512	3	55,59,73	1.30	10 (18%)	64,96,113	1.42	5 (7%)
25	MGE	D	410	25	48,48,48	0.93	3 (6%)	56,56,56	1.26	4 (7%)
26	DGD	C	517	-	48,48,67	1.03	2 (4%)	62,62,81	1.43	7 (11%)
20	BCR	T	102	-	41,41,41	1.19	4 (9%)	56,56,56	1.33	7 (12%)
20	BCR	t	5102	-	41,41,41	1.32	3 (7%)	56,56,56	1.23	7 (12%)
17	CLA	c	5510	3	69,73,73	1.19	9 (13%)	82,113,113	1.30	6 (7%)
25	MGE	D	409	-	41,41,48	1.02	2 (4%)	49,49,56	1.44	8 (16%)
25	MGE	m	5103	17	48,48,48	0.92	2 (4%)	56,56,56	1.03	3 (5%)
26	DGD	A	413	-	54,54,67	1.19	5 (9%)	68,68,81	1.43	8 (11%)
25	MGE	B	619	-	48,48,48	0.95	2 (4%)	56,56,56	1.15	4 (7%)
17	CLA	B	616	2	69,73,73	1.19	10 (14%)	82,113,113	1.35	7 (8%)
17	CLA	c	5506	3	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
21	LHG	A	408	-	38,38,48	0.78	1 (2%)	41,44,54	1.28	5 (12%)
17	CLA	B	605	2	69,73,73	1.20	10 (14%)	82,113,113	1.38	6 (7%)
17	CLA	b	5616	2	69,73,73	1.19	10 (14%)	82,113,113	1.35	7 (8%)
23	SQD	D	403	-	52,54,54	1.00	6 (11%)	62,65,65	1.49	12 (19%)
17	CLA	A	405	1	59,63,73	1.27	9 (15%)	70,101,113	1.40	5 (7%)
17	CLA	C	507	-	69,73,73	1.20	9 (13%)	82,113,113	1.34	5 (6%)
20	BCR	k	5502	-	41,41,41	1.21	3 (7%)	56,56,56	1.32	6 (10%)
17	CLA	c	5512	3	54,58,73	1.28	10 (18%)	64,95,113	1.37	6 (9%)
25	MGE	A	412	25	48,48,48	0.92	2 (4%)	56,56,56	1.22	5 (8%)
17	CLA	B	612	2	69,73,73	1.22	7 (10%)	82,113,113	1.41	8 (9%)

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
17	CLA	k	5501	3	1/1/15/20	12/39/115/115	-
29	HEM	f	5101	-	-	2/14/54/54	-
22	LMT	a	5410	-	-	8/21/61/61	0/2/2/2
17	CLA	d	5404	4	1/1/12/20	9/21/97/115	-
17	CLA	b	5609	2	1/1/15/20	17/39/115/115	-
17	CLA	c	5507	-	1/1/15/20	13/39/115/115	-
17	CLA	a	5403	-	1/1/15/20	14/39/115/115	-
20	BCR	c	5513	-	-	13/29/63/63	0/2/2/2
17	CLA	b	5606	-	1/1/10/20	4/12/88/115	-
18	PHO	D	402	-	-	11/37/103/103	0/5/6/6
17	CLA	b	5604	2	1/1/15/20	14/39/115/115	-
20	BCR	C	516	-	-	18/29/63/63	0/2/2/2
20	BCR	b	5617	-	-	14/29/63/63	0/2/2/2
22	LMT	A	409	-	-	10/21/61/61	0/2/2/2
23	SQD	d	5407	-	-	15/49/69/69	0/1/1/1
26	DGD	b	5621	-	-	21/43/83/95	0/2/2/2
17	CLA	C	513	3	1/1/12/20	3/21/97/115	-
17	CLA	c	5511	3	1/1/12/20	8/23/99/115	-
25	MGE	l	5101	-	-	12/43/63/63	0/1/1/1
17	CLA	A	403	-	1/1/15/20	13/39/115/115	-
17	CLA	c	5504	-	1/1/11/20	10/17/93/115	-
22	LMT	m	5102	-	-	9/21/61/61	0/2/2/2
29	HEM	F	101	6	-	2/14/54/54	-
19	PQ9	a	5407	-	-	7/23/43/61	0/1/1/1
17	CLA	c	5501	3	1/1/15/20	18/39/115/115	-
17	CLA	c	5503	3,17	1/1/15/20	22/39/115/115	-
17	CLA	c	5502	3,17	1/1/14/20	11/33/109/115	-
17	CLA	a	5402	1	1/1/15/20	13/39/115/115	-
17	CLA	B	603	2	1/1/15/20	15/39/115/115	-
17	CLA	C	511	3	1/1/15/20	12/39/115/115	-
26	DGD	c	5515	-	-	19/42/82/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMT	B	620	-	-	7/21/61/61	0/2/2/2
20	BCR	d	5406	-	-	16/29/63/63	0/2/2/2
20	BCR	b	5619	-	-	9/29/63/63	0/2/2/2
25	MGE	c	5517	-	-	11/43/63/63	0/1/1/1
17	CLA	B	606	-	1/1/15/20	16/39/115/115	-
17	CLA	b	5611	2	1/1/15/20	12/39/115/115	-
26	DGD	D	411	-	-	21/43/83/95	0/2/2/2
20	BCR	C	515	-	-	21/29/63/63	0/2/2/2
17	CLA	d	5403	4	1/1/15/20	24/39/115/115	-
17	CLA	b	5612	2	1/1/15/20	17/39/115/115	-
18	PHO	a	5405	-	-	16/37/103/103	0/5/6/6
21	LHG	a	5409	-	-	22/43/43/53	-
17	CLA	b	5602	2	1/1/15/20	19/39/115/115	-
19	PQ9	D	406	-	-	9/41/61/61	0/1/1/1
20	BCR	Y	101	-	-	9/29/63/63	0/2/2/2
26	DGD	a	5411	-	-	18/46/86/95	0/2/2/2
20	BCR	D	407	-	-	16/29/63/63	0/2/2/2
17	CLA	a	5406	1	1/1/13/20	6/27/103/115	-
25	MGE	m	5101	-	-	9/43/63/63	0/1/1/1
20	BCR	a	5408	-	-	13/29/63/63	0/2/2/2
20	BCR	C	514	-	-	12/29/63/63	0/2/2/2
17	CLA	C	501	3	1/1/15/20	18/39/115/115	-
17	CLA	B	611	2	1/1/15/20	12/39/115/115	-
17	CLA	A	401	1	1/1/15/20	13/39/115/115	-
17	CLA	b	5614	2	1/1/13/20	9/29/105/115	-
17	CLA	b	5605	2	1/1/15/20	19/39/115/115	-
17	CLA	b	5613	2	1/1/15/20	22/39/115/115	-
20	BCR	H	101	17	-	10/29/63/63	0/2/2/2
17	CLA	B	615	2	1/1/15/20	15/39/115/115	-
20	BCR	b	5618	-	-	14/29/63/63	0/2/2/2
25	MGE	C	519	-	-	11/43/63/63	0/1/1/1
18	PHO	A	404	-	-	16/37/103/103	0/5/6/6
20	BCR	h	5101	17	-	10/29/63/63	0/2/2/2
23	SQD	a	5401	-	-	10/19/39/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	MGE	d	5409	-	-	12/36/56/63	0/1/1/1
17	CLA	A	402	-	1/1/15/20	14/39/115/115	-
17	CLA	c	5509	3	1/1/11/20	4/18/94/115	-
17	CLA	B	607	-	1/1/15/20	18/39/115/115	-
17	CLA	b	5601	20	1/1/10/20	2/10/86/115	-
19	PQ9	d	5405	-	-	9/41/61/61	0/1/1/1
25	MGE	D	408	-	-	9/42/62/63	0/1/1/1
17	CLA	C	508	3	1/1/15/20	15/39/115/115	-
19	PQ9	A	406	-	-	12/41/61/61	0/1/1/1
17	CLA	b	5607	-	1/1/15/20	18/39/115/115	-
17	CLA	b	5603	2	1/1/15/20	15/39/115/115	-
20	BCR	c	5514	-	-	18/29/63/63	0/2/2/2
25	MGE	d	5408	-	-	15/42/62/63	0/1/1/1
25	MGE	d	5410	-	-	14/43/63/63	0/1/1/1
17	CLA	C	505	-	1/1/15/20	21/39/115/115	-
20	BCR	t	5101	-	-	9/29/63/63	0/2/2/2
22	LMT	T	101	-	-	10/21/61/61	0/2/2/2
22	LMT	M	101	-	-	8/21/61/61	0/2/2/2
17	CLA	B	608	2	1/1/15/20	9/39/115/115	-
17	CLA	C	509	3	1/1/11/20	4/18/94/115	-
20	BCR	B	618	-	-	14/29/63/63	0/2/2/2
17	CLA	B	601	20	1/1/10/20	2/10/86/115	-
17	CLA	B	602	2	1/1/15/20	19/39/115/115	-
17	CLA	B	604	2	1/1/15/20	14/39/115/115	-
20	BCR	A	407	-	-	13/29/63/63	0/2/2/2
17	CLA	C	504	-	1/1/11/20	10/17/93/115	-
17	CLA	C	503	3,17	1/1/15/20	22/39/115/115	-
17	CLA	C	506	3	1/1/15/20	19/39/115/115	-
18	PHO	d	5402	-	-	11/37/103/103	0/5/6/6
17	CLA	a	5404	-	1/1/15/20	13/39/115/115	-
17	CLA	b	5608	2	1/1/15/20	9/39/115/115	-
23	SQD	A	410	-	-	9/19/39/69	0/1/1/1
20	BCR	B	617	-	-	14/29/63/63	0/2/2/2
26	DGD	C	518	-	-	18/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	c	5516	-	-	17/36/76/95	0/2/2/2
25	MGE	b	5620	-	-	12/43/63/63	0/1/1/1
17	CLA	b	5615	2	1/1/15/20	15/39/115/115	-
17	CLA	C	502	3,17	1/1/14/20	11/33/109/115	-
17	CLA	b	5610	-	1/1/15/20	16/39/115/115	-
17	CLA	B	610	-	1/1/15/20	16/39/115/115	-
17	CLA	D	404	4	1/1/15/20	24/39/115/115	-
17	CLA	B	613	2	1/1/15/20	22/39/115/115	-
17	CLA	B	609	2	1/1/15/20	17/39/115/115	-
17	CLA	D	405	4	1/1/12/20	9/21/97/115	-
17	CLA	c	5508	3	1/1/15/20	15/39/115/115	-
20	BCR	z	5101	-	-	21/29/63/63	0/2/2/2
17	CLA	B	614	2,25	1/1/13/20	9/29/105/115	-
17	CLA	C	510	3	1/1/15/20	7/39/115/115	-
23	SQD	L	101	-	-	23/42/62/69	0/1/1/1
17	CLA	c	5505	-	1/1/15/20	21/39/115/115	-
23	SQD	l	5102	-	-	15/42/62/69	0/1/1/1
17	CLA	C	512	3	1/1/12/20	8/23/99/115	-
25	MGE	D	410	25	-	17/43/63/63	0/1/1/1
26	DGD	C	517	-	-	17/36/76/95	0/2/2/2
20	BCR	T	102	-	-	11/29/63/63	0/2/2/2
20	BCR	t	5102	-	-	13/29/63/63	0/2/2/2
17	CLA	c	5510	3	1/1/15/20	7/39/115/115	-
25	MGE	D	409	-	-	16/36/56/63	0/1/1/1
25	MGE	m	5103	17	-	22/43/63/63	0/1/1/1
26	DGD	A	413	-	-	19/42/82/95	0/2/2/2
25	MGE	B	619	-	-	12/43/63/63	0/1/1/1
17	CLA	B	616	2	1/1/15/20	6/39/115/115	-
17	CLA	c	5506	3	1/1/15/20	19/39/115/115	-
21	LHG	A	408	-	-	22/43/43/53	-
17	CLA	B	605	2	1/1/15/20	19/39/115/115	-
17	CLA	b	5616	2	1/1/15/20	6/39/115/115	-
23	SQD	D	403	-	-	24/49/69/69	0/1/1/1
17	CLA	A	405	1	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	C	507	-	1/1/15/20	13/39/115/115	-
20	BCR	k	5502	-	-	13/29/63/63	0/2/2/2
17	CLA	c	5512	3	1/1/12/20	3/21/97/115	-
25	MGE	A	412	25	-	12/43/63/63	0/1/1/1
17	CLA	B	612	2	1/1/15/20	16/39/115/115	-

All (857) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	402	PHO	C1B-C2B	8.40	1.48	1.39
18	d	5402	PHO	C1B-C2B	8.39	1.48	1.39
18	a	5405	PHO	C1B-C2B	8.01	1.48	1.39
18	A	404	PHO	C1B-C2B	7.99	1.48	1.39
18	A	404	PHO	C3B-C4B	7.20	1.48	1.41
18	a	5405	PHO	C3B-C4B	7.12	1.48	1.41
18	d	5402	PHO	C3B-C4B	6.25	1.47	1.41
18	D	402	PHO	C3B-C4B	6.22	1.47	1.41
20	B	617	BCR	C30-C25	-5.03	1.47	1.53
20	b	5617	BCR	C30-C25	-5.03	1.47	1.53
20	t	5101	BCR	C30-C25	-4.86	1.47	1.53
20	h	5101	BCR	C1-C6	-4.84	1.47	1.53
20	b	5619	BCR	C30-C25	-4.83	1.47	1.53
20	H	101	BCR	C1-C6	-4.77	1.47	1.53
20	D	407	BCR	C1-C6	-4.61	1.47	1.53
20	A	407	BCR	C30-C25	-4.59	1.47	1.53
20	a	5408	BCR	C30-C25	-4.56	1.47	1.53
20	d	5406	BCR	C1-C6	-4.56	1.47	1.53
20	t	5102	BCR	C30-C25	-4.53	1.48	1.53
20	c	5514	BCR	C1-C6	-4.49	1.48	1.53
20	C	516	BCR	C1-C6	-4.48	1.48	1.53
20	t	5101	BCR	C1-C6	-4.48	1.48	1.53
20	b	5619	BCR	C1-C6	-4.46	1.48	1.53
20	h	5101	BCR	C30-C25	-4.32	1.48	1.53
20	H	101	BCR	C30-C25	-4.27	1.48	1.53
20	c	5513	BCR	C1-C6	-4.25	1.48	1.53
20	z	5101	BCR	C1-C6	-4.23	1.48	1.53
20	A	407	BCR	C1-C6	-4.22	1.48	1.53
20	C	515	BCR	C1-C6	-4.21	1.48	1.53
25	D	409	MGE	O1G-C1A	4.21	1.45	1.33
25	b	5620	MGE	O1G-C1A	4.20	1.45	1.33
20	a	5408	BCR	C1-C6	-4.20	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	5408	MGE	O1G-C1A	4.20	1.45	1.33
25	d	5409	MGE	O1G-C1A	4.19	1.45	1.33
20	C	514	BCR	C1-C6	-4.18	1.48	1.53
25	B	619	MGE	O1G-C1A	4.18	1.45	1.33
20	z	5101	BCR	C30-C25	-4.18	1.48	1.53
25	D	408	MGE	O1G-C1A	4.16	1.45	1.33
20	C	515	BCR	C30-C25	-4.15	1.48	1.53
25	C	519	MGE	O2G-C1B	4.13	1.45	1.34
25	m	5101	MGE	O1G-C1A	4.13	1.45	1.33
25	m	5103	MGE	O1G-C1A	4.11	1.45	1.33
25	d	5408	MGE	O2G-C1B	4.11	1.45	1.34
25	C	519	MGE	O1G-C1A	4.11	1.45	1.33
25	c	5517	MGE	O1G-C1A	4.10	1.45	1.33
25	c	5517	MGE	O2G-C1B	4.10	1.45	1.34
25	l	5101	MGE	O2G-C1B	4.08	1.45	1.34
25	d	5410	MGE	O1G-C1A	4.06	1.45	1.33
20	b	5618	BCR	C30-C25	-4.05	1.48	1.53
20	b	5617	BCR	C1-C6	-4.05	1.48	1.53
25	D	410	MGE	O1G-C1A	4.04	1.45	1.33
25	A	412	MGE	O2G-C1B	4.04	1.45	1.34
20	B	618	BCR	C30-C25	-4.03	1.48	1.53
20	t	5102	BCR	C1-C6	-4.03	1.48	1.53
20	B	617	BCR	C1-C6	-4.01	1.48	1.53
25	B	619	MGE	O2G-C1B	4.00	1.45	1.34
20	C	514	BCR	C30-C25	-4.00	1.48	1.53
25	b	5620	MGE	O2G-C1B	3.99	1.45	1.34
20	c	5513	BCR	C30-C25	-3.98	1.48	1.53
20	c	5514	BCR	C30-C25	-3.97	1.48	1.53
20	C	516	BCR	C30-C25	-3.97	1.48	1.53
25	l	5101	MGE	O1G-C1A	3.96	1.44	1.33
20	k	5502	BCR	C1-C6	-3.94	1.48	1.53
25	D	408	MGE	O2G-C1B	3.94	1.45	1.34
25	A	412	MGE	O1G-C1A	3.92	1.44	1.33
25	d	5409	MGE	O2G-C1B	3.92	1.45	1.34
25	m	5103	MGE	O2G-C1B	3.89	1.45	1.34
25	m	5101	MGE	O2G-C1B	3.88	1.45	1.34
25	D	409	MGE	O2G-C1B	3.82	1.45	1.34
25	d	5410	MGE	O2G-C1B	3.79	1.45	1.34
20	B	618	BCR	C1-C6	-3.79	1.48	1.53
20	b	5618	BCR	C1-C6	-3.73	1.49	1.53
25	D	410	MGE	O2G-C1B	3.71	1.44	1.34
20	T	102	BCR	C1-C6	-3.66	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	101	BCR	C1-C6	-3.60	1.49	1.53
20	d	5406	BCR	C30-C25	-3.51	1.49	1.53
20	D	407	BCR	C30-C25	-3.50	1.49	1.53
20	Y	101	BCR	C30-C25	-3.47	1.49	1.53
18	a	5405	PHO	C3B-C2B	-3.44	1.35	1.40
18	A	404	PHO	C3B-C2B	-3.44	1.35	1.40
20	k	5502	BCR	C30-C25	-3.44	1.49	1.53
17	d	5403	CLA	MG-NB	-3.39	1.99	2.05
17	D	404	CLA	MG-NB	-3.38	1.99	2.05
18	d	5402	PHO	CAC-C3C	-3.34	1.45	1.51
18	D	402	PHO	CAC-C3C	-3.33	1.45	1.51
17	b	5611	CLA	CMC-C2C	-3.30	1.44	1.50
20	T	102	BCR	C30-C25	-3.29	1.49	1.53
17	B	611	CLA	CMC-C2C	-3.27	1.44	1.50
17	B	613	CLA	MG-NB	-3.27	1.99	2.05
23	a	5401	SQD	O47-C7	3.27	1.42	1.35
17	A	401	CLA	MG-NB	-3.26	1.99	2.05
17	a	5402	CLA	MG-NB	-3.25	1.99	2.05
17	b	5613	CLA	MG-NB	-3.25	1.99	2.05
17	b	5603	CLA	MG-NB	-3.24	1.99	2.05
17	b	5608	CLA	MG-NB	-3.23	1.99	2.05
17	B	608	CLA	MG-NB	-3.23	1.99	2.05
17	B	603	CLA	MG-NB	-3.21	1.99	2.05
23	A	410	SQD	O47-C7	3.21	1.42	1.35
18	A	404	PHO	CAC-C3C	-3.20	1.46	1.51
17	b	5612	CLA	MG-NB	-3.18	1.99	2.05
17	B	612	CLA	MG-NB	-3.17	1.99	2.05
18	a	5405	PHO	CAC-C3C	-3.16	1.46	1.51
29	F	101	HEM	FE-ND	3.16	2.04	1.94
17	B	604	CLA	MG-NB	-3.15	1.99	2.05
17	C	508	CLA	CMC-C2C	-3.15	1.44	1.50
29	f	5101	HEM	FE-ND	3.15	2.04	1.94
17	b	5604	CLA	MG-NB	-3.13	1.99	2.05
17	b	5610	CLA	MG-NB	-3.13	1.99	2.05
26	D	411	DGD	O1G-C1G	-3.13	1.38	1.45
18	A	404	PHO	CMC-C2C	-3.13	1.45	1.50
17	B	610	CLA	MG-NB	-3.12	1.99	2.05
17	c	5508	CLA	CMC-C2C	-3.12	1.44	1.50
17	C	508	CLA	MG-NB	-3.12	1.99	2.05
18	a	5405	PHO	CMC-C2C	-3.11	1.45	1.50
17	B	615	CLA	MG-NB	-3.11	1.99	2.05
17	C	502	CLA	MG-NB	-3.11	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5615	CLA	MG-NB	-3.11	1.99	2.05
26	b	5621	DGD	O1G-C1G	-3.10	1.38	1.45
17	c	5510	CLA	MG-NB	-3.10	1.99	2.05
23	D	403	SQD	O48-C23	3.10	1.42	1.33
17	c	5508	CLA	MG-NB	-3.09	1.99	2.05
18	D	402	PHO	CMC-C2C	-3.08	1.45	1.50
17	k	5501	CLA	MG-NB	-3.07	1.99	2.05
17	c	5502	CLA	MG-NB	-3.07	1.99	2.05
17	c	5507	CLA	MG-NB	-3.07	1.99	2.05
17	c	5509	CLA	MG-NB	-3.06	1.99	2.05
26	c	5515	DGD	O1G-C1G	-3.06	1.38	1.45
17	C	507	CLA	MG-NB	-3.06	1.99	2.05
17	D	404	CLA	CMD-C2D	-3.06	1.44	1.50
17	B	616	CLA	MG-NB	-3.05	1.99	2.05
23	d	5407	SQD	O48-C23	3.05	1.42	1.33
17	C	511	CLA	MG-NB	-3.05	1.99	2.05
17	C	510	CLA	MG-NB	-3.05	1.99	2.05
17	d	5403	CLA	CMD-C2D	-3.05	1.44	1.50
18	d	5402	PHO	CMC-C2C	-3.05	1.45	1.50
17	b	5614	CLA	MG-NB	-3.04	1.99	2.05
26	A	413	DGD	O1G-C1G	-3.04	1.38	1.45
18	D	402	PHO	C3B-C2B	-3.04	1.36	1.40
17	C	505	CLA	MG-NB	-3.04	1.99	2.05
18	d	5402	PHO	C3B-C2B	-3.03	1.36	1.40
17	a	5404	CLA	MG-NB	-3.03	1.99	2.05
17	B	614	CLA	MG-NB	-3.03	1.99	2.05
17	b	5606	CLA	MG-NB	-3.03	1.99	2.05
17	A	403	CLA	MG-NB	-3.02	1.99	2.05
17	D	405	CLA	MG-NB	-3.02	1.99	2.05
17	C	509	CLA	MG-NB	-3.01	1.99	2.05
18	a	5405	PHO	C1D-C2D	3.01	1.42	1.39
18	a	5405	PHO	CMD-C2D	-3.01	1.45	1.51
17	b	5616	CLA	MG-NB	-3.01	1.99	2.05
29	f	5101	HEM	CAC-C3C	3.00	1.55	1.47
17	d	5404	CLA	MG-NB	-3.00	1.99	2.05
17	B	606	CLA	MG-NB	-3.00	1.99	2.05
17	c	5505	CLA	MG-NB	-3.00	1.99	2.05
29	F	101	HEM	CAC-C3C	3.00	1.55	1.47
17	C	503	CLA	MG-NB	-2.99	1.99	2.05
18	A	404	PHO	CMD-C2D	-2.98	1.45	1.51
18	A	404	PHO	CBD-CGD	-2.98	1.48	1.52
17	b	5601	CLA	C1D-ND	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5503	CLA	MG-NB	-2.97	1.99	2.05
17	b	5607	CLA	MG-NB	-2.97	1.99	2.05
18	A	404	PHO	C1D-C2D	2.97	1.42	1.39
18	d	5402	PHO	CBD-CGD	-2.97	1.48	1.52
18	D	402	PHO	CBD-CGD	-2.96	1.48	1.52
18	a	5405	PHO	CMB-C2B	-2.96	1.45	1.51
17	A	402	CLA	MG-NB	-2.96	1.99	2.05
17	B	601	CLA	C1D-ND	2.96	1.41	1.37
23	L	101	SQD	O48-C23	2.95	1.42	1.33
17	b	5602	CLA	MG-NB	-2.95	1.99	2.05
23	l	5102	SQD	O48-C23	2.95	1.41	1.33
17	c	5506	CLA	MG-NB	-2.94	2.00	2.05
17	B	602	CLA	MG-NB	-2.94	2.00	2.05
17	B	605	CLA	MG-NB	-2.94	2.00	2.05
18	a	5405	PHO	CBD-CGD	-2.93	1.48	1.52
18	D	402	PHO	CMB-C2B	-2.93	1.45	1.51
21	A	408	LHG	O7-C5	-2.93	1.39	1.46
18	A	404	PHO	CMB-C2B	-2.93	1.45	1.51
17	B	607	CLA	MG-NB	-2.92	2.00	2.05
21	a	5409	LHG	O7-C5	-2.92	1.39	1.46
17	b	5611	CLA	MG-NB	-2.92	2.00	2.05
17	C	512	CLA	MG-NB	-2.92	2.00	2.05
17	a	5403	CLA	MG-NB	-2.91	2.00	2.05
17	b	5605	CLA	MG-NB	-2.91	2.00	2.05
18	d	5402	PHO	CMB-C2B	-2.91	1.45	1.51
29	F	101	HEM	CAB-C3B	2.91	1.55	1.47
17	B	611	CLA	MG-NB	-2.90	2.00	2.05
29	f	5101	HEM	CAB-C3B	2.90	1.55	1.47
17	c	5511	CLA	MG-NB	-2.89	2.00	2.05
17	c	5501	CLA	MG-NB	-2.88	2.00	2.05
17	C	506	CLA	MG-NB	-2.88	2.00	2.05
17	c	5512	CLA	MG-NB	-2.88	2.00	2.05
17	C	501	CLA	MG-NB	-2.87	2.00	2.05
17	a	5406	CLA	MG-NB	-2.87	2.00	2.05
17	A	405	CLA	MG-NB	-2.86	2.00	2.05
18	D	402	PHO	CMD-C2D	-2.85	1.45	1.51
18	d	5402	PHO	C4D-CHA	2.84	1.43	1.39
17	C	513	CLA	MG-NB	-2.84	2.00	2.05
18	d	5402	PHO	CMD-C2D	-2.84	1.46	1.51
23	l	5102	SQD	O47-C7	2.83	1.42	1.34
18	D	402	PHO	C4D-CHA	2.83	1.43	1.39
17	c	5504	CLA	MG-NB	-2.82	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	620	LMT	O3'-C3'	-2.82	1.36	1.43
17	B	604	CLA	C1B-NB	-2.81	1.34	1.37
18	D	402	PHO	C1D-C2D	2.81	1.42	1.39
18	a	5405	PHO	C4D-CHA	2.80	1.43	1.39
17	b	5609	CLA	MG-NB	-2.80	2.00	2.05
17	b	5603	CLA	C1B-NB	-2.79	1.34	1.37
17	C	504	CLA	MG-NB	-2.78	2.00	2.05
17	C	502	CLA	C1D-ND	2.78	1.41	1.37
17	B	609	CLA	MG-NB	-2.77	2.00	2.05
17	a	5402	CLA	MG-ND	-2.77	2.00	2.05
17	B	611	CLA	CMB-C2B	-2.77	1.45	1.50
23	d	5407	SQD	O47-C7	2.77	1.42	1.34
23	D	403	SQD	O47-C7	2.77	1.42	1.34
17	c	5502	CLA	C1D-ND	2.76	1.41	1.37
17	b	5604	CLA	C1B-NB	-2.76	1.34	1.37
17	B	603	CLA	C1B-NB	-2.75	1.34	1.37
17	b	5611	CLA	CMB-C2B	-2.75	1.45	1.50
17	B	612	CLA	C1B-NB	-2.75	1.34	1.37
17	b	5612	CLA	C1B-NB	-2.75	1.34	1.37
17	B	604	CLA	CMB-C2B	-2.74	1.45	1.50
17	b	5604	CLA	CMB-C2B	-2.74	1.45	1.50
17	B	613	CLA	C1B-NB	-2.74	1.34	1.37
17	A	401	CLA	MG-ND	-2.74	2.00	2.05
17	D	404	CLA	CMB-C2B	-2.74	1.45	1.50
17	B	612	CLA	CMD-C2D	-2.74	1.45	1.50
17	C	503	CLA	CMD-C2D	-2.74	1.45	1.50
17	B	608	CLA	CMB-C2B	-2.73	1.45	1.50
17	b	5608	CLA	CMB-C2B	-2.73	1.45	1.50
17	D	404	CLA	MG-ND	-2.73	2.00	2.05
17	b	5613	CLA	C1B-NB	-2.72	1.34	1.37
18	A	404	PHO	C4D-CHA	2.72	1.43	1.39
17	B	604	CLA	MG-ND	-2.72	2.00	2.05
17	B	613	CLA	CMD-C2D	-2.71	1.45	1.50
17	B	608	CLA	MG-ND	-2.71	2.00	2.05
17	d	5403	CLA	MG-ND	-2.71	2.00	2.05
17	B	602	CLA	MG-ND	-2.71	2.00	2.05
17	d	5403	CLA	CMB-C2B	-2.71	1.45	1.50
17	b	5604	CLA	MG-ND	-2.70	2.00	2.05
17	b	5611	CLA	CMD-C2D	-2.70	1.45	1.50
17	a	5403	CLA	CMB-C2B	-2.69	1.45	1.50
17	c	5509	CLA	CMD-C2D	-2.69	1.45	1.50
17	C	512	CLA	C1D-ND	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	5101	HEM	FE-NB	2.69	2.03	1.94
17	b	5608	CLA	MG-ND	-2.69	2.00	2.05
18	d	5402	PHO	C1D-C2D	2.69	1.42	1.39
17	B	611	CLA	CMD-C2D	-2.68	1.45	1.50
19	A	406	PQ9	C10-C5	2.68	1.48	1.35
17	c	5503	CLA	CMD-C2D	-2.68	1.45	1.50
17	b	5613	CLA	MG-ND	-2.68	2.00	2.05
17	b	5612	CLA	CMD-C2D	-2.68	1.45	1.50
17	b	5616	CLA	CMC-C2C	-2.68	1.45	1.50
19	a	5407	PQ9	C10-C5	2.68	1.48	1.35
17	b	5608	CLA	C1B-NB	-2.67	1.34	1.37
17	b	5602	CLA	MG-ND	-2.67	2.00	2.05
17	B	613	CLA	MG-ND	-2.67	2.00	2.05
17	b	5613	CLA	CMD-C2D	-2.67	1.45	1.50
17	C	509	CLA	CMD-C2D	-2.66	1.45	1.50
17	C	507	CLA	MG-ND	-2.66	2.00	2.05
17	C	511	CLA	C1D-ND	2.65	1.41	1.37
17	c	5507	CLA	MG-ND	-2.65	2.00	2.05
17	b	5610	CLA	CMD-C2D	-2.65	1.45	1.50
17	A	401	CLA	CMD-C2D	-2.65	1.45	1.50
29	F	101	HEM	FE-NB	2.65	2.03	1.94
17	B	616	CLA	CMC-C2C	-2.64	1.45	1.50
17	B	613	CLA	CMB-C2B	-2.64	1.45	1.50
22	B	620	LMT	O2'-C2'	-2.64	1.36	1.43
18	A	404	PHO	C4D-ND	-2.64	1.34	1.38
17	B	608	CLA	C1B-NB	-2.64	1.34	1.37
17	C	508	CLA	MG-ND	-2.64	2.00	2.05
17	B	610	CLA	MG-ND	-2.63	2.00	2.05
17	A	402	CLA	CMB-C2B	-2.63	1.45	1.50
18	D	402	PHO	C4D-ND	-2.63	1.34	1.38
17	b	5610	CLA	MG-ND	-2.63	2.00	2.05
17	a	5406	CLA	CMB-C2B	-2.63	1.45	1.50
17	k	5501	CLA	C1D-ND	2.63	1.41	1.37
17	A	401	CLA	CMB-C2B	-2.63	1.45	1.50
17	c	5511	CLA	C1D-ND	2.63	1.41	1.37
22	M	101	LMT	O2B-C2B	-2.63	1.36	1.43
17	c	5501	CLA	C1D-ND	2.62	1.41	1.37
17	B	612	CLA	MG-ND	-2.62	2.00	2.05
17	a	5402	CLA	CMD-C2D	-2.62	1.45	1.50
18	a	5405	PHO	C4D-ND	-2.62	1.34	1.38
17	b	5613	CLA	CMB-C2B	-2.62	1.45	1.50
17	B	607	CLA	CMC-C2C	-2.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5508	CLA	MG-ND	-2.62	2.00	2.05
17	b	5614	CLA	CMD-C2D	-2.61	1.45	1.50
17	a	5406	CLA	C1D-ND	2.61	1.41	1.37
22	B	620	LMT	O2B-C2B	-2.61	1.36	1.43
18	d	5402	PHO	C4D-ND	-2.61	1.34	1.38
17	B	610	CLA	CMD-C2D	-2.61	1.45	1.50
17	b	5607	CLA	CMC-C2C	-2.61	1.45	1.50
22	T	101	LMT	O3'-C3'	-2.61	1.36	1.43
17	C	502	CLA	CMB-C2B	-2.61	1.45	1.50
17	B	614	CLA	CMD-C2D	-2.61	1.45	1.50
17	a	5404	CLA	MG-ND	-2.60	2.00	2.05
17	a	5402	CLA	CMB-C2B	-2.60	1.45	1.50
17	A	403	CLA	CMD-C2D	-2.60	1.45	1.50
17	C	501	CLA	C1D-ND	2.60	1.41	1.37
17	B	603	CLA	CMB-C2B	-2.60	1.45	1.50
17	b	5606	CLA	CMD-C2D	-2.60	1.45	1.50
17	b	5615	CLA	CMB-C2B	-2.59	1.45	1.50
17	b	5612	CLA	MG-ND	-2.59	2.00	2.05
17	c	5502	CLA	CMB-C2B	-2.59	1.45	1.50
17	B	615	CLA	CMB-C2B	-2.59	1.45	1.50
17	A	403	CLA	MG-ND	-2.59	2.00	2.05
17	c	5507	CLA	CMD-C2D	-2.59	1.45	1.50
17	A	405	CLA	CMB-C2B	-2.59	1.45	1.50
17	b	5604	CLA	CMD-C2D	-2.59	1.45	1.50
17	c	5505	CLA	MG-ND	-2.58	2.00	2.05
17	C	509	CLA	C1D-ND	2.58	1.41	1.37
17	A	405	CLA	C1D-ND	2.58	1.41	1.37
17	B	604	CLA	CMD-C2D	-2.57	1.45	1.50
17	b	5603	CLA	CMB-C2B	-2.57	1.45	1.50
17	a	5403	CLA	C1D-ND	2.57	1.41	1.37
17	C	503	CLA	C1D-ND	2.57	1.41	1.37
17	B	602	CLA	C1D-ND	2.57	1.41	1.37
17	c	5512	CLA	C1D-ND	2.57	1.41	1.37
17	B	607	CLA	CMD-C2D	-2.56	1.45	1.50
17	C	505	CLA	MG-ND	-2.56	2.00	2.05
17	A	405	CLA	CMD-C2D	-2.56	1.45	1.50
17	a	5404	CLA	CMD-C2D	-2.56	1.45	1.50
17	a	5406	CLA	CMD-C2D	-2.56	1.45	1.50
17	B	606	CLA	CMD-C2D	-2.56	1.45	1.50
17	B	608	CLA	CMD-C2D	-2.56	1.45	1.50
17	D	404	CLA	CMC-C2C	-2.56	1.45	1.50
17	A	403	CLA	C1D-ND	2.55	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5615	CLA	C1B-NB	-2.55	1.34	1.37
17	C	509	CLA	MG-ND	-2.55	2.00	2.05
22	M	101	LMT	O3'-C3'	-2.55	1.36	1.43
17	c	5509	CLA	CMB-C2B	-2.55	1.45	1.50
17	c	5505	CLA	CMD-C2D	-2.55	1.45	1.50
17	c	5502	CLA	CMC-C2C	-2.55	1.45	1.50
17	B	610	CLA	CMC-C2C	-2.55	1.45	1.50
17	c	5507	CLA	CMB-C2B	-2.54	1.45	1.50
26	c	5515	DGD	O6D-C5D	-2.54	1.38	1.44
17	c	5503	CLA	C1D-ND	2.54	1.41	1.37
17	b	5608	CLA	CMD-C2D	-2.54	1.45	1.50
26	A	413	DGD	O6D-C5D	-2.54	1.38	1.44
17	c	5506	CLA	CMB-C2B	-2.54	1.45	1.50
17	b	5603	CLA	MG-ND	-2.54	2.00	2.05
17	C	507	CLA	CMD-C2D	-2.54	1.45	1.50
17	C	506	CLA	CMB-C2B	-2.54	1.45	1.50
17	c	5509	CLA	C1D-ND	2.54	1.41	1.37
17	D	404	CLA	C1B-NB	-2.53	1.34	1.37
17	a	5402	CLA	CMC-C2C	-2.53	1.45	1.50
17	b	5603	CLA	CMD-C2D	-2.53	1.45	1.50
17	a	5404	CLA	C1D-ND	2.53	1.41	1.37
17	B	610	CLA	CMB-C2B	-2.53	1.45	1.50
17	b	5607	CLA	CMD-C2D	-2.53	1.45	1.50
17	b	5610	CLA	CMC-C2C	-2.53	1.45	1.50
26	A	413	DGD	O2G-C2G	-2.53	1.40	1.46
17	b	5607	CLA	C1D-ND	2.53	1.41	1.37
17	b	5613	CLA	CMC-C2C	-2.53	1.45	1.50
17	c	5504	CLA	C1D-ND	2.53	1.41	1.37
17	b	5614	CLA	CMB-C2B	-2.53	1.45	1.50
17	b	5602	CLA	CMD-C2D	-2.53	1.45	1.50
17	A	402	CLA	C1D-ND	2.53	1.41	1.37
17	b	5616	CLA	CMB-C2B	-2.53	1.45	1.50
17	C	504	CLA	C1D-ND	2.52	1.41	1.37
17	b	5610	CLA	CMB-C2B	-2.52	1.45	1.50
17	A	401	CLA	CMC-C2C	-2.52	1.45	1.50
17	C	507	CLA	CMB-C2B	-2.52	1.45	1.50
17	a	5403	CLA	MG-ND	-2.52	2.00	2.05
17	C	513	CLA	C1D-ND	2.52	1.41	1.37
17	B	603	CLA	CMD-C2D	-2.52	1.45	1.50
17	A	402	CLA	CMD-C2D	-2.52	1.45	1.50
17	B	607	CLA	C1B-NB	-2.52	1.34	1.37
17	C	508	CLA	CMB-C2B	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	603	CLA	MG-ND	-2.51	2.00	2.05
17	C	509	CLA	CMB-C2B	-2.51	1.45	1.50
17	B	607	CLA	C1D-ND	2.51	1.41	1.37
17	C	510	CLA	C1D-ND	2.51	1.41	1.37
17	B	612	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	608	CLA	CMC-C2C	-2.51	1.45	1.50
17	b	5602	CLA	C1D-ND	2.51	1.41	1.37
17	B	605	CLA	CMB-C2B	-2.51	1.45	1.50
17	a	5403	CLA	CMD-C2D	-2.51	1.45	1.50
17	A	405	CLA	CMC-C2C	-2.51	1.45	1.50
17	B	614	CLA	CMB-C2B	-2.50	1.45	1.50
17	C	505	CLA	CMD-C2D	-2.50	1.45	1.50
17	b	5605	CLA	CMB-C2B	-2.50	1.45	1.50
17	B	613	CLA	CMC-C2C	-2.50	1.45	1.50
17	c	5510	CLA	C1D-ND	2.50	1.41	1.37
17	B	605	CLA	CMD-C2D	-2.50	1.45	1.50
17	d	5403	CLA	CMC-C2C	-2.50	1.45	1.50
17	C	502	CLA	CMC-C2C	-2.50	1.45	1.50
26	c	5515	DGD	O2G-C2G	-2.50	1.40	1.46
17	B	616	CLA	C1D-ND	2.50	1.41	1.37
17	c	5509	CLA	MG-ND	-2.50	2.00	2.05
17	a	5406	CLA	CMC-C2C	-2.50	1.45	1.50
17	B	612	CLA	CMB-C2B	-2.50	1.45	1.50
17	c	5508	CLA	CMD-C2D	-2.50	1.45	1.50
17	C	508	CLA	CMD-C2D	-2.50	1.45	1.50
17	B	615	CLA	C1B-NB	-2.49	1.34	1.37
17	b	5616	CLA	C1B-NB	-2.49	1.34	1.37
17	b	5612	CLA	CMC-C2C	-2.49	1.45	1.50
17	c	5508	CLA	CMB-C2B	-2.49	1.45	1.50
17	B	615	CLA	MG-ND	-2.49	2.00	2.05
17	b	5605	CLA	CMD-C2D	-2.49	1.45	1.50
22	A	409	LMT	O3'-C3'	-2.49	1.36	1.43
17	b	5606	CLA	C1D-ND	2.49	1.41	1.37
17	B	614	CLA	MG-ND	-2.49	2.00	2.05
17	b	5615	CLA	MG-ND	-2.49	2.00	2.05
17	D	405	CLA	C1D-ND	2.48	1.41	1.37
17	b	5612	CLA	CMB-C2B	-2.48	1.45	1.50
17	d	5403	CLA	C1B-NB	-2.48	1.34	1.37
17	d	5404	CLA	C1D-ND	2.48	1.41	1.37
17	B	616	CLA	CMB-C2B	-2.48	1.45	1.50
17	B	615	CLA	CMC-C2C	-2.48	1.45	1.50
17	b	5615	CLA	CMC-C2C	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5614	CLA	MG-ND	-2.48	2.00	2.05
17	b	5602	CLA	CMB-C2B	-2.48	1.45	1.50
17	B	611	CLA	C1B-NB	-2.48	1.34	1.37
17	B	602	CLA	CMD-C2D	-2.48	1.45	1.50
22	a	5410	LMT	O3'-C3'	-2.48	1.36	1.43
22	m	5102	LMT	O3'-C3'	-2.48	1.36	1.43
17	d	5404	CLA	CMB-C2B	-2.47	1.45	1.50
17	b	5609	CLA	CMB-C2B	-2.47	1.45	1.50
22	a	5410	LMT	O2'-C2'	-2.47	1.36	1.43
17	B	609	CLA	CMB-C2B	-2.47	1.45	1.50
17	b	5616	CLA	MG-ND	-2.47	2.00	2.05
17	A	402	CLA	MG-ND	-2.47	2.00	2.05
17	c	5507	CLA	CMC-C2C	-2.47	1.45	1.50
17	b	5601	CLA	MG-NB	-2.47	2.00	2.05
17	B	616	CLA	MG-ND	-2.46	2.00	2.05
17	c	5509	CLA	CMC-C2C	-2.46	1.45	1.50
17	b	5609	CLA	C4B-NB	2.46	1.41	1.37
17	C	507	CLA	CMC-C2C	-2.46	1.45	1.50
17	C	511	CLA	CMC-C2C	-2.46	1.45	1.50
17	k	5501	CLA	CMB-C2B	-2.46	1.45	1.50
17	C	507	CLA	C1D-ND	2.46	1.41	1.37
17	C	509	CLA	CMC-C2C	-2.46	1.45	1.50
17	k	5501	CLA	MG-ND	-2.46	2.00	2.05
17	D	405	CLA	CMB-C2B	-2.46	1.45	1.50
17	d	5404	CLA	MG-ND	-2.45	2.00	2.05
17	C	510	CLA	MG-ND	-2.45	2.00	2.05
17	C	511	CLA	MG-ND	-2.45	2.00	2.05
17	c	5510	CLA	CMD-C2D	-2.45	1.45	1.50
17	C	509	CLA	C1B-NB	-2.45	1.34	1.37
17	B	601	CLA	MG-NB	-2.45	2.00	2.05
17	B	611	CLA	MG-ND	-2.45	2.00	2.05
17	b	5616	CLA	C1D-ND	2.45	1.41	1.37
17	b	5606	CLA	CMB-C2B	-2.45	1.45	1.50
17	C	507	CLA	C1B-NB	-2.45	1.34	1.37
17	d	5404	CLA	CMD-C2D	-2.45	1.45	1.50
17	B	606	CLA	C1D-ND	2.45	1.41	1.37
17	B	606	CLA	CMB-C2B	-2.45	1.45	1.50
23	L	101	SQD	O47-C7	2.45	1.41	1.34
17	D	405	CLA	CMD-C2D	-2.45	1.45	1.50
17	c	5501	CLA	CMC-C2C	-2.45	1.45	1.50
17	B	616	CLA	C1B-NB	-2.45	1.34	1.37
17	C	506	CLA	MG-ND	-2.45	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5507	CLA	C1D-ND	2.45	1.41	1.37
17	c	5506	CLA	CMD-C2D	-2.45	1.45	1.50
17	b	5615	CLA	CMD-C2D	-2.44	1.45	1.50
17	D	405	CLA	MG-ND	-2.44	2.00	2.05
17	B	615	CLA	CMD-C2D	-2.44	1.45	1.50
17	B	605	CLA	MG-ND	-2.44	2.00	2.05
22	m	5102	LMT	O2B-C2B	-2.44	1.36	1.43
17	C	510	CLA	CMB-C2B	-2.44	1.45	1.50
17	B	607	CLA	MG-ND	-2.44	2.01	2.05
17	k	5501	CLA	CMC-C2C	-2.44	1.45	1.50
17	b	5606	CLA	C1B-NB	-2.44	1.34	1.37
17	b	5607	CLA	C1B-NB	-2.44	1.34	1.37
17	c	5509	CLA	C1B-NB	-2.44	1.34	1.37
17	B	602	CLA	CMB-C2B	-2.44	1.45	1.50
17	k	5501	CLA	CMD-C2D	-2.43	1.45	1.50
17	b	5603	CLA	CMC-C2C	-2.43	1.45	1.50
17	c	5511	CLA	CMD-C2D	-2.43	1.45	1.50
17	c	5510	CLA	MG-ND	-2.43	2.01	2.05
17	C	511	CLA	CMD-C2D	-2.43	1.45	1.50
17	C	506	CLA	CMD-C2D	-2.43	1.45	1.50
22	M	101	LMT	O2'-C2'	-2.43	1.36	1.43
17	b	5611	CLA	C1B-NB	-2.43	1.34	1.37
17	c	5507	CLA	C1B-NB	-2.43	1.34	1.37
17	c	5511	CLA	MG-ND	-2.43	2.01	2.05
17	C	512	CLA	CMD-C2D	-2.43	1.45	1.50
17	C	510	CLA	CMD-C2D	-2.42	1.45	1.50
17	b	5608	CLA	CMC-C2C	-2.42	1.45	1.50
17	b	5609	CLA	C1D-ND	2.42	1.41	1.37
17	B	603	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	402	CLA	C1B-NB	-2.42	1.34	1.37
17	b	5605	CLA	MG-ND	-2.41	2.01	2.05
17	b	5602	CLA	C1B-NB	-2.41	1.34	1.37
26	C	517	DGD	O2G-C2G	-2.41	1.40	1.46
17	b	5607	CLA	MG-ND	-2.41	2.01	2.05
17	C	511	CLA	CMB-C2B	-2.41	1.45	1.50
17	a	5404	CLA	CMB-C2B	-2.41	1.45	1.50
17	C	501	CLA	CMC-C2C	-2.41	1.45	1.50
17	c	5506	CLA	MG-ND	-2.41	2.01	2.05
17	C	512	CLA	MG-ND	-2.41	2.01	2.05
17	c	5510	CLA	CMB-C2B	-2.40	1.45	1.50
17	B	602	CLA	CMC-C2C	-2.40	1.45	1.50
26	c	5516	DGD	O2G-C2G	-2.40	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5604	CLA	CMC-C2C	-2.40	1.45	1.50
17	c	5506	CLA	C1B-NB	-2.40	1.34	1.37
17	b	5616	CLA	CMD-C2D	-2.40	1.45	1.50
17	c	5504	CLA	CMD-C2D	-2.40	1.45	1.50
17	C	504	CLA	CMD-C2D	-2.40	1.45	1.50
17	b	5602	CLA	CMC-C2C	-2.40	1.45	1.50
17	B	606	CLA	C1B-NB	-2.40	1.34	1.37
17	B	616	CLA	CMD-C2D	-2.40	1.45	1.50
17	b	5612	CLA	C1D-ND	2.40	1.41	1.37
26	c	5515	DGD	O6E-C5E	-2.39	1.38	1.44
17	A	403	CLA	CMB-C2B	-2.39	1.45	1.50
26	A	413	DGD	O6E-C5E	-2.39	1.38	1.44
17	c	5502	CLA	C1B-C2B	2.39	1.48	1.43
17	B	606	CLA	MG-ND	-2.39	2.01	2.05
17	c	5501	CLA	MG-ND	-2.39	2.01	2.05
17	c	5504	CLA	CMC-C2C	-2.39	1.45	1.50
17	C	505	CLA	CMB-C2B	-2.39	1.45	1.50
17	B	602	CLA	C1B-NB	-2.38	1.34	1.37
17	B	614	CLA	C1B-NB	-2.38	1.34	1.37
17	C	504	CLA	CMB-C2B	-2.38	1.45	1.50
17	C	513	CLA	MG-ND	-2.38	2.01	2.05
17	C	502	CLA	C1B-C2B	2.38	1.48	1.43
19	D	406	PQ9	C10-C5	2.38	1.47	1.35
17	B	602	CLA	C1B-C2B	2.37	1.48	1.43
17	C	506	CLA	C1B-NB	-2.37	1.34	1.37
17	B	614	CLA	C1D-ND	2.37	1.41	1.37
17	c	5512	CLA	MG-ND	-2.37	2.01	2.05
17	B	605	CLA	CMC-C2C	-2.37	1.45	1.50
17	C	504	CLA	CMC-C2C	-2.37	1.45	1.50
22	m	5102	LMT	O3B-C3B	-2.37	1.37	1.43
17	C	501	CLA	MG-ND	-2.37	2.01	2.05
17	c	5501	CLA	CMB-C2B	-2.37	1.45	1.50
22	M	101	LMT	O1'-C1'	-2.37	1.36	1.40
17	c	5504	CLA	CMB-C2B	-2.37	1.45	1.50
17	c	5505	CLA	CMB-C2B	-2.37	1.45	1.50
17	C	508	CLA	C1D-ND	2.37	1.41	1.37
17	C	505	CLA	CMC-C2C	-2.37	1.45	1.50
17	B	604	CLA	CMC-C2C	-2.36	1.45	1.50
17	C	506	CLA	C1D-ND	2.36	1.41	1.37
17	C	502	CLA	CMD-C2D	-2.36	1.45	1.50
17	B	609	CLA	CMC-C2C	-2.36	1.45	1.50
17	b	5606	CLA	MG-ND	-2.36	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5502	CLA	CMD-C2D	-2.36	1.45	1.50
17	b	5602	CLA	C1B-C2B	2.36	1.48	1.43
17	c	5505	CLA	CMC-C2C	-2.36	1.45	1.50
17	b	5606	CLA	CMC-C2C	-2.36	1.45	1.50
19	d	5405	PQ9	C10-C5	2.36	1.46	1.35
22	M	101	LMT	O3B-C3B	-2.36	1.37	1.43
17	B	609	CLA	C1D-ND	2.36	1.41	1.37
17	b	5611	CLA	MG-ND	-2.36	2.01	2.05
22	A	409	LMT	O2'-C2'	-2.35	1.37	1.43
17	B	609	CLA	C4B-NB	2.35	1.41	1.37
17	b	5609	CLA	CMC-C2C	-2.35	1.45	1.50
17	B	605	CLA	C1B-NB	-2.35	1.34	1.37
17	C	501	CLA	CMB-C2B	-2.35	1.45	1.50
17	b	5614	CLA	C1D-ND	2.35	1.41	1.37
17	C	511	CLA	C1B-NB	-2.35	1.34	1.37
17	a	5406	CLA	C1B-NB	-2.35	1.34	1.37
17	a	5403	CLA	C1B-NB	-2.35	1.34	1.37
17	a	5402	CLA	C1D-ND	2.35	1.40	1.37
26	C	517	DGD	O1G-C1G	-2.35	1.39	1.45
17	c	5511	CLA	CMB-C2B	-2.35	1.46	1.50
17	B	612	CLA	C1D-ND	2.35	1.40	1.37
17	c	5506	CLA	C1D-ND	2.35	1.40	1.37
17	b	5603	CLA	C1D-ND	2.34	1.40	1.37
17	c	5508	CLA	C1B-NB	-2.34	1.34	1.37
17	c	5510	CLA	CMC-C2C	-2.34	1.46	1.50
17	B	609	CLA	CMD-C2D	-2.34	1.46	1.50
17	B	601	CLA	C1B-C2B	2.34	1.48	1.43
17	k	5501	CLA	C1B-NB	-2.33	1.34	1.37
17	B	609	CLA	MG-ND	-2.33	2.01	2.05
17	b	5609	CLA	MG-ND	-2.33	2.01	2.05
17	C	501	CLA	C1B-C2B	2.33	1.48	1.43
17	b	5601	CLA	CMD-C2D	-2.33	1.46	1.50
17	B	605	CLA	C1D-ND	2.33	1.40	1.37
17	C	508	CLA	C1B-NB	-2.33	1.34	1.37
17	b	5605	CLA	C1B-NB	-2.33	1.34	1.37
17	C	510	CLA	CMC-C2C	-2.33	1.46	1.50
17	A	405	CLA	MG-ND	-2.33	2.01	2.05
17	c	5502	CLA	MG-ND	-2.33	2.01	2.05
17	B	603	CLA	C1D-ND	2.33	1.40	1.37
17	D	405	CLA	CMC-C2C	-2.32	1.46	1.50
17	a	5406	CLA	MG-ND	-2.32	2.01	2.05
17	c	5501	CLA	CMD-C2D	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	411	DGD	O2G-C2G	-2.32	1.41	1.46
17	A	405	CLA	C1B-NB	-2.32	1.34	1.37
17	c	5508	CLA	C1D-ND	2.32	1.40	1.37
22	m	5102	LMT	O2'-C2'	-2.31	1.37	1.43
17	b	5605	CLA	CMC-C2C	-2.31	1.46	1.50
17	b	5610	CLA	C1D-ND	2.31	1.40	1.37
26	c	5516	DGD	O1G-C1G	-2.31	1.40	1.45
17	B	613	CLA	CAA-C2A	-2.31	1.49	1.54
19	d	5405	PQ9	C3-C4	-2.31	1.38	1.44
17	b	5614	CLA	CMC-C2C	-2.31	1.46	1.50
17	C	504	CLA	MG-ND	-2.31	2.01	2.05
17	b	5601	CLA	C1B-C2B	2.31	1.48	1.43
19	D	406	PQ9	C3-C4	-2.31	1.38	1.44
22	T	101	LMT	O3B-C3B	-2.31	1.37	1.43
17	A	403	CLA	CMC-C2C	-2.31	1.46	1.50
17	B	601	CLA	CMD-C2D	-2.31	1.46	1.50
17	c	5501	CLA	C1B-C2B	2.30	1.48	1.43
17	c	5503	CLA	CMB-C2B	-2.30	1.46	1.50
26	a	5411	DGD	O5D-C6D	-2.30	1.39	1.43
17	C	512	CLA	CMB-C2B	-2.30	1.46	1.50
17	B	607	CLA	CMB-C2B	-2.30	1.46	1.50
20	A	407	BCR	C33-C5	-2.30	1.47	1.50
17	B	606	CLA	CMC-C2C	-2.30	1.46	1.50
17	b	5607	CLA	CMB-C2B	-2.30	1.46	1.50
26	b	5621	DGD	O2G-C2G	-2.29	1.41	1.46
17	C	502	CLA	MG-ND	-2.29	2.01	2.05
17	B	614	CLA	CMC-C2C	-2.29	1.46	1.50
17	c	5506	CLA	CMC-C2C	-2.29	1.46	1.50
17	C	510	CLA	C1B-NB	-2.29	1.34	1.37
23	d	5407	SQD	O2-C2	-2.29	1.37	1.43
17	c	5511	CLA	C1B-C2B	2.29	1.48	1.43
17	b	5613	CLA	CAA-C2A	-2.29	1.49	1.54
17	C	503	CLA	CMB-C2B	-2.29	1.46	1.50
17	b	5609	CLA	CMD-C2D	-2.29	1.46	1.50
17	C	513	CLA	CMC-C2C	-2.29	1.46	1.50
22	B	620	LMT	O3B-C3B	-2.29	1.37	1.43
17	C	513	CLA	C1B-NB	-2.29	1.34	1.37
17	a	5404	CLA	CMC-C2C	-2.29	1.46	1.50
17	d	5404	CLA	CMC-C2C	-2.29	1.46	1.50
17	C	513	CLA	C1B-C2B	2.28	1.48	1.43
17	c	5504	CLA	C1B-C2B	2.28	1.48	1.43
17	b	5601	CLA	C4B-NB	2.28	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	610	CLA	C1D-ND	2.28	1.40	1.37
17	b	5605	CLA	C1D-ND	2.28	1.40	1.37
17	C	504	CLA	C1B-C2B	2.28	1.48	1.43
17	C	501	CLA	CMD-C2D	-2.28	1.46	1.50
17	c	5504	CLA	MG-ND	-2.28	2.01	2.05
17	c	5512	CLA	C1B-C2B	2.28	1.48	1.43
17	C	506	CLA	CMC-C2C	-2.28	1.46	1.50
17	b	5608	CLA	C1D-ND	2.28	1.40	1.37
23	L	101	SQD	O47-C45	-2.27	1.41	1.46
26	C	518	DGD	O5D-C6D	-2.27	1.39	1.43
17	A	401	CLA	C1D-ND	2.27	1.40	1.37
17	b	5601	CLA	C3B-C4B	2.27	1.49	1.42
20	h	5101	BCR	C33-C5	-2.27	1.47	1.50
17	b	5610	CLA	C1B-NB	-2.27	1.34	1.37
17	c	5503	CLA	C1B-C2B	2.27	1.48	1.43
17	c	5512	CLA	CMC-C2C	-2.27	1.46	1.50
17	B	607	CLA	C1B-C2B	2.26	1.48	1.43
17	B	610	CLA	C1B-NB	-2.26	1.34	1.37
17	c	5504	CLA	C4B-NB	2.26	1.40	1.37
17	C	504	CLA	C4B-NB	2.26	1.40	1.37
20	H	101	BCR	C33-C5	-2.26	1.47	1.50
17	B	601	CLA	C3B-C4B	2.26	1.49	1.42
17	a	5404	CLA	C1B-NB	-2.26	1.34	1.37
17	B	608	CLA	C1D-ND	2.26	1.40	1.37
20	a	5408	BCR	C33-C5	-2.25	1.47	1.50
17	C	503	CLA	C1B-C2B	2.25	1.48	1.43
17	C	502	CLA	C1B-NB	-2.25	1.34	1.37
17	b	5614	CLA	C1B-NB	-2.25	1.34	1.37
17	B	601	CLA	C4B-NB	2.25	1.40	1.37
22	a	5410	LMT	O3B-C3B	-2.25	1.37	1.43
17	B	615	CLA	C1D-ND	2.25	1.40	1.37
26	C	518	DGD	O2G-C2G	-2.24	1.41	1.46
17	B	609	CLA	C1B-C2B	2.24	1.48	1.43
17	C	512	CLA	C1B-C2B	2.24	1.48	1.43
26	a	5411	DGD	O2G-C2G	-2.23	1.41	1.46
17	C	503	CLA	MG-ND	-2.23	2.01	2.05
17	A	403	CLA	C1B-NB	-2.23	1.34	1.37
17	C	503	CLA	CMC-C2C	-2.23	1.46	1.50
17	C	513	CLA	CMB-C2B	-2.23	1.46	1.50
17	c	5503	CLA	MG-ND	-2.23	2.01	2.05
17	b	5607	CLA	C1B-C2B	2.23	1.48	1.43
17	b	5615	CLA	C1D-ND	2.22	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	409	LMT	O3B-C3B	-2.22	1.37	1.43
17	c	5512	CLA	CMB-C2B	-2.22	1.46	1.50
17	A	402	CLA	CMC-C2C	-2.22	1.46	1.50
17	B	605	CLA	C1B-C2B	2.22	1.48	1.43
17	B	604	CLA	C1D-ND	2.22	1.40	1.37
17	c	5512	CLA	C1B-NB	-2.22	1.34	1.37
17	b	5604	CLA	C1D-ND	2.22	1.40	1.37
17	a	5406	CLA	C4B-NB	2.22	1.40	1.37
17	b	5609	CLA	C1B-C2B	2.21	1.48	1.43
17	b	5605	CLA	C1B-C2B	2.21	1.48	1.43
17	a	5403	CLA	CMC-C2C	-2.21	1.46	1.50
17	c	5502	CLA	C1B-NB	-2.21	1.35	1.37
17	C	512	CLA	CMC-C2C	-2.20	1.46	1.50
17	c	5503	CLA	CMC-C2C	-2.20	1.46	1.50
20	t	5102	BCR	C33-C5	-2.20	1.47	1.50
17	A	401	CLA	CAA-C2A	-2.20	1.50	1.54
17	B	611	CLA	C1D-ND	2.20	1.40	1.37
17	c	5510	CLA	C1B-NB	-2.20	1.35	1.37
17	c	5509	CLA	C1B-C2B	2.20	1.48	1.43
17	B	613	CLA	CAC-C3C	-2.19	1.45	1.51
17	C	505	CLA	C1D-ND	2.19	1.40	1.37
17	c	5511	CLA	CMC-C2C	-2.19	1.46	1.50
23	D	403	SQD	O2-C2	-2.19	1.37	1.43
17	B	605	CLA	C4B-NB	2.19	1.40	1.37
17	b	5605	CLA	CAC-C3C	-2.19	1.45	1.51
17	b	5613	CLA	CAC-C3C	-2.19	1.45	1.51
17	C	510	CLA	C1B-C2B	2.19	1.48	1.43
17	c	5505	CLA	C4B-NB	2.18	1.40	1.37
17	b	5604	CLA	CAC-C3C	-2.18	1.45	1.51
17	B	614	CLA	C1B-C2B	2.18	1.48	1.43
17	a	5402	CLA	C1B-NB	-2.18	1.35	1.37
17	B	604	CLA	CAC-C3C	-2.18	1.45	1.51
17	B	605	CLA	CAC-C3C	-2.18	1.45	1.51
17	A	401	CLA	C1B-NB	-2.18	1.35	1.37
17	B	611	CLA	CAC-C3C	-2.18	1.45	1.51
17	A	405	CLA	C4B-NB	2.17	1.40	1.37
17	k	5501	CLA	C1B-C2B	2.17	1.48	1.43
26	D	411	DGD	O6D-C5D	-2.17	1.39	1.44
17	c	5505	CLA	C1D-ND	2.17	1.40	1.37
17	C	509	CLA	C1B-C2B	2.17	1.48	1.43
17	c	5511	CLA	C1B-NB	-2.17	1.35	1.37
17	b	5614	CLA	C1B-C2B	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	512	CLA	C4B-NB	2.17	1.40	1.37
17	c	5506	CLA	C4B-NB	2.17	1.40	1.37
20	b	5618	BCR	C38-C26	-2.17	1.47	1.50
17	c	5512	CLA	C4B-NB	2.17	1.40	1.37
17	C	505	CLA	C4B-NB	2.16	1.40	1.37
17	B	609	CLA	C3B-C4B	2.16	1.49	1.42
22	a	5410	LMT	O2B-C2B	-2.16	1.37	1.43
17	a	5406	CLA	C3B-C4B	2.16	1.49	1.42
17	C	511	CLA	C1B-C2B	2.16	1.48	1.43
17	a	5403	CLA	C1B-C2B	2.16	1.48	1.43
20	D	407	BCR	C33-C5	-2.16	1.47	1.50
17	C	513	CLA	CMD-C2D	-2.15	1.46	1.50
17	b	5606	CLA	C1B-C2B	2.15	1.48	1.43
17	b	5611	CLA	CAC-C3C	-2.15	1.45	1.51
20	B	618	BCR	C38-C26	-2.15	1.47	1.50
17	A	405	CLA	C3B-C4B	2.15	1.49	1.42
17	c	5512	CLA	CMD-C2D	-2.15	1.46	1.50
26	b	5621	DGD	O6D-C5D	-2.15	1.39	1.44
17	C	506	CLA	C1B-C2B	2.15	1.48	1.43
22	M	101	LMT	O4'-C4B	-2.14	1.37	1.43
17	A	402	CLA	C1B-C2B	2.14	1.48	1.43
17	C	503	CLA	C1B-NB	-2.14	1.35	1.37
17	c	5507	CLA	C1B-C2B	2.14	1.48	1.43
17	C	512	CLA	C1B-NB	-2.14	1.35	1.37
17	b	5605	CLA	C4B-NB	2.14	1.40	1.37
17	c	5511	CLA	C4B-NB	2.14	1.40	1.37
17	a	5402	CLA	CAA-C2A	-2.14	1.50	1.54
17	B	606	CLA	C1B-C2B	2.14	1.48	1.43
22	a	5410	LMT	O1'-C1'	-2.14	1.36	1.40
23	D	403	SQD	O3-C3	-2.13	1.37	1.43
17	b	5609	CLA	C3B-C4B	2.13	1.48	1.42
17	c	5510	CLA	C1B-C2B	2.13	1.48	1.43
17	c	5506	CLA	C1B-C2B	2.13	1.48	1.43
17	B	608	CLA	C4B-NB	2.13	1.40	1.37
17	b	5616	CLA	C1B-C2B	2.13	1.48	1.43
23	D	403	SQD	O47-C45	-2.13	1.41	1.46
17	c	5503	CLA	C1B-NB	-2.13	1.35	1.37
17	D	405	CLA	C1B-NB	-2.12	1.35	1.37
17	b	5611	CLA	C1D-ND	2.12	1.40	1.37
17	b	5601	CLA	MG-ND	-2.12	2.01	2.05
20	d	5406	BCR	C33-C5	-2.12	1.47	1.50
20	t	5101	BCR	C33-C5	-2.12	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	513	CLA	C4B-NB	2.11	1.40	1.37
20	a	5408	BCR	C38-C26	-2.11	1.47	1.50
20	c	5514	BCR	C38-C26	-2.11	1.47	1.50
17	B	601	CLA	MG-ND	-2.11	2.01	2.05
20	C	516	BCR	C33-C5	-2.11	1.47	1.50
17	C	507	CLA	C1B-C2B	2.11	1.48	1.43
20	C	516	BCR	C38-C26	-2.10	1.47	1.50
20	C	514	BCR	C33-C5	-2.10	1.47	1.50
17	C	510	CLA	C4B-NB	2.10	1.40	1.37
23	A	410	SQD	O3-C3	-2.10	1.37	1.43
17	k	5501	CLA	C4B-NB	2.10	1.40	1.37
17	C	506	CLA	C4B-NB	2.10	1.40	1.37
17	B	616	CLA	C1B-C2B	2.09	1.48	1.43
20	b	5619	BCR	C33-C5	-2.09	1.47	1.50
17	D	404	CLA	C1D-ND	2.09	1.40	1.37
17	c	5508	CLA	CAC-C3C	-2.09	1.45	1.51
17	C	508	CLA	CAC-C3C	-2.09	1.45	1.51
26	c	5515	DGD	O3E-C3E	-2.09	1.37	1.43
17	d	5404	CLA	C1B-C2B	2.09	1.48	1.43
26	a	5411	DGD	O1G-C1G	-2.09	1.40	1.45
20	B	617	BCR	C38-C26	-2.09	1.47	1.50
26	A	413	DGD	O3E-C3E	-2.09	1.37	1.43
17	b	5613	CLA	C1D-ND	2.09	1.40	1.37
17	d	5404	CLA	C1B-NB	-2.08	1.35	1.37
17	D	405	CLA	C1B-C2B	2.08	1.48	1.43
17	A	403	CLA	C1B-C2B	2.08	1.48	1.43
20	b	5617	BCR	C33-C5	-2.08	1.47	1.50
20	T	102	BCR	C33-C5	-2.08	1.47	1.50
23	d	5407	SQD	O3-C3	-2.08	1.37	1.43
22	A	409	LMT	O1'-C1'	-2.08	1.36	1.40
17	c	5501	CLA	C4B-NB	2.07	1.40	1.37
20	k	5502	BCR	C33-C5	-2.07	1.47	1.50
17	c	5510	CLA	C4B-NB	2.07	1.40	1.37
23	A	410	SQD	O2-C2	-2.07	1.37	1.43
25	D	410	MGE	O2G-C2G	-2.07	1.41	1.46
23	a	5401	SQD	O3-C3	-2.07	1.37	1.43
17	a	5404	CLA	C1B-C2B	2.07	1.48	1.43
17	C	501	CLA	C1B-NB	-2.06	1.35	1.37
20	C	515	BCR	C38-C26	-2.06	1.47	1.50
17	b	5611	CLA	CAA-C2A	-2.06	1.50	1.54
17	B	611	CLA	CAA-C2A	-2.06	1.50	1.54
17	C	511	CLA	C4B-NB	2.06	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	d	5403	CLA	C1D-ND	2.06	1.40	1.37
23	a	5401	SQD	O4-C4	-2.06	1.37	1.43
22	M	101	LMT	O5'-C5'	-2.06	1.39	1.44
17	B	613	CLA	C1D-ND	2.05	1.40	1.37
20	c	5514	BCR	C33-C5	-2.05	1.47	1.50
17	c	5504	CLA	C1B-NB	-2.05	1.35	1.37
20	A	407	BCR	C38-C26	-2.05	1.47	1.50
23	a	5401	SQD	O2-C2	-2.05	1.37	1.43
18	A	404	PHO	C3D-CAD	-2.05	1.43	1.47
23	d	5407	SQD	O47-C45	-2.05	1.41	1.46
22	A	409	LMT	O4'-C4B	-2.05	1.37	1.43
17	b	5616	CLA	CAC-C3C	-2.05	1.45	1.51
20	b	5618	BCR	C33-C5	-2.05	1.47	1.50
17	b	5606	CLA	C4B-NB	2.05	1.40	1.37
20	b	5617	BCR	C38-C26	-2.05	1.47	1.50
20	B	617	BCR	C33-C5	-2.05	1.47	1.50
17	c	5501	CLA	C1B-NB	-2.04	1.35	1.37
17	B	601	CLA	CMC-C2C	-2.04	1.46	1.50
17	C	508	CLA	C4B-NB	2.04	1.40	1.37
22	T	101	LMT	O4'-C4B	-2.04	1.37	1.43
22	m	5102	LMT	O5'-C5'	-2.04	1.39	1.44
17	b	5607	CLA	C4B-NB	2.04	1.40	1.37
17	c	5511	CLA	C3B-C4B	2.04	1.48	1.42
18	a	5405	PHO	C3D-CAD	-2.04	1.43	1.47
17	a	5403	CLA	CHC-C4B	-2.04	1.34	1.39
17	B	606	CLA	C4B-NB	2.04	1.40	1.37
29	F	101	HEM	CMB-C2B	2.03	1.54	1.50
20	c	5513	BCR	C33-C5	-2.03	1.47	1.50
17	B	607	CLA	C4B-NB	2.03	1.40	1.37
17	A	402	CLA	CHC-C4B	-2.03	1.34	1.39
17	B	616	CLA	C4B-NB	2.03	1.40	1.37
23	A	410	SQD	O4-C4	-2.03	1.37	1.43
20	z	5101	BCR	C38-C26	-2.03	1.47	1.50
23	L	101	SQD	O2-C2	-2.03	1.37	1.43
17	C	504	CLA	C1B-NB	-2.03	1.35	1.37
22	T	101	LMT	O1'-C1'	-2.03	1.36	1.40
20	B	618	BCR	C33-C5	-2.03	1.47	1.50
17	C	509	CLA	C4B-NB	2.03	1.40	1.37
26	C	518	DGD	O1G-C1G	-2.03	1.40	1.45
23	a	5401	SQD	O47-C45	-2.03	1.41	1.46
17	B	616	CLA	CAC-C3C	-2.02	1.45	1.51
17	C	512	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	513	CLA	C3B-C4B	2.02	1.48	1.42
17	C	507	CLA	CHC-C4B	-2.02	1.34	1.39
17	B	602	CLA	CAC-C3C	-2.02	1.45	1.51
17	b	5601	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	603	CLA	CAC-C3C	-2.02	1.45	1.51
17	B	611	CLA	CAB-C3B	-2.02	1.42	1.47
17	b	5611	CLA	CAB-C3B	-2.01	1.42	1.47
17	c	5503	CLA	C4B-NB	2.01	1.40	1.37
17	b	5610	CLA	C1B-C2B	2.01	1.47	1.43
17	c	5509	CLA	C4B-NB	2.01	1.40	1.37
23	D	403	SQD	O4-C4	-2.01	1.38	1.43
20	T	102	BCR	C38-C26	-2.01	1.47	1.50
17	b	5612	CLA	C1B-C2B	2.01	1.47	1.43
17	c	5512	CLA	C3B-C4B	2.01	1.48	1.42
17	A	402	CLA	C4B-NB	2.01	1.40	1.37
17	a	5403	CLA	C4B-NB	2.01	1.40	1.37
20	C	514	BCR	C38-C26	-2.01	1.47	1.50
17	b	5603	CLA	CAC-C3C	-2.01	1.46	1.51
17	A	401	CLA	C1A-CHA	-2.01	1.34	1.43
23	d	5407	SQD	O4-C4	-2.01	1.38	1.43
17	b	5616	CLA	C4B-NB	2.01	1.40	1.37
23	L	101	SQD	O4-C4	-2.01	1.38	1.43
17	c	5505	CLA	C1B-NB	-2.01	1.35	1.37
23	l	5102	SQD	O4-C4	-2.00	1.38	1.43
17	b	5602	CLA	CAC-C3C	-2.00	1.46	1.51
17	c	5507	CLA	CHC-C4B	-2.00	1.34	1.39
17	c	5508	CLA	C4B-NB	2.00	1.40	1.37

All (923) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	5403	CLA	C4A-NA-C1A	7.79	110.23	106.68
17	A	402	CLA	C4A-NA-C1A	7.67	110.18	106.68
17	C	508	CLA	C4A-NA-C1A	7.51	110.11	106.68
17	c	5508	CLA	C4A-NA-C1A	7.51	110.11	106.68
17	b	5611	CLA	C4A-NA-C1A	7.41	110.06	106.68
17	B	607	CLA	C4A-NA-C1A	7.38	110.05	106.68
17	b	5607	CLA	C4A-NA-C1A	7.33	110.02	106.68
17	B	611	CLA	C4A-NA-C1A	7.29	110.00	106.68
17	C	511	CLA	C4A-NA-C1A	7.28	110.00	106.68
17	k	5501	CLA	C4A-NA-C1A	7.20	109.96	106.68
17	b	5615	CLA	C4A-NA-C1A	7.20	109.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	615	CLA	C4A-NA-C1A	7.18	109.95	106.68
17	b	5606	CLA	C4A-NA-C1A	7.12	109.93	106.68
17	A	405	CLA	C4A-NA-C1A	7.02	109.88	106.68
17	a	5406	CLA	C4A-NA-C1A	7.02	109.88	106.68
17	b	5614	CLA	C4A-NA-C1A	7.01	109.88	106.68
17	B	606	CLA	C4A-NA-C1A	7.00	109.87	106.68
17	C	501	CLA	C4A-NA-C1A	7.00	109.87	106.68
17	B	614	CLA	C4A-NA-C1A	6.98	109.86	106.68
17	B	613	CLA	C4A-NA-C1A	6.95	109.85	106.68
17	b	5612	CLA	C4A-NA-C1A	6.92	109.83	106.68
17	C	503	CLA	C4A-NA-C1A	6.89	109.82	106.68
17	c	5501	CLA	C4A-NA-C1A	6.88	109.82	106.68
17	c	5503	CLA	C4A-NA-C1A	6.87	109.81	106.68
17	A	403	CLA	C4A-NA-C1A	6.85	109.80	106.68
17	B	612	CLA	C4A-NA-C1A	6.84	109.80	106.68
17	b	5603	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	B	603	CLA	C4A-NA-C1A	6.78	109.77	106.68
17	b	5613	CLA	C4A-NA-C1A	6.75	109.76	106.68
17	B	604	CLA	C4A-NA-C1A	6.74	109.75	106.68
17	B	610	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	b	5604	CLA	C4A-NA-C1A	6.68	109.72	106.68
17	a	5404	CLA	C4A-NA-C1A	6.67	109.72	106.68
17	C	502	CLA	C4A-NA-C1A	6.63	109.70	106.68
17	b	5610	CLA	C4A-NA-C1A	6.58	109.68	106.68
17	b	5605	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	b	5609	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	B	609	CLA	C4A-NA-C1A	6.55	109.67	106.68
17	c	5502	CLA	C4A-NA-C1A	6.55	109.67	106.68
17	b	5602	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	B	605	CLA	C4A-NA-C1A	6.50	109.64	106.68
17	c	5511	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	C	506	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	B	602	CLA	C4A-NA-C1A	6.45	109.62	106.68
17	C	512	CLA	C4A-NA-C1A	6.43	109.61	106.68
17	C	504	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	c	5504	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	c	5506	CLA	C4A-NA-C1A	6.35	109.58	106.68
17	B	616	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	B	608	CLA	C4A-NA-C1A	6.32	109.56	106.68
17	b	5608	CLA	C4A-NA-C1A	6.30	109.55	106.68
17	d	5404	CLA	C4A-NA-C1A	6.29	109.55	106.68
17	D	405	CLA	C4A-NA-C1A	6.28	109.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5616	CLA	C4A-NA-C1A	6.22	109.52	106.68
17	C	510	CLA	C4A-NA-C1A	5.98	109.41	106.68
17	C	513	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	c	5512	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	c	5510	CLA	C4A-NA-C1A	5.89	109.36	106.68
17	C	507	CLA	C4A-NA-C1A	5.83	109.34	106.68
17	c	5507	CLA	C4A-NA-C1A	5.81	109.33	106.68
17	C	509	CLA	C4A-NA-C1A	5.57	109.22	106.68
18	a	5405	PHO	C4D-CHA-CBD	-5.52	105.81	108.45
17	d	5403	CLA	C4A-NA-C1A	5.52	109.20	106.68
17	c	5509	CLA	C4A-NA-C1A	5.50	109.19	106.68
17	B	601	CLA	C4A-NA-C1A	5.48	109.18	106.68
17	b	5601	CLA	C4A-NA-C1A	5.48	109.18	106.68
17	D	404	CLA	C4A-NA-C1A	5.43	109.16	106.68
18	d	5402	PHO	C4D-CHA-CBD	-5.41	105.86	108.45
26	b	5621	DGD	O3G-C3G-C2G	-5.38	97.73	110.82
26	D	411	DGD	O3G-C3G-C2G	-5.37	97.75	110.82
18	A	404	PHO	C4D-CHA-CBD	-5.36	105.88	108.45
17	c	5505	CLA	C4A-NA-C1A	5.34	109.11	106.68
18	D	402	PHO	C4D-CHA-CBD	-5.33	105.90	108.45
17	a	5402	CLA	C4A-NA-C1A	5.31	109.10	106.68
19	d	5405	PQ9	C11-C12-C13	-5.30	117.71	126.83
17	A	401	CLA	C4A-NA-C1A	5.28	109.09	106.68
19	D	406	PQ9	C11-C12-C13	-5.26	117.77	126.83
17	C	505	CLA	C4A-NA-C1A	5.24	109.07	106.68
23	a	5401	SQD	O47-C7-C8	5.15	120.28	111.09
17	c	5502	CLA	C6-C5-C3	-5.11	101.02	113.47
17	C	502	CLA	C6-C5-C3	-5.09	101.07	113.47
24	A	411	BCT	O2-C-O1	5.08	132.66	119.68
24	a	5412	BCT	O2-C-O1	5.07	132.66	119.68
23	A	410	SQD	O47-C7-C8	5.05	120.10	111.09
25	d	5408	MGE	O2G-C1B-C2B	4.78	121.83	111.48
23	d	5407	SQD	O5-C5-C4	4.67	118.11	109.70
26	c	5516	DGD	O3G-C3G-C2G	-4.55	99.75	110.82
26	C	517	DGD	O3G-C3G-C2G	-4.54	99.78	110.82
21	A	408	LHG	O4-P-O5	4.52	133.45	112.44
21	a	5409	LHG	O4-P-O5	4.52	133.45	112.44
25	B	619	MGE	O2G-C1B-C2B	4.44	121.08	111.48
25	b	5620	MGE	O2G-C1B-C2B	4.44	121.08	111.48
25	d	5410	MGE	O2G-C1B-C2B	4.43	121.07	111.48
25	D	410	MGE	O2G-C1B-C2B	4.43	121.07	111.48
26	a	5411	DGD	O3G-C3G-C2G	-4.37	100.20	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	5102	SQD	O47-C7-C8	4.36	120.91	111.48
26	C	518	DGD	O3G-C3G-C2G	-4.34	100.27	110.82
20	b	5618	BCR	C15-C14-C13	-4.30	121.25	127.28
20	B	618	BCR	C15-C14-C13	-4.29	121.26	127.28
25	D	409	MGE	O2G-C1B-C2B	4.20	120.56	111.48
23	L	101	SQD	O47-C7-C8	4.18	120.53	111.48
20	b	5618	BCR	C15-C16-C17	-4.15	115.03	123.52
20	B	618	BCR	C15-C16-C17	-4.13	115.07	123.52
25	D	410	MGE	C2G-O2G-C1B	-4.12	107.94	117.80
25	D	408	MGE	O2G-C1B-C2B	4.07	120.29	111.48
25	D	409	MGE	C3G-O3G-C1D	-4.06	105.10	113.80
25	A	412	MGE	O2G-C1B-C2B	4.02	120.17	111.48
25	l	5101	MGE	O2G-C1B-C2B	4.00	120.14	111.48
23	l	5102	SQD	O9-S-O7	-3.99	100.85	113.82
23	a	5401	SQD	O9-S-O7	-3.97	100.91	113.82
26	b	5621	DGD	O6D-C1D-O3G	-3.92	100.78	110.04
26	D	411	DGD	O6D-C1D-O3G	-3.92	100.79	110.04
17	C	505	CLA	CAA-C2A-C3A	-3.91	102.42	113.00
25	d	5410	MGE	C2G-O2G-C1B	-3.91	108.44	117.80
17	c	5505	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
23	l	5102	SQD	O7-S-C6	3.89	112.57	106.76
25	d	5409	MGE	O2G-C1B-C2B	3.88	119.88	111.48
23	L	101	SQD	O9-S-O7	-3.86	101.27	113.82
23	d	5407	SQD	O47-C7-C8	3.85	119.82	111.48
23	A	410	SQD	O9-S-O7	-3.85	101.31	113.82
20	t	5101	BCR	C24-C23-C22	-3.85	120.54	126.23
20	b	5619	BCR	C24-C23-C22	-3.85	120.55	126.23
20	c	5513	BCR	C15-C16-C17	-3.80	115.75	123.52
25	C	519	MGE	O2G-C1B-C2B	3.80	119.69	111.48
25	c	5517	MGE	O2G-C1B-C2B	3.79	119.68	111.48
25	m	5103	MGE	O2G-C1B-C2B	3.79	119.67	111.48
25	m	5101	MGE	O2G-C1B-C2B	3.78	119.67	111.48
20	C	514	BCR	C15-C16-C17	-3.78	115.78	123.52
17	D	404	CLA	C3B-C4B-NB	-3.71	107.22	110.53
17	d	5403	CLA	C3B-C4B-NB	-3.71	107.22	110.53
17	a	5402	CLA	C3B-C4B-NB	-3.69	107.24	110.53
17	B	609	CLA	C3B-C4B-NB	-3.69	107.24	110.53
26	C	518	DGD	O6D-C1D-O3G	-3.68	101.34	110.04
26	a	5411	DGD	O6D-C1D-O3G	-3.68	101.34	110.04
17	A	401	CLA	C3B-C4B-NB	-3.67	107.26	110.53
23	L	101	SQD	O8-S-C6	3.66	113.04	105.97
17	b	5609	CLA	C3B-C4B-NB	-3.65	107.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	SQD	O5-C5-C4	3.64	116.25	109.70
23	d	5407	SQD	O9-S-O7	-3.62	102.06	113.82
20	b	5617	BCR	C15-C16-C17	-3.61	116.13	123.52
17	C	510	CLA	C3B-C4B-NB	-3.61	107.31	110.53
20	B	617	BCR	C15-C16-C17	-3.60	116.15	123.52
23	D	403	SQD	O47-C7-C8	3.60	119.26	111.48
19	A	406	PQ9	C11-C2-C1	3.60	119.87	116.91
23	D	403	SQD	O9-S-O7	-3.59	102.14	113.82
22	M	101	LMT	C1'-O5'-C5'	-3.57	106.75	113.72
17	c	5508	CLA	C1-C2-C3	-3.55	120.37	126.20
25	d	5409	MGE	C3G-O3G-C1D	-3.54	106.20	113.80
17	C	508	CLA	C1-C2-C3	-3.54	120.40	126.20
19	D	406	PQ9	C36-C37-C38	-3.54	119.52	127.62
19	d	5405	PQ9	C36-C37-C38	-3.54	119.53	127.62
26	c	5515	DGD	O6D-C1D-O3G	-3.53	101.70	110.04
17	b	5609	CLA	C1-C2-C3	-3.53	120.42	126.20
17	c	5510	CLA	C3B-C4B-NB	-3.52	107.39	110.53
26	A	413	DGD	O6D-C1D-O3G	-3.52	101.72	110.04
17	B	609	CLA	C1-C2-C3	-3.52	120.43	126.20
25	d	5409	MGE	O1G-C1A-C2A	3.52	122.56	111.83
19	a	5407	PQ9	C11-C2-C1	3.51	119.80	116.91
18	d	5402	PHO	CBC-CAC-C3C	-3.50	107.86	112.87
23	d	5407	SQD	C3-C4-C5	3.50	116.58	110.23
17	b	5608	CLA	C1-C2-C3	-3.50	120.47	126.20
17	B	608	CLA	C1-C2-C3	-3.49	120.47	126.20
18	D	402	PHO	CBC-CAC-C3C	-3.49	107.87	112.87
17	C	503	CLA	C1-C2-C3	-3.49	120.48	126.20
17	c	5503	CLA	C1-C2-C3	-3.49	120.49	126.20
17	b	5611	CLA	C3B-C4B-NB	-3.48	107.42	110.53
17	a	5406	CLA	C3B-C4B-NB	-3.47	107.43	110.53
23	L	101	SQD	O6-C1-C2	3.47	113.54	108.27
20	C	516	BCR	C15-C16-C17	-3.47	116.42	123.52
20	c	5514	BCR	C15-C16-C17	-3.46	116.43	123.52
17	B	608	CLA	C3B-C4B-NB	-3.46	107.44	110.53
26	c	5516	DGD	O6D-C1D-O3G	-3.46	101.87	110.04
22	A	409	LMT	C1'-O5'-C5'	-3.46	106.97	113.72
17	b	5608	CLA	C3B-C4B-NB	-3.44	107.45	110.53
25	D	409	MGE	O1G-C1A-C2A	3.44	122.33	111.83
26	C	517	DGD	O6D-C1D-O3G	-3.43	101.93	110.04
20	b	5617	BCR	C15-C14-C13	-3.43	122.47	127.28
20	d	5406	BCR	C24-C23-C22	-3.43	121.16	126.23
19	d	5405	PQ9	C19-C18-C20	3.42	121.17	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	611	CLA	C3B-C4B-NB	-3.42	107.48	110.53
22	m	5102	LMT	C1'-O5'-C5'	-3.42	107.04	113.72
19	D	406	PQ9	C19-C18-C20	3.42	121.16	115.23
20	B	617	BCR	C15-C14-C13	-3.42	122.49	127.28
20	D	407	BCR	C24-C23-C22	-3.41	121.19	126.23
23	l	5102	SQD	O9-S-C6	3.40	111.83	106.76
17	A	405	CLA	C3B-C4B-NB	-3.39	107.50	110.53
17	d	5404	CLA	C3B-C4B-NB	-3.39	107.50	110.53
17	b	5613	CLA	C3B-C4B-NB	-3.38	107.51	110.53
17	B	603	CLA	C3B-C4B-NB	-3.35	107.54	110.53
17	D	405	CLA	C3B-C4B-NB	-3.35	107.54	110.53
23	l	5102	SQD	O5-C5-C4	3.33	115.69	109.70
17	B	613	CLA	C3B-C4B-NB	-3.32	107.57	110.53
20	k	5502	BCR	C24-C23-C22	-3.32	121.33	126.23
17	b	5615	CLA	C3B-C4B-NB	-3.30	107.58	110.53
20	Y	101	BCR	C24-C23-C22	-3.30	121.35	126.23
17	B	615	CLA	C3B-C4B-NB	-3.30	107.59	110.53
25	B	619	MGE	C2G-O2G-C1B	-3.29	109.92	117.80
17	B	614	CLA	C3B-C4B-NB	-3.29	107.59	110.53
17	b	5611	CLA	C1-C2-C3	-3.28	120.82	126.20
17	b	5614	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	b	5620	MGE	C2G-O2G-C1B	-3.28	109.95	117.80
19	d	5405	PQ9	C31-C32-C33	-3.27	120.13	127.62
25	A	412	MGE	C3G-O3G-C1D	-3.26	106.80	113.80
25	l	5101	MGE	C3G-O3G-C1D	-3.26	106.80	113.80
17	B	611	CLA	C1-C2-C3	-3.26	120.85	126.20
17	b	5603	CLA	C3B-C4B-NB	-3.25	107.62	110.53
17	k	5501	CLA	C3B-C4B-NB	-3.25	107.62	110.53
19	D	406	PQ9	C31-C32-C33	-3.25	120.18	127.62
20	H	101	BCR	C24-C23-C22	-3.24	121.44	126.23
17	B	606	CLA	C3B-C4B-NB	-3.24	107.64	110.53
20	A	407	BCR	C15-C16-C17	-3.23	116.91	123.52
17	C	511	CLA	C3B-C4B-NB	-3.23	107.65	110.53
20	a	5408	BCR	C15-C16-C17	-3.22	116.92	123.52
17	b	5610	CLA	C3B-C4B-NB	-3.22	107.65	110.53
20	h	5101	BCR	C24-C23-C22	-3.22	121.47	126.23
17	c	5511	CLA	C3B-C4B-NB	-3.21	107.66	110.53
19	D	406	PQ9	C21-C22-C23	-3.21	120.27	127.62
23	l	5102	SQD	C1-O5-C5	3.21	119.99	113.72
19	d	5405	PQ9	C21-C22-C23	-3.20	120.29	127.62
17	B	610	CLA	C3B-C4B-NB	-3.20	107.67	110.53
20	z	5101	BCR	C15-C16-C17	-3.20	116.97	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5606	CLA	C3B-C4B-NB	-3.19	107.68	110.53
23	d	5407	SQD	O7-S-C6	3.19	111.53	106.76
17	C	512	CLA	C3B-C4B-NB	-3.19	107.68	110.53
17	c	5503	CLA	C3B-C4B-NB	-3.19	107.68	110.53
20	C	515	BCR	C15-C16-C17	-3.18	117.00	123.52
17	C	503	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	d	5407	SQD	C4-C3-C2	3.16	116.39	110.83
23	D	403	SQD	O7-S-C6	3.16	111.48	106.76
19	D	406	PQ9	C24-C23-C25	3.15	120.69	115.23
19	d	5405	PQ9	C24-C23-C25	3.15	120.69	115.23
17	c	5508	CLA	C3B-C4B-NB	-3.14	107.72	110.53
17	B	606	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
26	C	518	DGD	CDB-CCB-CBB	-3.14	98.48	114.37
23	A	410	SQD	O7-S-C6	3.14	111.45	106.76
26	a	5411	DGD	CDB-CCB-CBB	-3.14	98.50	114.37
17	b	5606	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
17	C	504	CLA	C3B-C4B-NB	-3.13	107.74	110.53
20	c	5513	BCR	C15-C14-C13	-3.13	122.89	127.28
18	A	404	PHO	O1D-CGD-CBD	3.12	129.46	124.72
17	c	5504	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	A	406	PQ9	C11-C2-C3	-3.11	119.72	123.39
17	C	508	CLA	C3B-C4B-NB	-3.11	107.76	110.53
19	a	5407	PQ9	C11-C2-C3	-3.11	119.73	123.39
20	C	514	BCR	C15-C14-C13	-3.10	122.93	127.28
20	k	5502	BCR	C15-C16-C17	-3.10	117.18	123.52
18	a	5405	PHO	O1D-CGD-CBD	3.09	129.41	124.72
18	D	402	PHO	C2B-C1B-NB	-3.07	107.21	109.43
25	A	412	MGE	O1G-C1A-C2A	3.07	121.18	111.83
17	b	5604	CLA	C1-C2-C3	-3.06	121.19	126.20
17	B	604	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	A	406	PQ9	C34-C33-C35	3.05	120.51	115.23
25	l	5101	MGE	O1G-C1A-C2A	3.04	121.11	111.83
17	B	604	CLA	C1-C2-C3	-3.04	121.22	126.20
18	d	5402	PHO	C2B-C1B-NB	-3.03	107.24	109.43
20	a	5408	BCR	C15-C14-C13	-3.03	123.03	127.28
17	b	5604	CLA	C3B-C4B-NB	-3.03	107.83	110.53
17	b	5612	CLA	C3B-C4B-NB	-3.03	107.83	110.53
17	B	616	CLA	C3B-C4B-NB	-3.02	107.84	110.53
20	Y	101	BCR	C15-C16-C17	-3.01	117.35	123.52
17	B	612	CLA	C3B-C4B-NB	-3.01	107.84	110.53
17	C	506	CLA	C3B-C4B-NB	-3.01	107.84	110.53
17	c	5506	CLA	C3B-C4B-NB	-3.01	107.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	5101	BCR	C7-C8-C9	-3.00	121.79	126.23
17	B	602	CLA	C3B-C4B-NB	-3.00	107.86	110.53
20	A	407	BCR	C15-C14-C13	-2.99	123.08	127.28
26	a	5411	DGD	O6E-C1E-O5D	-2.99	102.98	110.04
26	C	518	DGD	O6E-C1E-O5D	-2.99	102.98	110.04
19	A	406	PQ9	C26-C27-C28	-2.99	120.78	127.62
20	H	101	BCR	C7-C8-C9	-2.99	121.81	126.23
18	A	404	PHO	C2B-C1B-NB	-2.99	107.27	109.43
17	C	509	CLA	C3B-C4B-NB	-2.99	107.86	110.53
17	b	5602	CLA	C3B-C4B-NB	-2.98	107.87	110.53
25	m	5101	MGE	C2G-O2G-C1B	-2.98	110.66	117.80
25	D	408	MGE	C2G-O2G-C1B	-2.98	110.67	117.80
20	b	5618	BCR	C27-C26-C25	2.98	126.73	122.70
20	B	618	BCR	C27-C26-C25	2.97	126.72	122.70
20	T	102	BCR	C27-C26-C25	2.97	126.72	122.70
17	c	5509	CLA	C3B-C4B-NB	-2.97	107.88	110.53
23	d	5407	SQD	O48-C23-C24	2.96	120.87	111.83
25	m	5101	MGE	O1G-C1A-C2A	2.96	120.85	111.83
23	D	403	SQD	C4-C3-C2	2.95	116.02	110.83
17	B	603	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
17	C	507	CLA	C3B-C4B-NB	-2.95	107.90	110.53
17	b	5616	CLA	C3B-C4B-NB	-2.95	107.90	110.53
26	a	5411	DGD	O5D-C6D-C5D	-2.94	102.79	109.42
22	B	620	LMT	C3'-C4'-C5'	-2.94	104.41	110.93
18	a	5405	PHO	C2B-C1B-NB	-2.94	107.31	109.43
26	C	518	DGD	O5D-C6D-C5D	-2.94	102.79	109.42
26	D	411	DGD	C3D-C4D-C5D	-2.92	104.93	110.23
17	B	613	CLA	CHB-C4A-NA	2.92	128.61	124.40
26	c	5515	DGD	O6D-C5D-C6D	-2.92	100.91	106.69
25	C	519	MGE	O1G-C1A-C2A	2.92	120.74	111.83
26	C	517	DGD	O5D-C6D-C5D	-2.92	102.84	109.42
17	B	605	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	c	5516	DGD	O5D-C6D-C5D	-2.92	102.84	109.42
17	b	5603	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	C	505	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
25	c	5517	MGE	O1G-C1A-C2A	2.91	120.72	111.83
17	c	5505	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	C	514	BCR	C33-C5-C6	-2.91	121.31	124.48
17	c	5507	CLA	C3B-C4B-NB	-2.91	107.93	110.53
17	b	5605	CLA	C3B-C4B-NB	-2.91	107.93	110.53
26	A	413	DGD	O6D-C5D-C6D	-2.91	100.93	106.69
20	T	102	BCR	C15-C16-C17	-2.90	117.59	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	608	CLA	CMB-C2B-C1B	-2.89	121.01	125.42
26	b	5621	DGD	C3D-C4D-C5D	-2.89	104.98	110.23
17	c	5511	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	b	5608	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
23	D	403	SQD	O6-C1-C2	2.89	112.66	108.27
17	b	5612	CLA	CHB-C4A-NA	2.89	128.57	124.40
17	b	5601	CLA	CAA-C2A-C3A	-2.88	109.63	116.23
20	B	617	BCR	C7-C8-C9	-2.88	121.98	126.23
17	B	601	CLA	CAA-C2A-C3A	-2.88	109.64	116.23
17	C	512	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	A	410	SQD	C44-O6-C1	2.87	119.94	113.80
17	B	612	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	B	617	BCR	C11-C10-C9	-2.86	123.26	127.28
17	b	5613	CLA	CHB-C4A-NA	2.86	128.53	124.40
17	b	5602	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	a	5401	SQD	O7-S-C6	2.86	111.02	106.76
20	b	5617	BCR	C7-C8-C9	-2.86	122.01	126.23
25	D	409	MGE	O3G-C1D-C2D	2.85	112.61	108.27
25	D	409	MGE	C2G-O2G-C1B	-2.85	110.97	117.80
20	t	5102	BCR	C27-C26-C25	2.85	126.56	122.70
17	c	5502	CLA	C4-C3-C5	2.85	120.18	115.23
20	b	5617	BCR	C11-C10-C9	-2.85	123.28	127.28
20	h	5101	BCR	C27-C26-C25	2.84	126.55	122.70
17	B	602	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	C	505	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	a	5411	DGD	C1D-C2D-C3D	-2.84	104.04	110.01
20	H	101	BCR	C27-C26-C25	2.83	126.53	122.70
26	C	518	DGD	C1D-C2D-C3D	-2.83	104.05	110.01
17	c	5508	CLA	CHB-C4A-NA	2.83	128.48	124.40
20	c	5513	BCR	C33-C5-C6	-2.83	121.40	124.48
17	C	508	CLA	CHB-C4A-NA	2.83	128.48	124.40
17	A	402	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
17	C	502	CLA	C4-C3-C5	2.82	120.12	115.23
17	a	5403	CLA	CHB-C4A-NA	2.82	128.46	124.40
17	b	5611	CLA	CHB-C4A-NA	2.81	128.46	124.40
17	a	5403	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	D	403	SQD	C3-C4-C5	2.81	115.33	110.23
17	c	5505	CLA	C3B-C4B-NB	-2.81	108.02	110.53
18	d	5402	PHO	C1-C2-C3	-2.81	121.60	126.20
19	D	406	PQ9	C26-C27-C28	-2.81	121.20	127.62
19	d	5405	PQ9	C26-C27-C28	-2.80	121.20	127.62
17	C	505	CLA	O2A-CGA-O1A	-2.80	116.61	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5505	CLA	O2A-CGA-O1A	-2.80	116.61	123.63
25	B	619	MGE	O1G-C1A-C2A	2.80	120.38	111.83
17	B	605	CLA	CHB-C4A-NA	2.80	128.44	124.40
23	l	5102	SQD	O48-C23-C24	2.80	120.38	111.83
17	c	5507	CLA	CAC-C3C-C4C	2.80	128.43	124.79
17	b	5605	CLA	CHB-C4A-NA	2.80	128.44	124.40
17	C	507	CLA	CAC-C3C-C4C	2.80	128.43	124.79
17	A	405	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	a	5412	BCT	O3-C-O1	-2.80	112.52	119.68
25	d	5410	MGE	O1G-C1A-C2A	2.79	120.36	111.83
17	B	607	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	t	5101	BCR	C27-C26-C25	2.79	126.47	122.70
24	A	411	BCT	O3-C-O1	-2.79	112.54	119.68
25	b	5620	MGE	O1G-C1A-C2A	2.79	120.34	111.83
17	C	511	CLA	CHB-C4A-NA	2.79	128.42	124.40
17	A	402	CLA	CHB-C4A-NA	2.79	128.42	124.40
17	k	5501	CLA	CHB-C4A-NA	2.78	128.42	124.40
19	A	406	PQ9	C11-C12-C13	-2.78	122.04	126.83
18	D	402	PHO	C1-C2-C3	-2.78	121.64	126.20
25	d	5408	MGE	O1G-C1A-C2A	2.78	120.31	111.83
23	a	5401	SQD	C44-O6-C1	2.78	119.75	113.80
20	D	407	BCR	C15-C14-C13	-2.78	123.38	127.28
20	d	5406	BCR	C33-C5-C6	-2.78	121.46	124.48
17	c	5503	CLA	CAA-C2A-C3A	-2.77	105.50	113.00
17	B	607	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	b	5619	BCR	C27-C26-C25	2.77	126.45	122.70
23	a	5401	SQD	O9-S-C6	2.77	110.89	106.76
17	B	608	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	D	403	SQD	O48-C23-C24	2.76	120.27	111.83
17	C	503	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
17	b	5607	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
17	b	5604	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
17	B	604	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
17	d	5403	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
19	a	5407	PQ9	C11-C12-C13	-2.75	122.08	126.83
22	a	5410	LMT	C1'-O5'-C5'	-2.75	108.34	113.72
17	B	611	CLA	CHB-C4A-NA	2.75	128.38	124.40
17	a	5406	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	D	406	PQ9	C6-C5-C4	2.75	120.91	115.28
20	d	5406	BCR	C15-C14-C13	-2.75	123.42	127.28
17	b	5607	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	d	5405	PQ9	C6-C5-C4	2.75	120.90	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	407	BCR	C33-C5-C6	-2.74	121.49	124.48
17	B	605	CLA	C1-C2-C3	-2.74	121.70	126.20
17	B	610	CLA	CHB-C4A-NA	2.74	128.36	124.40
17	b	5608	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	B	612	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	C	501	CLA	C1-C2-C3	-2.73	121.72	126.20
20	A	407	BCR	C24-C23-C22	-2.73	122.19	126.23
17	B	607	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	t	5101	BCR	C11-C10-C9	-2.73	123.45	127.28
17	C	511	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
17	C	502	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	b	5607	CLA	C3B-C4B-NB	-2.73	108.10	110.53
17	c	5502	CLA	C3B-C4B-NB	-2.73	108.10	110.53
17	D	404	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
17	B	614	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	d	5409	MGE	C3G-C2G-C1G	-2.72	105.44	111.78
20	c	5514	BCR	C15-C14-C13	-2.72	123.46	127.28
17	b	5610	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	k	5501	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
20	A	407	BCR	C27-C26-C25	2.71	126.37	122.70
17	C	501	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
17	b	5612	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
20	h	5101	BCR	C33-C5-C6	-2.71	121.53	124.48
20	C	516	BCR	C15-C14-C13	-2.71	123.48	127.28
20	b	5619	BCR	C11-C10-C9	-2.71	123.48	127.28
17	C	513	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	b	5605	CLA	C1-C2-C3	-2.71	121.77	126.20
20	b	5617	BCR	C27-C26-C25	2.70	126.36	122.70
17	c	5501	CLA	C1-C2-C3	-2.70	121.77	126.20
19	a	5407	PQ9	C14-C13-C15	2.70	119.92	115.23
26	A	413	DGD	O3G-C3G-C2G	-2.70	104.25	110.82
20	H	101	BCR	C33-C5-C6	-2.70	121.54	124.48
17	a	5403	CLA	C1-C2-C3	-2.70	121.78	126.20
20	a	5408	BCR	C24-C23-C22	-2.70	122.24	126.23
19	A	406	PQ9	C39-C38-C40	2.70	119.91	115.23
26	c	5515	DGD	O3G-C3G-C2G	-2.69	104.27	110.82
17	A	403	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
17	a	5404	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
17	A	402	CLA	C1-C2-C3	-2.69	121.79	126.20
17	c	5501	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
17	b	5614	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
20	z	5101	BCR	C27-C26-C25	2.69	126.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5501	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	C	514	BCR	C24-C23-C22	-2.68	122.26	126.23
19	A	406	PQ9	C14-C13-C15	2.68	119.89	115.23
17	c	5512	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	c	5507	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
23	d	5407	SQD	O6-C1-C2	2.68	112.34	108.27
17	C	507	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
17	C	509	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
17	c	5509	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
17	A	405	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
20	c	5513	BCR	C24-C23-C22	-2.66	122.30	126.23
25	c	5517	MGE	C3G-O3G-C1D	-2.66	108.10	113.80
20	B	617	BCR	C27-C26-C25	2.66	126.29	122.70
20	t	5101	BCR	C33-C5-C6	-2.65	121.59	124.48
20	a	5408	BCR	C27-C26-C25	2.65	126.29	122.70
20	t	5102	BCR	C33-C5-C6	-2.65	121.59	124.48
25	C	519	MGE	C3G-O3G-C1D	-2.65	108.12	113.80
17	B	613	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
17	b	5616	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
17	C	501	CLA	C3B-C4B-NB	-2.64	108.17	110.53
17	B	611	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
20	a	5408	BCR	C33-C5-C6	-2.64	121.60	124.48
17	b	5613	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
17	B	606	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	b	5606	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	C	517	DGD	C3D-C4D-C5D	-2.64	105.45	110.23
20	d	5406	BCR	C27-C26-C25	2.64	126.27	122.70
17	b	5614	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	B	616	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
26	A	413	DGD	O3E-C3E-C2E	-2.64	104.16	110.38
17	a	5406	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
20	C	515	BCR	C27-C26-C25	2.63	126.26	122.70
17	C	501	CLA	CHB-C4A-NA	2.63	128.20	124.40
23	L	101	SQD	O9-S-C6	2.63	110.69	106.76
26	c	5515	DGD	O3E-C3E-C2E	-2.63	104.18	110.38
17	b	5611	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
20	A	407	BCR	C33-C5-C6	-2.62	121.63	124.48
17	B	608	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	c	5516	DGD	C3D-C4D-C5D	-2.62	105.49	110.23
17	B	614	CLA	CHB-C4A-NA	2.61	128.17	124.40
20	C	515	BCR	C33-C5-C6	-2.61	121.63	124.48
19	A	406	PQ9	C19-C18-C20	2.61	119.76	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5619	BCR	C33-C5-C6	-2.61	121.64	124.48
20	k	5502	BCR	C33-C5-C6	-2.61	121.64	124.48
19	a	5407	PQ9	C19-C18-C20	2.60	119.75	115.23
17	c	5501	CLA	CHB-C4A-NA	2.60	128.16	124.40
20	c	5514	BCR	C7-C8-C9	-2.60	122.39	126.23
17	A	403	CLA	C3B-C4B-NB	-2.60	108.21	110.53
18	d	5402	PHO	O1D-CGD-CBD	2.60	128.66	124.72
17	a	5402	CLA	CAA-C2A-C1A	-2.60	103.46	111.97
20	D	407	BCR	C27-C26-C25	2.59	126.21	122.70
17	A	401	CLA	CAA-C2A-C1A	-2.59	103.48	111.97
19	d	5405	PQ9	C39-C38-C40	2.59	119.72	115.23
19	D	406	PQ9	C39-C38-C40	2.59	119.72	115.23
17	C	504	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
26	c	5516	DGD	C4E-C3E-C2E	-2.59	106.29	110.83
17	a	5404	CLA	C3B-C4B-NB	-2.58	108.22	110.53
17	c	5504	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
20	z	5101	BCR	C33-C5-C6	-2.58	121.67	124.48
17	b	5608	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	C	514	BCR	C27-C26-C25	2.58	126.19	122.70
23	L	101	SQD	O48-C23-O10	-2.57	117.19	123.63
20	C	516	BCR	C7-C8-C9	-2.57	122.43	126.23
26	c	5516	DGD	C3G-C2G-C1G	-2.57	105.78	111.78
23	A	410	SQD	O9-S-C6	2.57	110.60	106.76
19	A	406	PQ9	C31-C32-C33	-2.57	121.74	127.62
18	d	5402	PHO	O2D-CGD-O1D	-2.57	118.85	123.85
22	m	5102	LMT	C3B-C4B-C5B	-2.57	105.58	110.23
26	C	518	DGD	C3G-C2G-C1G	-2.57	105.80	111.78
20	b	5618	BCR	C35-C13-C14	-2.57	118.66	122.82
26	C	517	DGD	C3G-C2G-C1G	-2.56	105.81	111.78
26	a	5411	DGD	C3G-C2G-C1G	-2.56	105.81	111.78
20	c	5513	BCR	C27-C26-C25	2.56	126.17	122.70
19	d	5405	PQ9	C16-C17-C18	-2.56	121.76	127.62
18	D	402	PHO	O2D-CGD-O1D	-2.56	118.86	123.85
25	D	408	MGE	O1G-C1A-C2A	2.56	119.64	111.83
18	D	402	PHO	O1D-CGD-CBD	2.56	128.60	124.72
26	C	517	DGD	C4E-C3E-C2E	-2.56	106.34	110.83
19	D	406	PQ9	C29-C28-C30	2.56	119.66	115.23
17	A	403	CLA	C1-C2-C3	-2.55	122.01	126.20
20	B	618	BCR	C35-C13-C14	-2.55	118.68	122.82
17	d	5404	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	a	5404	CLA	C1-C2-C3	-2.55	122.02	126.20
19	D	406	PQ9	C16-C17-C18	-2.55	121.79	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	516	BCR	C11-C10-C9	-2.54	123.72	127.28
21	A	408	LHG	O8-C23-C24	2.54	119.57	111.83
17	b	5615	CLA	C1-C2-C3	-2.54	122.04	126.20
20	c	5514	BCR	C11-C10-C9	-2.53	123.72	127.28
17	A	403	CLA	CHB-C4A-NA	2.53	128.06	124.40
20	c	5514	BCR	C33-C5-C6	-2.53	121.72	124.48
23	l	5102	SQD	C4-C3-C2	2.53	115.27	110.83
23	L	101	SQD	C4-C3-C2	2.53	115.27	110.83
21	a	5409	LHG	O8-C23-C24	2.53	119.54	111.83
20	C	515	BCR	C15-C14-C13	-2.53	123.74	127.28
19	d	5405	PQ9	C29-C28-C30	2.53	119.61	115.23
17	D	405	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	C	506	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
17	B	601	CLA	C2A-C1A-CHA	2.52	128.22	123.86
17	C	501	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
17	c	5506	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
17	b	5615	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	b	5613	CLA	C1-C2-C3	-2.51	122.08	126.20
17	b	5601	CLA	C2A-C1A-CHA	2.51	128.21	123.86
17	b	5609	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	c	5501	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
19	a	5407	PQ9	C6-C5-C4	2.51	120.41	115.28
19	A	406	PQ9	C6-C5-C4	2.50	120.41	115.28
17	b	5606	CLA	O2D-CGD-CBD	2.50	115.61	111.23
23	A	410	SQD	O8-S-C6	2.50	110.80	105.97
20	z	5101	BCR	C15-C14-C13	-2.50	123.77	127.28
23	L	101	SQD	O48-C23-C24	2.50	119.45	111.83
26	c	5515	DGD	O2D-C2D-C1D	-2.50	104.12	110.08
17	B	613	CLA	C1-C2-C3	-2.50	122.11	126.20
17	a	5404	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	B	606	CLA	O2D-CGD-CBD	2.50	115.59	111.23
17	b	5605	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
26	A	413	DGD	O2D-C2D-C1D	-2.49	104.13	110.08
20	Y	101	BCR	C27-C26-C25	2.49	126.07	122.70
17	B	609	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	b	5604	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
17	B	605	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
17	B	616	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	b	5616	CLA	CHB-C4A-NA	2.49	127.99	124.40
26	b	5621	DGD	C4E-C3E-C2E	-2.49	106.47	110.83
17	C	502	CLA	CHB-C4A-NA	2.49	127.99	124.40
26	D	411	DGD	C4E-C3E-C2E	-2.48	106.48	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	615	CLA	C1-C2-C3	-2.48	122.14	126.20
20	C	515	BCR	C11-C10-C9	-2.48	123.80	127.28
17	C	511	CLA	C1-C2-C3	-2.48	122.14	126.20
18	a	5405	PHO	CMB-C2B-C3B	2.47	129.62	124.68
20	C	516	BCR	C33-C5-C6	-2.47	121.79	124.48
23	d	5407	SQD	O8-S-C6	2.47	110.74	105.97
20	A	407	BCR	C2-C1-C6	2.47	114.02	110.44
17	B	604	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
17	d	5404	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
20	D	407	BCR	C15-C16-C17	-2.47	118.47	123.52
17	B	615	CLA	CHB-C4A-NA	2.46	127.96	124.40
17	c	5511	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	C	509	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
20	z	5101	BCR	C11-C10-C9	-2.46	123.83	127.28
20	t	5101	BCR	C8-C7-C6	-2.46	120.43	127.00
25	m	5103	MGE	O1G-C1A-C2A	2.46	119.33	111.83
20	a	5408	BCR	C2-C1-C6	2.46	114.01	110.44
17	c	5502	CLA	CHB-C4A-NA	2.46	127.94	124.40
17	b	5615	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
18	A	404	PHO	CMB-C2B-C3B	2.46	129.59	124.68
25	D	410	MGE	O1G-C1A-C2A	2.45	119.31	111.83
17	C	506	CLA	CHB-C4A-NA	2.45	127.94	124.40
17	D	405	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
17	k	5501	CLA	C1-C2-C3	-2.45	122.18	126.20
23	a	5401	SQD	O8-S-C6	2.45	110.70	105.97
17	B	615	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
20	b	5619	BCR	C8-C7-C6	-2.45	120.46	127.00
18	d	5402	PHO	CMB-C2B-C3B	2.45	129.57	124.68
20	d	5406	BCR	C15-C16-C17	-2.44	118.52	123.52
17	c	5509	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
25	d	5409	MGE	O6D-C5D-C4D	2.44	114.10	109.70
20	T	102	BCR	C15-C14-C13	-2.44	123.85	127.28
17	C	512	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	b	5617	BCR	C33-C5-C6	-2.44	121.82	124.48
17	C	513	CLA	C1-C2-C3	-2.44	122.82	126.76
17	B	614	CLA	C1-C2-C3	-2.44	122.21	126.20
17	c	5506	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	b	5618	BCR	C24-C23-C22	-2.43	122.64	126.23
17	c	5512	CLA	C1-C2-C3	-2.43	122.83	126.76
20	k	5502	BCR	C27-C26-C25	2.43	125.98	122.70
18	D	402	PHO	CMB-C2B-C3B	2.43	129.53	124.68
17	C	505	CLA	CAC-C3C-C4C	2.43	127.95	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5505	CLA	CAC-C3C-C4C	2.42	127.94	124.79
17	D	405	CLA	C1-C2-C3	-2.42	122.84	126.76
20	c	5513	BCR	C7-C8-C9	-2.42	122.65	126.23
17	b	5614	CLA	C1-C2-C3	-2.42	122.23	126.20
20	B	617	BCR	C33-C5-C6	-2.42	121.84	124.48
20	D	407	BCR	C7-C8-C9	-2.42	122.66	126.23
17	c	5508	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
17	C	508	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
20	t	5102	BCR	C15-C14-C13	-2.41	123.89	127.28
17	B	610	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
17	d	5404	CLA	C1-C2-C3	-2.41	122.86	126.76
25	l	5101	MGE	C2G-O2G-C1B	-2.41	112.04	117.80
17	C	507	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	A	412	MGE	C2G-O2G-C1B	-2.41	112.04	117.80
20	C	514	BCR	C7-C8-C9	-2.40	122.68	126.23
17	b	5603	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
17	B	603	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
20	T	102	BCR	C40-C30-C25	2.40	114.01	110.24
17	b	5610	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	B	618	BCR	C24-C23-C22	-2.40	122.69	126.23
20	c	5514	BCR	C24-C23-C22	-2.39	122.69	126.23
20	d	5406	BCR	C7-C8-C9	-2.39	122.70	126.23
22	T	101	LMT	C3'-C4'-C5'	-2.39	105.63	110.93
19	A	406	PQ9	C29-C28-C30	2.39	119.38	115.23
17	c	5512	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
20	t	5101	BCR	C38-C26-C25	-2.39	121.88	124.48
17	c	5507	CLA	CHB-C4A-NA	2.39	127.84	124.40
20	b	5619	BCR	C38-C26-C25	-2.39	121.88	124.48
20	h	5101	BCR	C16-C15-C14	-2.38	118.64	123.52
18	A	404	PHO	O2D-CGD-O1D	-2.38	119.22	123.85
20	H	101	BCR	C16-C15-C14	-2.38	118.65	123.52
17	C	513	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
17	c	5509	CLA	CHB-C4A-NA	2.38	127.83	124.40
18	a	5405	PHO	O2D-CGD-O1D	-2.38	119.22	123.85
20	b	5617	BCR	C35-C13-C14	-2.37	118.97	122.82
17	B	604	CLA	CHB-C4A-NA	2.37	127.83	124.40
17	b	5604	CLA	CHB-C4A-NA	2.37	127.83	124.40
20	C	516	BCR	C24-C23-C22	-2.37	122.72	126.23
17	A	402	CLA	C3B-C4B-NB	-2.37	108.42	110.53
17	B	606	CLA	C1-C2-C3	-2.37	122.32	126.20
17	c	5505	CLA	CHB-C4A-NA	2.37	127.81	124.40
17	B	613	CLA	CAA-CBA-CGA	-2.36	106.49	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	503	CLA	CHB-C4A-NA	2.36	127.81	124.40
17	A	401	CLA	CAA-CBA-CGA	-2.36	106.50	113.21
17	C	509	CLA	CHB-C4A-NA	2.36	127.81	124.40
17	C	503	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
17	d	5403	CLA	CHB-C4A-NA	2.36	127.80	124.40
20	B	617	BCR	C35-C13-C14	-2.36	119.00	122.82
17	B	603	CLA	CHB-C4A-NA	2.36	127.80	124.40
17	B	610	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
17	c	5503	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
20	T	102	BCR	C30-C25-C26	-2.35	119.42	122.64
17	b	5601	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
20	C	515	BCR	C24-C23-C22	-2.35	122.76	126.23
17	B	611	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
19	A	406	PQ9	C36-C37-C38	-2.35	122.25	127.62
20	t	5101	BCR	C15-C14-C13	-2.35	123.99	127.28
17	c	5503	CLA	CHB-C4A-NA	2.34	127.78	124.40
17	B	601	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
17	a	5402	CLA	CAA-CBA-CGA	-2.34	106.56	113.21
17	b	5613	CLA	CAA-CBA-CGA	-2.34	106.56	113.21
17	B	610	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
17	D	404	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	f	5101	HEM	CHC-C1C-NC	2.34	127.00	124.45
17	C	513	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	C	518	DGD	O6D-C5D-C6D	-2.33	102.07	106.69
25	d	5410	MGE	O2G-C1B-O1B	-2.33	118.25	123.70
23	D	403	SQD	O8-S-C6	2.33	110.48	105.97
17	C	505	CLA	CHB-C4A-NA	2.33	127.77	124.40
17	b	5611	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
20	b	5619	BCR	C15-C14-C13	-2.33	124.01	127.28
17	b	5610	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
17	b	5610	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
17	b	5603	CLA	CHB-C4A-NA	2.33	127.76	124.40
17	a	5403	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	d	5408	MGE	C2G-O2G-C1B	-2.32	112.23	117.80
17	c	5506	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
18	a	5405	PHO	CMA-C3A-C4A	-2.32	109.61	114.61
20	z	5101	BCR	C24-C23-C22	-2.32	122.80	126.23
17	c	5512	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	L	101	SQD	O5-C5-C4	2.31	113.87	109.70
20	B	618	BCR	C2-C1-C6	2.31	113.80	110.44
17	a	5402	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
21	A	408	LHG	C27-C26-C25	-2.31	102.69	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	5409	LHG	C27-C26-C25	-2.31	102.70	114.37
17	C	506	CLA	CAA-C2A-C3A	-2.31	106.77	113.00
23	a	5401	SQD	O5-C5-C4	2.31	113.86	109.70
17	C	508	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
18	A	404	PHO	CMA-C3A-C4A	-2.30	109.65	114.61
20	Y	101	BCR	C33-C5-C6	-2.30	121.98	124.48
19	D	406	PQ9	C41-C42-C43	-2.30	119.99	127.64
26	a	5411	DGD	O6D-C5D-C6D	-2.29	102.14	106.69
26	b	5621	DGD	C3G-C2G-C1G	-2.29	106.44	111.78
17	B	609	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
19	d	5405	PQ9	C11-C2-C3	-2.29	120.68	123.39
17	b	5608	CLA	CMB-C2B-C3B	2.29	131.94	126.55
19	d	5405	PQ9	C41-C42-C43	-2.29	120.00	127.64
19	a	5407	PQ9	C16-C17-C18	-2.29	122.38	127.62
17	b	5612	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
20	b	5618	BCR	C2-C1-C6	2.29	113.77	110.44
26	C	518	DGD	CBB-CAB-C9B	-2.29	102.80	114.37
26	a	5411	DGD	CBB-CAB-C9B	-2.29	102.80	114.37
26	D	411	DGD	C3G-C2G-C1G	-2.28	106.46	111.78
17	C	510	CLA	CHB-C4A-NA	2.28	127.70	124.40
17	A	401	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
23	l	5102	SQD	C3-C4-C5	2.28	114.36	110.23
20	z	5101	BCR	C8-C7-C6	-2.28	120.91	127.00
29	F	101	HEM	CHC-C1C-NC	2.28	126.93	124.45
19	D	406	PQ9	C11-C2-C3	-2.28	120.70	123.39
19	A	406	PQ9	C16-C17-C18	-2.28	122.42	127.62
17	c	5508	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
20	t	5102	BCR	C30-C25-C26	-2.27	119.53	122.64
20	b	5617	BCR	C20-C21-C22	-2.27	124.09	127.28
19	A	406	PQ9	C45-C43-C44	2.27	119.81	114.59
17	B	608	CLA	CMB-C2B-C3B	2.27	131.89	126.55
17	C	513	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	D	409	MGE	C3G-C2G-C1G	-2.27	106.49	111.78
20	C	515	BCR	C8-C7-C6	-2.27	120.94	127.00
20	B	617	BCR	C20-C21-C22	-2.27	124.10	127.28
26	c	5515	DGD	O6E-C1E-O5D	-2.27	104.69	110.04
20	C	514	BCR	C11-C10-C9	-2.26	124.11	127.28
17	B	602	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	l	5102	SQD	C44-O6-C1	2.25	118.63	113.80
17	b	5609	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
17	C	510	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
17	C	503	CLA	O2D-CGD-O1D	-2.25	119.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5609	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
17	c	5512	CLA	CHB-C4A-NA	2.25	127.65	124.40
25	b	5620	MGE	O2G-C1B-O1B	-2.25	118.44	123.70
17	B	612	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
17	B	609	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
25	B	619	MGE	O2G-C1B-O1B	-2.25	118.45	123.70
20	b	5617	BCR	C2-C1-C6	2.25	113.70	110.44
17	b	5616	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
26	A	413	DGD	O6E-C1E-O5D	-2.24	104.74	110.04
17	c	5510	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
17	b	5602	CLA	CHB-C4A-NA	2.24	127.64	124.40
17	c	5504	CLA	CHB-C4A-NA	2.24	127.64	124.40
17	C	504	CLA	CHB-C4A-NA	2.24	127.63	124.40
20	c	5513	BCR	C11-C10-C9	-2.23	124.15	127.28
17	c	5503	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
23	l	5102	SQD	O5-C1-C2	2.23	114.95	110.37
17	B	616	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
17	b	5611	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
23	L	101	SQD	C44-O6-C1	2.23	118.57	113.80
17	d	5403	CLA	C1-C2-C3	-2.23	122.55	126.20
25	C	519	MGE	C2G-O2G-C1B	-2.23	112.47	117.80
25	c	5517	MGE	C2G-O2G-C1B	-2.22	112.48	117.80
17	b	5608	CLA	CHB-C1B-NB	2.22	127.38	124.05
20	t	5101	BCR	C16-C15-C14	-2.22	118.97	123.52
17	B	611	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
23	d	5407	SQD	C44-O6-C1	2.22	118.55	113.80
17	c	5510	CLA	CHB-C4A-NA	2.22	127.60	124.40
17	A	401	CLA	C1-C2-C3	-2.21	122.57	126.20
20	b	5619	BCR	C16-C15-C14	-2.21	118.99	123.52
23	A	410	SQD	O5-C5-C4	2.21	113.69	109.70
20	B	617	BCR	C2-C1-C6	2.21	113.65	110.44
20	T	102	BCR	C33-C5-C6	-2.21	122.07	124.48
20	h	5101	BCR	C30-C25-C26	-2.21	119.62	122.64
20	C	516	BCR	C27-C26-C25	2.21	125.69	122.70
17	D	404	CLA	C1-C2-C3	-2.21	122.58	126.20
17	B	608	CLA	CHB-C1B-NB	2.20	127.35	124.05
17	B	604	CLA	CHB-C1B-NB	2.20	127.35	124.05
17	B	603	CLA	C1-C2-C3	-2.19	122.60	126.20
20	b	5618	BCR	C8-C7-C6	-2.19	121.15	127.00
20	c	5514	BCR	C27-C26-C25	2.19	125.66	122.70
17	B	601	CLA	C3B-C4B-NB	-2.19	108.58	110.53
17	b	5612	CLA	CMB-C2B-C3B	2.19	131.69	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	BCR	C30-C25-C26	-2.18	119.65	122.64
20	b	5618	BCR	C33-C5-C6	-2.18	122.10	124.48
17	B	612	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
20	b	5619	BCR	C15-C16-C17	-2.18	119.06	123.52
17	b	5604	CLA	CHB-C1B-NB	2.18	127.32	124.05
25	d	5409	MGE	C2G-O2G-C1B	-2.18	112.58	117.80
17	b	5612	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
20	c	5514	BCR	C28-C27-C26	-2.18	110.17	114.06
20	B	618	BCR	C8-C7-C6	-2.18	121.19	127.00
20	k	5502	BCR	C7-C8-C9	-2.18	123.02	126.23
20	Y	101	BCR	C15-C14-C13	-2.17	124.23	127.28
23	A	410	SQD	O6-C1-C2	2.17	111.57	108.27
17	a	5402	CLA	C1-C2-C3	-2.17	122.64	126.20
25	c	5517	MGE	O1G-C1A-O1A	-2.17	118.20	123.63
21	A	408	LHG	C5-O7-C7	-2.17	112.60	117.80
20	B	618	BCR	C33-C5-C6	-2.17	122.12	124.48
17	b	5603	CLA	C1-C2-C3	-2.17	122.64	126.20
17	b	5601	CLA	C3B-C4B-NB	-2.17	108.59	110.53
25	C	519	MGE	O1G-C1A-O1A	-2.17	118.21	123.63
17	B	612	CLA	CMB-C2B-C3B	2.17	131.65	126.55
21	a	5409	LHG	C5-O7-C7	-2.17	112.61	117.80
20	b	5617	BCR	C24-C23-C22	-2.16	123.03	126.23
26	c	5515	DGD	C5B-C4B-C3B	-2.16	103.43	114.37
20	t	5101	BCR	C15-C16-C17	-2.16	119.09	123.52
20	T	102	BCR	C38-C26-C25	-2.16	122.12	124.48
17	a	5404	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
17	B	607	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
19	d	5405	PQ9	C14-C13-C15	2.16	118.98	115.23
17	b	5607	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
17	A	403	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
26	A	413	DGD	C5B-C4B-C3B	-2.16	103.46	114.37
26	c	5516	DGD	O2D-C2D-C1D	-2.16	104.94	110.08
22	A	409	LMT	C3'-C4'-C5'	-2.16	106.15	110.93
25	D	410	MGE	O2G-C1B-O1B	-2.16	118.67	123.70
20	C	516	BCR	C28-C27-C26	-2.15	110.22	114.06
25	l	5101	MGE	O1G-C1A-O1A	-2.15	118.24	123.63
19	a	5407	PQ9	C24-C23-C25	2.15	118.96	115.23
20	B	617	BCR	C24-C23-C22	-2.15	123.05	126.23
26	C	517	DGD	O2D-C2D-C1D	-2.15	104.96	110.08
17	B	616	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
19	A	406	PQ9	C24-C23-C25	2.15	118.95	115.23
17	d	5404	CLA	O2A-CGA-O1A	-2.14	118.26	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	412	MGE	O1G-C1A-O1A	-2.14	118.26	123.63
17	D	405	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
17	B	616	CLA	O2D-CGD-CBD	2.14	114.97	111.23
17	C	512	CLA	O2D-CGD-CBD	2.14	114.97	111.23
25	d	5409	MGE	O1G-C1A-O1A	-2.14	118.27	123.63
20	A	407	BCR	C38-C26-C25	-2.14	122.15	124.48
17	a	5403	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
17	b	5616	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
19	D	406	PQ9	C34-C33-C35	2.14	118.94	115.23
20	A	407	BCR	C8-C7-C6	-2.14	121.29	127.00
17	c	5511	CLA	O2D-CGD-CBD	2.13	114.96	111.23
25	d	5409	MGE	C1D-C2D-C3D	-2.13	105.52	110.01
18	D	402	PHO	O2A-CGA-O1A	-2.13	118.30	123.63
22	A	409	LMT	O5B-C5B-C4B	2.13	113.54	109.70
18	d	5402	PHO	O2A-CGA-O1A	-2.13	118.30	123.63
20	B	618	BCR	C10-C11-C12	-2.13	117.03	123.20
20	b	5618	BCR	C10-C11-C12	-2.13	117.03	123.20
19	d	5405	PQ9	C34-C33-C35	2.13	118.92	115.23
17	A	402	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
19	D	406	PQ9	C14-C13-C15	2.12	118.92	115.23
20	a	5408	BCR	C38-C26-C25	-2.12	122.17	124.48
23	l	5102	SQD	O47-C7-O49	-2.12	118.74	123.70
18	A	404	PHO	C3B-C4B-NB	-2.12	106.08	107.46
17	b	5616	CLA	O2D-CGD-CBD	2.12	114.93	111.23
17	C	506	CLA	O1D-CGD-CBD	2.11	128.68	124.52
23	L	101	SQD	O7-S-C6	2.11	109.91	106.76
17	b	5610	CLA	CMB-C2B-C3B	2.11	131.51	126.55
26	C	518	DGD	C6D-O5D-C1E	2.11	118.31	113.80
26	a	5411	DGD	C6D-O5D-C1E	2.11	118.31	113.80
17	c	5506	CLA	O1D-CGD-CBD	2.10	128.67	124.52
17	B	610	CLA	CMB-C2B-C3B	2.10	131.50	126.55
20	a	5408	BCR	C8-C7-C6	-2.10	121.38	127.00
17	c	5502	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
17	b	5606	CLA	CAA-C2A-C1A	-2.09	107.51	112.14
17	D	404	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
17	C	505	CLA	C1-C2-C3	-2.09	122.77	126.20
17	d	5403	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
19	a	5407	PQ9	C30-C28-C29	2.09	119.39	114.59
17	C	502	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
20	a	5408	BCR	C11-C10-C9	-2.08	124.36	127.28
17	A	405	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	B	605	CLA	O2A-CGA-O1A	-2.08	118.42	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5602	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	D	409	MGE	O2G-C1B-O1B	-2.08	118.84	123.70
17	a	5406	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	C	516	BCR	C8-C7-C6	-2.08	121.45	127.00
17	B	602	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
23	D	403	SQD	C44-O6-C1	2.08	118.25	113.80
20	A	407	BCR	C11-C10-C9	-2.07	124.37	127.28
18	a	5405	PHO	C3B-C4B-NB	-2.07	106.11	107.46
25	m	5101	MGE	C3G-O3G-C1D	-2.07	109.35	113.80
20	b	5618	BCR	C38-C26-C25	-2.07	122.22	124.48
25	d	5410	MGE	C4D-C3D-C2D	-2.07	107.20	110.83
25	D	409	MGE	O1G-C1A-O1A	-2.07	118.45	123.63
17	c	5505	CLA	C1-C2-C3	-2.07	122.81	126.20
22	m	5102	LMT	C3'-C4'-C5'	-2.07	106.35	110.93
20	B	618	BCR	C38-C26-C25	-2.07	122.23	124.48
17	c	5502	CLA	C6-C7-C8	-2.06	109.11	115.97
20	c	5513	BCR	C20-C21-C22	-2.06	124.39	127.28
20	d	5406	BCR	C38-C26-C25	-2.06	122.23	124.48
26	c	5515	DGD	O4D-C4D-C5D	-2.06	104.25	109.32
26	b	5621	DGD	C5B-C4B-C3B	-2.06	103.95	114.37
20	c	5514	BCR	C8-C7-C6	-2.06	121.49	127.00
17	C	502	CLA	C6-C7-C8	-2.06	109.12	115.97
23	D	403	SQD	O9-S-C6	2.06	109.83	106.76
26	C	518	DGD	C5B-C4B-C3B	-2.06	103.96	114.37
26	C	518	DGD	CAB-C9B-C8B	-2.06	103.96	114.37
19	a	5407	PQ9	C26-C27-C28	-2.06	120.79	127.64
20	t	5102	BCR	C15-C16-C17	-2.06	119.31	123.52
26	a	5411	DGD	CAB-C9B-C8B	-2.05	103.99	114.37
17	B	612	CLA	C11-C10-C8	-2.05	109.14	115.97
26	D	411	DGD	C5B-C4B-C3B	-2.05	104.00	114.37
17	C	510	CLA	C16-C15-C13	-2.05	109.15	115.97
26	D	411	DGD	O3E-C3E-C2E	-2.05	105.54	110.38
20	C	514	BCR	C20-C21-C22	-2.05	124.40	127.28
19	d	5405	PQ9	C45-C43-C44	2.05	119.30	114.59
25	m	5103	MGE	C2G-O2G-C1B	-2.05	112.89	117.80
19	D	406	PQ9	C45-C43-C44	2.05	119.30	114.59
26	a	5411	DGD	C5B-C4B-C3B	-2.05	104.02	114.37
23	D	403	SQD	O47-C7-O49	-2.05	118.92	123.70
17	b	5612	CLA	C11-C10-C8	-2.05	109.16	115.97
17	c	5510	CLA	C16-C15-C13	-2.04	109.17	115.97
20	t	5102	BCR	C11-C10-C9	-2.04	124.41	127.28
26	A	413	DGD	O4D-C4D-C5D	-2.04	104.29	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5605	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	D	407	BCR	C38-C26-C25	-2.04	122.26	124.48
26	b	5621	DGD	O3E-C3E-C2E	-2.04	105.57	110.38
23	d	5407	SQD	O47-C7-O49	-2.04	118.94	123.70
17	B	611	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
17	c	5509	CLA	CHA-C1A-NA	-2.03	121.78	126.39
20	t	5101	BCR	C20-C21-C22	-2.03	124.42	127.28
17	b	5611	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
17	b	5601	CLA	O2D-CGD-CBD	2.03	114.78	111.23
17	a	5402	CLA	CHB-C4A-NA	2.03	127.33	124.40
20	t	5102	BCR	C7-C8-C9	-2.03	123.23	126.23
17	C	510	CLA	CHB-C1B-NB	2.02	127.08	124.05
21	A	408	LHG	O8-C6-C5	-2.02	102.56	108.40
17	c	5510	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
17	B	601	CLA	O2D-CGD-CBD	2.02	114.77	111.23
17	k	5501	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
21	a	5409	LHG	O8-C6-C5	-2.02	102.59	108.40
17	C	509	CLA	CHA-C1A-NA	-2.02	121.83	126.39
17	A	401	CLA	CHB-C4A-NA	2.01	127.31	124.40
20	k	5502	BCR	C15-C14-C13	-2.01	124.45	127.28
17	d	5403	CLA	C2D-C1D-ND	-2.01	108.13	110.13
17	b	5614	CLA	O2D-CGD-CBD	2.01	114.75	111.23
17	b	5607	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
17	c	5506	CLA	C1-C2-C3	-2.01	122.91	126.20
20	Y	101	BCR	C8-C7-C6	-2.01	121.63	127.00
17	B	613	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	A	407	BCR	C7-C8-C9	-2.00	123.27	126.23
26	a	5411	DGD	O5E-C6E-C5E	-2.00	104.52	111.33
20	t	5101	BCR	C2-C1-C6	2.00	113.34	110.44
17	c	5507	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	401	CLA	ND
17	A	402	CLA	ND
17	A	403	CLA	ND
17	A	405	CLA	ND
17	B	601	CLA	ND
17	B	602	CLA	ND
17	B	603	CLA	ND
17	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	605	CLA	ND
17	B	606	CLA	ND
17	B	607	CLA	ND
17	B	608	CLA	ND
17	B	609	CLA	ND
17	B	610	CLA	ND
17	B	611	CLA	ND
17	B	612	CLA	ND
17	B	613	CLA	ND
17	B	614	CLA	ND
17	B	615	CLA	ND
17	B	616	CLA	ND
17	C	501	CLA	ND
17	C	502	CLA	ND
17	C	503	CLA	ND
17	C	504	CLA	ND
17	C	505	CLA	ND
17	C	506	CLA	ND
17	C	507	CLA	ND
17	C	508	CLA	ND
17	C	509	CLA	ND
17	C	510	CLA	ND
17	C	511	CLA	ND
17	C	512	CLA	ND
17	C	513	CLA	ND
17	D	404	CLA	ND
17	D	405	CLA	ND
17	a	5402	CLA	ND
17	a	5403	CLA	ND
17	a	5404	CLA	ND
17	a	5406	CLA	ND
17	b	5601	CLA	ND
17	b	5602	CLA	ND
17	b	5603	CLA	ND
17	b	5604	CLA	ND
17	b	5605	CLA	ND
17	b	5606	CLA	ND
17	b	5607	CLA	ND
17	b	5608	CLA	ND
17	b	5609	CLA	ND
17	b	5610	CLA	ND
17	b	5611	CLA	ND

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Mol	Chain	Res	Type	Atom
17	b	5612	CLA	ND
17	b	5613	CLA	ND
17	b	5614	CLA	ND
17	b	5615	CLA	ND
17	b	5616	CLA	ND
17	c	5501	CLA	ND
17	c	5502	CLA	ND
17	c	5503	CLA	ND
17	c	5504	CLA	ND
17	c	5505	CLA	ND
17	c	5506	CLA	ND
17	c	5507	CLA	ND
17	c	5508	CLA	ND
17	c	5509	CLA	ND
17	c	5510	CLA	ND
17	c	5511	CLA	ND
17	c	5512	CLA	ND
17	d	5403	CLA	ND
17	d	5404	CLA	ND
17	k	5501	CLA	ND

All (1845) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	602	CLA	C4-C3-C5-C6
17	B	603	CLA	CBD-CGD-O2D-CED
17	B	605	CLA	CAD-CBD-CGD-O2D
17	B	605	CLA	C14-C13-C15-C16
17	B	606	CLA	C1A-C2A-CAA-CBA
17	B	606	CLA	C3A-C2A-CAA-CBA
17	B	608	CLA	C1A-C2A-CAA-CBA
17	B	609	CLA	C1A-C2A-CAA-CBA
17	B	609	CLA	C3A-C2A-CAA-CBA
17	B	609	CLA	CAD-CBD-CGD-O1D
17	B	609	CLA	CAD-CBD-CGD-O2D
17	B	609	CLA	CBD-CGD-O2D-CED
17	B	609	CLA	C11-C10-C8-C9
17	B	610	CLA	CHA-CBD-CGD-O1D
17	B	610	CLA	CHA-CBD-CGD-O2D
17	B	612	CLA	C1A-C2A-CAA-CBA
17	B	612	CLA	C3A-C2A-CAA-CBA
17	B	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	616	CLA	C1A-C2A-CAA-CBA
17	B	616	CLA	C3A-C2A-CAA-CBA
17	C	502	CLA	C4B-C3B-CAB-CBB
17	C	503	CLA	C1A-C2A-CAA-CBA
17	C	503	CLA	C4B-C3B-CAB-CBB
17	C	503	CLA	CHA-CBD-CGD-O1D
17	C	503	CLA	CHA-CBD-CGD-O2D
17	C	504	CLA	CBA-CGA-O2A-C1
17	C	504	CLA	O1A-CGA-O2A-C1
17	C	505	CLA	CAD-CBD-CGD-O1D
17	C	505	CLA	CAD-CBD-CGD-O2D
17	C	506	CLA	C1A-C2A-CAA-CBA
17	C	507	CLA	CHA-CBD-CGD-O1D
17	C	507	CLA	CHA-CBD-CGD-O2D
17	C	508	CLA	C2B-C3B-CAB-CBB
17	C	508	CLA	C4B-C3B-CAB-CBB
17	C	508	CLA	CHA-CBD-CGD-O1D
17	C	508	CLA	CHA-CBD-CGD-O2D
17	C	510	CLA	CBD-CGD-O2D-CED
17	D	404	CLA	C1A-C2A-CAA-CBA
17	D	405	CLA	C1A-C2A-CAA-CBA
17	D	405	CLA	C3A-C2A-CAA-CBA
17	D	405	CLA	CBD-CGD-O2D-CED
17	b	5602	CLA	C4-C3-C5-C6
17	b	5603	CLA	CBD-CGD-O2D-CED
17	b	5605	CLA	CAD-CBD-CGD-O2D
17	b	5605	CLA	C14-C13-C15-C16
17	b	5606	CLA	C1A-C2A-CAA-CBA
17	b	5606	CLA	C3A-C2A-CAA-CBA
17	b	5608	CLA	C1A-C2A-CAA-CBA
17	b	5609	CLA	C1A-C2A-CAA-CBA
17	b	5609	CLA	C3A-C2A-CAA-CBA
17	b	5609	CLA	CAD-CBD-CGD-O1D
17	b	5609	CLA	CAD-CBD-CGD-O2D
17	b	5609	CLA	CBD-CGD-O2D-CED
17	b	5609	CLA	C11-C10-C8-C9
17	b	5610	CLA	CHA-CBD-CGD-O1D
17	b	5610	CLA	CHA-CBD-CGD-O2D
17	b	5612	CLA	C1A-C2A-CAA-CBA
17	b	5612	CLA	C3A-C2A-CAA-CBA
17	b	5615	CLA	CBD-CGD-O2D-CED
17	b	5616	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	b	5616	CLA	C3A-C2A-CAA-CBA
17	c	5502	CLA	C4B-C3B-CAB-CBB
17	c	5503	CLA	C1A-C2A-CAA-CBA
17	c	5503	CLA	C4B-C3B-CAB-CBB
17	c	5503	CLA	CHA-CBD-CGD-O1D
17	c	5503	CLA	CHA-CBD-CGD-O2D
17	c	5504	CLA	CBA-CGA-O2A-C1
17	c	5504	CLA	O1A-CGA-O2A-C1
17	c	5505	CLA	CAD-CBD-CGD-O1D
17	c	5505	CLA	CAD-CBD-CGD-O2D
17	c	5506	CLA	C1A-C2A-CAA-CBA
17	c	5507	CLA	CHA-CBD-CGD-O1D
17	c	5507	CLA	CHA-CBD-CGD-O2D
17	c	5508	CLA	C2B-C3B-CAB-CBB
17	c	5508	CLA	C4B-C3B-CAB-CBB
17	c	5508	CLA	CHA-CBD-CGD-O1D
17	c	5508	CLA	CHA-CBD-CGD-O2D
17	c	5510	CLA	CBD-CGD-O2D-CED
17	d	5403	CLA	C1A-C2A-CAA-CBA
17	d	5404	CLA	C1A-C2A-CAA-CBA
17	d	5404	CLA	C3A-C2A-CAA-CBA
17	d	5404	CLA	CBD-CGD-O2D-CED
18	D	402	PHO	C1A-C2A-CAA-CBA
18	D	402	PHO	C3A-C2A-CAA-CBA
18	D	402	PHO	CBD-CGD-O2D-CED
18	d	5402	PHO	C1A-C2A-CAA-CBA
18	d	5402	PHO	C3A-C2A-CAA-CBA
18	d	5402	PHO	CBD-CGD-O2D-CED
20	A	407	BCR	C9-C10-C11-C12
20	A	407	BCR	C18-C19-C20-C21
20	B	617	BCR	C11-C12-C13-C35
20	B	617	BCR	C14-C15-C16-C17
20	B	617	BCR	C21-C22-C23-C24
20	B	617	BCR	C37-C22-C23-C24
20	B	618	BCR	C11-C10-C9-C8
20	B	618	BCR	C10-C11-C12-C13
20	B	618	BCR	C21-C22-C23-C24
20	C	514	BCR	C7-C8-C9-C34
20	C	514	BCR	C14-C15-C16-C17
20	C	515	BCR	C6-C7-C8-C9
20	C	515	BCR	C11-C10-C9-C8
20	C	515	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	C	515	BCR	C12-C13-C14-C15
20	C	515	BCR	C14-C15-C16-C17
20	C	515	BCR	C16-C17-C18-C19
20	C	515	BCR	C16-C17-C18-C36
20	C	515	BCR	C18-C19-C20-C21
20	C	515	BCR	C22-C23-C24-C25
20	C	516	BCR	C6-C7-C8-C9
20	C	516	BCR	C7-C8-C9-C34
20	C	516	BCR	C10-C11-C12-C13
20	C	516	BCR	C12-C13-C14-C15
20	C	516	BCR	C35-C13-C14-C15
20	C	516	BCR	C20-C21-C22-C37
20	C	516	BCR	C21-C22-C23-C24
20	C	516	BCR	C22-C23-C24-C25
20	D	407	BCR	C7-C8-C9-C10
20	D	407	BCR	C11-C12-C13-C35
20	H	101	BCR	C6-C7-C8-C9
20	H	101	BCR	C16-C17-C18-C19
20	H	101	BCR	C16-C17-C18-C36
20	T	102	BCR	C16-C17-C18-C19
20	T	102	BCR	C16-C17-C18-C36
20	T	102	BCR	C23-C24-C25-C26
20	T	102	BCR	C23-C24-C25-C30
20	a	5408	BCR	C9-C10-C11-C12
20	a	5408	BCR	C18-C19-C20-C21
20	b	5617	BCR	C11-C12-C13-C35
20	b	5617	BCR	C14-C15-C16-C17
20	b	5617	BCR	C21-C22-C23-C24
20	b	5617	BCR	C37-C22-C23-C24
20	b	5618	BCR	C11-C10-C9-C8
20	b	5618	BCR	C10-C11-C12-C13
20	b	5618	BCR	C21-C22-C23-C24
20	b	5619	BCR	C6-C7-C8-C9
20	b	5619	BCR	C7-C8-C9-C34
20	b	5619	BCR	C22-C23-C24-C25
20	c	5513	BCR	C7-C8-C9-C34
20	c	5513	BCR	C14-C15-C16-C17
20	c	5514	BCR	C6-C7-C8-C9
20	c	5514	BCR	C7-C8-C9-C34
20	c	5514	BCR	C10-C11-C12-C13
20	c	5514	BCR	C12-C13-C14-C15
20	c	5514	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	c	5514	BCR	C20-C21-C22-C37
20	c	5514	BCR	C21-C22-C23-C24
20	c	5514	BCR	C22-C23-C24-C25
20	d	5406	BCR	C7-C8-C9-C10
20	d	5406	BCR	C11-C12-C13-C35
20	h	5101	BCR	C6-C7-C8-C9
20	h	5101	BCR	C16-C17-C18-C19
20	h	5101	BCR	C16-C17-C18-C36
20	k	5502	BCR	C6-C7-C8-C9
20	k	5502	BCR	C14-C15-C16-C17
20	k	5502	BCR	C18-C19-C20-C21
20	k	5502	BCR	C19-C20-C21-C22
20	k	5502	BCR	C20-C21-C22-C37
20	k	5502	BCR	C21-C22-C23-C24
20	k	5502	BCR	C22-C23-C24-C25
20	t	5101	BCR	C6-C7-C8-C9
20	t	5101	BCR	C7-C8-C9-C34
20	t	5101	BCR	C22-C23-C24-C25
20	t	5102	BCR	C9-C10-C11-C12
20	t	5102	BCR	C14-C15-C16-C17
20	t	5102	BCR	C16-C17-C18-C36
20	t	5102	BCR	C21-C22-C23-C24
20	t	5102	BCR	C37-C22-C23-C24
20	t	5102	BCR	C22-C23-C24-C25
20	z	5101	BCR	C6-C7-C8-C9
20	z	5101	BCR	C11-C10-C9-C8
20	z	5101	BCR	C11-C12-C13-C14
20	z	5101	BCR	C12-C13-C14-C15
20	z	5101	BCR	C14-C15-C16-C17
20	z	5101	BCR	C16-C17-C18-C19
20	z	5101	BCR	C16-C17-C18-C36
20	z	5101	BCR	C18-C19-C20-C21
20	z	5101	BCR	C22-C23-C24-C25
20	Y	101	BCR	C11-C12-C13-C14
20	Y	101	BCR	C14-C15-C16-C17
20	Y	101	BCR	C17-C18-C19-C20
20	Y	101	BCR	C18-C19-C20-C21
20	Y	101	BCR	C22-C23-C24-C25
21	A	408	LHG	O1-C1-C2-C3
21	A	408	LHG	C3-O3-P-O4
21	A	408	LHG	C3-O3-P-O5
21	A	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
21	A	408	LHG	C4-O6-P-O3
21	A	408	LHG	C4-O6-P-O4
21	A	408	LHG	C4-O6-P-O5
21	a	5409	LHG	O1-C1-C2-C3
21	a	5409	LHG	C3-O3-P-O4
21	a	5409	LHG	C3-O3-P-O5
21	a	5409	LHG	C3-O3-P-O6
21	a	5409	LHG	C4-O6-P-O3
21	a	5409	LHG	C4-O6-P-O4
21	a	5409	LHG	C4-O6-P-O5
22	B	620	LMT	O5'-C1'-O1'-C1
22	m	5102	LMT	O5'-C1'-O1'-C1
23	A	410	SQD	O5-C5-C6-S
23	D	403	SQD	O5-C5-C6-S
23	L	101	SQD	O47-C45-C46-O48
23	L	101	SQD	O49-C7-O47-C45
23	L	101	SQD	C5-C6-S-O7
23	L	101	SQD	C5-C6-S-O8
23	L	101	SQD	C5-C6-S-O9
23	a	5401	SQD	C8-C7-O47-C45
23	a	5401	SQD	O5-C5-C6-S
23	a	5401	SQD	C5-C6-S-O7
23	a	5401	SQD	C5-C6-S-O8
23	a	5401	SQD	C5-C6-S-O9
23	d	5407	SQD	O5-C1-O6-C44
23	d	5407	SQD	O5-C5-C6-S
23	l	5102	SQD	O5-C1-O6-C44
23	l	5102	SQD	O5-C5-C6-S
25	C	519	MGE	O2G-C2G-C3G-O3G
25	D	409	MGE	O2G-C2G-C3G-O3G
25	D	410	MGE	O6D-C1D-O3G-C3G
25	c	5517	MGE	O2G-C2G-C3G-O3G
25	d	5410	MGE	O6D-C1D-O3G-C3G
25	m	5103	MGE	C2B-C1B-O2G-C2G
25	m	5103	MGE	O6D-C1D-O3G-C3G
26	A	413	DGD	O6E-C1E-O5D-C6D
26	C	517	DGD	C2E-C1E-O5D-C6D
26	C	517	DGD	O6E-C1E-O5D-C6D
26	C	518	DGD	O2G-C2G-C3G-O3G
26	C	518	DGD	O6E-C1E-O5D-C6D
26	D	411	DGD	O1G-C1G-C2G-O2G
26	a	5411	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
26	a	5411	DGD	O6E-C1E-O5D-C6D
26	b	5621	DGD	O1G-C1G-C2G-O2G
26	c	5515	DGD	O6E-C1E-O5D-C6D
26	c	5516	DGD	C2E-C1E-O5D-C6D
26	c	5516	DGD	O6E-C1E-O5D-C6D
17	B	607	CLA	O1D-CGD-O2D-CED
17	B	609	CLA	O1D-CGD-O2D-CED
17	B	611	CLA	O1D-CGD-O2D-CED
17	B	613	CLA	O1D-CGD-O2D-CED
17	B	615	CLA	O1D-CGD-O2D-CED
17	C	511	CLA	O1D-CGD-O2D-CED
17	b	5607	CLA	O1D-CGD-O2D-CED
17	b	5609	CLA	O1D-CGD-O2D-CED
17	b	5611	CLA	O1D-CGD-O2D-CED
17	b	5615	CLA	O1D-CGD-O2D-CED
17	k	5501	CLA	O1D-CGD-O2D-CED
17	C	502	CLA	O1D-CGD-O2D-CED
17	b	5613	CLA	O1D-CGD-O2D-CED
17	c	5502	CLA	O1D-CGD-O2D-CED
23	a	5401	SQD	O49-C7-O47-C45
17	A	405	CLA	CBD-CGD-O2D-CED
17	B	605	CLA	CBD-CGD-O2D-CED
17	B	606	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	CBD-CGD-O2D-CED
17	B	611	CLA	CBD-CGD-O2D-CED
17	B	613	CLA	CBD-CGD-O2D-CED
17	B	614	CLA	CBD-CGD-O2D-CED
17	B	616	CLA	CBD-CGD-O2D-CED
17	C	501	CLA	CBD-CGD-O2D-CED
17	C	502	CLA	CBD-CGD-O2D-CED
17	C	503	CLA	CBD-CGD-O2D-CED
17	C	506	CLA	CBD-CGD-O2D-CED
17	C	509	CLA	CBD-CGD-O2D-CED
17	C	511	CLA	CBD-CGD-O2D-CED
17	a	5406	CLA	CBD-CGD-O2D-CED
17	b	5605	CLA	CBD-CGD-O2D-CED
17	b	5606	CLA	CBD-CGD-O2D-CED
17	b	5607	CLA	CBD-CGD-O2D-CED
17	b	5611	CLA	CBD-CGD-O2D-CED
17	b	5613	CLA	CBD-CGD-O2D-CED
17	b	5614	CLA	CBD-CGD-O2D-CED
17	b	5616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	c	5501	CLA	CBD-CGD-O2D-CED
17	c	5502	CLA	CBD-CGD-O2D-CED
17	c	5503	CLA	CBD-CGD-O2D-CED
17	c	5506	CLA	CBD-CGD-O2D-CED
17	c	5509	CLA	CBD-CGD-O2D-CED
17	k	5501	CLA	CBD-CGD-O2D-CED
22	T	101	LMT	O5B-C1B-O1B-C4'
22	T	101	LMT	C4B-C5B-C6B-O6B
17	C	501	CLA	O1D-CGD-O2D-CED
17	c	5501	CLA	O1D-CGD-O2D-CED
17	C	507	CLA	CBD-CGD-O2D-CED
17	c	5507	CLA	CBD-CGD-O2D-CED
17	C	507	CLA	O1A-CGA-O2A-C1
17	D	405	CLA	O1A-CGA-O2A-C1
17	c	5507	CLA	O1A-CGA-O2A-C1
17	d	5404	CLA	O1A-CGA-O2A-C1
23	L	101	SQD	O10-C23-O48-C46
17	C	509	CLA	O1D-CGD-O2D-CED
17	c	5509	CLA	O1D-CGD-O2D-CED
18	D	402	PHO	O1D-CGD-O2D-CED
18	d	5402	PHO	O1D-CGD-O2D-CED
22	T	101	LMT	C2B-C1B-O1B-C4'
17	B	603	CLA	O1D-CGD-O2D-CED
17	C	510	CLA	O1D-CGD-O2D-CED
17	b	5603	CLA	O1D-CGD-O2D-CED
17	c	5510	CLA	O1D-CGD-O2D-CED
25	D	409	MGE	C4D-C5D-C6D-O5D
17	C	512	CLA	CBD-CGD-O2D-CED
17	c	5511	CLA	CBD-CGD-O2D-CED
25	m	5103	MGE	O1B-C1B-O2G-C2G
26	A	413	DGD	O1B-C1B-O2G-C2G
26	C	517	DGD	O1B-C1B-O2G-C2G
26	c	5515	DGD	O1B-C1B-O2G-C2G
26	c	5516	DGD	O1B-C1B-O2G-C2G
17	B	602	CLA	C3-C5-C6-C7
17	B	606	CLA	C3-C5-C6-C7
17	B	608	CLA	C3-C5-C6-C7
17	B	614	CLA	C3-C5-C6-C7
17	b	5602	CLA	C3-C5-C6-C7
17	b	5608	CLA	C3-C5-C6-C7
17	b	5614	CLA	C3-C5-C6-C7
17	C	507	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	D	405	CLA	CBA-CGA-O2A-C1
17	c	5507	CLA	CBA-CGA-O2A-C1
17	d	5404	CLA	CBA-CGA-O2A-C1
26	C	518	DGD	C2A-C1A-O1G-C1G
26	a	5411	DGD	C2A-C1A-O1G-C1G
17	B	602	CLA	CBD-CGD-O2D-CED
17	C	508	CLA	CBD-CGD-O2D-CED
17	b	5602	CLA	CBD-CGD-O2D-CED
17	c	5508	CLA	CBD-CGD-O2D-CED
23	L	101	SQD	C8-C7-O47-C45
17	D	405	CLA	O1D-CGD-O2D-CED
17	d	5404	CLA	O1D-CGD-O2D-CED
17	B	606	CLA	C4-C3-C5-C6
17	B	607	CLA	C4-C3-C5-C6
17	C	503	CLA	C4-C3-C5-C6
17	b	5607	CLA	C4-C3-C5-C6
17	c	5503	CLA	C4-C3-C5-C6
19	A	406	PQ9	C19-C18-C20-C21
19	A	406	PQ9	C29-C28-C30-C31
19	A	406	PQ9	C34-C33-C35-C36
19	D	406	PQ9	C24-C23-C25-C26
19	D	406	PQ9	C34-C33-C35-C36
19	a	5407	PQ9	C19-C18-C20-C21
19	d	5405	PQ9	C24-C23-C25-C26
19	d	5405	PQ9	C34-C33-C35-C36
17	B	602	CLA	C2-C3-C5-C6
17	B	607	CLA	C2-C3-C5-C6
17	C	503	CLA	C2-C3-C5-C6
17	b	5602	CLA	C2-C3-C5-C6
17	b	5607	CLA	C2-C3-C5-C6
17	c	5503	CLA	C2-C3-C5-C6
19	A	406	PQ9	C27-C28-C30-C31
17	B	604	CLA	CBD-CGD-O2D-CED
17	b	5604	CLA	CBD-CGD-O2D-CED
17	A	402	CLA	C3-C5-C6-C7
17	B	612	CLA	C3-C5-C6-C7
17	C	505	CLA	C3-C5-C6-C7
17	a	5403	CLA	C3-C5-C6-C7
17	b	5612	CLA	C3-C5-C6-C7
17	c	5505	CLA	C3-C5-C6-C7
17	c	5505	CLA	C2C-C3C-CAC-CBC
23	L	101	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
17	C	505	CLA	C2C-C3C-CAC-CBC
26	D	411	DGD	C4D-C5D-C6D-O5D
26	b	5621	DGD	C4D-C5D-C6D-O5D
20	A	407	BCR	C13-C14-C15-C16
20	C	514	BCR	C9-C10-C11-C12
20	C	515	BCR	C19-C20-C21-C22
20	D	407	BCR	C9-C10-C11-C12
20	T	102	BCR	C9-C10-C11-C12
20	a	5408	BCR	C13-C14-C15-C16
20	c	5513	BCR	C9-C10-C11-C12
20	d	5406	BCR	C9-C10-C11-C12
20	t	5102	BCR	C15-C16-C17-C18
20	z	5101	BCR	C19-C20-C21-C22
20	Y	101	BCR	C19-C20-C21-C22
17	C	506	CLA	O1D-CGD-O2D-CED
17	c	5506	CLA	O1D-CGD-O2D-CED
25	D	409	MGE	O6D-C5D-C6D-O5D
17	A	401	CLA	CBD-CGD-O2D-CED
17	a	5402	CLA	CBD-CGD-O2D-CED
17	B	605	CLA	O1D-CGD-O2D-CED
17	b	5605	CLA	O1D-CGD-O2D-CED
22	A	409	LMT	O5B-C5B-C6B-O6B
22	B	620	LMT	O5'-C5'-C6'-O6'
22	a	5410	LMT	O5'-C5'-C6'-O6'
23	a	5401	SQD	C24-C23-O48-C46
22	m	5102	LMT	O5B-C5B-C6B-O6B
22	A	409	LMT	C4B-C5B-C6B-O6B
22	m	5102	LMT	C4B-C5B-C6B-O6B
25	D	409	MGE	C2B-C1B-O2G-C2G
22	M	101	LMT	O5B-C5B-C6B-O6B
17	A	405	CLA	O1D-CGD-O2D-CED
17	B	614	CLA	O1D-CGD-O2D-CED
17	a	5406	CLA	O1D-CGD-O2D-CED
17	b	5614	CLA	O1D-CGD-O2D-CED
17	A	403	CLA	C3-C5-C6-C7
17	a	5404	CLA	C3-C5-C6-C7
17	B	601	CLA	CBD-CGD-O2D-CED
17	C	513	CLA	CBD-CGD-O2D-CED
17	b	5601	CLA	CBD-CGD-O2D-CED
17	c	5512	CLA	CBD-CGD-O2D-CED
22	T	101	LMT	O5B-C5B-C6B-O6B
17	c	5503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	406	PQ9	C14-C13-C15-C16
19	a	5407	PQ9	C14-C13-C15-C16
17	B	606	CLA	C2-C3-C5-C6
19	A	406	PQ9	C12-C13-C15-C16
19	A	406	PQ9	C17-C18-C20-C21
19	A	406	PQ9	C32-C33-C35-C36
19	D	406	PQ9	C32-C33-C35-C36
19	a	5407	PQ9	C12-C13-C15-C16
19	a	5407	PQ9	C17-C18-C20-C21
19	d	5405	PQ9	C32-C33-C35-C36
23	a	5401	SQD	O10-C23-O48-C46
22	T	101	LMT	O5'-C5'-C6'-O6'
17	C	503	CLA	O1D-CGD-O2D-CED
19	A	406	PQ9	C18-C20-C21-C22
19	A	406	PQ9	C23-C25-C26-C27
19	A	406	PQ9	C38-C40-C41-C42
19	a	5407	PQ9	C18-C20-C21-C22
19	a	5407	PQ9	C23-C25-C26-C27
17	C	507	CLA	O1D-CGD-O2D-CED
17	c	5507	CLA	O1D-CGD-O2D-CED
17	B	602	CLA	C2A-CAA-CBA-CGA
17	b	5602	CLA	C2A-CAA-CBA-CGA
17	b	5616	CLA	O1D-CGD-O2D-CED
22	A	409	LMT	O5'-C1'-O1'-C1
23	D	403	SQD	O5-C1-O6-C44
26	A	413	DGD	O6D-C1D-O3G-C3G
26	D	411	DGD	O6D-C1D-O3G-C3G
26	D	411	DGD	O6E-C1E-O5D-C6D
26	b	5621	DGD	O6D-C1D-O3G-C3G
26	b	5621	DGD	O6E-C1E-O5D-C6D
26	c	5515	DGD	O6D-C1D-O3G-C3G
26	C	518	DGD	O6E-C5E-C6E-O5E
26	a	5411	DGD	O6E-C5E-C6E-O5E
17	B	616	CLA	O1D-CGD-O2D-CED
17	C	504	CLA	CBD-CGD-O2D-CED
17	D	404	CLA	CBD-CGD-O2D-CED
17	c	5504	CLA	CBD-CGD-O2D-CED
17	d	5403	CLA	CBD-CGD-O2D-CED
17	C	505	CLA	C5-C6-C7-C8
17	c	5505	CLA	C5-C6-C7-C8
20	B	617	BCR	C9-C10-C11-C12
20	C	516	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	C	516	BCR	C13-C14-C15-C16
20	b	5617	BCR	C9-C10-C11-C12
20	c	5514	BCR	C9-C10-C11-C12
20	c	5514	BCR	C13-C14-C15-C16
17	A	401	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	CBA-CGA-O2A-C1
17	C	506	CLA	CBA-CGA-O2A-C1
17	a	5402	CLA	CBA-CGA-O2A-C1
17	b	5607	CLA	CBA-CGA-O2A-C1
17	c	5506	CLA	CBA-CGA-O2A-C1
22	B	620	LMT	C4'-C5'-C6'-O6'
17	B	606	CLA	O1D-CGD-O2D-CED
17	C	512	CLA	O1D-CGD-O2D-CED
17	b	5606	CLA	O1D-CGD-O2D-CED
17	c	5511	CLA	O1D-CGD-O2D-CED
26	C	518	DGD	O1A-C1A-O1G-C1G
26	a	5411	DGD	O1A-C1A-O1G-C1G
17	B	605	CLA	C4-C3-C5-C6
17	D	404	CLA	C4-C3-C5-C6
17	b	5605	CLA	C4-C3-C5-C6
17	d	5403	CLA	C4-C3-C5-C6
19	D	406	PQ9	C19-C18-C20-C21
19	d	5405	PQ9	C19-C18-C20-C21
17	B	605	CLA	C2-C3-C5-C6
17	D	404	CLA	C2-C3-C5-C6
17	b	5605	CLA	C2-C3-C5-C6
17	d	5403	CLA	C2-C3-C5-C6
19	D	406	PQ9	C17-C18-C20-C21
19	D	406	PQ9	C22-C23-C25-C26
19	d	5405	PQ9	C17-C18-C20-C21
19	d	5405	PQ9	C22-C23-C25-C26
17	C	505	CLA	C4C-C3C-CAC-CBC
17	c	5505	CLA	C4C-C3C-CAC-CBC
17	B	604	CLA	C14-C13-C15-C16
17	C	501	CLA	C11-C12-C13-C14
17	C	506	CLA	C11-C10-C8-C9
17	C	507	CLA	C11-C10-C8-C9
17	C	508	CLA	C11-C10-C8-C9
17	C	511	CLA	C6-C7-C8-C9
17	D	404	CLA	C6-C7-C8-C9
17	b	5604	CLA	C14-C13-C15-C16
17	c	5501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	c	5506	CLA	C11-C10-C8-C9
17	c	5507	CLA	C11-C10-C8-C9
17	c	5508	CLA	C11-C10-C8-C9
17	d	5403	CLA	C6-C7-C8-C9
17	k	5501	CLA	C6-C7-C8-C9
18	A	404	PHO	C11-C10-C8-C9
18	a	5405	PHO	C11-C10-C8-C9
22	M	101	LMT	O5'-C5'-C6'-O6'
22	A	409	LMT	C2'-C1'-O1'-C1
22	B	620	LMT	C2'-C1'-O1'-C1
22	m	5102	LMT	C2'-C1'-O1'-C1
23	A	410	SQD	C2-C1-O6-C44
26	A	413	DGD	C2D-C1D-O3G-C3G
26	C	518	DGD	C2E-C1E-O5D-C6D
26	D	411	DGD	C2D-C1D-O3G-C3G
26	D	411	DGD	C2E-C1E-O5D-C6D
26	a	5411	DGD	C2E-C1E-O5D-C6D
26	b	5621	DGD	C2D-C1D-O3G-C3G
26	b	5621	DGD	C2E-C1E-O5D-C6D
26	c	5515	DGD	C2D-C1D-O3G-C3G
26	D	411	DGD	O6D-C5D-C6D-O5D
26	b	5621	DGD	O6D-C5D-C6D-O5D
17	B	607	CLA	O1A-CGA-O2A-C1
17	b	5607	CLA	O1A-CGA-O2A-C1
17	C	508	CLA	O1D-CGD-O2D-CED
17	c	5508	CLA	O1D-CGD-O2D-CED
20	A	407	BCR	C11-C12-C13-C35
20	B	618	BCR	C37-C22-C23-C24
20	C	515	BCR	C7-C8-C9-C34
20	C	515	BCR	C11-C12-C13-C35
20	C	516	BCR	C11-C12-C13-C35
20	D	407	BCR	C7-C8-C9-C34
20	a	5408	BCR	C11-C12-C13-C35
20	b	5618	BCR	C37-C22-C23-C24
20	c	5514	BCR	C11-C12-C13-C35
20	d	5406	BCR	C7-C8-C9-C34
20	z	5101	BCR	C7-C8-C9-C34
20	z	5101	BCR	C11-C12-C13-C35
20	Y	101	BCR	C11-C12-C13-C35
20	C	515	BCR	C7-C8-C9-C10
20	T	102	BCR	C7-C8-C9-C10
20	z	5101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
17	C	509	CLA	C2A-CAA-CBA-CGA
17	c	5509	CLA	C2A-CAA-CBA-CGA
22	a	5410	LMT	C4'-C5'-C6'-O6'
25	D	409	MGE	O1B-C1B-O2G-C2G
23	d	5407	SQD	C8-C7-O47-C45
23	l	5102	SQD	O47-C45-C46-O48
25	d	5409	MGE	C1B-C2B-C3B-C4B
17	A	401	CLA	O1A-CGA-O2A-C1
17	a	5402	CLA	O1A-CGA-O2A-C1
17	B	602	CLA	O1D-CGD-O2D-CED
17	b	5602	CLA	O1D-CGD-O2D-CED
22	m	5102	LMT	O5'-C5'-C6'-O6'
17	C	506	CLA	O1A-CGA-O2A-C1
17	c	5506	CLA	O1A-CGA-O2A-C1
17	B	606	CLA	C12-C13-C15-C16
17	C	503	CLA	C12-C13-C15-C16
17	c	5503	CLA	C12-C13-C15-C16
18	A	404	PHO	C12-C13-C15-C16
18	a	5405	PHO	C12-C13-C15-C16
17	B	603	CLA	C4-C3-C5-C6
17	b	5603	CLA	C4-C3-C5-C6
17	C	510	CLA	C15-C16-C17-C18
17	c	5510	CLA	C15-C16-C17-C18
20	k	5502	BCR	C9-C10-C11-C12
19	D	406	PQ9	C13-C15-C16-C17
19	d	5405	PQ9	C13-C15-C16-C17
17	C	503	CLA	C10-C11-C12-C13
17	c	5503	CLA	C10-C11-C12-C13
18	D	402	PHO	C5-C6-C7-C8
18	d	5402	PHO	C5-C6-C7-C8
23	A	410	SQD	O10-C23-O48-C46
21	A	408	LHG	C23-C24-C25-C26
21	a	5409	LHG	C23-C24-C25-C26
25	D	409	MGE	C1B-C2B-C3B-C4B
17	A	403	CLA	CBD-CGD-O2D-CED
17	a	5404	CLA	CBD-CGD-O2D-CED
26	A	413	DGD	C2B-C1B-O2G-C2G
26	c	5515	DGD	C2B-C1B-O2G-C2G
17	A	402	CLA	C15-C16-C17-C18
17	B	609	CLA	C10-C11-C12-C13
17	C	506	CLA	C15-C16-C17-C18
17	a	5403	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	c	5506	CLA	C15-C16-C17-C18
17	A	405	CLA	C2A-CAA-CBA-CGA
17	C	508	CLA	C2A-CAA-CBA-CGA
17	a	5406	CLA	C2A-CAA-CBA-CGA
17	c	5508	CLA	C2A-CAA-CBA-CGA
20	H	101	BCR	C18-C19-C20-C21
20	h	5101	BCR	C18-C19-C20-C21
20	k	5502	BCR	C10-C11-C12-C13
17	B	609	CLA	C13-C15-C16-C17
17	B	611	CLA	C13-C15-C16-C17
17	C	505	CLA	C13-C15-C16-C17
17	D	404	CLA	C13-C15-C16-C17
17	b	5609	CLA	C10-C11-C12-C13
17	b	5611	CLA	C13-C15-C16-C17
17	c	5505	CLA	C13-C15-C16-C17
17	d	5403	CLA	C13-C15-C16-C17
25	A	412	MGE	C1B-C2B-C3B-C4B
25	l	5101	MGE	C1B-C2B-C3B-C4B
25	m	5103	MGE	C1A-C2A-C3A-C4A
20	T	102	BCR	C22-C23-C24-C25
22	M	101	LMT	O5'-C1'-O1'-C1
23	L	101	SQD	C9-C10-C11-C12
17	A	402	CLA	C5-C6-C7-C8
17	A	403	CLA	C8-C10-C11-C12
17	A	405	CLA	C5-C6-C7-C8
17	B	611	CLA	C15-C16-C17-C18
17	C	508	CLA	C10-C11-C12-C13
17	C	511	CLA	C10-C11-C12-C13
17	a	5403	CLA	C5-C6-C7-C8
17	a	5404	CLA	C8-C10-C11-C12
17	a	5406	CLA	C5-C6-C7-C8
17	b	5609	CLA	C13-C15-C16-C17
17	b	5611	CLA	C15-C16-C17-C18
17	c	5508	CLA	C10-C11-C12-C13
17	k	5501	CLA	C10-C11-C12-C13
25	A	412	MGE	C1A-C2A-C3A-C4A
25	l	5101	MGE	C1A-C2A-C3A-C4A
17	B	603	CLA	C10-C11-C12-C13
17	D	404	CLA	C15-C16-C17-C18
17	b	5603	CLA	C10-C11-C12-C13
17	d	5403	CLA	C15-C16-C17-C18
18	D	402	PHO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	d	5402	PHO	C15-C16-C17-C18
22	M	101	LMT	O1'-C1-C2-C3
17	B	601	CLA	O1D-CGD-O2D-CED
17	b	5601	CLA	O1D-CGD-O2D-CED
17	A	401	CLA	O1D-CGD-O2D-CED
17	a	5402	CLA	O1D-CGD-O2D-CED
17	b	5604	CLA	O1D-CGD-O2D-CED
17	B	611	CLA	C5-C6-C7-C8
17	b	5611	CLA	C5-C6-C7-C8
23	D	403	SQD	C24-C23-O48-C46
17	B	612	CLA	CBD-CGD-O2D-CED
17	b	5612	CLA	CBD-CGD-O2D-CED
26	C	517	DGD	C2B-C1B-O2G-C2G
26	c	5516	DGD	C2B-C1B-O2G-C2G
17	B	604	CLA	O1D-CGD-O2D-CED
23	l	5102	SQD	C23-C24-C25-C26
17	C	506	CLA	C3-C5-C6-C7
17	c	5506	CLA	C3-C5-C6-C7
17	B	610	CLA	C15-C16-C17-C18
17	b	5610	CLA	C15-C16-C17-C18
17	B	606	CLA	C2A-CAA-CBA-CGA
17	B	605	CLA	CBA-CGA-O2A-C1
17	C	512	CLA	CBA-CGA-O2A-C1
17	b	5605	CLA	CBA-CGA-O2A-C1
17	c	5511	CLA	CBA-CGA-O2A-C1
25	d	5410	MGE	C2A-C3A-C4A-C5A
17	A	401	CLA	C13-C15-C16-C17
17	B	602	CLA	C15-C16-C17-C18
17	C	508	CLA	C15-C16-C17-C18
17	a	5402	CLA	C13-C15-C16-C17
17	b	5602	CLA	C15-C16-C17-C18
17	c	5508	CLA	C15-C16-C17-C18
17	A	401	CLA	C5-C6-C7-C8
17	B	612	CLA	C10-C11-C12-C13
17	B	616	CLA	C13-C15-C16-C17
17	a	5402	CLA	C5-C6-C7-C8
17	b	5612	CLA	C10-C11-C12-C13
17	b	5616	CLA	C13-C15-C16-C17
23	D	403	SQD	C8-C7-O47-C45
25	D	410	MGE	C2B-C1B-O2G-C2G
25	d	5408	MGE	C2B-C1B-O2G-C2G
25	d	5410	MGE	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	d	5408	MGE	O1B-C1B-O2G-C2G
25	d	5410	MGE	O1B-C1B-O2G-C2G
23	L	101	SQD	C2-C1-O6-C44
19	A	406	PQ9	C13-C15-C16-C17
19	a	5407	PQ9	C13-C15-C16-C17
23	L	101	SQD	C14-C15-C16-C17
26	A	413	DGD	O1A-C1A-O1G-C1G
20	A	407	BCR	C11-C10-C9-C34
20	A	407	BCR	C16-C17-C18-C36
20	B	618	BCR	C11-C10-C9-C34
20	C	515	BCR	C11-C10-C9-C34
20	D	407	BCR	C35-C13-C14-C15
20	H	101	BCR	C20-C21-C22-C37
20	T	102	BCR	C20-C21-C22-C37
20	a	5408	BCR	C11-C10-C9-C34
20	a	5408	BCR	C16-C17-C18-C36
20	b	5618	BCR	C11-C10-C9-C34
20	d	5406	BCR	C35-C13-C14-C15
20	h	5101	BCR	C20-C21-C22-C37
20	z	5101	BCR	C11-C10-C9-C34
20	Y	101	BCR	C20-C21-C22-C37
20	T	102	BCR	C7-C8-C9-C34
22	A	409	LMT	C5'-C4'-O1B-C1B
25	C	519	MGE	O6D-C5D-C6D-O5D
20	A	407	BCR	C11-C12-C13-C14
20	B	617	BCR	C7-C8-C9-C10
20	B	617	BCR	C11-C12-C13-C14
20	C	514	BCR	C7-C8-C9-C10
20	C	516	BCR	C7-C8-C9-C10
20	a	5408	BCR	C11-C12-C13-C14
20	b	5617	BCR	C7-C8-C9-C10
20	b	5617	BCR	C11-C12-C13-C14
20	c	5513	BCR	C7-C8-C9-C10
20	c	5514	BCR	C7-C8-C9-C10
26	c	5515	DGD	O1A-C1A-O1G-C1G
17	B	610	CLA	C2A-CAA-CBA-CGA
17	b	5610	CLA	C2A-CAA-CBA-CGA
26	A	413	DGD	C4D-C5D-C6D-O5D
26	c	5515	DGD	C4D-C5D-C6D-O5D
25	D	410	MGE	C1B-C2B-C3B-C4B
17	B	609	CLA	C16-C17-C18-C20
17	b	5609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
17	B	605	CLA	C3-C5-C6-C7
17	D	404	CLA	C3-C5-C6-C7
17	b	5605	CLA	C3-C5-C6-C7
17	d	5403	CLA	C3-C5-C6-C7
25	c	5517	MGE	O6D-C5D-C6D-O5D
20	B	618	BCR	C12-C13-C14-C15
20	C	514	BCR	C16-C17-C18-C19
20	C	516	BCR	C20-C21-C22-C23
20	T	102	BCR	C20-C21-C22-C23
20	b	5618	BCR	C12-C13-C14-C15
20	c	5513	BCR	C16-C17-C18-C19
20	c	5514	BCR	C20-C21-C22-C23
20	k	5502	BCR	C20-C21-C22-C23
20	t	5102	BCR	C12-C13-C14-C15
25	D	410	MGE	O1B-C1B-O2G-C2G
23	L	101	SQD	O5-C1-O6-C44
17	C	513	CLA	O1D-CGD-O2D-CED
17	c	5512	CLA	O1D-CGD-O2D-CED
17	B	613	CLA	CBA-CGA-O2A-C1
17	b	5613	CLA	CBA-CGA-O2A-C1
17	A	402	CLA	C8-C10-C11-C12
17	a	5403	CLA	C8-C10-C11-C12
17	B	615	CLA	C2-C1-O2A-CGA
17	b	5615	CLA	C2-C1-O2A-CGA
17	A	403	CLA	C16-C17-C18-C19
17	a	5404	CLA	C16-C17-C18-C19
17	B	605	CLA	O1A-CGA-O2A-C1
17	b	5605	CLA	O1A-CGA-O2A-C1
17	C	503	CLA	C13-C15-C16-C17
17	c	5503	CLA	C13-C15-C16-C17
20	B	618	BCR	C14-C15-C16-C17
20	b	5618	BCR	C14-C15-C16-C17
23	l	5102	SQD	C24-C25-C26-C27
26	A	413	DGD	C4A-C5A-C6A-C7A
26	c	5515	DGD	C4A-C5A-C6A-C7A
26	c	5516	DGD	C8A-C9A-CAA-CBA
17	C	504	CLA	O1D-CGD-O2D-CED
17	D	404	CLA	O1D-CGD-O2D-CED
17	c	5504	CLA	O1D-CGD-O2D-CED
17	d	5403	CLA	O1D-CGD-O2D-CED
26	C	517	DGD	C8A-C9A-CAA-CBA
26	C	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
26	a	5411	DGD	C5A-C6A-C7A-C8A
17	B	611	CLA	CBA-CGA-O2A-C1
17	b	5611	CLA	CBA-CGA-O2A-C1
22	B	620	LMT	C4-C5-C6-C7
21	A	408	LHG	O1-C1-C2-O2
21	a	5409	LHG	O1-C1-C2-O2
17	B	605	CLA	C8-C10-C11-C12
17	b	5605	CLA	C8-C10-C11-C12
17	A	402	CLA	C4B-C3B-CAB-CBB
17	A	403	CLA	C4B-C3B-CAB-CBB
17	B	605	CLA	C4B-C3B-CAB-CBB
17	C	501	CLA	C4B-C3B-CAB-CBB
17	a	5403	CLA	C4B-C3B-CAB-CBB
17	a	5404	CLA	C4B-C3B-CAB-CBB
17	b	5605	CLA	C4B-C3B-CAB-CBB
17	c	5501	CLA	C4B-C3B-CAB-CBB
17	A	403	CLA	C16-C17-C18-C20
17	B	606	CLA	C16-C17-C18-C19
17	B	609	CLA	C16-C17-C18-C19
17	a	5404	CLA	C16-C17-C18-C20
17	b	5609	CLA	C16-C17-C18-C19
18	A	404	PHO	C16-C17-C18-C19
18	A	404	PHO	C16-C17-C18-C20
18	a	5405	PHO	C16-C17-C18-C19
18	a	5405	PHO	C16-C17-C18-C20
17	B	614	CLA	C2A-CAA-CBA-CGA
17	b	5614	CLA	C2A-CAA-CBA-CGA
17	B	615	CLA	C5-C6-C7-C8
17	b	5615	CLA	C5-C6-C7-C8
25	A	412	MGE	C2B-C1B-O2G-C2G
25	l	5101	MGE	C2B-C1B-O2G-C2G
26	C	518	DGD	C2B-C1B-O2G-C2G
26	a	5411	DGD	C2B-C1B-O2G-C2G
17	A	402	CLA	C11-C12-C13-C15
17	a	5403	CLA	C11-C12-C13-C15
23	l	5102	SQD	C27-C28-C29-C30
26	C	518	DGD	C4E-C5E-C6E-O5E
26	a	5411	DGD	C4E-C5E-C6E-O5E
17	C	508	CLA	C3-C5-C6-C7
17	c	5508	CLA	C3-C5-C6-C7
17	C	503	CLA	C3A-C2A-CAA-CBA
17	C	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	D	404	CLA	C3A-C2A-CAA-CBA
17	c	5503	CLA	C3A-C2A-CAA-CBA
17	c	5511	CLA	C3A-C2A-CAA-CBA
17	d	5403	CLA	C3A-C2A-CAA-CBA
22	T	101	LMT	C1-C2-C3-C4
17	C	506	CLA	C13-C15-C16-C17
17	D	404	CLA	C5-C6-C7-C8
17	c	5506	CLA	C13-C15-C16-C17
17	d	5403	CLA	C5-C6-C7-C8
22	M	101	LMT	C4B-C5B-C6B-O6B
26	C	517	DGD	C1A-C2A-C3A-C4A
26	c	5516	DGD	C1A-C2A-C3A-C4A
26	c	5515	DGD	C2B-C3B-C4B-C5B
17	B	606	CLA	C16-C17-C18-C20
26	A	413	DGD	O6D-C5D-C6D-O5D
26	c	5515	DGD	O6D-C5D-C6D-O5D
17	C	512	CLA	O1A-CGA-O2A-C1
17	c	5511	CLA	O1A-CGA-O2A-C1
26	A	413	DGD	C2B-C3B-C4B-C5B
26	c	5515	DGD	C3A-C4A-C5A-C6A
17	C	505	CLA	CBA-CGA-O2A-C1
17	c	5505	CLA	CBA-CGA-O2A-C1
21	A	408	LHG	C4-C5-C6-O8
21	a	5409	LHG	C4-C5-C6-O8
23	L	101	SQD	O6-C44-C45-C46
25	D	409	MGE	O1G-C1G-C2G-C3G
25	d	5409	MGE	C1G-C2G-C3G-O3G
25	d	5410	MGE	O1G-C1G-C2G-C3G
25	D	410	MGE	C2B-C3B-C4B-C5B
26	A	413	DGD	C3A-C4A-C5A-C6A
22	a	5410	LMT	C4-C5-C6-C7
23	d	5407	SQD	C11-C12-C13-C14
26	C	518	DGD	C2B-C3B-C4B-C5B
26	a	5411	DGD	C2B-C3B-C4B-C5B
23	D	403	SQD	C15-C16-C17-C18
23	D	403	SQD	C27-C28-C29-C30
26	b	5621	DGD	C2A-C3A-C4A-C5A
22	T	101	LMT	C4'-C5'-C6'-O6'
23	D	403	SQD	C11-C12-C13-C14
26	D	411	DGD	C2A-C3A-C4A-C5A
17	B	613	CLA	O1A-CGA-O2A-C1
17	b	5613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	402	CLA	C2B-C3B-CAB-CBB
17	B	605	CLA	C2B-C3B-CAB-CBB
17	C	502	CLA	C2B-C3B-CAB-CBB
17	C	503	CLA	C2B-C3B-CAB-CBB
17	D	405	CLA	C2B-C3B-CAB-CBB
17	a	5403	CLA	C2B-C3B-CAB-CBB
17	b	5605	CLA	C2B-C3B-CAB-CBB
17	c	5502	CLA	C2B-C3B-CAB-CBB
17	c	5503	CLA	C2B-C3B-CAB-CBB
17	d	5404	CLA	C2B-C3B-CAB-CBB
20	C	514	BCR	C1-C6-C7-C8
20	D	407	BCR	C1-C6-C7-C8
20	D	407	BCR	C5-C6-C7-C8
20	b	5619	BCR	C23-C24-C25-C26
20	b	5619	BCR	C23-C24-C25-C30
20	c	5513	BCR	C1-C6-C7-C8
20	d	5406	BCR	C1-C6-C7-C8
20	d	5406	BCR	C5-C6-C7-C8
20	t	5101	BCR	C23-C24-C25-C26
20	t	5101	BCR	C23-C24-C25-C30
17	B	608	CLA	CBD-CGD-O2D-CED
17	b	5608	CLA	CBD-CGD-O2D-CED
25	d	5408	MGE	C7A-C8A-C9A-CAA
25	D	409	MGE	C9B-CAB-CBB-CCB
26	C	517	DGD	C2A-C3A-C4A-C5A
23	D	403	SQD	C17-C18-C19-C20
25	m	5103	MGE	C2A-C3A-C4A-C5A
26	c	5516	DGD	C2A-C3A-C4A-C5A
17	B	611	CLA	O1A-CGA-O2A-C1
17	b	5611	CLA	O1A-CGA-O2A-C1
23	A	410	SQD	C24-C23-O48-C46
17	B	604	CLA	C4-C3-C5-C6
17	b	5604	CLA	C4-C3-C5-C6
20	B	617	BCR	C10-C11-C12-C13
20	B	618	BCR	C18-C19-C20-C21
20	D	407	BCR	C10-C11-C12-C13
20	b	5617	BCR	C10-C11-C12-C13
20	b	5618	BCR	C18-C19-C20-C21
20	d	5406	BCR	C10-C11-C12-C13
17	B	603	CLA	C2-C3-C5-C6
17	b	5603	CLA	C2-C3-C5-C6
23	D	403	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	d	5409	MGE	C9B-CAB-CBB-CCB
17	B	609	CLA	CBA-CGA-O2A-C1
17	B	615	CLA	CBA-CGA-O2A-C1
17	b	5609	CLA	CBA-CGA-O2A-C1
17	b	5615	CLA	CBA-CGA-O2A-C1
26	C	518	DGD	C6A-C7A-C8A-C9A
26	a	5411	DGD	C6A-C7A-C8A-C9A
20	B	617	BCR	C6-C7-C8-C9
20	B	618	BCR	C6-C7-C8-C9
20	b	5617	BCR	C6-C7-C8-C9
20	b	5618	BCR	C6-C7-C8-C9
26	D	411	DGD	C4A-C5A-C6A-C7A
26	b	5621	DGD	C4A-C5A-C6A-C7A
25	D	410	MGE	O6D-C5D-C6D-O5D
25	d	5409	MGE	O6D-C5D-C6D-O5D
25	A	412	MGE	C2D-C1D-O3G-C3G
25	l	5101	MGE	C2D-C1D-O3G-C3G
17	C	511	CLA	C8-C10-C11-C12
17	k	5501	CLA	C8-C10-C11-C12
18	D	402	PHO	C10-C11-C12-C13
18	d	5402	PHO	C10-C11-C12-C13
26	A	413	DGD	C3B-C4B-C5B-C6B
26	c	5515	DGD	C3B-C4B-C5B-C6B
17	k	5501	CLA	C5-C6-C7-C8
23	L	101	SQD	C25-C26-C27-C28
25	d	5408	MGE	C5B-C6B-C7B-C8B
17	C	503	CLA	C8-C10-C11-C12
17	C	511	CLA	C5-C6-C7-C8
17	c	5503	CLA	C8-C10-C11-C12
20	B	618	BCR	C17-C18-C19-C20
20	b	5618	BCR	C17-C18-C19-C20
25	d	5408	MGE	C2G-C3G-O3G-C1D
17	C	511	CLA	C16-C17-C18-C19
17	k	5501	CLA	C16-C17-C18-C19
17	B	612	CLA	C5-C6-C7-C8
17	b	5612	CLA	C5-C6-C7-C8
25	m	5103	MGE	C3A-C4A-C5A-C6A
17	c	5505	CLA	O1A-CGA-O2A-C1
23	D	403	SQD	O10-C23-O48-C46
25	d	5410	MGE	O6D-C5D-C6D-O5D
17	B	613	CLA	C5-C6-C7-C8
17	C	507	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	b	5613	CLA	C5-C6-C7-C8
17	c	5507	CLA	C10-C11-C12-C13
17	B	608	CLA	C8-C10-C11-C12
17	b	5608	CLA	C8-C10-C11-C12
17	C	511	CLA	C16-C17-C18-C20
17	k	5501	CLA	C16-C17-C18-C20
23	d	5407	SQD	C24-C25-C26-C27
17	C	505	CLA	O1A-CGA-O2A-C1
17	B	611	CLA	C10-C11-C12-C13
17	B	612	CLA	C8-C10-C11-C12
17	b	5611	CLA	C10-C11-C12-C13
17	b	5612	CLA	C8-C10-C11-C12
17	B	604	CLA	C3-C5-C6-C7
17	b	5604	CLA	C3-C5-C6-C7
25	D	410	MGE	O1G-C1G-C2G-O2G
25	d	5410	MGE	O1G-C1G-C2G-O2G
21	A	408	LHG	C25-C26-C27-C28
21	a	5409	LHG	C25-C26-C27-C28
26	A	413	DGD	C6A-C7A-C8A-C9A
26	c	5515	DGD	C6A-C7A-C8A-C9A
25	m	5101	MGE	O6D-C5D-C6D-O5D
26	C	518	DGD	C4A-C5A-C6A-C7A
26	a	5411	DGD	C4A-C5A-C6A-C7A
17	A	403	CLA	C2-C1-O2A-CGA
17	a	5404	CLA	C2-C1-O2A-CGA
25	D	409	MGE	C2B-C3B-C4B-C5B
25	D	408	MGE	O6D-C5D-C6D-O5D
25	m	5103	MGE	C6B-C7B-C8B-C9B
18	A	404	PHO	C4-C3-C5-C6
18	a	5405	PHO	C4-C3-C5-C6
25	A	412	MGE	O1B-C1B-O2G-C2G
25	l	5101	MGE	O1B-C1B-O2G-C2G
26	C	518	DGD	O1B-C1B-O2G-C2G
26	a	5411	DGD	O1B-C1B-O2G-C2G
17	C	504	CLA	C2A-CAA-CBA-CGA
17	c	5504	CLA	C2A-CAA-CBA-CGA
23	D	403	SQD	C13-C14-C15-C16
25	B	619	MGE	C8A-C9A-CAA-CBA
25	C	519	MGE	C6A-C7A-C8A-C9A
25	b	5620	MGE	C8A-C9A-CAA-CBA
25	c	5517	MGE	C6A-C7A-C8A-C9A
26	D	411	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
26	b	5621	DGD	CBA-CCA-CDA-CEA
18	A	404	PHO	C5-C6-C7-C8
18	a	5405	PHO	C5-C6-C7-C8
17	B	609	CLA	O1A-CGA-O2A-C1
17	A	405	CLA	C1A-C2A-CAA-CBA
17	C	504	CLA	C1A-C2A-CAA-CBA
17	C	512	CLA	C1A-C2A-CAA-CBA
17	a	5406	CLA	C1A-C2A-CAA-CBA
17	c	5504	CLA	C1A-C2A-CAA-CBA
17	c	5511	CLA	C1A-C2A-CAA-CBA
17	B	610	CLA	C8-C10-C11-C12
17	b	5610	CLA	C8-C10-C11-C12
26	D	411	DGD	C8A-C9A-CAA-CBA
26	b	5621	DGD	C8A-C9A-CAA-CBA
17	b	5609	CLA	O1A-CGA-O2A-C1
17	B	613	CLA	C10-C11-C12-C13
17	B	603	CLA	C6-C7-C8-C10
17	B	603	CLA	C12-C13-C15-C16
17	B	608	CLA	C12-C13-C15-C16
17	B	609	CLA	C11-C10-C8-C7
17	B	610	CLA	C6-C7-C8-C10
17	B	612	CLA	C12-C13-C15-C16
17	B	615	CLA	C12-C13-C15-C16
17	C	501	CLA	C11-C12-C13-C15
17	C	501	CLA	C12-C13-C15-C16
17	C	505	CLA	C11-C10-C8-C7
17	C	506	CLA	C6-C7-C8-C10
17	D	404	CLA	C12-C13-C15-C16
17	b	5603	CLA	C6-C7-C8-C10
17	b	5603	CLA	C12-C13-C15-C16
17	b	5608	CLA	C12-C13-C15-C16
17	b	5609	CLA	C11-C10-C8-C7
17	b	5610	CLA	C6-C7-C8-C10
17	b	5612	CLA	C12-C13-C15-C16
17	b	5615	CLA	C12-C13-C15-C16
17	c	5501	CLA	C11-C12-C13-C15
17	c	5501	CLA	C12-C13-C15-C16
17	c	5505	CLA	C11-C10-C8-C7
17	c	5506	CLA	C6-C7-C8-C10
17	d	5403	CLA	C12-C13-C15-C16
22	a	5410	LMT	C3-C4-C5-C6
17	b	5613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	T	101	LMT	O1'-C1-C2-C3
17	B	615	CLA	O1A-CGA-O2A-C1
17	b	5615	CLA	O1A-CGA-O2A-C1
17	C	505	CLA	C2A-CAA-CBA-CGA
17	c	5505	CLA	C2A-CAA-CBA-CGA
17	B	602	CLA	C11-C10-C8-C9
17	B	602	CLA	C11-C12-C13-C14
17	B	602	CLA	C14-C13-C15-C16
17	B	603	CLA	C6-C7-C8-C9
17	B	603	CLA	C14-C13-C15-C16
17	B	610	CLA	C6-C7-C8-C9
17	C	501	CLA	C14-C13-C15-C16
17	C	503	CLA	C6-C7-C8-C9
17	C	503	CLA	C14-C13-C15-C16
17	C	505	CLA	C11-C10-C8-C9
17	C	508	CLA	C14-C13-C15-C16
17	D	404	CLA	C14-C13-C15-C16
17	b	5602	CLA	C11-C10-C8-C9
17	b	5602	CLA	C11-C12-C13-C14
17	b	5602	CLA	C14-C13-C15-C16
17	b	5603	CLA	C6-C7-C8-C9
17	b	5603	CLA	C14-C13-C15-C16
17	b	5610	CLA	C6-C7-C8-C9
17	c	5501	CLA	C14-C13-C15-C16
17	c	5503	CLA	C6-C7-C8-C9
17	c	5505	CLA	C11-C10-C8-C9
17	c	5508	CLA	C14-C13-C15-C16
17	d	5403	CLA	C14-C13-C15-C16
17	C	505	CLA	C16-C17-C18-C20
17	c	5505	CLA	C16-C17-C18-C20
17	D	404	CLA	CBA-CGA-O2A-C1
17	d	5403	CLA	CBA-CGA-O2A-C1
26	D	411	DGD	O6E-C5E-C6E-O5E
26	b	5621	DGD	O6E-C5E-C6E-O5E
22	M	101	LMT	C4'-C5'-C6'-O6'
23	d	5407	SQD	O49-C7-O47-C45
23	D	403	SQD	O6-C44-C45-C46
23	L	101	SQD	C44-C45-C46-O48
23	l	5102	SQD	C44-C45-C46-O48
25	d	5408	MGE	C1G-C2G-C3G-O3G
25	m	5103	MGE	C1G-C2G-C3G-O3G
26	C	518	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
26	D	411	DGD	O1G-C1G-C2G-C3G
26	a	5411	DGD	C1G-C2G-C3G-O3G
26	b	5621	DGD	O1G-C1G-C2G-C3G
23	l	5102	SQD	C11-C12-C13-C14
23	L	101	SQD	C27-C28-C29-C30
22	T	101	LMT	C4-C5-C6-C7
20	B	618	BCR	C20-C21-C22-C37
20	C	514	BCR	C11-C10-C9-C34
20	C	515	BCR	C35-C13-C14-C15
20	b	5618	BCR	C20-C21-C22-C37
20	b	5619	BCR	C16-C17-C18-C36
20	c	5513	BCR	C11-C10-C9-C34
20	t	5101	BCR	C16-C17-C18-C36
20	t	5102	BCR	C11-C10-C9-C34
20	z	5101	BCR	C35-C13-C14-C15
23	l	5102	SQD	C9-C10-C11-C12
23	d	5407	SQD	C14-C15-C16-C17
17	A	403	CLA	C2-C3-C5-C6
17	a	5404	CLA	C2-C3-C5-C6
17	B	605	CLA	C13-C15-C16-C17
25	d	5408	MGE	O6D-C5D-C6D-O5D
21	a	5409	LHG	C24-C25-C26-C27
23	D	403	SQD	C14-C15-C16-C17
25	D	410	MGE	C6B-C7B-C8B-C9B
20	D	407	BCR	C11-C12-C13-C14
20	d	5406	BCR	C11-C12-C13-C14
17	b	5605	CLA	C13-C15-C16-C17
26	A	413	DGD	C5B-C6B-C7B-C8B
21	A	408	LHG	C24-C25-C26-C27
26	c	5515	DGD	C5B-C6B-C7B-C8B
22	A	409	LMT	C3'-C4'-O1B-C1B
17	b	5613	CLA	C13-C15-C16-C17
23	D	403	SQD	C32-C33-C34-C35
26	b	5621	DGD	C3B-C4B-C5B-C6B
23	L	101	SQD	C11-C10-C9-C8
26	D	411	DGD	C3B-C4B-C5B-C6B
25	d	5409	MGE	C2A-C1A-O1G-C1G
17	B	613	CLA	C13-C15-C16-C17
22	a	5410	LMT	C2-C3-C4-C5
17	A	403	CLA	O1D-CGD-O2D-CED
20	B	617	BCR	C12-C13-C14-C15
20	b	5617	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	a	5404	CLA	O1D-CGD-O2D-CED
26	A	413	DGD	C2A-C1A-O1G-C1G
26	c	5515	DGD	C2A-C1A-O1G-C1G
23	d	5407	SQD	C12-C13-C14-C15
26	c	5516	DGD	C5A-C6A-C7A-C8A
26	C	517	DGD	C5A-C6A-C7A-C8A
26	D	411	DGD	C5B-C6B-C7B-C8B
26	b	5621	DGD	C5B-C6B-C7B-C8B
25	d	5410	MGE	C3A-C4A-C5A-C6A
21	A	408	LHG	O7-C5-C6-O8
21	a	5409	LHG	O7-C5-C6-O8
25	d	5408	MGE	O1G-C1G-C2G-O2G
26	C	517	DGD	O1G-C1G-C2G-O2G
26	c	5516	DGD	O1G-C1G-C2G-O2G
23	L	101	SQD	C11-C12-C13-C14
17	c	5507	CLA	C2A-CAA-CBA-CGA
18	D	402	PHO	C3-C5-C6-C7
18	d	5402	PHO	C3-C5-C6-C7
22	B	620	LMT	C2-C3-C4-C5
23	l	5102	SQD	C19-C20-C21-C22
17	b	5607	CLA	C15-C16-C17-C18
17	B	607	CLA	C15-C16-C17-C18
25	C	519	MGE	C2B-C1B-O2G-C2G
25	c	5517	MGE	C2B-C1B-O2G-C2G
17	B	604	CLA	C15-C16-C17-C18
17	B	607	CLA	C5-C6-C7-C8
17	C	508	CLA	C8-C10-C11-C12
17	b	5604	CLA	C15-C16-C17-C18
17	c	5508	CLA	C8-C10-C11-C12
25	D	408	MGE	C1B-C2B-C3B-C4B
23	d	5407	SQD	C17-C18-C19-C20
17	b	5607	CLA	C5-C6-C7-C8
17	A	403	CLA	C4-C3-C5-C6
17	a	5404	CLA	C4-C3-C5-C6
22	T	101	LMT	C2-C1-O1'-C1'
17	A	402	CLA	C14-C13-C15-C16
17	B	605	CLA	C11-C12-C13-C14
17	B	606	CLA	C14-C13-C15-C16
17	B	611	CLA	C6-C7-C8-C9
17	B	612	CLA	C14-C13-C15-C16
17	B	615	CLA	C14-C13-C15-C16
17	C	501	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	C	506	CLA	C6-C7-C8-C9
17	a	5403	CLA	C14-C13-C15-C16
17	b	5605	CLA	C11-C12-C13-C14
17	b	5611	CLA	C6-C7-C8-C9
17	b	5612	CLA	C14-C13-C15-C16
17	b	5615	CLA	C14-C13-C15-C16
17	c	5501	CLA	C6-C7-C8-C9
17	c	5503	CLA	C14-C13-C15-C16
17	c	5506	CLA	C6-C7-C8-C9
18	D	402	PHO	C11-C12-C13-C14
18	d	5402	PHO	C11-C12-C13-C14
17	A	401	CLA	C4B-C3B-CAB-CBB
17	B	603	CLA	C4B-C3B-CAB-CBB
17	B	604	CLA	C4B-C3B-CAB-CBB
17	D	405	CLA	C4B-C3B-CAB-CBB
17	a	5402	CLA	C4B-C3B-CAB-CBB
17	b	5603	CLA	C4B-C3B-CAB-CBB
17	b	5604	CLA	C4B-C3B-CAB-CBB
17	d	5404	CLA	C4B-C3B-CAB-CBB
17	C	507	CLA	C2A-CAA-CBA-CGA
25	D	409	MGE	C2D-C1D-O3G-C3G
25	m	5103	MGE	C2D-C1D-O3G-C3G
25	B	619	MGE	C7A-C8A-C9A-CAA
25	b	5620	MGE	C7A-C8A-C9A-CAA
17	A	402	CLA	C12-C13-C15-C16
17	B	602	CLA	C11-C10-C8-C7
17	B	602	CLA	C11-C12-C13-C15
17	B	602	CLA	C12-C13-C15-C16
17	B	611	CLA	C6-C7-C8-C10
17	B	615	CLA	C6-C7-C8-C10
17	C	501	CLA	C6-C7-C8-C10
17	C	503	CLA	C6-C7-C8-C10
17	C	508	CLA	C12-C13-C15-C16
17	a	5403	CLA	C12-C13-C15-C16
17	b	5602	CLA	C11-C10-C8-C7
17	b	5602	CLA	C11-C12-C13-C15
17	b	5602	CLA	C12-C13-C15-C16
17	b	5611	CLA	C6-C7-C8-C10
17	b	5615	CLA	C6-C7-C8-C10
17	c	5501	CLA	C6-C7-C8-C10
17	c	5503	CLA	C6-C7-C8-C10
17	c	5508	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	D	404	CLA	O1A-CGA-O2A-C1
17	d	5403	CLA	O1A-CGA-O2A-C1
17	C	505	CLA	C16-C17-C18-C19
17	c	5505	CLA	C16-C17-C18-C19
25	D	408	MGE	C5B-C6B-C7B-C8B
25	d	5409	MGE	C2B-C3B-C4B-C5B
26	C	517	DGD	O1A-C1A-O1G-C1G
26	c	5516	DGD	O1A-C1A-O1G-C1G
17	A	405	CLA	C3A-C2A-CAA-CBA
17	B	607	CLA	C3A-C2A-CAA-CBA
17	a	5406	CLA	C3A-C2A-CAA-CBA
17	b	5607	CLA	C3A-C2A-CAA-CBA
18	A	404	PHO	C3A-C2A-CAA-CBA
18	a	5405	PHO	C3A-C2A-CAA-CBA
17	B	615	CLA	C15-C16-C17-C18
18	A	404	PHO	C15-C16-C17-C18
18	a	5405	PHO	C15-C16-C17-C18
17	b	5615	CLA	C15-C16-C17-C18
20	A	407	BCR	C19-C20-C21-C22
20	a	5408	BCR	C19-C20-C21-C22
17	C	510	CLA	C3-C5-C6-C7
17	c	5510	CLA	C3-C5-C6-C7
21	A	408	LHG	C33-C34-C35-C36
25	d	5410	MGE	C8B-C9B-CAB-CBB
21	a	5409	LHG	C33-C34-C35-C36
17	B	607	CLA	C8-C10-C11-C12
17	b	5607	CLA	C8-C10-C11-C12
23	A	410	SQD	C44-C45-C46-O48
23	d	5407	SQD	O6-C44-C45-C46
25	C	519	MGE	C1G-C2G-C3G-O3G
25	D	410	MGE	O1G-C1G-C2G-C3G
25	c	5517	MGE	C1G-C2G-C3G-O3G
25	d	5409	MGE	O1G-C1G-C2G-C3G
26	C	518	DGD	O1G-C1G-C2G-C3G
26	a	5411	DGD	O1G-C1G-C2G-C3G
21	a	5409	LHG	C32-C33-C34-C35
25	m	5103	MGE	O6D-C5D-C6D-O5D
21	A	408	LHG	C32-C33-C34-C35
23	l	5102	SQD	C11-C10-C9-C8
22	a	5410	LMT	C7-C8-C9-C10
25	d	5409	MGE	O1A-C1A-O1G-C1G
25	A	412	MGE	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
25	l	5101	MGE	C2A-C3A-C4A-C5A
23	D	403	SQD	C33-C34-C35-C36
17	B	615	CLA	C16-C17-C18-C19
17	b	5615	CLA	C16-C17-C18-C19
17	C	511	CLA	C2B-C3B-CAB-CBB
17	k	5501	CLA	C2B-C3B-CAB-CBB
20	A	407	BCR	C1-C6-C7-C8
20	C	515	BCR	C1-C6-C7-C8
20	D	407	BCR	C23-C24-C25-C30
20	a	5408	BCR	C1-C6-C7-C8
20	b	5619	BCR	C1-C6-C7-C8
20	d	5406	BCR	C23-C24-C25-C30
20	t	5101	BCR	C1-C6-C7-C8
20	t	5102	BCR	C1-C6-C7-C8
20	z	5101	BCR	C1-C6-C7-C8
26	C	517	DGD	C1B-C2B-C3B-C4B
26	c	5516	DGD	C1B-C2B-C3B-C4B
25	D	408	MGE	C2A-C3A-C4A-C5A
17	B	609	CLA	C5-C6-C7-C8
17	b	5609	CLA	C5-C6-C7-C8
25	m	5103	MGE	C4A-C5A-C6A-C7A
17	C	501	CLA	C10-C11-C12-C13
17	c	5501	CLA	C10-C11-C12-C13
23	A	410	SQD	O6-C44-C45-O47
23	a	5401	SQD	O6-C44-C45-O47
25	d	5409	MGE	O1G-C1G-C2G-O2G
22	m	5102	LMT	C4'-C5'-C6'-O6'
22	A	409	LMT	C5-C6-C7-C8
22	B	620	LMT	C5-C6-C7-C8
17	b	5613	CLA	C8-C10-C11-C12
17	A	401	CLA	C11-C10-C8-C9
17	A	402	CLA	C11-C10-C8-C9
17	a	5402	CLA	C11-C10-C8-C9
17	a	5403	CLA	C11-C10-C8-C9
25	A	412	MGE	C7A-C8A-C9A-CAA
26	D	411	DGD	CCA-CDA-CEA-CFA
26	b	5621	DGD	CCA-CDA-CEA-CFA
17	B	613	CLA	C8-C10-C11-C12
25	l	5101	MGE	C7A-C8A-C9A-CAA
20	D	407	BCR	C6-C7-C8-C9
20	H	101	BCR	C14-C15-C16-C17
20	h	5101	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	409	LMT	C1-C2-C3-C4
22	m	5102	LMT	C1-C2-C3-C4
17	B	612	CLA	O1D-CGD-O2D-CED
17	b	5612	CLA	O1D-CGD-O2D-CED
17	C	501	CLA	CBA-CGA-O2A-C1
17	c	5501	CLA	CBA-CGA-O2A-C1
23	l	5102	SQD	C24-C23-O48-C46
25	D	410	MGE	C5A-C6A-C7A-C8A
20	A	407	BCR	C35-C13-C14-C15
20	B	618	BCR	C16-C17-C18-C36
20	a	5408	BCR	C35-C13-C14-C15
20	b	5618	BCR	C16-C17-C18-C36
25	c	5517	MGE	C1A-C2A-C3A-C4A
17	B	603	CLA	C15-C16-C17-C18
17	B	615	CLA	C16-C17-C18-C20
17	b	5615	CLA	C16-C17-C18-C20
17	b	5610	CLA	CBD-CGD-O2D-CED
17	b	5603	CLA	C15-C16-C17-C18
17	A	401	CLA	C6-C7-C8-C10
17	A	402	CLA	C11-C10-C8-C7
17	B	606	CLA	C11-C12-C13-C15
17	C	506	CLA	C11-C10-C8-C7
17	C	506	CLA	C11-C12-C13-C15
17	a	5402	CLA	C6-C7-C8-C10
17	a	5403	CLA	C11-C10-C8-C7
17	c	5506	CLA	C11-C10-C8-C7
17	c	5506	CLA	C11-C12-C13-C15
25	C	519	MGE	C1A-C2A-C3A-C4A
17	B	610	CLA	CBD-CGD-O2D-CED
20	k	5502	BCR	C11-C12-C13-C14
25	D	408	MGE	C2G-C3G-O3G-C1D
25	m	5103	MGE	CCB-CDB-CEB-CFB
17	D	404	CLA	C8-C10-C11-C12
17	d	5403	CLA	C8-C10-C11-C12
17	C	501	CLA	C13-C15-C16-C17
17	c	5501	CLA	C13-C15-C16-C17
25	b	5620	MGE	C3A-C4A-C5A-C6A
22	a	5410	LMT	C1-C2-C3-C4
25	B	619	MGE	C3A-C4A-C5A-C6A
20	t	5102	BCR	C16-C17-C18-C19
21	A	408	LHG	O6-C4-C5-O7
21	a	5409	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
25	D	410	MGE	C6A-C7A-C8A-C9A
25	A	412	MGE	O6D-C1D-O3G-C3G
25	l	5101	MGE	O6D-C1D-O3G-C3G
23	A	410	SQD	O6-C44-C45-C46
25	D	409	MGE	C1G-C2G-C3G-O3G
25	d	5408	MGE	O1G-C1G-C2G-C3G
26	A	413	DGD	C1G-C2G-C3G-O3G
26	c	5515	DGD	C1G-C2G-C3G-O3G
29	F	101	HEM	C4C-C3C-CAC-CBC
29	f	5101	HEM	C4C-C3C-CAC-CBC
21	A	408	LHG	C29-C30-C31-C32
21	a	5409	LHG	C29-C30-C31-C32
17	B	604	CLA	C2-C3-C5-C6
17	b	5604	CLA	C2-C3-C5-C6
17	B	607	CLA	C3-C5-C6-C7
23	L	101	SQD	O6-C44-C45-O47
25	B	619	MGE	O2G-C2G-C3G-O3G
25	D	409	MGE	O1G-C1G-C2G-O2G
25	b	5620	MGE	O2G-C2G-C3G-O3G
25	d	5408	MGE	O2G-C2G-C3G-O3G
25	m	5103	MGE	O2G-C2G-C3G-O3G
26	A	413	DGD	O2G-C2G-C3G-O3G
26	c	5515	DGD	O2G-C2G-C3G-O3G
17	A	401	CLA	C6-C7-C8-C9
17	B	612	CLA	C6-C7-C8-C9
17	a	5402	CLA	C6-C7-C8-C9
17	b	5612	CLA	C6-C7-C8-C9
23	L	101	SQD	C28-C29-C30-C31
25	l	5101	MGE	C3A-C4A-C5A-C6A
17	C	502	CLA	C10-C11-C12-C13
17	c	5502	CLA	C10-C11-C12-C13
25	A	412	MGE	C3A-C4A-C5A-C6A
17	C	501	CLA	O1A-CGA-O2A-C1
17	c	5501	CLA	O1A-CGA-O2A-C1
17	b	5607	CLA	C3-C5-C6-C7
22	M	101	LMT	C9-C10-C11-C12
25	d	5410	MGE	C3B-C4B-C5B-C6B
20	D	407	BCR	C14-C15-C16-C17
20	d	5406	BCR	C14-C15-C16-C17
25	D	410	MGE	CCB-CDB-CEB-CFB
23	A	410	SQD	C4-C5-C6-S
23	D	403	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
17	B	602	CLA	C4B-C3B-CAB-CBB
17	B	604	CLA	C1A-C2A-CAA-CBA
17	C	504	CLA	C4B-C3B-CAB-CBB
17	C	505	CLA	C4B-C3B-CAB-CBB
17	C	511	CLA	C4B-C3B-CAB-CBB
17	C	513	CLA	C1A-C2A-CAA-CBA
17	D	404	CLA	C4B-C3B-CAB-CBB
17	b	5602	CLA	C4B-C3B-CAB-CBB
17	b	5604	CLA	C1A-C2A-CAA-CBA
17	c	5504	CLA	C4B-C3B-CAB-CBB
17	c	5505	CLA	C4B-C3B-CAB-CBB
17	c	5512	CLA	C1A-C2A-CAA-CBA
17	d	5403	CLA	C4B-C3B-CAB-CBB
17	k	5501	CLA	C4B-C3B-CAB-CBB
17	B	608	CLA	O1D-CGD-O2D-CED
17	b	5608	CLA	O1D-CGD-O2D-CED
26	D	411	DGD	C5A-C6A-C7A-C8A
26	b	5621	DGD	C5A-C6A-C7A-C8A
20	A	407	BCR	C22-C23-C24-C25
20	a	5408	BCR	C22-C23-C24-C25
20	d	5406	BCR	C6-C7-C8-C9
25	d	5408	MGE	O2G-C1B-C2B-C3B
21	A	408	LHG	O6-C4-C5-C6
21	a	5409	LHG	O6-C4-C5-C6
25	C	519	MGE	O1B-C1B-O2G-C2G
25	c	5517	MGE	O1B-C1B-O2G-C2G
25	m	5101	MGE	C4A-C5A-C6A-C7A
17	B	604	CLA	C12-C13-C15-C16
17	B	607	CLA	C11-C10-C8-C7
17	C	505	CLA	C11-C12-C13-C15
17	b	5604	CLA	C12-C13-C15-C16
17	b	5607	CLA	C11-C10-C8-C7
17	c	5505	CLA	C11-C12-C13-C15
18	D	402	PHO	C12-C13-C15-C16
18	d	5402	PHO	C12-C13-C15-C16
25	A	412	MGE	C7B-C8B-C9B-CAB
25	l	5101	MGE	C7B-C8B-C9B-CAB
23	l	5102	SQD	C28-C29-C30-C31
23	D	403	SQD	C11-C10-C9-C8
23	d	5407	SQD	C11-C10-C9-C8
17	B	604	CLA	C16-C17-C18-C20
17	b	5604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	d	5408	MGE	C4B-C5B-C6B-C7B
23	D	403	SQD	O49-C7-O47-C45
23	D	403	SQD	C26-C27-C28-C29
17	B	615	CLA	C6-C7-C8-C9
17	b	5615	CLA	C6-C7-C8-C9
20	B	617	BCR	C15-C16-C17-C18
20	C	514	BCR	C13-C14-C15-C16
20	b	5617	BCR	C15-C16-C17-C18
20	c	5513	BCR	C13-C14-C15-C16
17	b	5616	CLA	C10-C11-C12-C13
25	B	619	MGE	CAA-CBA-CCA-CDA
17	B	610	CLA	C5-C6-C7-C8
17	b	5610	CLA	C5-C6-C7-C8
25	b	5620	MGE	CAA-CBA-CCA-CDA
25	m	5103	MGE	O1A-C1A-O1G-C1G
23	D	403	SQD	O6-C44-C45-O47
23	d	5407	SQD	O6-C44-C45-O47
25	d	5409	MGE	O2G-C2G-C3G-O3G
26	C	517	DGD	O2G-C2G-C3G-O3G
26	C	518	DGD	O1G-C1G-C2G-O2G
26	a	5411	DGD	O1G-C1G-C2G-O2G
26	c	5516	DGD	O2G-C2G-C3G-O3G
26	a	5411	DGD	C5B-C6B-C7B-C8B
17	B	616	CLA	C10-C11-C12-C13
26	C	518	DGD	C5B-C6B-C7B-C8B
26	c	5516	DGD	C4A-C5A-C6A-C7A
25	C	519	MGE	C5A-C6A-C7A-C8A
26	C	517	DGD	C4A-C5A-C6A-C7A
26	D	411	DGD	C3A-C4A-C5A-C6A
26	b	5621	DGD	C3A-C4A-C5A-C6A
18	a	5405	PHO	C2-C3-C5-C6
25	c	5517	MGE	C5A-C6A-C7A-C8A
17	B	603	CLA	CAD-CBD-CGD-O2D
17	B	613	CLA	CAD-CBD-CGD-O2D
17	C	501	CLA	CAD-CBD-CGD-O2D
17	C	502	CLA	CAD-CBD-CGD-O2D
17	C	506	CLA	CAD-CBD-CGD-O2D
17	C	510	CLA	CAD-CBD-CGD-O2D
17	b	5603	CLA	CAD-CBD-CGD-O2D
17	b	5613	CLA	CAD-CBD-CGD-O2D
17	c	5501	CLA	CAD-CBD-CGD-O2D
17	c	5502	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	c	5506	CLA	CAD-CBD-CGD-O2D
17	c	5510	CLA	CAD-CBD-CGD-O2D
25	m	5103	MGE	C2A-C1A-O1G-C1G
17	D	405	CLA	C2A-CAA-CBA-CGA
17	d	5404	CLA	C2A-CAA-CBA-CGA
17	B	603	CLA	CAD-CBD-CGD-O1D
17	B	605	CLA	CAD-CBD-CGD-O1D
17	B	607	CLA	CAD-CBD-CGD-O1D
17	B	613	CLA	CAD-CBD-CGD-O1D
17	C	501	CLA	CAD-CBD-CGD-O1D
17	C	502	CLA	CAD-CBD-CGD-O1D
17	C	506	CLA	CAD-CBD-CGD-O1D
17	C	510	CLA	CAD-CBD-CGD-O1D
17	b	5603	CLA	CAD-CBD-CGD-O1D
17	b	5605	CLA	CAD-CBD-CGD-O1D
17	b	5607	CLA	CAD-CBD-CGD-O1D
17	b	5613	CLA	CAD-CBD-CGD-O1D
17	c	5501	CLA	CAD-CBD-CGD-O1D
17	c	5502	CLA	CAD-CBD-CGD-O1D
17	c	5506	CLA	CAD-CBD-CGD-O1D
17	c	5510	CLA	CAD-CBD-CGD-O1D
18	A	404	PHO	CHA-CBD-CGD-O1D
18	A	404	PHO	CHA-CBD-CGD-O2D
18	a	5405	PHO	CHA-CBD-CGD-O1D
18	a	5405	PHO	CHA-CBD-CGD-O2D
20	H	101	BCR	C15-C16-C17-C18
20	h	5101	BCR	C15-C16-C17-C18
20	k	5502	BCR	C16-C17-C18-C36
21	a	5409	LHG	O10-C23-O8-C6
17	C	510	CLA	C13-C15-C16-C17
17	A	403	CLA	C2B-C3B-CAB-CBB
17	C	501	CLA	C2B-C3B-CAB-CBB
17	C	504	CLA	C2B-C3B-CAB-CBB
17	a	5404	CLA	C2B-C3B-CAB-CBB
17	c	5501	CLA	C2B-C3B-CAB-CBB
17	c	5504	CLA	C2B-C3B-CAB-CBB
20	C	516	BCR	C1-C6-C7-C8
20	C	516	BCR	C23-C24-C25-C30
20	c	5514	BCR	C1-C6-C7-C8
20	c	5514	BCR	C23-C24-C25-C30
18	A	404	PHO	C2-C3-C5-C6
17	c	5510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	A	408	LHG	C2-C3-O3-P
21	a	5409	LHG	C2-C3-O3-P
21	A	408	LHG	O10-C23-O8-C6
22	A	409	LMT	C3-C4-C5-C6
23	L	101	SQD	C17-C18-C19-C20
25	D	410	MGE	CBB-CCB-CDB-CEB
17	A	402	CLA	C10-C11-C12-C13
17	a	5403	CLA	C10-C11-C12-C13
25	B	619	MGE	C1B-C2B-C3B-C4B
25	b	5620	MGE	C1B-C2B-C3B-C4B
20	H	101	BCR	C9-C10-C11-C12
20	h	5101	BCR	C9-C10-C11-C12
17	B	606	CLA	C11-C12-C13-C14
17	B	607	CLA	C11-C10-C8-C9
17	B	609	CLA	C14-C13-C15-C16
17	B	610	CLA	C14-C13-C15-C16
17	C	503	CLA	C11-C12-C13-C14
17	C	506	CLA	C11-C12-C13-C14
17	b	5607	CLA	C11-C10-C8-C9
17	b	5608	CLA	C6-C7-C8-C9
17	b	5609	CLA	C14-C13-C15-C16
17	c	5503	CLA	C11-C12-C13-C14
17	c	5506	CLA	C11-C12-C13-C14
17	B	609	CLA	C12-C13-C15-C16
17	C	503	CLA	C11-C12-C13-C15
17	b	5609	CLA	C12-C13-C15-C16
17	c	5503	CLA	C11-C12-C13-C15
17	C	503	CLA	CBA-CGA-O2A-C1
17	c	5503	CLA	CBA-CGA-O2A-C1
26	C	517	DGD	C9A-CAA-CBA-CCA
26	c	5516	DGD	C9A-CAA-CBA-CCA
25	D	410	MGE	C2D-C1D-O3G-C3G
17	B	604	CLA	C16-C17-C18-C19
17	b	5604	CLA	C16-C17-C18-C19
17	c	5505	CLA	C15-C16-C17-C18
17	C	505	CLA	C15-C16-C17-C18
25	B	619	MGE	O1G-C1G-C2G-O2G
25	D	408	MGE	O1G-C1G-C2G-O2G
25	b	5620	MGE	O1G-C1G-C2G-O2G
17	b	5615	CLA	C13-C15-C16-C17
23	l	5102	SQD	C18-C19-C20-C21
23	D	403	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
17	B	612	CLA	C2-C1-O2A-CGA
17	C	502	CLA	C2-C1-O2A-CGA
17	b	5612	CLA	C2-C1-O2A-CGA
17	c	5502	CLA	C2-C1-O2A-CGA
17	B	613	CLA	C4-C3-C5-C6
17	b	5613	CLA	C4-C3-C5-C6
17	B	615	CLA	C13-C15-C16-C17
25	d	5409	MGE	C6B-C7B-C8B-C9B
17	C	511	CLA	C15-C16-C17-C18
17	D	404	CLA	C2A-CAA-CBA-CGA
17	d	5403	CLA	C2A-CAA-CBA-CGA
20	C	515	BCR	C13-C14-C15-C16
20	D	407	BCR	C19-C20-C21-C22
20	d	5406	BCR	C19-C20-C21-C22
20	z	5101	BCR	C13-C14-C15-C16
20	Y	101	BCR	C9-C10-C11-C12
25	B	619	MGE	C1A-C2A-C3A-C4A
25	b	5620	MGE	C1A-C2A-C3A-C4A
17	k	5501	CLA	C15-C16-C17-C18
17	B	608	CLA	C6-C7-C8-C9
17	B	613	CLA	C14-C13-C15-C16
17	b	5610	CLA	C14-C13-C15-C16
17	b	5613	CLA	C14-C13-C15-C16
18	A	404	PHO	C6-C7-C8-C9
18	a	5405	PHO	C6-C7-C8-C9
17	C	503	CLA	O1A-CGA-O2A-C1
17	c	5503	CLA	O1A-CGA-O2A-C1
25	m	5103	MGE	C5B-C6B-C7B-C8B
19	D	406	PQ9	C18-C20-C21-C22
19	d	5405	PQ9	C18-C20-C21-C22
17	C	502	CLA	C6-C7-C8-C10
17	D	404	CLA	C11-C10-C8-C7
17	c	5502	CLA	C6-C7-C8-C10
17	d	5403	CLA	C11-C10-C8-C7
25	m	5101	MGE	O1G-C1G-C2G-O2G
25	c	5517	MGE	C5B-C6B-C7B-C8B
17	B	608	CLA	C3A-C2A-CAA-CBA
17	C	502	CLA	C4-C3-C5-C6
17	C	505	CLA	C3A-C2A-CAA-CBA
17	C	506	CLA	C3A-C2A-CAA-CBA
17	b	5608	CLA	C3A-C2A-CAA-CBA
17	c	5502	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	c	5505	CLA	C3A-C2A-CAA-CBA
17	c	5506	CLA	C3A-C2A-CAA-CBA
25	C	519	MGE	C5B-C6B-C7B-C8B
20	b	5619	BCR	C20-C21-C22-C37
20	t	5101	BCR	C20-C21-C22-C37
25	C	519	MGE	O6D-C1D-O3G-C3G
25	c	5517	MGE	O6D-C1D-O3G-C3G
18	D	402	PHO	C13-C15-C16-C17
18	d	5402	PHO	C13-C15-C16-C17
20	C	514	BCR	C15-C16-C17-C18
20	C	515	BCR	C15-C16-C17-C18
20	c	5513	BCR	C15-C16-C17-C18
25	B	619	MGE	C1G-C2G-C3G-O3G
26	C	517	DGD	C1G-C2G-C3G-O3G
26	c	5516	DGD	C1G-C2G-C3G-O3G
17	B	607	CLA	C6-C7-C8-C9
17	B	611	CLA	C14-C13-C15-C16
17	b	5607	CLA	C6-C7-C8-C9
17	b	5611	CLA	C14-C13-C15-C16
18	A	404	PHO	C14-C13-C15-C16
18	a	5405	PHO	C14-C13-C15-C16
17	B	613	CLA	C16-C17-C18-C20
17	b	5613	CLA	C16-C17-C18-C20
17	A	403	CLA	CBA-CGA-O2A-C1
17	C	507	CLA	C8-C10-C11-C12
17	c	5507	CLA	C8-C10-C11-C12
21	A	408	LHG	C26-C27-C28-C29
25	m	5101	MGE	C2B-C3B-C4B-C5B
21	a	5409	LHG	C26-C27-C28-C29
25	D	410	MGE	C5B-C6B-C7B-C8B
17	a	5404	CLA	CBA-CGA-O2A-C1
26	C	518	DGD	O2G-C1B-C2B-C3B
26	a	5411	DGD	O2G-C1B-C2B-C3B
17	B	607	CLA	C2A-CAA-CBA-CGA
17	C	501	CLA	C2A-CAA-CBA-CGA
17	b	5607	CLA	C2A-CAA-CBA-CGA
17	c	5501	CLA	C2A-CAA-CBA-CGA
17	b	5610	CLA	O1D-CGD-O2D-CED
17	B	607	CLA	C1A-C2A-CAA-CBA
17	C	501	CLA	C1A-C2A-CAA-CBA
17	b	5607	CLA	C1A-C2A-CAA-CBA
17	c	5501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	C	516	BCR	C16-C17-C18-C19
20	c	5514	BCR	C16-C17-C18-C19
17	A	402	CLA	C2C-C3C-CAC-CBC
17	A	401	CLA	C2B-C3B-CAB-CBB
17	B	602	CLA	C2B-C3B-CAB-CBB
17	B	603	CLA	C2B-C3B-CAB-CBB
17	C	505	CLA	C2B-C3B-CAB-CBB
17	D	404	CLA	C2B-C3B-CAB-CBB
17	a	5402	CLA	C2B-C3B-CAB-CBB
17	b	5602	CLA	C2B-C3B-CAB-CBB
17	b	5603	CLA	C2B-C3B-CAB-CBB
17	c	5505	CLA	C2B-C3B-CAB-CBB
17	d	5403	CLA	C2B-C3B-CAB-CBB
20	A	407	BCR	C5-C6-C7-C8
20	B	618	BCR	C23-C24-C25-C30
20	C	514	BCR	C5-C6-C7-C8
20	C	515	BCR	C5-C6-C7-C8
20	C	515	BCR	C23-C24-C25-C30
20	D	407	BCR	C23-C24-C25-C26
20	a	5408	BCR	C5-C6-C7-C8
20	b	5618	BCR	C23-C24-C25-C30
20	b	5619	BCR	C5-C6-C7-C8
20	c	5513	BCR	C5-C6-C7-C8
20	d	5406	BCR	C23-C24-C25-C26
20	t	5101	BCR	C5-C6-C7-C8
20	t	5102	BCR	C5-C6-C7-C8
20	z	5101	BCR	C5-C6-C7-C8
20	z	5101	BCR	C23-C24-C25-C30
26	D	411	DGD	C6B-C7B-C8B-C9B
26	b	5621	DGD	C6B-C7B-C8B-C9B
25	d	5408	MGE	C2A-C3A-C4A-C5A
17	A	403	CLA	O1A-CGA-O2A-C1
25	l	5101	MGE	C5A-C6A-C7A-C8A
17	a	5404	CLA	O1A-CGA-O2A-C1
17	C	502	CLA	C2-C3-C5-C6
17	c	5502	CLA	C2-C3-C5-C6
26	A	413	DGD	CBA-CCA-CDA-CEA
26	c	5515	DGD	CBA-CCA-CDA-CEA
17	a	5403	CLA	C2C-C3C-CAC-CBC
25	A	412	MGE	C5A-C6A-C7A-C8A
17	A	401	CLA	C15-C16-C17-C18
20	z	5101	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	B	613	CLA	C12-C13-C15-C16
17	C	507	CLA	C11-C10-C8-C7
17	b	5613	CLA	C12-C13-C15-C16
17	c	5507	CLA	C11-C10-C8-C7
18	A	404	PHO	C6-C7-C8-C10
18	a	5405	PHO	C6-C7-C8-C10
17	B	603	CLA	C2A-CAA-CBA-CGA
17	b	5603	CLA	C2A-CAA-CBA-CGA
22	m	5102	LMT	O1'-C1-C2-C3
17	a	5402	CLA	C15-C16-C17-C18
17	B	610	CLA	O1D-CGD-O2D-CED
17	C	506	CLA	C16-C17-C18-C20
17	c	5506	CLA	C16-C17-C18-C20
25	d	5409	MGE	C2A-C3A-C4A-C5A
17	B	612	CLA	C11-C10-C8-C9
17	b	5612	CLA	C11-C10-C8-C9
17	B	610	CLA	O1A-CGA-O2A-C1
25	D	409	MGE	C6B-C7B-C8B-C9B
17	b	5610	CLA	O1A-CGA-O2A-C1
25	B	619	MGE	O1G-C1G-C2G-C3G
25	b	5620	MGE	O1G-C1G-C2G-C3G
25	b	5620	MGE	C1G-C2G-C3G-O3G
26	C	517	DGD	O1G-C1G-C2G-C3G
26	c	5516	DGD	O1G-C1G-C2G-C3G
17	B	602	CLA	CAA-CBA-CGA-O2A
23	d	5407	SQD	C10-C11-C12-C13
17	b	5602	CLA	CAA-CBA-CGA-O2A
17	B	612	CLA	C11-C10-C8-C7
17	b	5612	CLA	C11-C10-C8-C7
18	A	404	PHO	C11-C10-C8-C7
18	a	5405	PHO	C11-C10-C8-C7
23	A	410	SQD	C45-C44-O6-C1
25	m	5101	MGE	C2G-C3G-O3G-C1D
23	l	5102	SQD	O48-C23-C24-C25
17	B	608	CLA	C2-C1-O2A-CGA
17	b	5608	CLA	C2-C1-O2A-CGA
17	B	610	CLA	CBA-CGA-O2A-C1
17	b	5610	CLA	CBA-CGA-O2A-C1
17	B	605	CLA	C16-C17-C18-C20
17	b	5605	CLA	C16-C17-C18-C20
25	m	5103	MGE	C1G-C2G-O2G-C1B
25	m	5103	MGE	C3G-C2G-O2G-C1B

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Mol	Chain	Res	Type	Atoms
17	A	402	CLA	C4C-C3C-CAC-CBC
22	M	101	LMT	C1-C2-C3-C4
17	a	5403	CLA	C4C-C3C-CAC-CBC
17	B	614	CLA	CBA-CGA-O2A-C1
17	b	5614	CLA	CBA-CGA-O2A-C1
25	d	5410	MGE	C6B-C7B-C8B-C9B
23	a	5401	SQD	O6-C44-C45-C46
25	D	408	MGE	O1G-C1G-C2G-C3G
25	D	409	MGE	C2A-C3A-C4A-C5A
26	D	411	DGD	C4B-C5B-C6B-C7B
17	B	613	CLA	C2-C3-C5-C6
20	B	617	BCR	C19-C20-C21-C22
20	b	5617	BCR	C19-C20-C21-C22
20	k	5502	BCR	C15-C16-C17-C18
26	b	5621	DGD	C4B-C5B-C6B-C7B
17	B	610	CLA	C16-C17-C18-C19
17	b	5610	CLA	C16-C17-C18-C19
25	m	5101	MGE	C4B-C5B-C6B-C7B
17	C	506	CLA	C10-C11-C12-C13
25	m	5103	MGE	O1G-C1G-C2G-O2G
17	B	614	CLA	O1A-CGA-O2A-C1
17	c	5506	CLA	C10-C11-C12-C13
17	B	602	CLA	C6-C7-C8-C9
17	C	505	CLA	C11-C12-C13-C14
17	b	5602	CLA	C6-C7-C8-C9
17	c	5505	CLA	C11-C12-C13-C14
17	C	507	CLA	CAA-CBA-CGA-O2A
17	c	5507	CLA	CAA-CBA-CGA-O2A
20	D	407	BCR	C17-C18-C19-C20
20	d	5406	BCR	C17-C18-C19-C20
23	D	403	SQD	C12-C13-C14-C15
17	B	611	CLA	C4-C3-C5-C6
17	B	612	CLA	C4-C3-C5-C6
17	b	5611	CLA	C4-C3-C5-C6
17	b	5612	CLA	C4-C3-C5-C6
17	B	614	CLA	C4C-C3C-CAC-CBC
17	b	5614	CLA	C4C-C3C-CAC-CBC
17	b	5613	CLA	C2-C3-C5-C6
17	B	602	CLA	C6-C7-C8-C10
17	B	605	CLA	C12-C13-C15-C16
17	C	505	CLA	C12-C13-C15-C16
17	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	D	404	CLA	C6-C7-C8-C10
17	b	5602	CLA	C6-C7-C8-C10
17	b	5605	CLA	C12-C13-C15-C16
17	c	5505	CLA	C12-C13-C15-C16
17	c	5508	CLA	C11-C10-C8-C7
17	d	5403	CLA	C6-C7-C8-C10
25	D	409	MGE	C3B-C4B-C5B-C6B
17	b	5614	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C2B-C3B-CAB-CBB
17	B	613	CLA	C2B-C3B-CAB-CBB
17	b	5604	CLA	C2B-C3B-CAB-CBB
17	b	5613	CLA	C2B-C3B-CAB-CBB
20	A	407	BCR	C23-C24-C25-C30
20	B	617	BCR	C1-C6-C7-C8
20	B	617	BCR	C5-C6-C7-C8
20	B	618	BCR	C1-C6-C7-C8
20	C	514	BCR	C23-C24-C25-C26
20	C	514	BCR	C23-C24-C25-C30
20	C	515	BCR	C23-C24-C25-C26
20	C	516	BCR	C5-C6-C7-C8
20	H	101	BCR	C1-C6-C7-C8
20	H	101	BCR	C5-C6-C7-C8
20	T	102	BCR	C1-C6-C7-C8
20	a	5408	BCR	C23-C24-C25-C30
20	b	5617	BCR	C1-C6-C7-C8
20	b	5617	BCR	C5-C6-C7-C8
20	b	5618	BCR	C1-C6-C7-C8
20	c	5513	BCR	C23-C24-C25-C26
20	c	5513	BCR	C23-C24-C25-C30
20	c	5514	BCR	C5-C6-C7-C8
20	h	5101	BCR	C1-C6-C7-C8
20	h	5101	BCR	C5-C6-C7-C8
20	z	5101	BCR	C23-C24-C25-C26
25	D	408	MGE	C2B-C1B-O2G-C2G
25	m	5103	MGE	O2G-C1B-C2B-C3B
25	d	5408	MGE	C9A-CAA-CBA-CCA
17	B	610	CLA	C16-C17-C18-C20
17	b	5610	CLA	C16-C17-C18-C20
23	L	101	SQD	O48-C23-C24-C25
17	B	612	CLA	C2-C3-C5-C6
17	b	5612	CLA	C2-C3-C5-C6
25	m	5101	MGE	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	m	5101	MGE	C2B-C1B-O2G-C2G
17	C	503	CLA	CAA-CBA-CGA-O2A
23	L	101	SQD	C4-C5-C6-S
23	d	5407	SQD	C4-C5-C6-S
19	D	406	PQ9	C39-C38-C40-C41
17	c	5503	CLA	CAA-CBA-CGA-O2A
20	c	5513	BCR	C16-C17-C18-C36
25	d	5410	MGE	C9B-CAB-CBB-CCB
17	B	605	CLA	C11-C10-C8-C9
17	D	404	CLA	C11-C10-C8-C9
17	b	5605	CLA	C11-C10-C8-C9
17	d	5403	CLA	C11-C10-C8-C9
20	C	516	BCR	C37-C22-C23-C24
20	c	5514	BCR	C37-C22-C23-C24
17	B	613	CLA	C4B-C3B-CAB-CBB
17	C	509	CLA	C1A-C2A-CAA-CBA
17	b	5613	CLA	C4B-C3B-CAB-CBB
17	c	5509	CLA	C1A-C2A-CAA-CBA
17	b	5613	CLA	C3-C5-C6-C7
19	d	5405	PQ9	C39-C38-C40-C41
22	a	5410	LMT	O5'-C1'-O1'-C1
25	D	409	MGE	O6D-C1D-O3G-C3G
26	C	517	DGD	O6D-C1D-O3G-C3G
26	c	5516	DGD	O6D-C1D-O3G-C3G
17	C	512	CLA	CAA-CBA-CGA-O2A
17	c	5511	CLA	CAA-CBA-CGA-O2A
26	D	411	DGD	O2G-C1B-C2B-C3B
26	b	5621	DGD	O2G-C1B-C2B-C3B
17	B	613	CLA	CAA-CBA-CGA-O2A
17	B	614	CLA	CAA-CBA-CGA-O2A
17	b	5613	CLA	CAA-CBA-CGA-O2A
17	b	5614	CLA	CAA-CBA-CGA-O2A
17	A	401	CLA	C2A-CAA-CBA-CGA
17	a	5402	CLA	C2A-CAA-CBA-CGA
25	B	619	MGE	C7B-C8B-C9B-CAB
25	d	5410	MGE	C2D-C1D-O3G-C3G
17	B	613	CLA	C3-C5-C6-C7
25	b	5620	MGE	C7B-C8B-C9B-CAB
17	B	613	CLA	C2-C1-O2A-CGA
17	D	404	CLA	C2-C1-O2A-CGA
17	b	5613	CLA	C2-C1-O2A-CGA
17	d	5403	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	C	504	CLA	CAA-CBA-CGA-O2A
17	c	5504	CLA	CAA-CBA-CGA-O2A
17	B	605	CLA	C11-C10-C8-C7
17	C	511	CLA	C6-C7-C8-C10
17	b	5605	CLA	C11-C10-C8-C7
17	k	5501	CLA	C6-C7-C8-C10
17	B	604	CLA	C2C-C3C-CAC-CBC
17	b	5604	CLA	C2C-C3C-CAC-CBC
21	A	408	LHG	C30-C31-C32-C33
21	a	5409	LHG	C30-C31-C32-C33
25	C	519	MGE	C8A-C9A-CAA-CBA
22	m	5102	LMT	C11-C10-C9-C8
25	c	5517	MGE	C8A-C9A-CAA-CBA
17	C	507	CLA	CAA-CBA-CGA-O1A
17	c	5507	CLA	CAA-CBA-CGA-O1A
25	d	5408	MGE	O1B-C1B-C2B-C3B
17	B	615	CLA	C11-C10-C8-C9
17	b	5615	CLA	C11-C10-C8-C9
17	B	602	CLA	C10-C11-C12-C13
17	b	5602	CLA	C10-C11-C12-C13
17	b	5610	CLA	C4-C3-C5-C6
25	m	5103	MGE	O1B-C1B-C2B-C3B
22	A	409	LMT	C9-C10-C11-C12
25	b	5620	MGE	C2B-C3B-C4B-C5B
25	B	619	MGE	C2B-C3B-C4B-C5B
25	D	410	MGE	C9A-CAA-CBA-CCA
23	D	403	SQD	C45-C44-O6-C1
23	d	5407	SQD	C45-C44-O6-C1
25	m	5103	MGE	C2G-C3G-O3G-C1D
25	D	410	MGE	O2G-C1B-C2B-C3B
25	m	5101	MGE	O1G-C1G-C2G-C3G
17	B	614	CLA	CAA-CBA-CGA-O1A
17	C	504	CLA	CAA-CBA-CGA-O1A
17	C	512	CLA	CAA-CBA-CGA-O1A
17	b	5614	CLA	CAA-CBA-CGA-O1A
17	c	5504	CLA	CAA-CBA-CGA-O1A
17	c	5511	CLA	CAA-CBA-CGA-O1A
17	B	610	CLA	C4-C3-C5-C6
29	F	101	HEM	C2B-C3B-CAB-CBB
29	f	5101	HEM	C2B-C3B-CAB-CBB
25	D	408	MGE	O1B-C1B-O2G-C2G
25	l	5101	MGE	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
17	B	607	CLA	CAD-CBD-CGD-O2D
17	b	5607	CLA	CAD-CBD-CGD-O2D
17	B	606	CLA	C8-C10-C11-C12
26	c	5515	DGD	C9A-CAA-CBA-CCA
25	A	412	MGE	CDB-CEB-CFB-CGB
25	d	5410	MGE	CBB-CCB-CDB-CEB
26	A	413	DGD	C9A-CAA-CBA-CCA
20	D	407	BCR	C22-C23-C24-C25
20	d	5406	BCR	C22-C23-C24-C25
20	t	5102	BCR	C6-C7-C8-C9
18	A	404	PHO	C1A-C2A-CAA-CBA
18	a	5405	PHO	C1A-C2A-CAA-CBA
23	D	403	SQD	C31-C32-C33-C34
17	b	5613	CLA	CAA-CBA-CGA-O1A
17	B	606	CLA	C10-C11-C12-C13
17	B	613	CLA	C15-C16-C17-C18
17	b	5613	CLA	C15-C16-C17-C18
17	D	404	CLA	CAA-CBA-CGA-O2A
17	d	5403	CLA	CAA-CBA-CGA-O2A
17	B	613	CLA	CAA-CBA-CGA-O1A
17	b	5612	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

133 monomers are involved in 701 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	k	5501	CLA	7	0
29	f	5101	HEM	4	0
17	d	5404	CLA	1	0
17	b	5609	CLA	8	0
17	c	5507	CLA	5	0
17	a	5403	CLA	12	0
20	c	5513	BCR	4	0
17	b	5606	CLA	3	0
18	D	402	PHO	7	0
17	b	5604	CLA	7	0
20	C	516	BCR	5	0
20	b	5617	BCR	8	0
22	A	409	LMT	3	0
23	d	5407	SQD	2	0
26	b	5621	DGD	7	0
17	C	513	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c	5511	CLA	3	0
25	l	5101	MGE	9	0
17	A	403	CLA	1	0
22	m	5102	LMT	1	0
29	F	101	HEM	8	0
19	a	5407	PQ9	2	0
17	c	5501	CLA	8	0
17	c	5503	CLA	8	0
17	c	5502	CLA	3	0
17	a	5402	CLA	13	0
17	B	603	CLA	12	0
17	C	511	CLA	9	0
26	c	5515	DGD	7	0
22	B	620	LMT	1	0
20	d	5406	BCR	4	0
20	b	5619	BCR	3	0
24	a	5412	BCT	6	0
25	c	5517	MGE	5	0
17	B	606	CLA	9	0
17	b	5611	CLA	8	0
26	D	411	DGD	7	0
20	C	515	BCR	3	0
17	d	5403	CLA	8	0
17	b	5612	CLA	11	0
18	a	5405	PHO	9	0
21	a	5409	LHG	3	0
17	b	5602	CLA	10	0
19	D	406	PQ9	7	0
20	Y	101	BCR	9	0
26	a	5411	DGD	2	0
20	D	407	BCR	5	0
17	a	5406	CLA	1	0
25	m	5101	MGE	10	0
20	a	5408	BCR	5	0
20	C	514	BCR	4	0
17	C	501	CLA	8	0
17	B	611	CLA	8	0
17	A	401	CLA	15	0
17	b	5614	CLA	6	0
17	b	5605	CLA	5	0
17	b	5613	CLA	10	0
20	H	101	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	615	CLA	4	0
20	b	5618	BCR	1	0
25	C	519	MGE	5	0
18	A	404	PHO	7	0
20	h	5101	BCR	7	0
25	d	5409	MGE	8	0
17	A	402	CLA	9	0
17	c	5509	CLA	1	0
17	B	607	CLA	10	0
17	b	5601	CLA	6	0
19	d	5405	PQ9	8	0
25	D	408	MGE	6	0
17	C	508	CLA	7	0
24	A	411	BCT	8	0
19	A	406	PQ9	7	0
17	b	5607	CLA	10	0
17	b	5603	CLA	11	0
20	c	5514	BCR	5	0
25	d	5408	MGE	4	0
25	d	5410	MGE	13	0
17	C	505	CLA	10	0
20	t	5101	BCR	3	0
22	M	101	LMT	2	0
17	B	608	CLA	7	0
17	C	509	CLA	1	0
20	B	618	BCR	1	0
17	B	601	CLA	5	0
17	B	602	CLA	5	0
17	B	604	CLA	7	0
20	A	407	BCR	3	0
17	C	504	CLA	1	0
17	C	503	CLA	8	0
17	C	506	CLA	4	0
18	d	5402	PHO	14	0
17	a	5404	CLA	4	0
17	b	5608	CLA	8	0
20	B	617	BCR	6	0
26	C	518	DGD	3	0
25	b	5620	MGE	6	0
17	b	5615	CLA	3	0
17	C	502	CLA	3	0
17	b	5610	CLA	4	0

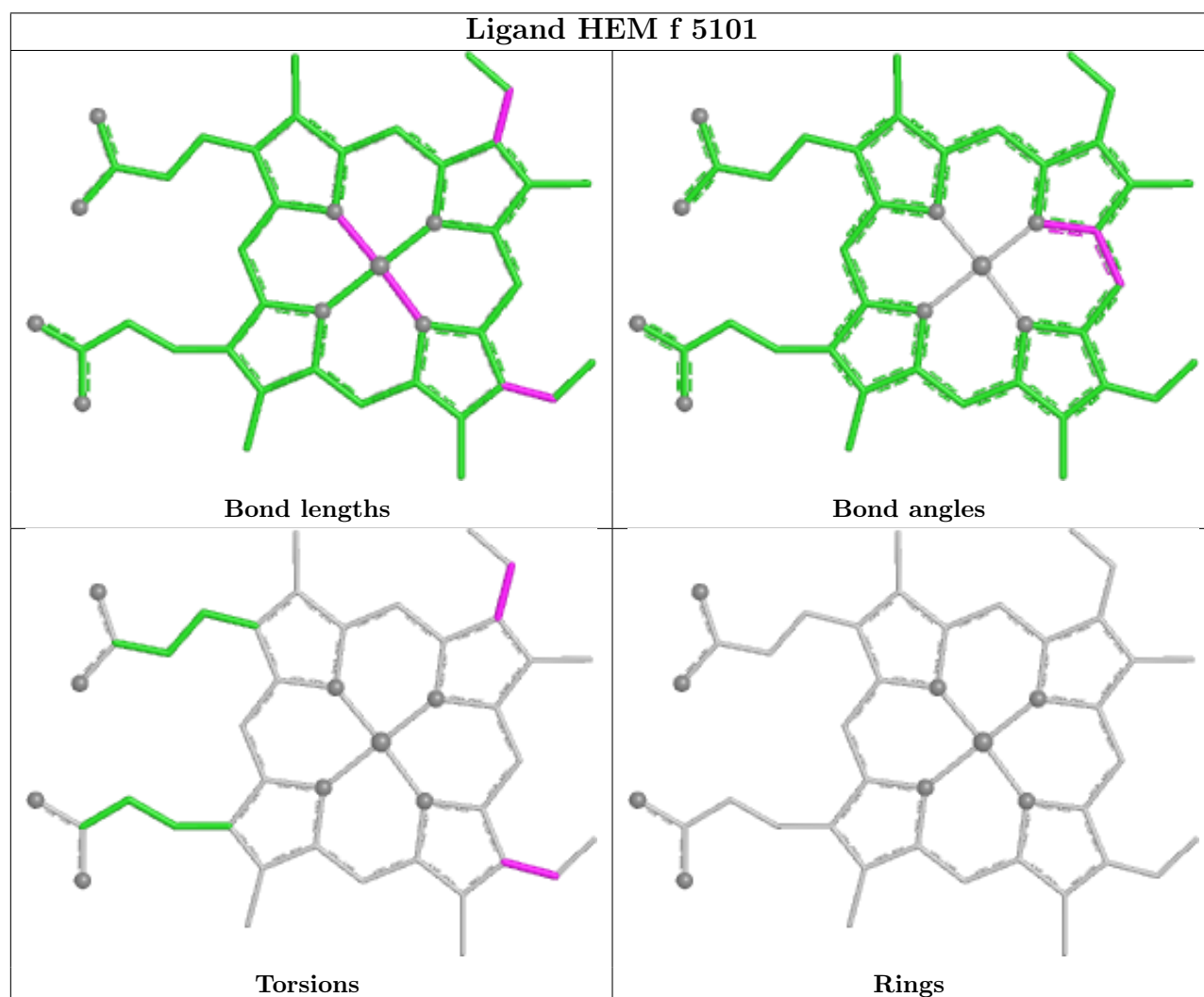
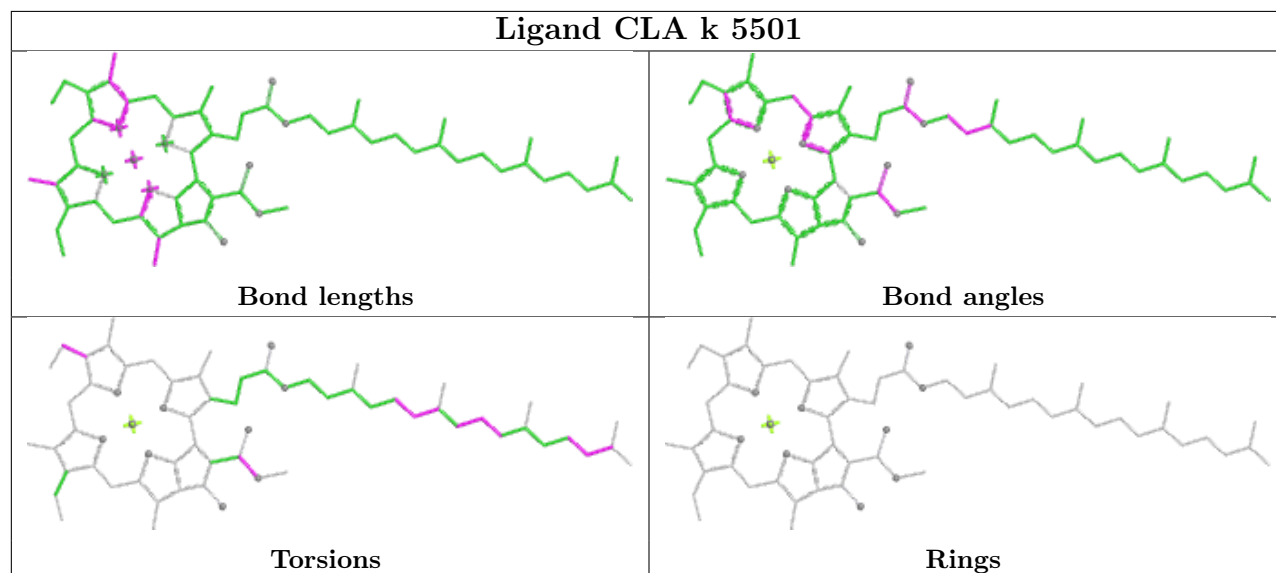
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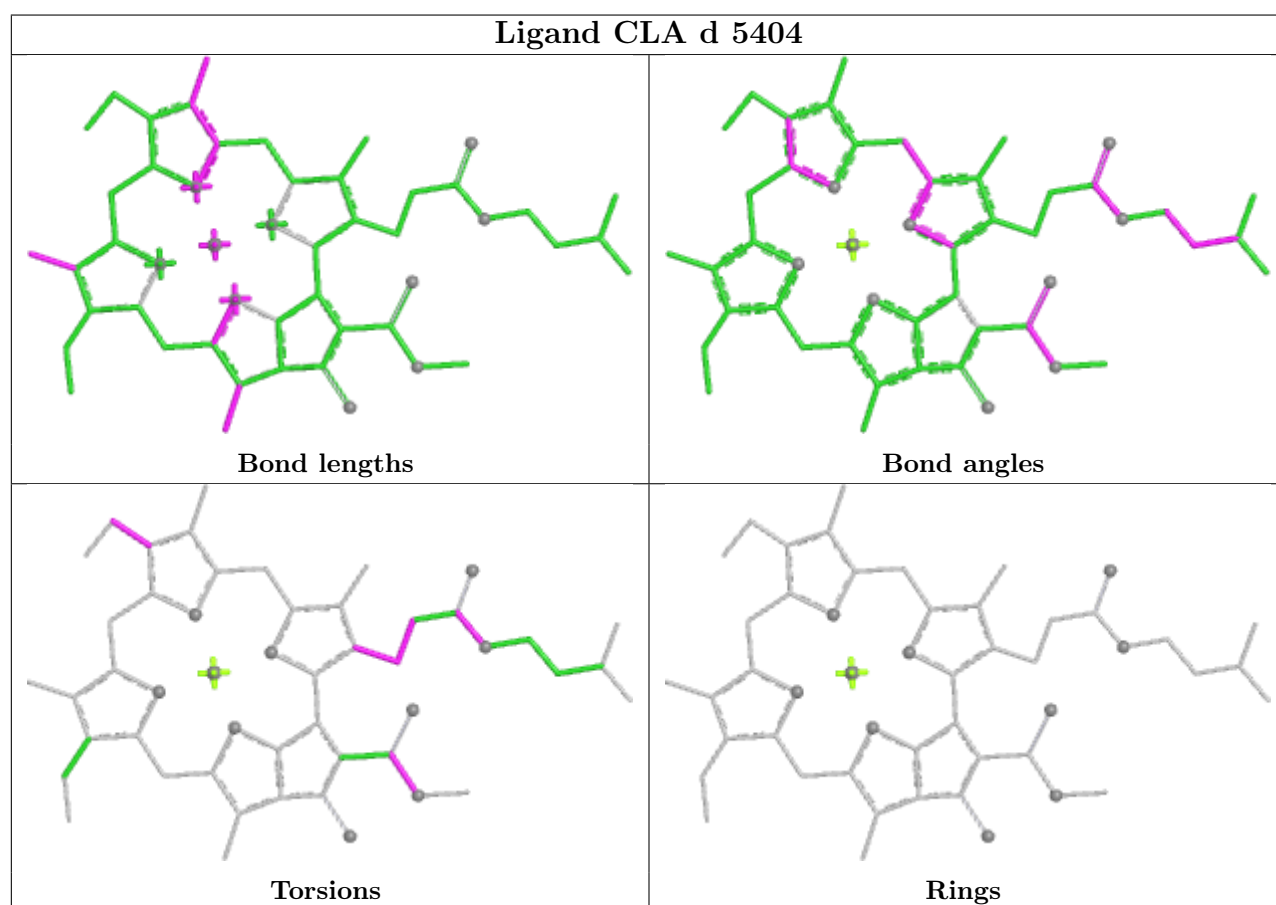
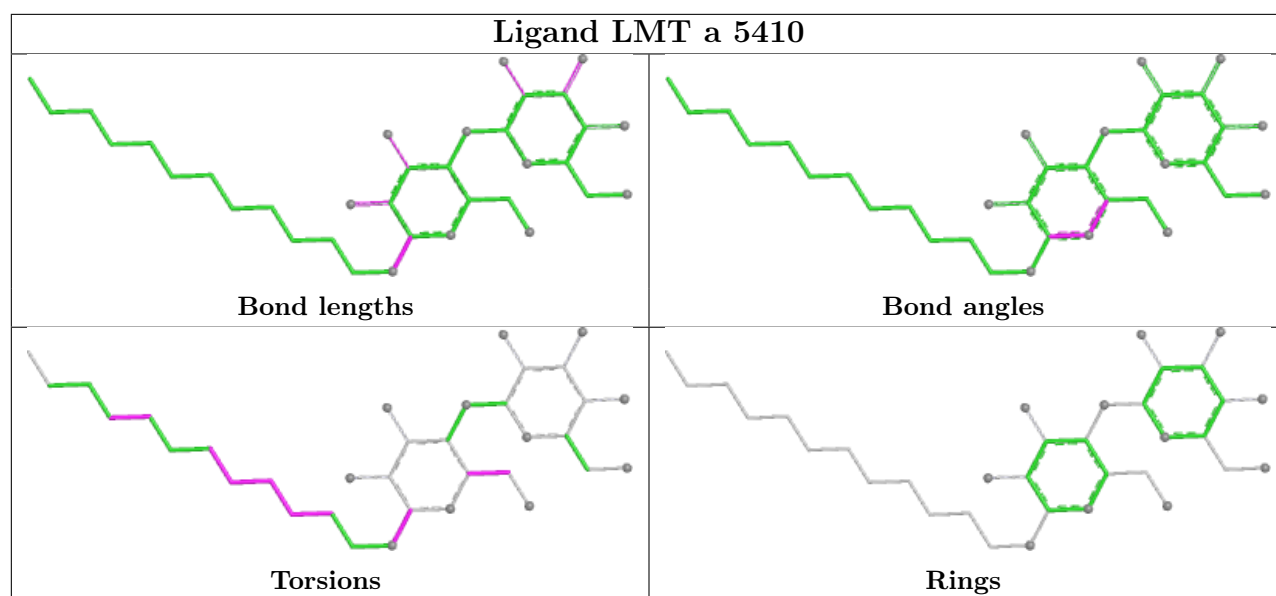
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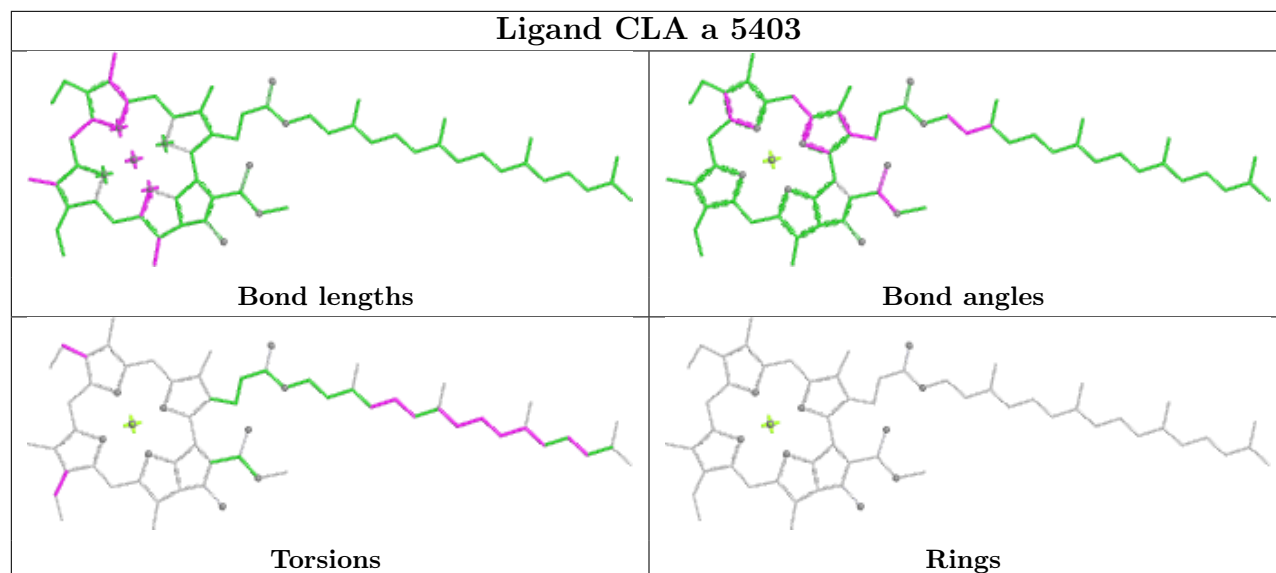
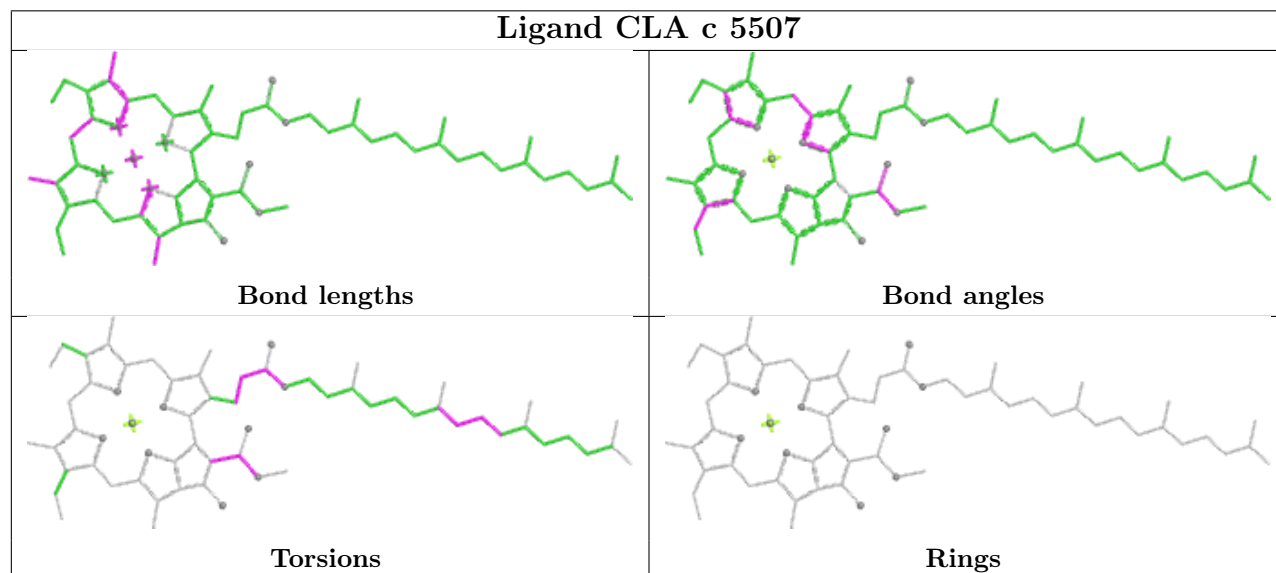
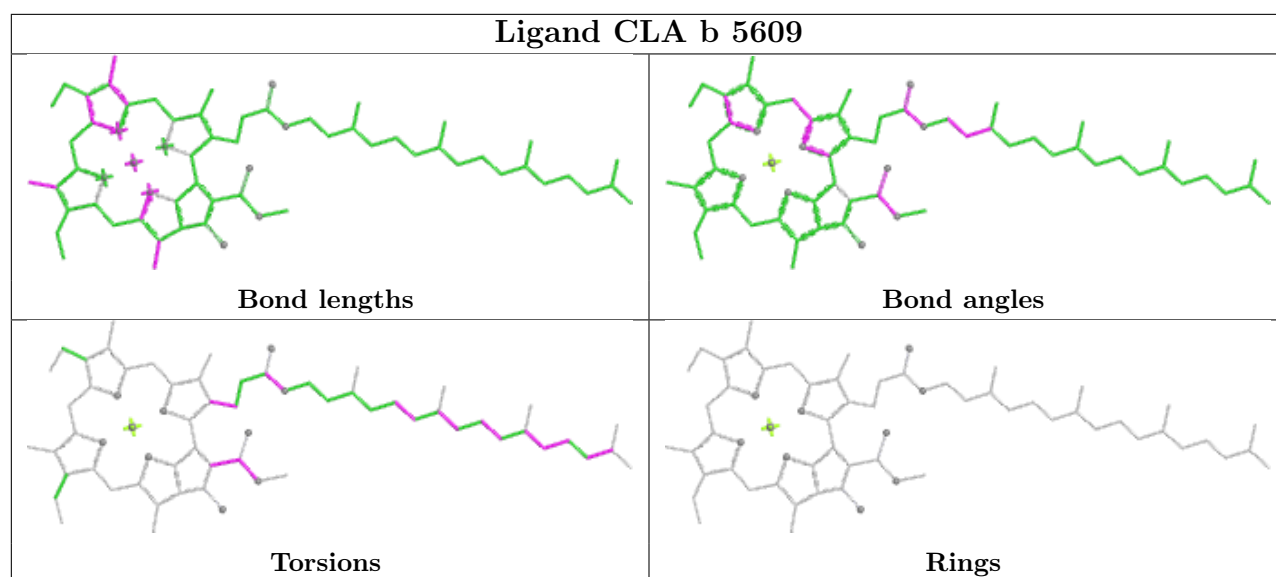
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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17	D	404	CLA	10	0
17	B	613	CLA	12	0
17	B	609	CLA	9	0
17	D	405	CLA	2	0
17	c	5508	CLA	6	0
20	z	5101	BCR	4	0
17	B	614	CLA	6	0
17	C	510	CLA	3	0
23	L	101	SQD	16	0
17	c	5505	CLA	11	0
23	l	5102	SQD	13	0
17	C	512	CLA	3	0
25	D	410	MGE	13	0
20	T	102	BCR	6	0
20	t	5102	BCR	6	0
17	c	5510	CLA	3	0
25	D	409	MGE	5	0
25	m	5103	MGE	9	0
26	A	413	DGD	7	0
25	B	619	MGE	6	0
17	B	616	CLA	4	0
17	c	5506	CLA	5	0
21	A	408	LHG	2	0
17	B	605	CLA	6	0
17	b	5616	CLA	5	0
23	D	403	SQD	6	0
17	A	405	CLA	5	0
17	C	507	CLA	6	0
20	k	5502	BCR	9	0
17	c	5512	CLA	6	0
25	A	412	MGE	12	0
17	B	612	CLA	12	0

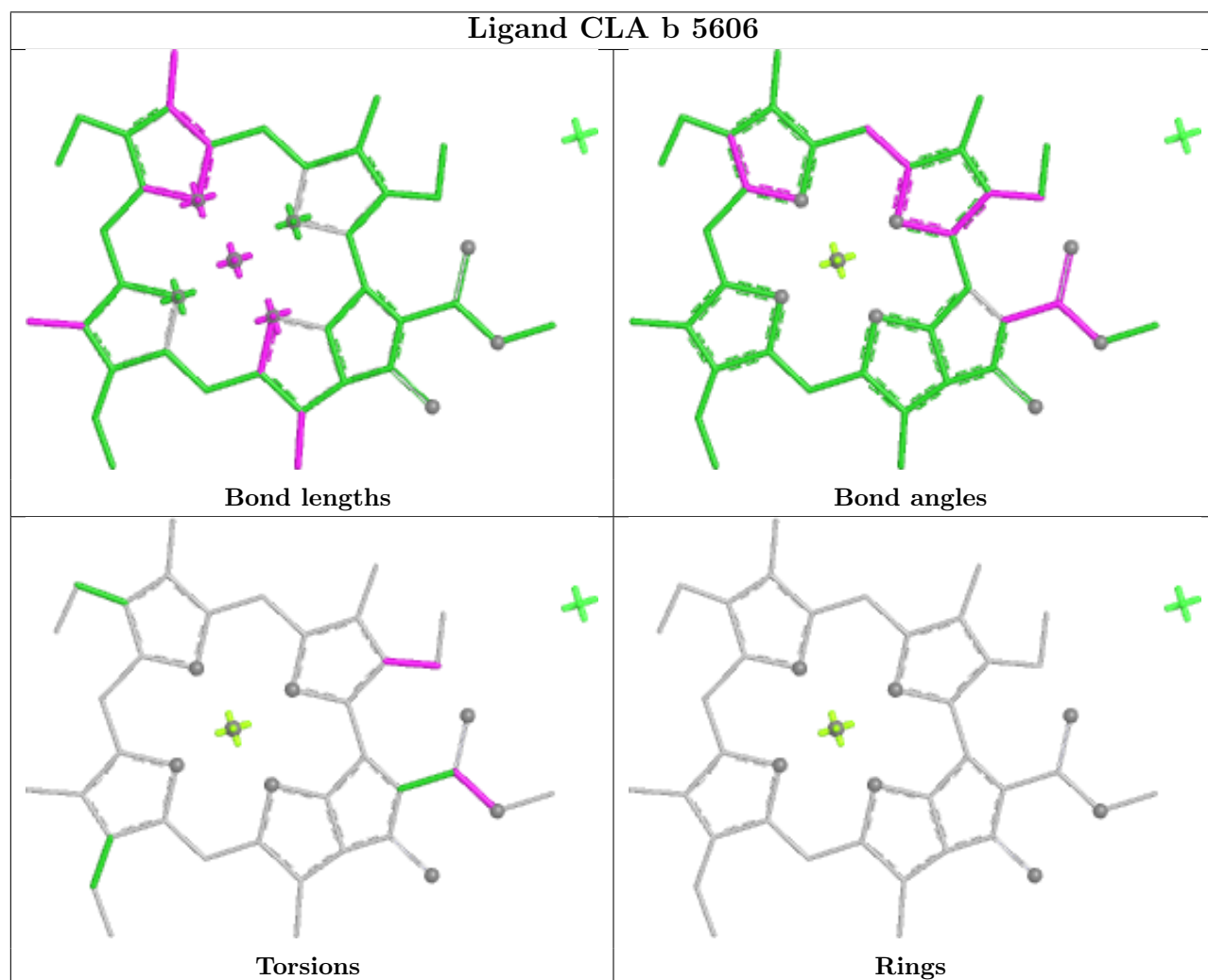
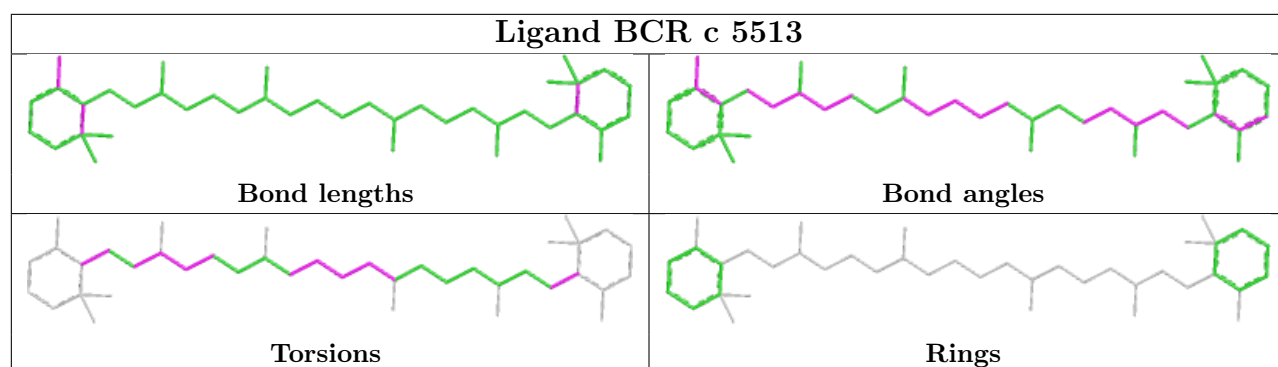
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

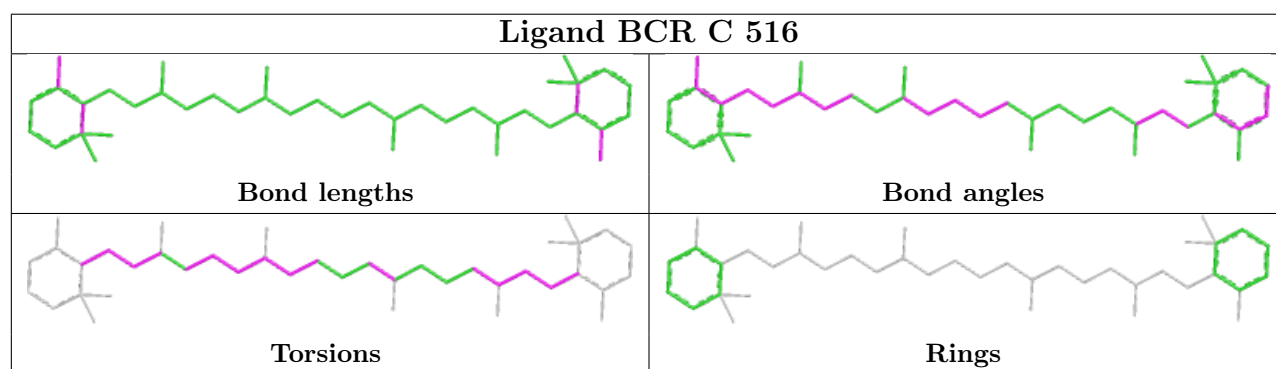
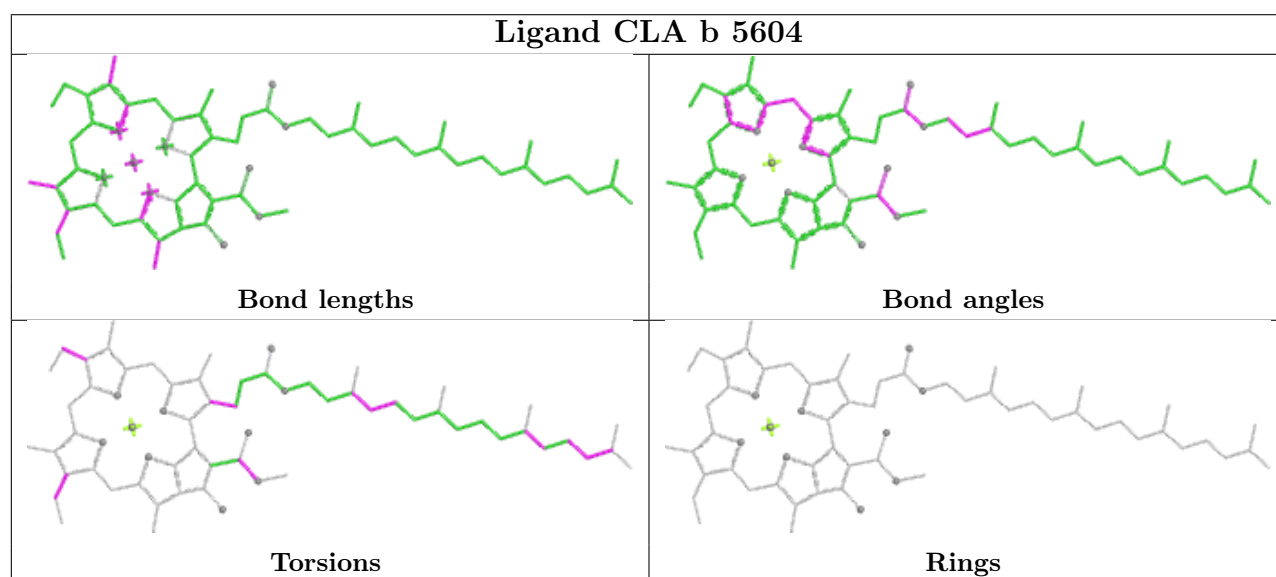
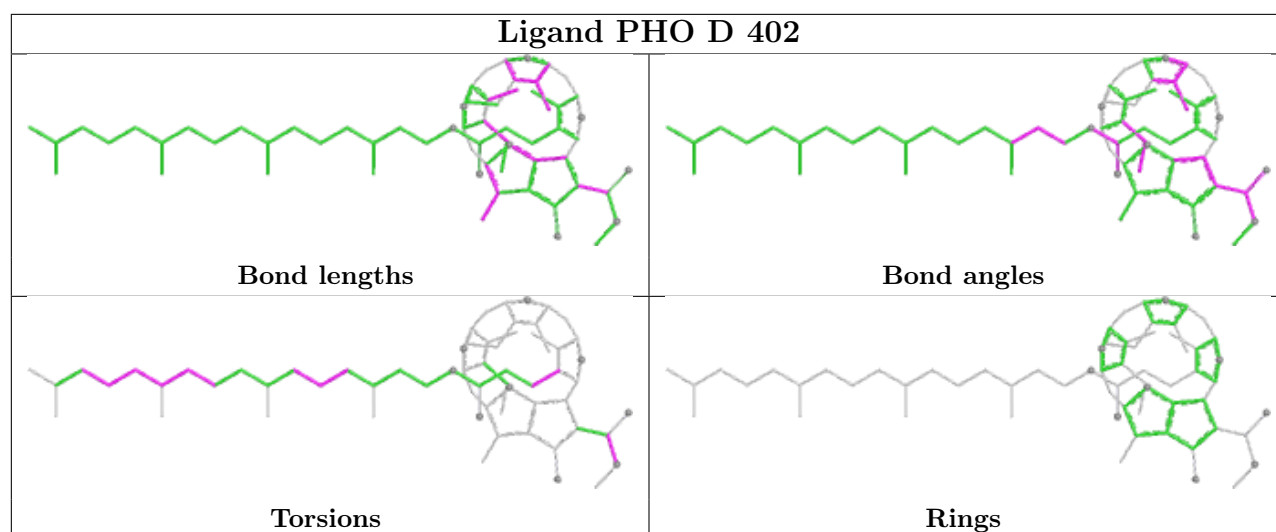
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

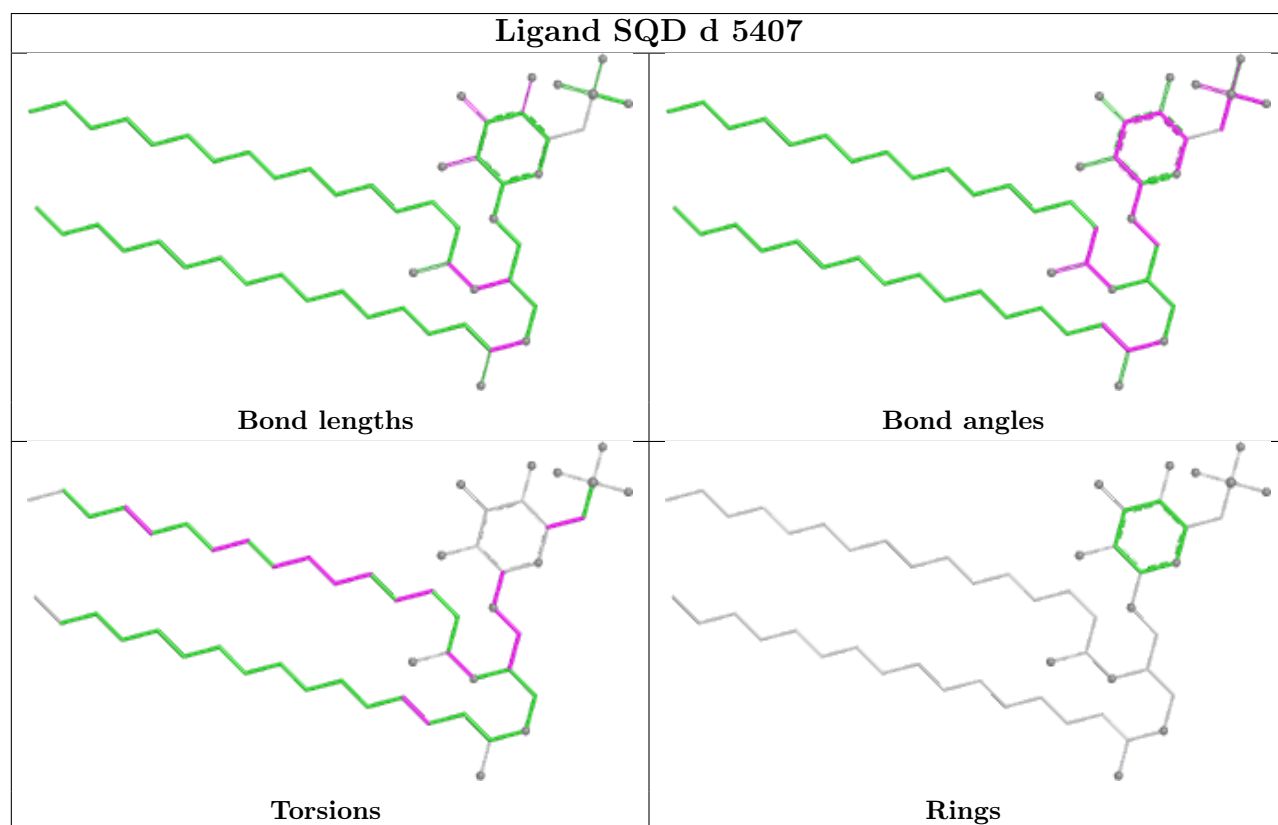
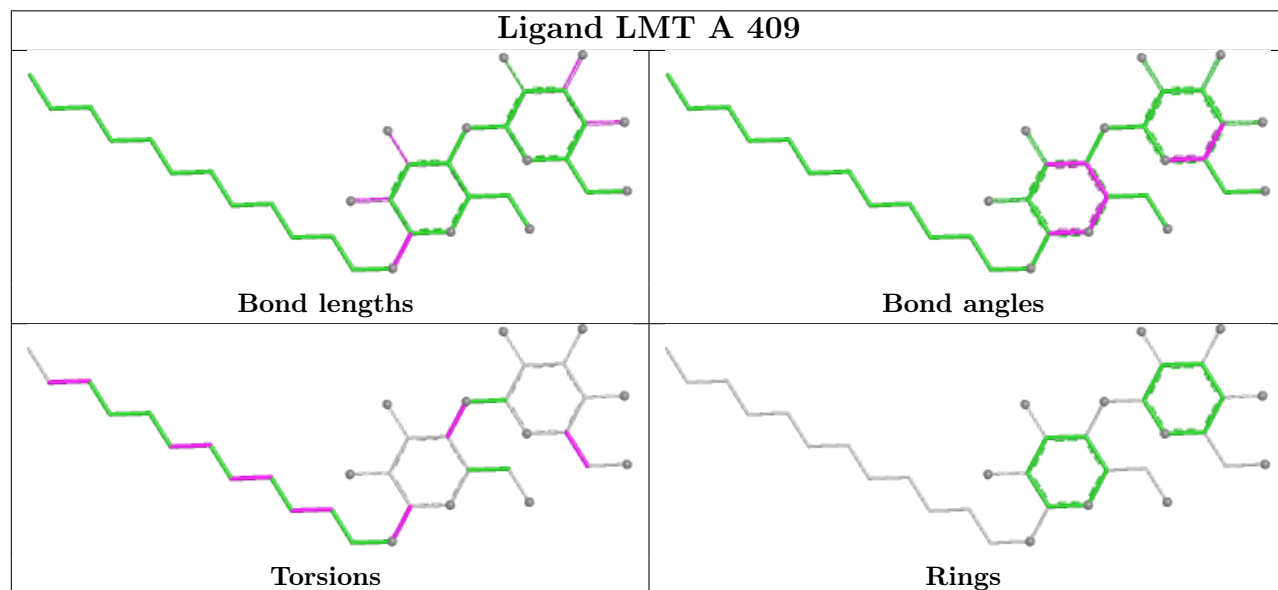
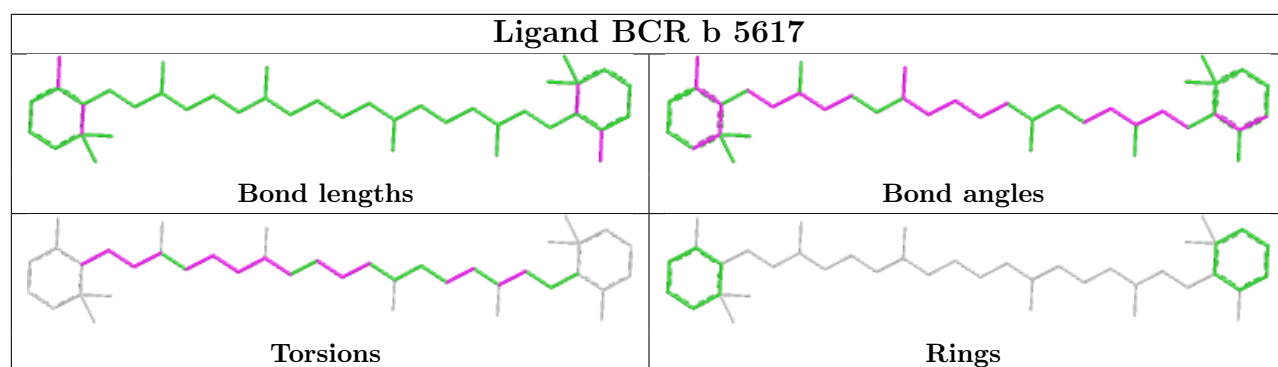




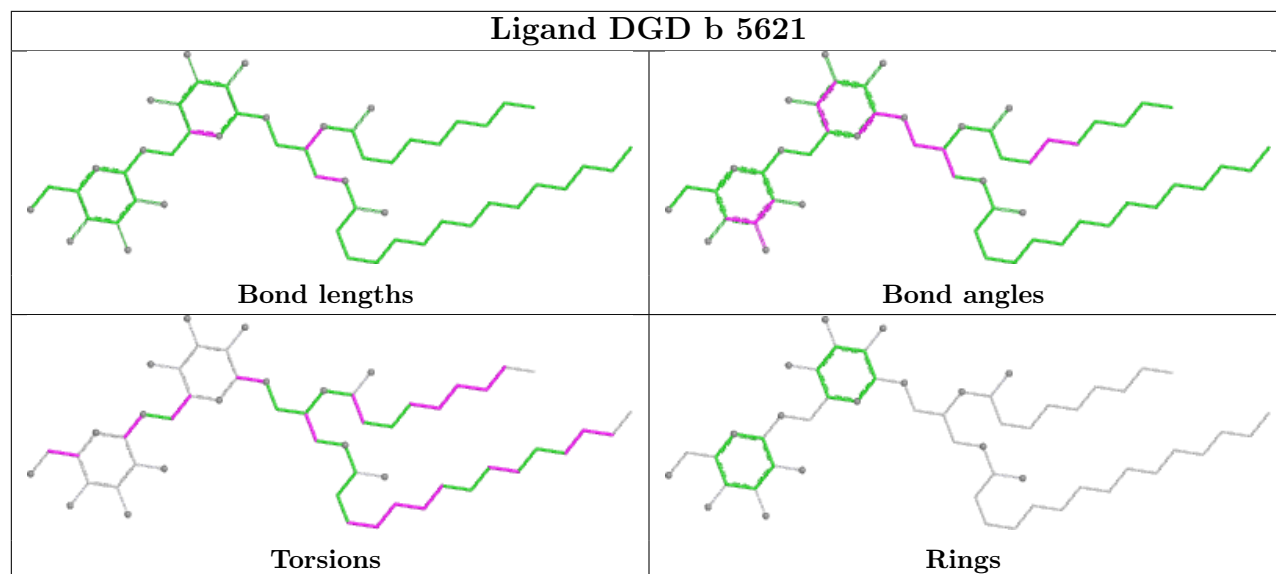




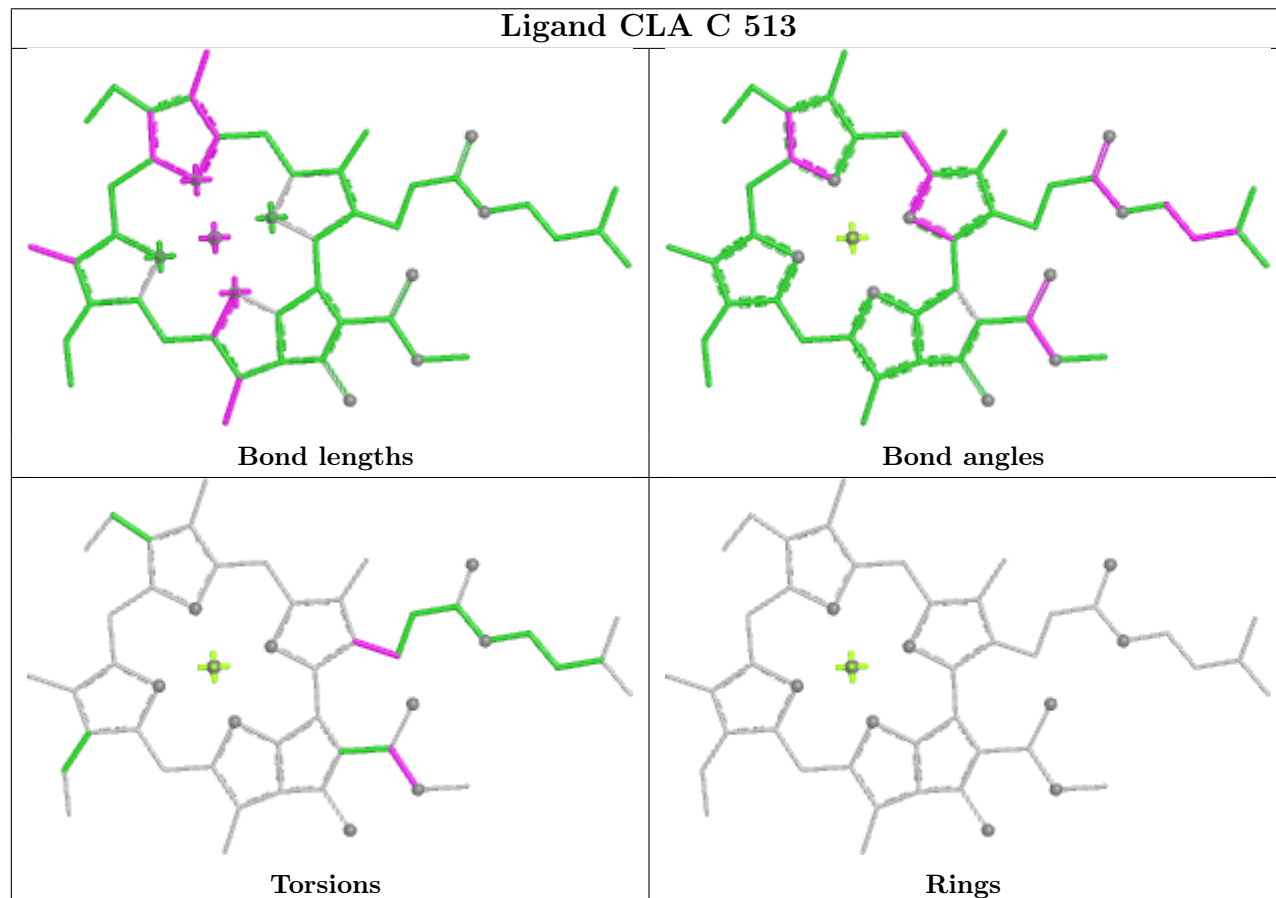


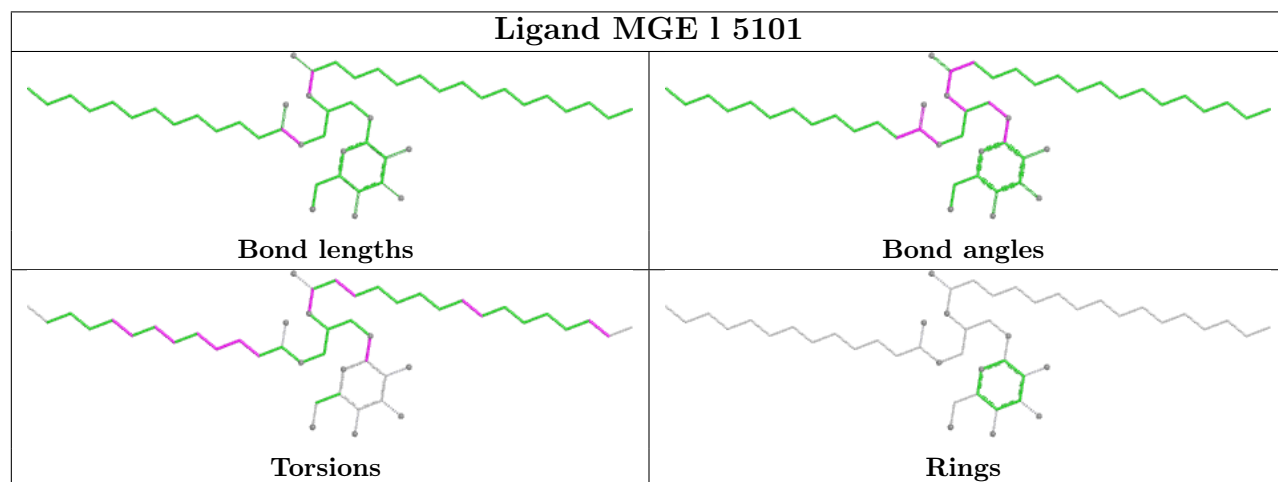
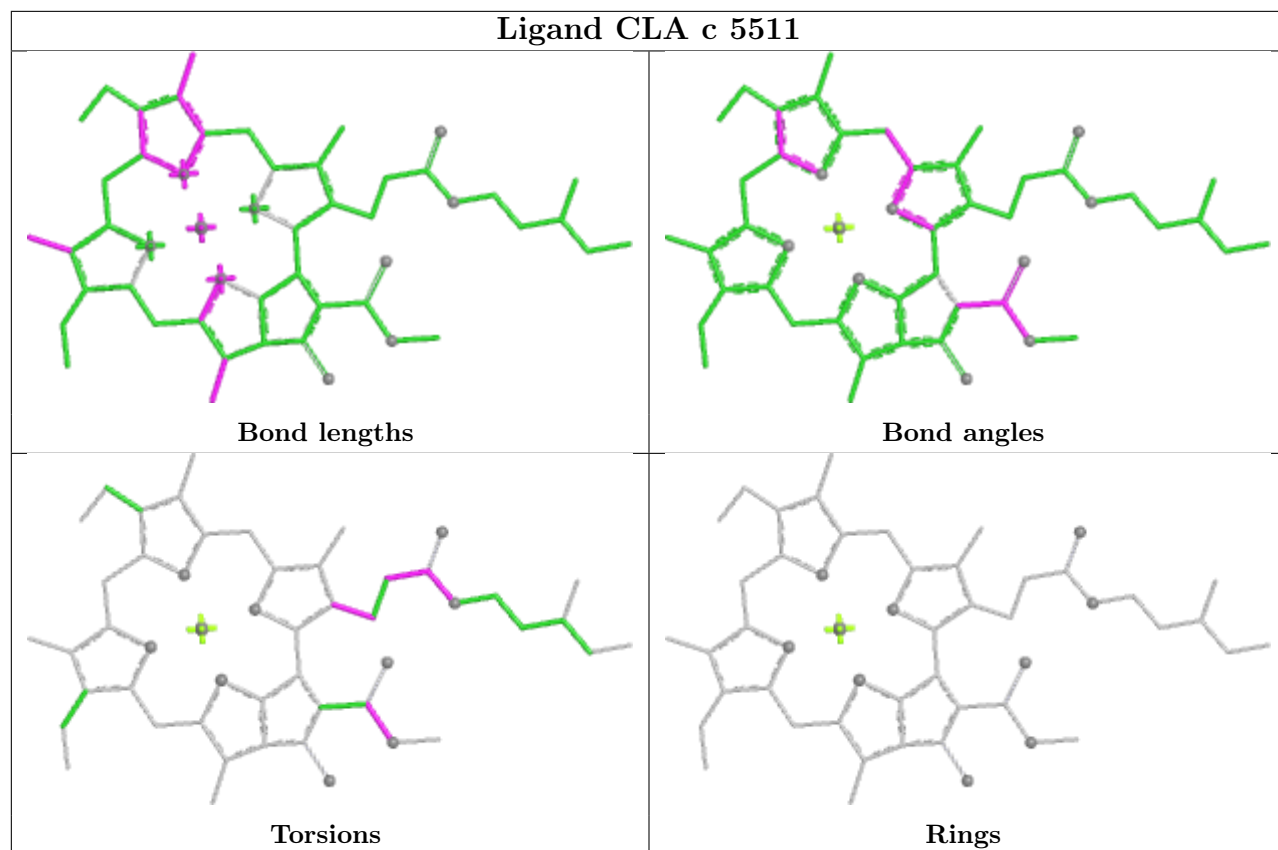


Ligand DGD b 5621

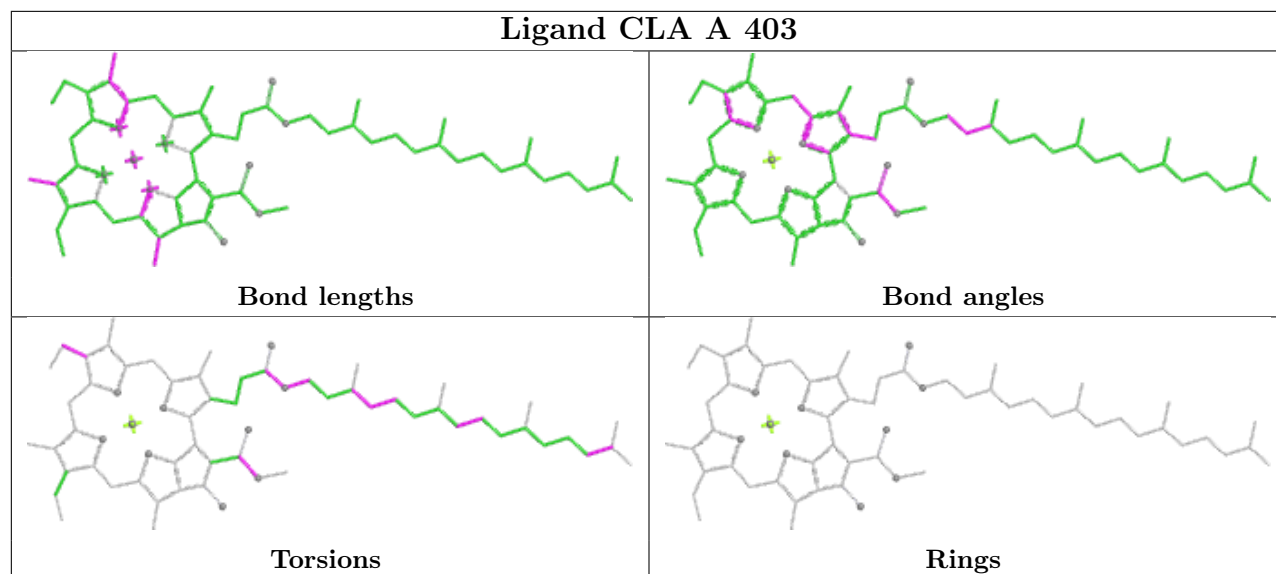


Ligand CLA C 513

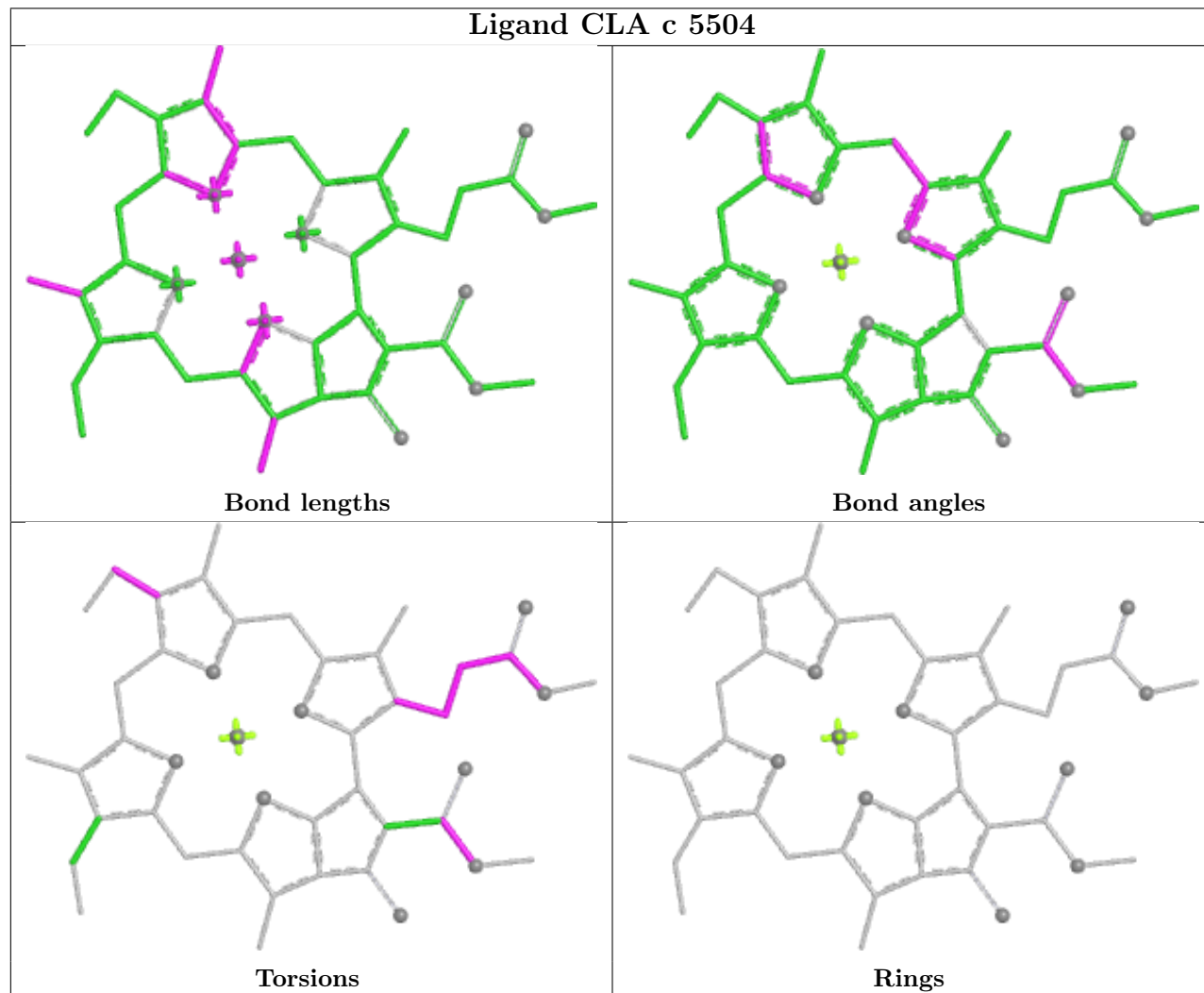


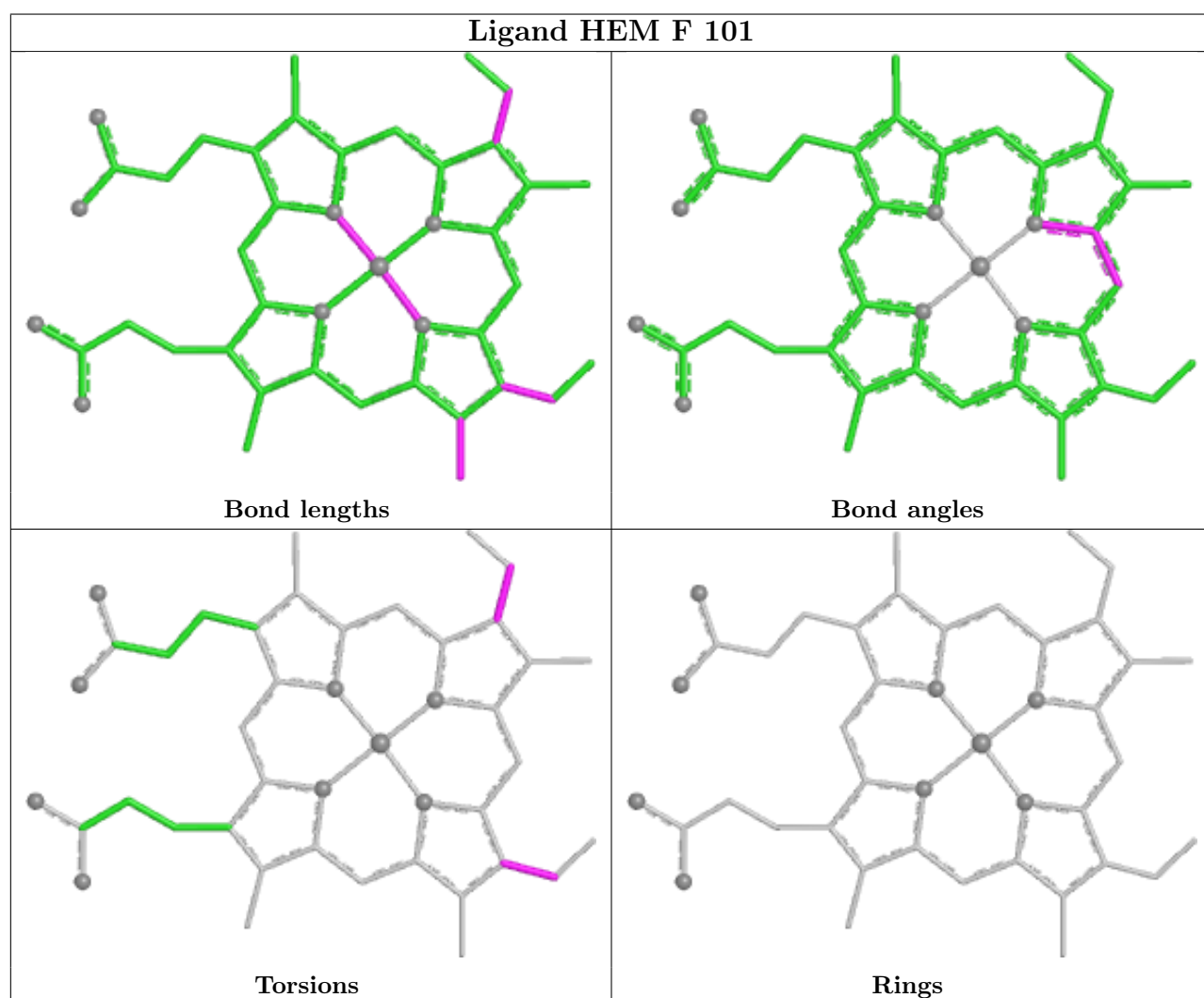
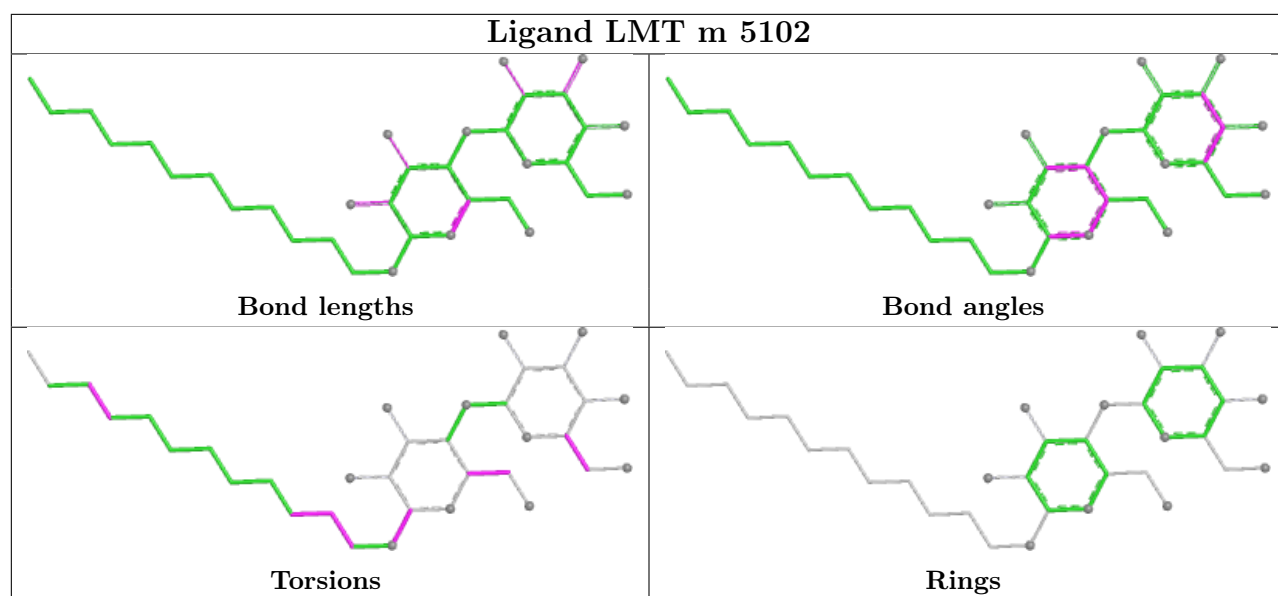


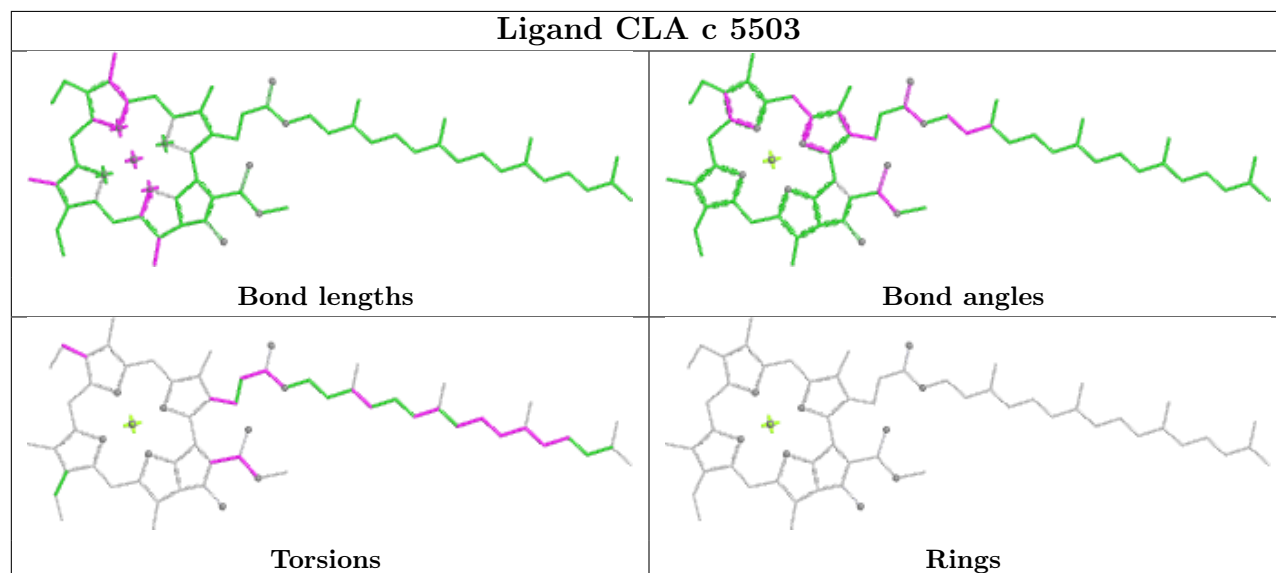
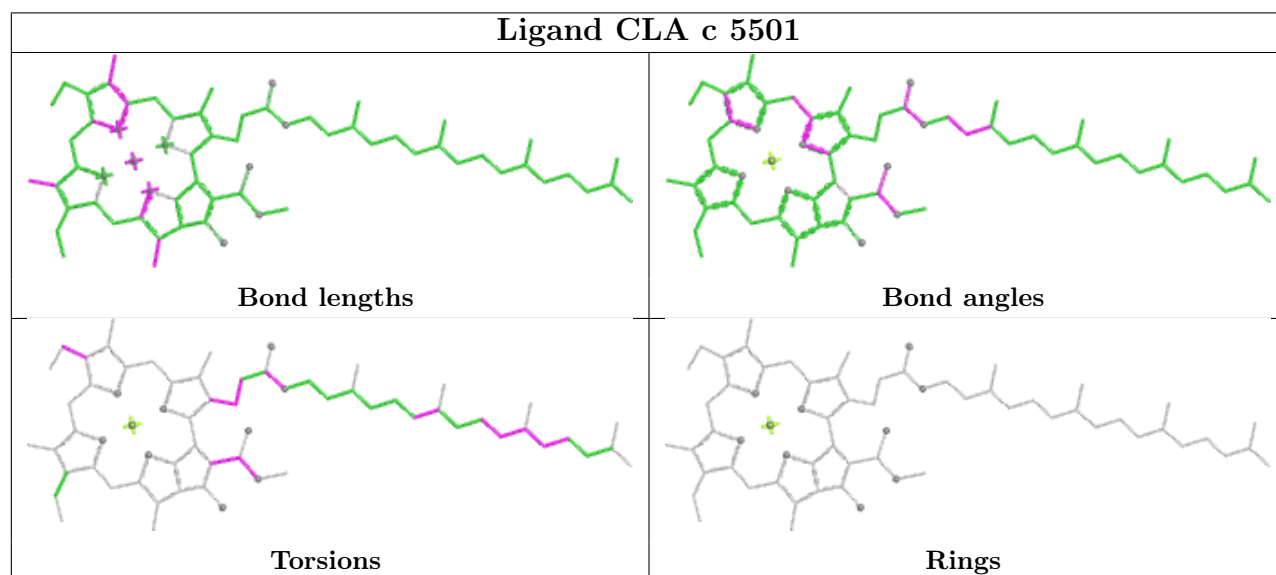
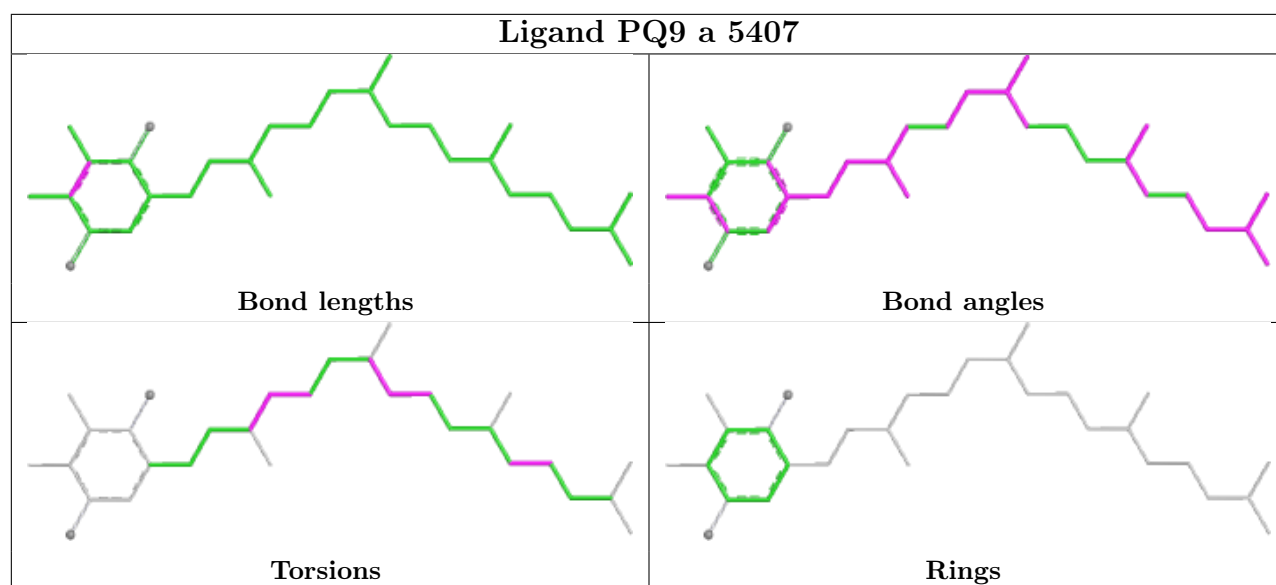
Ligand CLA A 403

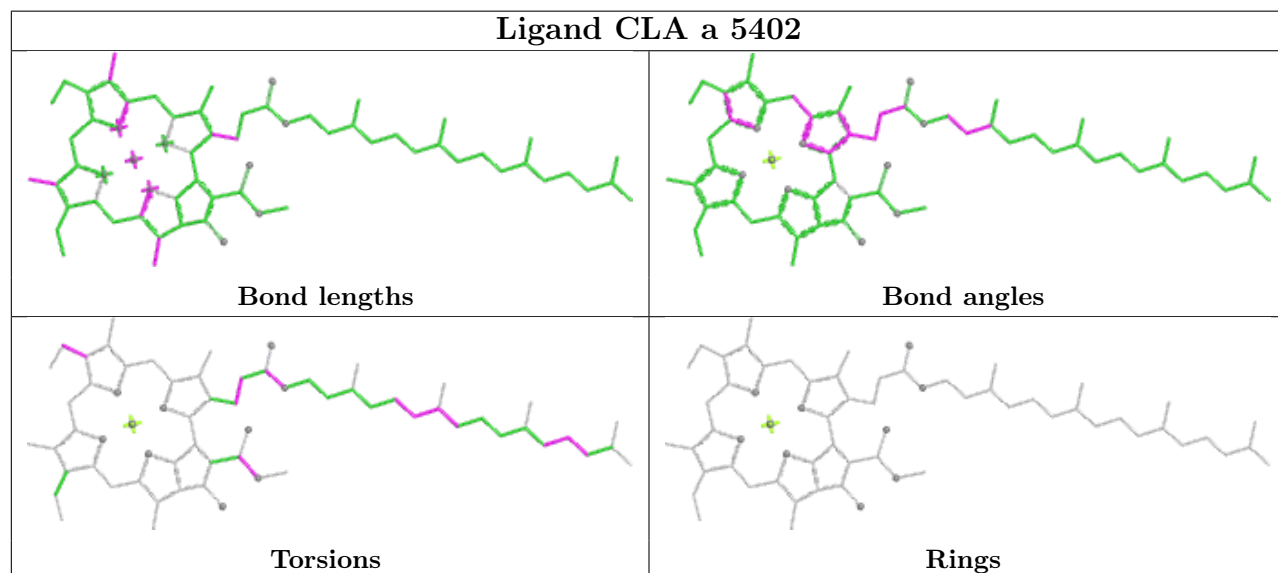
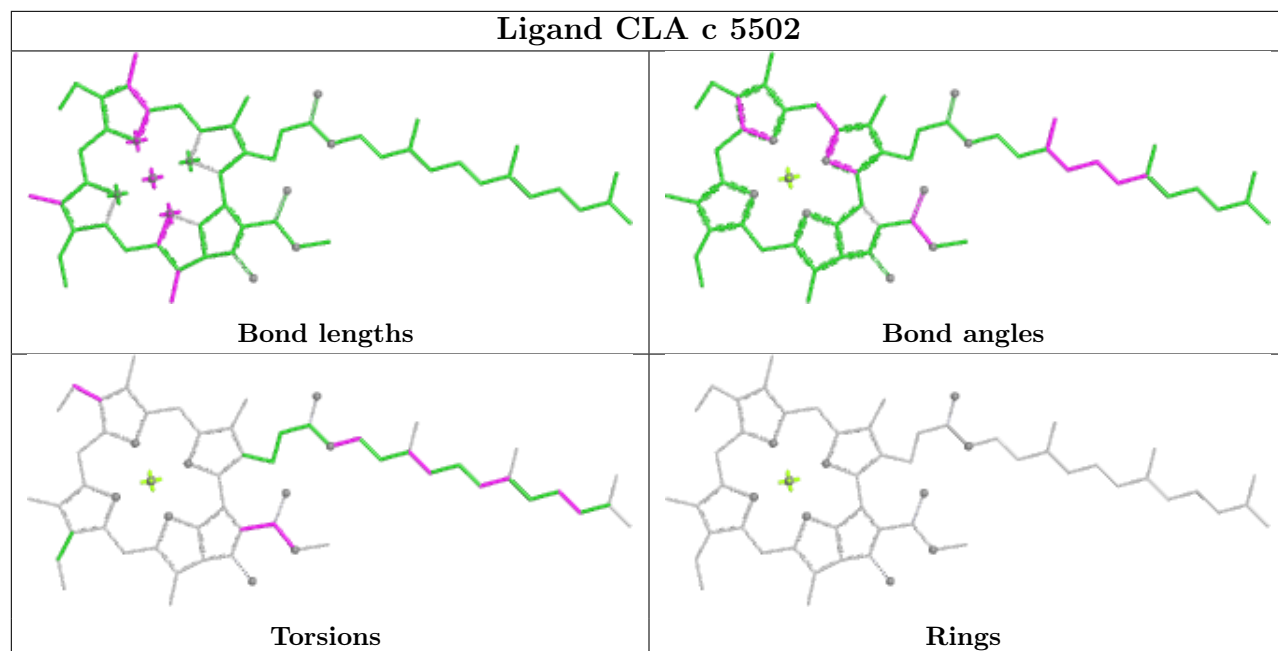


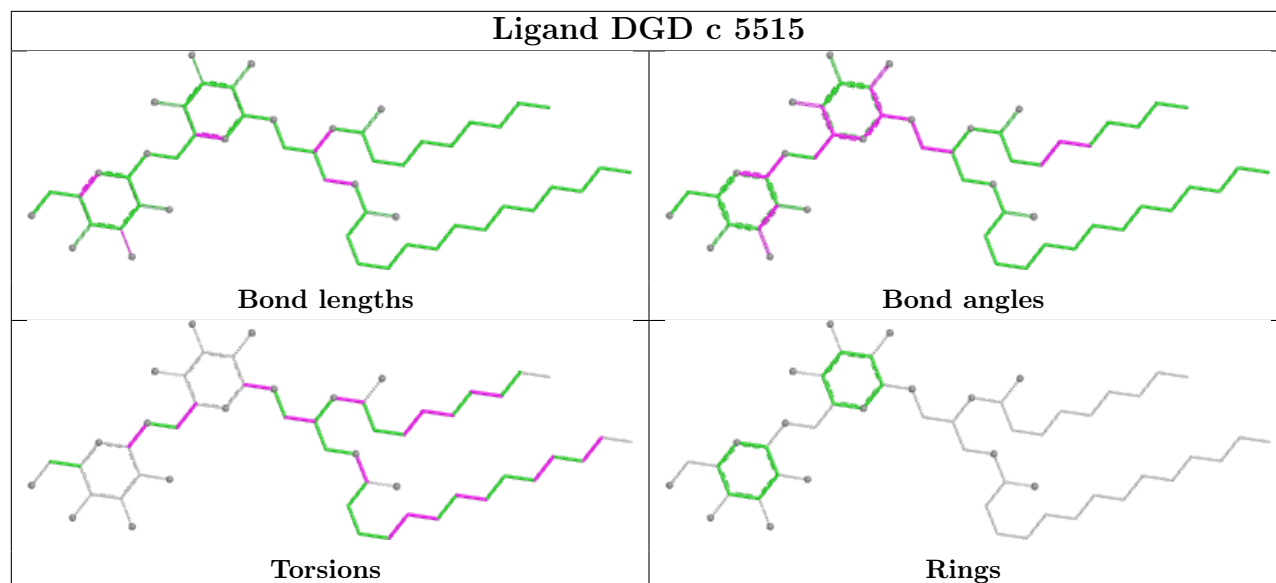
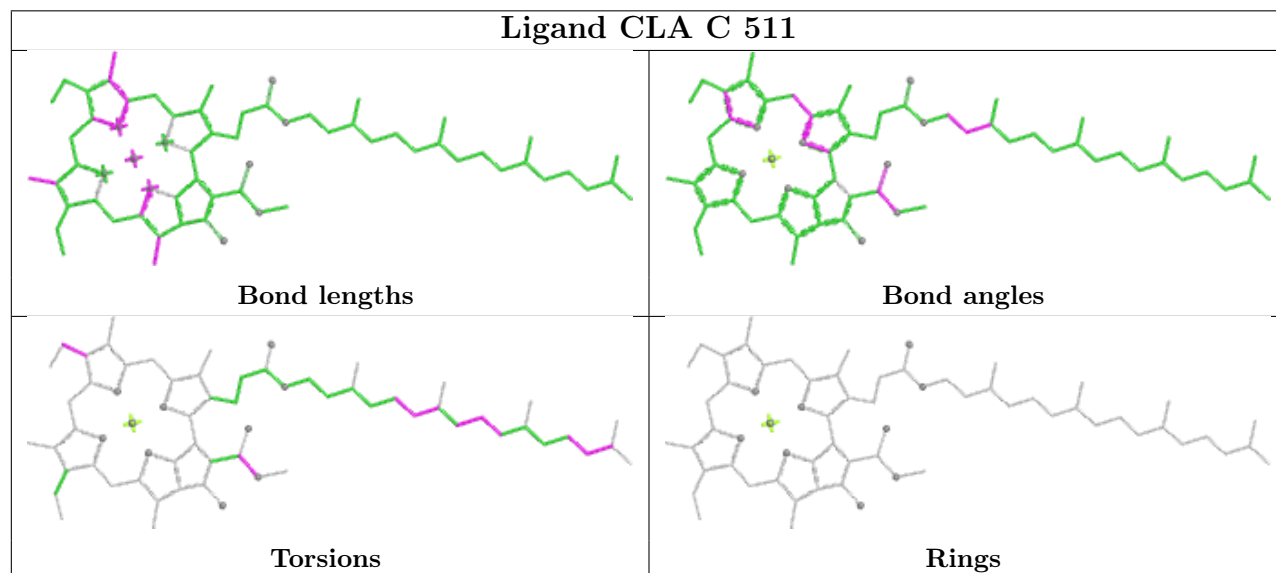
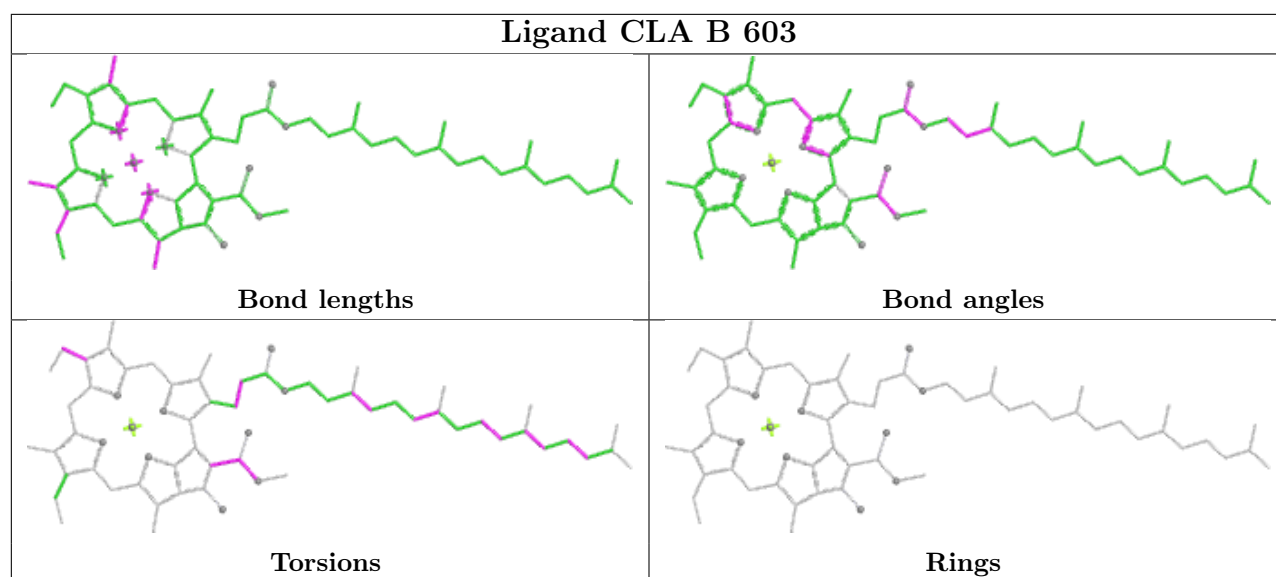
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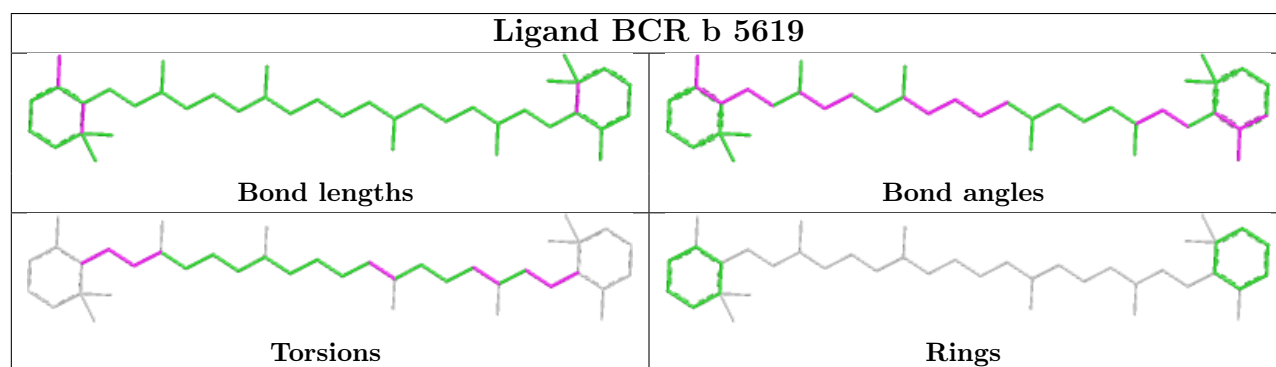
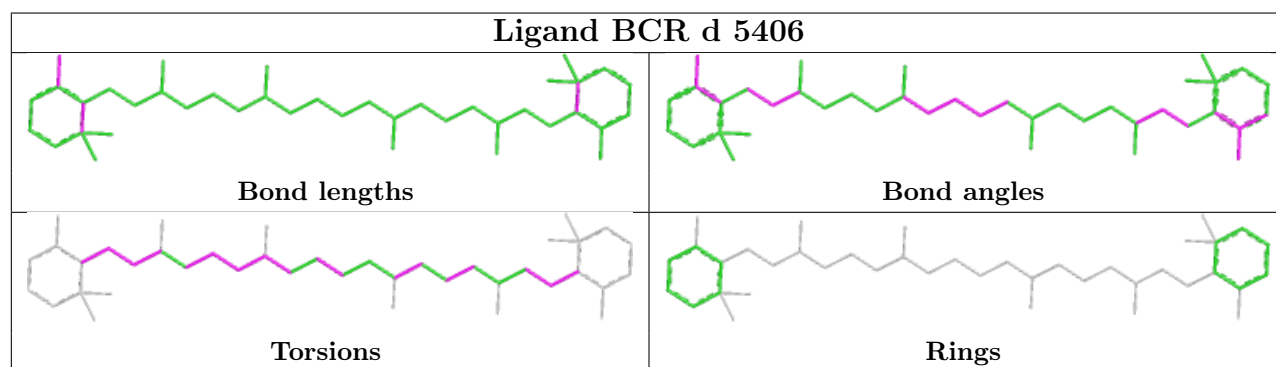
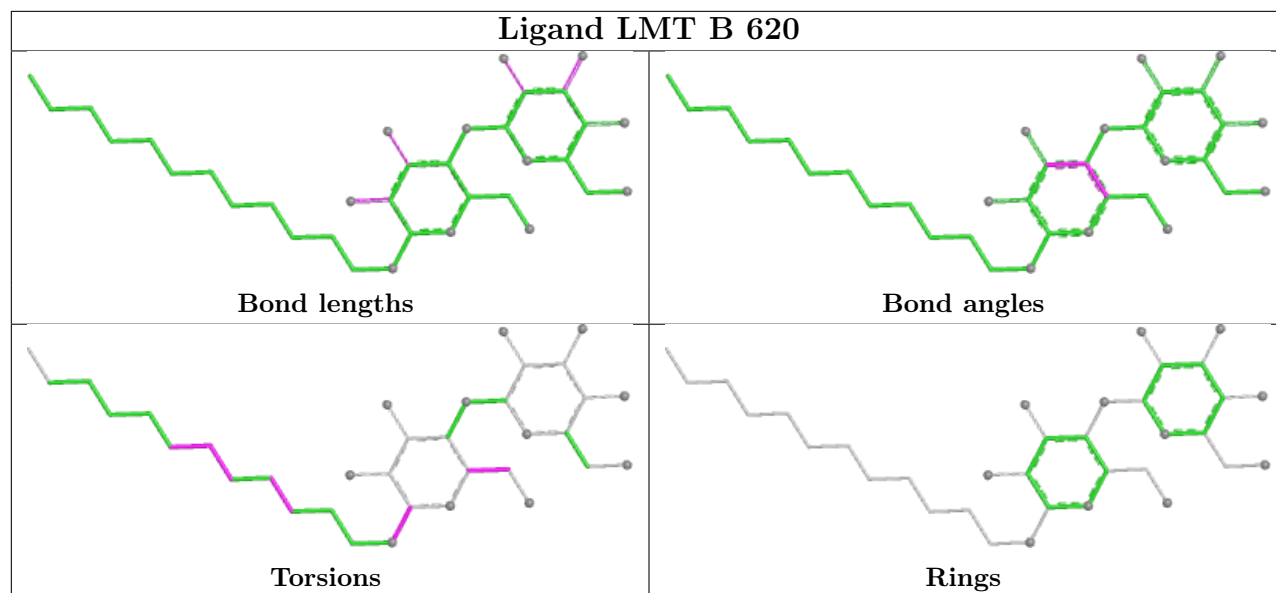


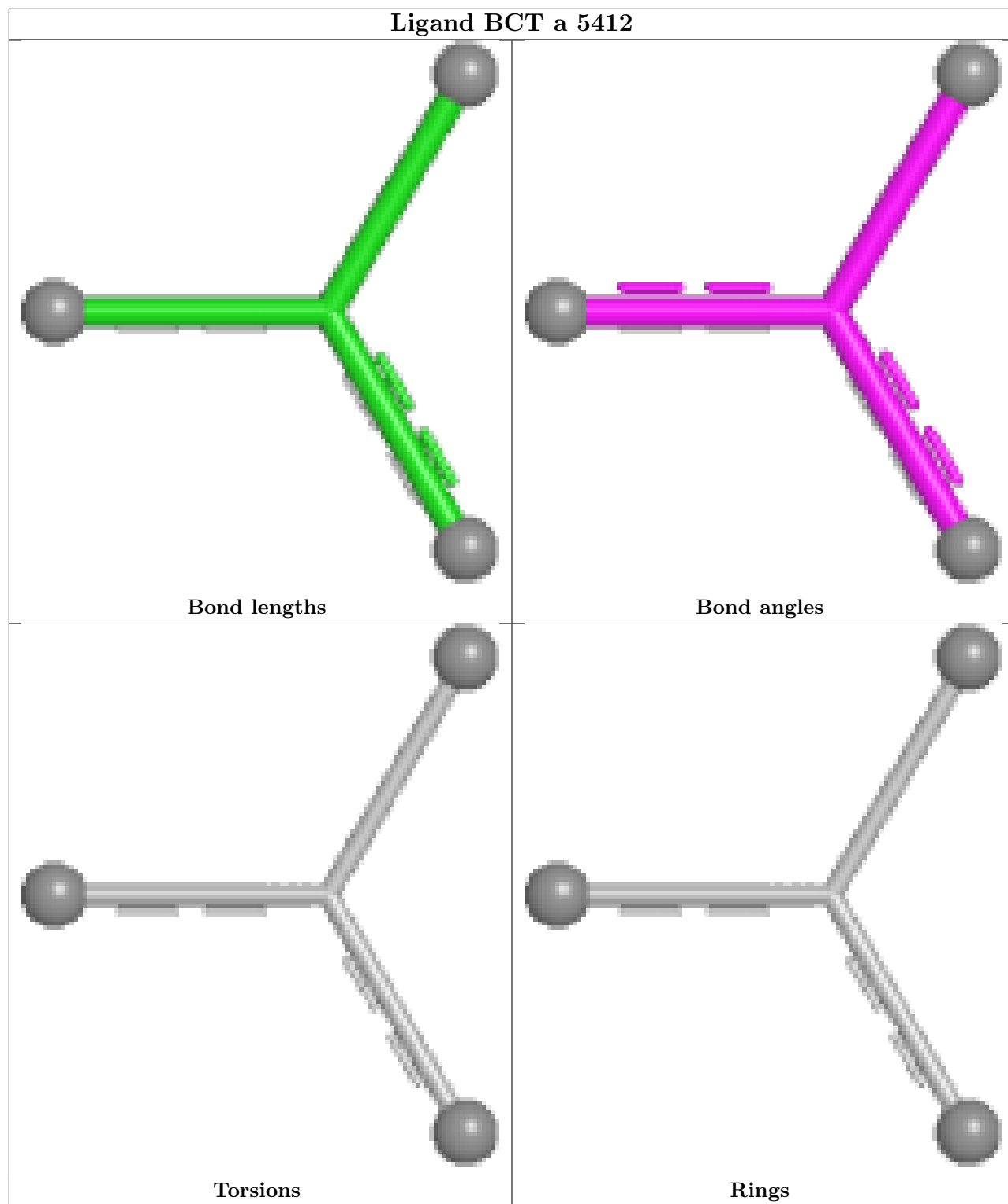


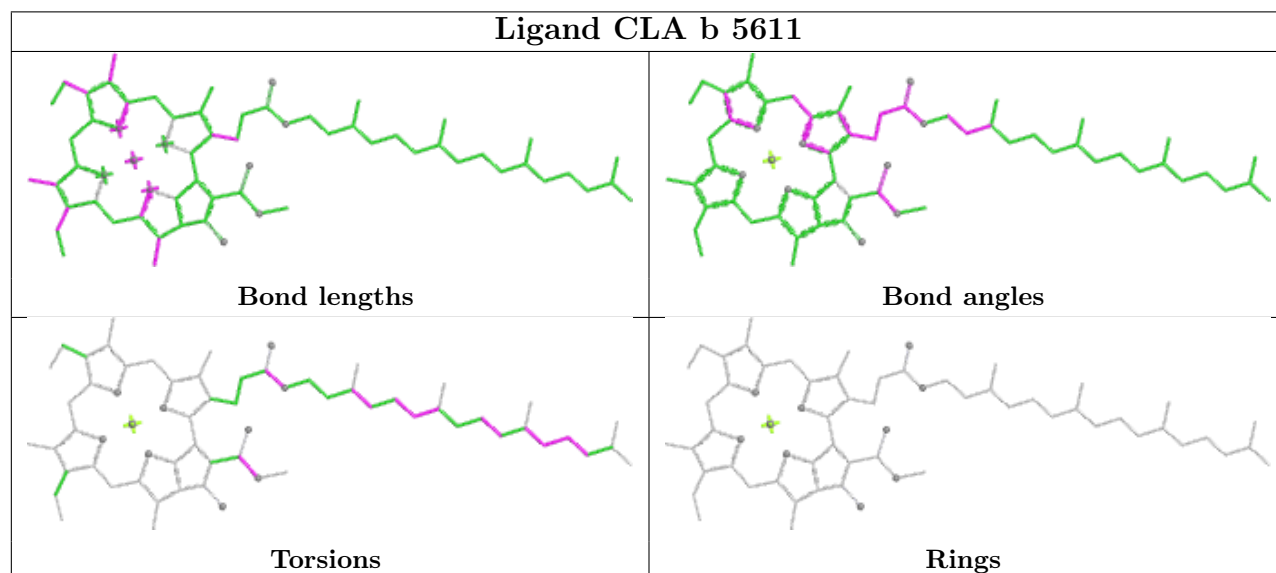
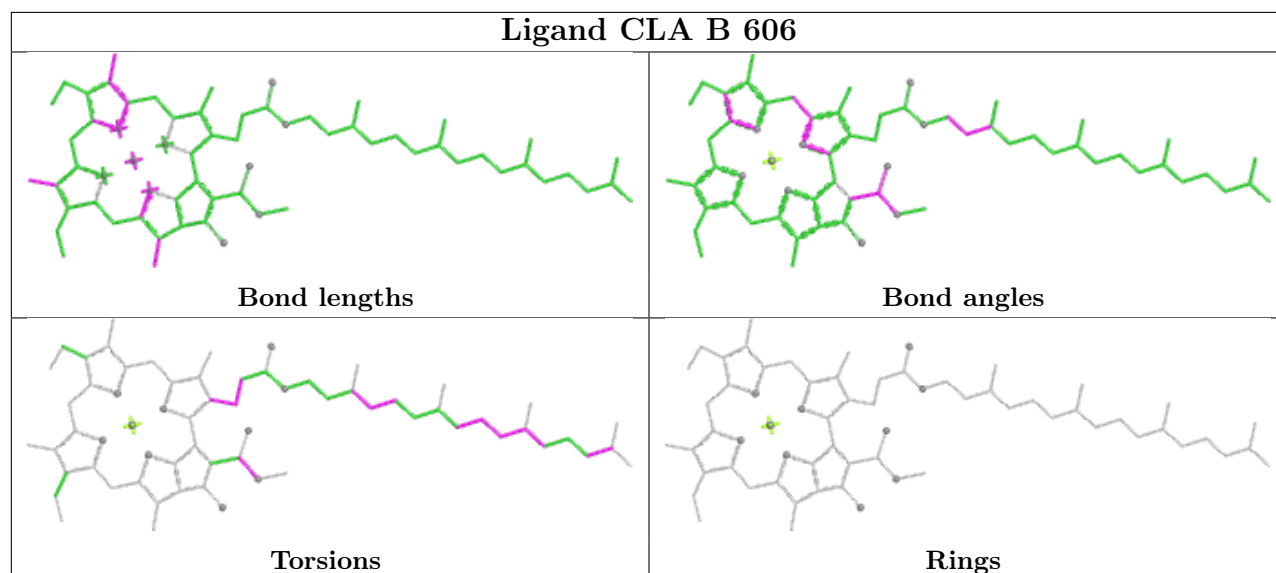
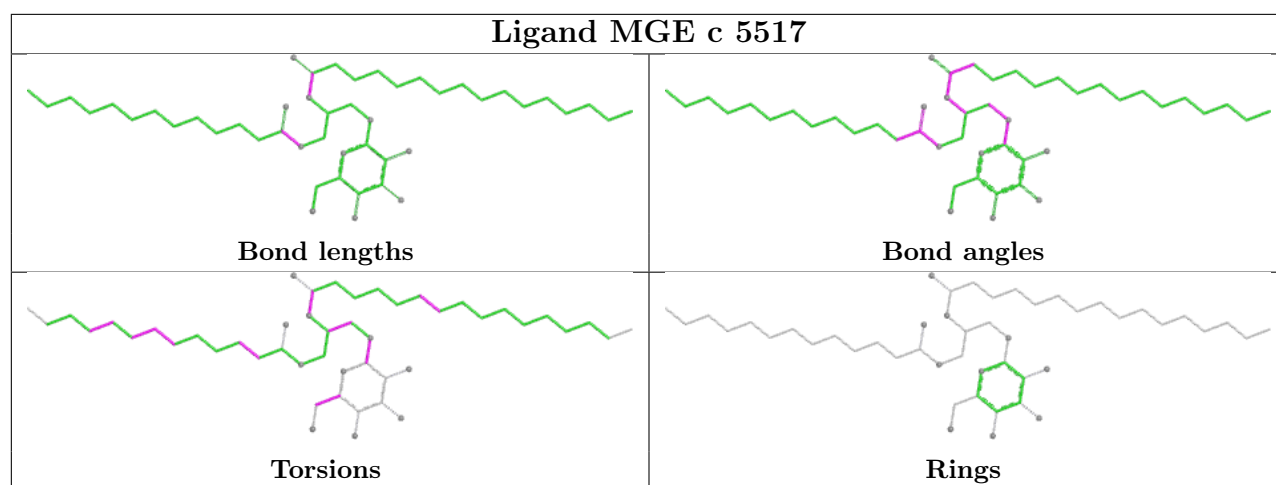


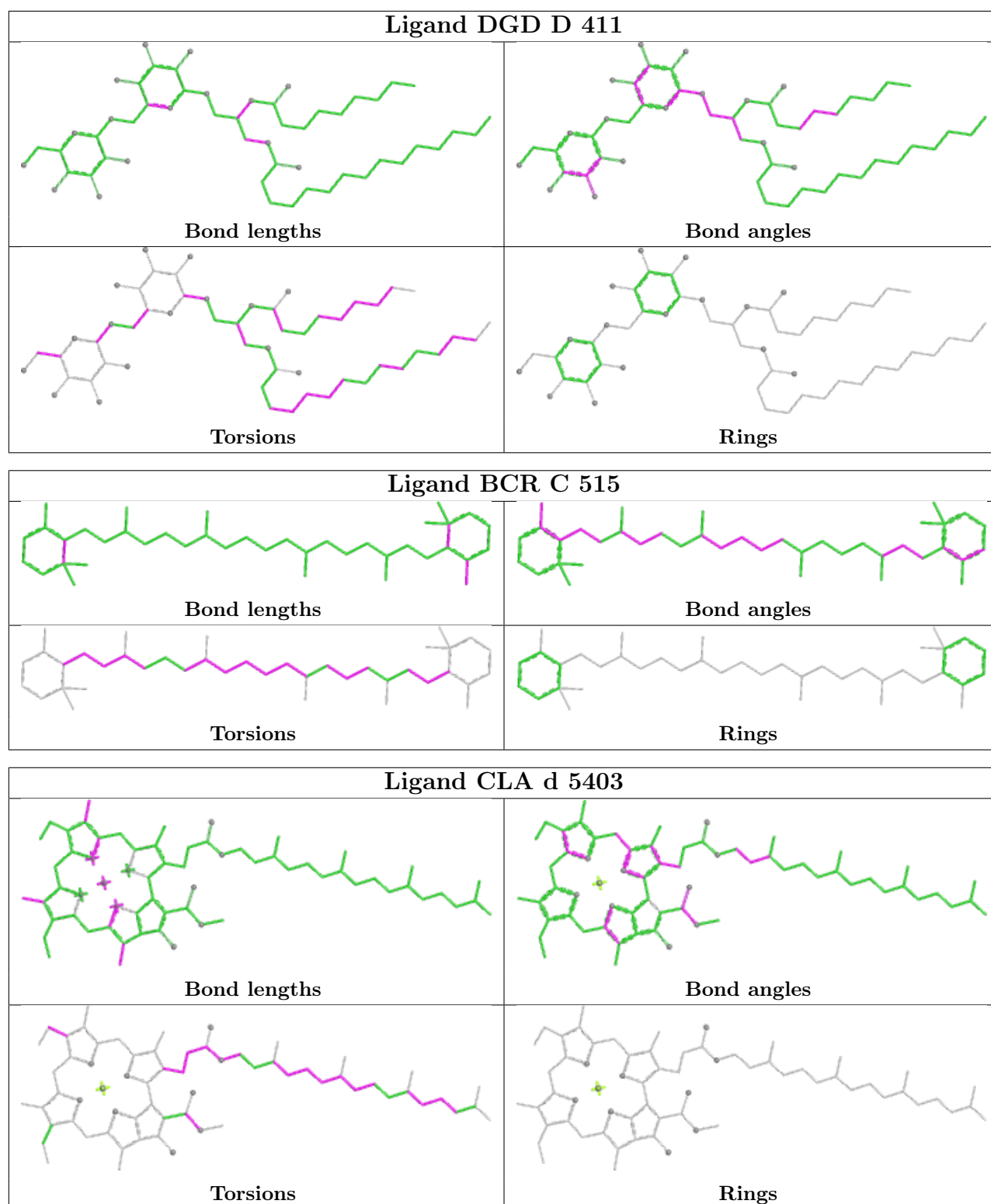


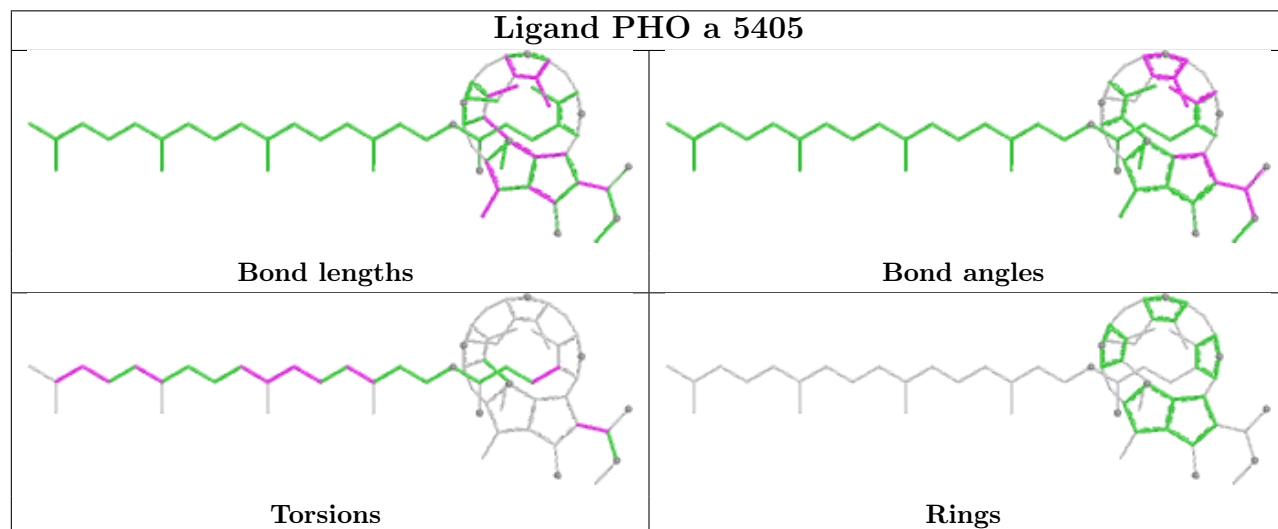
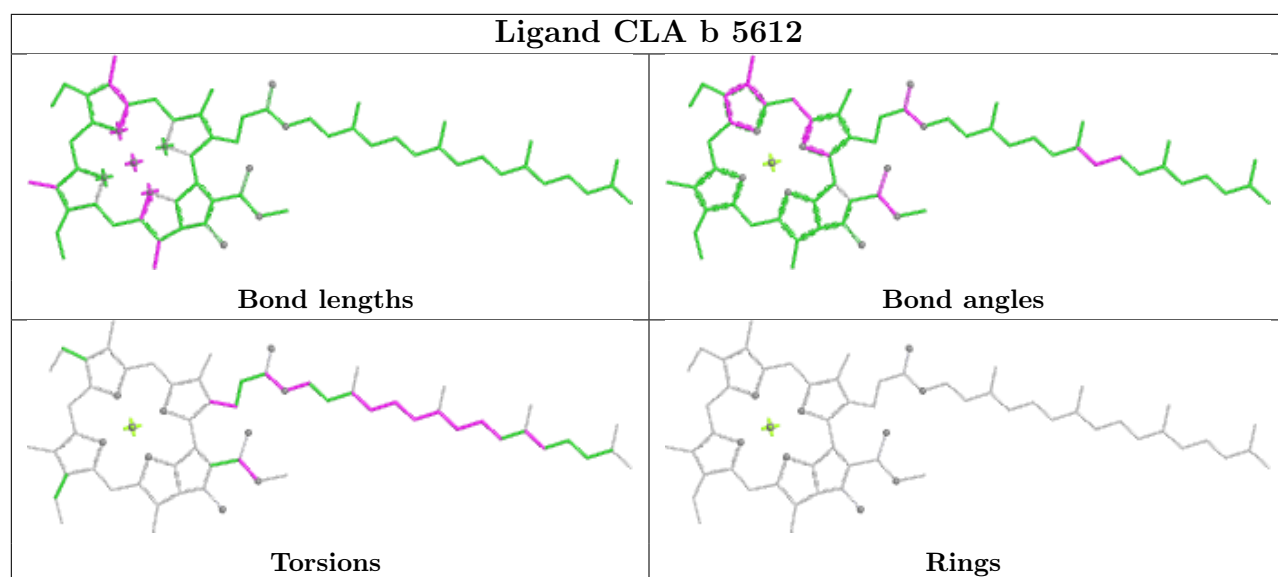


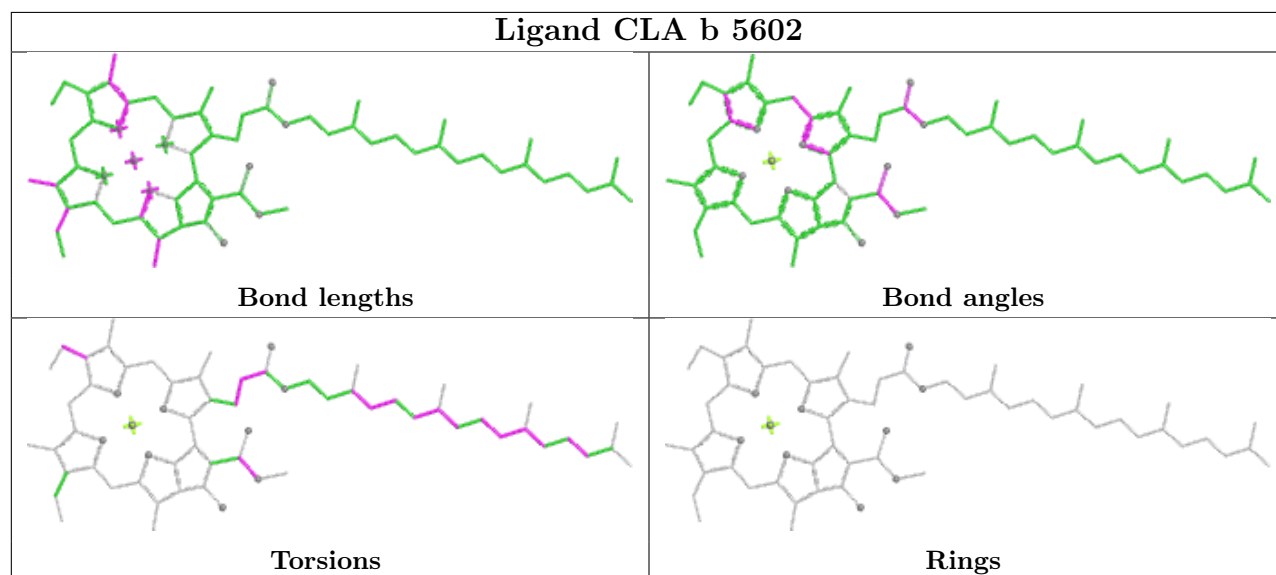
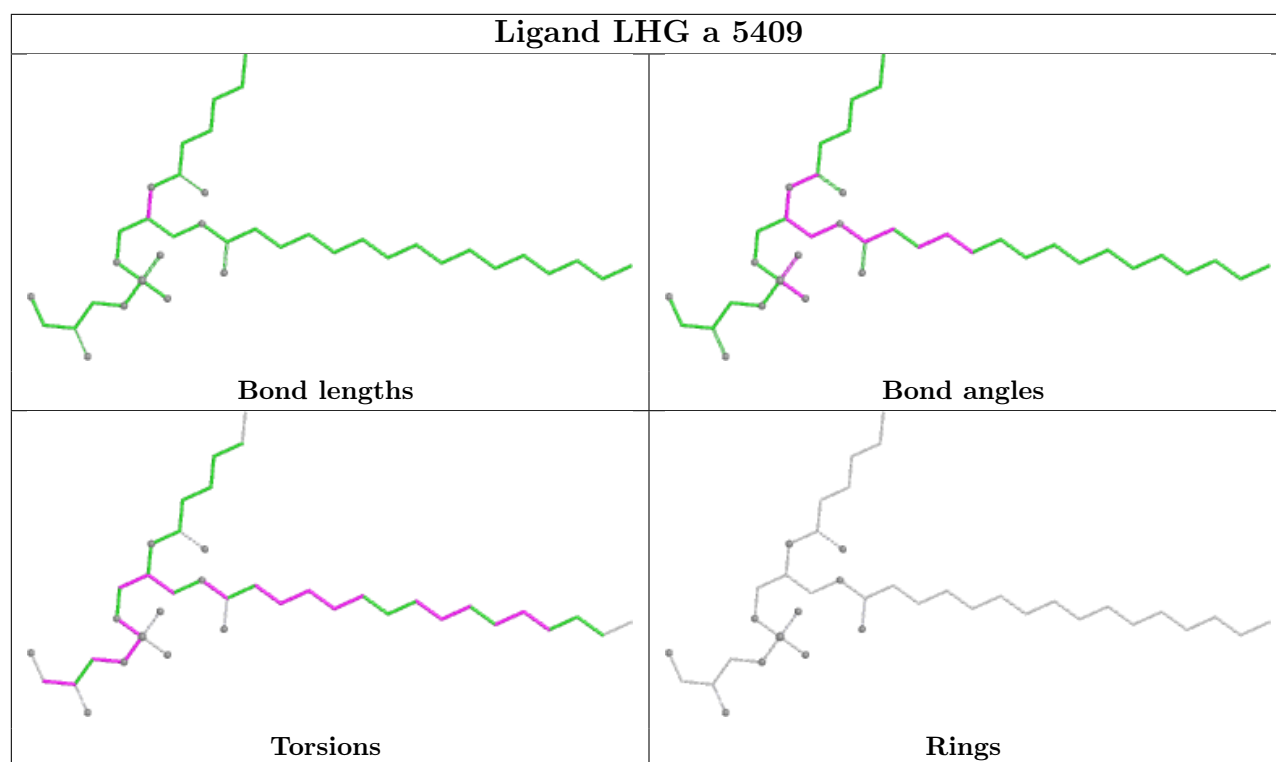


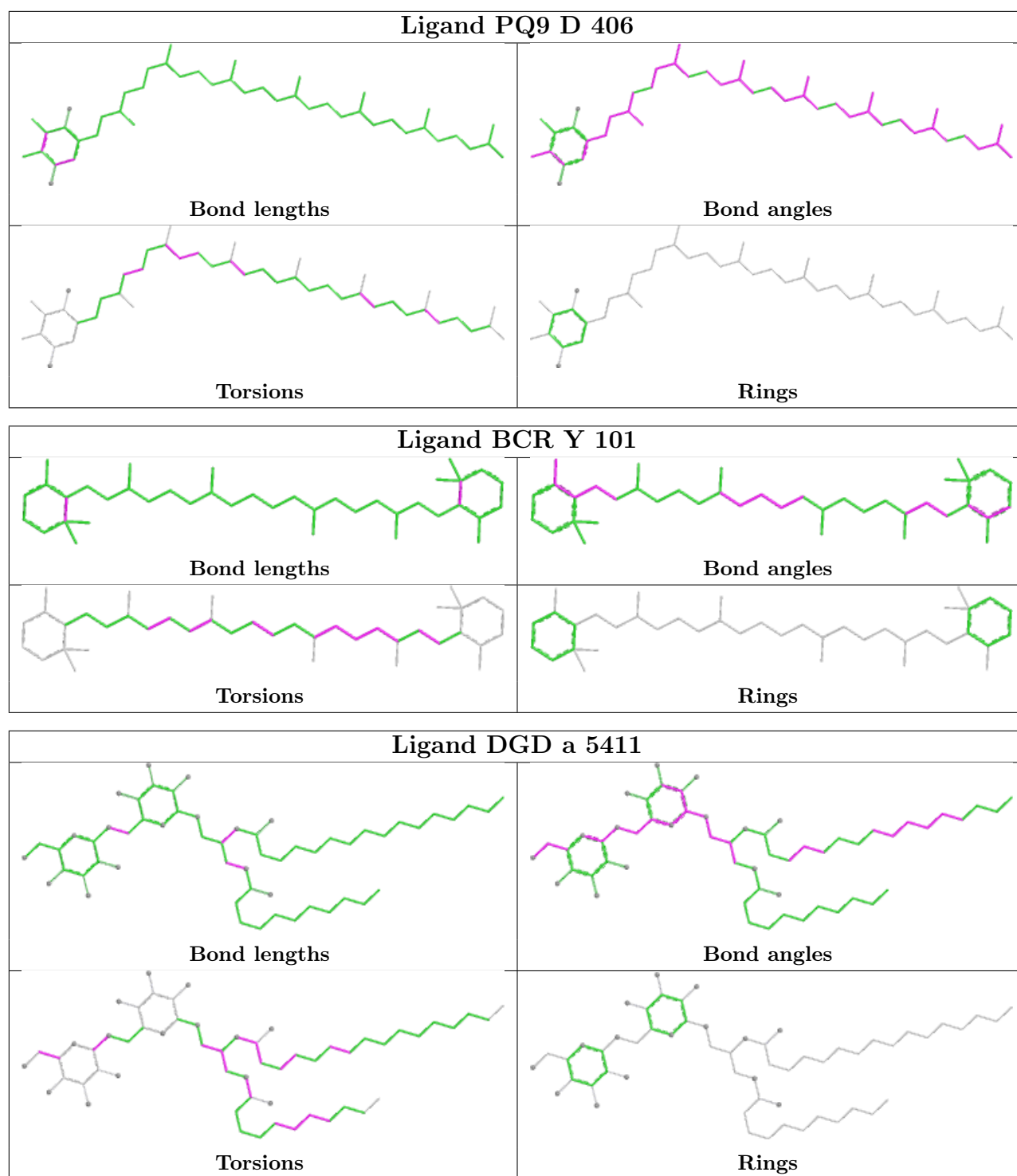


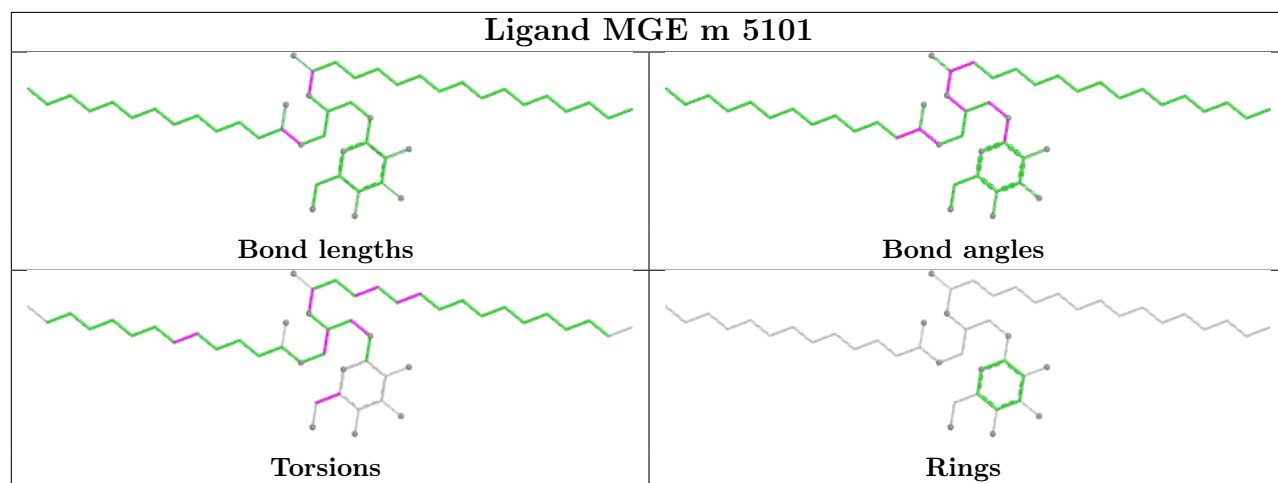
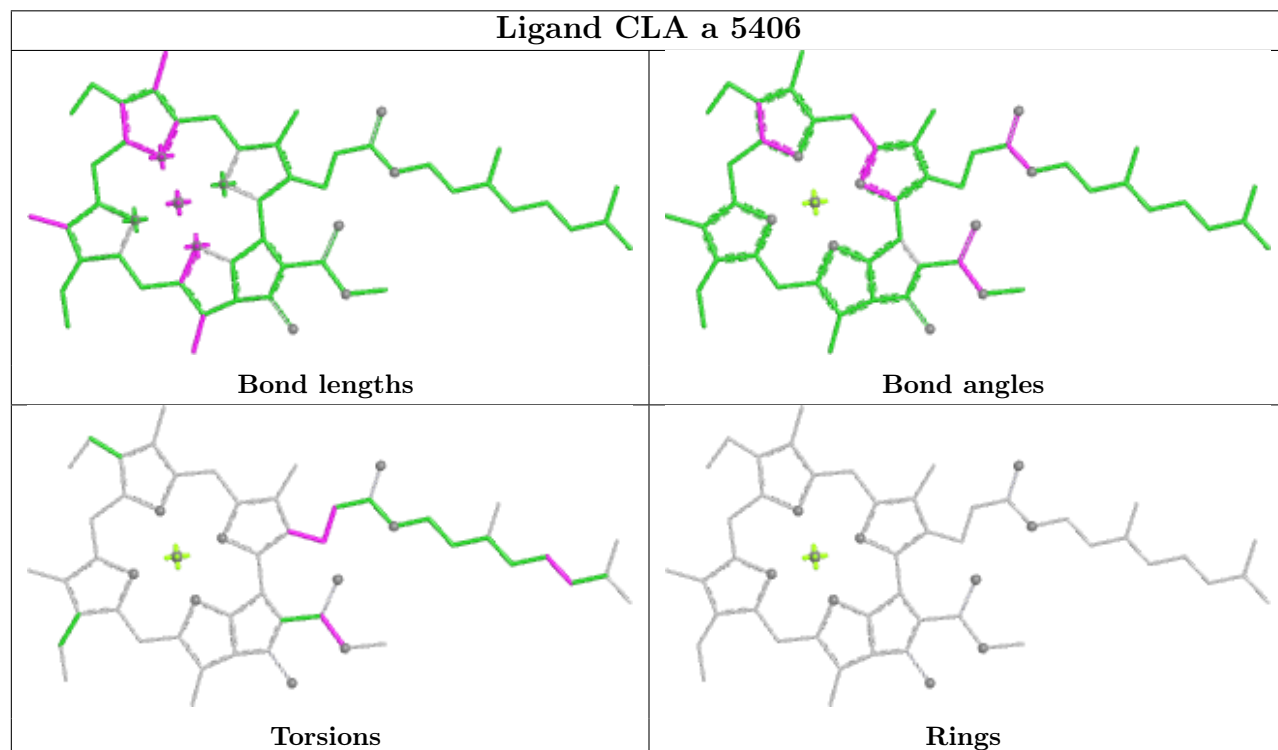
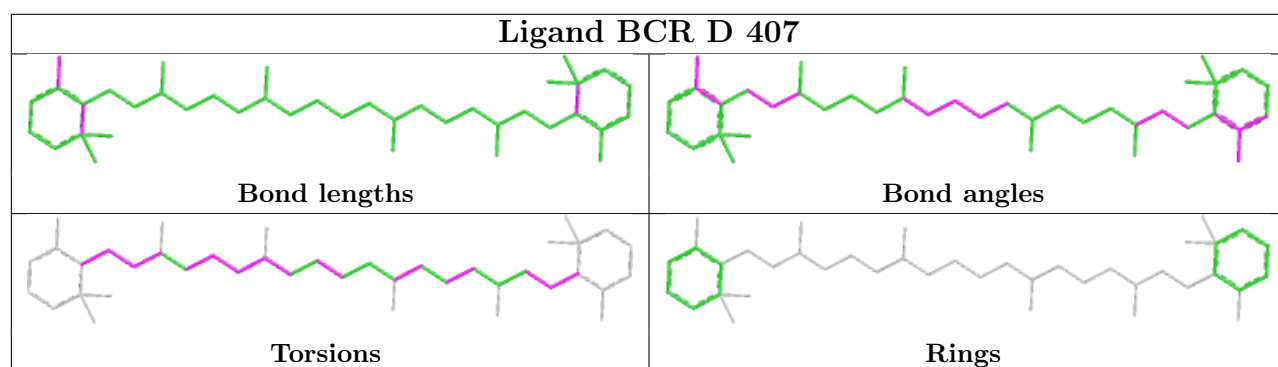


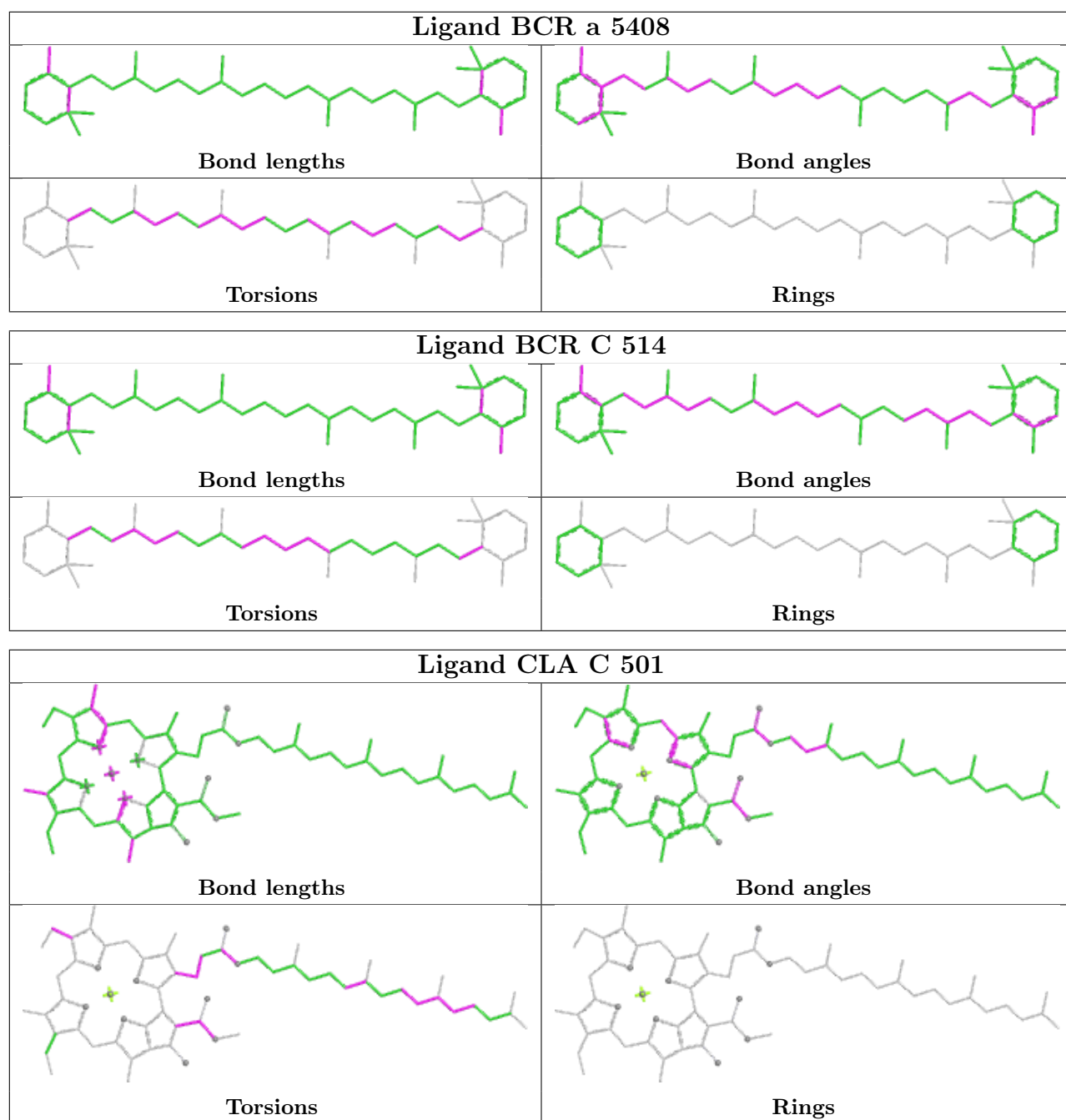


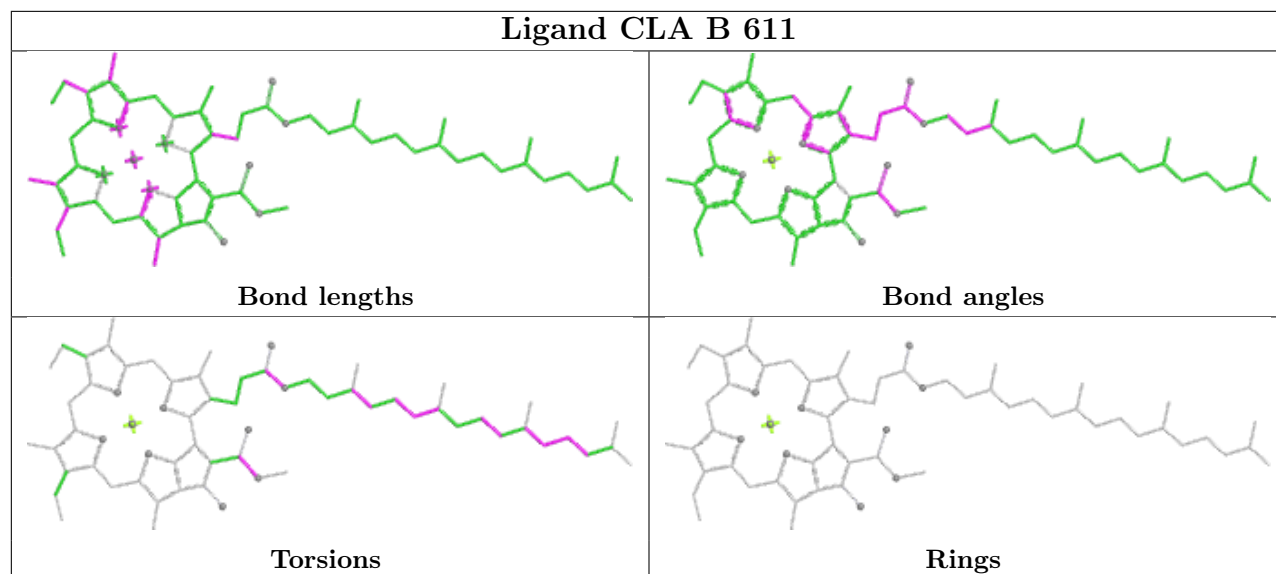
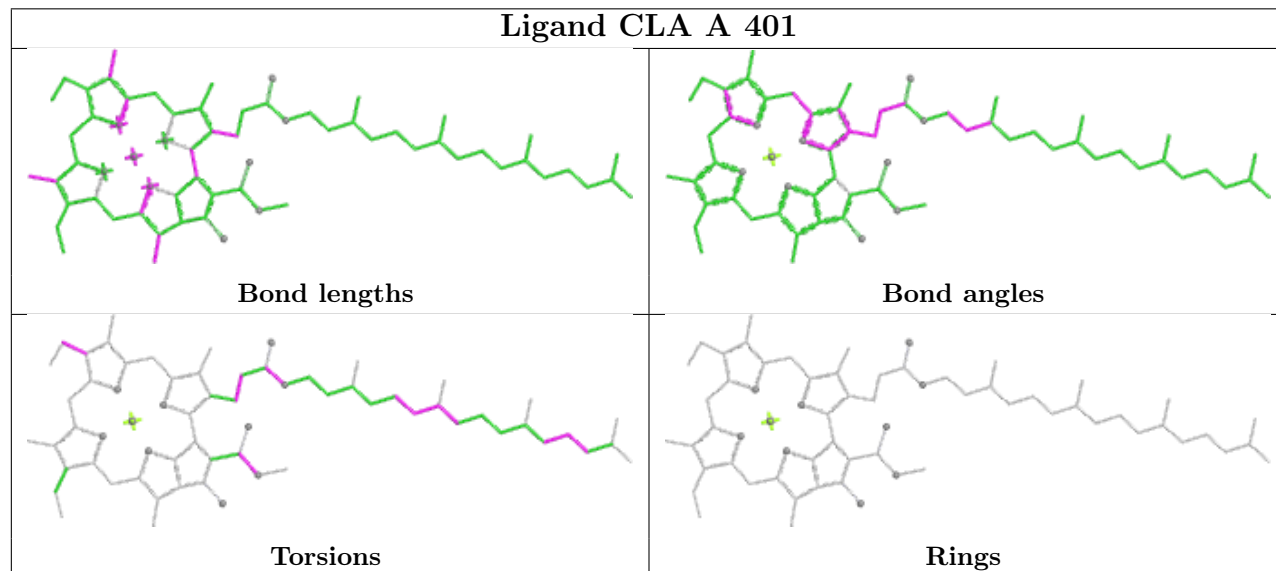


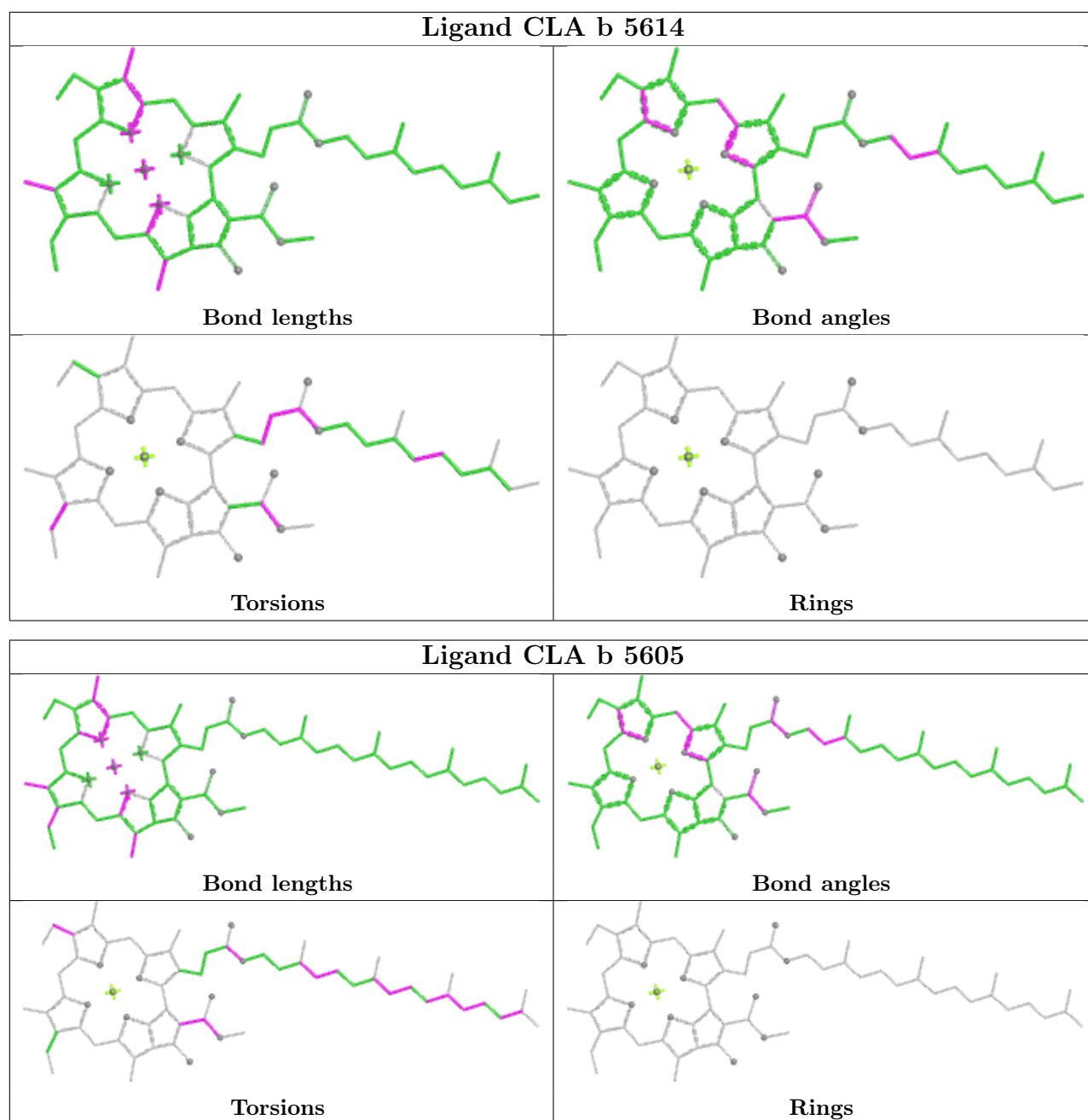


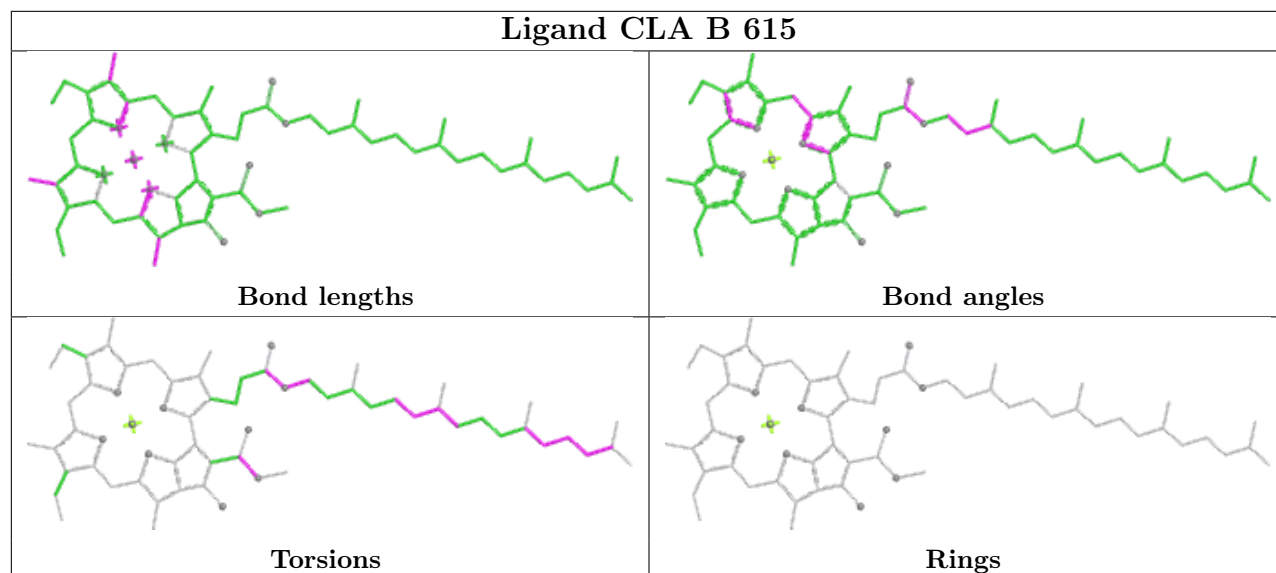
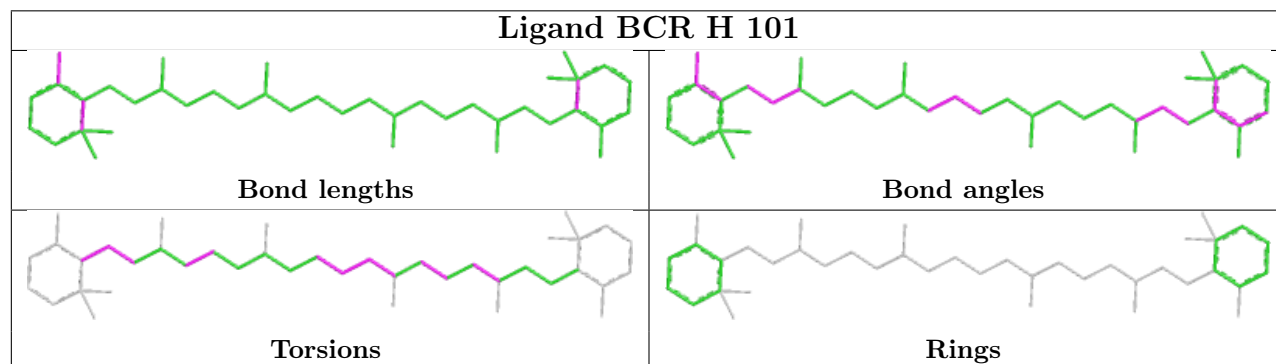
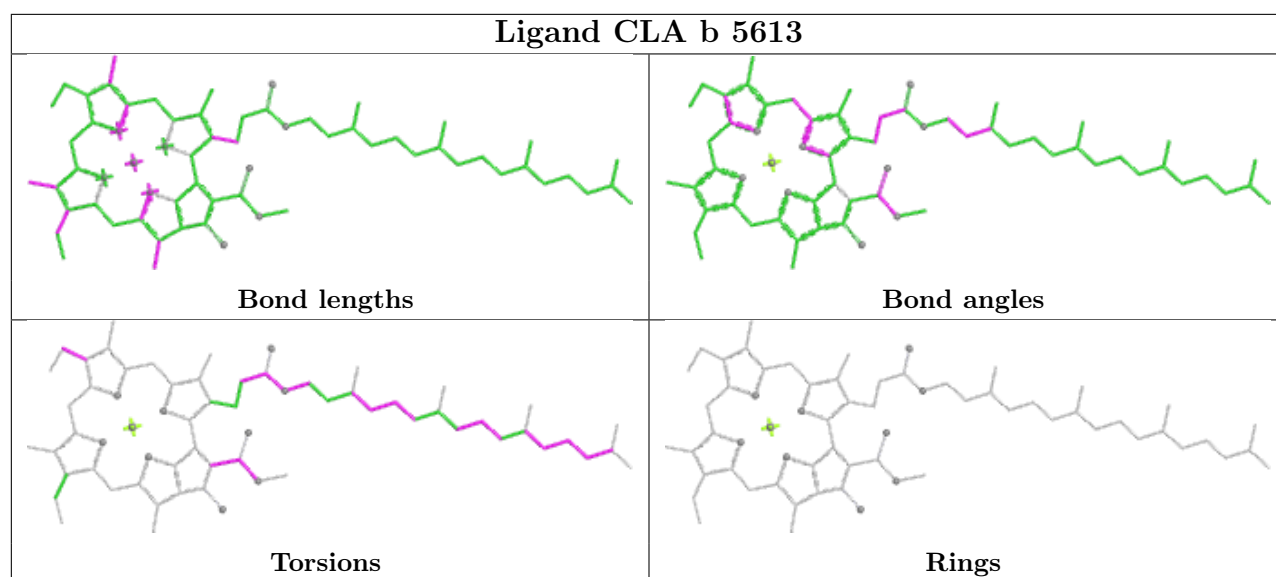


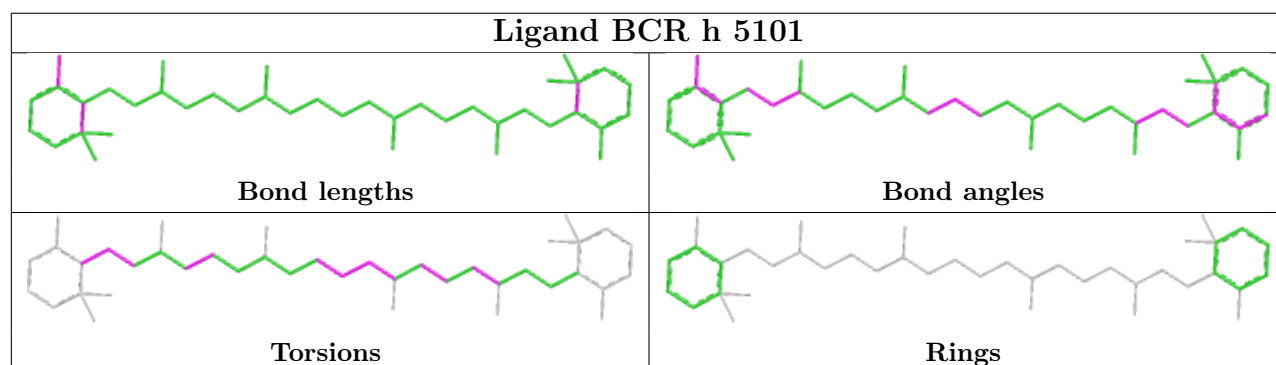
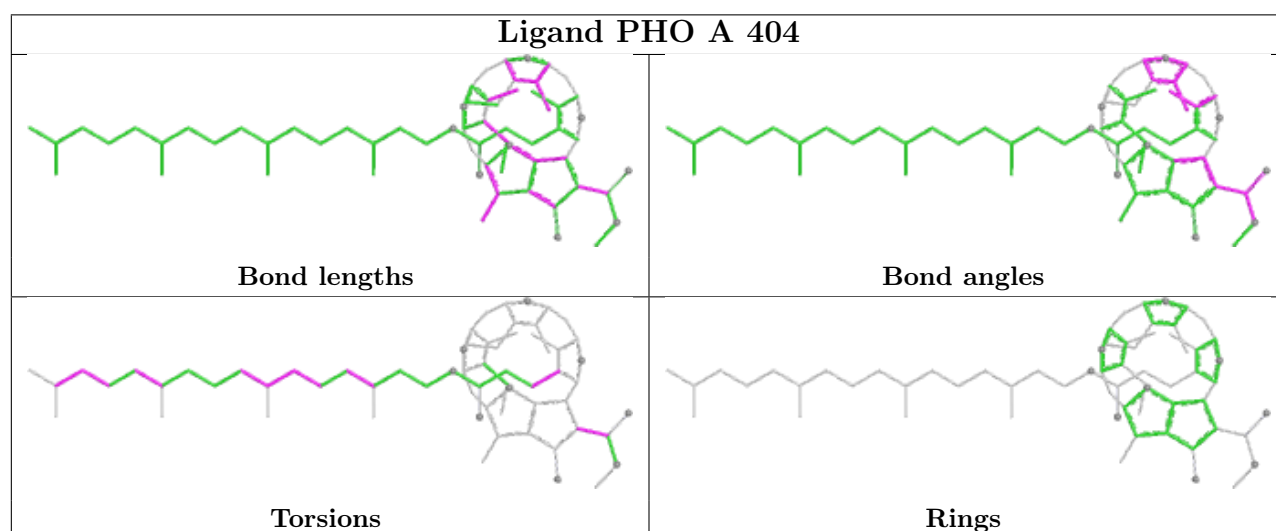
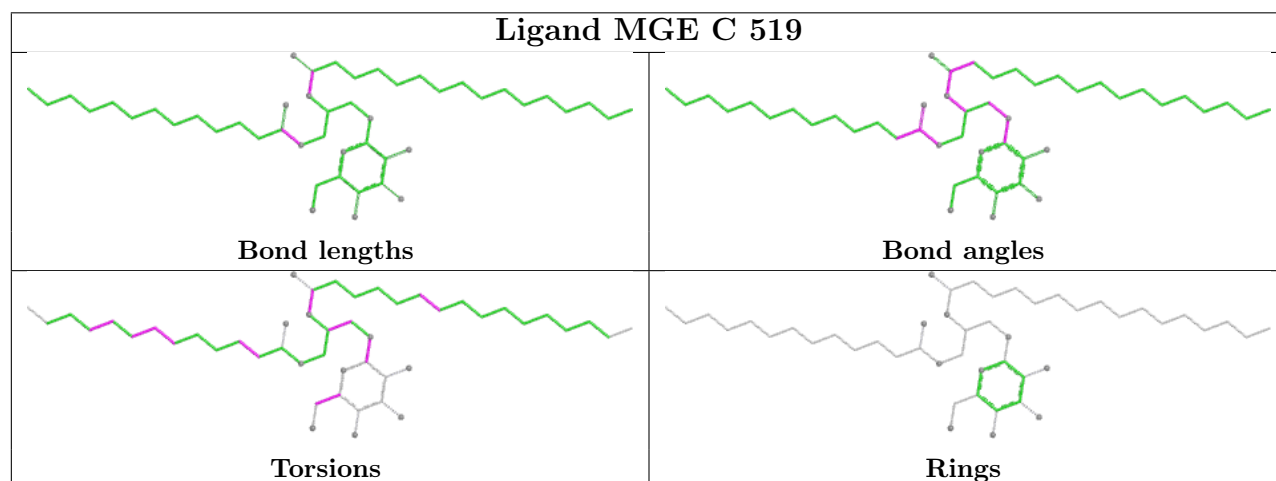
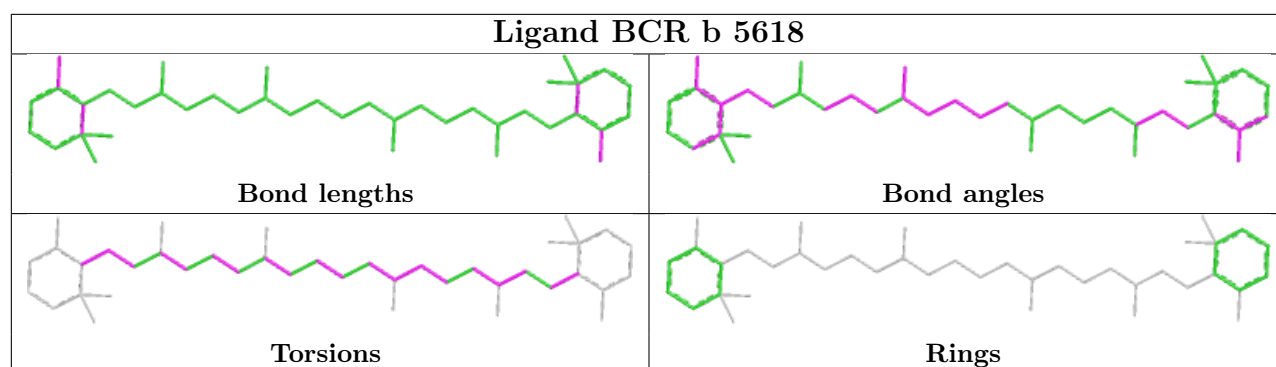


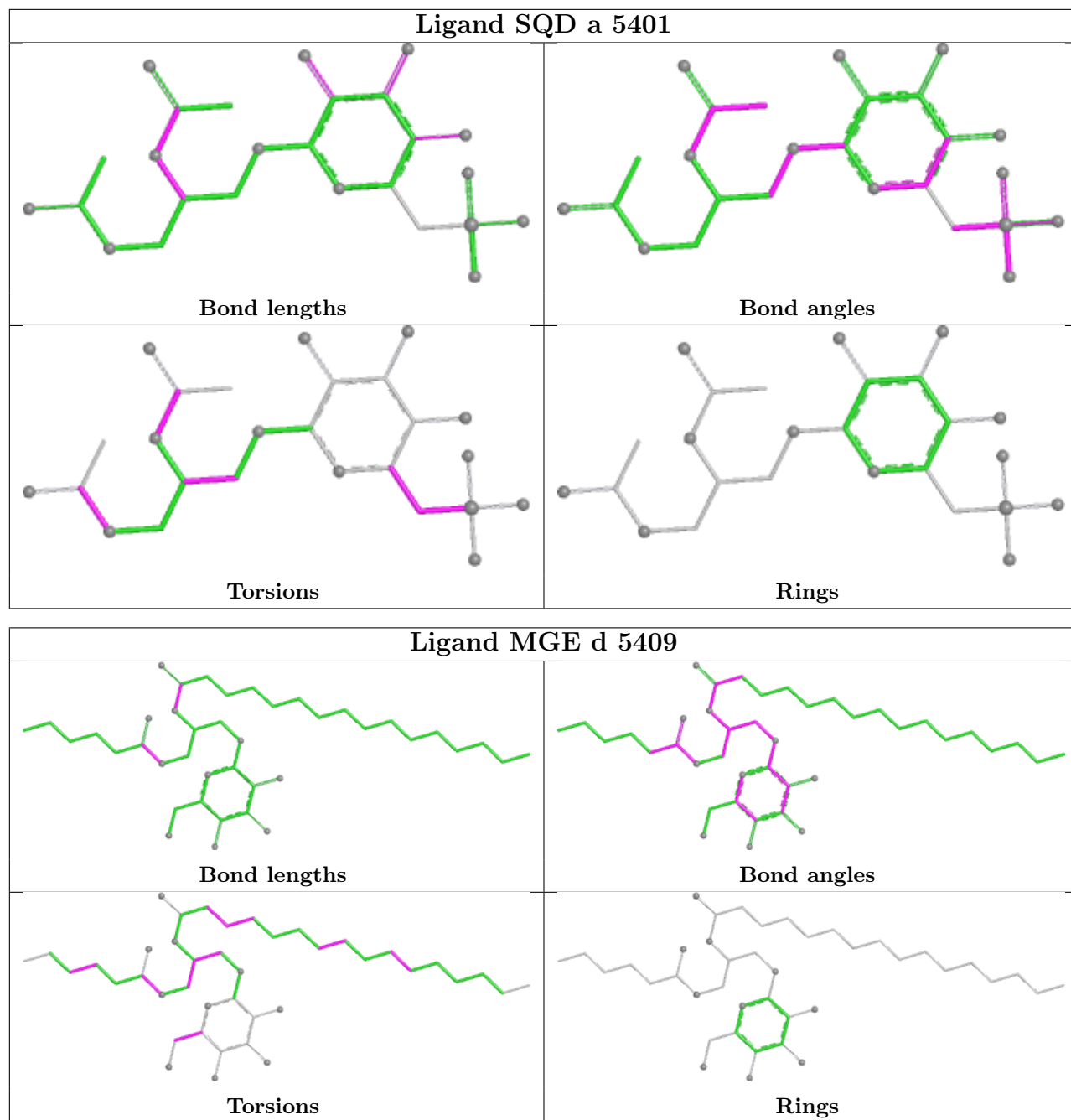


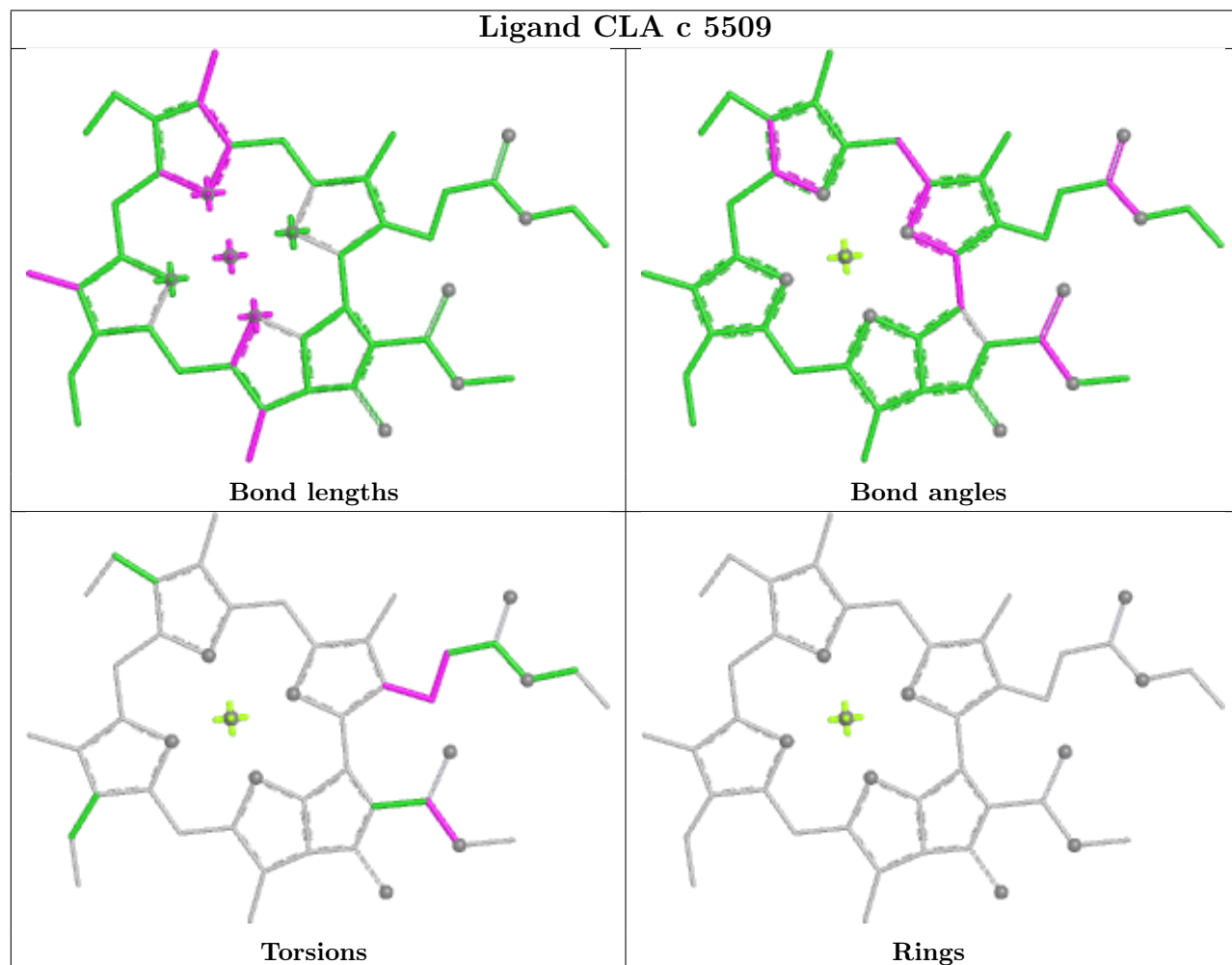
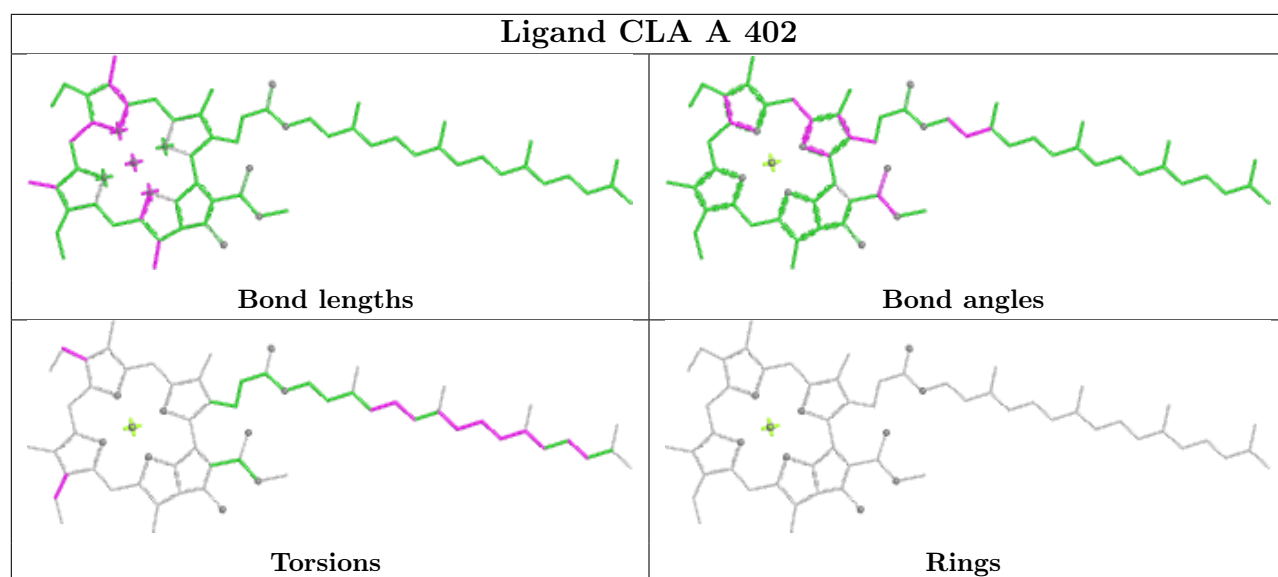
Ligand CLA B 611**Ligand CLA A 401**



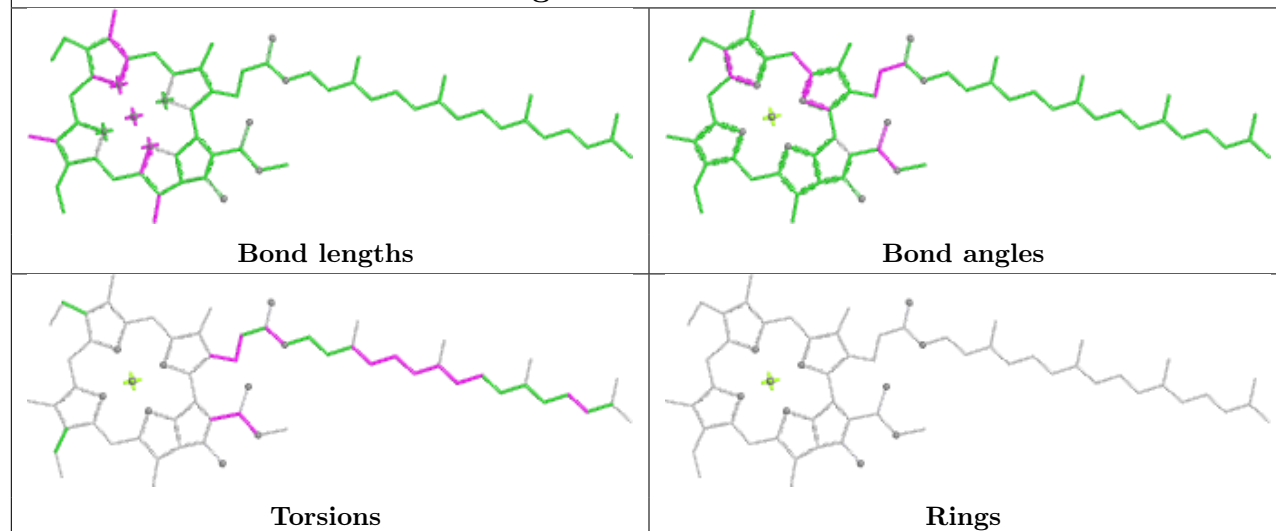




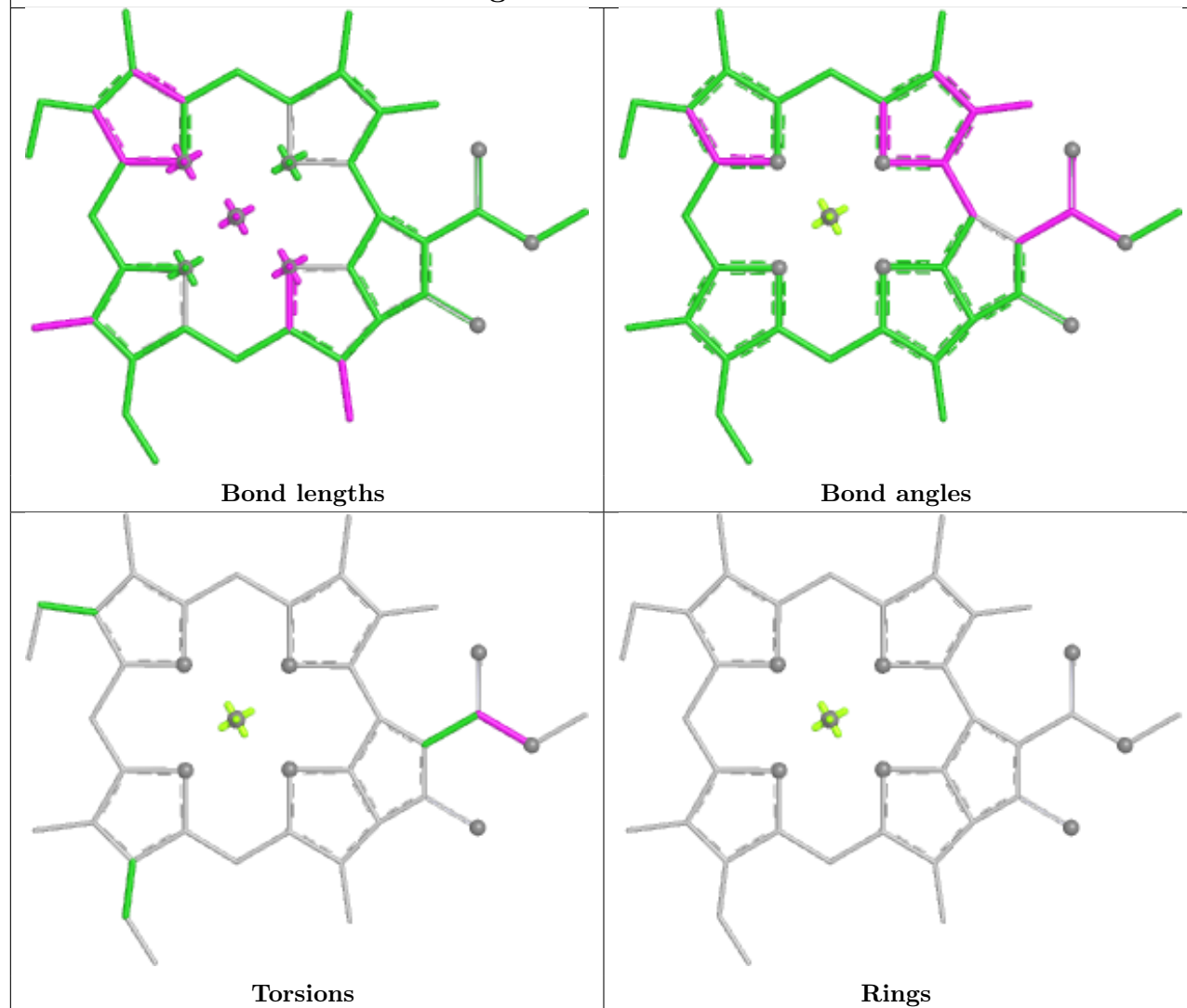


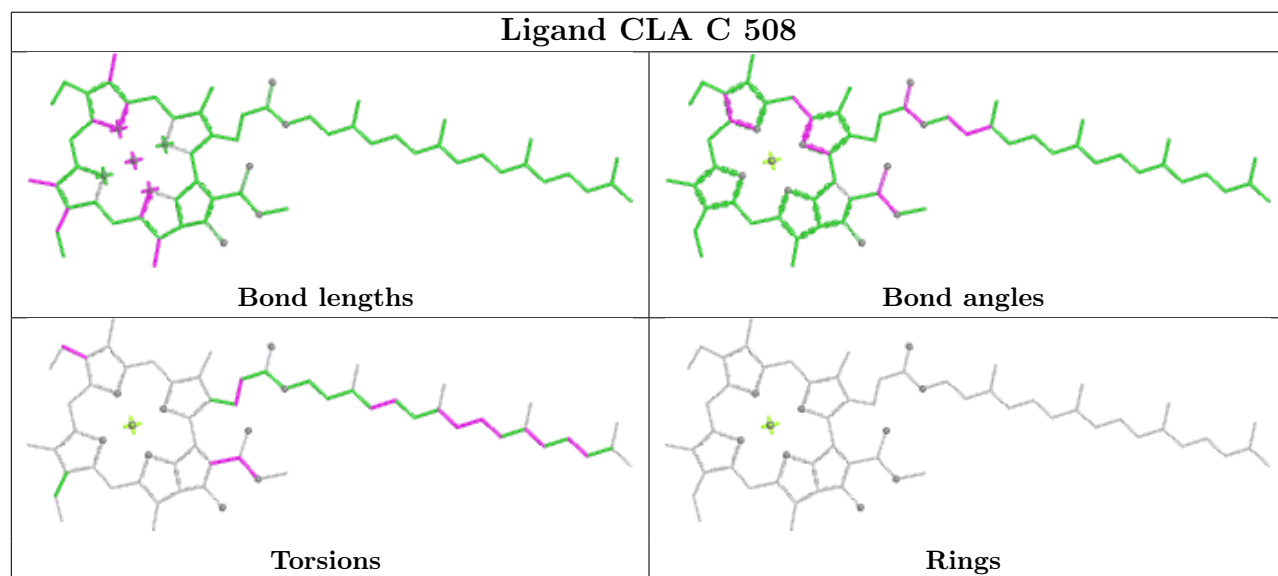
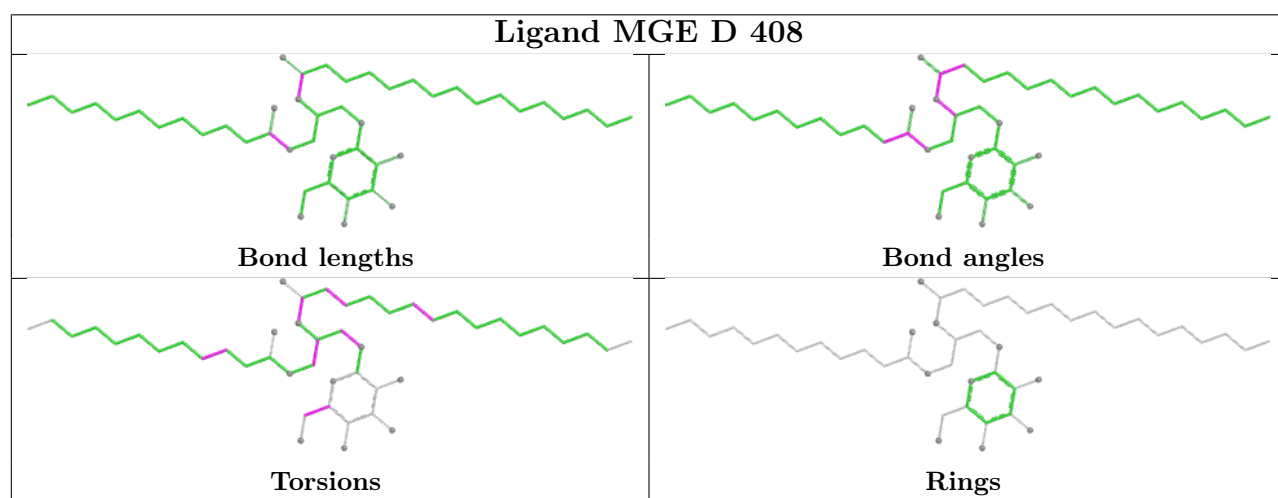
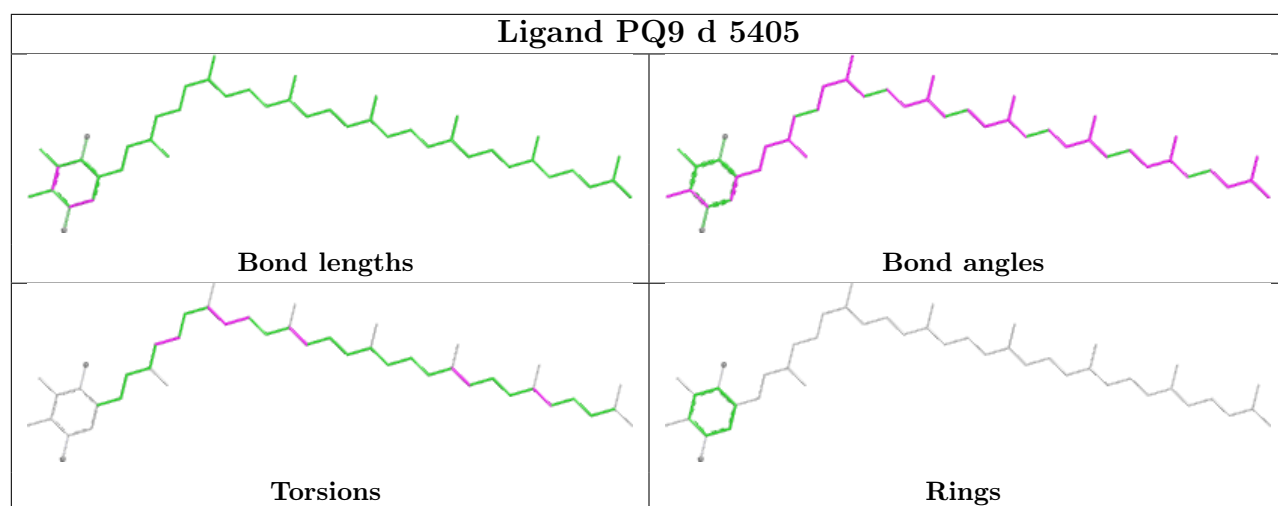


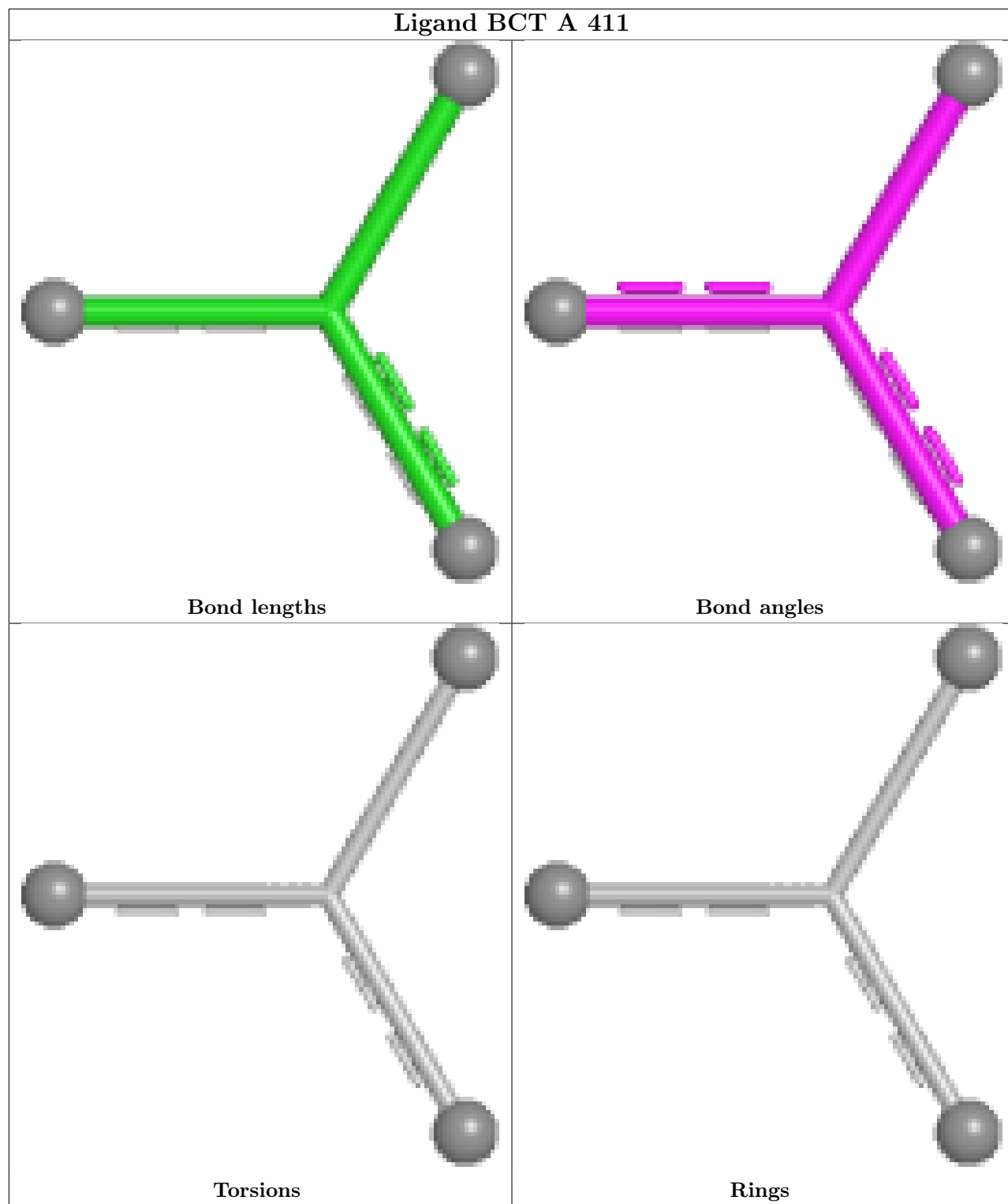
Ligand CLA B 607

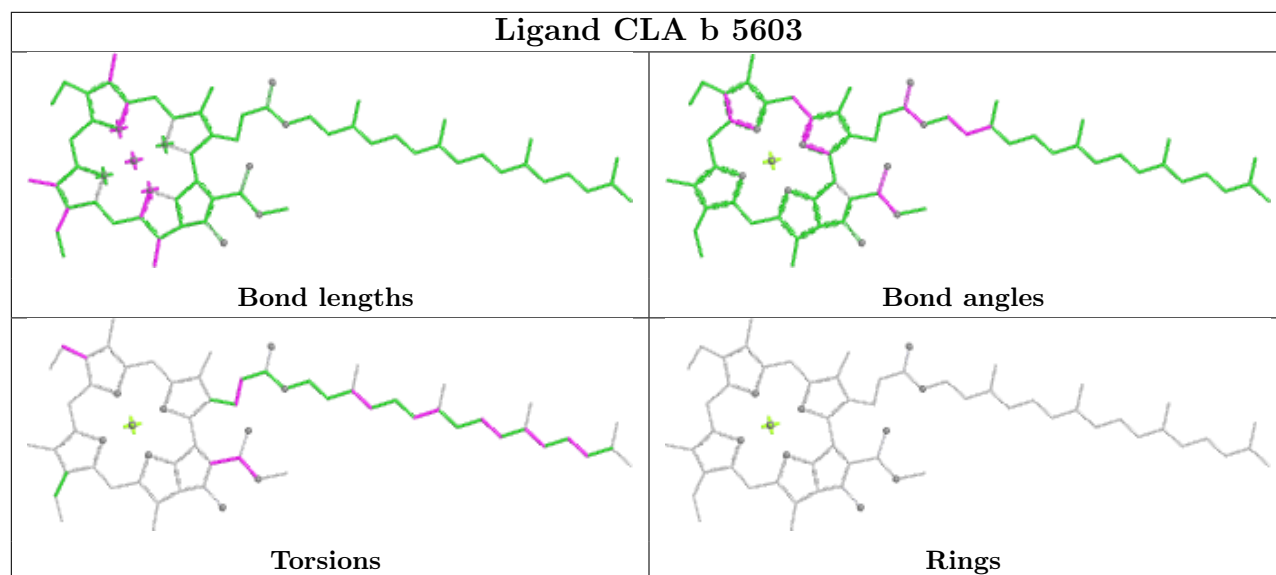
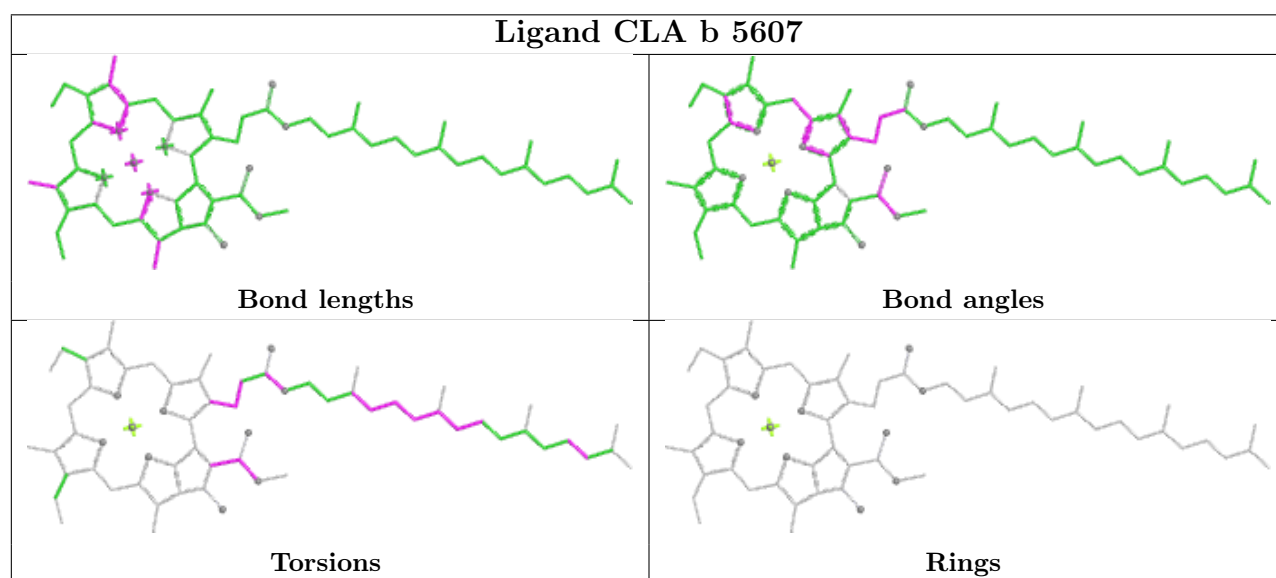
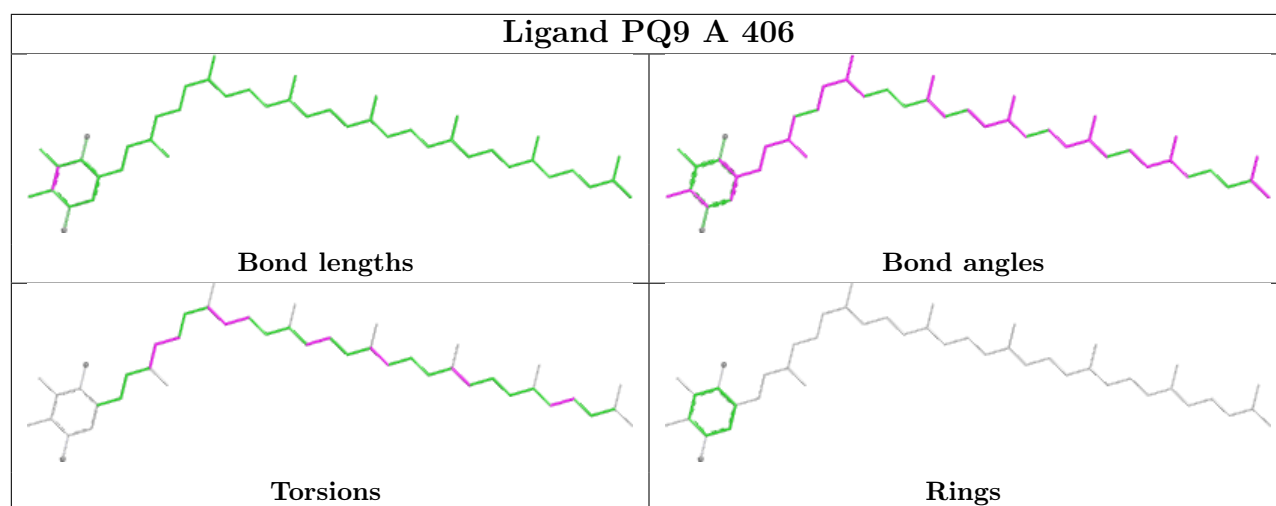


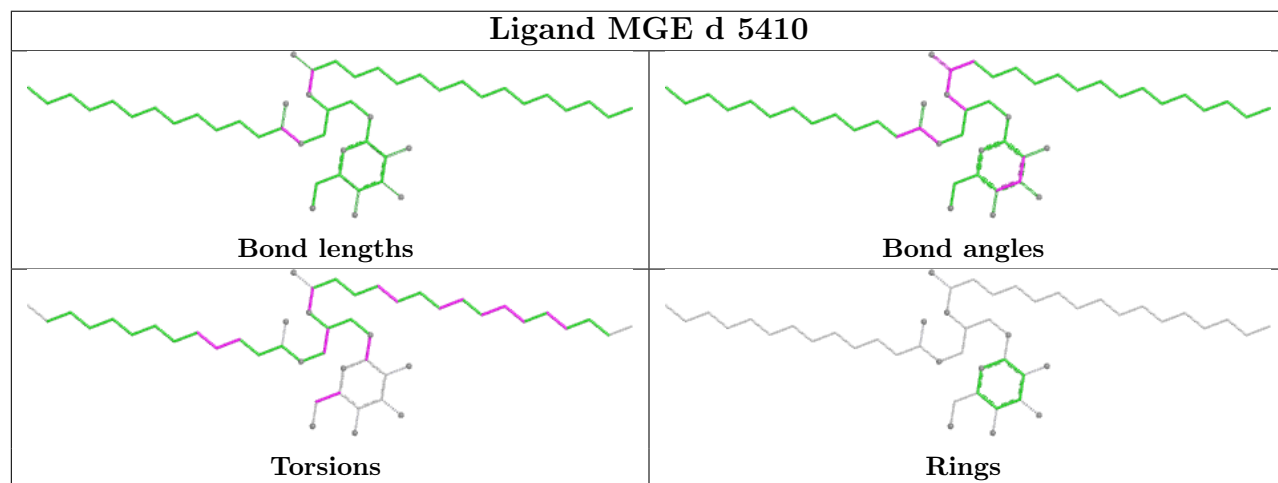
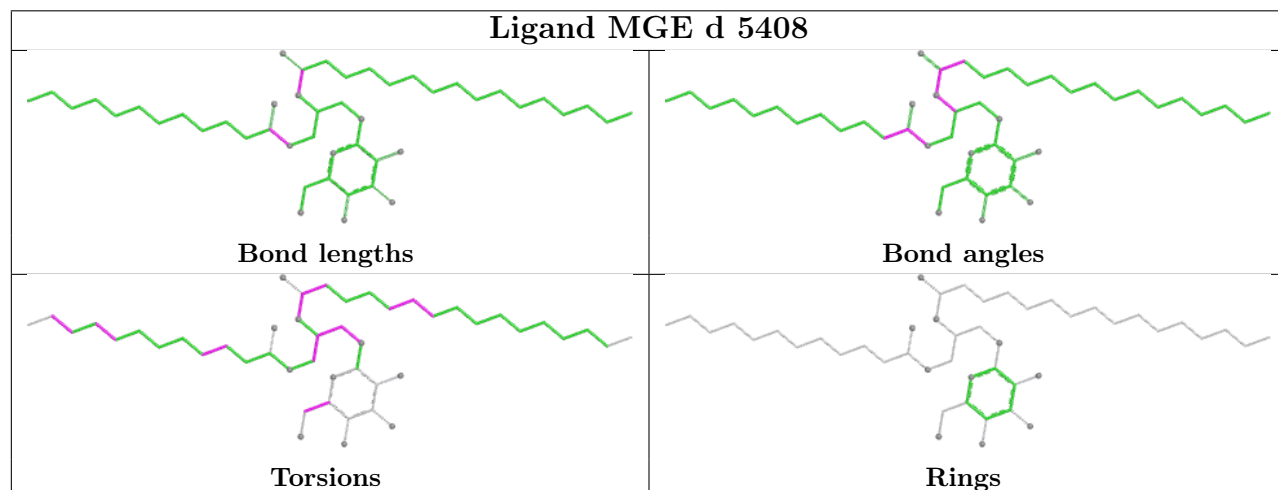
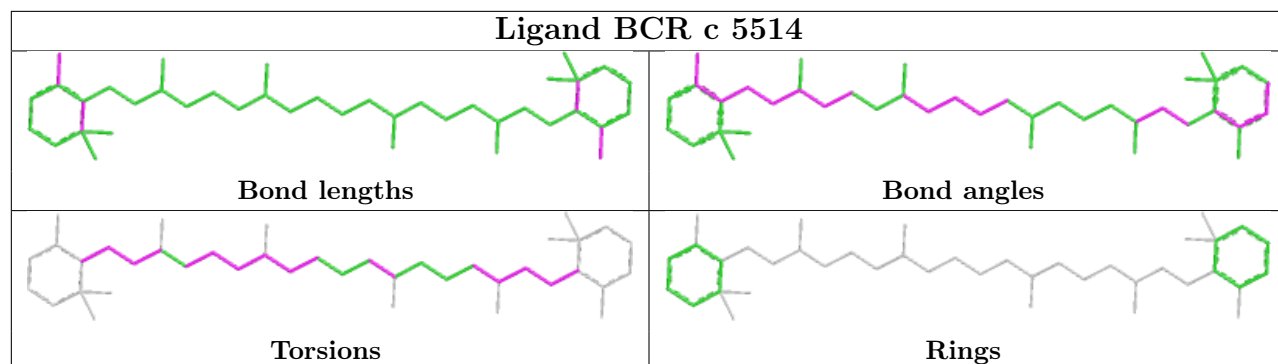
Ligand CLA b 5601

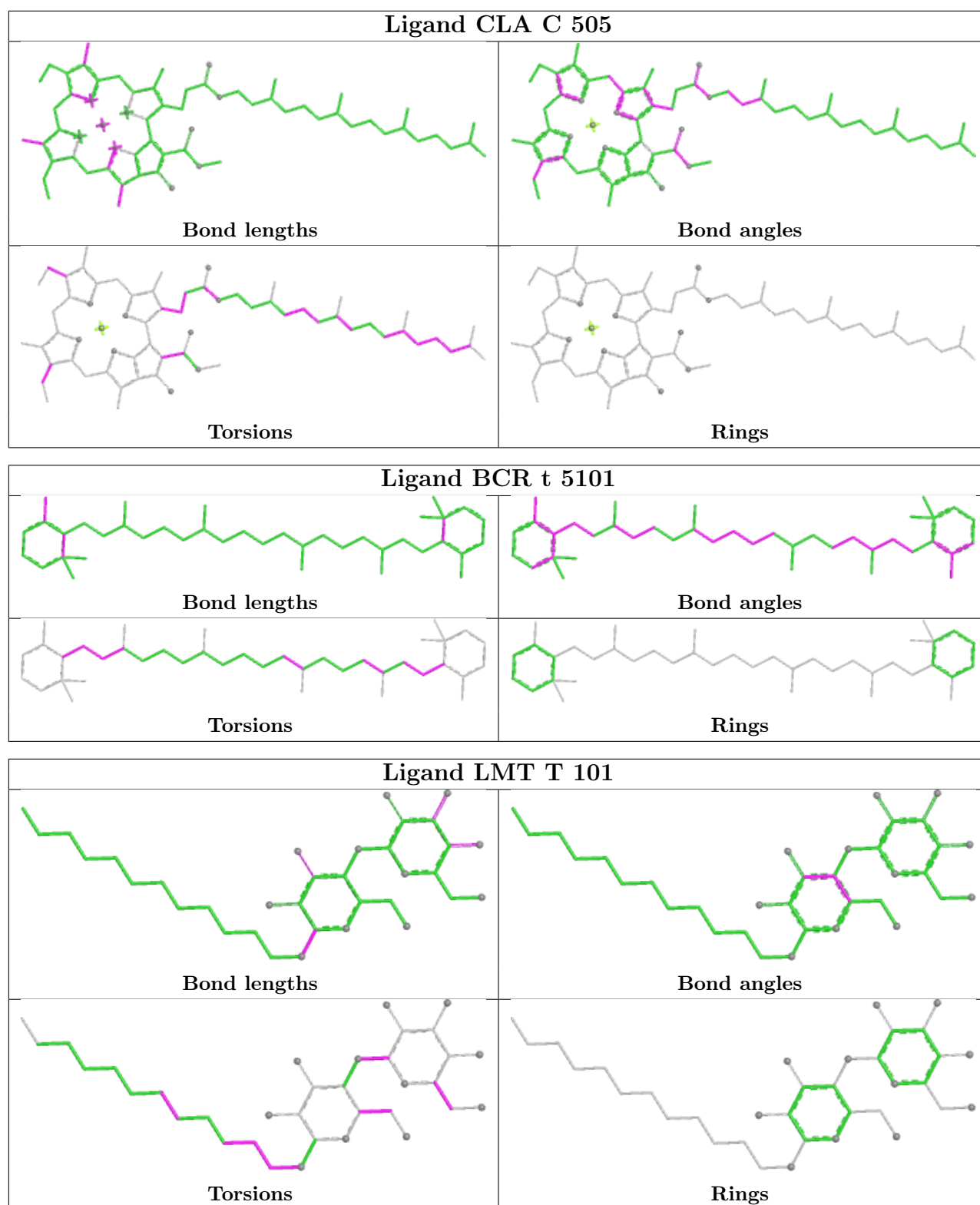


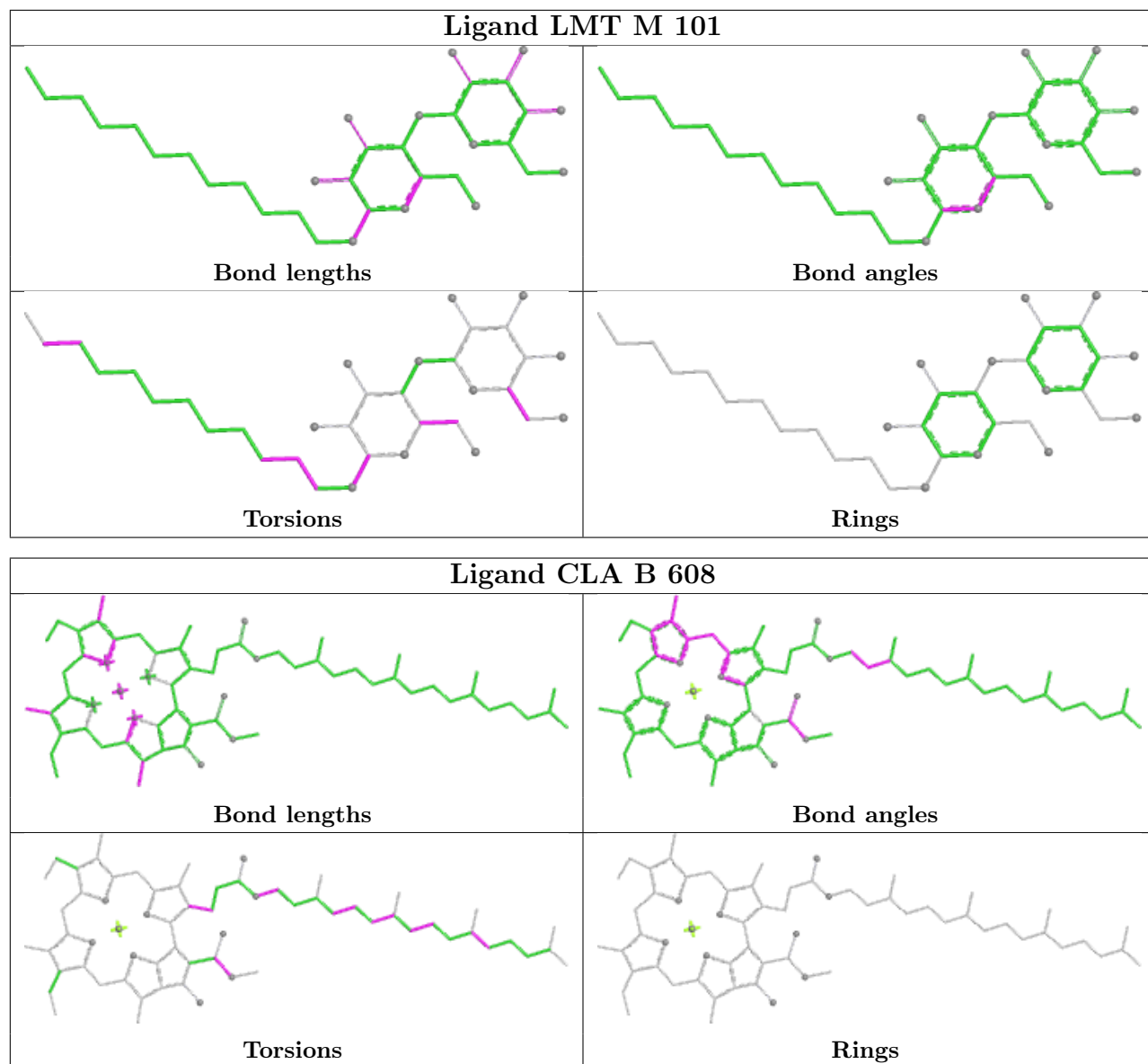




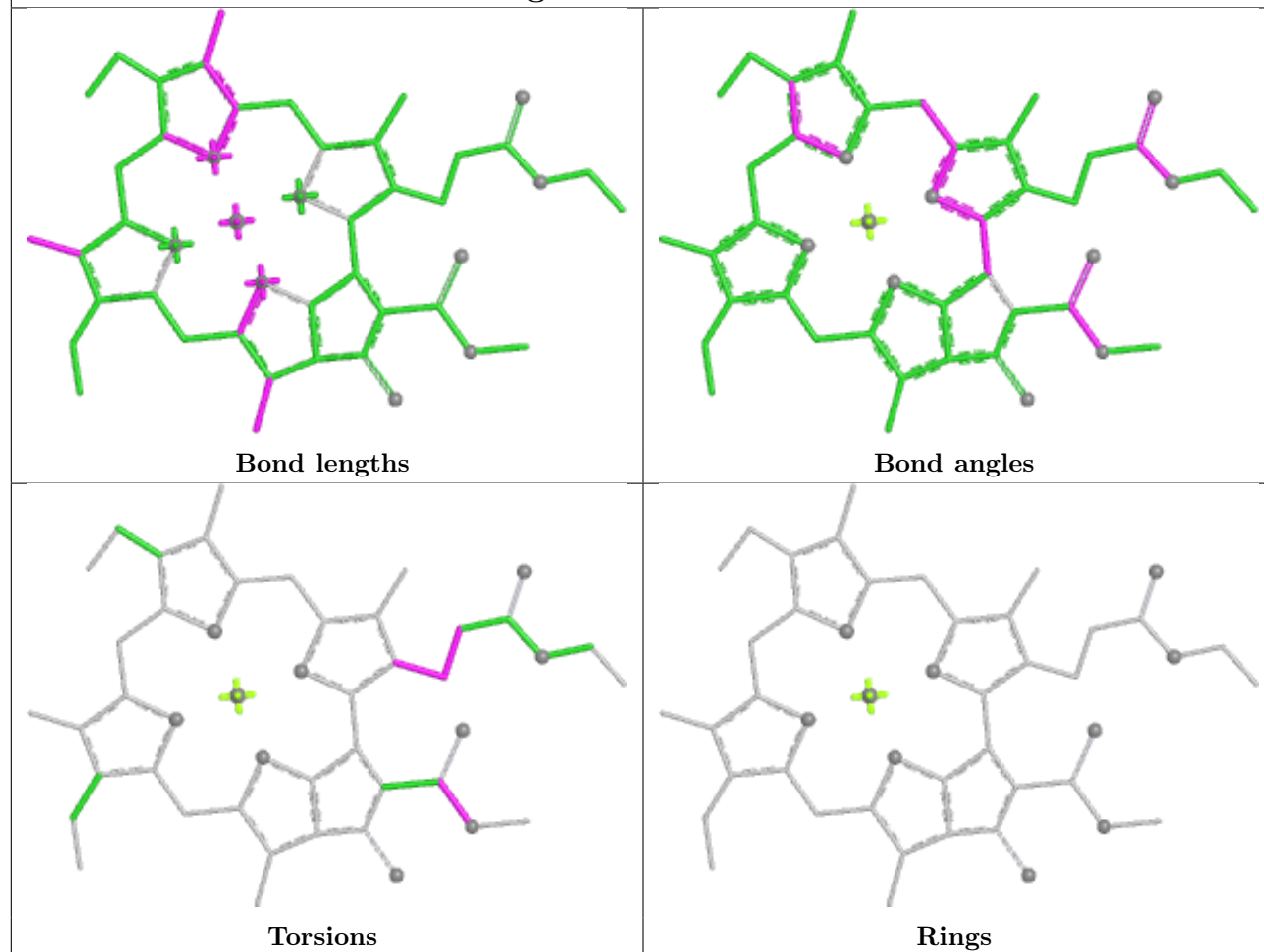




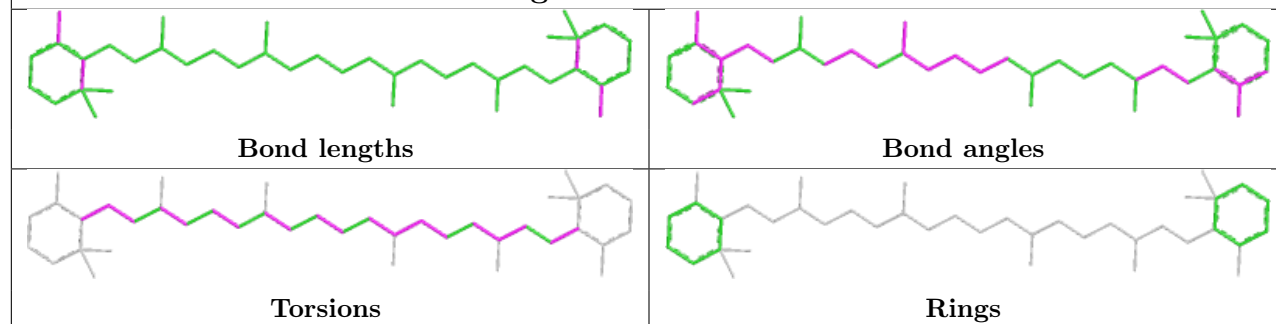




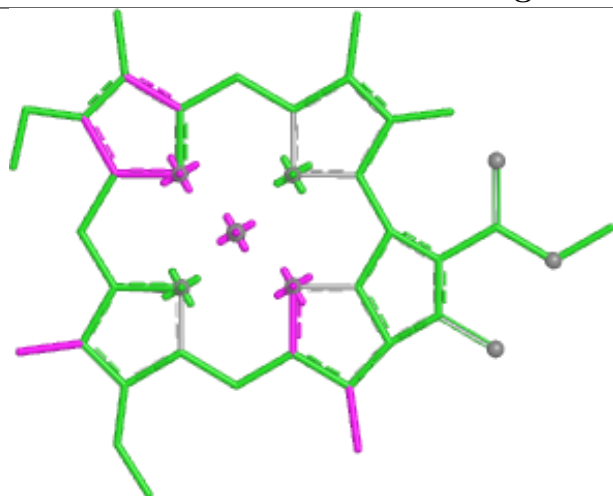
Ligand CLA C 509



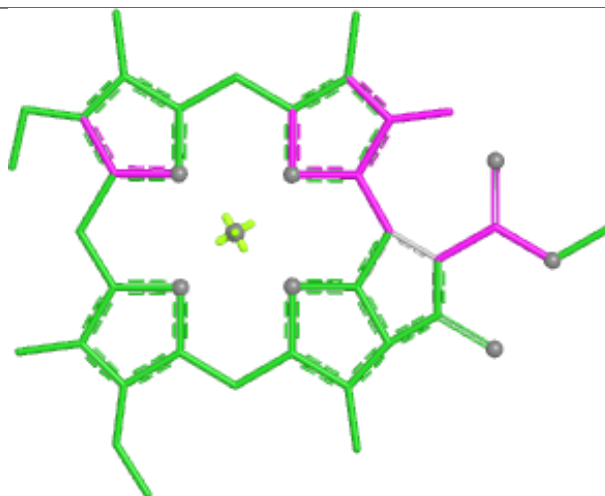
Ligand BCR B 618



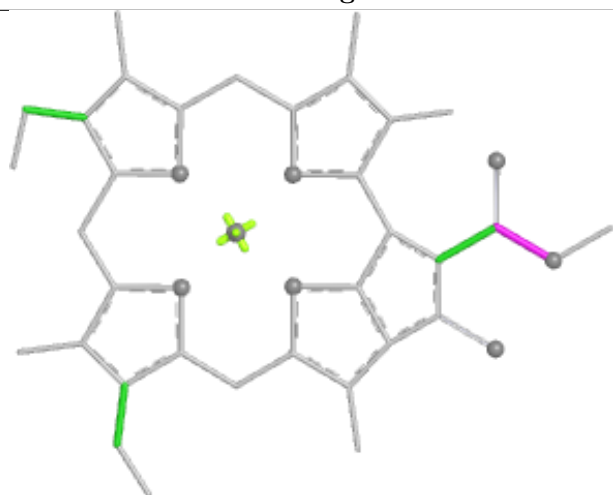
Ligand CLA B 601



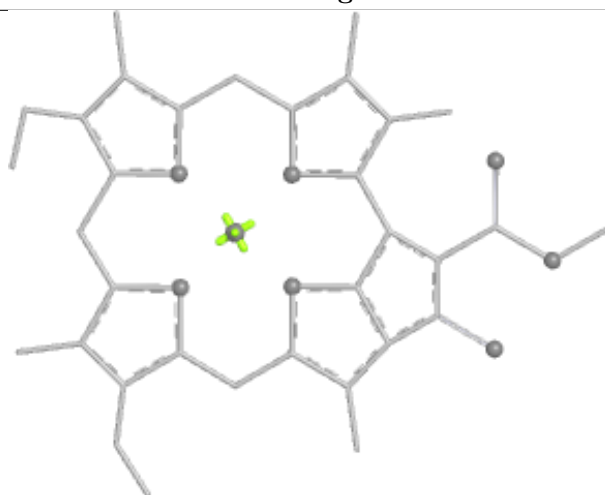
Bond lengths



Bond angles

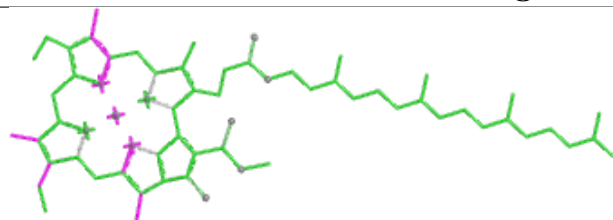


Torsions

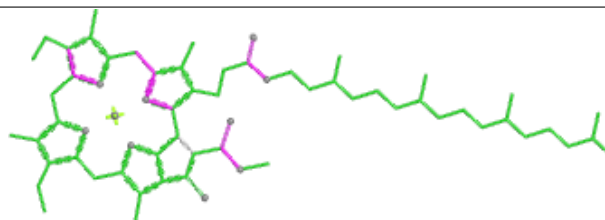


Rings

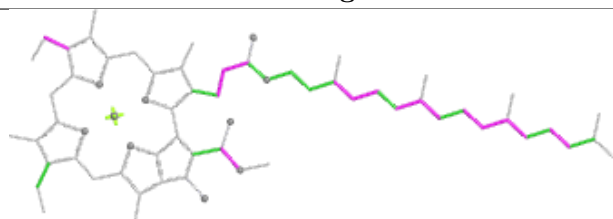
Ligand CLA B 602



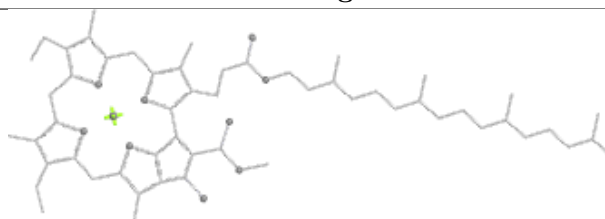
Bond lengths



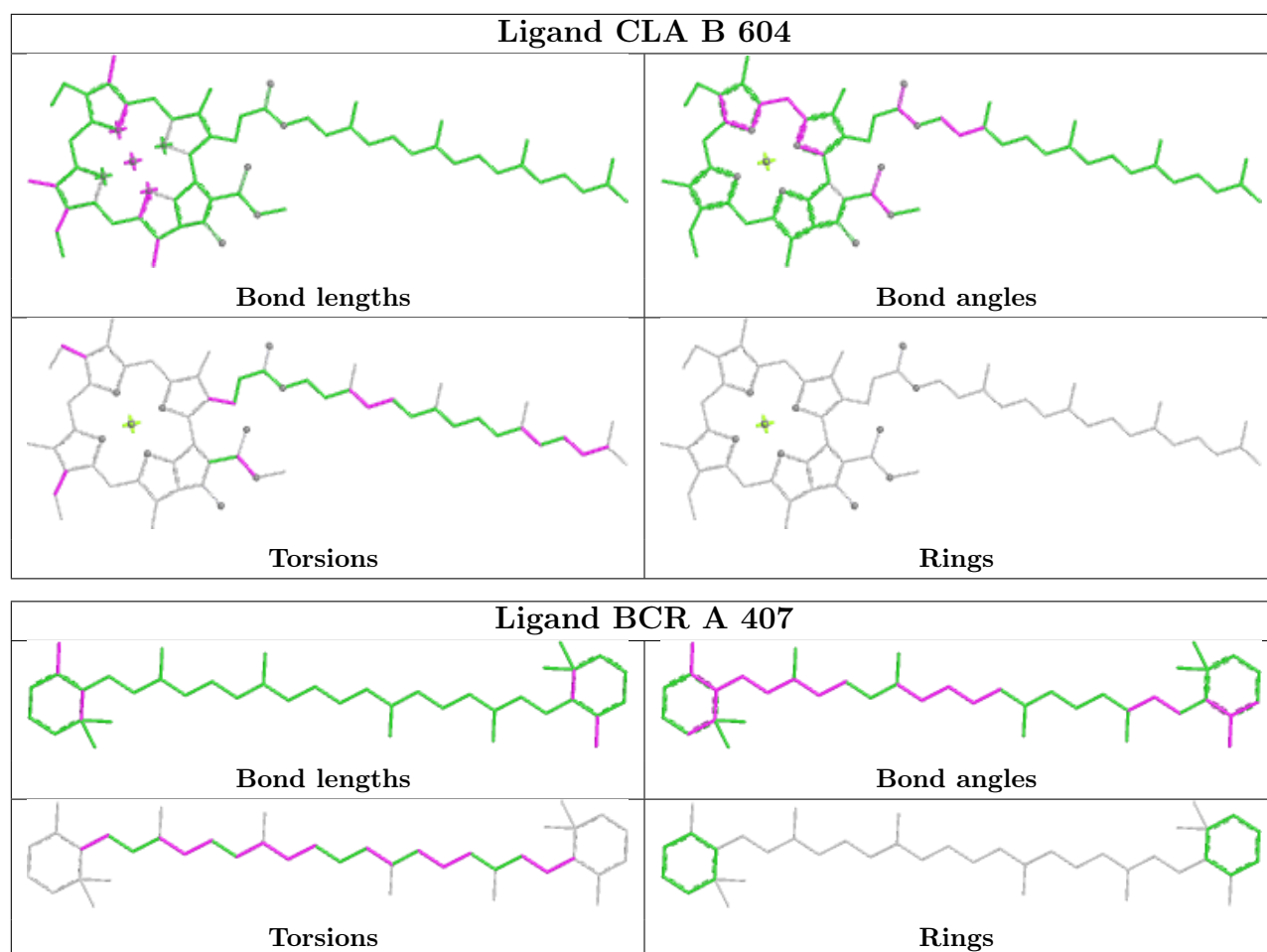
Bond angles



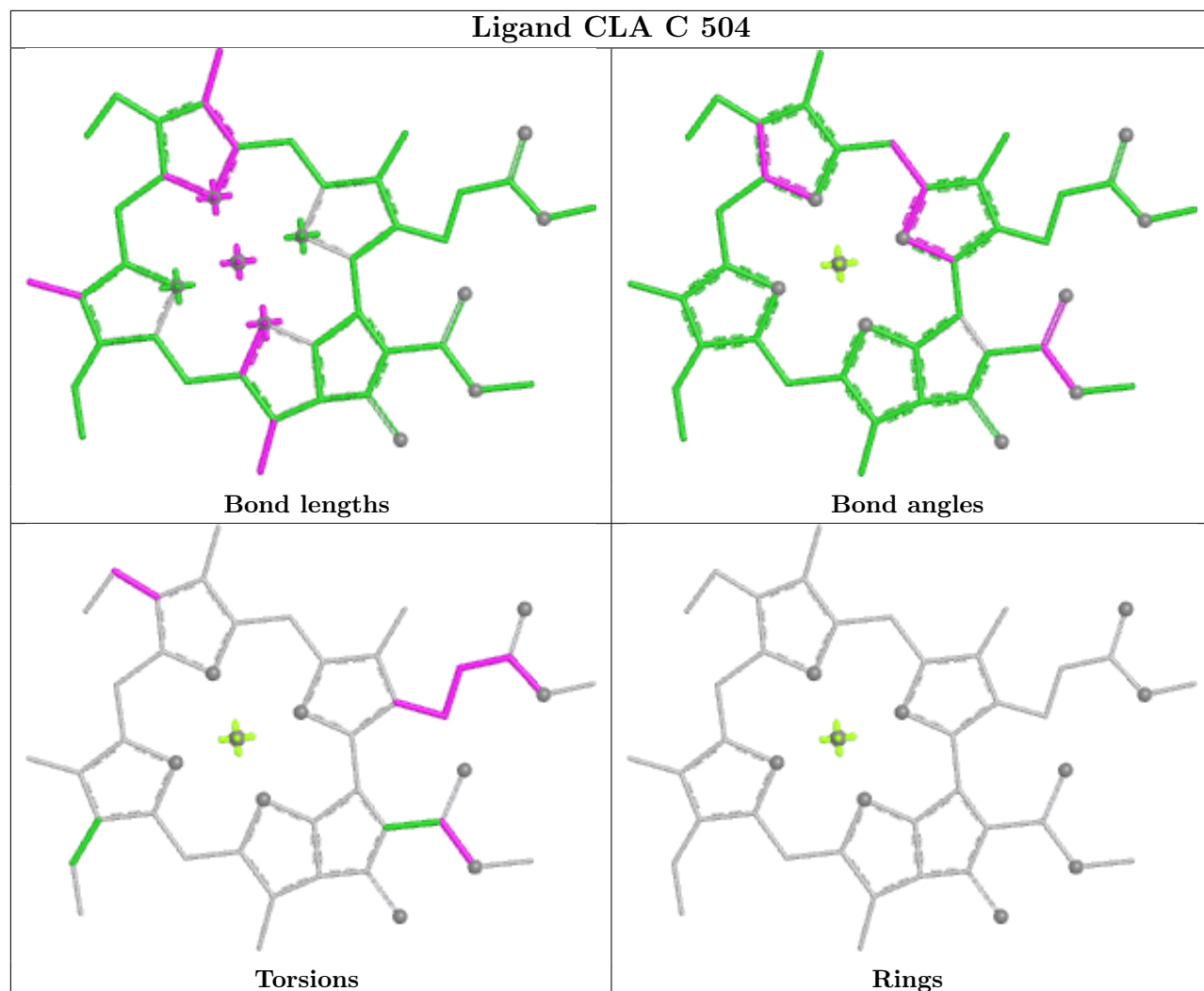
Torsions



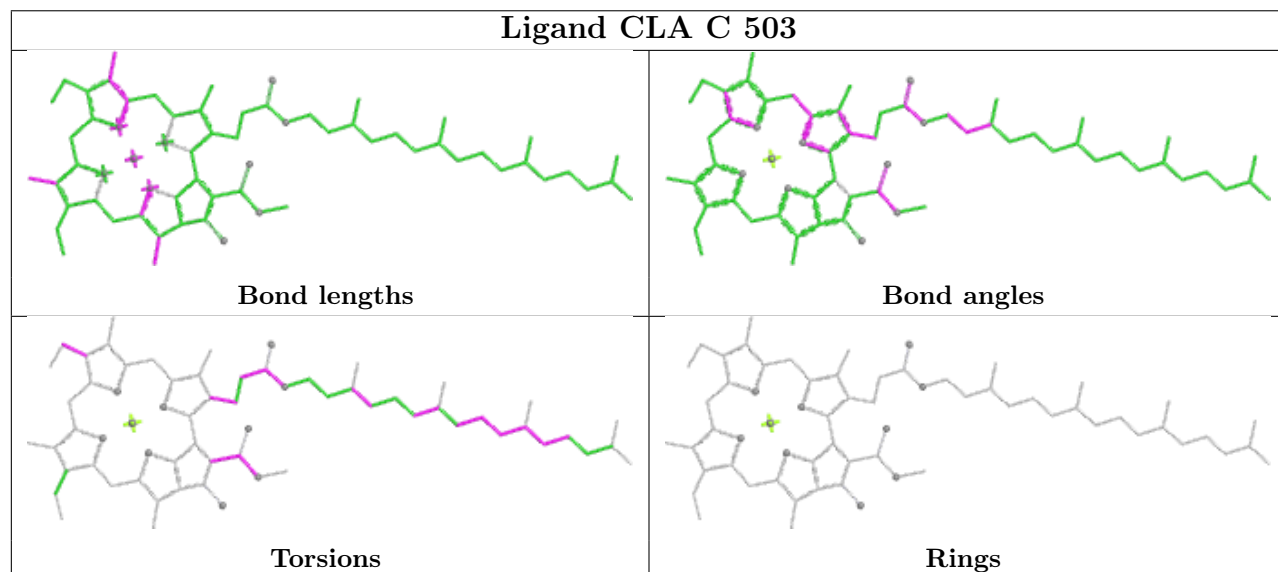
Rings

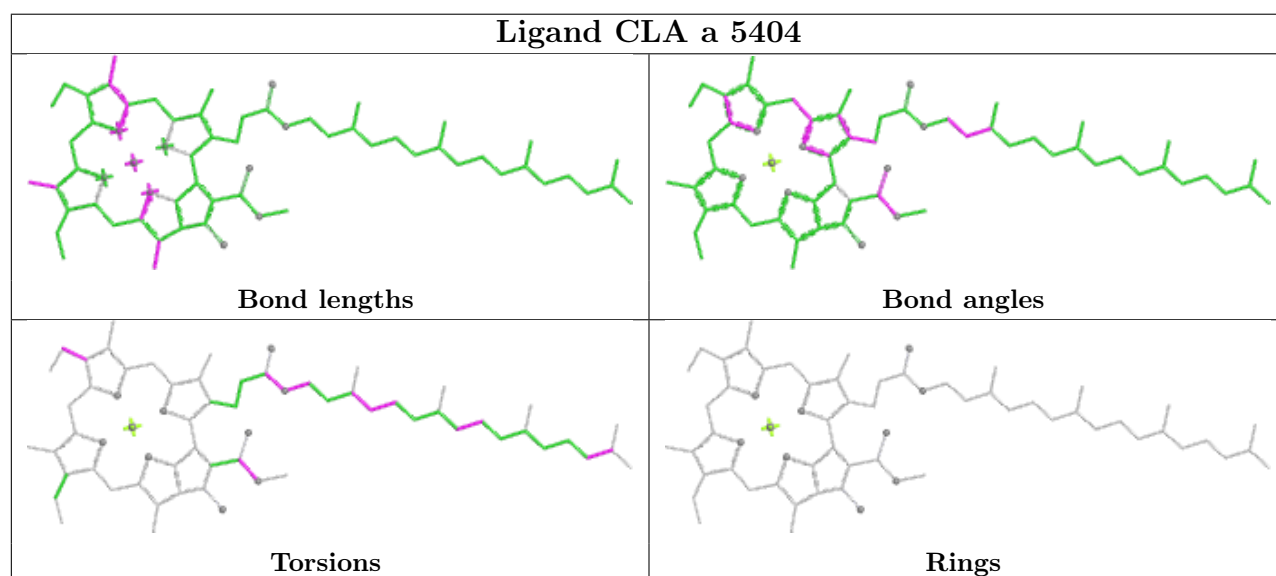
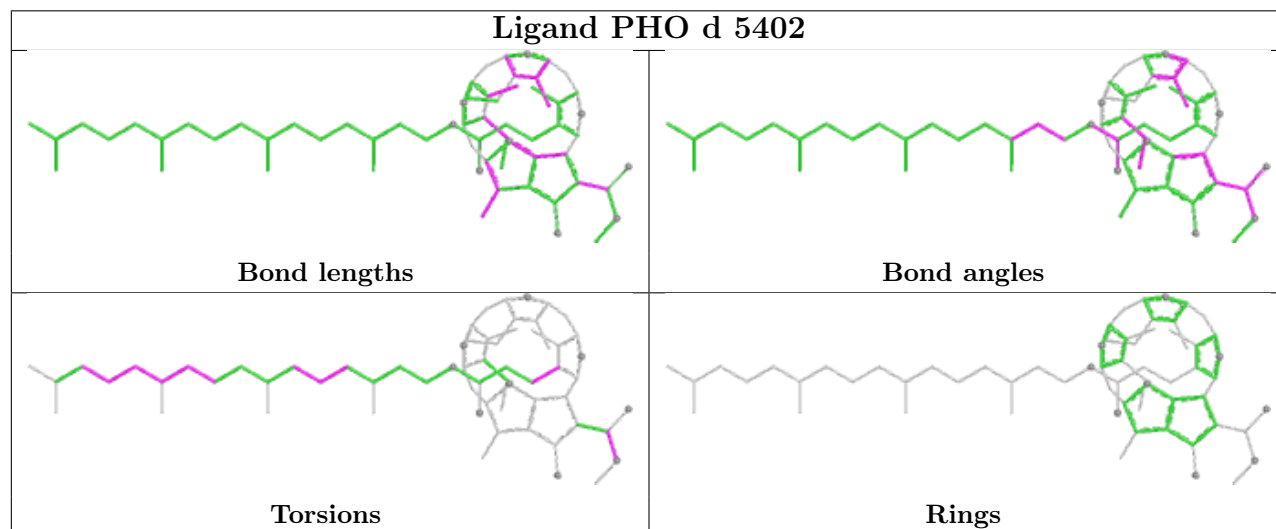
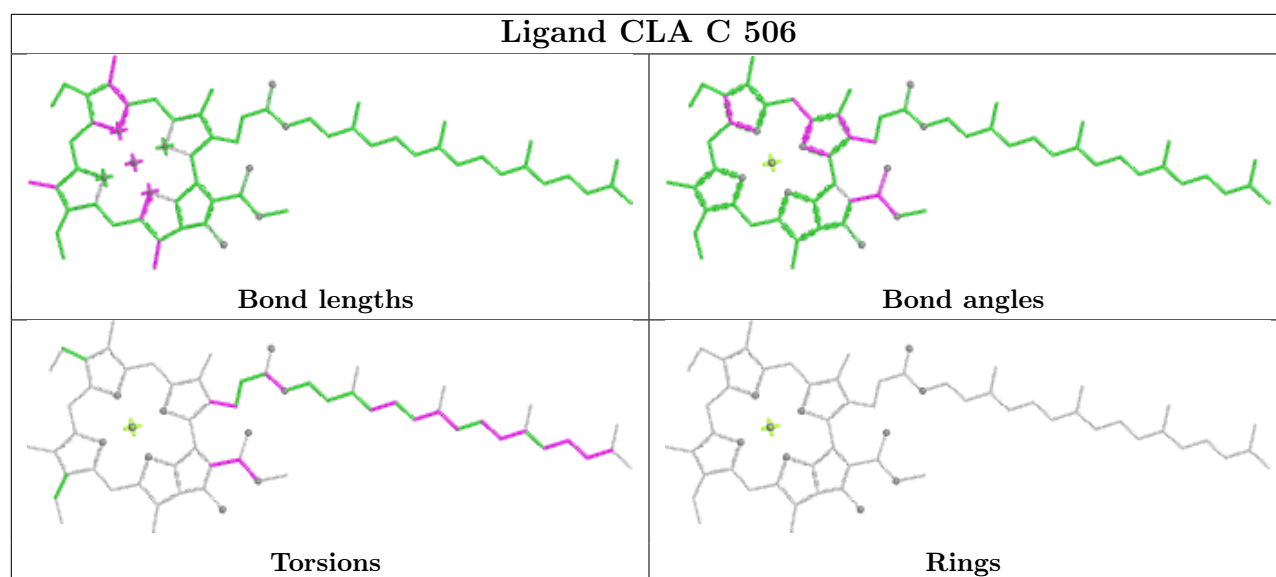


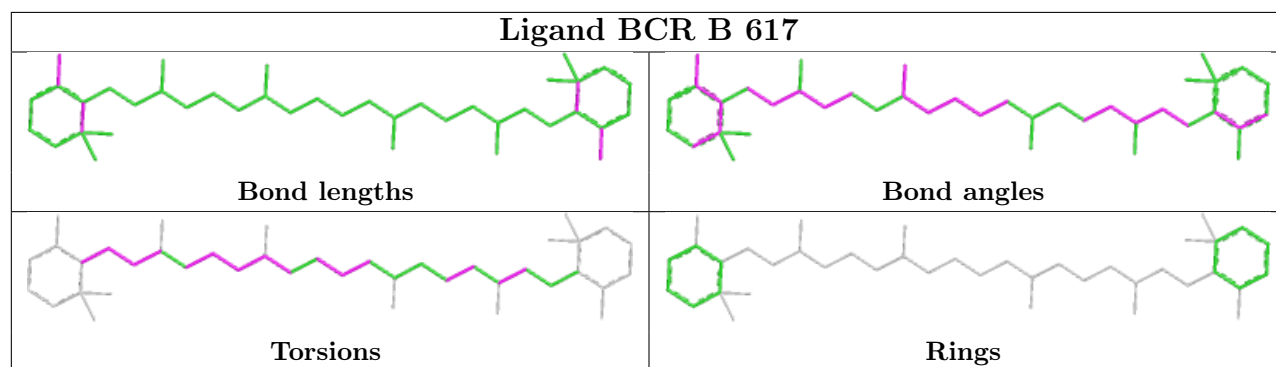
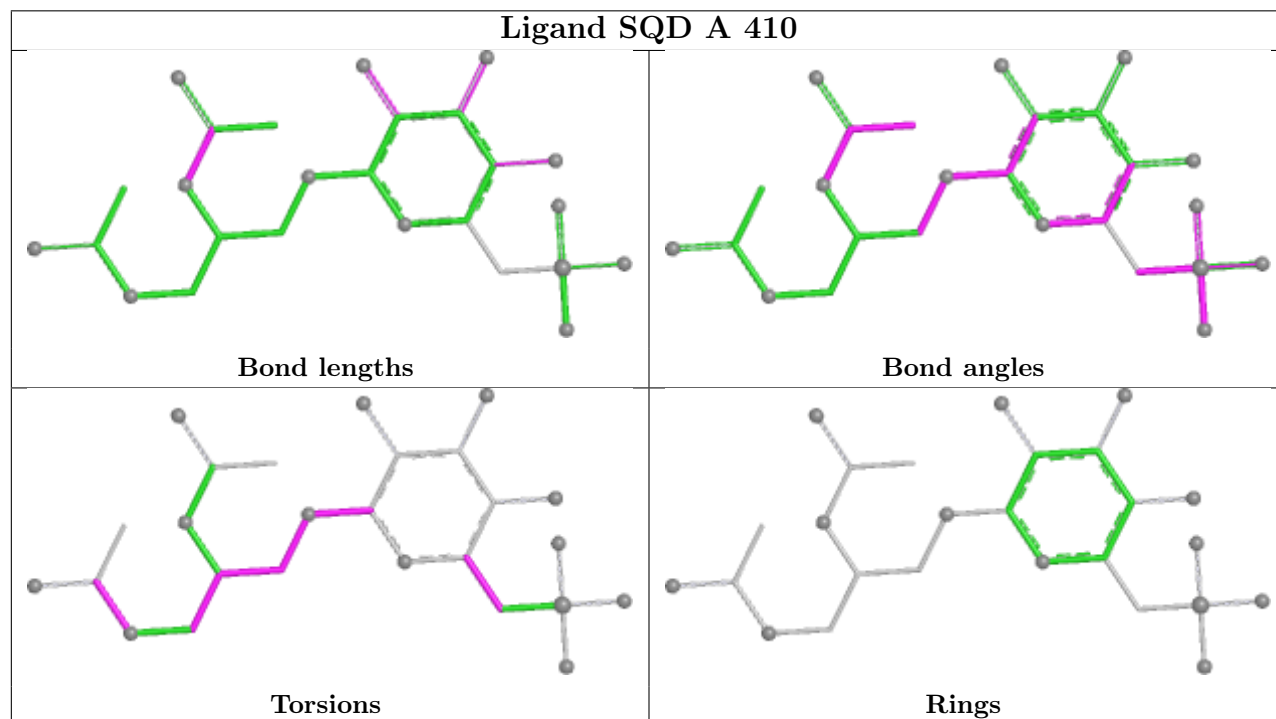
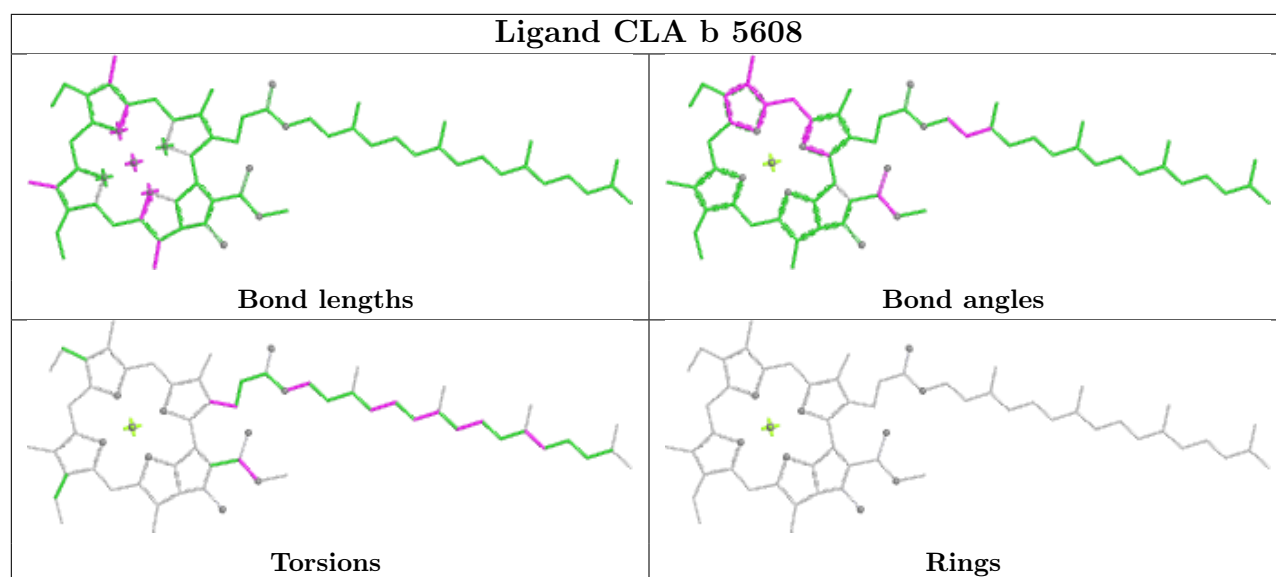
Ligand CLA C 504

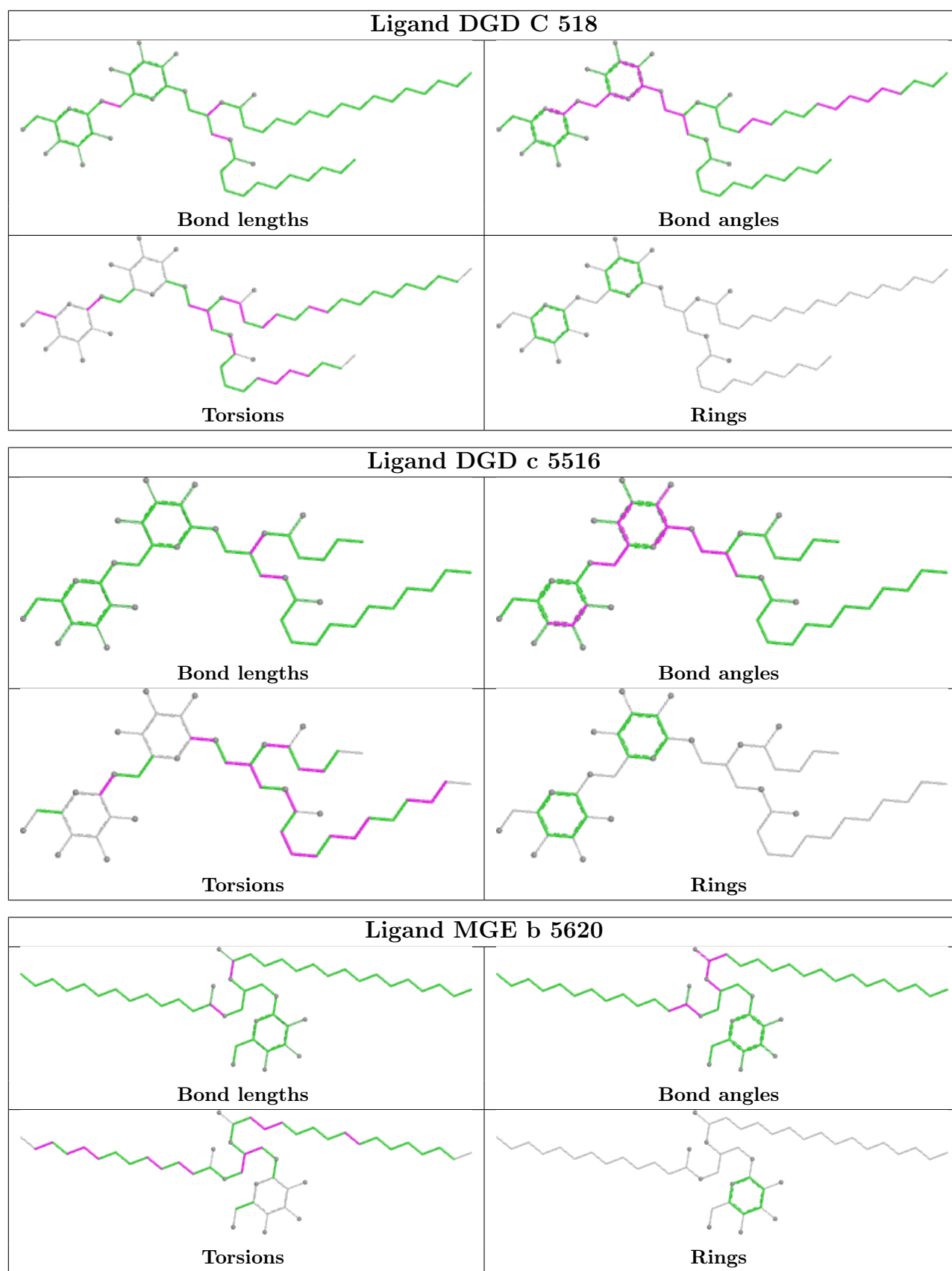


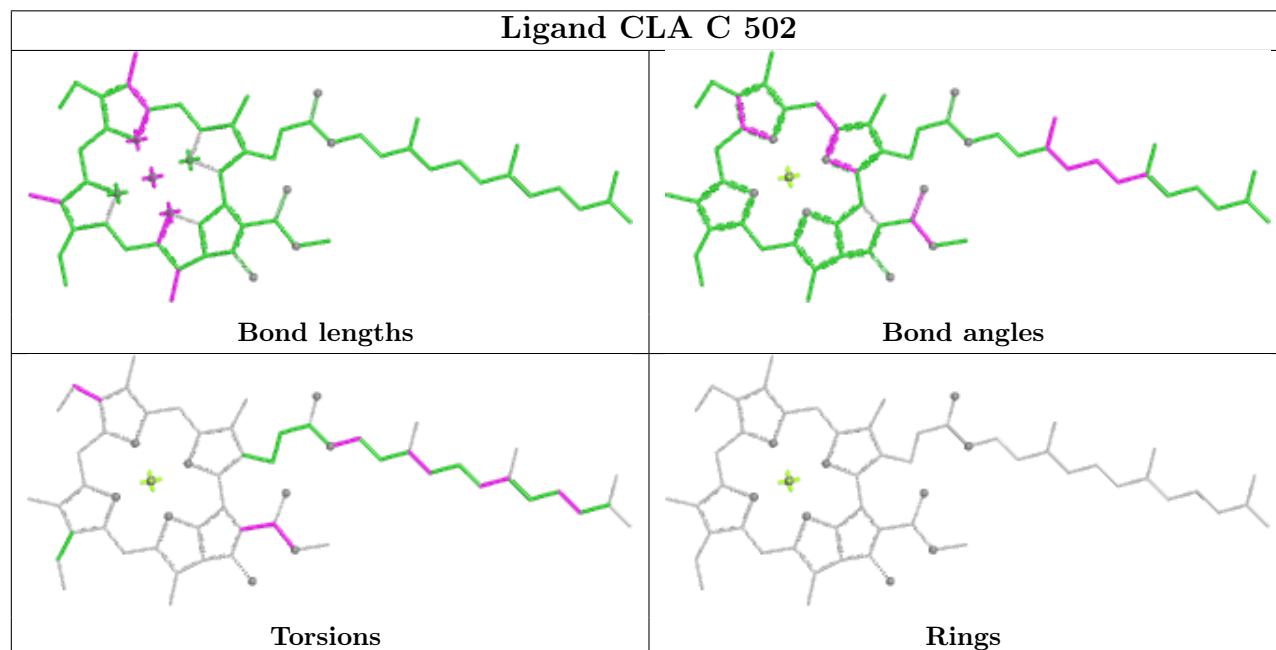
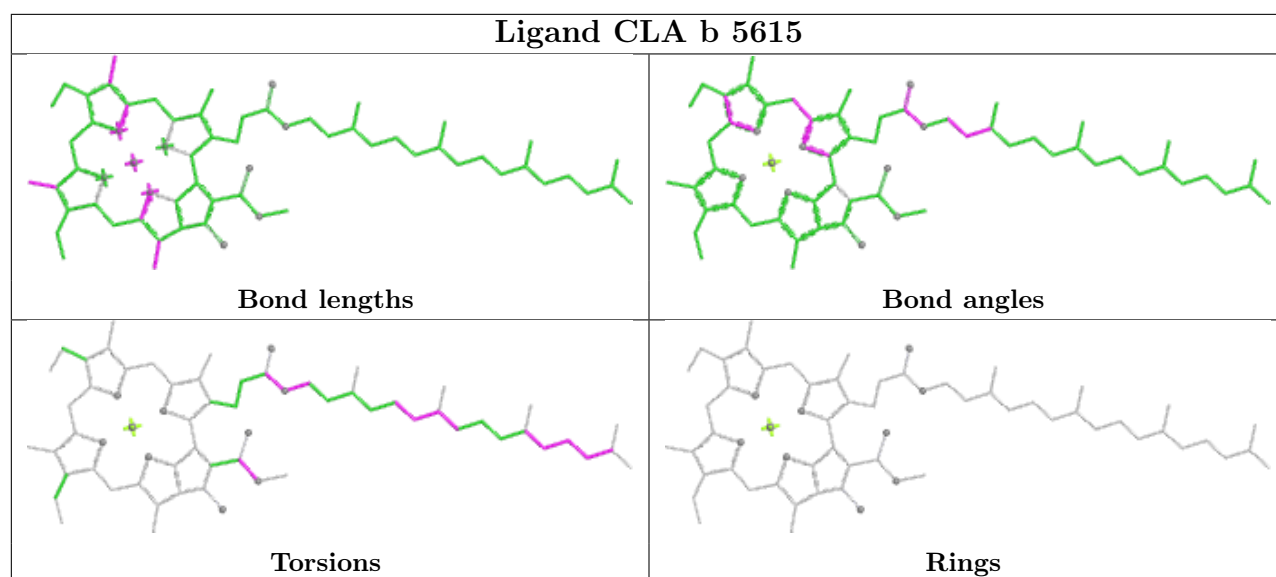
Ligand CLA C 503

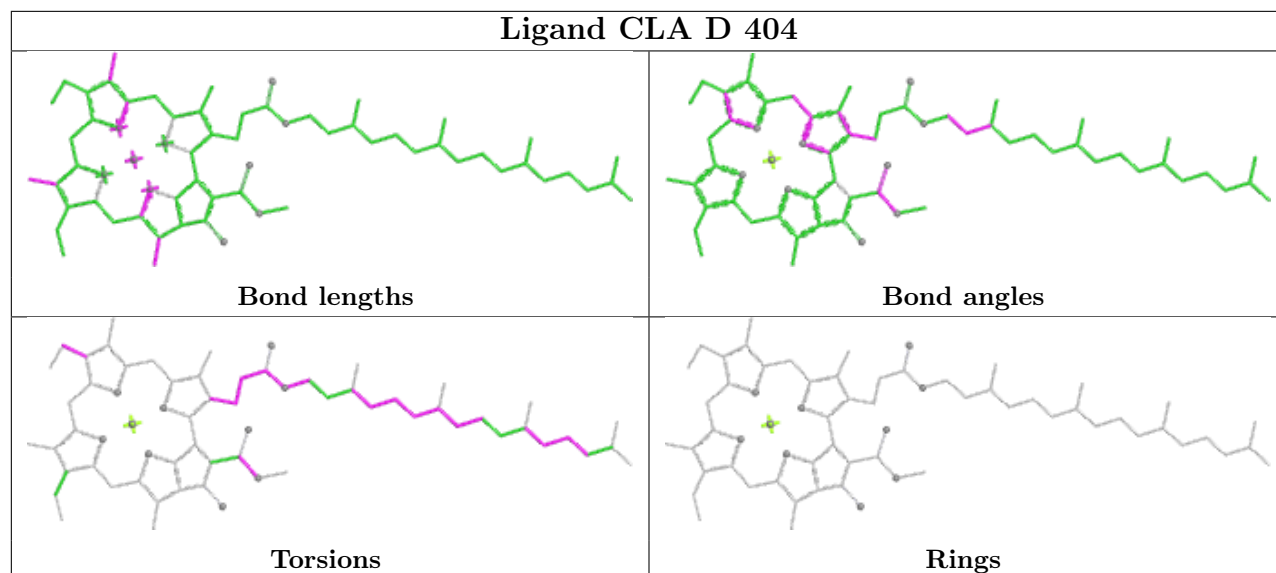
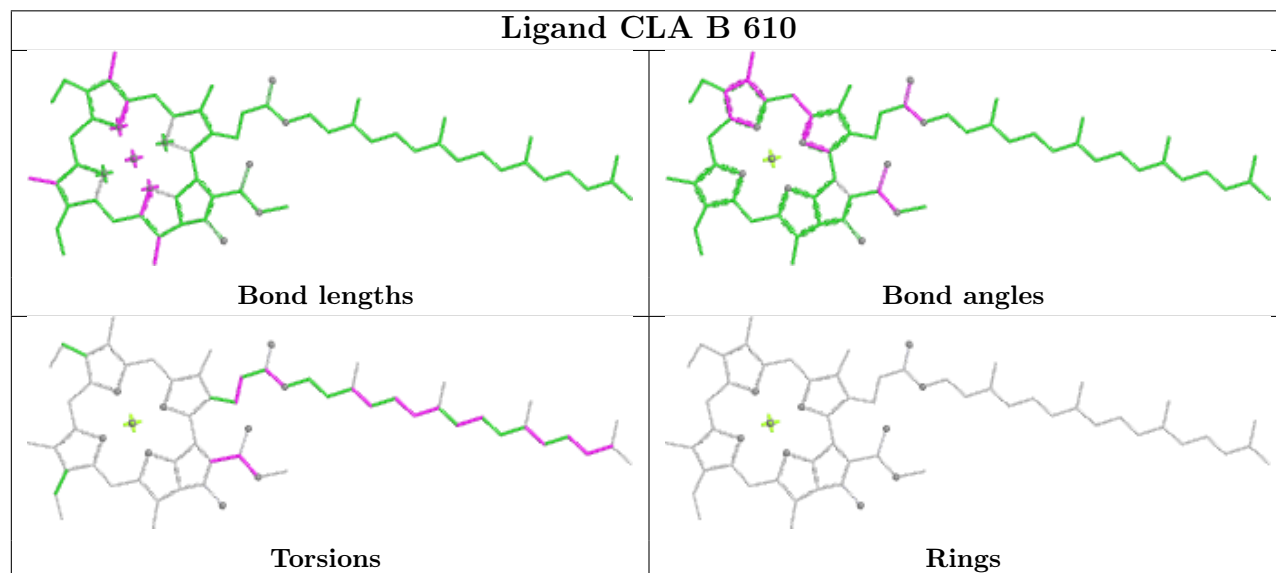
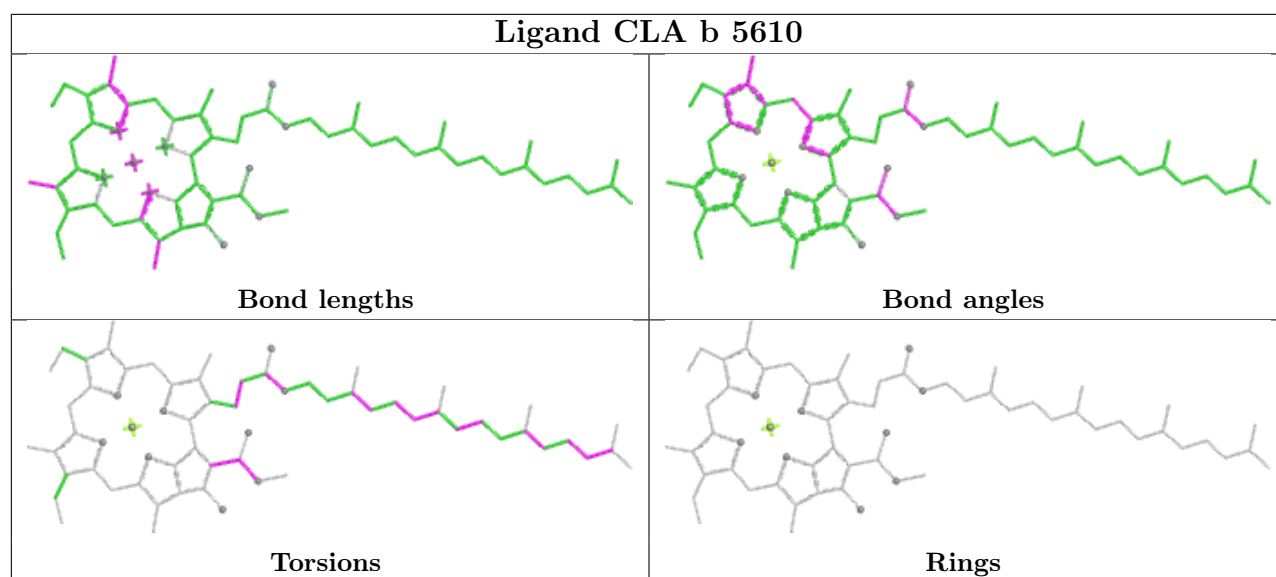


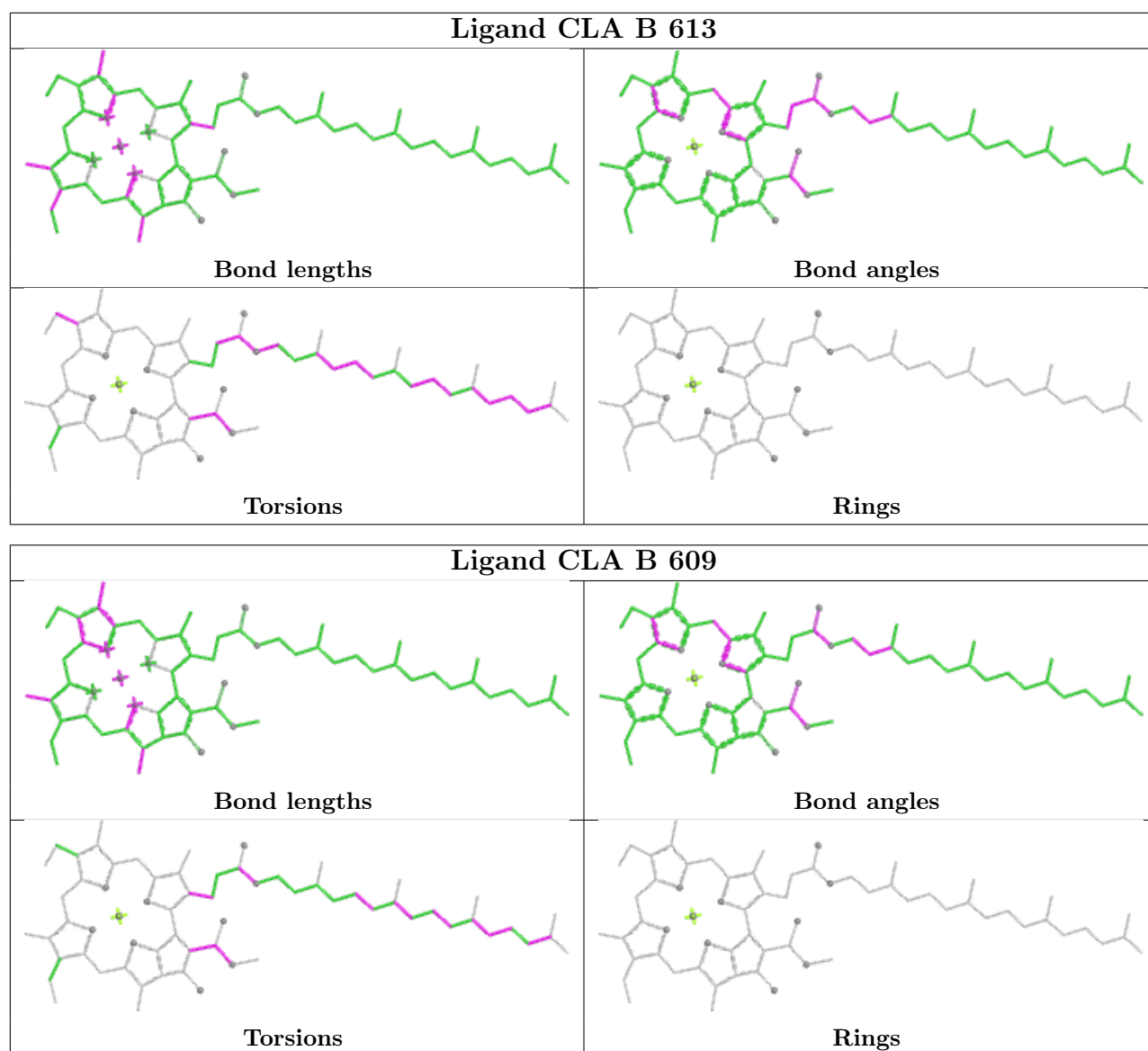




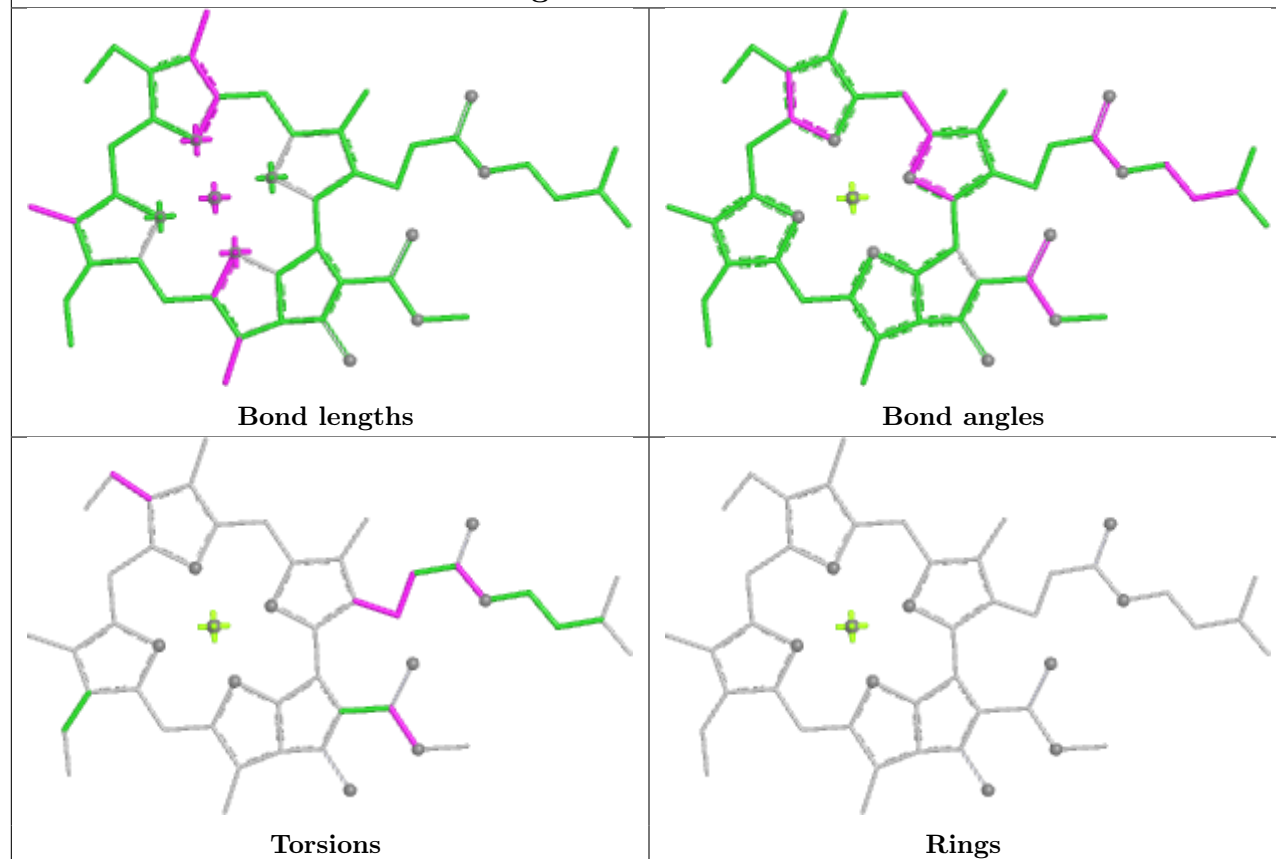




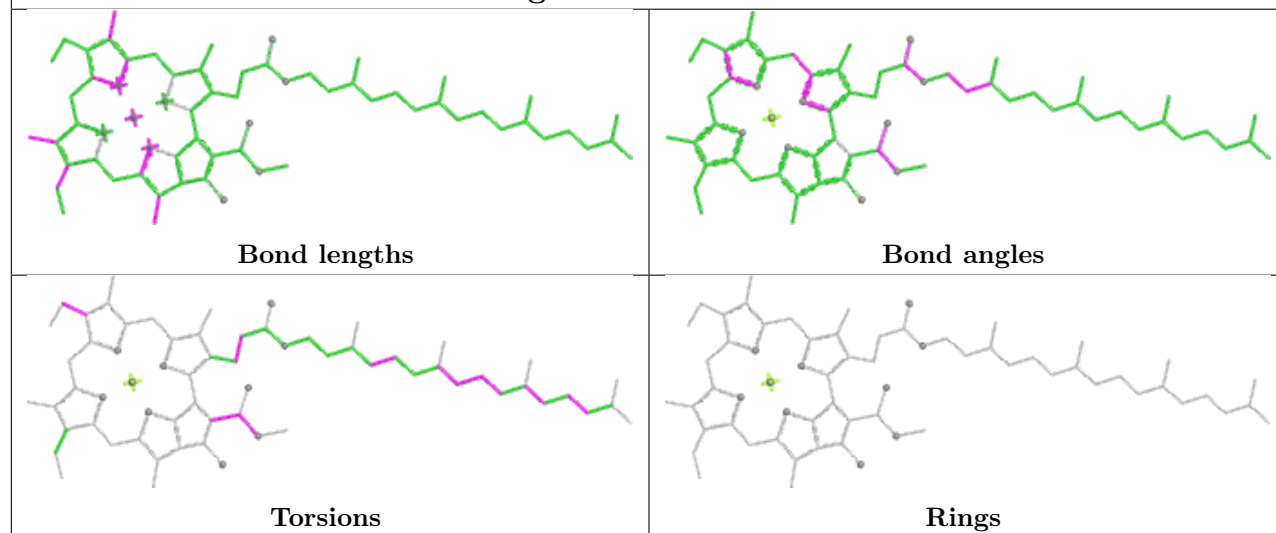


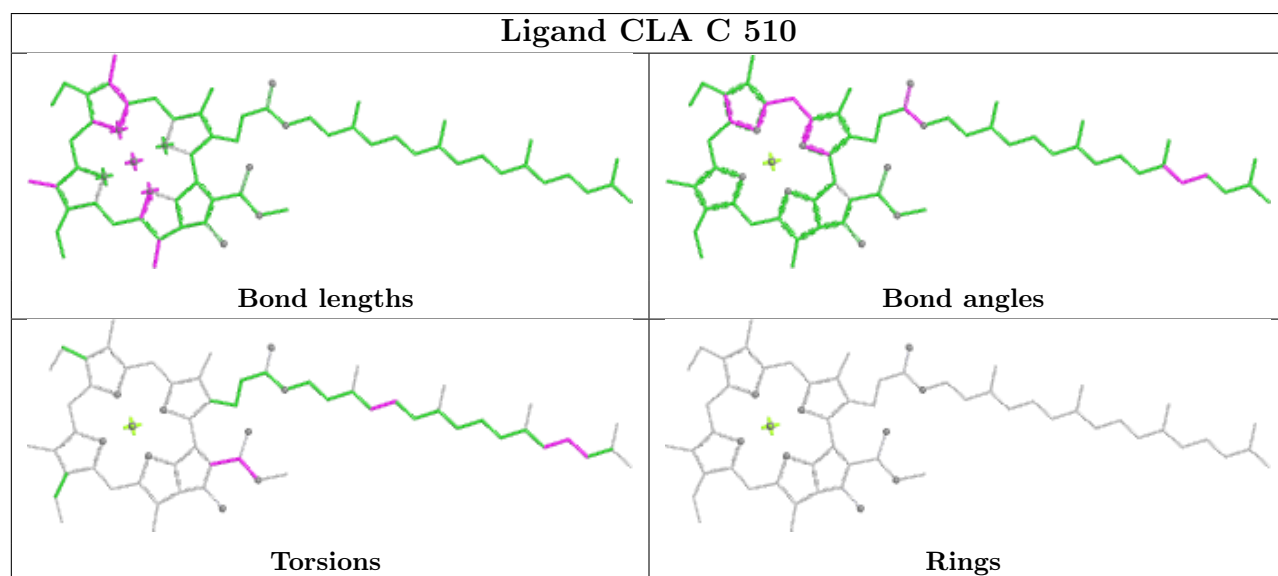
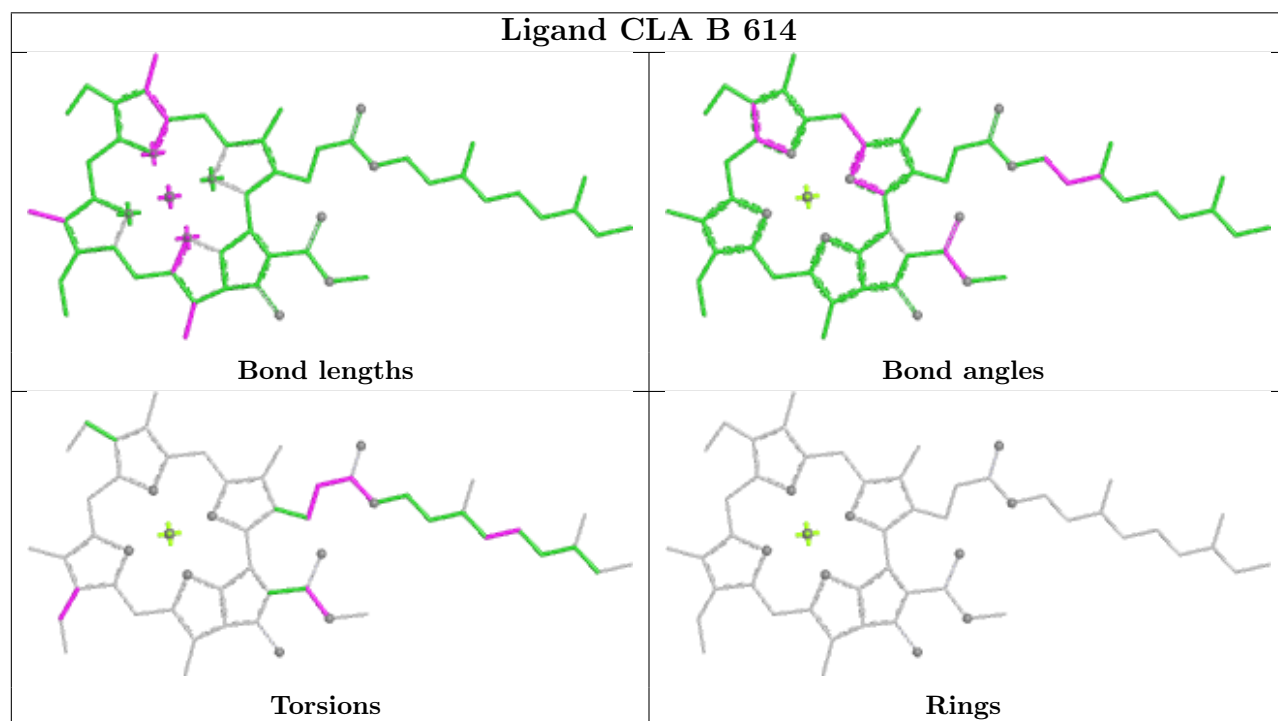
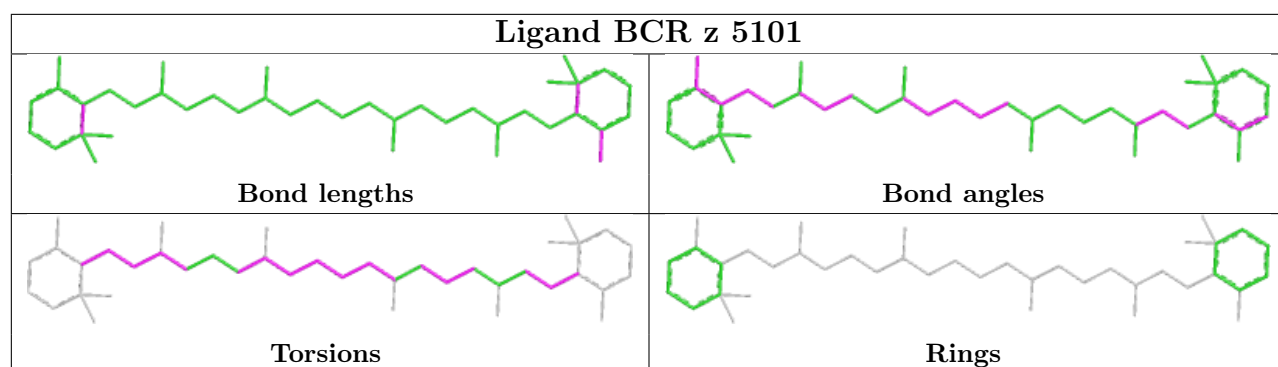


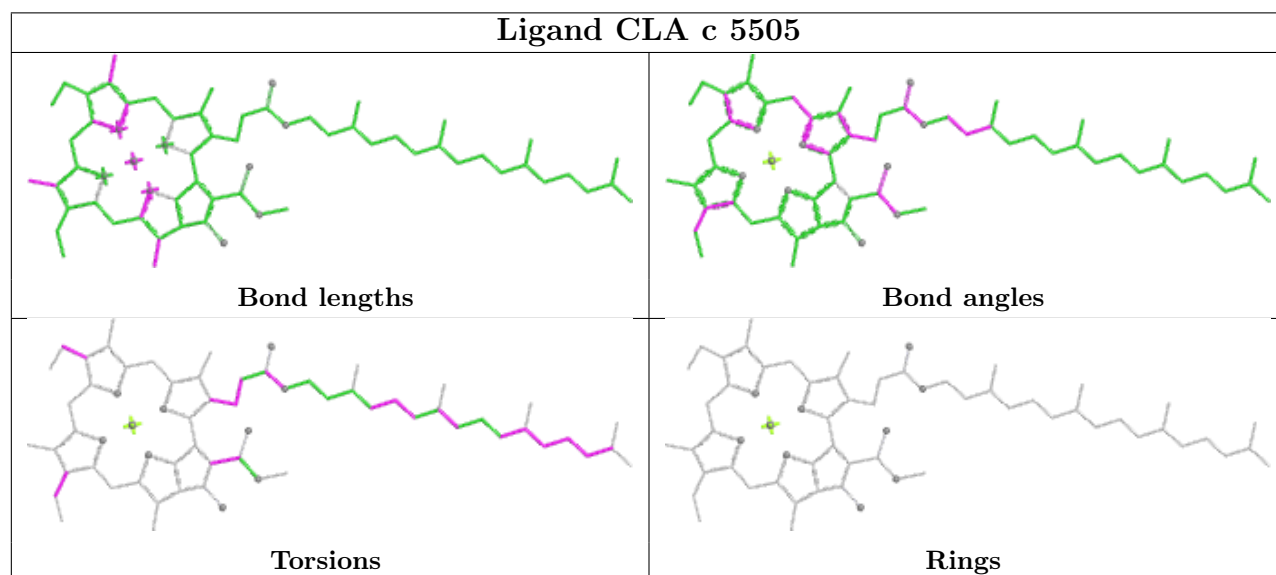
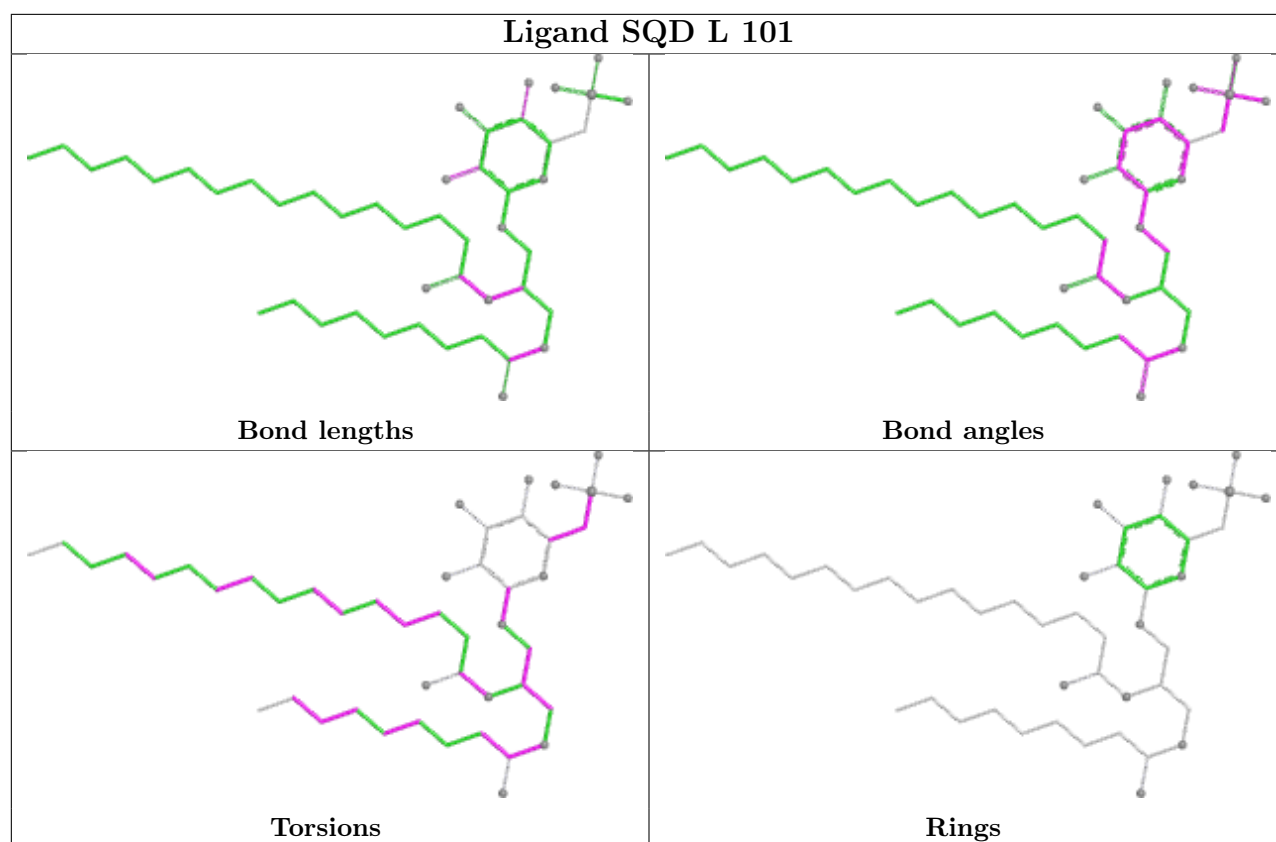
Ligand CLA D 405

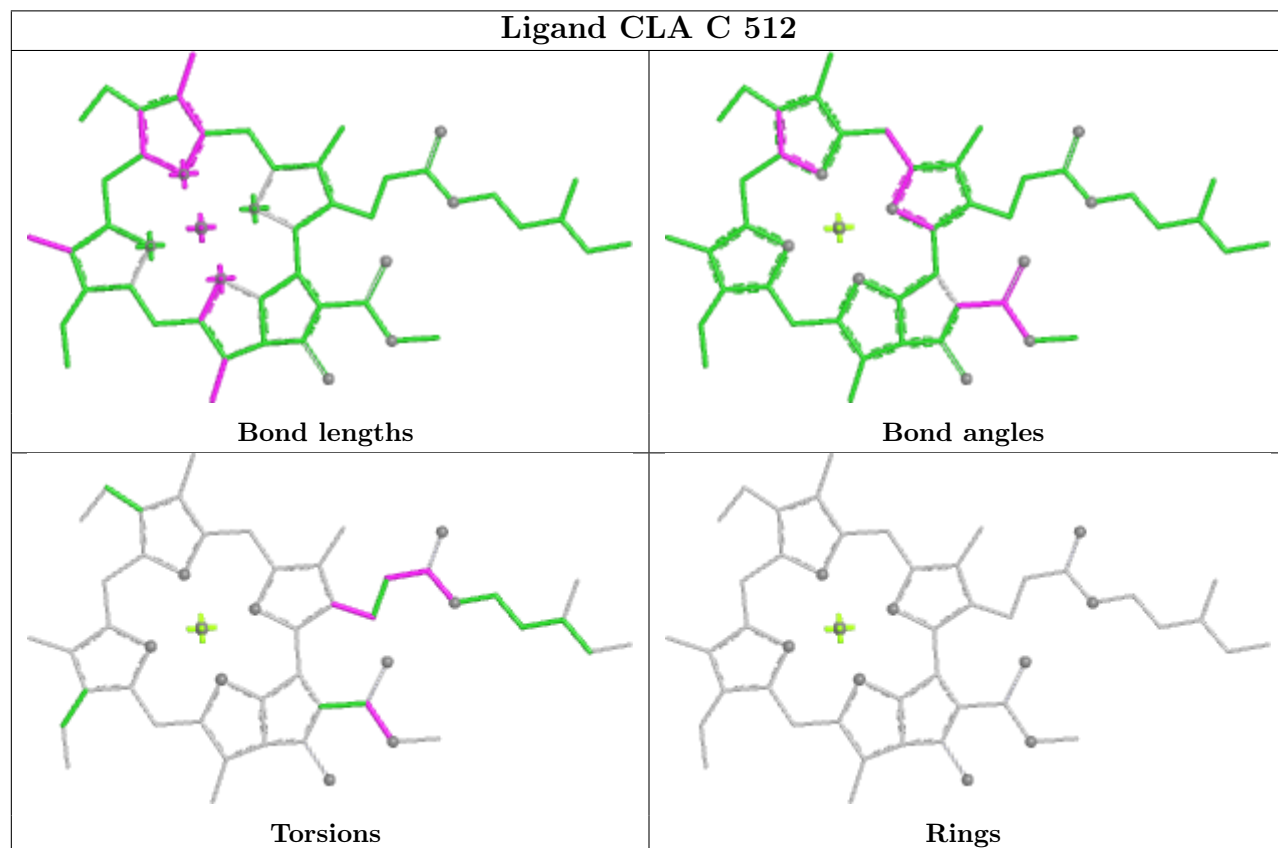
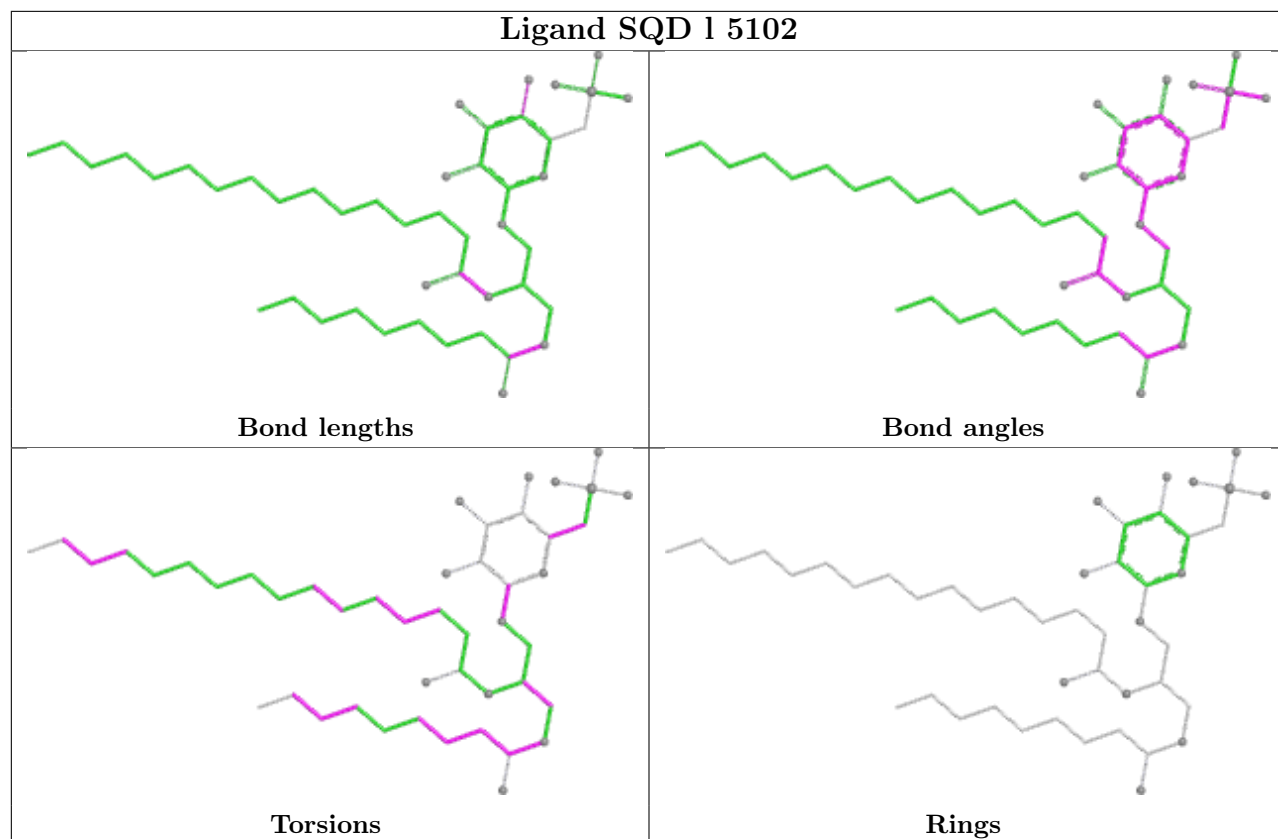


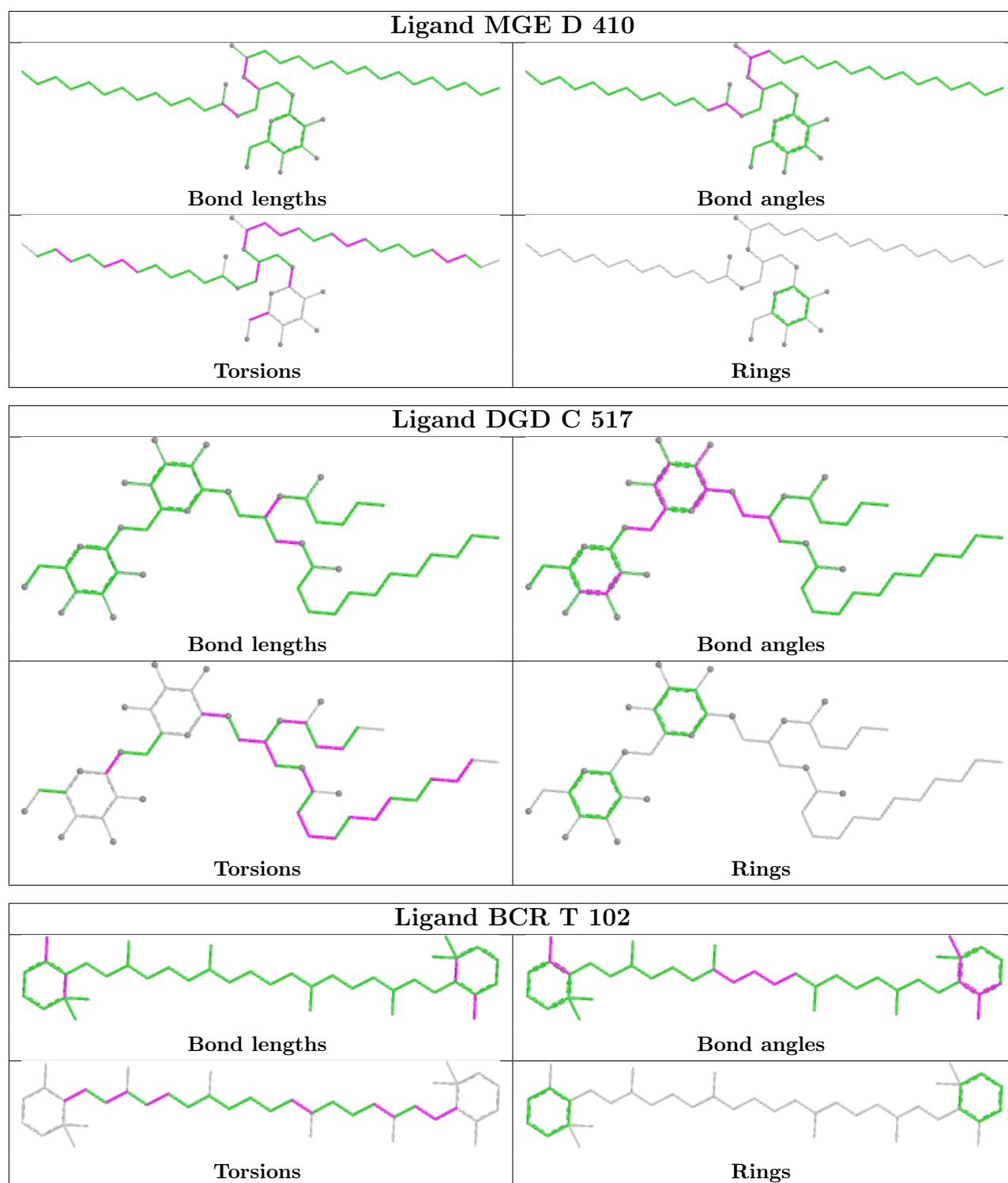
Ligand CLA c 5508

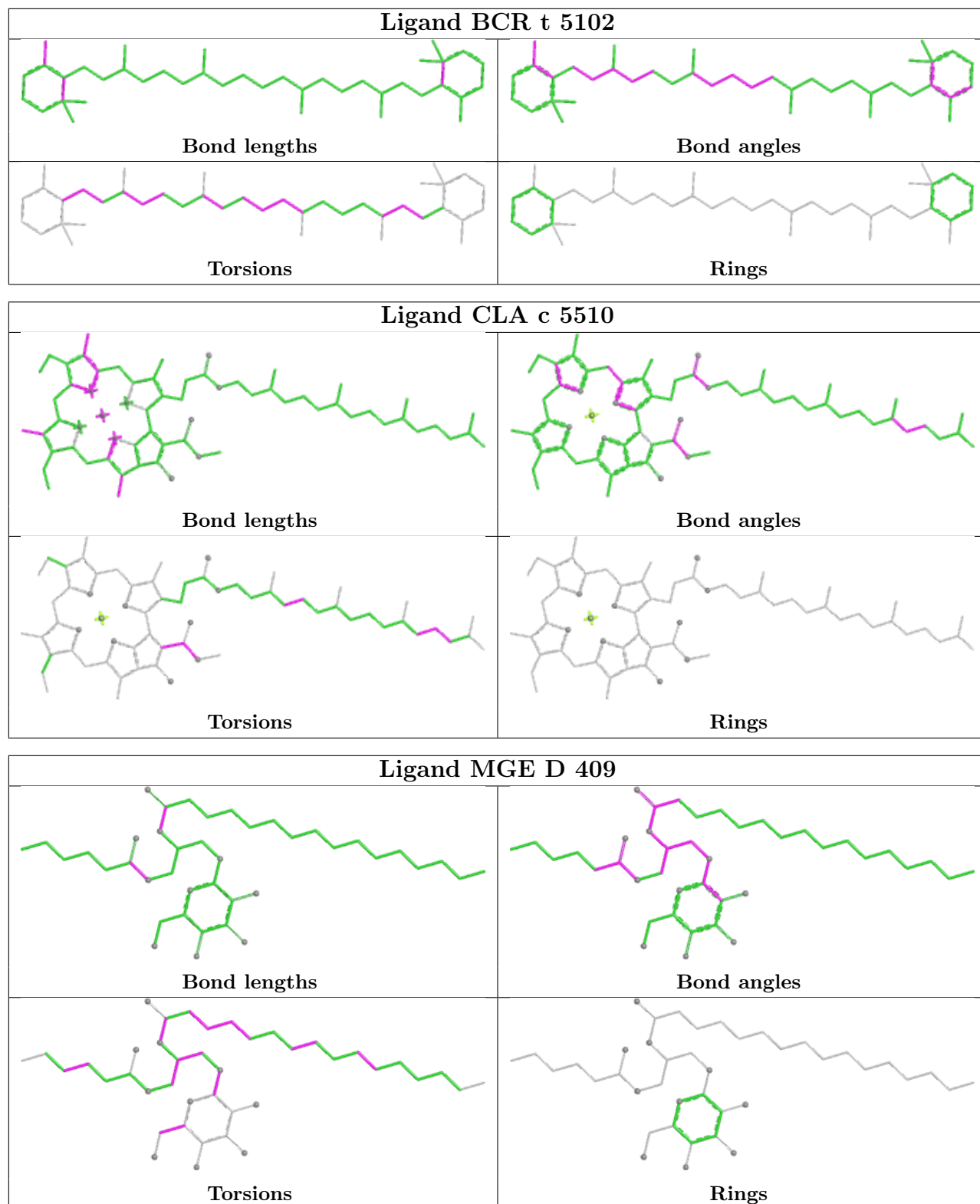




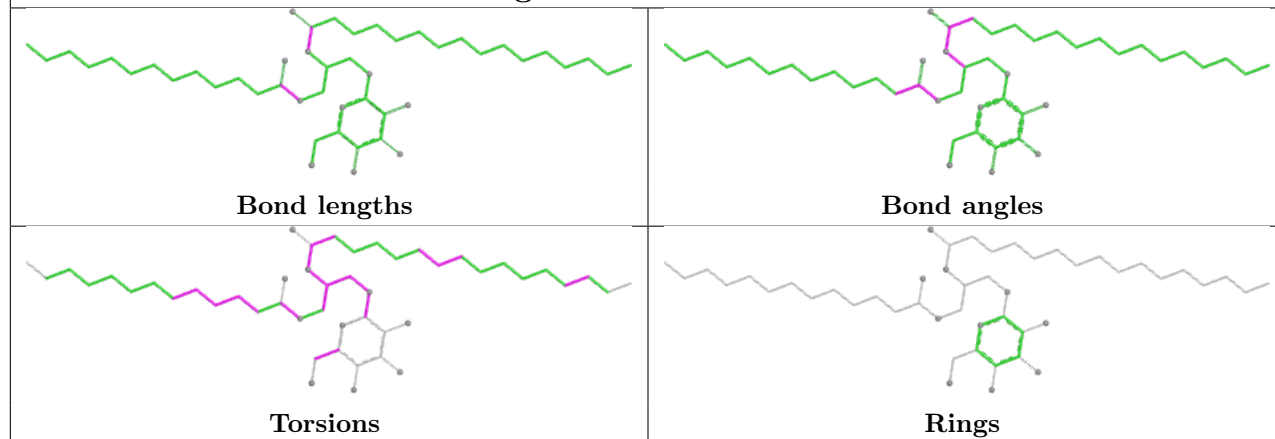




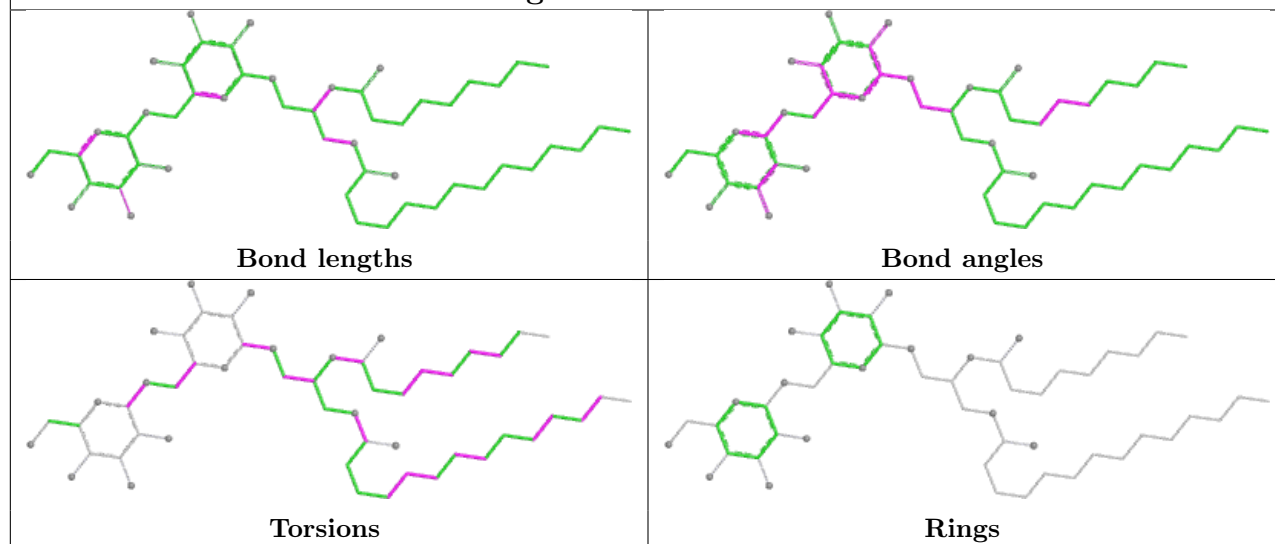




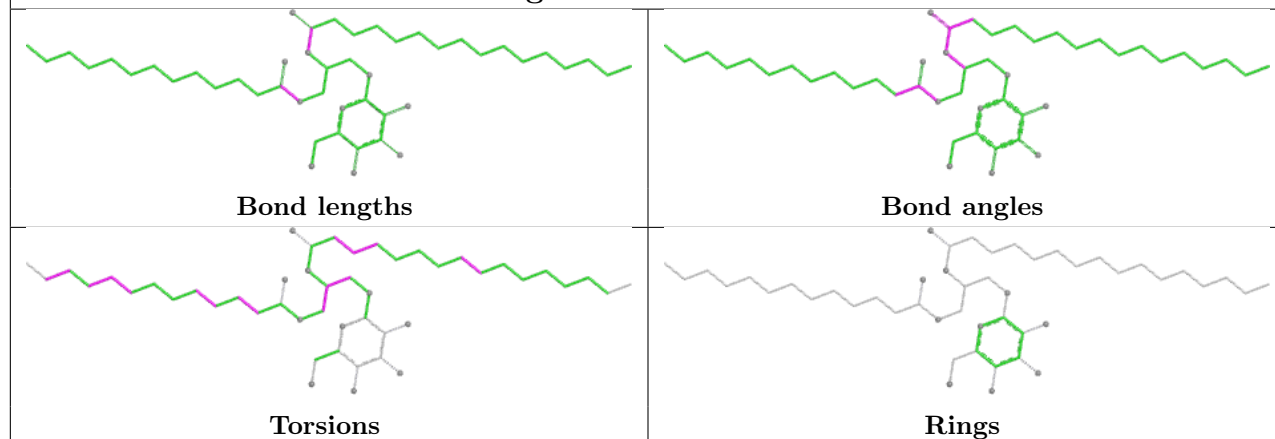
Ligand MGE m 5103

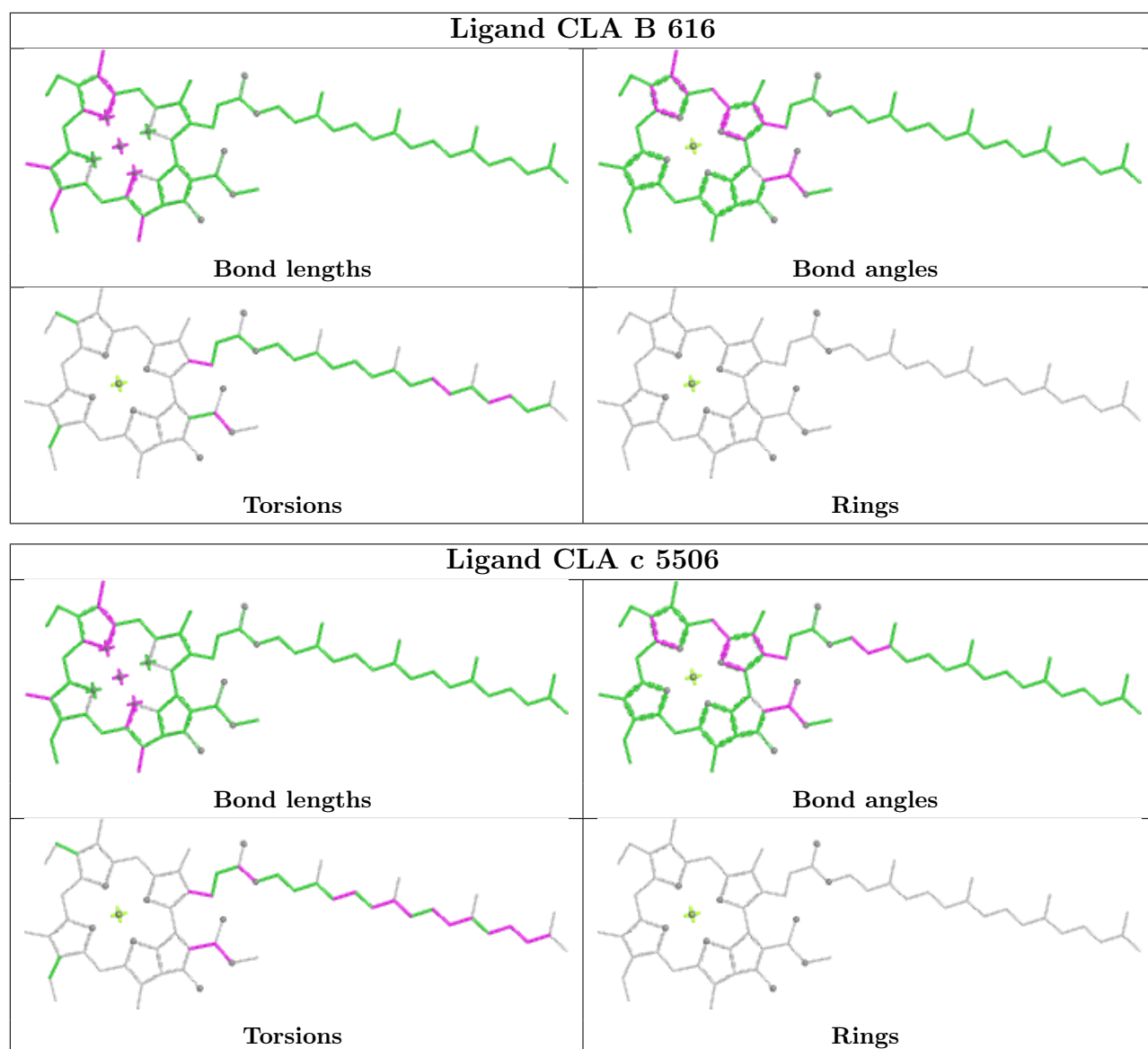


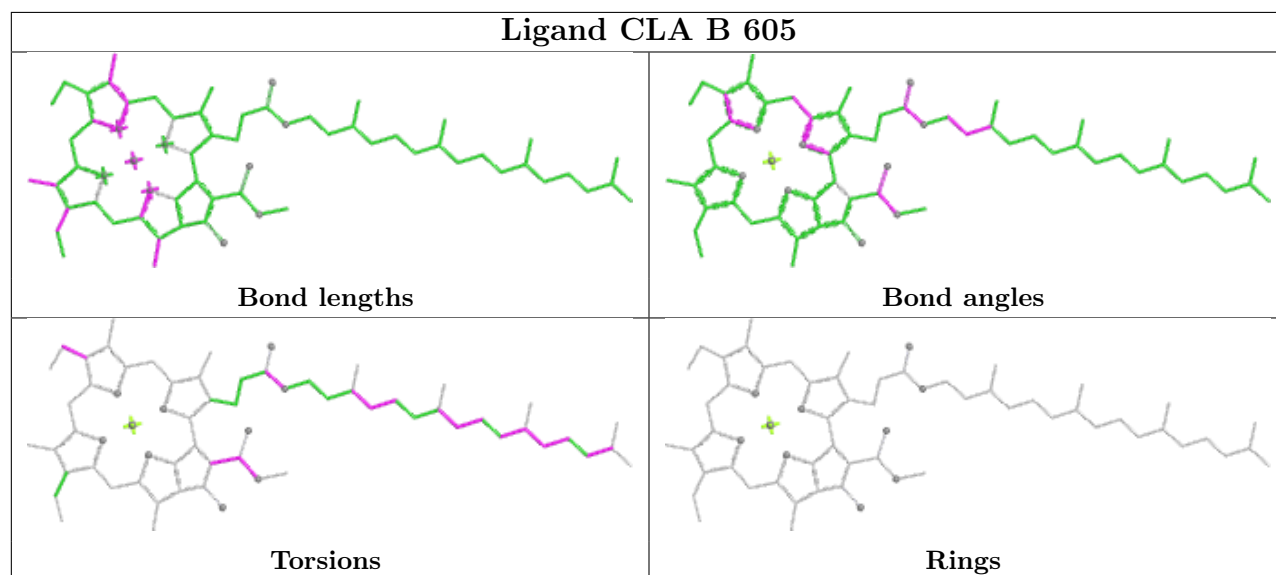
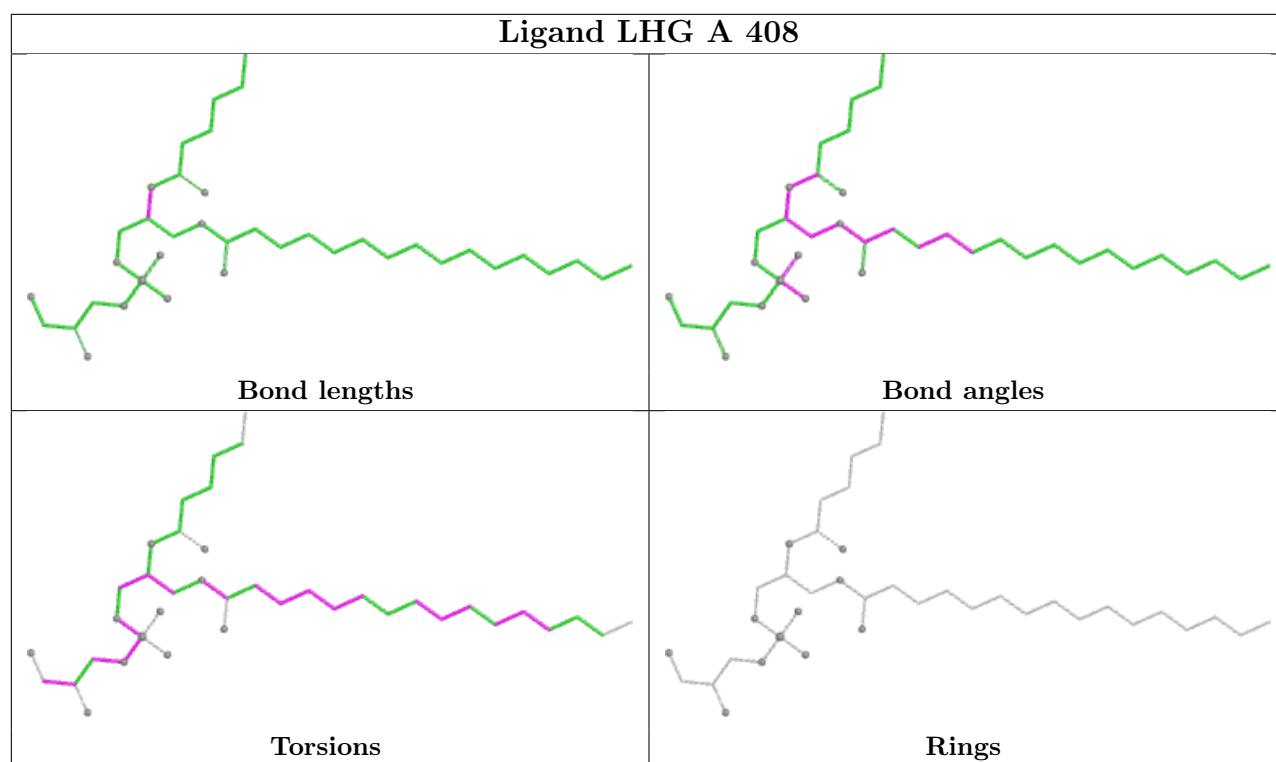
Ligand DGD A 413

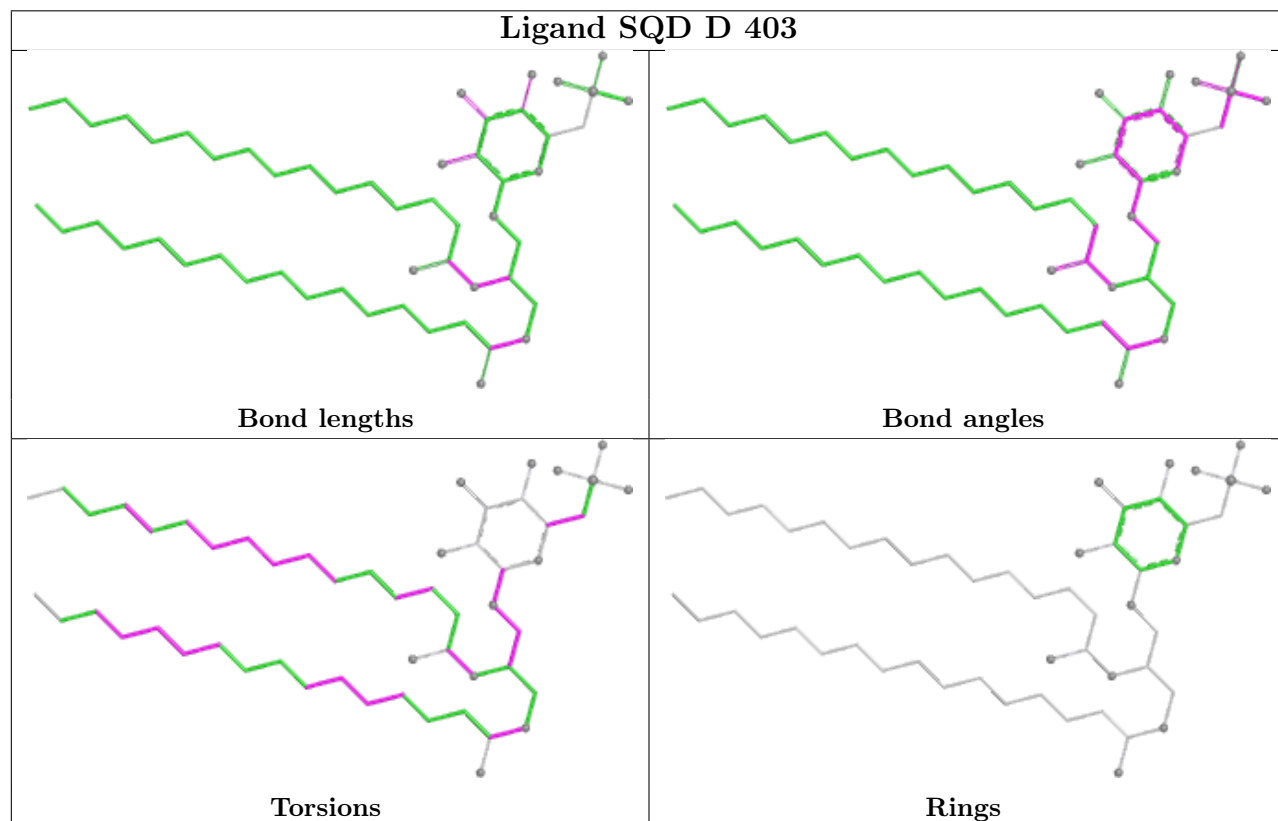
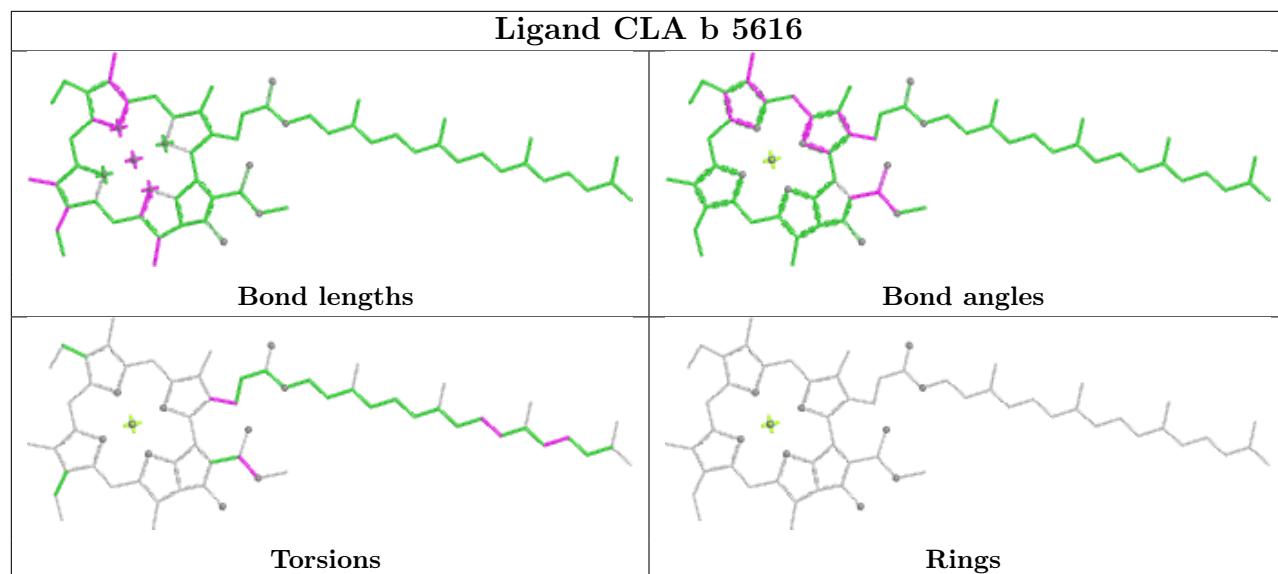


Ligand MGE B 619

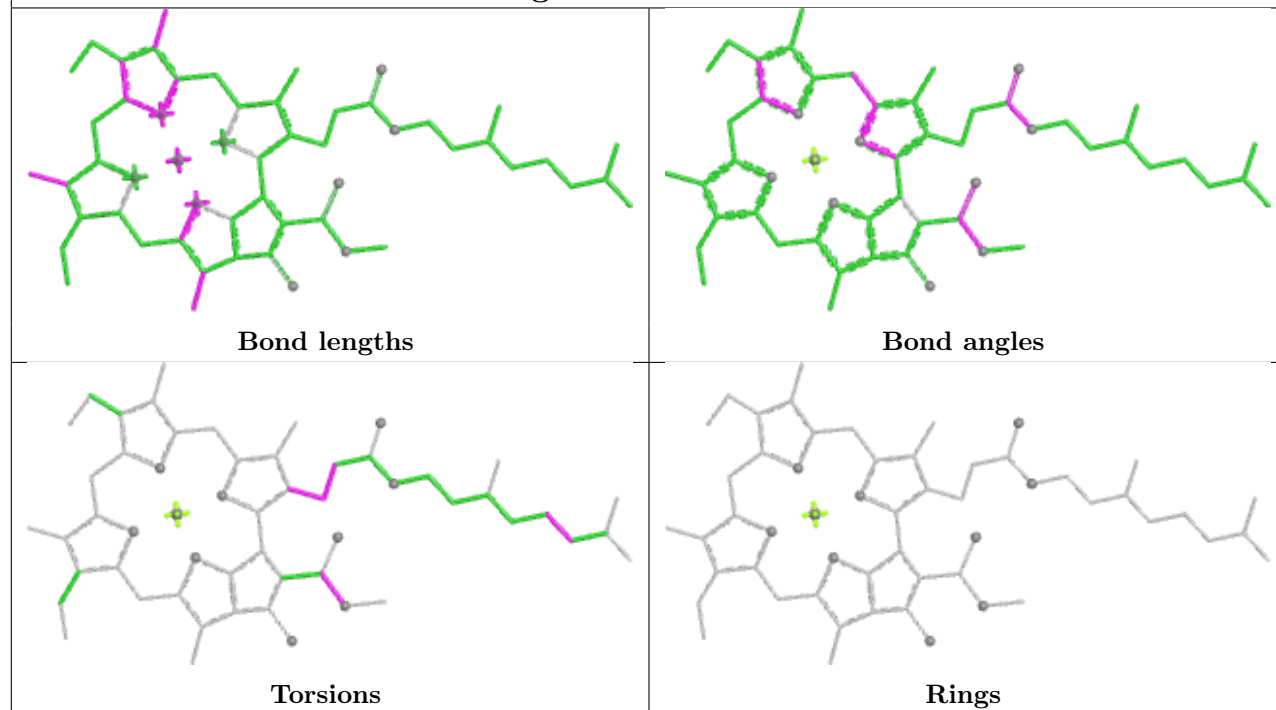




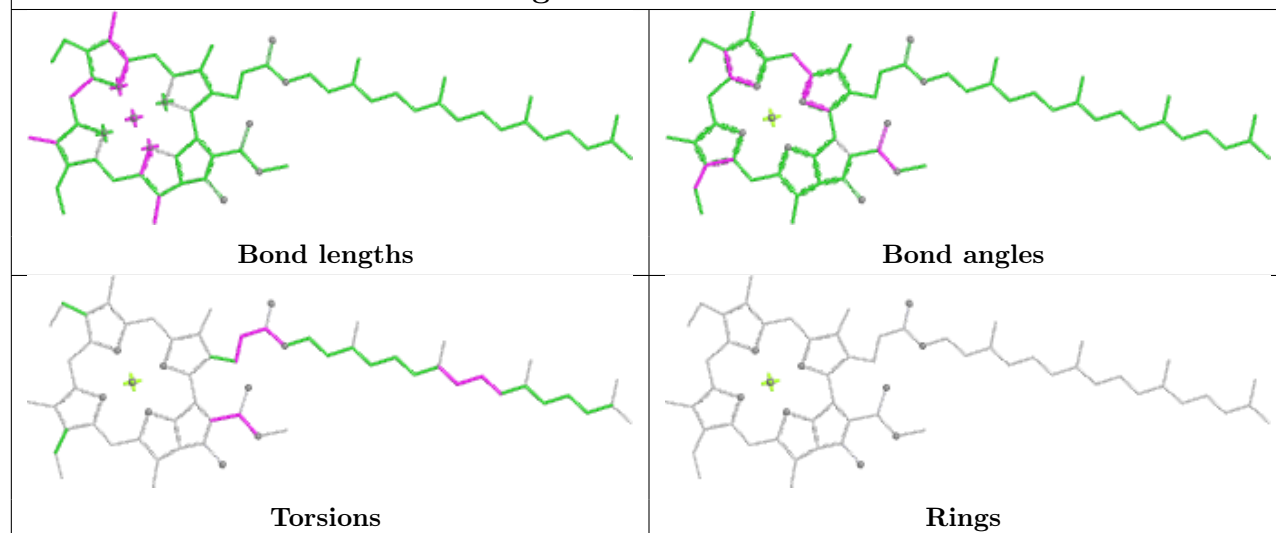




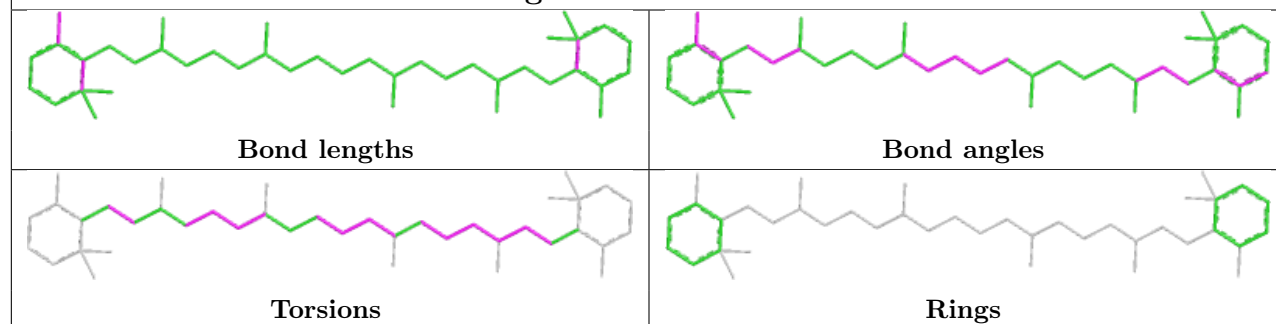
Ligand CLA A 405

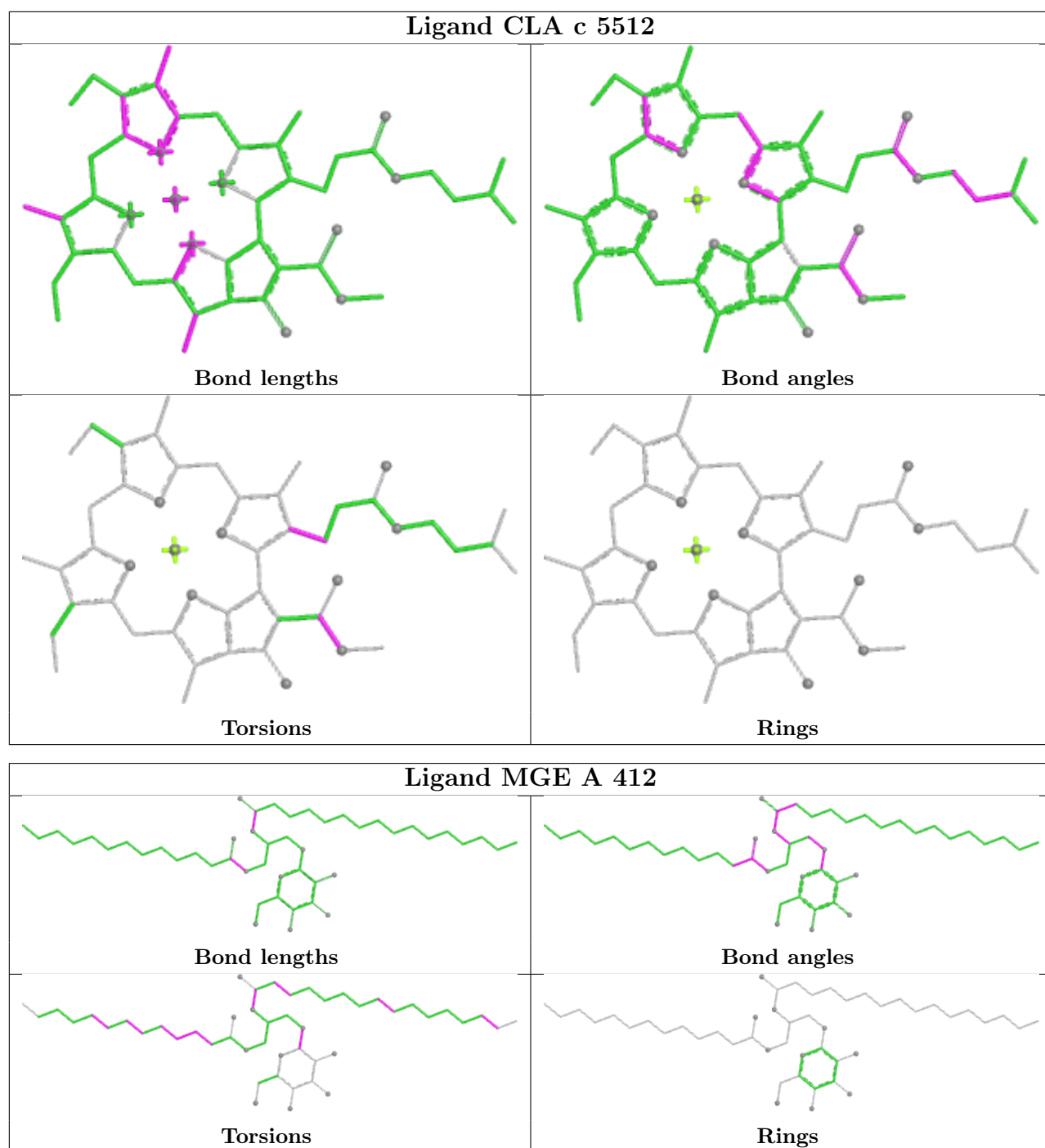


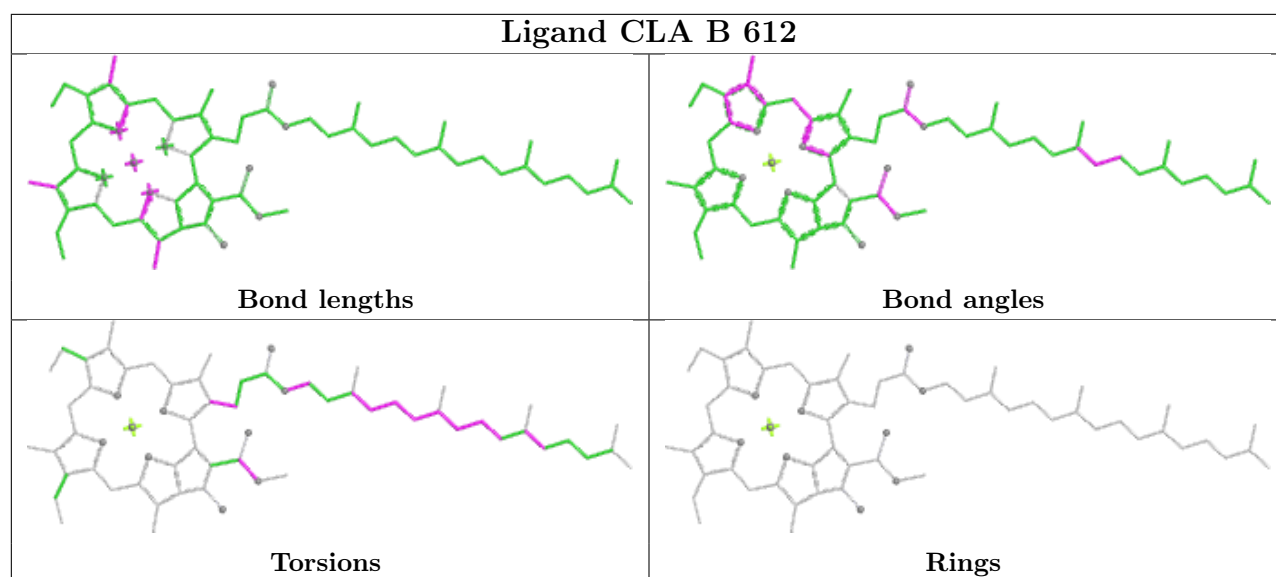
Ligand CLA C 507



Ligand BCR k 5502







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.

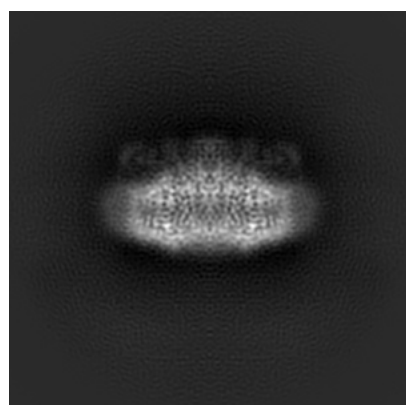
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30511. These allow visual inspection of the internal detail of the map and identification of artifacts.

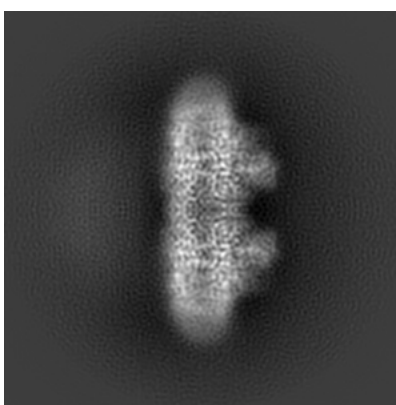
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

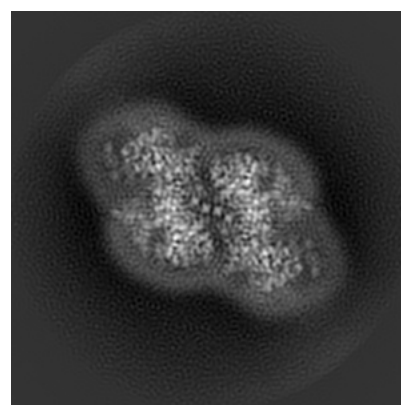
6.1.1 Primary map



X



Y

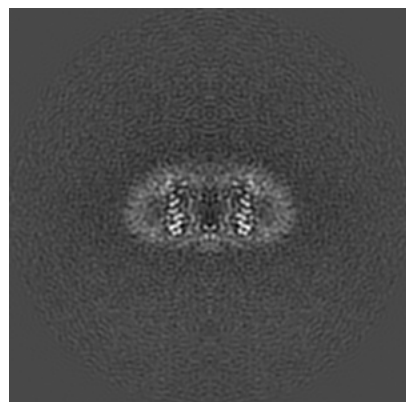


Z

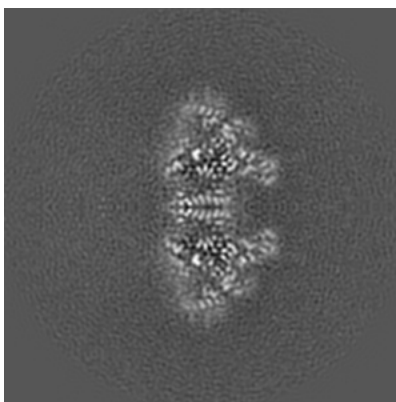
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

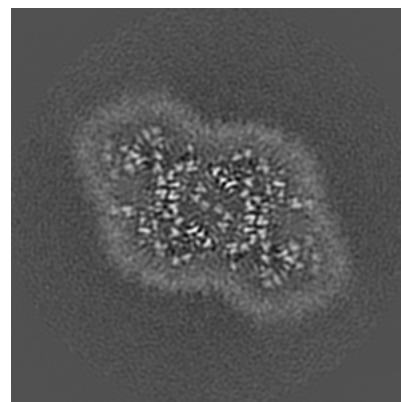
6.2.1 Primary map



X Index: 120



Y Index: 120

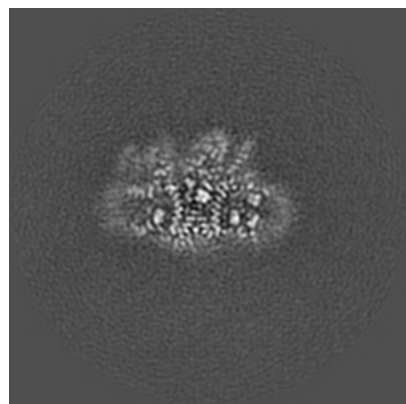


Z Index: 120

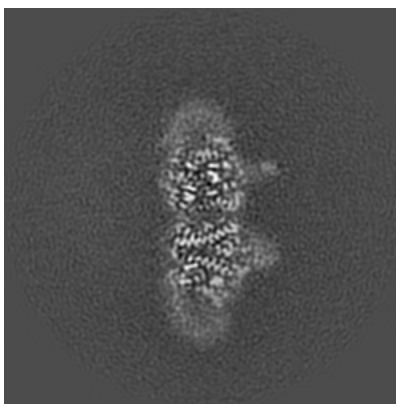
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

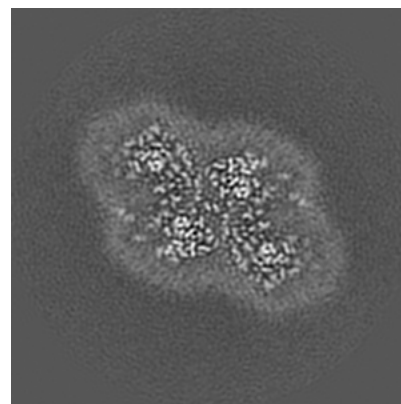
6.3.1 Primary map



X Index: 146



Y Index: 144

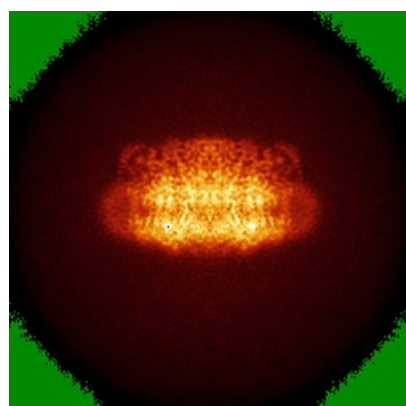


Z Index: 111

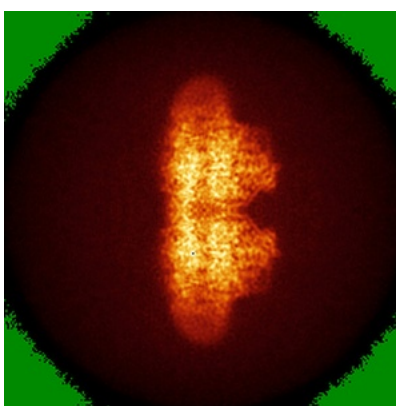
The images above show the largest variance slices of the map in three orthogonal directions.

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

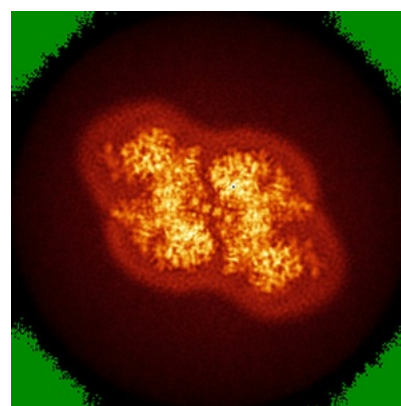
6.4.1 Primary map



X



Y

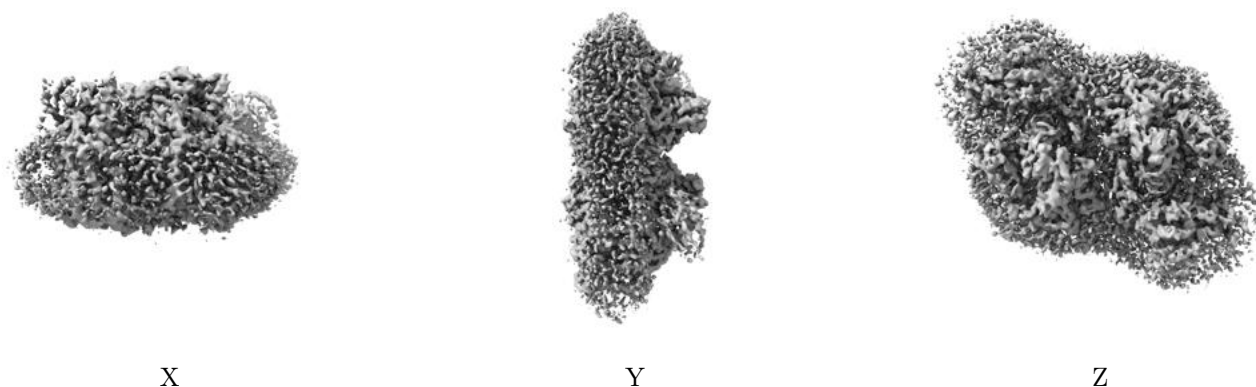


Z

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 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

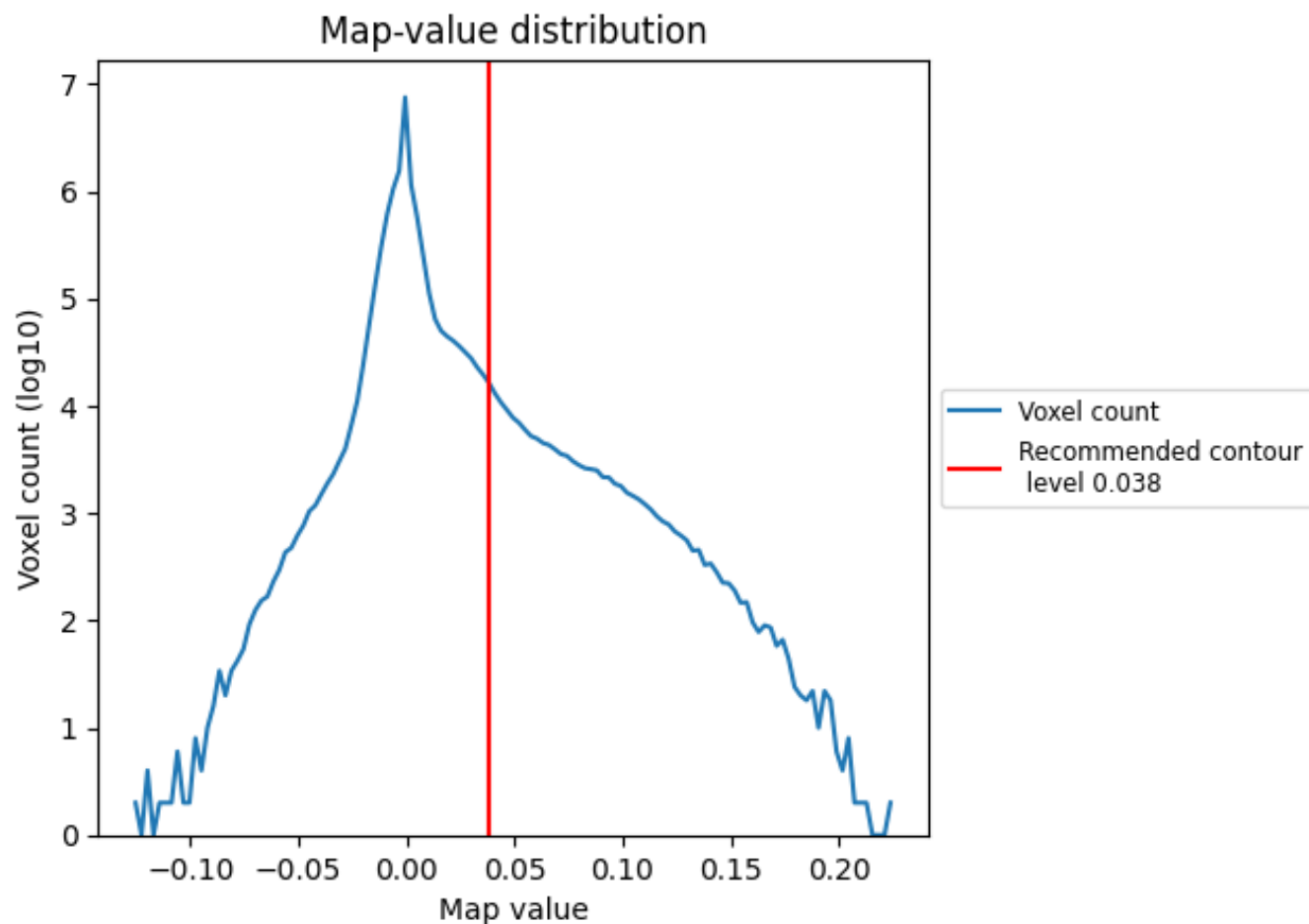
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

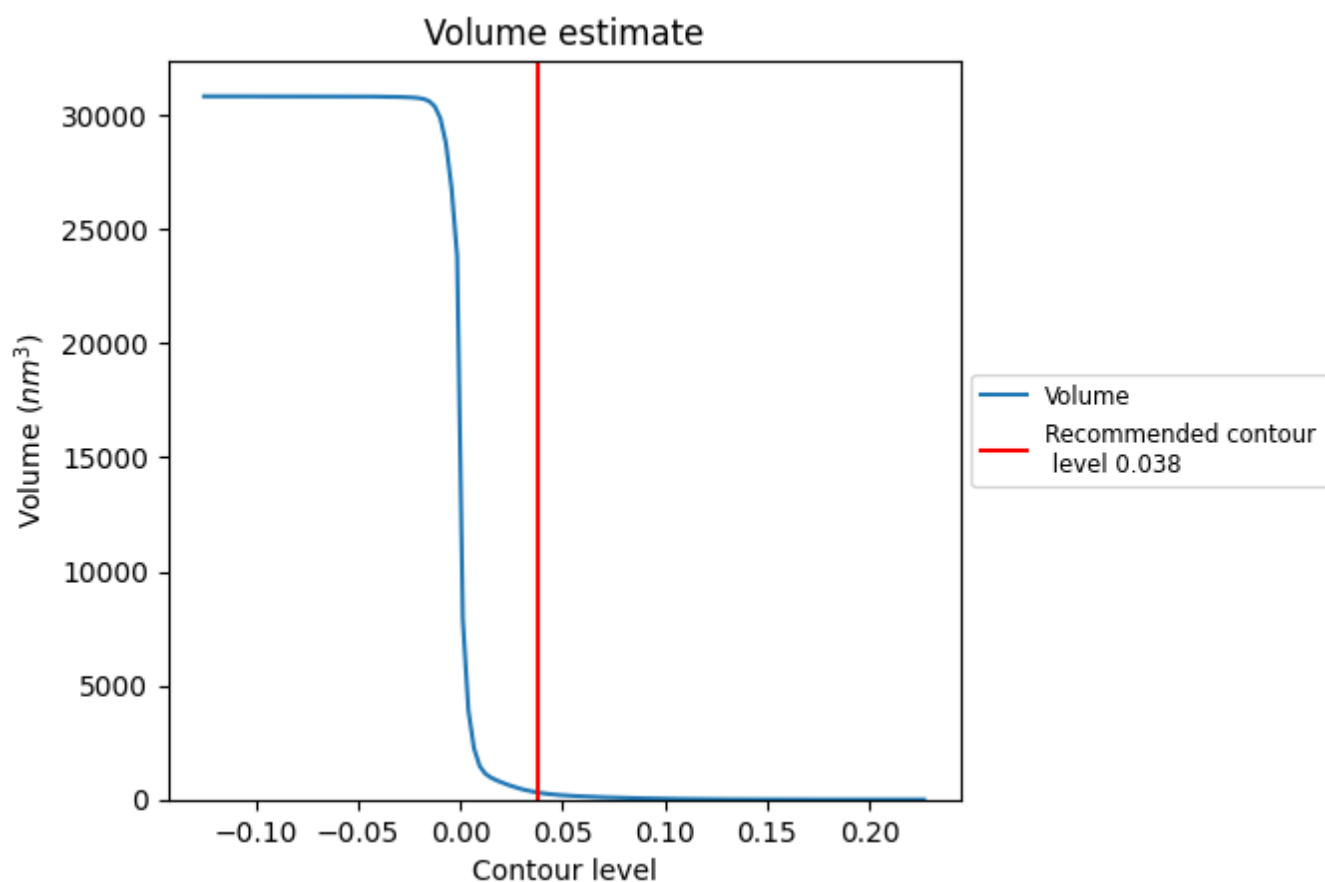
This section contains the results of statistical analysis of the map.

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.

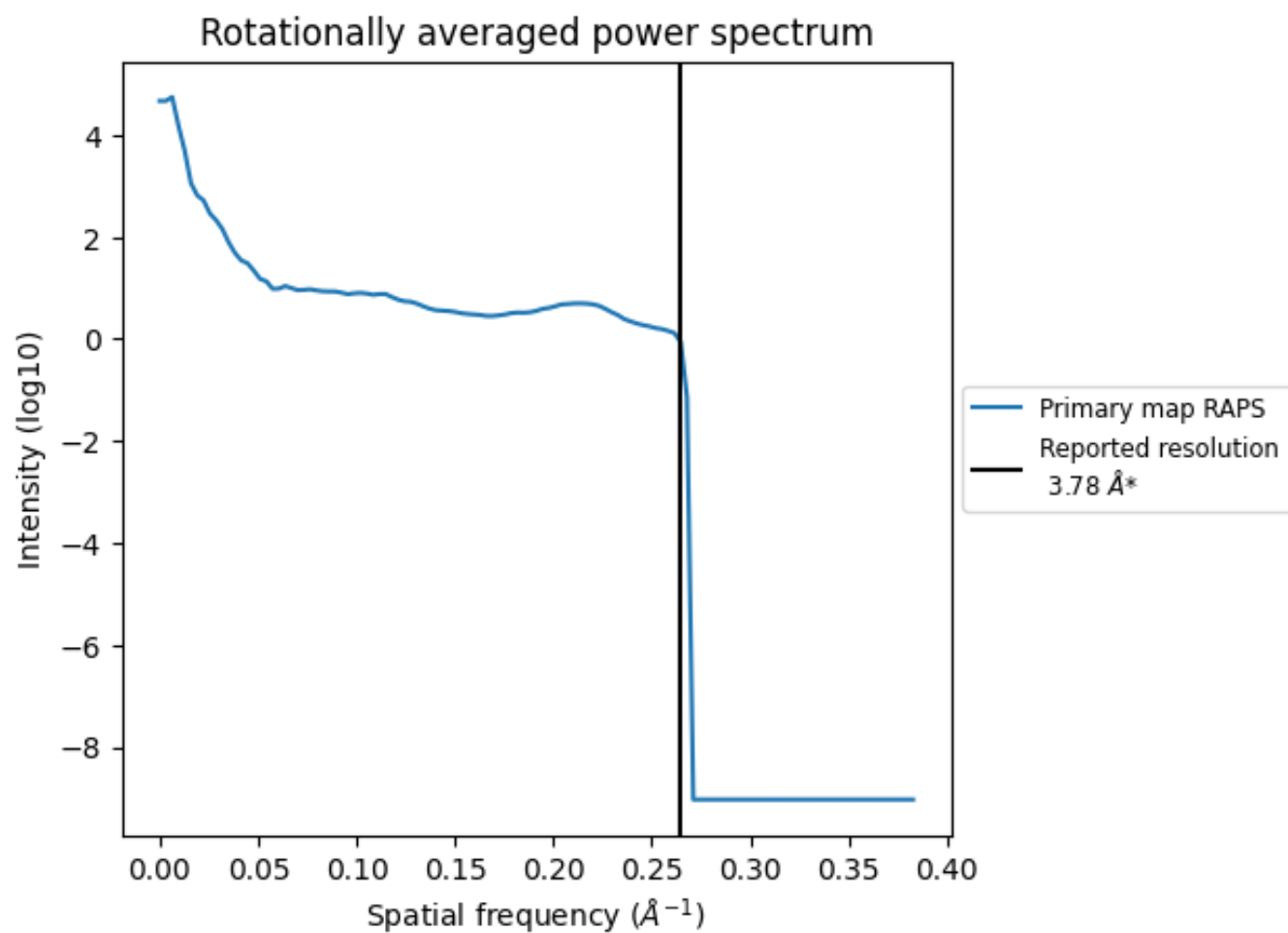
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 277 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 0.265 Å⁻¹

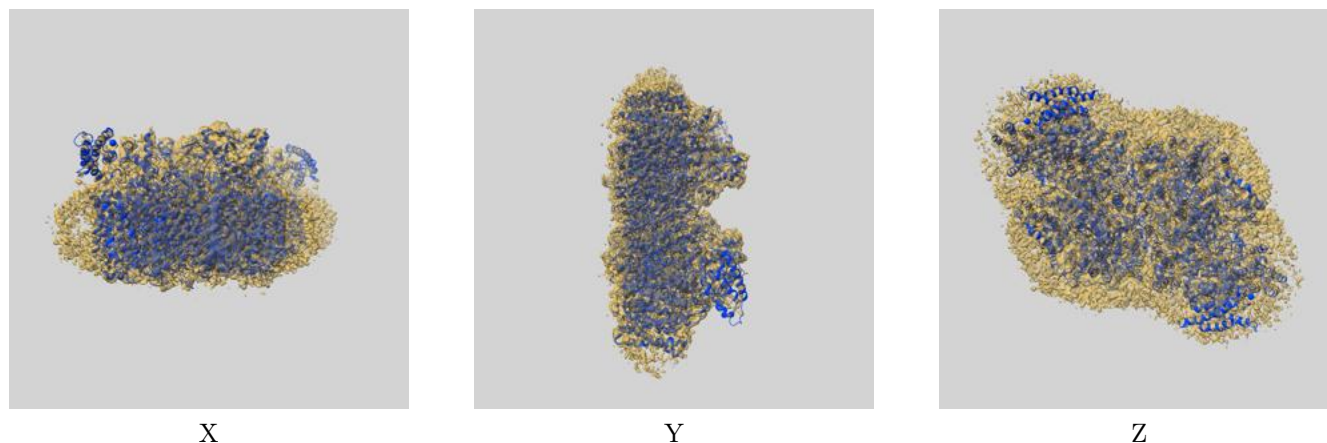
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

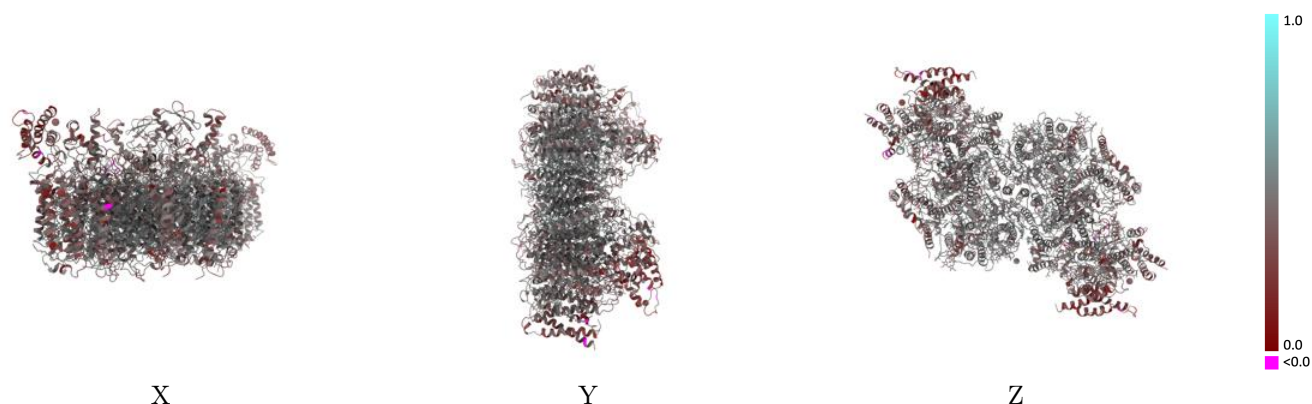
This section contains information regarding the fit between EMDB map EMD-30511 and PDB model 7CZL. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



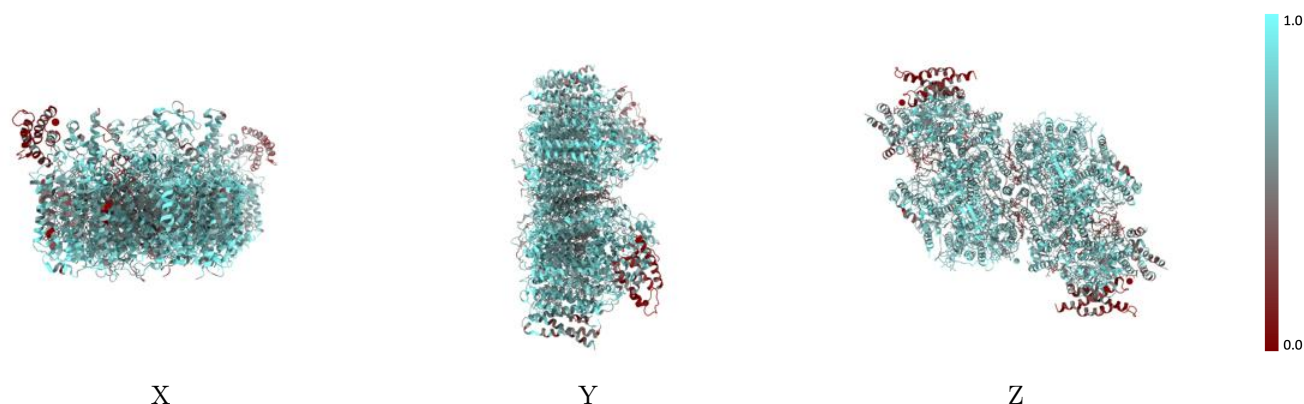
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



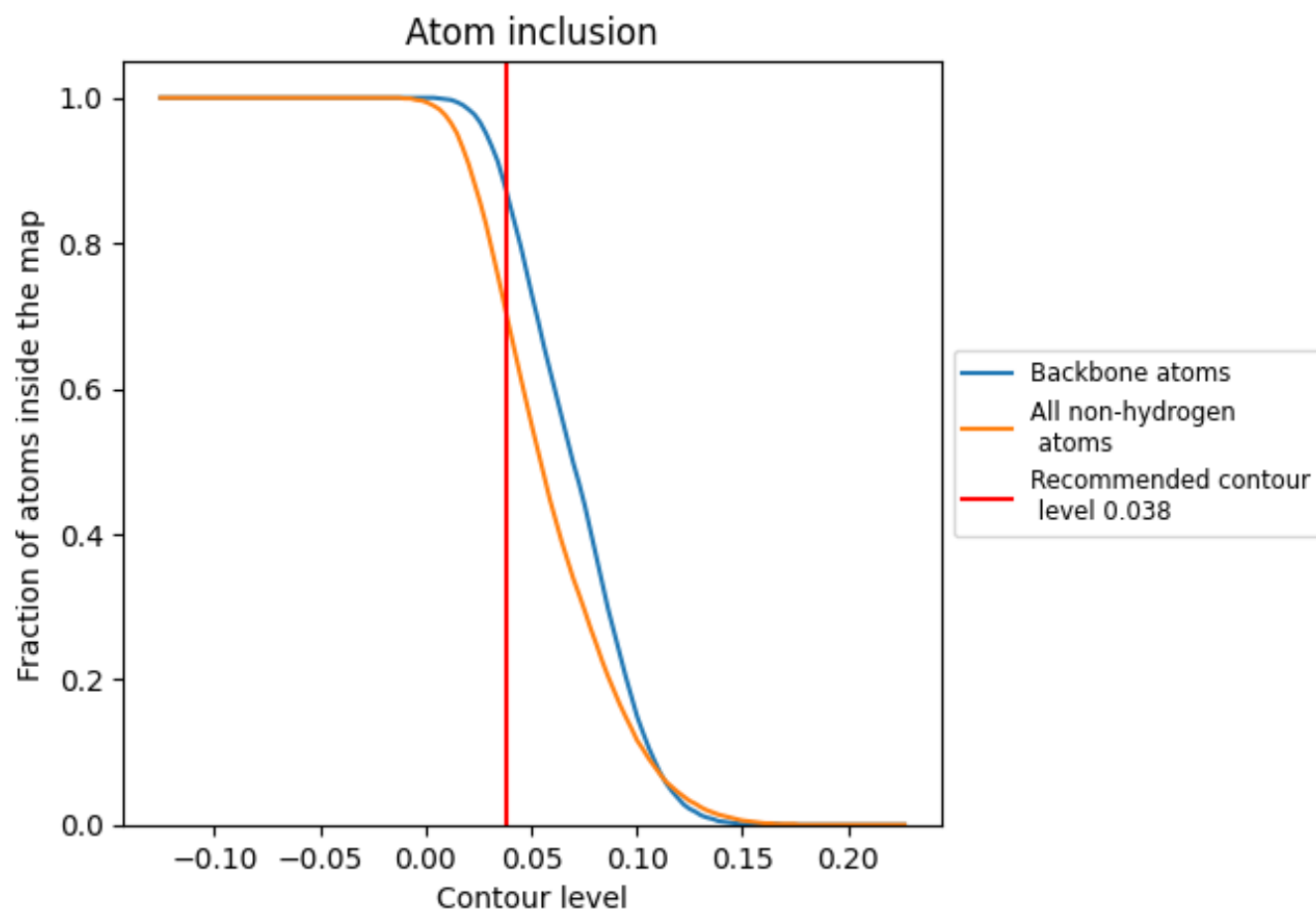
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4220
A	 0.7320	 0.4420
B	 0.7710	 0.4490
C	 0.6990	 0.4070
D	 0.7690	 0.4500
E	 0.6800	 0.3720
F	 0.7410	 0.3800
H	 0.8110	 0.4300
I	 0.7650	 0.4150
K	 0.6700	 0.3670
L	 0.6960	 0.4470
M	 0.6060	 0.4270
N	 0.2210	 0.2790
T	 0.6080	 0.4550
X	 0.7360	 0.3700
Y	 0.4900	 0.3980
Z	 0.5290	 0.3190
a	 0.7330	 0.4390
b	 0.7750	 0.4510
c	 0.7080	 0.4070
d	 0.7670	 0.4470
e	 0.6860	 0.3680
f	 0.7410	 0.3550
h	 0.7890	 0.4260
i	 0.7680	 0.4200
k	 0.6530	 0.4010
l	 0.6610	 0.4700
m	 0.5950	 0.4350
n	 0.2060	 0.2740
t	 0.6630	 0.4710
x	 0.7640	 0.3980
y	 0.5020	 0.3350
z	 0.5150	 0.3210

