



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:01 AM UTC

PDB ID : 8ZK2 / pdb_00008zk2
EMDB ID : EMD-60165
Title : Cryo-EM structure of photosynthetic LH1-RC core complex of *Roseospirillum parvum*
Authors : Wang, G.-L.; Wang, X.-P.; Yu, L.-J.
Deposited on : 2024-05-15
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

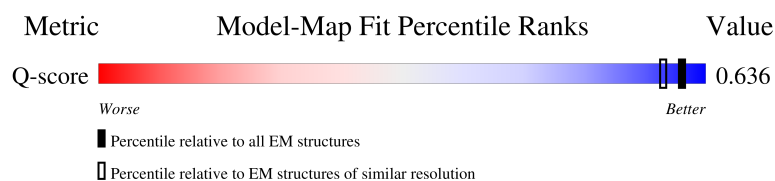
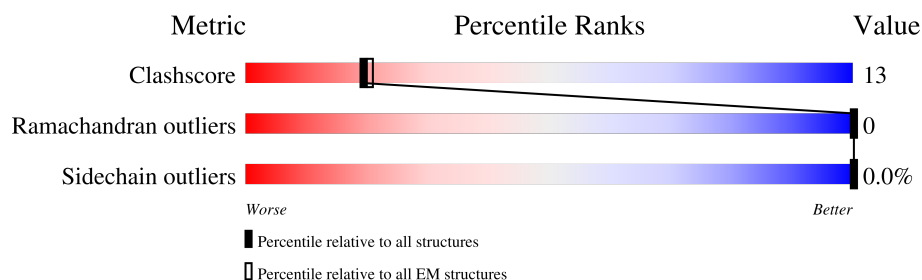
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

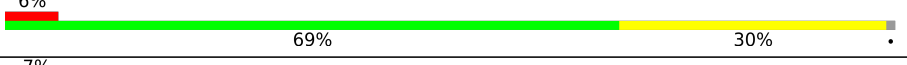
The reported resolution of this entry is 2.65 Å.

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	9050 (2.15 - 3.15)

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	C	362	
2	L	275	
3	M	323	
4	H	254	

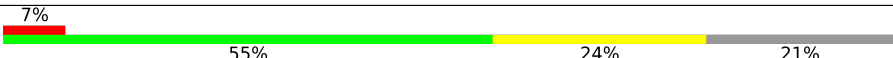
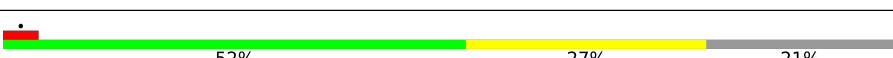
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Mol	Chain	Length	Quality of chain
5	B	68	
5	D	68	
5	F	68	
5	I	68	
5	K	68	
5	O	68	
5	Q	68	
5	S	68	
5	U	68	
5	W	68	
5	Y	68	
5	a	68	
5	c	68	
5	e	68	
5	g	68	
5	i	68	
6	A	67	
6	E	67	
6	G	67	
6	J	67	
6	N	67	
6	P	67	
6	R	67	
6	T	67	
6	V	67	

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Mol	Chain	Length	Quality of chain
6	X	67	
6	Z	67	
6	b	67	
6	d	67	
6	f	67	
6	h	67	
6	j	67	

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
9	PGV	L	410	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26948 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	342	Total	C	N	O	S	0	0
			2618	1646	446	501	25		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	273	Total	C	N	O	S	0	0
			2163	1458	344	350	11		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	287	Total	C	N	O	S	0	0
			2269	1514	369	376	10		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	245	Total	C	N	O	S	0	0
			1906	1214	327	357	8		

- Molecule 5 is a protein called Beta subunit of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	D	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	F	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	I	49	Total	C	N	O	S	0	0
			377	248	62	65	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	O	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	Q	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	S	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	U	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	W	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	Y	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	a	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	c	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	e	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	g	49	Total	C	N	O	S	0	0
			377	248	62	65	2		
5	i	49	Total	C	N	O	S	0	0
			377	248	62	65	2		

- Molecule 6 is a protein called Alpha subunit of light-harvesting 1 complex.

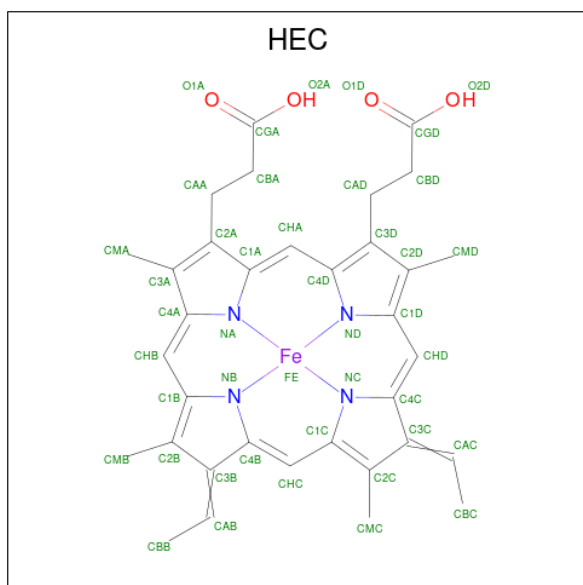
Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	E	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	G	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	J	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	N	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	P	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	R	53	Total	C	N	O	S	0	0
			424	283	71	67	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	V	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	X	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	Z	46	Total	C	N	O	S	0	0
			369	248	63	56	2		
6	b	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	d	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	f	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	h	53	Total	C	N	O	S	0	0
			424	283	71	67	3		
6	j	53	Total	C	N	O	S	0	0
			424	283	71	67	3		

- Molecule 7 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

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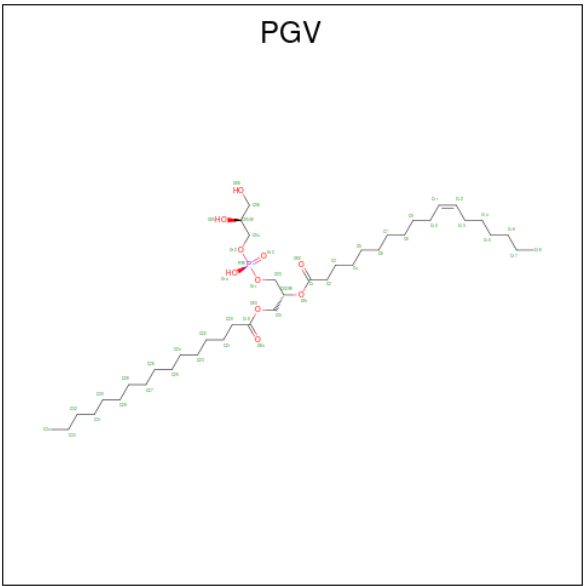
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Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	C	3	Total	Mg	0
			3	3	
8	H	1	Total	Mg	0
			1	1	

- Molecule 9 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



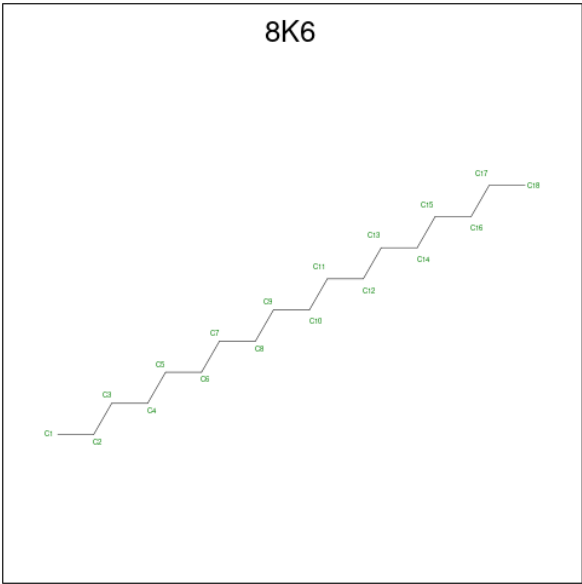
Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	O	P	0
			38	27	10	1	
9	L	1	Total	C	O		0
			22	17	5		
9	M	1	Total	C	O	P	0
			46	37	8	1	
9	M	1	Total	C	O	P	0
			42	33	8	1	

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Mol	Chain	Residues	Atoms				AltConf
9	H	1	Total	C	O	P	0
			51	40	10	1	
9	H	1	Total	C	O	P	0
			51	40	10	1	
9	R	1	Total	C	O	P	0
			51	40	10	1	
9	Z	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 10 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).



Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	C	0
			16	16	
10	L	1	Total	C	0
			15	15	
10	L	1	Total	C	0
			18	18	
10	L	1	Total	C	0
			18	18	
10	L	1	Total	C	0
			18	18	
10	L	1	Total	C	0
			18	18	
10	M	1	Total	C	0
			18	18	

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Mol	Chain	Residues	Atoms	AltConf
10	H	1	Total C 17 17	0
10	H	1	Total C 18 18	0
10	H	1	Total C 18 18	0
10	H	1	Total C 15 15	0
10	J	1	Total C 13 13	0
10	J	1	Total C 18 18	0
10	N	1	Total C 18 18	0
10	P	1	Total C 18 18	0
10	V	1	Total C 18 18	0
10	V	1	Total C 18 18	0
10	X	1	Total C 18 18	0
10	d	1	Total C 18 18	0
10	f	1	Total C 18 18	0
10	j	1	Total C 18 18	0
10	j	1	Total C 18 18	0

- Molecule 11 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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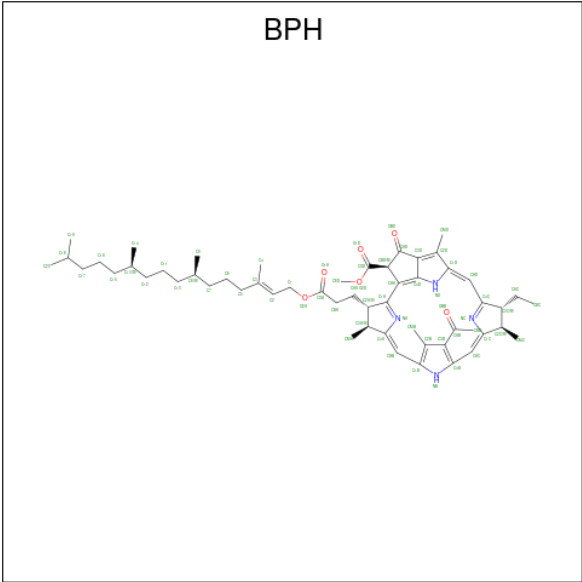
Mol	Chain	Residues	Atoms					AltConf
11	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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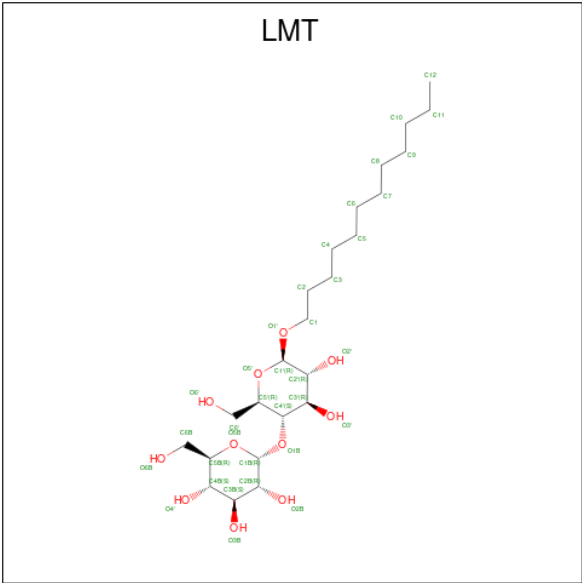
Mol	Chain	Residues	Atoms					AltConf
11	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 12 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			65	55	4	6	
12	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 13 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



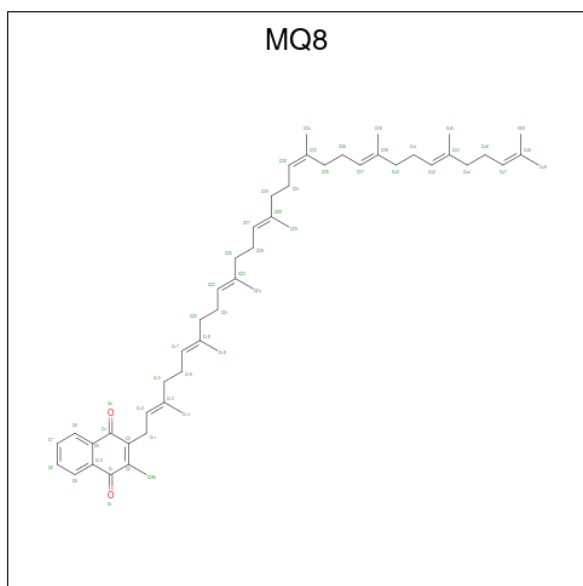
Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			32	21	11	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest")

by depositor).

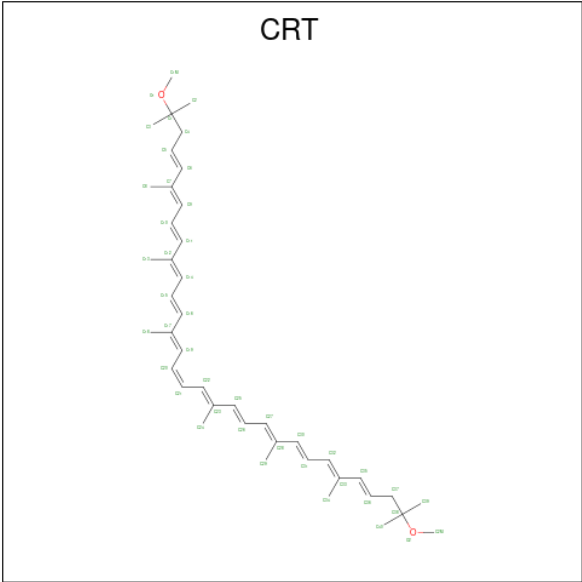
Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			53	51	2	

- Molecule 16 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			44	42	2	
16	B	1	Total	C	O	0
			44	42	2	
16	A	1	Total	C	O	0
			44	42	2	
16	E	1	Total	C	O	0
			44	42	2	
16	I	1	Total	C	O	0
			44	42	2	
16	K	1	Total	C	O	0
			44	42	2	
16	N	1	Total	C	O	0
			44	42	2	
16	P	1	Total	C	O	0
			44	42	2	
16	R	1	Total	C	O	0
			44	42	2	
16	U	1	Total	C	O	0
			44	42	2	
16	W	1	Total	C	O	0
			44	42	2	
16	Y	1	Total	C	O	0
			44	42	2	
16	Z	1	Total	C	O	0
			44	42	2	
16	a	1	Total	C	O	0
			44	42	2	

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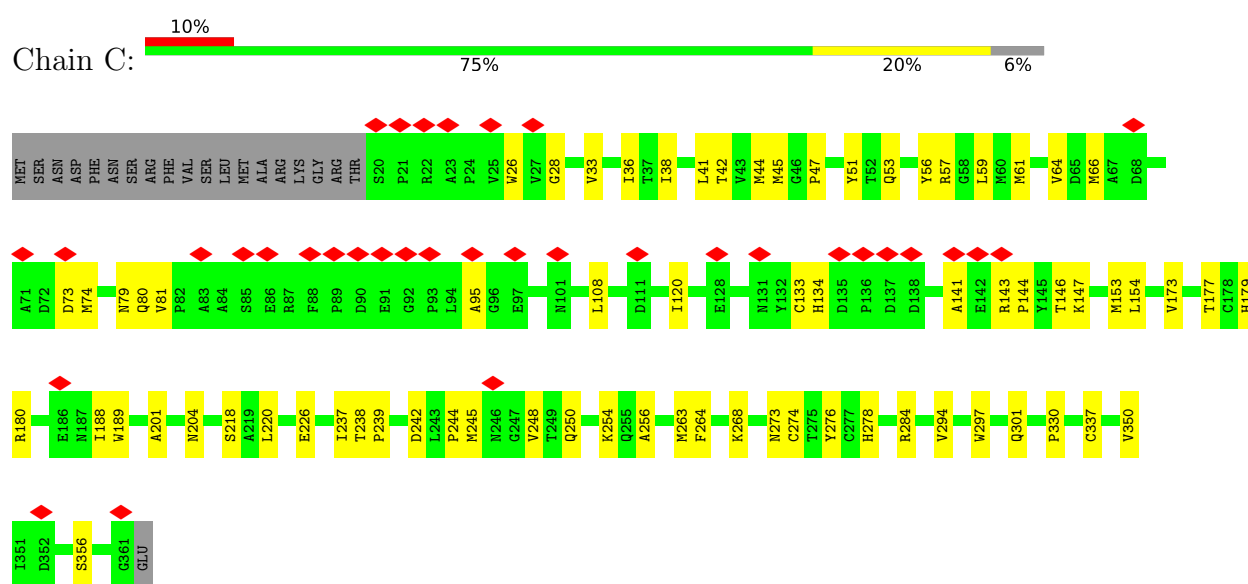
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Mol	Chain	Residues	Atoms			AltConf
16	e	1	Total	C	O	0
			44	42	2	
16	i	1	Total	C	O	0
			44	42	2	
16	j	1	Total	C	O	0
			44	42	2	

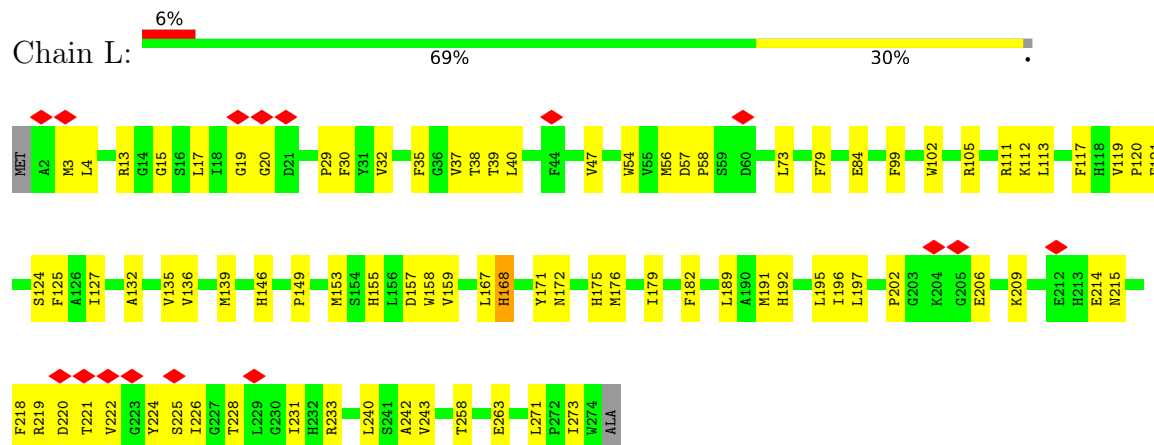
3 Residue-property plots

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

- Molecule 1: Photosynthetic reaction center cytochrome c subunit

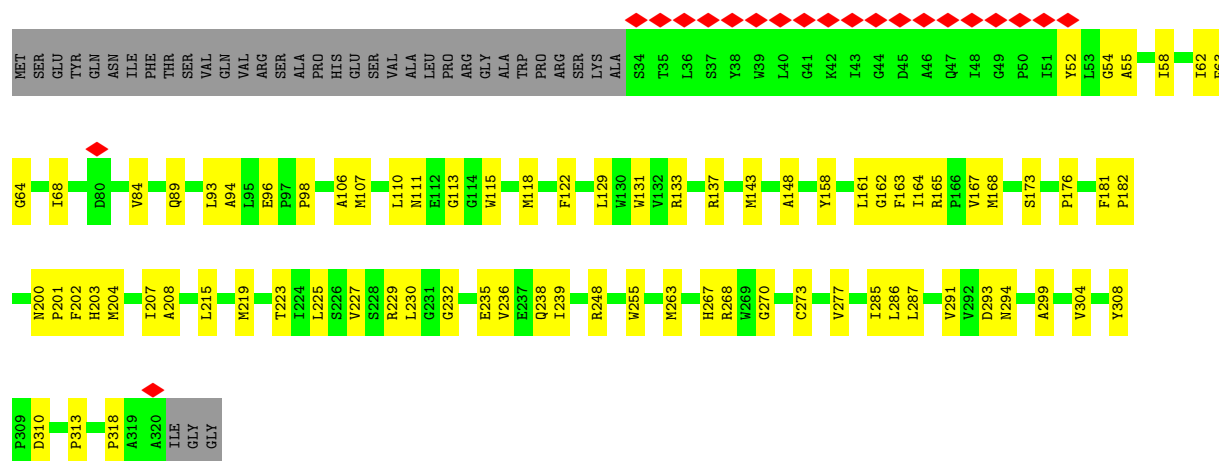


- Molecule 2: Reaction center protein L chain

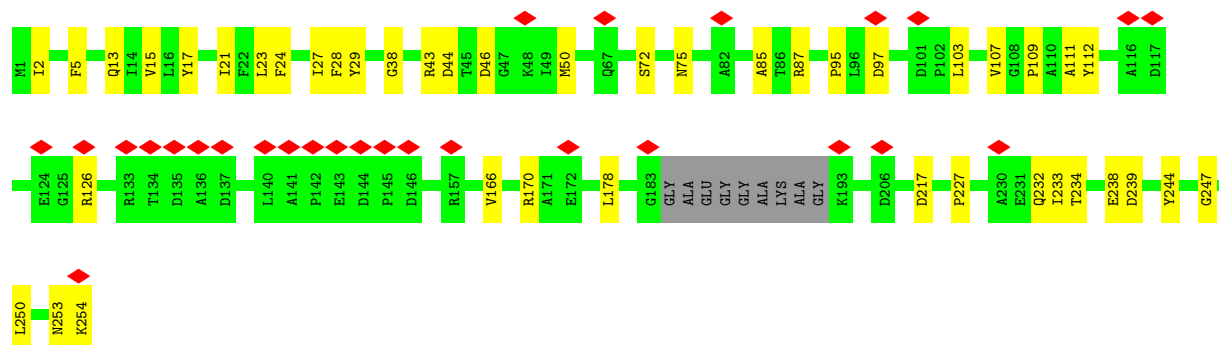
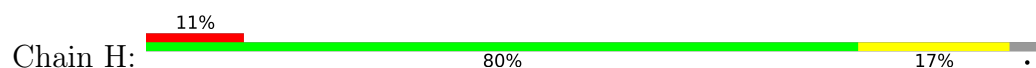


- Molecule 3: Reaction center protein M chain

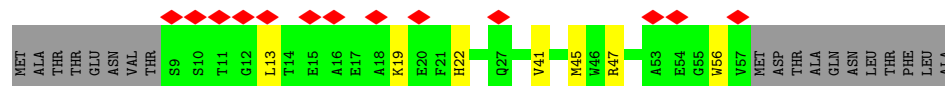




• Molecule 4: Photosynthetic reaction center H subunit



• Molecule 5: Beta subunit of light-harvesting 1 complex



• Molecule 5: Beta subunit of light-harvesting 1 complex

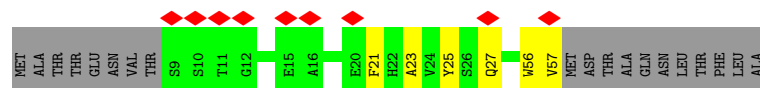


• Molecule 5: Beta subunit of light-harvesting 1 complex





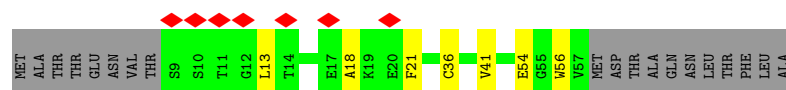
- Molecule 5: Beta subunit of light-harvesting 1 complex



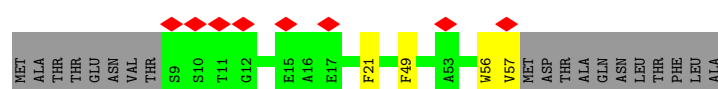
- Molecule 5: Beta subunit of light-harvesting 1 complex



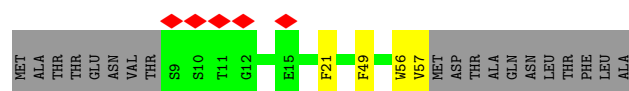
- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



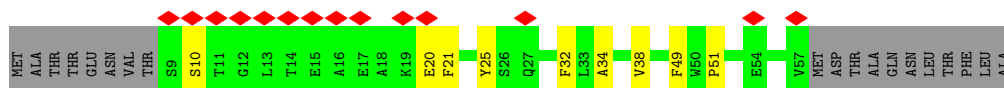
- Molecule 5: Beta subunit of light-harvesting 1 complex



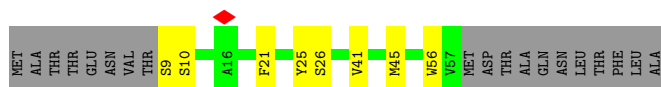
- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



- Molecule 5: Beta subunit of light-harvesting 1 complex



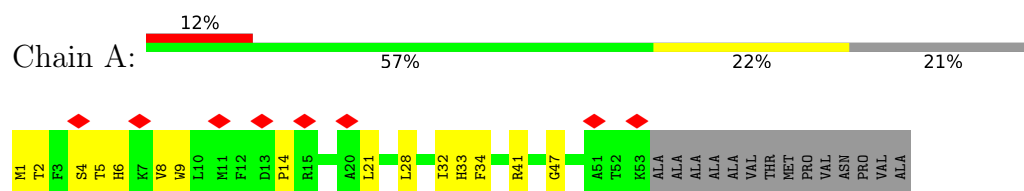
- Molecule 5: Beta subunit of light-harvesting 1 complex



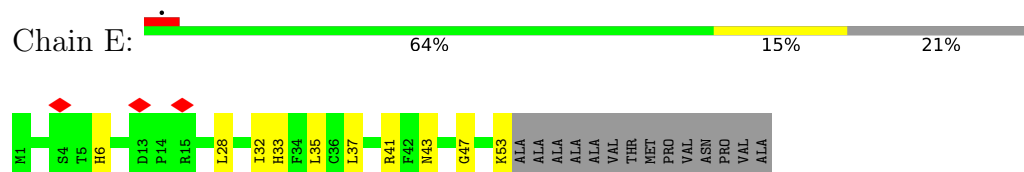
- Molecule 5: Beta subunit of light-harvesting 1 complex



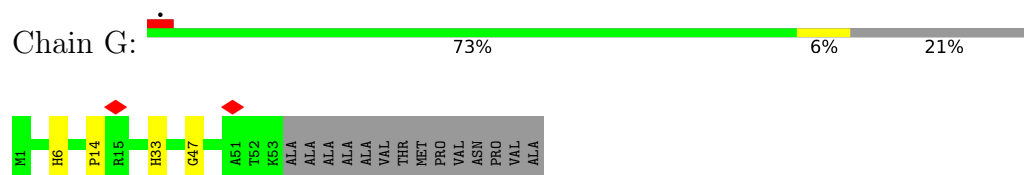
- Molecule 6: Alpha subunit of light-harvesting 1 complex



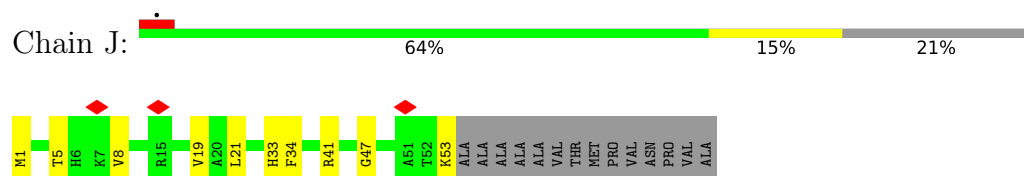
- Molecule 6: Alpha subunit of light-harvesting 1 complex



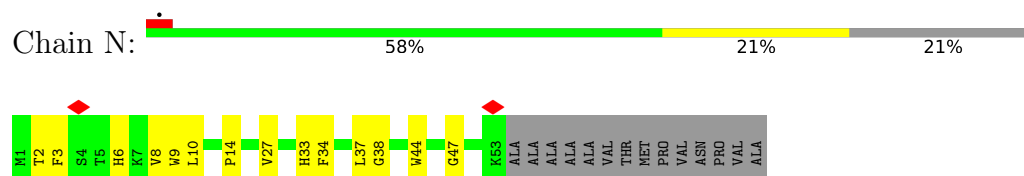
- Molecule 6: Alpha subunit of light-harvesting 1 complex



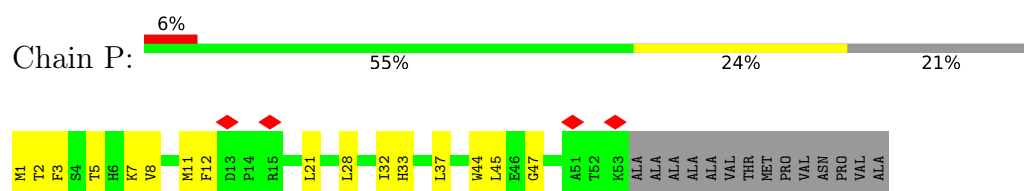
- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex

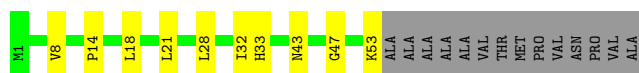


- Molecule 6: Alpha subunit of light-harvesting 1 complex

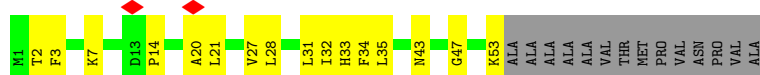


- Molecule 6: Alpha subunit of light-harvesting 1 complex





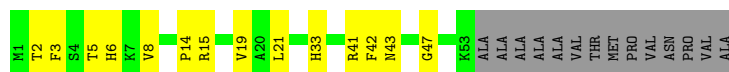
- Molecule 6: Alpha subunit of light-harvesting 1 complex



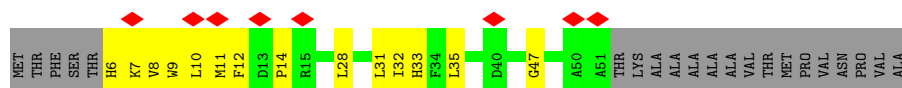
- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



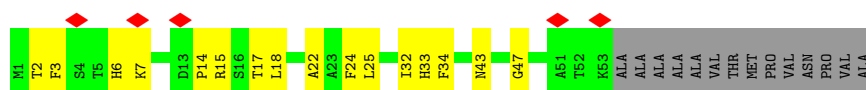
- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



- Molecule 6: Alpha subunit of light-harvesting 1 complex



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.289	Depositor
Minimum map value	-1.682	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.562	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FE, 8K6, PGV, BPH, MG, MQ8, LMT, BCL, CRT

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	C	0.19	0/2693	0.42	0/3681
2	L	0.26	0/2250	0.45	0/3075
3	M	0.26	0/2357	0.43	0/3230
4	H	0.18	0/1952	0.37	0/2658
5	B	0.15	0/392	0.42	0/537
5	D	0.15	0/392	0.36	0/537
5	F	0.16	0/392	0.42	0/537
5	I	0.18	0/392	0.47	0/537
5	K	0.15	0/392	0.36	0/537
5	O	0.15	0/392	0.40	0/537
5	Q	0.17	0/392	0.38	0/537
5	S	0.25	0/392	0.39	0/537
5	U	0.16	0/392	0.34	0/537
5	W	0.19	0/392	0.43	0/537
5	Y	0.14	0/392	0.37	0/537
5	a	0.16	0/392	0.34	0/537
5	c	0.15	0/392	0.34	0/537
5	e	0.18	0/392	0.42	0/537
5	g	0.15	0/392	0.37	0/537
5	i	0.17	0/392	0.36	0/537
6	A	0.36	0/437	0.59	0/595
6	E	0.37	0/437	0.53	0/595
6	G	0.25	0/437	0.44	0/595
6	J	0.20	0/437	0.41	0/595
6	N	0.20	0/437	0.41	0/595
6	P	0.22	0/437	0.46	0/595
6	R	0.19	0/437	0.40	0/595
6	T	0.16	0/437	0.37	0/595
6	V	0.19	0/437	0.38	0/595
6	X	0.20	0/437	0.41	0/595
6	Z	0.27	0/381	0.59	1/520 (0.2%)
6	b	0.17	0/437	0.38	0/595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	d	0.18	0/437	0.42	0/595
6	f	0.20	0/437	0.42	0/595
6	h	0.19	0/437	0.38	0/595
6	j	0.26	0/437	0.44	0/595
All	All	0.21	0/22460	0.42	1/30681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	10	LEU	N-CA-C	-5.62	106.09	113.17

There are no chirality outliers.

There are no planarity outliers.

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	C	2618	0	2465	65	0
2	L	2163	0	2111	118	0
3	M	2269	0	2210	67	0
4	H	1906	0	1894	32	0
5	B	377	0	349	6	0
5	D	377	0	349	5	0
5	F	377	0	349	12	0
5	I	377	0	349	8	0
5	K	377	0	349	12	0
5	O	377	0	349	7	0
5	Q	377	0	349	5	0
5	S	377	0	349	4	0
5	U	377	0	349	7	0
5	W	377	0	349	6	0
5	Y	377	0	349	11	0
5	a	377	0	349	7	0
5	c	377	0	349	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	377	0	349	5	0
5	g	377	0	349	9	0
5	i	377	0	349	9	0
6	A	424	0	434	15	0
6	E	424	0	434	9	0
6	G	424	0	434	5	0
6	J	424	0	434	12	0
6	N	424	0	434	15	0
6	P	424	0	434	12	0
6	R	424	0	434	10	0
6	T	424	0	434	16	0
6	V	424	0	434	15	0
6	X	424	0	434	13	0
6	Z	369	0	374	14	0
6	b	424	0	434	17	0
6	d	424	0	434	20	0
6	f	424	0	434	14	0
6	h	424	0	434	17	0
6	j	424	0	434	19	0
7	C	172	0	120	16	0
8	C	3	0	0	0	0
8	H	1	0	0	0	0
9	C	38	0	47	0	0
9	H	102	0	152	12	0
9	L	22	0	25	40	0
9	M	88	0	127	11	0
9	R	51	0	76	2	0
9	Z	42	0	55	3	0
10	C	16	0	31	2	0
10	H	68	0	138	4	0
10	J	31	0	63	2	0
10	L	87	0	181	12	0
10	M	18	0	38	0	0
10	N	18	0	38	4	0
10	P	18	0	38	2	0
10	V	36	0	76	2	0
10	X	18	0	38	1	0
10	d	18	0	38	1	0
10	f	18	0	38	3	0
10	j	36	0	76	2	0
11	A	132	0	148	7	0
11	B	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	66	0	74	4	0
11	E	132	0	148	4	0
11	F	66	0	74	3	0
11	G	132	0	148	6	0
11	I	66	0	74	5	0
11	J	132	0	148	5	0
11	K	66	0	74	5	0
11	L	132	0	148	10	0
11	M	132	0	148	2	0
11	N	132	0	148	4	0
11	O	66	0	74	6	0
11	P	132	0	148	6	0
11	Q	66	0	74	4	0
11	R	132	0	148	5	0
11	S	66	0	74	2	0
11	T	132	0	148	7	0
11	U	66	0	74	5	0
11	V	132	0	148	3	0
11	W	66	0	74	3	0
11	X	132	0	148	8	0
11	Y	66	0	74	4	0
11	Z	66	0	74	3	0
11	a	66	0	74	4	0
11	b	132	0	148	7	0
11	c	66	0	74	7	0
11	d	132	0	148	7	0
11	e	66	0	74	1	0
11	f	132	0	148	11	0
11	g	66	0	74	5	0
11	h	132	0	148	8	0
11	i	66	0	74	7	0
11	j	132	0	148	6	0
12	L	65	0	76	4	0
12	M	65	0	76	3	0
13	L	32	0	37	0	0
14	M	1	0	0	0	0
15	M	53	0	72	7	0
16	A	44	0	60	6	0
16	B	44	0	60	4	0
16	E	44	0	60	10	0
16	I	44	0	60	10	0
16	K	44	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	44	0	60	3	0
16	N	44	0	60	6	0
16	P	44	0	60	7	0
16	R	44	0	60	8	0
16	U	44	0	60	8	0
16	W	44	0	60	5	0
16	Y	44	0	60	7	0
16	Z	44	0	60	15	0
16	a	44	0	60	5	0
16	e	44	0	60	5	0
16	i	44	0	60	8	0
16	j	44	0	60	8	0
All	All	26948	0	27598	686	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 13.

All (686) 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)
2:L:195:LEU:HD23	9:L:410:PGV:H221	1.30	1.11
2:L:228:THR:HG22	9:L:410:PGV:H241	1.33	1.08
4:H:250:LEU:O	4:H:254:LYS:HD2	1.51	1.06
2:L:195:LEU:HD13	2:L:218:PHE:CE2	1.97	1.00
2:L:192:HIS:HA	9:L:410:PGV:H202	1.43	0.97
2:L:231:ILE:HG12	9:L:410:PGV:H211	1.47	0.97
2:L:191:MET:HE3	2:L:218:PHE:HE1	1.35	0.91
2:L:191:MET:CE	2:L:218:PHE:HE1	1.83	0.91
2:L:192:HIS:HD1	9:L:410:PGV:H222	1.36	0.91
2:L:191:MET:HE3	2:L:218:PHE:CE1	2.10	0.87
2:L:192:HIS:HE1	9:L:410:PGV:H251	1.44	0.83
2:L:195:LEU:HD22	9:L:410:PGV:H201	1.62	0.81
9:L:410:PGV:O02	9:L:410:PGV:H212	1.80	0.81
9:L:410:PGV:H232	9:L:410:PGV:H42	1.62	0.81
2:L:228:THR:HG23	9:L:410:PGV:H51	1.61	0.81
9:H:302:PGV:H21	6:T:34:PHE:HB3	1.63	0.80
2:L:228:THR:CG2	9:L:410:PGV:H51	2.11	0.79
5:Q:57:VAL:HG12	6:R:53:LYS:HG2	1.66	0.78
11:Y:101:BCL:H3A	11:Y:101:BCL:H2	1.66	0.77
2:L:192:HIS:ND1	9:L:410:PGV:H222	2.01	0.76
6:Z:8:VAL:HG22	16:Z:102:CRT:H5	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:101:BCL:H3A	11:Q:101:BCL:H2	1.67	0.76
3:M:94:ALA:HB2	3:M:182:PRO:HG2	1.67	0.75
2:L:214:GLU:HB3	9:L:410:PGV:H41	1.68	0.75
16:U:102:CRT:H82	6:X:8:VAL:HG22	1.69	0.74
2:L:195:LEU:CD2	9:L:410:PGV:H221	2.16	0.73
16:R:103:CRT:H82	6:V:8:VAL:HB	1.69	0.73
16:E:103:CRT:H182	11:G:101:BCL:H72	1.70	0.73
11:I:101:BCL:H3A	11:I:101:BCL:H2	1.70	0.73
16:Z:102:CRT:H21A	5:c:24:VAL:HG21	1.72	0.72
2:L:195:LEU:HD22	2:L:218:PHE:HE2	1.56	0.71
2:L:226:ILE:HG22	9:L:410:PGV:O02	1.91	0.71
1:C:268:LYS:NZ	2:L:263:GLU:OE2	2.24	0.69
2:L:228:THR:HG22	9:L:410:PGV:C24	2.18	0.69
11:c:101:BCL:H2	11:c:101:BCL:H3A	1.74	0.69
2:L:228:THR:HG23	9:L:410:PGV:C5	2.23	0.69
11:R:101:BCL:HED1	11:T:102:BCL:H11	1.75	0.69
6:d:22:ALA:HB2	11:d:101:BCL:H8	1.75	0.68
11:i:101:BCL:H12	16:i:102:CRT:H27	1.76	0.68
16:i:102:CRT:H182	11:j:102:BCL:H72	1.76	0.67
1:C:254:LYS:HD3	3:M:173:SER:HB2	1.78	0.66
5:W:41:VAL:HG12	5:W:45:MET:HE2	1.78	0.66
4:H:15:VAL:HG13	9:R:104:PGV:H152	1.78	0.65
1:C:264:PHE:HZ	2:L:168:HIS:HB2	1.61	0.65
2:L:3:MET:HE1	4:H:50:MET:HE1	1.77	0.65
2:L:195:LEU:HD22	2:L:218:PHE:CE2	2.32	0.64
2:L:195:LEU:HD13	2:L:218:PHE:HE2	1.55	0.64
1:C:153:MET:HG3	7:C:502:HEC:C1B	2.28	0.64
10:L:409:8K6:H112	15:M:405:MQ8:H271	1.80	0.64
6:N:37:LEU:HD13	10:N:104:8K6:H142	1.80	0.64
3:M:52:TYR:O	3:M:133:ARG:NH2	2.31	0.64
1:C:330:PRO:HB2	7:C:502:HEC:HAD2	1.80	0.63
5:K:24:VAL:HG11	16:K:102:CRT:H81	1.79	0.63
9:H:302:PGV:H061	6:T:43:ASN:HD22	1.61	0.63
9:M:407:PGV:H231	9:M:407:PGV:H42	1.80	0.63
1:C:273:ASN:HA	2:L:167:LEU:HD21	1.78	0.63
9:M:407:PGV:H261	9:R:104:PGV:H221	1.79	0.63
2:L:192:HIS:HD1	9:L:410:PGV:C22	2.10	0.63
2:L:135:VAL:HG12	2:L:139:MET:HE2	1.81	0.63
5:K:49:PHE:CE1	11:K:101:BCL:H141	2.34	0.62
2:L:219:ARG:HG3	2:L:225:SER:HB3	1.80	0.62
2:L:214:GLU:HB3	9:L:410:PGV:C4	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:13:LEU:HD11	6:A:14:PRO:HG2	1.80	0.62
5:U:41:VAL:HG12	5:U:45:MET:HE2	1.82	0.61
5:c:14:THR:HB	5:c:17:GLU:HG3	1.82	0.61
5:c:21:PHE:HZ	6:d:18:LEU:HD11	1.64	0.61
1:C:73:ASP:O	1:C:79:ASN:ND2	2.34	0.61
5:i:41:VAL:HG12	5:i:45:MET:HE2	1.81	0.61
4:H:109:PRO:HB2	4:H:247:GLY:HA2	1.82	0.61
6:h:7:LYS:HE2	16:i:102:CRT:H22A	1.82	0.61
16:I:102:CRT:H82	6:N:8:VAL:HG22	1.83	0.61
2:L:121:PHE:HB2	10:L:405:8K6:H61C	1.82	0.61
16:B:102:CRT:H372	6:Z:33:HIS:CG	2.35	0.61
2:L:117:PHE:HB2	10:L:405:8K6:H52C	1.83	0.60
5:a:41:VAL:HG12	5:a:45:MET:HE2	1.83	0.60
4:H:217:ASP:OD1	4:H:253:ASN:ND2	2.35	0.60
16:Y:102:CRT:H182	11:Z:101:BCL:H71	1.83	0.60
16:e:102:CRT:H243	6:f:21:LEU:HD11	1.82	0.60
2:L:39:THR:HG21	2:L:102:TRP:HE3	1.67	0.60
5:D:41:VAL:HG12	5:D:45:MET:HE2	1.83	0.60
2:L:32:VAL:HG22	15:M:405:MQ8:H411	1.84	0.60
10:L:407:8K6:H162	10:V:103:8K6:H162	1.84	0.60
5:D:57:VAL:HG22	6:E:53:LYS:HG2	1.84	0.59
11:a:101:BCL:H2	11:a:101:BCL:H3A	1.82	0.59
2:L:231:ILE:HG21	9:L:410:PGV:H231	1.84	0.59
2:L:19:GLY:O	6:j:15:ARG:NH1	2.35	0.59
2:L:195:LEU:CD2	9:L:410:PGV:H201	2.31	0.58
12:M:404:BPH:H4C1	12:M:404:BPH:H7C1	1.84	0.58
11:h:101:BCL:H72	16:j:101:CRT:H182	1.84	0.58
1:C:189:TRP:HZ3	1:C:226:GLU:HG3	1.67	0.58
16:Z:102:CRT:H1M2	5:c:21:PHE:HD2	1.68	0.58
11:f:102:BCL:H102	11:f:102:BCL:H2	1.84	0.58
3:M:62:ILE:HG23	10:J:104:8K6:H152	1.85	0.58
6:A:33:HIS:CG	16:A:103:CRT:H372	2.39	0.58
16:E:103:CRT:H41	5:F:24:VAL:HG21	1.86	0.58
5:K:41:VAL:HG12	5:K:45:MET:HE2	1.86	0.58
1:C:244:PRO:HB2	4:H:2:ILE:HD12	1.84	0.58
6:N:33:HIS:CG	16:N:103:CRT:H372	2.38	0.58
16:R:103:CRT:H22A	6:V:7:LYS:HB2	1.85	0.58
6:Z:7:LYS:H	16:Z:102:CRT:H23	1.68	0.58
6:h:2:THR:HG22	6:h:3:PHE:H	1.68	0.58
5:Y:49:PHE:CE1	11:Y:101:BCL:H141	2.39	0.58
6:Z:9:TRP:HB3	6:Z:14:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:102:CRT:H182	11:J:101:BCL:H72	1.85	0.58
11:T:101:BCL:H18	6:V:17:THR:HG23	1.85	0.58
6:V:47:GLY:HA3	5:W:56:TRP:CD1	2.39	0.58
5:B:56:TRP:CD1	6:Z:47:GLY:HA3	2.39	0.57
16:Z:102:CRT:H81	16:Z:102:CRT:H11	1.85	0.57
9:L:410:PGV:H232	9:L:410:PGV:C4	2.33	0.57
5:i:47:ARG:NH1	6:j:41:ARG:O	2.32	0.57
6:A:8:VAL:HG22	16:Y:102:CRT:H82	1.86	0.57
6:E:47:GLY:HA3	5:F:56:TRP:CD1	2.39	0.57
6:h:19:VAL:HG23	11:h:101:BCL:H193	1.87	0.57
1:C:179:HIS:HE1	7:C:502:HEC:C1A	2.16	0.57
6:d:25:LEU:HD12	11:d:101:BCL:H62	1.86	0.57
1:C:153:MET:HE3	7:C:502:HEC:C4D	2.33	0.57
6:b:46:GLU:O	6:j:53:LYS:NZ	2.38	0.57
3:M:107:MET:HE1	3:M:118:MET:HG3	1.87	0.57
6:J:1:MET:HE2	6:J:8:VAL:HG11	1.87	0.57
5:e:47:ARG:NH1	6:f:41:ARG:O	2.37	0.56
5:c:19:LYS:HA	6:d:6:HIS:HB2	1.87	0.56
5:e:23:ALA:O	5:e:27:GLN:HG3	2.05	0.56
6:A:2:THR:HG22	6:A:5:THR:HG23	1.85	0.56
5:e:41:VAL:HG12	5:e:45:MET:HE2	1.87	0.56
6:f:1:MET:SD	6:f:8:VAL:HG11	2.44	0.56
11:W:101:BCL:H12	16:W:102:CRT:H27	1.87	0.56
3:M:106:ALA:HB2	6:N:38:GLY:HA3	1.88	0.56
6:P:47:GLY:HA3	5:Q:56:TRP:CD1	2.40	0.56
5:D:47:ARG:NH1	6:E:41:ARG:O	2.35	0.56
3:M:158:TYR:CZ	16:M:406:CRT:H293	2.40	0.55
3:M:55:ALA:HB3	9:M:408:PGV:H332	1.88	0.55
6:Z:6:HIS:HB3	6:Z:8:VAL:HG23	1.89	0.55
5:B:41:VAL:HG12	5:B:45:MET:HE2	1.88	0.55
6:J:33:HIS:CG	16:K:102:CRT:H372	2.41	0.55
6:h:11:MET:O	6:j:15:ARG:NE	2.36	0.55
5:F:54:GLU:OE1	5:F:57:VAL:HG22	2.06	0.55
2:L:29:PRO:HG3	10:L:409:8K6:H42C	1.87	0.55
11:L:401:BCL:H142	9:H:301:PGV:H141	1.89	0.55
6:E:33:HIS:CG	16:E:103:CRT:H372	2.42	0.55
5:Y:10:SER:HB2	6:Z:11:MET:HA	1.89	0.55
6:d:2:THR:HG22	6:d:3:PHE:H	1.70	0.55
6:Z:31:LEU:HD13	9:Z:103:PGV:H62	1.89	0.55
2:L:226:ILE:HG22	9:L:410:PGV:H02	1.88	0.55
6:T:2:THR:HG22	6:T:3:PHE:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:101:BCL:H143	6:j:1:MET:HE3	1.89	0.55
6:d:7:LYS:HE3	16:e:102:CRT:H22A	1.88	0.55
11:i:101:BCL:H3A	11:i:101:BCL:H2	1.88	0.55
3:M:299:ALA:HB1	3:M:304:VAL:HB	1.90	0.54
16:U:102:CRT:H243	6:V:21:LEU:HD11	1.89	0.54
2:L:195:LEU:CD1	2:L:218:PHE:CE2	2.84	0.54
2:L:215:ASN:OD1	9:L:410:PGV:H32	2.08	0.54
3:M:131:TRP:NE1	3:M:148:ALA:O	2.40	0.54
2:L:228:THR:HG22	9:L:410:PGV:H51	1.89	0.54
5:F:41:VAL:O	5:F:45:MET:HG3	2.07	0.54
5:g:56:TRP:CD1	6:j:47:GLY:HA3	2.43	0.54
1:C:276:TYR:OH	7:C:504:HEC:O1A	2.25	0.54
5:g:20:GLU:HB3	16:j:101:CRT:H1M1	1.88	0.54
16:j:101:CRT:H392	11:j:102:BCL:HBB2	1.89	0.54
2:L:175:HIS:CE1	2:L:179:ILE:HD11	2.43	0.54
1:C:41:LEU:O	1:C:45:MET:HG2	2.08	0.53
2:L:218:PHE:CE2	9:L:410:PGV:O03	2.61	0.53
5:e:15:GLU:OE2	6:f:7:LYS:NZ	2.36	0.53
4:H:227:PRO:HG3	4:H:233:ILE:HD12	1.91	0.53
1:C:254:LYS:NZ	3:M:96:GLU:OE2	2.42	0.53
2:L:121:PHE:O	2:L:124:SER:OG	2.21	0.53
6:X:15:ARG:O	6:X:19:VAL:HG23	2.08	0.53
4:H:233:ILE:HG12	4:H:238:GLU:HG3	1.91	0.53
3:M:203:HIS:CE1	3:M:207:ILE:HD11	2.43	0.53
11:B:101:BCL:H3A	11:B:101:BCL:H2	1.91	0.53
6:G:33:HIS:CG	16:I:102:CRT:H372	2.44	0.53
1:C:263:MET:HE3	7:C:503:HEC:C1A	2.38	0.53
2:L:40:LEU:HD11	15:M:405:MQ8:H401	1.90	0.53
3:M:236:VAL:HA	3:M:239:ILE:HD12	1.91	0.53
4:H:5:PHE:O	6:R:43:ASN:ND2	2.42	0.53
1:C:297:TRP:O	1:C:301:GLN:HG2	2.09	0.52
10:J:103:8K6:H61C	10:J:104:8K6:H72C	1.91	0.52
12:M:404:BPH:HBC3	12:M:404:BPH:HHD	1.90	0.52
16:B:102:CRT:H243	6:A:21:LEU:HD11	1.91	0.52
6:T:47:GLY:HA3	5:U:56:TRP:CD1	2.44	0.52
16:e:102:CRT:H372	6:h:33:HIS:CG	2.45	0.52
5:g:49:PHE:HE1	11:g:101:BCL:H141	1.74	0.52
4:H:13:GLN:NE2	9:H:301:PGV:O13	2.41	0.52
6:A:1:MET:HE2	6:A:8:VAL:HG11	1.91	0.52
6:V:35:LEU:HD23	10:V:104:8K6:H142	1.90	0.52
11:X:101:BCL:CHB	16:a:102:CRT:H35	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:102:CRT:H182	11:N:101:BCL:H71	1.91	0.52
5:U:47:ARG:NH1	6:V:41:ARG:O	2.36	0.52
2:L:172:ASN:HB3	2:L:175:HIS:HB2	1.92	0.52
2:L:196:ILE:HD11	9:L:410:PGV:H242	1.92	0.52
5:I:25:TYR:CD2	16:I:102:CRT:H14	2.44	0.52
5:K:20:GLU:HB3	16:K:102:CRT:H1M1	1.89	0.52
6:N:34:PHE:HD2	10:N:104:8K6:H111	1.74	0.52
5:Q:49:PHE:HE1	11:Q:101:BCL:H141	1.75	0.52
5:e:56:TRP:CD1	6:h:47:GLY:HA3	2.45	0.52
1:C:204:ASN:ND2	3:M:111:ASN:O	2.42	0.52
1:C:239:PRO:HG2	3:M:294:ASN:HB2	1.92	0.52
16:B:102:CRT:H182	11:A:101:BCL:H71	1.92	0.52
5:a:9:SER:OG	5:a:10:SER:N	2.41	0.52
6:b:18:LEU:HD12	6:j:12:PHE:HZ	1.74	0.52
4:H:24:PHE:HB3	10:H:304:8K6:H172	1.90	0.51
6:P:37:LEU:HD21	6:P:45:LEU:HD12	1.92	0.51
11:d:102:BCL:HAA1	11:d:102:BCL:HBD	1.93	0.51
4:H:43:ARG:NH2	4:H:46:ASP:OD2	2.38	0.51
6:b:1:MET:HE3	6:b:8:VAL:HG11	1.91	0.51
16:R:103:CRT:H243	6:T:21:LEU:HD11	1.92	0.51
6:d:17:THR:HG21	11:f:101:BCL:H18	1.91	0.51
1:C:179:HIS:HE1	7:C:502:HEC:NA	1.98	0.51
2:L:113:LEU:HD22	3:M:248:ARG:HG2	1.91	0.51
6:R:47:GLY:HA3	5:S:56:TRP:CD1	2.46	0.51
6:T:33:HIS:CD2	16:U:102:CRT:H372	2.46	0.51
11:T:101:BCL:HBB2	16:U:102:CRT:H392	1.91	0.51
6:b:2:THR:HG22	6:b:3:PHE:H	1.74	0.51
6:b:33:HIS:CG	16:i:102:CRT:H372	2.45	0.51
5:B:19:LYS:HA	6:A:6:HIS:HB2	1.92	0.51
2:L:196:ILE:HD11	9:L:410:PGV:C25	2.41	0.51
4:H:126:ARG:HH21	4:H:170:ARG:NH1	2.09	0.51
6:J:47:GLY:HA3	5:K:56:TRP:CD1	2.45	0.51
16:Z:102:CRT:H371	11:f:101:BCL:C2B	2.41	0.51
11:f:102:BCL:HMA1	5:g:28:SER:HB3	1.93	0.51
5:F:33:LEU:HD11	11:G:102:BCL:H91	1.93	0.51
6:X:15:ARG:NH1	6:b:11:MET:O	2.42	0.51
16:Z:102:CRT:H42	5:c:21:PHE:HA	1.93	0.51
11:K:101:BCL:H2	11:K:101:BCL:H3A	1.92	0.51
5:Y:10:SER:OG	6:d:15:ARG:NH1	2.43	0.51
6:Z:7:LYS:HB2	16:Z:102:CRT:H32A	1.92	0.51
6:P:33:HIS:CG	16:P:103:CRT:H372	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:VAL:HG22	15:M:405:MQ8:H492	1.91	0.50
2:L:233:ARG:HG2	3:M:225:LEU:HD21	1.92	0.50
11:L:401:BCL:HBB2	11:L:402:BCL:H112	1.92	0.50
16:E:103:CRT:H6	6:J:8:VAL:HA	1.92	0.50
6:T:2:THR:HG22	6:T:3:PHE:N	2.26	0.50
6:V:33:HIS:CD2	16:W:102:CRT:H372	2.45	0.50
11:i:101:BCL:HAA1	11:i:101:BCL:H71	1.93	0.50
2:L:153:MET:HE2	3:M:304:VAL:HG12	1.94	0.50
2:L:171:TYR:HA	2:L:176:MET:HE3	1.93	0.50
11:L:401:BCL:H162	11:L:402:BCL:H141	1.93	0.50
3:M:248:ARG:NH2	4:H:111:ALA:O	2.41	0.50
11:A:102:BCL:HAA1	11:A:102:BCL:HBD	1.93	0.50
1:C:51:TYR:CE2	1:C:64:VAL:HG22	2.46	0.50
1:C:278:HIS:CE1	7:C:503:HEC:NA	2.79	0.50
6:N:47:GLY:HA3	5:O:56:TRP:CD1	2.47	0.50
11:B:101:BCL:H12	16:B:102:CRT:H27	1.92	0.50
6:V:28:LEU:O	6:V:32:ILE:HG13	2.12	0.50
6:h:28:LEU:O	6:h:32:ILE:HG13	2.11	0.50
16:e:102:CRT:H182	11:f:101:BCL:H72	1.94	0.50
6:V:33:HIS:CG	16:W:102:CRT:H372	2.47	0.50
11:a:101:BCL:HMD3	6:b:33:HIS:CE1	2.46	0.50
2:L:218:PHE:CZ	9:L:410:PGV:O03	2.65	0.49
6:P:11:MET:HE3	6:P:12:PHE:CE2	2.47	0.49
5:c:56:TRP:CD1	6:f:47:GLY:HA3	2.48	0.49
1:C:179:HIS:CD2	7:C:502:HEC:NB	2.78	0.49
2:L:243:VAL:HG21	12:L:403:BPH:HBC3	1.94	0.49
1:C:28:GLY:HA3	6:f:19:VAL:HG11	1.93	0.49
6:j:33:HIS:CD2	16:j:101:CRT:H372	2.47	0.49
7:C:503:HEC:HBB1	2:L:167:LEU:HD22	1.94	0.49
4:H:44:ASP:O	4:H:87:ARG:NH2	2.44	0.49
16:Y:102:CRT:H372	6:d:33:HIS:CG	2.48	0.49
16:a:102:CRT:H82	6:j:8:VAL:HB	1.95	0.49
3:M:200:ASN:O	3:M:204:MET:HG3	2.13	0.49
11:E:102:BCL:HAA1	11:E:102:BCL:HBD	1.93	0.49
5:O:13:LEU:HD23	5:O:18:ALA:HA	1.94	0.49
6:b:23:ALA:O	6:b:27:VAL:HG23	2.13	0.49
2:L:192:HIS:CE1	9:L:410:PGV:H222	2.46	0.49
2:L:220:ASP:OD2	3:M:137:ARG:NH2	2.46	0.49
16:R:103:CRT:H21A	16:R:103:CRT:H6	1.95	0.49
6:T:33:HIS:CG	16:U:102:CRT:H372	2.47	0.49
2:L:228:THR:HG23	9:L:410:PGV:C6	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:166:VAL:HG12	4:H:178:LEU:HD23	1.94	0.49
6:j:33:HIS:CG	16:j:101:CRT:H372	2.48	0.48
2:L:132:ALA:HA	2:L:136:VAL:HB	1.94	0.48
16:K:102:CRT:H22A	6:P:7:LYS:HE3	1.94	0.48
6:P:33:HIS:CD2	16:P:103:CRT:H372	2.49	0.48
2:L:195:LEU:CD1	2:L:218:PHE:HE2	2.23	0.48
2:L:226:ILE:HG22	9:L:410:PGV:C02	2.43	0.48
5:F:21:PHE:CZ	6:G:14:PRO:HB3	2.49	0.48
6:R:33:HIS:CG	16:R:103:CRT:H372	2.48	0.48
6:X:47:GLY:HA3	5:a:56:TRP:CD1	2.47	0.48
5:g:36:CYS:SG	11:g:101:BCL:HBA1	2.53	0.48
11:i:101:BCL:HMD3	6:j:33:HIS:CE1	2.48	0.48
2:L:195:LEU:CD2	2:L:218:PHE:HE2	2.23	0.48
2:L:221:THR:HA	3:M:133:ARG:HH12	1.79	0.48
16:P:103:CRT:H243	6:R:21:LEU:HD11	1.96	0.48
1:C:244:PRO:HG3	3:M:293:ASP:HB2	1.95	0.48
5:I:57:VAL:HG22	6:J:53:LYS:HG2	1.95	0.48
10:f:103:8K6:H131	10:f:103:8K6:H172	1.95	0.48
2:L:105:ARG:NH2	3:M:255:TRP:O	2.46	0.48
3:M:162:GLY:HA3	16:M:406:CRT:H292	1.95	0.48
9:M:408:PGV:H101	6:N:27:VAL:HG11	1.94	0.48
5:F:19:LYS:HA	6:G:6:HIS:HB2	1.96	0.48
11:X:102:BCL:HAA1	11:X:102:BCL:HBD	1.96	0.48
3:M:248:ARG:NH1	4:H:109:PRO:O	2.47	0.48
6:T:28:LEU:O	6:T:32:ILE:HG13	2.14	0.48
5:a:9:SER:HG	5:a:10:SER:H	1.61	0.48
6:b:47:GLY:HA3	5:i:56:TRP:CD1	2.49	0.48
6:G:47:GLY:HA3	5:I:56:TRP:NE1	2.28	0.48
1:C:188:ILE:HD12	1:C:330:PRO:HB3	1.95	0.48
2:L:20:GLY:HA3	6:j:16:SER:OG	2.14	0.48
11:L:401:BCL:H112	9:H:301:PGV:H142	1.96	0.48
5:K:49:PHE:CZ	11:K:101:BCL:H141	2.49	0.48
5:Y:25:TYR:CE1	16:Y:102:CRT:H16	2.49	0.48
2:L:111:ARG:HG3	2:L:117:PHE:HE1	1.79	0.47
3:M:64:GLY:O	3:M:68:ILE:HG12	2.14	0.47
5:F:31:GLY:HA3	11:J:102:BCL:HED3	1.95	0.47
16:e:102:CRT:H372	6:h:33:HIS:CD2	2.50	0.47
4:H:85:ALA:HB2	4:H:107:VAL:HG11	1.97	0.47
6:T:31:LEU:O	6:T:35:LEU:HG	2.14	0.47
6:Z:7:LYS:N	16:Z:102:CRT:H23	2.30	0.47
10:H:303:8K6:H62C	6:T:20:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9:TRP:HB3	6:A:14:PRO:HG3	1.96	0.47
6:A:47:GLY:HA3	5:D:56:TRP:CD1	2.50	0.47
6:h:22:ALA:HB2	11:h:101:BCL:H8	1.96	0.47
2:L:202:PRO:HB2	2:L:206:GLU:HB2	1.97	0.47
16:A:103:CRT:H27	11:D:101:BCL:H12	1.96	0.47
1:C:237:ILE:HD13	1:C:256:ALA:HA	1.96	0.47
3:M:54:GLY:O	3:M:58:ILE:HG12	2.15	0.47
16:Z:102:CRT:C4	5:c:21:PHE:HA	2.44	0.47
2:L:111:ARG:HG3	2:L:117:PHE:CE1	2.50	0.47
2:L:197:LEU:HD21	3:M:268:ARG:HG2	1.97	0.47
6:A:33:HIS:CD2	16:A:103:CRT:H372	2.50	0.47
5:K:21:PHE:CE2	6:N:14:PRO:HB3	2.50	0.47
1:C:95:ALA:N	1:C:108:LEU:O	2.43	0.47
1:C:201:ALA:O	3:M:115:TRP:NE1	2.44	0.47
6:E:28:LEU:O	6:E:32:ILE:HG13	2.15	0.47
11:R:101:BCL:H161	11:R:101:BCL:H141	1.64	0.47
11:X:102:BCL:H102	11:X:102:BCL:H62	1.68	0.47
6:Z:12:PHE:CZ	6:d:18:LEU:HD12	2.50	0.47
4:H:72:SER:O	4:H:75:ASN:HB3	2.14	0.47
11:G:101:BCL:H62	11:G:101:BCL:H41	1.34	0.47
11:Y:101:BCL:HAA1	11:Y:101:BCL:H71	1.96	0.47
10:C:509:8K6:H111	10:f:103:8K6:H62C	1.96	0.47
3:M:164:ILE:HG12	10:P:104:8K6:H41C	1.97	0.47
6:R:33:HIS:CD2	16:R:103:CRT:H372	2.49	0.47
1:C:44:MET:HE2	6:d:34:PHE:CE2	2.49	0.46
16:W:102:CRT:H243	6:X:21:LEU:HD11	1.96	0.46
11:Z:101:BCL:H161	11:Z:101:BCL:H141	1.60	0.46
6:d:2:THR:HG22	6:d:3:PHE:N	2.29	0.46
3:M:163:PHE:O	3:M:167:VAL:HG23	2.15	0.46
5:U:21:PHE:CZ	6:V:14:PRO:HB3	2.50	0.46
5:B:47:ARG:NH1	6:A:41:ARG:O	2.37	0.46
11:E:102:BCL:HAA1	11:E:102:BCL:CBF	2.45	0.46
16:N:103:CRT:H42	5:O:21:PHE:HD1	1.81	0.46
6:R:28:LEU:O	6:R:32:ILE:HG13	2.15	0.46
5:S:21:PHE:CZ	6:T:14:PRO:HB3	2.50	0.46
5:U:11:THR:HG22	5:U:13:LEU:HD13	1.98	0.46
11:U:101:BCL:HBB	11:U:101:BCL:H71	1.98	0.46
11:X:101:BCL:H151	11:X:101:BCL:H111	1.36	0.46
6:f:1:MET:HE2	11:f:102:BCL:HBB3	1.97	0.46
1:C:47:PRO:HG2	1:C:66:MET:HE1	1.98	0.46
2:L:13:ARG:HD2	4:H:97:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:11:THR:HG22	5:F:13:LEU:H	1.80	0.46
11:X:101:BCL:H62	11:X:101:BCL:H41	1.32	0.46
5:g:19:LYS:HA	6:h:6:HIS:HB2	1.96	0.46
1:C:141:ALA:HB1	1:C:143:ARG:HG2	1.96	0.46
1:C:263:MET:HE3	7:C:503:HEC:NA	2.30	0.46
1:C:274:CYS:HA	7:C:503:HEC:HHC	1.97	0.46
4:H:29:TYR:HB2	10:H:304:8K6:H72C	1.96	0.46
11:A:101:BCL:H151	11:A:101:BCL:H112	1.47	0.46
5:S:49:PHE:CE1	11:S:101:BCL:H141	2.51	0.46
11:f:101:BCL:H62	11:f:101:BCL:H41	1.50	0.46
5:K:15:GLU:HG3	6:N:10:LEU:HD11	1.97	0.46
5:c:14:THR:HG22	5:c:16:ALA:H	1.80	0.46
6:h:9:TRP:HB3	6:h:14:PRO:HG3	1.97	0.46
3:M:110:LEU:HD13	3:M:115:TRP:CZ2	2.51	0.46
11:I:101:BCL:H112	11:I:101:BCL:H152	1.67	0.46
11:W:101:BCL:HMD3	6:X:33:HIS:CE1	2.51	0.46
2:L:30:PHE:HZ	10:L:409:8K6:H81C	1.80	0.46
6:h:38:GLY:HA3	10:j:104:8K6:H62C	1.98	0.46
4:H:17:TYR:O	4:H:21:ILE:HG12	2.16	0.46
5:O:36:CYS:SG	11:O:101:BCL:HBA1	2.56	0.46
6:P:28:LEU:O	6:P:32:ILE:HG13	2.16	0.46
6:j:2:THR:HG22	6:j:3:PHE:N	2.31	0.46
10:L:409:8K6:H151	15:M:405:MQ8:H241	1.97	0.45
3:M:201:PRO:HB3	9:H:301:PGV:H22	1.97	0.45
5:a:25:TYR:CD2	16:a:102:CRT:H14	2.51	0.45
1:C:180:ARG:NH2	1:C:337:CYS:O	2.50	0.45
2:L:30:PHE:CE2	15:M:405:MQ8:H321	2.52	0.45
3:M:215:LEU:O	3:M:219:MET:HG3	2.16	0.45
5:K:49:PHE:HE1	11:K:101:BCL:H141	1.80	0.45
16:N:103:CRT:H82	6:R:8:VAL:HG22	1.97	0.45
5:Y:51:PRO:HG3	6:d:47:GLY:HA2	1.98	0.45
16:i:102:CRT:H243	6:j:21:LEU:HD11	1.97	0.45
5:c:41:VAL:O	5:c:45:MET:HG3	2.16	0.45
11:h:101:BCL:H111	11:h:101:BCL:H152	1.68	0.45
11:h:102:BCL:H3A	11:h:102:BCL:HBA2	1.33	0.45
1:C:38:ILE:O	1:C:42:THR:HG23	2.17	0.45
1:C:294:VAL:HG13	3:M:318:PRO:HG3	1.97	0.45
3:M:229:ARG:HG3	3:M:230:LEU:HG	1.98	0.45
9:H:302:PGV:H182	6:T:27:VAL:HG21	1.97	0.45
11:D:101:BCL:H112	11:D:101:BCL:H71	1.56	0.45
11:F:101:BCL:H162	11:F:101:BCL:H141	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:101:BCL:H62	11:P:101:BCL:H41	1.41	0.45
5:Y:21:PHE:CZ	6:Z:14:PRO:HB3	2.51	0.45
11:f:102:BCL:H2	11:f:102:BCL:H62	1.66	0.45
1:C:53:GLN:HB2	2:L:73:LEU:HD12	1.99	0.45
3:M:129:LEU:HD21	9:M:408:PGV:H232	1.99	0.45
3:M:201:PRO:HA	3:M:204:MET:SD	2.56	0.45
11:A:101:BCL:H62	11:A:101:BCL:H41	1.37	0.45
1:C:33:VAL:HG22	6:d:24:PHE:HB2	1.97	0.45
6:G:47:GLY:HA3	5:I:56:TRP:CD1	2.52	0.45
5:Y:49:PHE:CZ	11:Y:101:BCL:H141	2.51	0.45
6:b:28:LEU:O	6:b:32:ILE:HG13	2.17	0.45
6:b:33:HIS:CD2	16:i:102:CRT:H372	2.51	0.45
5:i:49:PHE:CE1	11:i:101:BCL:H141	2.51	0.45
5:a:21:PHE:CZ	6:b:14:PRO:HB3	2.52	0.45
5:i:21:PHE:CZ	6:j:14:PRO:HB3	2.51	0.45
2:L:172:ASN:HB3	2:L:175:HIS:CB	2.47	0.45
2:L:222:VAL:HG23	2:L:224:TYR:H	1.82	0.45
12:L:403:BPH:CBB	12:L:403:BPH:HHC	2.47	0.45
3:M:208:ALA:HB1	9:H:301:PGV:H332	1.99	0.45
3:M:235:GLU:HG2	3:M:263:MET:SD	2.57	0.45
11:N:101:BCL:H141	11:N:101:BCL:H161	1.66	0.45
6:Z:28:LEU:O	6:Z:32:ILE:HG13	2.17	0.45
16:a:102:CRT:H243	6:b:21:LEU:HD11	1.99	0.45
11:b:101:BCL:H203	11:b:101:BCL:H162	1.69	0.45
11:f:101:BCL:H193	11:f:101:BCL:H161	1.75	0.45
11:F:101:BCL:H161	11:F:101:BCL:H192	1.68	0.45
5:Y:20:GLU:HB2	16:Y:102:CRT:H1M1	1.98	0.45
11:d:101:BCL:H141	11:d:101:BCL:H162	1.81	0.45
1:C:64:VAL:HG12	2:L:258:THR:HB	1.99	0.45
4:H:250:LEU:O	4:H:254:LYS:CD	2.42	0.45
6:N:9:TRP:HB3	6:N:14:PRO:HG3	1.99	0.45
11:O:101:BCL:H112	11:O:101:BCL:H143	1.55	0.45
6:b:2:THR:HG22	6:b:3:PHE:N	2.31	0.45
6:b:18:LEU:HD12	6:j:12:PHE:CZ	2.52	0.45
11:d:102:BCL:H111	11:d:102:BCL:H91	1.60	0.45
2:L:153:MET:HE1	3:M:204:MET:HE2	2.00	0.44
9:M:407:PGV:H281	9:M:407:PGV:H82	1.99	0.44
4:H:232:GLN:HE22	4:H:234:THR:HG22	1.82	0.44
5:D:22:HIS:CG	6:E:6:HIS:HA	2.52	0.44
11:R:102:BCL:H2	11:R:102:BCL:H62	1.77	0.44
16:R:103:CRT:H83	6:V:5:THR:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:41:ARG:NH1	6:V:50:ALA:O	2.49	0.44
6:X:5:THR:O	6:X:8:VAL:HG23	2.16	0.44
11:X:101:BCL:H3A	16:a:102:CRT:H32	1.98	0.44
6:b:19:VAL:HG22	11:b:101:BCL:H193	1.98	0.44
5:O:54:GLU:OE1	5:O:54:GLU:N	2.50	0.44
11:T:102:BCL:H3A	11:T:102:BCL:HBA2	1.31	0.44
11:a:101:BCL:H91	11:a:101:BCL:H112	1.78	0.44
1:C:173:VAL:HG12	1:C:177:THR:HG21	1.99	0.44
2:L:54:TRP:CE2	10:L:407:8K6:H131	2.52	0.44
2:L:99:PHE:HB3	2:L:127:ILE:HG12	1.99	0.44
11:L:402:BCL:H161	11:L:402:BCL:H192	1.64	0.44
3:M:165:ARG:HD2	3:M:285:ILE:HG22	1.98	0.44
5:W:22:HIS:CG	6:X:6:HIS:HA	2.52	0.44
11:j:102:BCL:H62	11:j:102:BCL:H41	1.52	0.44
2:L:30:PHE:CZ	10:L:409:8K6:H81C	2.52	0.44
3:M:310:ASP:OD2	3:M:313:PRO:HA	2.16	0.44
11:M:402:BCL:H11	12:M:404:BPH:HBB2	1.99	0.44
11:U:101:BCL:H102	11:U:101:BCL:H62	1.50	0.44
1:C:51:TYR:CG	2:L:146:HIS:HE1	2.36	0.44
2:L:176:MET:HE1	3:M:181:PHE:CE1	2.53	0.44
2:L:218:PHE:CD1	9:L:410:PGV:H011	2.53	0.44
3:M:98:PRO:HG3	3:M:113:GLY:HA3	1.99	0.44
1:C:143:ARG:HB2	1:C:144:PRO:HD3	1.98	0.44
1:C:179:HIS:CD2	7:C:502:HEC:NC	2.82	0.44
11:L:401:BCL:H13	11:L:401:BCL:H172	1.48	0.44
11:c:101:BCL:H112	11:c:101:BCL:H143	1.51	0.44
1:C:57:ARG:NH1	2:L:84:GLU:HA	2.32	0.44
9:M:408:PGV:H81	9:M:408:PGV:H221	2.00	0.44
5:Q:21:PHE:CE2	6:R:14:PRO:HB3	2.53	0.44
1:C:120:ILE:HD11	1:C:154:LEU:HD21	1.99	0.44
2:L:4:LEU:HD22	4:H:38:GLY:HA3	2.00	0.44
6:A:28:LEU:O	6:A:32:ILE:HG13	2.17	0.44
16:E:103:CRT:H14	5:F:25:TYR:CD2	2.53	0.44
5:I:21:PHE:HD1	16:I:102:CRT:H42	1.83	0.44
6:P:2:THR:HG22	6:P:3:PHE:N	2.33	0.44
6:Z:35:LEU:HB2	9:Z:103:PGV:H31	2.00	0.44
5:g:29:ALA:O	5:g:33:LEU:HG	2.18	0.44
6:j:22:ALA:HB2	11:j:102:BCL:H8	2.00	0.44
11:A:102:BCL:HBA1	5:Y:32:PHE:HA	2.00	0.44
5:K:21:PHE:HE1	16:K:102:CRT:H9	1.82	0.44
16:U:102:CRT:H182	11:V:101:BCL:H71	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:102:CRT:H372	6:f:33:HIS:CG	2.53	0.44
11:D:101:BCL:H43	11:E:102:BCL:H8	2.00	0.43
16:P:103:CRT:H22A	6:T:7:LYS:HE2	1.99	0.43
11:S:101:BCL:HMD1	6:T:33:HIS:CE1	2.53	0.43
11:V:101:BCL:H142	11:V:101:BCL:H111	1.73	0.43
2:L:191:MET:CE	2:L:218:PHE:CE1	2.74	0.43
11:J:101:BCL:H143	11:J:101:BCL:H162	1.84	0.43
6:N:2:THR:HG22	6:N:3:PHE:N	2.33	0.43
3:M:167:VAL:HG11	10:N:104:8K6:H132	1.99	0.43
9:M:408:PGV:H291	9:M:408:PGV:H262	1.83	0.43
6:A:2:THR:HG23	6:A:4:SER:H	1.82	0.43
6:E:37:LEU:O	6:E:43:ASN:ND2	2.52	0.43
11:O:101:BCL:H3A	11:O:101:BCL:H2	2.00	0.43
16:W:102:CRT:H31A	16:W:102:CRT:H5	1.85	0.43
11:b:102:BCL:H91	11:b:102:BCL:H111	1.57	0.43
10:j:105:8K6:H91C	10:j:105:8K6:H52C	2.00	0.43
3:M:118:MET:SD	6:J:34:PHE:HB3	2.58	0.43
5:W:21:PHE:CZ	6:X:14:PRO:HB3	2.53	0.43
11:a:101:BCL:H112	11:a:101:BCL:H152	1.78	0.43
11:b:101:BCL:H41	11:b:101:BCL:H62	1.47	0.43
1:C:108:LEU:HD11	1:C:356:SER:HB2	1.99	0.43
3:M:63:PHE:HD1	3:M:122:PHE:HD1	1.65	0.43
16:A:103:CRT:H182	11:E:101:BCL:H71	2.01	0.43
5:c:21:PHE:CZ	6:d:14:PRO:HB3	2.53	0.43
6:h:41:ARG:NH1	6:h:50:ALA:O	2.51	0.43
1:C:242:ASP:HA	3:M:294:ASN:HB3	1.99	0.43
12:L:403:BPH:HHC	12:L:403:BPH:HBB3	2.01	0.43
3:M:161:LEU:HD13	11:M:402:BCL:HMC2	2.01	0.43
11:A:102:BCL:HMA1	11:A:102:BCL:HHB	1.87	0.43
11:N:101:BCL:H62	11:N:101:BCL:H41	1.58	0.43
11:c:101:BCL:H192	11:c:101:BCL:H161	1.70	0.43
11:j:103:BCL:HBA2	11:j:103:BCL:H3A	1.35	0.43
11:G:101:BCL:H151	11:G:101:BCL:H111	1.51	0.43
6:P:44:TRP:CZ2	11:P:101:BCL:HHC	2.54	0.43
11:e:101:BCL:HMD1	6:f:33:HIS:CE1	2.54	0.43
1:C:133:CYS:O	1:C:147:LYS:HB2	2.19	0.43
11:J:102:BCL:HBA2	11:J:102:BCL:H3A	1.21	0.43
6:N:44:TRP:CD2	11:N:101:BCL:H2C	2.53	0.43
16:N:103:CRT:H243	6:P:21:LEU:HD11	2.00	0.43
4:H:23:LEU:O	4:H:27:ILE:HG12	2.19	0.43
11:I:101:BCL:H62	11:I:101:BCL:H101	1.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:1:MET:HE2	6:P:8:VAL:HG11	2.01	0.43
11:U:101:BCL:HMD1	6:V:33:HIS:CE1	2.54	0.43
5:W:29:ALA:O	5:W:33:LEU:HG	2.19	0.43
2:L:38:THR:HG22	10:L:406:8K6:H82C	2.01	0.43
2:L:209:LYS:HG3	3:M:143:MET:HG2	2.01	0.43
11:L:401:BCL:H161	11:L:401:BCL:H192	1.63	0.43
5:U:48:PRO:HD2	6:V:41:ARG:HH21	1.84	0.43
2:L:13:ARG:HG3	4:H:95:PRO:HB2	2.00	0.42
2:L:189:LEU:HD11	3:M:270:GLY:HA3	2.01	0.42
5:I:25:TYR:CE2	16:I:102:CRT:H16	2.54	0.42
11:P:101:BCL:H151	11:P:101:BCL:H112	1.28	0.42
16:R:103:CRT:H182	11:T:101:BCL:H71	2.01	0.42
11:c:101:BCL:H111	11:c:101:BCL:H71	1.54	0.42
2:L:79:PHE:HB2	6:j:38:GLY:HA2	2.00	0.42
3:M:89:GLN:O	3:M:93:LEU:HG	2.19	0.42
4:H:28:PHE:CE1	10:H:303:8K6:H22C	2.54	0.42
4:H:112:TYR:HB2	4:H:239:ASP:OD2	2.19	0.42
11:h:102:BCL:H62	11:h:102:BCL:H2	1.55	0.42
1:C:218:SER:OG	1:C:220:LEU:HD12	2.20	0.42
2:L:159:VAL:HG13	11:L:402:BCL:C2D	2.50	0.42
11:L:401:BCL:H92	11:L:401:BCL:H62	1.81	0.42
11:U:101:BCL:H71	11:U:101:BCL:CHB	2.48	0.42
11:W:101:BCL:H111	11:W:101:BCL:H143	1.65	0.42
6:h:2:THR:HG22	6:h:3:PHE:N	2.34	0.42
4:H:103:LEU:HB3	4:H:244:TYR:CE2	2.54	0.42
16:E:103:CRT:H83	6:J:5:THR:HB	2.01	0.42
5:i:25:TYR:CD1	16:i:102:CRT:H14	2.54	0.42
2:L:218:PHE:HD2	9:L:410:PGV:H22	1.84	0.42
3:M:55:ALA:HB1	6:J:19:VAL:HG11	2.00	0.42
16:E:103:CRT:H6	6:J:8:VAL:CB	2.50	0.42
5:F:36:CYS:SG	11:F:101:BCL:HBA1	2.60	0.42
5:g:21:PHE:CE2	6:h:14:PRO:HB3	2.54	0.42
1:C:42:THR:HG22	10:C:509:8K6:H72C	2.02	0.42
1:C:238:THR:HB	1:C:284:ARG:HG3	2.02	0.42
2:L:47:VAL:HG22	11:L:401:BCL:H191	2.02	0.42
2:L:271:LEU:HD23	2:L:273:ILE:HD12	2.02	0.42
3:M:287:LEU:HD22	3:M:291:VAL:HG21	2.02	0.42
9:M:407:PGV:H31	10:P:104:8K6:H111	2.02	0.42
16:I:102:CRT:H6	6:N:8:VAL:HA	2.01	0.42
11:P:102:BCL:H2	11:P:102:BCL:H62	1.89	0.42
11:i:101:BCL:H101	11:i:101:BCL:H62	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:125:PHE:CE1	2:L:240:LEU:HD13	2.55	0.42
2:L:228:THR:HA	9:L:410:PGV:H252	2.01	0.42
3:M:238:GLN:HB2	3:M:263:MET:HG2	2.02	0.42
9:H:301:PGV:H131	9:H:301:PGV:H102	1.69	0.42
16:Z:102:CRT:H372	6:f:33:HIS:CD2	2.55	0.42
16:Z:102:CRT:H26	16:Z:102:CRT:H241	1.85	0.42
1:C:133:CYS:HA	1:C:146:THR:OG1	2.19	0.42
2:L:182:PHE:CD2	2:L:242:ALA:HB1	2.54	0.42
3:M:84:VAL:HG22	6:A:34:PHE:CD1	2.55	0.42
11:J:101:BCL:H62	11:J:101:BCL:H41	1.39	0.42
6:X:41:ARG:HD3	6:X:42:PHE:CZ	2.54	0.42
11:X:102:BCL:H141	11:X:102:BCL:H161	1.63	0.42
2:L:40:LEU:HD13	15:M:405:MQ8:H503	2.01	0.42
2:L:149:PRO:HD2	2:L:158:TRP:HB2	2.01	0.42
2:L:226:ILE:HG22	9:L:410:PGV:C1	2.48	0.42
3:M:168:MET:HE1	3:M:286:LEU:HD22	2.02	0.42
16:I:102:CRT:H20	16:I:102:CRT:H181	1.96	0.42
16:P:103:CRT:H27	11:Q:101:BCL:H12	2.02	0.42
11:R:101:BCL:H41	11:R:101:BCL:H62	1.40	0.42
11:T:101:BCL:H111	11:T:101:BCL:H143	1.68	0.42
16:Z:102:CRT:H291	16:Z:102:CRT:H31	1.84	0.42
2:L:157:ASP:OD2	3:M:308:TYR:OH	2.27	0.42
3:M:223:THR:O	3:M:227:VAL:HG22	2.19	0.42
4:H:13:GLN:NE2	9:H:302:PGV:H31	2.35	0.42
2:L:155:HIS:O	2:L:159:VAL:HG23	2.20	0.41
11:G:102:BCL:H3A	11:G:102:BCL:HBA2	1.25	0.41
5:Q:49:PHE:CE1	11:Q:101:BCL:H141	2.53	0.41
5:Y:34:ALA:O	5:Y:38:VAL:HG23	2.19	0.41
5:a:26:SER:HB3	6:b:3:PHE:CD1	2.55	0.41
11:g:101:BCL:H91	11:g:101:BCL:H112	1.91	0.41
11:g:101:BCL:H12	16:j:101:CRT:H27	2.01	0.41
11:h:101:BCL:H41	11:h:101:BCL:H62	1.53	0.41
5:i:49:PHE:HE1	11:i:101:BCL:H141	1.84	0.41
2:L:192:HIS:HD1	9:L:410:PGV:C21	2.33	0.41
2:L:196:ILE:HD11	9:L:410:PGV:H251	2.02	0.41
5:B:22:HIS:CG	6:A:6:HIS:HA	2.55	0.41
16:E:103:CRT:H82	6:J:8:VAL:HB	2.02	0.41
5:K:22:HIS:CG	6:N:6:HIS:HA	2.56	0.41
5:i:25:TYR:CE1	16:i:102:CRT:H16	2.54	0.41
1:C:56:TYR:HB3	1:C:59:LEU:HD12	2.02	0.41
1:C:74:MET:O	1:C:80:GLN:NE2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:LEU:HB2	2:L:35:PHE:HE2	1.85	0.41
9:M:408:PGV:H231	9:M:408:PGV:H202	1.86	0.41
16:E:103:CRT:H10	16:E:103:CRT:H81	1.81	0.41
16:E:103:CRT:H42	5:F:21:PHE:HD1	1.85	0.41
5:K:21:PHE:CE1	16:K:102:CRT:H9	2.56	0.41
5:S:57:VAL:HG22	6:T:53:LYS:HG2	2.02	0.41
11:Z:101:BCL:H62	11:Z:101:BCL:H41	1.44	0.41
11:f:102:BCL:HBA2	11:f:102:BCL:H3A	1.17	0.41
6:j:7:LYS:HA	6:j:10:LEU:HD13	2.01	0.41
2:L:15:GLY:HA2	2:L:111:ARG:HB3	2.02	0.41
2:L:112:LYS:HE2	2:L:112:LYS:HB2	1.83	0.41
3:M:273:CYS:O	3:M:277:VAL:HG23	2.21	0.41
5:I:23:ALA:O	5:I:27:GLN:OE1	2.38	0.41
6:X:2:THR:HG22	6:X:3:PHE:N	2.35	0.41
11:d:101:BCL:H162	11:d:101:BCL:H202	1.83	0.41
3:M:227:VAL:HG23	3:M:232:GLY:HA3	2.02	0.41
11:T:101:BCL:H62	11:T:101:BCL:H41	1.59	0.41
6:f:12:PHE:CZ	6:h:15:ARG:HG2	2.56	0.41
16:j:101:CRT:H36	16:j:101:CRT:H341	1.94	0.41
12:L:403:BPH:H7C2	12:L:403:BPH:H112	1.87	0.41
3:M:110:LEU:HD23	3:M:110:LEU:HA	1.90	0.41
3:M:176:PRO:HG2	16:M:406:CRT:H242	2.02	0.41
16:A:103:CRT:H391	6:E:35:LEU:HD13	2.03	0.41
16:N:103:CRT:H36	16:N:103:CRT:H341	1.94	0.41
11:X:102:BCL:H3A	11:X:102:BCL:HBA2	1.19	0.41
11:c:101:BCL:H162	11:c:101:BCL:H141	1.78	0.41
6:f:15:ARG:O	6:f:19:VAL:HG23	2.20	0.41
11:K:101:BCL:H12	16:K:102:CRT:H27	2.02	0.41
6:P:2:THR:HB	6:P:5:THR:HG23	2.03	0.41
11:V:101:BCL:H41	11:V:101:BCL:H62	1.39	0.41
5:W:21:PHE:CE2	6:X:14:PRO:HB3	2.56	0.41
11:c:101:BCL:O1D	6:d:32:ILE:HD12	2.21	0.41
1:C:26:TRP:CZ3	6:d:17:THR:HG23	2.56	0.41
2:L:196:ILE:HG21	3:M:267:HIS:CE1	2.55	0.41
2:L:231:ILE:CG1	9:L:410:PGV:H211	2.34	0.41
11:A:102:BCL:H2	11:A:102:BCL:H62	1.82	0.41
11:O:101:BCL:H111	11:O:101:BCL:H71	1.74	0.41
1:C:33:VAL:O	1:C:36:ILE:HG22	2.21	0.41
1:C:81:VAL:HG11	1:C:350:VAL:HG12	2.03	0.41
1:C:134:HIS:CE1	7:C:501:HEC:ND	2.88	0.41
1:C:278:HIS:CE1	7:C:503:HEC:ND	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:57:ASP:HA	2:L:58:PRO:HD3	1.96	0.41
2:L:119:VAL:HB	2:L:120:PRO:HD3	2.02	0.41
2:L:139:MET:HE3	10:L:404:8K6:H22C	2.03	0.41
10:L:404:8K6:H41C	10:f:103:8K6:H52C	2.01	0.41
9:M:408:PGV:H262	9:M:408:PGV:H231	1.71	0.41
11:U:101:BCL:H12	16:U:102:CRT:H27	2.03	0.41
10:X:103:8K6:H111	10:X:103:8K6:H71C	2.01	0.41
11:c:101:BCL:HMD3	6:d:33:HIS:CE1	2.56	0.41
6:h:41:ARG:HD3	6:h:42:PHE:CZ	2.55	0.41
1:C:153:MET:HG3	7:C:502:HEC:CHB	2.50	0.41
1:C:244:PRO:HB3	1:C:250:GLN:HG2	2.02	0.41
3:M:202:PHE:CZ	4:H:15:VAL:HG12	2.56	0.41
11:D:101:BCL:HMD3	6:E:33:HIS:CE1	2.56	0.41
5:I:56:TRP:CD2	6:J:41:ARG:HD2	2.56	0.41
11:O:101:BCL:H141	11:O:101:BCL:H162	1.94	0.41
16:P:103:CRT:H36	16:P:103:CRT:H341	1.94	0.41
1:C:245:MET:HB2	1:C:248:VAL:HB	2.03	0.40
11:P:102:BCL:H91	11:P:102:BCL:H111	1.86	0.40
16:P:103:CRT:H11	6:R:18:LEU:HD21	2.03	0.40
5:U:21:PHE:CE1	16:U:102:CRT:H9	2.57	0.40
16:Y:102:CRT:H372	6:d:33:HIS:CD2	2.56	0.40
16:j:101:CRT:H20	16:j:101:CRT:H181	1.96	0.40
1:C:44:MET:HE1	9:Z:103:PGV:H11	2.03	0.40
9:H:301:PGV:H51	9:H:301:PGV:H81	1.87	0.40
9:H:302:PGV:H272	9:H:302:PGV:H241	1.87	0.40
6:N:34:PHE:CD2	10:N:104:8K6:H111	2.56	0.40
11:b:102:BCL:HAA1	11:b:102:BCL:HBD	2.02	0.40
1:C:61:MET:HE2	1:C:61:MET:HB3	1.84	0.40
2:L:56:MET:HE1	6:X:43:ASN:HD21	1.86	0.40
11:I:101:BCL:H12	16:I:102:CRT:H27	2.03	0.40
11:P:102:BCL:H3A	11:P:102:BCL:HBA2	1.38	0.40
11:R:102:BCL:HBA2	11:R:102:BCL:H3A	1.33	0.40
11:h:102:BCL:H62	11:h:102:BCL:H102	1.90	0.40
5:i:13:LEU:HD22	5:i:17:GLU:HB3	2.02	0.40
16:I:102:CRT:H243	6:J:21:LEU:HD11	2.02	0.40
5:O:41:VAL:HG22	11:O:101:BCL:H203	2.03	0.40
5:Y:25:TYR:HD1	16:Y:102:CRT:H14	1.85	0.40
11:b:102:BCL:HBA2	11:b:102:BCL:H3A	1.26	0.40
6:f:2:THR:HB	6:f:5:THR:HG23	2.03	0.40
6:f:2:THR:HG22	6:f:3:PHE:N	2.37	0.40
5:g:49:PHE:CE1	11:g:101:BCL:H141	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:j:103:BCL:HMA1	11:j:103:BCL:HHB	1.87	0.40
1:C:57:ARG:HH12	2:L:84:GLU:HA	1.86	0.40
2:L:214:GLU:C	9:L:410:PGV:H41	2.47	0.40
16:A:103:CRT:H15	16:A:103:CRT:H131	1.94	0.40
11:G:101:BCL:OBB	11:I:101:BCL:HMC3	2.21	0.40
16:N:103:CRT:H1M3	5:O:21:PHE:HB2	2.04	0.40
16:Z:102:CRT:H41	5:c:24:VAL:HB	2.04	0.40
6:d:43:ASN:HD21	10:d:103:8K6:H152	1.85	0.40
11:d:102:BCL:H11	11:f:101:BCL:HED1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	340/362 (94%)	325 (96%)	15 (4%)	0	100	100
2	L	271/275 (98%)	265 (98%)	6 (2%)	0	100	100
3	M	285/323 (88%)	277 (97%)	8 (3%)	0	100	100
4	H	241/254 (95%)	237 (98%)	4 (2%)	0	100	100
5	B	47/68 (69%)	47 (100%)	0	0	100	100
5	D	47/68 (69%)	47 (100%)	0	0	100	100
5	F	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	I	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	K	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	O	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	Q	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	S	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	U	47/68 (69%)	46 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	W	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	Y	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	a	47/68 (69%)	47 (100%)	0	0	100	100
5	c	47/68 (69%)	47 (100%)	0	0	100	100
5	e	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	g	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	i	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
6	A	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
6	E	51/67 (76%)	51 (100%)	0	0	100	100
6	G	51/67 (76%)	51 (100%)	0	0	100	100
6	J	51/67 (76%)	51 (100%)	0	0	100	100
6	N	51/67 (76%)	51 (100%)	0	0	100	100
6	P	51/67 (76%)	51 (100%)	0	0	100	100
6	R	51/67 (76%)	51 (100%)	0	0	100	100
6	T	51/67 (76%)	51 (100%)	0	0	100	100
6	V	51/67 (76%)	51 (100%)	0	0	100	100
6	X	51/67 (76%)	51 (100%)	0	0	100	100
6	Z	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
6	b	51/67 (76%)	51 (100%)	0	0	100	100
6	d	51/67 (76%)	51 (100%)	0	0	100	100
6	f	51/67 (76%)	51 (100%)	0	0	100	100
6	h	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
6	j	51/67 (76%)	51 (100%)	0	0	100	100
All	All	2698/3374 (80%)	2645 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	278/296 (94%)	278 (100%)	0	100	100
2	L	218/219 (100%)	217 (100%)	1 (0%)	81	91
3	M	225/254 (89%)	225 (100%)	0	100	100
4	H	200/202 (99%)	200 (100%)	0	100	100
5	B	35/51 (69%)	35 (100%)	0	100	100
5	D	35/51 (69%)	35 (100%)	0	100	100
5	F	35/51 (69%)	35 (100%)	0	100	100
5	I	35/51 (69%)	35 (100%)	0	100	100
5	K	35/51 (69%)	35 (100%)	0	100	100
5	O	35/51 (69%)	35 (100%)	0	100	100
5	Q	35/51 (69%)	35 (100%)	0	100	100
5	S	35/51 (69%)	35 (100%)	0	100	100
5	U	35/51 (69%)	35 (100%)	0	100	100
5	W	35/51 (69%)	35 (100%)	0	100	100
5	Y	35/51 (69%)	35 (100%)	0	100	100
5	a	35/51 (69%)	35 (100%)	0	100	100
5	c	35/51 (69%)	35 (100%)	0	100	100
5	e	35/51 (69%)	35 (100%)	0	100	100
5	g	35/51 (69%)	35 (100%)	0	100	100
5	i	35/51 (69%)	35 (100%)	0	100	100
6	A	45/53 (85%)	45 (100%)	0	100	100
6	E	45/53 (85%)	45 (100%)	0	100	100
6	G	45/53 (85%)	45 (100%)	0	100	100
6	J	45/53 (85%)	45 (100%)	0	100	100
6	N	45/53 (85%)	45 (100%)	0	100	100
6	P	45/53 (85%)	45 (100%)	0	100	100
6	R	45/53 (85%)	45 (100%)	0	100	100
6	T	45/53 (85%)	45 (100%)	0	100	100
6	V	45/53 (85%)	45 (100%)	0	100	100
6	X	45/53 (85%)	45 (100%)	0	100	100
6	Z	38/53 (72%)	38 (100%)	0	100	100
6	b	45/53 (85%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	d	45/53 (85%)	45 (100%)	0	100	100
6	f	45/53 (85%)	45 (100%)	0	100	100
6	h	45/53 (85%)	45 (100%)	0	100	100
6	j	45/53 (85%)	45 (100%)	0	100	100
All	All	2194/2635 (83%)	2193 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	168	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	233	GLN
1	C	349	ASN
2	L	165	GLN
3	M	260	ASN
4	H	232	GLN
4	H	242	GLN
4	H	253	ASN
6	J	6	HIS
6	R	48	ASN
6	T	39	HIS
6	X	43	ASN
6	Z	48	ASN
6	f	6	HIS
6	j	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 111 ligands modelled in this entry, 5 are monoatomic - leaving 106 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
16	CRT	M	406	-	43,43,43	1.50	11 (25%)	48,54,54	1.40	11 (22%)
11	BCL	E	102	6	69,74,74	1.79	19 (27%)	79,115,115	2.27	22 (27%)
16	CRT	a	102	-	43,43,43	1.49	11 (25%)	48,54,54	1.61	13 (27%)
9	PGV	M	407	-	45,45,50	0.99	2 (4%)	48,50,56	1.05	4 (8%)
11	BCL	U	101	-	69,74,74	1.89	18 (26%)	79,115,115	2.09	23 (29%)
10	8K6	H	306	-	14,14,17	0.11	0	13,13,16	0.18	0
11	BCL	Q	101	-	69,74,74	1.84	17 (24%)	79,115,115	2.05	25 (31%)
11	BCL	R	101	-	69,74,74	1.89	16 (23%)	79,115,115	2.19	24 (30%)
9	PGV	H	301	-	50,50,50	0.92	2 (4%)	53,56,56	1.11	4 (7%)
16	CRT	E	103	-	43,43,43	1.49	11 (25%)	48,54,54	1.84	17 (35%)
10	8K6	L	409	-	17,17,17	0.10	0	16,16,16	0.16	0
11	BCL	V	102	6	69,74,74	1.76	20 (28%)	79,115,115	2.26	25 (31%)
11	BCL	P	102	6	69,74,74	1.75	17 (24%)	79,115,115	2.37	26 (32%)
13	LMT	L	408	-	33,33,36	0.39	0	44,44,47	0.78	0
16	CRT	U	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.66	12 (25%)
11	BCL	A	102	6	69,74,74	1.80	20 (28%)	79,115,115	2.33	27 (34%)
10	8K6	J	103	-	12,12,17	0.09	0	11,11,16	0.11	0
10	8K6	N	104	-	17,17,17	0.11	0	16,16,16	0.11	0
16	CRT	i	102	-	43,43,43	1.49	10 (23%)	48,54,54	1.60	14 (29%)
10	8K6	P	104	-	17,17,17	0.11	0	16,16,16	0.10	0
9	PGV	R	104	-	50,50,50	0.92	2 (4%)	53,56,56	0.96	2 (3%)
9	PGV	Z	103	-	41,41,50	1.01	2 (4%)	44,47,56	1.08	4 (9%)
10	8K6	H	304	-	17,17,17	0.11	0	16,16,16	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	X	101	-	69,74,74	1.84	20 (28%)	79,115,115	2.40	27 (34%)
11	BCL	h	102	6	69,74,74	1.77	18 (26%)	79,115,115	2.31	22 (27%)
16	CRT	W	102	-	43,43,43	1.50	11 (25%)	48,54,54	1.57	12 (25%)
11	BCL	d	102	6	69,74,74	1.77	18 (26%)	79,115,115	2.24	24 (30%)
11	BCL	R	102	6	69,74,74	1.77	18 (26%)	79,115,115	2.31	24 (30%)
9	PGV	M	408	-	41,41,50	1.05	2 (4%)	44,46,56	1.21	5 (11%)
10	8K6	d	103	-	17,17,17	0.11	0	16,16,16	0.07	0
16	CRT	j	101	-	43,43,43	1.50	11 (25%)	48,54,54	1.64	13 (27%)
7	HEC	C	502	1	46,50,50	1.84	4 (8%)	58,82,82	1.80	4 (6%)
12	BPH	L	403	-	59,70,70	1.14	3 (5%)	59,101,101	1.89	9 (15%)
9	PGV	L	410	-	21,21,50	1.29	2 (9%)	23,23,56	1.70	5 (21%)
11	BCL	P	101	-	69,74,74	1.82	16 (23%)	79,115,115	2.48	23 (29%)
16	CRT	I	102	-	43,43,43	1.48	12 (27%)	48,54,54	1.90	17 (35%)
10	8K6	X	103	-	17,17,17	0.10	0	16,16,16	0.08	0
11	BCL	M	402	-	69,74,74	1.83	16 (23%)	79,115,115	2.33	21 (26%)
11	BCL	g	101	-	69,74,74	1.81	16 (23%)	79,115,115	2.14	22 (27%)
11	BCL	M	403	-	69,74,74	1.93	19 (27%)	79,115,115	2.65	26 (32%)
11	BCL	Y	101	-	69,74,74	1.84	20 (28%)	79,115,115	2.10	28 (35%)
11	BCL	D	101	-	69,74,74	1.87	18 (26%)	79,115,115	2.13	26 (32%)
16	CRT	Y	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.71	17 (35%)
11	BCL	N	101	-	69,74,74	1.82	18 (26%)	79,115,115	2.42	26 (32%)
16	CRT	A	103	-	43,43,43	1.50	10 (23%)	48,54,54	1.63	12 (25%)
9	PGV	C	508	-	37,37,50	1.06	2 (5%)	40,43,56	1.17	4 (10%)
16	CRT	P	103	-	43,43,43	1.50	11 (25%)	48,54,54	1.58	13 (27%)
10	8K6	V	104	-	17,17,17	0.12	0	16,16,16	0.07	0
11	BCL	I	101	-	69,74,74	1.84	17 (24%)	79,115,115	2.09	23 (29%)
11	BCL	Z	101	-	69,74,74	1.83	18 (26%)	79,115,115	2.25	25 (31%)
11	BCL	G	101	-	69,74,74	1.84	18 (26%)	79,115,115	2.37	24 (30%)
11	BCL	i	101	-	69,74,74	1.83	17 (24%)	79,115,115	2.09	23 (29%)
11	BCL	J	101	-	69,74,74	1.86	19 (27%)	79,115,115	2.34	24 (30%)
11	BCL	K	101	-	69,74,74	1.85	17 (24%)	79,115,115	2.10	24 (30%)
10	8K6	M	409	-	17,17,17	0.09	0	16,16,16	0.11	0
11	BCL	A	101	-	69,74,74	1.87	17 (24%)	79,115,115	2.38	25 (31%)
11	BCL	h	101	-	69,74,74	1.82	15 (21%)	79,115,115	2.31	23 (29%)
10	8K6	H	303	-	16,16,17	0.09	0	15,15,16	0.13	0
11	BCL	d	101	-	69,74,74	1.84	18 (26%)	79,115,115	2.36	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	8K6	H	305	-	17,17,17	0.12	0	16,16,16	0.10	0
11	BCL	G	102	6	69,74,74	1.75	18 (26%)	79,115,115	2.27	26 (32%)
11	BCL	X	102	6	69,74,74	1.79	17 (24%)	79,115,115	2.25	22 (27%)
11	BCL	a	101	-	69,74,74	1.86	15 (21%)	79,115,115	2.06	24 (30%)
11	BCL	T	101	-	69,74,74	1.84	17 (24%)	79,115,115	2.29	23 (29%)
16	CRT	K	102	-	43,43,43	1.51	11 (25%)	48,54,54	1.71	15 (31%)
10	8K6	j	105	-	17,17,17	0.10	0	16,16,16	0.10	0
10	8K6	C	509	-	15,15,17	0.12	0	14,14,16	0.11	0
16	CRT	R	103	-	43,43,43	1.50	11 (25%)	48,54,54	1.64	14 (29%)
11	BCL	S	101	-	69,74,74	1.85	19 (27%)	79,115,115	1.98	26 (32%)
11	BCL	c	101	-	69,74,74	1.83	18 (26%)	79,115,115	2.13	23 (29%)
10	8K6	L	404	-	14,14,17	0.10	0	13,13,16	0.14	0
12	BPH	M	404	-	59,70,70	1.11	4 (6%)	59,101,101	1.94	8 (13%)
11	BCL	b	102	6	69,74,74	1.77	18 (26%)	79,115,115	2.33	26 (32%)
11	BCL	F	101	-	69,74,74	1.87	17 (24%)	79,115,115	2.06	27 (34%)
10	8K6	L	406	-	17,17,17	0.11	0	16,16,16	0.10	0
11	BCL	e	101	-	69,74,74	1.85	15 (21%)	79,115,115	2.14	23 (29%)
7	HEC	C	501	1	46,50,50	1.82	5 (10%)	58,82,82	1.80	5 (8%)
10	8K6	J	104	-	17,17,17	0.10	0	16,16,16	0.12	0
11	BCL	W	101	-	69,74,74	1.83	17 (24%)	79,115,115	2.09	22 (27%)
9	PGV	H	302	-	50,50,50	0.91	2 (4%)	53,56,56	1.06	3 (5%)
11	BCL	j	103	6	69,74,74	1.79	18 (26%)	79,115,115	2.29	25 (31%)
11	BCL	J	102	6	69,74,74	1.77	17 (24%)	79,115,115	2.30	27 (34%)
11	BCL	N	102	6	69,74,74	1.76	18 (26%)	79,115,115	2.45	29 (36%)
11	BCL	j	102	-	69,74,74	1.87	18 (26%)	79,115,115	2.38	24 (30%)
15	MQ8	M	405	-	54,54,54	0.41	0	67,69,69	0.45	1 (1%)
10	8K6	j	104	-	17,17,17	0.12	0	16,16,16	0.11	0
10	8K6	L	405	-	17,17,17	0.12	0	16,16,16	0.11	0
7	HEC	C	504	1	46,50,50	1.83	5 (10%)	58,82,82	1.88	5 (8%)
16	CRT	Z	102	-	43,43,43	1.51	12 (27%)	48,54,54	2.01	18 (37%)
11	BCL	L	402	-	69,74,74	1.85	17 (24%)	79,115,115	2.30	26 (32%)
16	CRT	N	103	-	43,43,43	1.49	12 (27%)	48,54,54	1.59	13 (27%)
10	8K6	f	103	-	17,17,17	0.10	0	16,16,16	0.11	0
16	CRT	e	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.62	12 (25%)
11	BCL	T	102	6	69,74,74	1.78	18 (26%)	79,115,115	2.32	26 (32%)
10	8K6	V	103	-	17,17,17	0.11	0	16,16,16	0.07	0
11	BCL	f	101	-	69,74,74	1.85	17 (24%)	79,115,115	2.36	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	f	102	6	69,74,74	1.76	17 (24%)	79,115,115	2.23	22 (27%)
7	HEC	C	503	1	46,50,50	1.82	5 (10%)	58,82,82	1.83	6 (10%)
10	8K6	L	407	-	17,17,17	0.11	0	16,16,16	0.08	0
11	BCL	V	101	-	69,74,74	1.82	16 (23%)	79,115,115	2.32	24 (30%)
11	BCL	B	101	-	69,74,74	1.83	16 (23%)	79,115,115	2.03	24 (30%)
11	BCL	L	401	-	69,74,74	1.83	17 (24%)	79,115,115	2.40	24 (30%)
11	BCL	O	101	-	69,74,74	1.86	18 (26%)	79,115,115	2.07	24 (30%)
16	CRT	B	102	-	43,43,43	1.50	11 (25%)	48,54,54	1.63	11 (22%)
11	BCL	E	101	-	69,74,74	1.85	21 (30%)	79,115,115	2.40	25 (31%)
11	BCL	b	101	-	69,74,74	1.85	18 (26%)	79,115,115	2.26	25 (31%)

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
16	CRT	M	406	-	-	0/51/51/51	-
11	BCL	E	102	6	-	16/41/137/137	-
16	CRT	a	102	-	-	5/51/51/51	-
9	PGV	M	407	-	-	13/47/47/55	-
11	BCL	U	101	-	-	17/41/137/137	-
10	8K6	H	306	-	-	0/12/12/15	-
11	BCL	Q	101	-	-	16/41/137/137	-
11	BCL	R	101	-	-	17/41/137/137	-
9	PGV	H	301	-	-	21/55/55/55	-
16	CRT	E	103	-	-	3/51/51/51	-
10	8K6	L	409	-	-	0/15/15/15	-
11	BCL	V	102	6	-	19/41/137/137	-
11	BCL	P	102	6	-	18/41/137/137	-
13	LMT	L	408	-	-	7/18/58/61	0/2/2/2
16	CRT	U	102	-	-	7/51/51/51	-
11	BCL	A	102	6	-	15/41/137/137	-
10	8K6	J	103	-	-	0/10/10/15	-
10	8K6	N	104	-	-	0/15/15/15	-
16	CRT	i	102	-	-	4/51/51/51	-
10	8K6	P	104	-	-	1/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGV	R	104	-	-	14/55/55/55	-
9	PGV	Z	103	-	-	10/46/46/55	-
10	8K6	H	304	-	-	0/15/15/15	-
11	BCL	X	101	-	-	18/41/137/137	-
11	BCL	h	102	6	-	22/41/137/137	-
16	CRT	W	102	-	-	7/51/51/51	-
11	BCL	d	102	6	-	21/41/137/137	-
11	BCL	R	102	6	-	15/41/137/137	-
9	PGV	M	408	-	-	11/43/43/55	-
10	8K6	d	103	-	-	3/15/15/15	-
16	CRT	j	101	-	-	5/51/51/51	-
7	HEC	C	502	1	-	5/14/54/54	-
12	BPH	L	403	-	-	3/37/105/105	0/5/6/6
9	PGV	L	410	-	-	9/23/23/55	-
11	BCL	P	101	-	-	19/41/137/137	-
16	CRT	I	102	-	-	5/51/51/51	-
10	8K6	X	103	-	-	1/15/15/15	-
11	BCL	M	402	-	-	13/41/137/137	-
11	BCL	g	101	-	-	14/41/137/137	-
11	BCL	M	403	-	-	15/41/137/137	-
11	BCL	Y	101	-	-	17/41/137/137	-
11	BCL	D	101	-	-	17/41/137/137	-
16	CRT	Y	102	-	-	3/51/51/51	-
11	BCL	N	101	-	-	16/41/137/137	-
16	CRT	A	103	-	-	4/51/51/51	-
9	PGV	C	508	-	-	6/42/42/55	-
16	CRT	P	103	-	-	5/51/51/51	-
10	8K6	V	104	-	-	0/15/15/15	-
11	BCL	I	101	-	-	16/41/137/137	-
11	BCL	Z	101	-	-	21/41/137/137	-
11	BCL	G	101	-	-	15/41/137/137	-
11	BCL	i	101	-	-	16/41/137/137	-
11	BCL	J	101	-	-	19/41/137/137	-
11	BCL	K	101	-	-	15/41/137/137	-
10	8K6	M	409	-	-	0/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	A	101	-	-	22/41/137/137	-
11	BCL	h	101	-	-	12/41/137/137	-
10	8K6	H	303	-	-	2/14/14/15	-
11	BCL	d	101	-	-	12/41/137/137	-
10	8K6	H	305	-	-	0/15/15/15	-
11	BCL	G	102	6	-	19/41/137/137	-
11	BCL	X	102	6	-	20/41/137/137	-
11	BCL	a	101	-	-	14/41/137/137	-
11	BCL	T	101	-	-	19/41/137/137	-
16	CRT	K	102	-	-	3/51/51/51	-
10	8K6	j	105	-	-	2/15/15/15	-
10	8K6	C	509	-	-	2/13/13/15	-
16	CRT	R	103	-	-	4/51/51/51	-
11	BCL	S	101	-	-	13/41/137/137	-
11	BCL	c	101	-	-	13/41/137/137	-
10	8K6	L	404	-	-	0/12/12/15	-
12	BPH	M	404	-	-	7/37/105/105	0/5/6/6
11	BCL	b	102	6	-	24/41/137/137	-
11	BCL	F	101	-	-	16/41/137/137	-
10	8K6	L	406	-	-	2/15/15/15	-
11	BCL	e	101	-	-	20/41/137/137	-
7	HEC	C	501	1	-	4/14/54/54	-
10	8K6	J	104	-	-	1/15/15/15	-
11	BCL	W	101	-	-	17/41/137/137	-
9	PGV	H	302	-	-	12/55/55/55	-
11	BCL	j	103	6	-	14/41/137/137	-
11	BCL	J	102	6	-	16/41/137/137	-
11	BCL	N	102	6	-	15/41/137/137	-
11	BCL	j	102	-	-	13/41/137/137	-
15	MQ8	M	405	-	-	12/47/67/67	0/2/2/2
10	8K6	j	104	-	-	2/15/15/15	-
10	8K6	L	405	-	-	1/15/15/15	-
7	HEC	C	504	1	-	8/14/54/54	-
16	CRT	Z	102	-	-	11/51/51/51	-
11	BCL	L	402	-	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CRT	N	103	-	-	5/51/51/51	-
10	8K6	f	103	-	-	1/15/15/15	-
16	CRT	e	102	-	-	6/51/51/51	-
11	BCL	T	102	6	-	17/41/137/137	-
10	8K6	V	103	-	-	1/15/15/15	-
11	BCL	f	101	-	-	21/41/137/137	-
11	BCL	f	102	6	-	18/41/137/137	-
7	HEC	C	503	1	-	4/14/54/54	-
10	8K6	L	407	-	-	1/15/15/15	-
11	BCL	V	101	-	-	20/41/137/137	-
11	BCL	B	101	-	-	15/41/137/137	-
11	BCL	L	401	-	-	9/41/137/137	-
11	BCL	O	101	-	-	12/41/137/137	-
16	CRT	B	102	-	-	5/51/51/51	-
11	BCL	E	101	-	-	21/41/137/137	-
11	BCL	b	101	-	-	20/41/137/137	-

All (1130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	HEC	CAC-C3C	6.35	1.55	1.35
7	C	502	HEC	CAC-C3C	6.32	1.55	1.35
7	C	501	HEC	CAC-C3C	6.26	1.55	1.35
7	C	504	HEC	CAC-C3C	6.24	1.55	1.35
7	C	502	HEC	CAB-C3B	6.22	1.55	1.35
7	C	504	HEC	CAB-C3B	6.17	1.55	1.35
7	C	503	HEC	CAB-C3B	6.13	1.54	1.35
7	C	501	HEC	CAB-C3B	6.12	1.54	1.35
7	C	502	HEC	C3D-C2D	5.74	1.53	1.38
7	C	504	HEC	C3D-C2D	5.63	1.53	1.38
7	C	501	HEC	C3D-C2D	5.51	1.53	1.38
11	L	401	BCL	C3D-C4D	-5.50	1.31	1.44
7	C	503	HEC	C3D-C2D	5.48	1.53	1.38
11	U	101	BCL	C3D-C4D	-5.47	1.31	1.44
11	L	402	BCL	C3D-C4D	-5.46	1.31	1.44
11	M	402	BCL	C3D-C4D	-5.34	1.32	1.44
11	M	403	BCL	C3D-C4D	-5.34	1.32	1.44
11	i	101	BCL	C3D-C4D	-5.25	1.32	1.44
11	b	102	BCL	C3D-C4D	-5.22	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	101	BCL	C3D-C4D	-5.16	1.32	1.44
11	A	101	BCL	C3D-C4D	-5.16	1.32	1.44
11	T	101	BCL	C3D-C4D	-5.15	1.32	1.44
11	N	101	BCL	C3D-C4D	-5.14	1.32	1.44
11	g	101	BCL	C3D-C4D	-5.14	1.32	1.44
11	b	101	BCL	C3D-C4D	-5.12	1.32	1.44
11	W	101	BCL	C3D-C4D	-5.12	1.32	1.44
11	f	101	BCL	C3D-C4D	-5.11	1.32	1.44
11	V	101	BCL	C3D-C4D	-5.10	1.32	1.44
11	T	102	BCL	C3D-C4D	-5.06	1.32	1.44
11	J	101	BCL	C3D-C4D	-5.06	1.32	1.44
11	j	103	BCL	C3D-C4D	-5.06	1.32	1.44
11	G	101	BCL	C3D-C4D	-5.05	1.32	1.44
11	c	101	BCL	C3D-C4D	-5.05	1.32	1.44
11	F	101	BCL	C3D-C4D	-5.04	1.32	1.44
11	d	101	BCL	C3D-C4D	-5.02	1.32	1.44
11	Y	101	BCL	C3D-C4D	-5.02	1.32	1.44
11	E	101	BCL	C3D-C4D	-5.02	1.32	1.44
11	P	102	BCL	C3D-C4D	-5.01	1.32	1.44
11	P	101	BCL	C3D-C4D	-4.99	1.33	1.44
11	d	102	BCL	C3D-C4D	-4.99	1.33	1.44
11	O	101	BCL	C3D-C4D	-4.98	1.33	1.44
11	J	102	BCL	C3D-C4D	-4.98	1.33	1.44
11	e	101	BCL	C3D-C4D	-4.97	1.33	1.44
11	R	101	BCL	C3D-C4D	-4.97	1.33	1.44
11	a	101	BCL	C3D-C4D	-4.95	1.33	1.44
11	S	101	BCL	C3D-C4D	-4.95	1.33	1.44
11	R	102	BCL	C3D-C4D	-4.94	1.33	1.44
11	G	102	BCL	C3D-C4D	-4.93	1.33	1.44
11	X	102	BCL	C3D-C4D	-4.93	1.33	1.44
11	f	102	BCL	C3D-C4D	-4.92	1.33	1.44
11	V	102	BCL	C3D-C4D	-4.92	1.33	1.44
11	Q	101	BCL	C3D-C4D	-4.88	1.33	1.44
11	X	101	BCL	C3D-C4D	-4.88	1.33	1.44
11	E	102	BCL	C3D-C4D	-4.87	1.33	1.44
11	D	101	BCL	C3D-C4D	-4.86	1.33	1.44
11	j	102	BCL	C3D-C4D	-4.86	1.33	1.44
11	h	101	BCL	C3D-C4D	-4.83	1.33	1.44
11	E	102	BCL	O2D-CGD	4.83	1.45	1.33
11	h	102	BCL	C3D-C4D	-4.82	1.33	1.44
11	A	102	BCL	O2D-CGD	4.80	1.45	1.33
11	L	402	BCL	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	101	BCL	C1D-ND	-4.78	1.31	1.37
11	B	101	BCL	C3D-C4D	-4.78	1.33	1.44
11	M	403	BCL	O2D-CGD	4.76	1.44	1.33
11	Z	101	BCL	C3D-C4D	-4.75	1.33	1.44
11	d	101	BCL	O2D-CGD	4.75	1.44	1.33
11	j	103	BCL	O2D-CGD	4.75	1.44	1.33
11	I	101	BCL	C3D-C4D	-4.72	1.33	1.44
11	d	102	BCL	O2D-CGD	4.72	1.44	1.33
11	N	102	BCL	C3D-C4D	-4.70	1.33	1.44
11	A	102	BCL	C3D-C4D	-4.70	1.33	1.44
11	M	403	BCL	C4B-NB	-4.68	1.31	1.37
11	F	101	BCL	O2D-CGD	4.65	1.44	1.33
11	N	102	BCL	O2D-CGD	4.65	1.44	1.33
11	f	102	BCL	O2D-CGD	4.62	1.44	1.33
11	E	101	BCL	C4B-NB	-4.61	1.31	1.37
11	P	102	BCL	O2D-CGD	4.58	1.44	1.33
11	V	102	BCL	O2D-CGD	4.57	1.44	1.33
11	K	101	BCL	O2D-CGD	4.57	1.44	1.33
11	B	101	BCL	C1D-ND	-4.56	1.31	1.37
11	a	101	BCL	O2A-CGA	4.56	1.46	1.33
11	G	102	BCL	O2D-CGD	4.56	1.44	1.33
11	Y	101	BCL	O2D-CGD	4.55	1.44	1.33
11	X	102	BCL	O2D-CGD	4.55	1.44	1.33
11	h	102	BCL	O2D-CGD	4.54	1.44	1.33
11	T	102	BCL	O2D-CGD	4.53	1.44	1.33
11	A	101	BCL	C4B-NB	-4.50	1.32	1.37
11	F	101	BCL	C1D-ND	-4.49	1.32	1.37
11	R	102	BCL	O2D-CGD	4.49	1.44	1.33
11	R	101	BCL	C1D-ND	-4.49	1.32	1.37
11	S	101	BCL	O2D-CGD	4.47	1.44	1.33
11	U	101	BCL	O2D-CGD	4.46	1.44	1.33
11	c	101	BCL	O2A-CGA	4.46	1.46	1.33
11	U	101	BCL	C1D-ND	-4.46	1.32	1.37
11	e	101	BCL	O2D-CGD	4.45	1.44	1.33
11	B	101	BCL	O2D-CGD	4.45	1.44	1.33
11	g	101	BCL	O2D-CGD	4.44	1.44	1.33
11	c	101	BCL	O2D-CGD	4.44	1.44	1.33
11	R	101	BCL	O2D-CGD	4.43	1.44	1.33
11	L	401	BCL	O2D-CGD	4.40	1.44	1.33
11	h	101	BCL	O2D-CGD	4.40	1.44	1.33
11	h	101	BCL	C4B-NB	-4.40	1.32	1.37
11	J	101	BCL	C4B-NB	-4.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	101	BCL	O2D-CGD	4.38	1.44	1.33
11	U	101	BCL	O2A-CGA	4.37	1.46	1.33
11	a	101	BCL	O2D-CGD	4.37	1.44	1.33
11	D	101	BCL	C1D-ND	-4.36	1.32	1.37
11	O	101	BCL	O2D-CGD	4.36	1.43	1.33
11	G	101	BCL	O2D-CGD	4.35	1.43	1.33
11	b	101	BCL	O2D-CGD	4.34	1.43	1.33
11	I	101	BCL	O2D-CGD	4.34	1.43	1.33
11	X	101	BCL	O2D-CGD	4.34	1.43	1.33
11	j	102	BCL	C4B-NB	-4.33	1.32	1.37
11	L	401	BCL	C4B-NB	-4.32	1.32	1.37
11	f	101	BCL	O2D-CGD	4.32	1.43	1.33
11	I	101	BCL	O2A-CGA	4.32	1.45	1.33
11	P	101	BCL	O2D-CGD	4.31	1.43	1.33
11	J	102	BCL	O2D-CGD	4.31	1.43	1.33
11	j	102	BCL	O2D-CGD	4.31	1.43	1.33
11	T	101	BCL	O2D-CGD	4.30	1.43	1.33
11	e	101	BCL	C1D-ND	-4.30	1.32	1.37
11	Q	101	BCL	O2A-CGA	4.29	1.45	1.33
11	e	101	BCL	O2A-CGA	4.27	1.45	1.33
11	A	101	BCL	O2D-CGD	4.27	1.43	1.33
12	M	404	BPH	CBD-CGD	-4.26	1.47	1.52
9	R	104	PGV	O01-C1	4.26	1.46	1.34
11	W	101	BCL	O2D-CGD	4.26	1.43	1.33
11	L	402	BCL	C3B-C4B	4.25	1.49	1.41
11	b	101	BCL	C1D-ND	-4.25	1.32	1.37
11	N	101	BCL	O2D-CGD	4.24	1.43	1.33
11	a	101	BCL	C1D-ND	-4.24	1.32	1.37
9	M	407	PGV	O03-C19	4.23	1.45	1.33
11	R	101	BCL	C4B-NB	-4.23	1.32	1.37
9	C	508	PGV	O03-C19	4.22	1.45	1.33
11	L	402	BCL	O2A-CGA	4.22	1.45	1.33
11	h	102	BCL	O2A-CGA	4.21	1.45	1.33
11	f	101	BCL	O2A-CGA	4.21	1.45	1.33
11	S	101	BCL	O2A-CGA	4.21	1.45	1.33
9	M	408	PGV	O03-C19	4.20	1.45	1.33
9	Z	103	PGV	O03-C19	4.20	1.45	1.33
11	E	101	BCL	O2D-CGD	4.19	1.43	1.33
11	Z	101	BCL	O2D-CGD	4.18	1.43	1.33
9	H	302	PGV	O03-C19	4.18	1.45	1.33
11	i	101	BCL	O2D-CGD	4.18	1.43	1.33
11	b	102	BCL	C4B-NB	-4.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	101	BCL	C1D-ND	-4.18	1.32	1.37
9	R	104	PGV	O03-C19	4.18	1.45	1.33
9	M	408	PGV	O01-C1	4.18	1.46	1.34
11	A	101	BCL	C1D-ND	-4.17	1.32	1.37
11	F	101	BCL	O2A-CGA	4.17	1.45	1.33
11	V	101	BCL	O2D-CGD	4.16	1.43	1.33
11	Q	101	BCL	C1D-ND	-4.16	1.32	1.37
11	J	101	BCL	O2D-CGD	4.16	1.43	1.33
11	X	102	BCL	O2A-CGA	4.16	1.45	1.33
9	H	301	PGV	O03-C19	4.14	1.45	1.33
11	b	102	BCL	O2A-CGA	4.14	1.45	1.33
11	i	101	BCL	O2A-CGA	4.14	1.45	1.33
11	Y	101	BCL	O2A-CGA	4.14	1.45	1.33
11	j	103	BCL	O2A-CGA	4.14	1.45	1.33
11	D	101	BCL	O2D-CGD	4.13	1.43	1.33
11	A	102	BCL	O2A-CGA	4.13	1.45	1.33
11	b	102	BCL	O2D-CGD	4.11	1.43	1.33
11	G	101	BCL	C4B-NB	-4.10	1.32	1.37
11	M	403	BCL	C1D-ND	-4.10	1.32	1.37
11	R	102	BCL	O2A-CGA	4.09	1.45	1.33
11	D	101	BCL	C4B-NB	-4.09	1.32	1.37
11	O	101	BCL	O2A-CGA	4.09	1.45	1.33
11	j	102	BCL	C1D-ND	-4.09	1.32	1.37
9	C	508	PGV	O01-C1	4.09	1.45	1.34
11	B	101	BCL	O2A-CGA	4.08	1.45	1.33
9	Z	103	PGV	O01-C1	4.08	1.45	1.34
11	e	101	BCL	C3B-C4B	4.08	1.49	1.41
11	J	102	BCL	C4B-NB	-4.08	1.32	1.37
11	D	101	BCL	C3B-C4B	4.08	1.49	1.41
11	R	101	BCL	O2A-CGA	4.08	1.45	1.33
11	f	101	BCL	C4B-NB	-4.07	1.32	1.37
11	D	101	BCL	O2A-CGA	4.07	1.45	1.33
11	K	101	BCL	O2A-CGA	4.06	1.45	1.33
11	M	402	BCL	C1D-ND	-4.06	1.32	1.37
11	N	101	BCL	C1D-ND	-4.05	1.32	1.37
11	g	101	BCL	C3B-C4B	4.04	1.49	1.41
11	g	101	BCL	O2A-CGA	4.04	1.45	1.33
9	H	301	PGV	O01-C1	4.04	1.45	1.34
9	H	302	PGV	O01-C1	4.04	1.45	1.34
9	M	407	PGV	O01-C1	4.03	1.45	1.34
11	G	102	BCL	O2A-CGA	4.02	1.45	1.33
12	L	403	BPH	CBD-CGD	-4.02	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	101	BCL	C4B-NB	-4.02	1.32	1.37
11	j	102	BCL	O2A-CGA	4.01	1.45	1.33
11	V	101	BCL	C1D-ND	-4.00	1.32	1.37
11	B	101	BCL	C4B-NB	-4.00	1.32	1.37
11	M	402	BCL	O2D-CGD	4.00	1.43	1.33
11	c	101	BCL	C1D-ND	-4.00	1.32	1.37
11	Z	101	BCL	O2A-CGA	3.99	1.45	1.33
11	P	101	BCL	C1D-ND	-3.99	1.32	1.37
11	W	101	BCL	C1D-ND	-3.99	1.32	1.37
11	U	101	BCL	C3B-C4B	3.99	1.49	1.41
11	K	101	BCL	C3B-C4B	3.97	1.49	1.41
11	T	101	BCL	O2A-CGA	3.96	1.44	1.33
11	W	101	BCL	O2A-CGA	3.96	1.44	1.33
11	a	101	BCL	C3B-C4B	3.96	1.48	1.41
11	M	403	BCL	C3B-C4B	3.96	1.48	1.41
11	B	101	BCL	C3B-C4B	3.96	1.48	1.41
11	T	101	BCL	C1D-ND	-3.96	1.32	1.37
11	E	102	BCL	C3B-C4B	3.96	1.48	1.41
11	d	101	BCL	O2A-CGA	3.95	1.44	1.33
11	J	102	BCL	O2A-CGA	3.94	1.44	1.33
11	g	101	BCL	C1D-ND	-3.94	1.32	1.37
11	G	101	BCL	C1D-ND	-3.94	1.32	1.37
11	V	101	BCL	O2A-CGA	3.94	1.44	1.33
11	K	101	BCL	C1D-ND	-3.93	1.32	1.37
11	d	101	BCL	C1D-ND	-3.93	1.32	1.37
11	G	102	BCL	C4B-NB	-3.92	1.32	1.37
11	M	402	BCL	C3B-C4B	3.92	1.48	1.41
11	S	101	BCL	C1D-ND	-3.92	1.32	1.37
11	X	101	BCL	C4B-NB	-3.92	1.32	1.37
11	i	101	BCL	C1D-ND	-3.92	1.32	1.37
11	S	101	BCL	C4B-NB	-3.91	1.32	1.37
11	b	101	BCL	O2A-CGA	3.91	1.44	1.33
11	V	102	BCL	O2A-CGA	3.91	1.44	1.33
11	I	101	BCL	C1D-ND	-3.91	1.32	1.37
11	W	101	BCL	C3B-C4B	3.90	1.48	1.41
11	R	102	BCL	C4B-NB	-3.90	1.32	1.37
11	T	102	BCL	O2A-CGA	3.90	1.44	1.33
11	f	102	BCL	O2A-CGA	3.89	1.44	1.33
11	M	402	BCL	O2A-CGA	3.88	1.44	1.33
11	d	102	BCL	O2A-CGA	3.88	1.44	1.33
11	Q	101	BCL	C3B-C4B	3.88	1.48	1.41
11	J	101	BCL	O2A-CGA	3.87	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	f	101	BCL	C1D-ND	-3.87	1.32	1.37
11	L	401	BCL	O2A-CGA	3.87	1.44	1.33
11	G	101	BCL	O2A-CGA	3.86	1.44	1.33
11	P	102	BCL	O2A-CGA	3.86	1.44	1.33
11	X	101	BCL	O2A-CGA	3.86	1.44	1.33
11	A	101	BCL	O2A-CGA	3.86	1.44	1.33
11	I	101	BCL	C3B-C4B	3.86	1.48	1.41
11	P	101	BCL	C4B-NB	-3.85	1.32	1.37
11	E	101	BCL	O2A-CGA	3.85	1.44	1.33
11	M	403	BCL	O2A-CGA	3.85	1.44	1.33
11	i	101	BCL	C4B-NB	-3.84	1.32	1.37
11	h	101	BCL	O2A-CGA	3.84	1.44	1.33
11	V	101	BCL	C4B-NB	-3.84	1.32	1.37
11	N	101	BCL	C4B-NB	-3.83	1.32	1.37
11	b	101	BCL	C4B-NB	-3.82	1.32	1.37
11	N	101	BCL	C3B-C4B	3.82	1.48	1.41
9	L	410	PGV	O01-C1	3.81	1.45	1.34
11	N	102	BCL	C4B-NB	-3.81	1.32	1.37
11	O	101	BCL	C4B-NB	-3.77	1.32	1.37
9	L	410	PGV	O03-C19	3.77	1.44	1.33
11	X	101	BCL	C1D-ND	-3.76	1.32	1.37
11	J	101	BCL	C1D-ND	-3.76	1.32	1.37
11	E	102	BCL	O2A-CGA	3.76	1.44	1.33
11	Z	101	BCL	C1D-ND	-3.74	1.32	1.37
12	L	403	BPH	C3B-C4B	3.74	1.47	1.41
11	Y	101	BCL	C4B-NB	-3.74	1.33	1.37
11	L	402	BCL	C1D-ND	-3.73	1.33	1.37
11	A	102	BCL	C4B-NB	-3.73	1.33	1.37
11	h	102	BCL	C3B-C4B	3.72	1.48	1.41
11	D	101	BCL	C1B-NB	-3.72	1.33	1.37
11	h	102	BCL	C4B-NB	-3.72	1.33	1.37
11	E	102	BCL	C4B-NB	-3.71	1.33	1.37
11	X	102	BCL	C4B-NB	-3.70	1.33	1.37
11	h	101	BCL	C1D-ND	-3.70	1.33	1.37
11	j	103	BCL	C4B-NB	-3.70	1.33	1.37
11	T	102	BCL	C3B-C4B	3.70	1.48	1.41
11	N	102	BCL	O2A-CGA	3.69	1.44	1.33
11	A	102	BCL	OBD-CAD	3.69	1.28	1.22
11	j	103	BCL	C3B-C4B	3.68	1.48	1.41
11	V	102	BCL	C3B-C4B	3.66	1.48	1.41
11	Z	101	BCL	C3B-C4B	3.65	1.48	1.41
11	d	102	BCL	C4B-NB	-3.65	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	101	BCL	C3C-C4C	-3.64	1.47	1.51
11	N	101	BCL	O2A-CGA	3.64	1.44	1.33
11	c	101	BCL	C3B-C4B	3.62	1.48	1.41
11	X	102	BCL	C3B-C4B	3.61	1.48	1.41
11	f	102	BCL	C3B-C4B	3.60	1.48	1.41
11	Y	101	BCL	C3B-C4B	3.60	1.48	1.41
11	F	101	BCL	C3B-C4B	3.60	1.48	1.41
11	d	101	BCL	C3B-C4B	3.59	1.48	1.41
11	M	402	BCL	C4B-NB	-3.58	1.33	1.37
11	i	101	BCL	C3B-C4B	3.58	1.48	1.41
11	L	401	BCL	C3B-C4B	3.57	1.48	1.41
11	X	101	BCL	C3C-C4C	-3.56	1.47	1.51
11	T	102	BCL	C4B-NB	-3.55	1.33	1.37
11	Z	101	BCL	C4B-NB	-3.54	1.33	1.37
11	g	101	BCL	CHC-C4B	3.54	1.47	1.39
11	d	102	BCL	C3B-C4B	3.54	1.48	1.41
11	O	101	BCL	C3B-C4B	3.53	1.48	1.41
11	L	401	BCL	C1D-ND	-3.53	1.33	1.37
11	N	102	BCL	C3B-C4B	3.53	1.48	1.41
11	L	402	BCL	CHB-C1B	3.53	1.47	1.39
11	j	102	BCL	C3B-C4B	3.52	1.48	1.41
11	E	101	BCL	C1D-ND	-3.52	1.33	1.37
11	S	101	BCL	C1B-NB	-3.52	1.33	1.37
11	j	102	BCL	C1B-NB	-3.52	1.33	1.37
11	F	101	BCL	C1B-NB	-3.50	1.33	1.37
11	b	102	BCL	C1D-ND	-3.50	1.33	1.37
11	d	101	BCL	C4B-NB	-3.50	1.33	1.37
11	P	101	BCL	O2A-CGA	3.50	1.43	1.33
11	P	102	BCL	C3B-C4B	3.50	1.48	1.41
11	F	101	BCL	C4B-NB	-3.49	1.33	1.37
11	h	101	BCL	C3B-C4B	3.48	1.48	1.41
11	R	101	BCL	C3B-C4B	3.48	1.48	1.41
11	B	101	BCL	C3C-C4C	-3.47	1.47	1.51
11	Q	101	BCL	C4B-NB	-3.46	1.33	1.37
11	V	101	BCL	C3B-C4B	3.46	1.47	1.41
11	j	102	BCL	C3C-C4C	-3.45	1.47	1.51
11	K	101	BCL	CHC-C4B	3.44	1.47	1.39
11	b	101	BCL	C3B-C4B	3.43	1.47	1.41
11	U	101	BCL	C1B-NB	-3.42	1.33	1.37
11	J	101	BCL	C3B-C4B	3.42	1.47	1.41
11	e	101	BCL	CHC-C4B	3.42	1.47	1.39
11	N	101	BCL	C3C-C4C	-3.42	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	j	103	BCL	C1D-ND	-3.41	1.33	1.37
11	E	102	BCL	CHD-C1D	3.41	1.45	1.38
11	a	101	BCL	C4B-NB	-3.41	1.33	1.37
11	M	403	BCL	MG-NA	-3.41	1.98	2.06
11	I	101	BCL	C1B-NB	-3.40	1.33	1.37
11	W	101	BCL	C4B-NB	-3.40	1.33	1.37
11	P	102	BCL	C4B-NB	-3.40	1.33	1.37
11	j	103	BCL	OBD-CAD	3.40	1.28	1.22
11	d	102	BCL	CHD-C1D	3.39	1.45	1.38
11	A	101	BCL	C3B-C4B	3.38	1.47	1.41
11	A	101	BCL	C1B-NB	-3.38	1.33	1.37
11	R	101	BCL	C3C-C4C	-3.37	1.47	1.51
11	a	101	BCL	CHC-C4B	3.37	1.47	1.39
11	N	102	BCL	OBD-CAD	3.37	1.28	1.22
11	F	101	BCL	CHC-C4B	3.35	1.46	1.39
11	f	102	BCL	C4B-NB	-3.34	1.33	1.37
11	R	102	BCL	C3B-C4B	3.34	1.47	1.41
11	P	101	BCL	C3C-C4C	-3.33	1.47	1.51
11	X	101	BCL	C3B-C4B	3.33	1.47	1.41
11	d	101	BCL	CHB-C1B	3.33	1.46	1.39
11	a	101	BCL	C3C-C4C	-3.32	1.47	1.51
11	T	102	BCL	C1D-ND	-3.32	1.33	1.37
11	g	101	BCL	C3C-C4C	-3.32	1.47	1.51
11	h	102	BCL	OBD-CAD	3.32	1.28	1.22
11	P	101	BCL	CHB-C1B	3.31	1.46	1.39
11	J	101	BCL	C3C-C4C	-3.31	1.47	1.51
11	G	102	BCL	CHD-C1D	3.31	1.44	1.38
12	L	403	BPH	C3D-CAD	-3.31	1.41	1.47
11	W	101	BCL	CHC-C4B	3.30	1.46	1.39
11	g	101	BCL	C1B-NB	-3.30	1.33	1.37
11	f	101	BCL	C3B-C4B	3.30	1.47	1.41
11	S	101	BCL	C3B-C4B	3.30	1.47	1.41
11	U	101	BCL	C3C-C4C	-3.30	1.47	1.51
11	E	101	BCL	C3C-C4C	-3.29	1.47	1.51
11	d	102	BCL	OBD-CAD	3.29	1.28	1.22
11	U	101	BCL	C4B-NB	-3.28	1.33	1.37
11	b	102	BCL	C3B-C4B	3.28	1.47	1.41
11	J	102	BCL	C1D-ND	-3.28	1.33	1.37
11	D	101	BCL	CHC-C4B	3.28	1.46	1.39
11	P	102	BCL	C1D-ND	-3.27	1.33	1.37
11	Z	101	BCL	C3C-C4C	-3.27	1.47	1.51
11	B	101	BCL	CHC-C4B	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	101	BCL	CHB-C1B	3.27	1.46	1.39
11	c	101	BCL	C1B-NB	-3.27	1.33	1.37
11	J	102	BCL	C3B-C4B	3.27	1.47	1.41
11	V	102	BCL	C1D-ND	-3.27	1.33	1.37
11	V	102	BCL	C4B-NB	-3.26	1.33	1.37
11	R	101	BCL	CHB-C1B	3.26	1.46	1.39
11	K	101	BCL	C4B-NB	-3.25	1.33	1.37
11	A	101	BCL	C3C-C4C	-3.25	1.47	1.51
11	E	101	BCL	C3B-C4B	3.25	1.47	1.41
11	U	101	BCL	CHC-C4B	3.24	1.46	1.39
11	X	102	BCL	CHD-C1D	3.24	1.44	1.38
11	M	403	BCL	CHB-C1B	3.24	1.46	1.39
11	M	402	BCL	CHC-C4B	3.24	1.46	1.39
11	c	101	BCL	C4B-NB	-3.24	1.33	1.37
11	J	102	BCL	OBD-CAD	3.23	1.28	1.22
11	T	101	BCL	C3B-C4B	3.23	1.47	1.41
11	L	402	BCL	C1B-NB	-3.23	1.33	1.37
11	K	101	BCL	C1B-NB	-3.22	1.33	1.37
11	L	401	BCL	CHD-C1D	3.22	1.44	1.38
11	X	102	BCL	C1D-ND	-3.22	1.33	1.37
11	L	402	BCL	CHC-C4B	3.22	1.46	1.39
11	X	102	BCL	C1B-NB	-3.21	1.33	1.37
11	M	403	BCL	C1B-NB	-3.21	1.33	1.37
11	e	101	BCL	C4B-NB	-3.21	1.33	1.37
11	N	102	BCL	C1B-NB	-3.21	1.33	1.37
11	E	102	BCL	C1D-ND	-3.21	1.33	1.37
11	T	101	BCL	C1B-NB	-3.21	1.33	1.37
11	a	101	BCL	C1B-NB	-3.21	1.33	1.37
11	P	101	BCL	C3B-C4B	3.21	1.47	1.41
11	I	101	BCL	C3C-C4C	-3.20	1.47	1.51
11	E	101	BCL	C1B-NB	-3.20	1.33	1.37
11	a	101	BCL	CHB-C1B	3.20	1.46	1.39
11	O	101	BCL	CHC-C4B	3.20	1.46	1.39
11	e	101	BCL	C3C-C4C	-3.20	1.47	1.51
11	b	101	BCL	CHB-C1B	3.19	1.46	1.39
11	J	101	BCL	CHB-C1B	3.19	1.46	1.39
11	R	102	BCL	CHD-C1D	3.18	1.44	1.38
11	S	101	BCL	CHC-C4B	3.18	1.46	1.39
11	I	101	BCL	C4B-NB	-3.18	1.33	1.37
11	f	101	BCL	CHB-C1B	3.18	1.46	1.39
11	G	101	BCL	MG-NA	-3.18	1.98	2.06
11	G	101	BCL	C3C-C4C	-3.17	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	101	BCL	C1B-NB	-3.17	1.33	1.37
11	Q	101	BCL	C3C-C4C	-3.17	1.47	1.51
11	i	101	BCL	CHC-C4B	3.17	1.46	1.39
11	T	102	BCL	OBD-CAD	3.16	1.27	1.22
11	F	101	BCL	C3C-C4C	-3.16	1.47	1.51
11	Z	101	BCL	CHB-C1B	3.16	1.46	1.39
11	b	101	BCL	C3C-C4C	-3.15	1.47	1.51
11	P	101	BCL	MG-NA	-3.15	1.98	2.06
11	P	101	BCL	C1B-NB	-3.15	1.33	1.37
11	T	102	BCL	CHD-C1D	3.15	1.44	1.38
11	h	101	BCL	CHB-C1B	3.15	1.46	1.39
11	W	101	BCL	C3C-C4C	-3.14	1.47	1.51
11	V	102	BCL	CHD-C1D	3.14	1.44	1.38
11	g	101	BCL	C4B-NB	-3.14	1.33	1.37
11	G	102	BCL	C3B-C4B	3.14	1.47	1.41
11	R	102	BCL	OBD-CAD	3.13	1.27	1.22
11	T	101	BCL	CHB-C1B	3.13	1.46	1.39
11	B	101	BCL	CHB-C1B	3.13	1.46	1.39
11	Y	101	BCL	CHB-C1B	3.13	1.46	1.39
11	M	402	BCL	MG-NA	-3.13	1.98	2.06
11	G	102	BCL	C1B-NB	-3.13	1.33	1.37
11	e	101	BCL	CHB-C1B	3.13	1.46	1.39
11	d	102	BCL	C1D-ND	-3.12	1.33	1.37
11	A	102	BCL	CHD-C1D	3.12	1.44	1.38
11	N	102	BCL	C3D-C2D	3.12	1.47	1.39
11	c	101	BCL	CHB-C1B	3.11	1.46	1.39
11	f	102	BCL	OBD-CAD	3.11	1.27	1.22
11	Q	101	BCL	C3D-C2D	3.11	1.47	1.39
11	A	101	BCL	CHB-C1B	3.11	1.46	1.39
11	h	101	BCL	C1B-NB	-3.10	1.33	1.37
11	V	102	BCL	OBD-CAD	3.10	1.27	1.22
11	M	402	BCL	C3D-C2D	3.09	1.47	1.39
11	f	101	BCL	MG-NA	-3.09	1.98	2.06
11	i	101	BCL	C1B-NB	-3.09	1.33	1.37
11	G	101	BCL	C3B-C4B	3.09	1.47	1.41
11	Q	101	BCL	CHC-C4B	3.09	1.46	1.39
11	f	101	BCL	C1B-NB	-3.09	1.33	1.37
11	D	101	BCL	CHB-C1B	3.09	1.46	1.39
11	W	101	BCL	CHB-C1B	3.09	1.46	1.39
11	d	101	BCL	C1B-NB	-3.08	1.33	1.37
11	V	101	BCL	C3C-C4C	-3.07	1.47	1.51
11	h	101	BCL	C3C-C4C	-3.07	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	102	BCL	C1B-NB	-3.07	1.33	1.37
11	W	101	BCL	C1B-NB	-3.07	1.33	1.37
11	N	101	BCL	CHC-C4B	3.06	1.46	1.39
11	Y	101	BCL	CHC-C4B	3.06	1.46	1.39
11	X	102	BCL	OBD-CAD	3.05	1.27	1.22
11	i	101	BCL	CHB-C1B	3.05	1.46	1.39
11	S	101	BCL	CHD-C1D	3.04	1.44	1.38
11	c	101	BCL	CHC-C4B	3.04	1.46	1.39
11	G	102	BCL	C3D-C2D	3.04	1.47	1.39
11	P	102	BCL	OBD-CAD	3.03	1.27	1.22
11	G	102	BCL	OBD-CAD	3.03	1.27	1.22
11	A	102	BCL	C3B-C4B	3.03	1.47	1.41
11	J	101	BCL	C1B-NB	-3.03	1.33	1.37
11	L	401	BCL	CHB-C1B	3.03	1.46	1.39
11	I	101	BCL	CHB-C1B	3.02	1.46	1.39
11	f	102	BCL	C1D-ND	-3.02	1.33	1.37
11	O	101	BCL	C1B-NB	-3.02	1.33	1.37
11	R	102	BCL	CHB-C1B	3.02	1.46	1.39
11	X	101	BCL	CHB-C1B	3.02	1.46	1.39
11	f	102	BCL	CHD-C1D	3.02	1.44	1.38
11	M	402	BCL	C1B-NB	-3.02	1.33	1.37
11	Z	101	BCL	OBD-CAD	3.02	1.27	1.22
11	G	102	BCL	C1D-ND	-3.02	1.33	1.37
11	E	102	BCL	OBD-CAD	3.01	1.27	1.22
11	N	102	BCL	CHD-C1D	3.01	1.44	1.38
11	G	101	BCL	CHB-C1B	3.01	1.46	1.39
11	h	102	BCL	CHD-C1D	3.01	1.44	1.38
11	d	101	BCL	MG-NA	-3.00	1.99	2.06
11	K	101	BCL	C3C-C4C	-2.99	1.47	1.51
11	J	101	BCL	MG-NA	-2.99	1.99	2.06
11	K	101	BCL	CHD-C1D	2.99	1.44	1.38
11	L	401	BCL	MG-NA	-2.99	1.99	2.06
11	e	101	BCL	C1B-NB	-2.99	1.33	1.37
11	I	101	BCL	CHC-C4B	2.98	1.46	1.39
11	Z	101	BCL	C3D-C2D	2.98	1.47	1.39
11	V	101	BCL	CHC-C4B	2.97	1.46	1.39
12	M	404	BPH	C3D-CAD	-2.97	1.42	1.47
11	j	102	BCL	MG-NA	-2.97	1.99	2.06
11	j	103	BCL	C3D-C2D	2.97	1.47	1.39
11	j	103	BCL	C1B-NB	-2.97	1.34	1.37
11	J	102	BCL	C3D-C2D	2.96	1.47	1.39
11	Q	101	BCL	C1B-NB	-2.96	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	102	BCL	C3D-C2D	2.96	1.47	1.39
11	J	102	BCL	CHC-C4B	2.96	1.46	1.39
11	Y	101	BCL	C3D-C2D	2.96	1.47	1.39
11	O	101	BCL	CHB-C1B	2.96	1.46	1.39
11	T	101	BCL	C3D-C2D	2.96	1.47	1.39
11	h	101	BCL	MG-NA	-2.96	1.99	2.06
11	S	101	BCL	C3C-C4C	-2.96	1.47	1.51
11	M	403	BCL	CHC-C4B	2.96	1.46	1.39
11	P	102	BCL	C3D-C2D	2.96	1.47	1.39
11	S	101	BCL	CHB-C1B	2.95	1.46	1.39
11	R	101	BCL	C3D-C2D	2.94	1.47	1.39
11	X	102	BCL	CHC-C4B	2.94	1.46	1.39
11	B	101	BCL	C1B-NB	-2.94	1.34	1.37
11	b	102	BCL	CHD-C1D	2.94	1.44	1.38
11	d	101	BCL	C3C-C4C	-2.93	1.47	1.51
11	Q	101	BCL	CHB-C1B	2.93	1.46	1.39
11	T	102	BCL	CHC-C4B	2.93	1.46	1.39
11	I	101	BCL	CHD-C1D	2.93	1.44	1.38
11	b	101	BCL	C1B-NB	-2.92	1.34	1.37
11	d	101	BCL	CHC-C4B	2.92	1.46	1.39
11	F	101	BCL	CHB-C1B	2.92	1.46	1.39
11	I	101	BCL	C3D-C2D	2.92	1.47	1.39
11	j	102	BCL	CHB-C1B	2.92	1.46	1.39
11	E	102	BCL	C3D-C2D	2.91	1.46	1.39
11	E	102	BCL	C1B-NB	-2.91	1.34	1.37
11	L	401	BCL	C3D-C2D	2.90	1.46	1.39
11	c	101	BCL	OBD-CAD	2.90	1.27	1.22
11	b	101	BCL	C3D-C2D	2.90	1.46	1.39
11	X	101	BCL	MG-NA	-2.90	1.99	2.06
11	X	102	BCL	C3D-C2D	2.90	1.46	1.39
11	h	102	BCL	C1D-ND	-2.89	1.34	1.37
11	O	101	BCL	C3D-C2D	2.89	1.46	1.39
11	b	101	BCL	MG-NA	-2.89	1.99	2.06
11	S	101	BCL	C3D-C2D	2.89	1.46	1.39
11	A	102	BCL	C3D-C2D	2.88	1.46	1.39
11	E	102	BCL	CHC-C4B	2.88	1.45	1.39
11	V	102	BCL	C3D-C2D	2.88	1.46	1.39
11	h	102	BCL	C3D-C2D	2.88	1.46	1.39
11	W	101	BCL	C3D-C2D	2.88	1.46	1.39
11	X	101	BCL	CHC-C4B	2.88	1.45	1.39
11	f	102	BCL	CHC-C4B	2.88	1.45	1.39
11	F	101	BCL	C3D-C2D	2.87	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	j	102	BCL	C3D-C2D	2.87	1.46	1.39
11	a	101	BCL	C3D-C2D	2.87	1.46	1.39
11	X	101	BCL	C3D-C2D	2.87	1.46	1.39
11	R	102	BCL	C1D-ND	-2.87	1.34	1.37
11	T	101	BCL	MG-NA	-2.87	1.99	2.06
11	i	101	BCL	C3D-C2D	2.87	1.46	1.39
11	c	101	BCL	CHD-C1D	2.87	1.44	1.38
11	K	101	BCL	CHB-C1B	2.86	1.45	1.39
11	V	101	BCL	C1B-NB	-2.86	1.34	1.37
11	P	102	BCL	CHD-C1D	2.86	1.44	1.38
11	B	101	BCL	C3D-C2D	2.86	1.46	1.39
11	V	102	BCL	C1B-NB	-2.86	1.34	1.37
11	X	101	BCL	C1B-NB	-2.86	1.34	1.37
11	J	102	BCL	CHD-C1D	2.86	1.44	1.38
11	G	101	BCL	CHC-C4B	2.86	1.45	1.39
11	T	102	BCL	C3D-C2D	2.85	1.46	1.39
11	R	102	BCL	C3D-C2D	2.85	1.46	1.39
11	h	102	BCL	C1B-NB	-2.85	1.34	1.37
11	N	102	BCL	C1D-ND	-2.85	1.34	1.37
11	N	101	BCL	CHB-C1B	2.85	1.45	1.39
11	M	402	BCL	OBD-CAD	2.84	1.27	1.22
11	f	102	BCL	C3D-C2D	2.84	1.46	1.39
11	c	101	BCL	C3D-C2D	2.84	1.46	1.39
11	E	101	BCL	CHB-C1B	2.83	1.45	1.39
11	L	402	BCL	C4B-NB	-2.83	1.34	1.37
11	K	101	BCL	C3D-C2D	2.83	1.46	1.39
11	M	402	BCL	CHB-C1B	2.82	1.45	1.39
11	Z	101	BCL	C1B-NB	-2.82	1.34	1.37
11	b	102	BCL	C1B-NB	-2.82	1.34	1.37
11	g	101	BCL	CHB-C1B	2.82	1.45	1.39
11	A	102	BCL	C1D-ND	-2.81	1.34	1.37
11	b	102	BCL	OBD-CAD	2.81	1.27	1.22
11	d	101	BCL	C3D-C2D	2.81	1.46	1.39
11	J	101	BCL	C3D-C2D	2.80	1.46	1.39
11	D	101	BCL	C3D-C2D	2.80	1.46	1.39
11	Z	101	BCL	MG-NA	-2.80	1.99	2.06
11	Z	101	BCL	CHC-C4B	2.80	1.45	1.39
11	L	401	BCL	CHC-C4B	2.80	1.45	1.39
11	J	102	BCL	CHB-C1B	2.80	1.45	1.39
11	A	102	BCL	C1B-NB	-2.80	1.34	1.37
11	G	101	BCL	C1B-NB	-2.80	1.34	1.37
11	P	102	BCL	MG-NA	-2.79	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	101	BCL	C3C-C4C	-2.79	1.48	1.51
11	E	101	BCL	MG-NA	-2.79	1.99	2.06
11	V	102	BCL	CHC-C4B	2.79	1.45	1.39
11	A	101	BCL	MG-NA	-2.79	1.99	2.06
11	A	102	BCL	CHB-C1B	2.78	1.45	1.39
11	j	103	BCL	CHD-C1D	2.78	1.43	1.38
11	f	102	BCL	CHB-C1B	2.78	1.45	1.39
11	G	101	BCL	C3D-C2D	2.78	1.46	1.39
11	c	101	BCL	C3C-C4C	-2.78	1.48	1.51
11	d	102	BCL	CHC-C4B	2.78	1.45	1.39
11	N	101	BCL	C3D-C2D	2.77	1.46	1.39
11	P	101	BCL	C3D-C2D	2.77	1.46	1.39
11	e	101	BCL	MG-NA	-2.77	1.99	2.06
11	K	101	BCL	OBD-CAD	2.77	1.27	1.22
11	h	102	BCL	CHC-C4B	2.76	1.45	1.39
11	d	102	BCL	C3D-C2D	2.76	1.46	1.39
11	U	101	BCL	MG-NA	-2.75	1.99	2.06
11	e	101	BCL	C3D-C2D	2.75	1.46	1.39
11	f	101	BCL	C3D-C2D	2.75	1.46	1.39
11	f	101	BCL	C3C-C4C	-2.75	1.48	1.51
11	X	102	BCL	CHB-C4A	-2.74	1.30	1.37
11	E	101	BCL	C3D-C2D	2.74	1.46	1.39
11	A	102	BCL	C3C-C4C	-2.73	1.48	1.51
11	A	102	BCL	MG-NA	-2.73	1.99	2.06
11	R	101	BCL	CHC-C4B	2.72	1.45	1.39
11	W	101	BCL	CHD-C1D	2.72	1.43	1.38
11	L	402	BCL	C3D-C2D	2.72	1.46	1.39
11	N	101	BCL	C1B-NB	-2.72	1.34	1.37
11	U	101	BCL	C3D-C2D	2.72	1.46	1.39
11	T	102	BCL	CHB-C1B	2.71	1.45	1.39
11	J	102	BCL	C1B-NB	-2.71	1.34	1.37
11	V	101	BCL	C3D-C2D	2.71	1.46	1.39
11	R	101	BCL	MG-NA	-2.71	1.99	2.06
16	A	103	CRT	C30-C28	-2.71	1.40	1.46
11	E	101	BCL	CHC-C4B	2.71	1.45	1.39
11	e	101	BCL	OBD-CAD	2.70	1.27	1.22
16	M	406	CRT	C30-C28	-2.70	1.40	1.46
11	h	101	BCL	CHC-C4B	2.70	1.45	1.39
11	T	102	BCL	MG-NA	-2.70	1.99	2.06
16	E	103	CRT	C25-C23	-2.70	1.40	1.46
11	Q	101	BCL	MG-NA	-2.70	1.99	2.06
11	b	102	BCL	CHC-C4B	2.70	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	101	BCL	MG-NA	-2.69	1.99	2.06
11	b	102	BCL	MG-NA	-2.69	1.99	2.06
16	A	103	CRT	C25-C23	-2.69	1.40	1.46
11	j	103	BCL	CHB-C4A	-2.69	1.31	1.37
11	U	101	BCL	CHB-C1B	2.68	1.45	1.39
11	j	103	BCL	CHC-C4B	2.68	1.45	1.39
11	J	101	BCL	CHC-C1C	-2.68	1.31	1.37
11	i	101	BCL	C3C-C4C	-2.68	1.48	1.51
11	N	102	BCL	CHC-C4B	2.68	1.45	1.39
11	A	101	BCL	CHC-C4B	2.67	1.45	1.39
11	N	102	BCL	MG-NA	-2.67	1.99	2.06
11	i	101	BCL	MG-NA	-2.67	1.99	2.06
11	A	101	BCL	OBD-CAD	2.67	1.27	1.22
11	L	402	BCL	C3C-C4C	-2.67	1.48	1.51
11	j	102	BCL	CHC-C1C	-2.67	1.31	1.37
11	M	402	BCL	CHD-C1D	2.67	1.43	1.38
11	L	402	BCL	CHD-C1D	2.67	1.43	1.38
11	Y	101	BCL	C1B-NB	-2.67	1.34	1.37
11	P	102	BCL	CHC-C4B	2.66	1.45	1.39
11	h	101	BCL	CHC-C1C	-2.66	1.31	1.37
11	Z	101	BCL	CHD-C1D	2.66	1.43	1.38
16	R	103	CRT	C25-C23	-2.65	1.40	1.46
11	I	101	BCL	OBD-CAD	2.65	1.27	1.22
11	h	101	BCL	C3D-C2D	2.65	1.46	1.39
16	P	103	CRT	C30-C28	-2.65	1.40	1.46
11	G	102	BCL	CHC-C4B	2.65	1.45	1.39
11	f	101	BCL	CHC-C4B	2.65	1.45	1.39
11	R	102	BCL	C1B-NB	-2.64	1.34	1.37
11	d	102	BCL	CHD-C4C	2.64	1.46	1.39
16	E	103	CRT	C30-C28	-2.64	1.40	1.46
11	D	101	BCL	C3C-C4C	-2.64	1.48	1.51
16	R	103	CRT	C30-C28	-2.63	1.40	1.46
11	f	102	BCL	C1B-NB	-2.63	1.34	1.37
11	Y	101	BCL	C3C-C4C	-2.63	1.48	1.51
11	G	102	BCL	CHD-C4C	2.63	1.46	1.39
11	A	101	BCL	C3D-C2D	2.62	1.46	1.39
11	g	101	BCL	C3D-C2D	2.62	1.46	1.39
11	P	101	BCL	OBD-CAD	2.62	1.27	1.22
16	i	102	CRT	C30-C28	-2.62	1.40	1.46
16	B	102	CRT	C25-C23	-2.62	1.40	1.46
16	i	102	CRT	C25-C23	-2.62	1.40	1.46
11	b	101	BCL	CHC-C4B	2.62	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	102	BCL	CHD-C4C	2.61	1.46	1.39
16	P	103	CRT	C25-C23	-2.61	1.40	1.46
11	I	101	BCL	MG-NA	-2.61	2.00	2.06
11	i	101	BCL	CHD-C1D	2.61	1.43	1.38
16	B	102	CRT	C30-C28	-2.60	1.40	1.46
11	R	102	BCL	MG-NA	-2.60	2.00	2.06
16	e	102	CRT	C30-C28	-2.60	1.40	1.46
16	e	102	CRT	C25-C23	-2.60	1.40	1.46
16	a	102	CRT	C30-C28	-2.60	1.40	1.46
11	F	101	BCL	MG-NA	-2.60	2.00	2.06
11	S	101	BCL	OBD-CAD	2.59	1.26	1.22
11	L	402	BCL	MG-NA	-2.59	2.00	2.06
16	j	101	CRT	C30-C28	-2.59	1.40	1.46
11	E	102	BCL	CHD-C4C	2.59	1.46	1.39
11	V	101	BCL	MG-NA	-2.59	2.00	2.06
16	W	102	CRT	C25-C23	-2.59	1.40	1.46
11	J	101	BCL	CHC-C4B	2.59	1.45	1.39
11	E	102	BCL	CHB-C4A	-2.59	1.31	1.37
16	I	102	CRT	C25-C23	-2.58	1.40	1.46
11	V	102	BCL	CHB-C1B	2.58	1.45	1.39
11	Y	101	BCL	CHD-C1D	2.58	1.43	1.38
11	h	102	BCL	CHB-C1B	2.58	1.45	1.39
11	R	102	BCL	CHC-C4B	2.58	1.45	1.39
16	K	102	CRT	C30-C28	-2.57	1.40	1.46
11	G	101	BCL	OBD-CAD	2.57	1.26	1.22
11	f	102	BCL	CHD-C4C	2.57	1.46	1.39
11	A	102	BCL	CHD-C4C	2.57	1.46	1.39
11	O	101	BCL	MG-NA	-2.57	2.00	2.06
16	A	103	CRT	C16-C17	-2.57	1.40	1.46
11	J	101	BCL	OBD-CAD	2.57	1.26	1.22
16	M	406	CRT	C35-C33	-2.56	1.40	1.46
16	W	102	CRT	C35-C33	-2.56	1.40	1.46
16	a	102	CRT	C16-C17	-2.56	1.40	1.46
11	M	403	BCL	CBD-CAD	-2.56	1.45	1.56
12	M	404	BPH	C3B-C4B	2.56	1.45	1.41
16	W	102	CRT	C30-C28	-2.56	1.40	1.46
11	J	102	BCL	MG-NA	-2.56	2.00	2.06
16	P	103	CRT	C35-C33	-2.56	1.40	1.46
16	i	102	CRT	C35-C33	-2.55	1.40	1.46
11	M	403	BCL	CHD-C1D	2.55	1.43	1.38
11	V	102	BCL	MG-NA	-2.55	2.00	2.06
16	K	102	CRT	C25-C23	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	103	CRT	C35-C33	-2.54	1.40	1.46
11	d	102	BCL	CHB-C1B	2.54	1.45	1.39
16	K	102	CRT	C35-C33	-2.54	1.40	1.46
11	U	101	BCL	OBD-CAD	2.54	1.26	1.22
11	Y	101	BCL	OBD-CAD	2.54	1.26	1.22
11	d	101	BCL	CHD-C1D	2.54	1.43	1.38
11	X	101	BCL	OBD-CAD	2.54	1.26	1.22
11	T	101	BCL	CHC-C4B	2.54	1.45	1.39
16	P	103	CRT	C16-C17	-2.54	1.40	1.46
16	R	103	CRT	C16-C17	-2.54	1.40	1.46
16	j	101	CRT	C35-C33	-2.53	1.40	1.46
16	R	103	CRT	C35-C33	-2.53	1.40	1.46
11	G	102	BCL	CHB-C4A	-2.53	1.31	1.37
16	U	102	CRT	C25-C23	-2.53	1.40	1.46
16	I	102	CRT	C30-C28	-2.53	1.40	1.46
16	j	101	CRT	C25-C23	-2.53	1.40	1.46
11	U	101	BCL	CHD-C1D	2.53	1.43	1.38
11	R	101	BCL	CHC-C1C	-2.53	1.31	1.37
16	A	103	CRT	C35-C33	-2.53	1.40	1.46
11	P	101	BCL	CHC-C4B	2.53	1.45	1.39
16	W	102	CRT	C16-C17	-2.53	1.40	1.46
11	O	101	BCL	CHD-C1D	2.53	1.43	1.38
11	b	101	BCL	CHD-C1D	2.53	1.43	1.38
16	a	102	CRT	C25-C23	-2.52	1.40	1.46
11	d	102	BCL	MG-NA	-2.52	2.00	2.06
11	a	101	BCL	CHD-C1D	2.52	1.43	1.38
11	L	401	BCL	C1B-NB	-2.52	1.34	1.37
11	D	101	BCL	OBD-CAD	2.52	1.26	1.22
16	N	103	CRT	C25-C23	-2.52	1.40	1.46
11	P	101	BCL	CHC-C1C	-2.52	1.31	1.37
11	e	101	BCL	CHD-C1D	2.51	1.43	1.38
11	T	102	BCL	C1B-NB	-2.51	1.34	1.37
16	I	102	CRT	C35-C33	-2.51	1.40	1.46
11	j	103	BCL	MG-NA	-2.51	2.00	2.06
11	Q	101	BCL	CHD-C1D	2.51	1.43	1.38
16	Z	102	CRT	C9-C7	2.51	1.41	1.35
16	M	406	CRT	C16-C17	-2.51	1.40	1.46
16	N	103	CRT	C30-C28	-2.51	1.40	1.46
11	d	102	BCL	CHB-C4A	-2.51	1.31	1.37
16	i	102	CRT	C16-C17	-2.51	1.40	1.46
16	a	102	CRT	C11-C12	-2.51	1.40	1.46
16	U	102	CRT	C30-C28	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	103	CRT	C16-C17	-2.50	1.40	1.46
11	Q	101	BCL	OBD-CAD	2.50	1.26	1.22
11	V	101	BCL	CHD-C1D	2.50	1.43	1.38
11	h	102	BCL	CHC-C1C	-2.50	1.31	1.37
16	N	103	CRT	C16-C17	-2.50	1.40	1.46
16	e	102	CRT	C35-C33	-2.49	1.40	1.46
16	B	102	CRT	C16-C17	-2.49	1.40	1.46
11	b	101	BCL	OBD-CAD	2.49	1.26	1.22
16	i	102	CRT	C11-C12	-2.48	1.40	1.46
11	T	102	BCL	CHD-C4C	2.48	1.46	1.39
11	R	101	BCL	OBD-CAD	2.48	1.26	1.22
16	B	102	CRT	C35-C33	-2.48	1.40	1.46
11	U	101	BCL	CHB-C4A	-2.48	1.31	1.37
16	U	102	CRT	C35-C33	-2.48	1.40	1.46
11	b	102	BCL	CHB-C1B	2.48	1.45	1.39
16	a	102	CRT	C35-C33	-2.48	1.40	1.46
11	V	102	BCL	CHD-C4C	2.48	1.46	1.39
11	j	102	BCL	CHC-C4B	2.48	1.45	1.39
11	f	101	BCL	CHC-C1C	-2.47	1.31	1.37
11	g	101	BCL	CHD-C1D	2.47	1.43	1.38
16	N	103	CRT	C35-C33	-2.47	1.40	1.46
11	F	101	BCL	CHD-C1D	2.47	1.43	1.38
16	A	103	CRT	C11-C12	-2.46	1.40	1.46
11	E	101	BCL	CHD-C1D	2.46	1.43	1.38
11	E	102	BCL	CHB-C1B	2.46	1.44	1.39
11	L	401	BCL	OBD-CAD	2.46	1.26	1.22
11	f	101	BCL	CHD-C1D	2.46	1.43	1.38
16	Z	102	CRT	C11-C12	-2.46	1.40	1.46
16	U	102	CRT	C16-C17	-2.46	1.40	1.46
16	P	103	CRT	C11-C12	-2.46	1.40	1.46
11	E	101	BCL	CHC-C1C	-2.45	1.31	1.37
11	f	102	BCL	CHB-C4A	-2.45	1.31	1.37
11	h	102	BCL	CHD-C4C	2.45	1.46	1.39
11	R	101	BCL	CHD-C1D	2.45	1.43	1.38
11	N	102	BCL	CHD-C4C	2.45	1.46	1.39
11	Y	101	BCL	MG-NA	-2.45	2.00	2.06
11	P	102	BCL	CHB-C1B	2.45	1.44	1.39
16	E	103	CRT	C11-C12	-2.44	1.40	1.46
11	i	101	BCL	OBD-CAD	2.44	1.26	1.22
16	j	101	CRT	C16-C17	-2.44	1.40	1.46
11	c	101	BCL	MG-NA	-2.44	2.00	2.06
11	V	102	BCL	CHB-C4A	-2.44	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	102	CRT	C11-C12	-2.43	1.40	1.46
16	W	102	CRT	C11-C12	-2.43	1.40	1.46
16	j	101	CRT	C11-C12	-2.43	1.40	1.46
11	d	102	BCL	C1B-NB	-2.43	1.34	1.37
11	R	102	BCL	CHD-C4C	2.43	1.46	1.39
11	G	101	BCL	CHC-C1C	-2.43	1.31	1.37
11	b	102	BCL	CHB-C4A	-2.43	1.31	1.37
11	A	101	BCL	CHC-C1C	-2.43	1.31	1.37
11	d	101	BCL	OBD-CAD	2.43	1.26	1.22
16	Z	102	CRT	C16-C17	-2.43	1.40	1.46
16	e	102	CRT	C16-C17	-2.42	1.40	1.46
16	Y	102	CRT	C30-C28	-2.42	1.40	1.46
16	N	103	CRT	C11-C12	-2.42	1.40	1.46
11	J	102	BCL	CHB-C4A	-2.42	1.31	1.37
11	T	101	BCL	CHC-C1C	-2.41	1.31	1.37
16	e	102	CRT	C11-C12	-2.41	1.40	1.46
11	a	101	BCL	CHB-C4A	-2.41	1.31	1.37
11	g	101	BCL	CHB-C4A	-2.41	1.31	1.37
16	R	103	CRT	C11-C12	-2.41	1.40	1.46
16	I	102	CRT	C16-C17	-2.41	1.40	1.46
16	M	406	CRT	C25-C23	-2.41	1.40	1.46
16	M	406	CRT	C11-C12	-2.41	1.40	1.46
11	J	102	BCL	CHD-C4C	2.41	1.46	1.39
11	M	402	BCL	CHD-C4C	2.41	1.46	1.39
11	X	102	BCL	CHB-C1B	2.40	1.44	1.39
11	d	101	BCL	CHC-C1C	-2.40	1.31	1.37
11	g	101	BCL	OBD-CAD	2.40	1.26	1.22
11	M	403	BCL	C3D-C2D	2.40	1.45	1.39
11	L	401	BCL	CHD-C4C	2.40	1.45	1.39
11	G	102	BCL	MG-NA	-2.40	2.00	2.06
11	S	101	BCL	CHB-C4A	-2.40	1.31	1.37
11	h	102	BCL	CHB-C4A	-2.39	1.31	1.37
11	M	402	BCL	CHB-C4A	-2.39	1.31	1.37
11	f	101	BCL	OBD-CAD	2.39	1.26	1.22
16	U	102	CRT	C11-C12	-2.39	1.40	1.46
16	Y	102	CRT	C35-C33	-2.39	1.40	1.46
11	O	101	BCL	CHB-C4A	-2.39	1.31	1.37
11	R	102	BCL	CHC-C1C	-2.38	1.31	1.37
11	F	101	BCL	OBD-CAD	2.38	1.26	1.22
16	Y	102	CRT	C25-C23	-2.38	1.40	1.46
11	G	101	BCL	CHD-C1D	2.38	1.43	1.38
11	j	103	BCL	CHB-C1B	2.38	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	102	BCL	CHB-C4A	-2.37	1.31	1.37
11	D	101	BCL	MG-NA	-2.37	2.00	2.06
11	W	101	BCL	MG-NA	-2.37	2.00	2.06
11	R	101	BCL	CHB-C4A	-2.36	1.31	1.37
16	Z	102	CRT	C30-C28	-2.36	1.40	1.46
11	a	101	BCL	MG-NA	-2.35	2.00	2.06
11	N	101	BCL	CHD-C1D	2.35	1.43	1.38
11	E	102	BCL	MG-NA	-2.35	2.00	2.06
16	K	102	CRT	C16-C17	-2.35	1.40	1.46
16	K	102	CRT	C9-C7	2.35	1.41	1.35
11	A	102	BCL	C1D-C2D	2.34	1.50	1.45
11	j	103	BCL	CHD-C4C	2.34	1.45	1.39
11	M	403	BCL	C3C-C4C	-2.34	1.48	1.51
11	X	101	BCL	CHD-C1D	2.34	1.43	1.38
11	L	401	BCL	CHB-C4A	-2.34	1.31	1.37
11	G	102	BCL	CHC-C1C	-2.34	1.31	1.37
11	Z	101	BCL	CHC-C1C	-2.34	1.31	1.37
16	Z	102	CRT	C35-C33	-2.34	1.41	1.46
11	f	102	BCL	MG-NA	-2.34	2.00	2.06
11	b	101	BCL	CHC-C1C	-2.34	1.31	1.37
11	L	401	BCL	CHC-C1C	-2.33	1.31	1.37
11	T	101	BCL	CHD-C1D	2.33	1.42	1.38
11	B	101	BCL	CHD-C1D	2.33	1.42	1.38
11	K	101	BCL	CHB-C4A	-2.33	1.31	1.37
11	J	101	BCL	CHD-C1D	2.32	1.42	1.38
11	b	102	BCL	C3C-C4C	-2.32	1.48	1.51
16	Z	102	CRT	C19-C17	2.32	1.41	1.35
16	Z	102	CRT	C22-C23	2.32	1.41	1.35
16	K	102	CRT	C6-C7	-2.32	1.41	1.46
16	Y	102	CRT	C16-C17	-2.32	1.41	1.46
11	E	101	BCL	CHB-C4A	-2.32	1.31	1.37
11	D	101	BCL	CHC-C1C	-2.31	1.31	1.37
16	M	406	CRT	C6-C7	-2.31	1.41	1.46
16	W	102	CRT	C6-C7	-2.31	1.41	1.46
11	A	102	BCL	MG-NC	-2.31	2.00	2.06
11	f	102	BCL	MG-NC	-2.30	2.00	2.06
11	P	102	BCL	CHD-C4C	2.30	1.45	1.39
16	Z	102	CRT	C14-C12	2.30	1.41	1.35
11	h	102	BCL	MG-NA	-2.30	2.00	2.06
11	P	101	BCL	CHD-C1D	2.30	1.42	1.38
11	g	101	BCL	MG-NA	-2.30	2.00	2.06
11	I	101	BCL	MG-NC	-2.30	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	102	BCL	CHD-C4C	2.29	1.45	1.39
11	M	403	BCL	OBD-CAD	2.29	1.26	1.22
11	c	101	BCL	CHB-C4A	-2.29	1.32	1.37
11	D	101	BCL	CHD-C1D	2.29	1.42	1.38
16	Y	102	CRT	C22-C23	2.28	1.41	1.35
11	X	101	BCL	CHC-C1C	-2.28	1.32	1.37
11	D	101	BCL	C2C-C3C	-2.28	1.48	1.54
11	O	101	BCL	CHC-C1C	-2.28	1.32	1.37
11	V	101	BCL	OBD-CAD	2.28	1.26	1.22
11	F	101	BCL	CHB-C4A	-2.28	1.32	1.37
11	N	102	BCL	CHC-C1C	-2.27	1.32	1.37
11	M	403	BCL	C2C-C3C	-2.27	1.48	1.54
16	Y	102	CRT	C9-C7	2.27	1.41	1.35
11	E	101	BCL	C2C-C3C	-2.27	1.48	1.54
11	Q	101	BCL	C2C-C3C	-2.26	1.48	1.54
11	O	101	BCL	OBD-CAD	2.26	1.26	1.22
11	j	102	BCL	OBD-CAD	2.26	1.26	1.22
16	K	102	CRT	C11-C12	-2.26	1.41	1.46
16	Y	102	CRT	C27-C28	2.26	1.41	1.35
11	D	101	BCL	CHB-C4A	-2.26	1.32	1.37
16	Y	102	CRT	C11-C12	-2.26	1.41	1.46
11	f	101	BCL	CHB-C4A	-2.26	1.32	1.37
16	Z	102	CRT	C6-C7	-2.25	1.41	1.46
11	W	101	BCL	OBD-CAD	2.25	1.26	1.22
16	Y	102	CRT	C19-C17	2.25	1.41	1.35
16	Z	102	CRT	C27-C28	2.25	1.41	1.35
11	F	101	BCL	MG-NC	-2.25	2.00	2.06
16	Z	102	CRT	C25-C23	-2.25	1.41	1.46
11	W	101	BCL	CHB-C4A	-2.25	1.32	1.37
16	E	103	CRT	C6-C7	-2.25	1.41	1.46
11	I	101	BCL	CHB-C4A	-2.24	1.32	1.37
16	Z	102	CRT	C32-C33	2.24	1.41	1.35
11	X	102	BCL	MG-NA	-2.24	2.00	2.06
7	C	503	HEC	C3B-C2B	-2.24	1.33	1.41
11	M	403	BCL	CHC-C1C	-2.24	1.32	1.37
11	h	101	BCL	CHD-C1D	2.24	1.42	1.38
16	Y	102	CRT	C14-C12	2.24	1.41	1.35
11	N	101	BCL	OBD-CAD	2.24	1.26	1.22
11	Q	101	BCL	CHB-C4A	-2.24	1.32	1.37
11	Y	101	BCL	C1B-C2B	2.23	1.48	1.43
11	P	102	BCL	CHC-C1C	-2.23	1.32	1.37
11	N	102	BCL	CHB-C1B	2.23	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	406	CRT	C22-C23	2.23	1.41	1.35
11	R	102	BCL	MG-NC	-2.23	2.01	2.06
11	N	102	BCL	CHB-C4A	-2.23	1.32	1.37
11	f	101	BCL	C2C-C3C	-2.23	1.48	1.54
16	N	103	CRT	C6-C7	-2.23	1.41	1.46
11	Z	101	BCL	CHD-C4C	2.23	1.45	1.39
11	A	102	BCL	CHB-C4A	-2.23	1.32	1.37
16	B	102	CRT	C6-C7	-2.23	1.41	1.46
16	I	102	CRT	C11-C12	-2.22	1.41	1.46
11	A	101	BCL	CHB-C4A	-2.22	1.32	1.37
11	j	102	BCL	C2C-C3C	-2.22	1.48	1.54
16	e	102	CRT	C6-C7	-2.22	1.41	1.46
11	B	101	BCL	MG-NA	-2.22	2.01	2.06
11	b	101	BCL	CHB-C4A	-2.22	1.32	1.37
16	a	102	CRT	C6-C7	-2.22	1.41	1.46
11	Y	101	BCL	CHC-C1C	-2.22	1.32	1.37
11	A	102	BCL	C1B-C2B	2.21	1.48	1.43
11	X	101	BCL	CHB-C4A	-2.21	1.32	1.37
11	R	102	BCL	CHB-C4A	-2.21	1.32	1.37
11	V	101	BCL	CHB-C4A	-2.20	1.32	1.37
16	j	101	CRT	C22-C23	2.20	1.40	1.35
16	R	103	CRT	C6-C7	-2.20	1.41	1.46
11	J	101	BCL	C2C-C3C	-2.20	1.48	1.54
11	d	102	BCL	CHC-C1C	-2.20	1.32	1.37
11	E	101	BCL	CHD-C4C	2.20	1.45	1.39
16	B	102	CRT	C22-C23	2.20	1.40	1.35
11	h	101	BCL	C2C-C3C	-2.20	1.48	1.54
16	K	102	CRT	C19-C17	2.20	1.40	1.35
16	Y	102	CRT	C32-C33	2.19	1.40	1.35
11	L	402	BCL	OBD-CAD	2.19	1.26	1.22
11	K	101	BCL	CHD-C4C	2.18	1.45	1.39
11	G	101	BCL	C2C-C3C	-2.18	1.48	1.54
11	P	102	BCL	C4D-CHA	2.18	1.45	1.38
16	U	102	CRT	C9-C7	2.18	1.40	1.35
11	B	101	BCL	CHC-C1C	-2.18	1.32	1.37
16	U	102	CRT	C6-C7	-2.18	1.41	1.46
11	X	101	BCL	C2C-C3C	-2.18	1.48	1.54
11	V	102	BCL	C3C-C4C	-2.18	1.48	1.51
16	U	102	CRT	C19-C17	2.18	1.40	1.35
11	E	102	BCL	C1D-C2D	2.17	1.49	1.45
11	K	101	BCL	MG-NA	-2.17	2.01	2.06
11	A	101	BCL	C2C-C3C	-2.17	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	U	102	CRT	C22-C23	2.17	1.40	1.35
16	I	102	CRT	C22-C23	2.17	1.40	1.35
16	N	103	CRT	C22-C23	2.17	1.40	1.35
11	Z	101	BCL	CHB-C4A	-2.16	1.32	1.37
16	A	103	CRT	C6-C7	-2.16	1.41	1.46
11	j	103	BCL	C4D-CHA	2.16	1.45	1.38
11	X	102	BCL	C4D-CHA	2.15	1.45	1.38
11	V	101	BCL	CHC-C1C	-2.15	1.32	1.37
11	X	102	BCL	MG-NC	-2.15	2.01	2.06
11	N	101	BCL	C2C-C3C	-2.15	1.48	1.54
16	M	406	CRT	C27-C28	2.15	1.40	1.35
16	K	102	CRT	C22-C23	2.15	1.40	1.35
16	j	101	CRT	C14-C12	2.15	1.40	1.35
16	j	101	CRT	C6-C7	-2.15	1.41	1.46
11	i	101	BCL	CHC-C1C	-2.15	1.32	1.37
16	j	101	CRT	C27-C28	2.14	1.40	1.35
16	K	102	CRT	C27-C28	2.14	1.40	1.35
16	i	102	CRT	C6-C7	-2.14	1.41	1.46
16	K	102	CRT	C14-C12	2.14	1.40	1.35
11	h	102	BCL	C4D-CHA	2.14	1.45	1.38
16	Y	102	CRT	C6-C7	-2.14	1.41	1.46
16	P	103	CRT	C6-C7	-2.14	1.41	1.46
16	e	102	CRT	C22-C23	2.14	1.40	1.35
16	j	101	CRT	C19-C17	2.14	1.40	1.35
11	B	101	BCL	CHB-C4A	-2.14	1.32	1.37
16	I	102	CRT	C9-C7	2.14	1.40	1.35
11	B	101	BCL	OBD-CAD	2.14	1.26	1.22
11	b	102	BCL	C4D-CHA	2.14	1.45	1.38
16	W	102	CRT	C9-C7	2.13	1.40	1.35
16	N	103	CRT	C9-C7	2.13	1.40	1.35
11	P	101	BCL	C2C-C3C	-2.13	1.48	1.54
11	j	103	BCL	CHC-C1C	-2.13	1.32	1.37
11	N	101	BCL	CAA-C2A	-2.13	1.50	1.54
11	A	102	BCL	C4D-CHA	2.13	1.45	1.38
16	e	102	CRT	C14-C12	2.13	1.40	1.35
11	j	102	BCL	MG-NC	-2.13	2.01	2.06
11	i	101	BCL	CHB-C4A	-2.13	1.32	1.37
11	P	102	BCL	C3C-C4C	-2.13	1.48	1.51
11	O	101	BCL	C2C-C3C	-2.13	1.48	1.54
11	a	101	BCL	OBD-CAD	2.13	1.26	1.22
11	j	102	BCL	CHB-C4A	-2.13	1.32	1.37
11	d	102	BCL	C1D-C2D	2.13	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	102	BCL	C1D-C2D	2.13	1.49	1.45
11	V	102	BCL	MG-NC	-2.12	2.01	2.06
11	A	101	BCL	CHD-C1D	2.12	1.42	1.38
11	W	101	BCL	C2C-C3C	-2.12	1.48	1.54
11	K	101	BCL	MG-NC	-2.12	2.01	2.06
11	J	102	BCL	CHC-C1C	-2.12	1.32	1.37
16	U	102	CRT	C27-C28	2.12	1.40	1.35
11	L	402	BCL	C2C-C3C	-2.12	1.48	1.54
16	M	406	CRT	C9-C7	2.12	1.40	1.35
11	M	403	BCL	CHB-C4A	-2.12	1.32	1.37
11	U	101	BCL	MG-ND	-2.12	2.01	2.05
16	j	101	CRT	C9-C7	2.12	1.40	1.35
16	e	102	CRT	C9-C7	2.12	1.40	1.35
16	B	102	CRT	C9-C7	2.11	1.40	1.35
16	P	103	CRT	C22-C23	2.11	1.40	1.35
11	L	402	BCL	CHB-C4A	-2.11	1.32	1.37
16	R	103	CRT	C9-C7	2.11	1.40	1.35
16	R	103	CRT	C22-C23	2.11	1.40	1.35
16	I	102	CRT	C19-C17	2.11	1.40	1.35
11	h	102	BCL	MG-NC	-2.11	2.01	2.06
11	j	102	BCL	OBB-CAB	-2.11	1.18	1.23
16	A	103	CRT	C9-C7	2.11	1.40	1.35
11	J	101	BCL	CHB-C4A	-2.11	1.32	1.37
16	U	102	CRT	C14-C12	2.10	1.40	1.35
16	i	102	CRT	C22-C23	2.10	1.40	1.35
11	b	102	BCL	CHC-C1C	-2.10	1.32	1.37
16	I	102	CRT	C6-C7	-2.10	1.41	1.46
11	S	101	BCL	CHC-C1C	-2.10	1.32	1.37
11	E	101	BCL	OBD-CAD	2.10	1.26	1.22
11	c	101	BCL	C2C-C3C	-2.10	1.48	1.54
11	Z	101	BCL	C2C-C3C	-2.10	1.48	1.54
11	J	101	BCL	CAA-C2A	-2.10	1.50	1.54
11	Y	101	BCL	CHB-C4A	-2.10	1.32	1.37
11	E	102	BCL	C4D-CHA	2.10	1.45	1.38
16	A	103	CRT	C22-C23	2.10	1.40	1.35
16	a	102	CRT	C22-C23	2.09	1.40	1.35
11	G	101	BCL	CHB-C4A	-2.09	1.32	1.37
16	N	103	CRT	C27-C28	2.09	1.40	1.35
16	e	102	CRT	C27-C28	2.09	1.40	1.35
11	S	101	BCL	CAA-C2A	-2.09	1.50	1.54
11	E	101	BCL	C3A-C2A	-2.09	1.48	1.54
16	i	102	CRT	C9-C7	2.09	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	d	101	BCL	CHD-C4C	2.09	1.45	1.39
11	d	101	BCL	CHB-C4A	-2.09	1.32	1.37
11	Y	101	BCL	C2C-C3C	-2.09	1.48	1.54
16	M	406	CRT	C19-C17	2.09	1.40	1.35
16	B	102	CRT	C19-C17	2.09	1.40	1.35
11	g	101	BCL	MG-NC	-2.08	2.01	2.06
16	N	103	CRT	C14-C12	2.08	1.40	1.35
16	a	102	CRT	C19-C17	2.08	1.40	1.35
11	d	101	BCL	C2C-C3C	-2.08	1.48	1.54
7	C	501	HEC	C3B-C2B	-2.08	1.34	1.41
11	T	101	BCL	OBD-CAD	2.08	1.26	1.22
16	W	102	CRT	C22-C23	2.08	1.40	1.35
16	a	102	CRT	C9-C7	2.08	1.40	1.35
11	E	101	BCL	C4D-CHA	2.08	1.45	1.38
11	E	102	BCL	MG-NC	-2.08	2.01	2.06
16	E	103	CRT	C22-C23	2.08	1.40	1.35
16	M	406	CRT	C14-C12	2.08	1.40	1.35
11	S	101	BCL	MG-NC	-2.08	2.01	2.06
16	a	102	CRT	C14-C12	2.07	1.40	1.35
11	D	101	BCL	CAA-C2A	-2.07	1.50	1.54
11	c	101	BCL	CHD-C4C	2.07	1.45	1.39
16	P	103	CRT	C9-C7	2.07	1.40	1.35
16	P	103	CRT	C14-C12	2.07	1.40	1.35
11	I	101	BCL	C2C-C3C	-2.07	1.48	1.54
16	e	102	CRT	C19-C17	2.07	1.40	1.35
11	Q	101	BCL	CHC-C1C	-2.07	1.32	1.37
11	N	102	BCL	C1D-C2D	2.07	1.49	1.45
11	e	101	BCL	CHB-C4A	-2.07	1.32	1.37
11	G	102	BCL	CHB-C1B	2.07	1.44	1.39
7	C	503	HEC	C3C-C2C	-2.07	1.34	1.41
11	b	101	BCL	C2C-C3C	-2.06	1.48	1.54
11	X	101	BCL	CAA-C2A	-2.06	1.50	1.54
16	P	103	CRT	C19-C17	2.06	1.40	1.35
11	N	102	BCL	MG-NC	-2.06	2.01	2.06
12	M	404	BPH	OBD-CAD	2.06	1.25	1.22
16	I	102	CRT	C32-C33	2.06	1.40	1.35
11	Y	101	BCL	CHD-C4C	2.06	1.45	1.39
11	X	101	BCL	MG-NC	-2.06	2.01	2.06
16	U	102	CRT	C32-C33	2.05	1.40	1.35
16	I	102	CRT	C14-C12	2.05	1.40	1.35
16	W	102	CRT	C27-C28	2.05	1.40	1.35
7	C	502	HEC	CMC-C2C	2.05	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	504	HEC	CMC-C2C	2.05	1.55	1.50
16	R	103	CRT	C14-C12	2.05	1.40	1.35
11	G	102	BCL	MG-NC	-2.05	2.01	2.06
11	b	101	BCL	CHD-C4C	2.05	1.44	1.39
16	R	103	CRT	C19-C17	2.05	1.40	1.35
16	N	103	CRT	C19-C17	2.05	1.40	1.35
11	N	101	BCL	CHB-C4A	-2.05	1.32	1.37
16	B	102	CRT	C14-C12	2.04	1.40	1.35
16	W	102	CRT	C14-C12	2.04	1.40	1.35
11	T	102	BCL	CHC-C1C	-2.04	1.32	1.37
11	S	101	BCL	MG-NA	-2.04	2.01	2.06
16	B	102	CRT	C27-C28	2.04	1.40	1.35
11	S	101	BCL	CHD-C4C	2.04	1.44	1.39
11	j	103	BCL	MG-NC	-2.04	2.01	2.06
11	T	101	BCL	C4D-CHA	2.04	1.45	1.38
16	a	102	CRT	C27-C28	2.04	1.40	1.35
11	E	101	BCL	CAA-C2A	-2.04	1.50	1.54
11	A	102	BCL	C2C-C3C	-2.04	1.49	1.54
16	i	102	CRT	C19-C17	2.04	1.40	1.35
11	T	102	BCL	C4D-CHA	2.03	1.45	1.38
16	N	103	CRT	C32-C33	2.03	1.40	1.35
16	E	103	CRT	C14-C12	2.03	1.40	1.35
7	C	501	HEC	C3C-C2C	-2.03	1.34	1.41
11	F	101	BCL	C2C-C3C	-2.03	1.49	1.54
11	W	101	BCL	O2D-CED	-2.03	1.40	1.45
16	W	102	CRT	C19-C17	2.03	1.40	1.35
7	C	504	HEC	C3B-C2B	-2.03	1.34	1.41
16	P	103	CRT	C27-C28	2.03	1.40	1.35
16	i	102	CRT	C14-C12	2.03	1.40	1.35
16	E	103	CRT	C19-C17	2.03	1.40	1.35
16	R	103	CRT	C27-C28	2.03	1.40	1.35
11	J	101	BCL	C3A-C2A	-2.03	1.49	1.54
11	O	101	BCL	CAA-C2A	-2.02	1.50	1.54
16	I	102	CRT	C27-C28	2.02	1.40	1.35
16	A	103	CRT	C19-C17	2.02	1.40	1.35
11	X	101	BCL	CHD-C4C	2.02	1.44	1.39
11	Y	101	BCL	C4D-CHA	2.02	1.45	1.38
11	V	102	BCL	C1D-C2D	2.02	1.49	1.45
11	T	101	BCL	CHB-C4A	-2.01	1.32	1.37
11	i	101	BCL	C2C-C3C	-2.01	1.49	1.54
16	E	103	CRT	C9-C7	2.01	1.40	1.35
11	L	401	BCL	MG-NC	-2.01	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	U	101	BCL	MG-NC	-2.01	2.01	2.06
11	d	102	BCL	C4D-CHA	2.01	1.45	1.38
11	c	101	BCL	CHC-C1C	-2.01	1.32	1.37
11	M	402	BCL	MG-NC	-2.01	2.01	2.06
16	A	103	CRT	C14-C12	2.01	1.40	1.35
11	L	402	BCL	MG-NC	-2.01	2.01	2.06
11	V	102	BCL	CHC-C1C	-2.01	1.32	1.37
16	E	103	CRT	C27-C28	2.01	1.40	1.35
11	U	101	BCL	CHD-C4C	2.01	1.44	1.39
11	M	403	BCL	C3A-C2A	-2.01	1.49	1.54
16	e	102	CRT	C32-C33	2.01	1.40	1.35
11	N	101	BCL	C3A-C2A	-2.01	1.49	1.54
11	E	102	BCL	CHC-C1C	-2.00	1.32	1.37
11	G	102	BCL	C4D-CHA	2.00	1.45	1.38
11	V	102	BCL	C4D-CHA	2.00	1.45	1.38
11	f	102	BCL	CHC-C1C	-2.00	1.32	1.37
11	J	102	BCL	C4D-CHA	2.00	1.45	1.38
11	G	101	BCL	CHD-C4C	2.00	1.44	1.39
11	R	102	BCL	C1D-C2D	2.00	1.49	1.45

All (1551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	404	BPH	C4D-CHA-CBD	-10.72	103.31	108.45
12	L	403	BPH	C4D-CHA-CBD	-10.41	103.46	108.45
11	L	401	BCL	O2D-CGD-CBD	8.88	126.75	111.23
11	N	102	BCL	C2B-C1B-NB	8.54	119.18	110.33
7	C	503	HEC	CBB-CAB-C3B	-8.52	110.40	127.43
7	C	501	HEC	CBB-CAB-C3B	-8.19	111.07	127.43
11	d	102	BCL	CMD-C2D-C1D	8.15	139.08	124.73
11	j	103	BCL	C2B-C1B-NB	7.99	118.61	110.33
11	E	102	BCL	C2B-C1B-NB	7.93	118.55	110.33
11	A	102	BCL	CMD-C2D-C1D	7.90	138.64	124.73
7	C	502	HEC	CBB-CAB-C3B	-7.90	111.64	127.43
11	f	102	BCL	CMD-C2D-C1D	7.89	138.62	124.73
11	R	102	BCL	CMD-C2D-C1D	7.85	138.55	124.73
7	C	504	HEC	CBC-CAC-C3C	-7.83	111.78	127.43
11	P	102	BCL	C2B-C1B-NB	7.83	118.44	110.33
11	M	403	BCL	O2D-CGD-CBD	7.80	124.86	111.23
7	C	504	HEC	CBB-CAB-C3B	-7.78	111.88	127.43
11	G	102	BCL	C2B-C1B-NB	7.74	118.35	110.33
11	X	102	BCL	CMD-C2D-C1D	7.73	138.33	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	CMD-C2D-C1D	7.72	138.32	124.73
11	J	102	BCL	CMD-C2D-C1D	7.71	138.31	124.73
11	X	102	BCL	C2B-C1B-NB	7.68	118.29	110.33
11	h	102	BCL	CMD-C2D-C1D	7.66	138.22	124.73
11	P	102	BCL	CMD-C2D-C1D	7.64	138.18	124.73
11	G	102	BCL	CMD-C2D-C1D	7.63	138.16	124.73
11	T	102	BCL	CMD-C2D-C1D	7.62	138.15	124.73
11	h	102	BCL	C2B-C1B-NB	7.60	118.20	110.33
11	L	402	BCL	CMD-C2D-C1D	7.56	138.05	124.73
11	E	102	BCL	CMD-C2D-C1D	7.51	137.96	124.73
11	b	102	BCL	CMD-C2D-C1D	7.51	137.95	124.73
11	d	102	BCL	C2B-C1B-NB	7.45	118.06	110.33
11	j	103	BCL	CMD-C2D-C1D	7.44	137.83	124.73
11	V	102	BCL	CMD-C2D-C1D	7.38	137.73	124.73
11	U	101	BCL	C2B-C1B-NB	7.38	117.98	110.33
7	C	502	HEC	CBC-CAC-C3C	-7.38	112.68	127.43
11	b	102	BCL	C2B-C1B-NB	7.37	117.97	110.33
11	T	102	BCL	C2B-C1B-NB	7.29	117.89	110.33
7	C	501	HEC	CBC-CAC-C3C	-7.27	112.89	127.43
11	A	102	BCL	C2B-C1B-NB	7.24	117.83	110.33
11	J	102	BCL	C2B-C1B-NB	7.24	117.83	110.33
11	N	102	BCL	CMD-C2D-C1D	7.23	137.47	124.73
11	V	102	BCL	C2B-C1B-NB	7.23	117.82	110.33
11	K	101	BCL	C2B-C1B-NB	7.15	117.74	110.33
11	M	402	BCL	CMD-C2D-C1D	7.14	137.31	124.73
11	M	402	BCL	C2B-C1B-NB	7.14	117.73	110.33
11	M	403	BCL	C4A-NA-C1A	7.11	109.92	106.68
11	L	401	BCL	CMD-C2D-C1D	7.03	137.11	124.73
11	g	101	BCL	C2B-C1B-NB	6.97	117.55	110.33
11	D	101	BCL	C2B-C1B-NB	6.94	117.52	110.33
11	N	101	BCL	C2B-C1B-NB	6.85	117.43	110.33
11	R	102	BCL	C2B-C1B-NB	6.83	117.41	110.33
11	E	101	BCL	CMD-C2D-C1D	6.83	136.76	124.73
11	f	102	BCL	C2B-C1B-NB	6.79	117.36	110.33
11	O	101	BCL	C2B-C1B-NB	6.78	117.36	110.33
11	M	403	BCL	C2B-C1B-NB	6.72	117.30	110.33
11	W	101	BCL	C2B-C1B-NB	6.70	117.28	110.33
11	L	401	BCL	C2B-C1B-NB	6.67	117.25	110.33
11	E	101	BCL	C2B-C1B-NB	6.67	117.24	110.33
11	F	101	BCL	C2B-C1B-NB	6.64	117.21	110.33
11	Q	101	BCL	C2B-C1B-NB	6.63	117.20	110.33
11	I	101	BCL	C2B-C1B-NB	6.58	117.15	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	101	BCL	C2B-C1B-NB	6.56	117.13	110.33
11	e	101	BCL	C2B-C1B-NB	6.56	117.13	110.33
11	M	402	BCL	O2D-CGD-CBD	6.55	122.68	111.23
11	P	101	BCL	CMD-C2D-C1D	6.55	136.25	124.73
11	j	102	BCL	C4A-NA-C1A	6.51	109.65	106.68
11	B	101	BCL	C2B-C1B-NB	6.50	117.07	110.33
11	d	101	BCL	O2D-CGD-CBD	6.49	122.57	111.23
11	f	101	BCL	CMD-C2D-C1D	6.47	136.12	124.73
11	M	402	BCL	CHD-C1D-ND	-6.42	115.77	124.80
11	G	101	BCL	C2B-C1B-NB	6.41	116.98	110.33
11	A	101	BCL	CMD-C2D-C1D	6.40	135.99	124.73
11	X	101	BCL	C2B-C1B-NB	6.39	116.95	110.33
11	c	101	BCL	C2B-C1B-NB	6.38	116.94	110.33
11	a	101	BCL	C2B-C1B-NB	6.30	116.86	110.33
11	J	101	BCL	C1C-NC-C4C	-6.26	103.82	106.68
7	C	503	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
11	V	101	BCL	C2B-C1B-NB	6.24	116.80	110.33
11	S	101	BCL	C2B-C1B-NB	6.24	116.79	110.33
11	i	101	BCL	C2B-C1B-NB	6.24	116.79	110.33
11	P	101	BCL	C1C-NC-C4C	-6.21	103.85	106.68
11	A	101	BCL	O2D-CGD-CBD	6.16	122.00	111.23
11	X	101	BCL	O2D-CGD-CBD	6.16	122.00	111.23
11	j	102	BCL	C2B-C1B-NB	6.16	116.71	110.33
11	f	101	BCL	C2B-C1B-NB	6.15	116.71	110.33
11	Z	101	BCL	C2B-C1B-NB	6.10	116.65	110.33
11	X	101	BCL	CMD-C2D-C1D	6.08	135.43	124.73
11	A	101	BCL	C2B-C1B-NB	6.07	116.62	110.33
11	b	101	BCL	C2B-C1B-NB	6.05	116.60	110.33
11	P	101	BCL	C4A-NA-C1A	6.04	109.44	106.68
11	h	101	BCL	CMD-C2D-C1D	6.01	135.31	124.73
11	h	101	BCL	C2B-C1B-NB	6.01	116.55	110.33
11	J	101	BCL	CMD-C2D-C1D	5.94	135.19	124.73
11	b	101	BCL	O2D-CGD-CBD	5.93	121.60	111.23
11	V	101	BCL	CMD-C2D-C1D	5.93	135.18	124.73
11	T	101	BCL	C2B-C1B-NB	5.92	116.47	110.33
11	Z	101	BCL	CMD-C2D-C1D	5.92	135.15	124.73
11	R	101	BCL	C2B-C1B-NB	5.92	116.47	110.33
11	L	402	BCL	C2B-C1B-NB	5.91	116.46	110.33
11	b	101	BCL	CMD-C2D-C1D	5.91	135.13	124.73
11	T	101	BCL	CMD-C2D-C1D	5.89	135.10	124.73
11	A	102	BCL	CHD-C1D-ND	-5.87	116.54	124.80
11	h	101	BCL	C1C-NC-C4C	-5.87	104.00	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	101	BCL	O2D-CGD-CBD	5.85	121.46	111.23
11	d	101	BCL	C2B-C1B-NB	5.85	116.39	110.33
11	M	403	BCL	O2D-CGD-O1D	-5.85	112.47	123.85
11	A	101	BCL	C3C-C4C-CHD	-5.84	111.08	123.39
11	d	101	BCL	CMD-C2D-C1D	5.84	135.00	124.73
11	J	101	BCL	C2B-C1B-NB	5.83	116.37	110.33
11	N	101	BCL	CMD-C2D-C1D	5.83	134.99	124.73
11	G	101	BCL	O2D-CGD-CBD	5.82	121.41	111.23
11	V	101	BCL	O2D-CGD-CBD	5.81	121.39	111.23
11	P	101	BCL	C3D-C2D-C1D	-5.75	97.99	105.83
11	G	101	BCL	CMD-C2D-C1D	5.74	134.84	124.73
11	P	101	BCL	C3C-C4C-CHD	-5.71	111.36	123.39
11	d	102	BCL	CHD-C1D-ND	-5.70	116.78	124.80
11	T	101	BCL	O2D-CGD-CBD	5.69	121.18	111.23
11	X	101	BCL	C3D-C2D-C1D	-5.69	98.07	105.83
11	P	102	BCL	CHD-C1D-ND	-5.68	116.81	124.80
11	N	102	BCL	CHD-C1D-ND	-5.67	116.82	124.80
11	j	102	BCL	C3C-C4C-CHD	-5.67	111.44	123.39
11	g	101	BCL	CMD-C2D-C1D	5.66	134.70	124.73
11	N	101	BCL	C3C-C4C-CHD	-5.66	111.47	123.39
11	Z	101	BCL	O2D-CGD-CBD	5.65	121.11	111.23
11	N	101	BCL	O2D-CGD-CBD	5.64	121.09	111.23
11	E	101	BCL	C3D-C2D-C1D	-5.64	98.14	105.83
11	J	102	BCL	CHD-C1D-ND	-5.63	116.88	124.80
11	M	403	BCL	CHD-C1D-ND	-5.61	116.90	124.80
11	R	101	BCL	C3C-C4C-CHD	-5.61	111.56	123.39
11	X	101	BCL	C3C-C4C-CHD	-5.60	111.57	123.39
11	X	102	BCL	O2D-CGD-CBD	5.60	121.02	111.23
11	X	102	BCL	CHD-C1D-ND	-5.58	116.95	124.80
11	T	102	BCL	CHD-C1D-ND	-5.56	116.97	124.80
11	V	101	BCL	C3C-C4C-CHD	-5.56	111.67	123.39
11	f	101	BCL	O2D-CGD-CBD	5.55	120.94	111.23
11	g	101	BCL	C3C-C4C-CHD	-5.55	111.69	123.39
11	T	101	BCL	C3C-C4C-CHD	-5.54	111.72	123.39
11	M	403	BCL	C3D-C2D-C1D	-5.53	98.28	105.83
11	R	102	BCL	CHD-C1D-ND	-5.53	117.02	124.80
11	b	102	BCL	CHD-C1D-ND	-5.53	117.03	124.80
11	d	101	BCL	C3C-C4C-CHD	-5.53	111.74	123.39
11	P	101	BCL	C2B-C1B-NB	5.52	116.06	110.33
11	a	101	BCL	C3C-C4C-CHD	-5.52	111.75	123.39
11	B	101	BCL	C3C-C4C-CHD	-5.51	111.77	123.39
11	G	101	BCL	C3C-C4C-CHD	-5.49	111.81	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	f	101	BCL	C1C-NC-C4C	-5.49	104.17	106.68
11	G	102	BCL	O2D-CGD-CBD	5.49	120.82	111.23
11	E	102	BCL	CHD-C1D-ND	-5.48	117.09	124.80
11	K	101	BCL	CMD-C2D-C1D	5.48	134.38	124.73
11	V	102	BCL	CHD-C1D-ND	-5.48	117.09	124.80
11	P	101	BCL	O2D-CGD-CBD	5.47	120.80	111.23
11	R	101	BCL	O2D-CGD-CBD	5.47	120.79	111.23
11	G	102	BCL	CHD-C1D-ND	-5.46	117.12	124.80
11	J	101	BCL	C3C-C4C-CHD	-5.46	111.89	123.39
11	j	103	BCL	CHD-C1D-ND	-5.46	117.12	124.80
11	D	101	BCL	C3C-C4C-CHD	-5.44	111.92	123.39
11	E	101	BCL	CHD-C1D-ND	-5.44	117.15	124.80
11	f	102	BCL	CHD-C1D-ND	-5.42	117.18	124.80
11	e	101	BCL	C3C-C4C-CHD	-5.39	112.03	123.39
11	b	101	BCL	C3C-C4C-CHD	-5.39	112.03	123.39
11	h	102	BCL	CHD-C1D-ND	-5.38	117.23	124.80
11	P	101	BCL	CHD-C1D-ND	-5.38	117.23	124.80
11	U	101	BCL	C3C-C4C-CHD	-5.38	112.05	123.39
11	L	402	BCL	C3C-C4C-CHD	-5.37	112.06	123.39
11	T	101	BCL	C3D-C2D-C1D	-5.35	98.54	105.83
11	h	102	BCL	C3D-C2D-C1D	-5.34	98.54	105.83
11	j	102	BCL	O2D-CGD-CBD	5.34	120.56	111.23
11	J	101	BCL	C3D-C2D-C1D	-5.34	98.55	105.83
11	h	101	BCL	C3C-C4C-CHD	-5.34	112.14	123.39
11	E	101	BCL	C3C-C4C-CHD	-5.32	112.18	123.39
11	Q	101	BCL	C3C-C4C-CHD	-5.31	112.20	123.39
11	X	101	BCL	CHD-C1D-ND	-5.31	117.33	124.80
11	F	101	BCL	C3C-C4C-CHD	-5.31	112.20	123.39
11	R	101	BCL	CMD-C2D-C1D	5.31	134.07	124.73
11	L	401	BCL	CHD-C1D-ND	-5.29	117.35	124.80
11	j	102	BCL	C3D-C2D-C1D	-5.29	98.62	105.83
11	d	101	BCL	C3D-C2D-C1D	-5.29	98.62	105.83
11	f	101	BCL	C3C-C4C-CHD	-5.28	112.25	123.39
11	c	101	BCL	C3C-C4C-CHD	-5.28	112.25	123.39
11	N	101	BCL	C3D-C2D-C1D	-5.26	98.66	105.83
11	A	101	BCL	C3D-C2D-C1D	-5.25	98.66	105.83
11	j	102	BCL	CMD-C2D-C1D	5.25	133.97	124.73
11	V	101	BCL	C3D-C2D-C1D	-5.23	98.70	105.83
11	O	101	BCL	C3C-C4C-CHD	-5.23	112.37	123.39
11	d	102	BCL	C3D-C2D-C1D	-5.22	98.71	105.83
11	i	101	BCL	C3C-C4C-CHD	-5.22	112.39	123.39
11	Z	101	BCL	CHD-C1D-ND	-5.21	117.48	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	f	101	BCL	C3D-C2D-C1D	-5.20	98.74	105.83
9	L	410	PGV	O01-C1-C2	5.20	122.72	111.48
11	P	101	BCL	C2D-C1D-ND	5.19	115.26	110.13
11	X	101	BCL	C2D-C1D-ND	5.19	115.26	110.13
11	h	101	BCL	C3D-C2D-C1D	-5.18	98.76	105.83
11	R	101	BCL	C1C-NC-C4C	-5.17	104.32	106.68
11	f	101	BCL	CHD-C1D-ND	-5.17	117.53	124.80
11	G	101	BCL	C1C-NC-C4C	-5.17	104.32	106.68
11	R	102	BCL	C3D-C2D-C1D	-5.16	98.79	105.83
11	I	101	BCL	C3C-C4C-CHD	-5.15	112.52	123.39
11	J	101	BCL	O2D-CGD-CBD	5.14	120.22	111.23
11	G	101	BCL	C3D-C2D-C1D	-5.13	98.83	105.83
11	Z	101	BCL	C3C-C4C-CHD	-5.12	112.59	123.39
11	j	103	BCL	C3D-C2D-C1D	-5.11	98.86	105.83
11	c	101	BCL	CMD-C2D-C1D	5.10	133.71	124.73
11	V	101	BCL	CHD-C1D-ND	-5.07	117.66	124.80
11	R	101	BCL	CHD-C1D-ND	-5.07	117.67	124.80
11	W	101	BCL	C3C-C4C-CHD	-5.07	112.70	123.39
11	A	102	BCL	C3D-C2D-C1D	-5.07	98.92	105.83
11	T	102	BCL	O2D-CGD-CBD	5.06	120.07	111.23
11	R	102	BCL	O2D-CGD-CBD	5.06	120.07	111.23
11	L	402	BCL	C3D-C2D-C1D	-5.06	98.93	105.83
11	f	102	BCL	O2D-CGD-CBD	5.06	120.07	111.23
11	b	102	BCL	C3D-C2D-C1D	-5.04	98.95	105.83
11	g	101	BCL	C3D-C2D-C1D	-5.04	98.96	105.83
11	f	102	BCL	C3D-C2D-C1D	-5.04	98.96	105.83
11	K	101	BCL	C3C-C4C-CHD	-5.03	112.78	123.39
11	j	102	BCL	C2D-C1D-ND	5.03	115.11	110.13
11	b	101	BCL	C3D-C2D-C1D	-5.03	98.97	105.83
11	N	101	BCL	C1-C2-C3	-5.01	117.99	126.20
11	T	101	BCL	CHD-C1D-ND	-5.00	117.76	124.80
11	P	102	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
11	V	102	BCL	O2D-CGD-CBD	5.00	119.97	111.23
11	L	402	BCL	CHD-C1D-ND	-4.99	117.78	124.80
11	f	101	BCL	C4A-NA-C1A	4.98	108.95	106.68
11	X	102	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
11	J	102	BCL	C3D-C2D-C1D	-4.98	99.03	105.83
11	Y	101	BCL	C3C-C4C-CHD	-4.98	112.90	123.39
11	P	102	BCL	C4A-NA-C1A	4.97	108.95	106.68
11	M	403	BCL	C3C-C4C-CHD	-4.97	112.92	123.39
11	j	102	BCL	C1C-NC-C4C	-4.96	104.42	106.68
11	N	102	BCL	C3D-C2D-C1D	-4.96	99.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	101	BCL	CHD-C1D-ND	-4.96	117.83	124.80
11	S	101	BCL	C3C-C4C-CHD	-4.95	112.96	123.39
11	V	102	BCL	C3D-C2D-C1D	-4.94	99.08	105.83
11	N	102	BCL	O2D-CGD-CBD	4.94	119.86	111.23
11	Y	101	BCL	CMD-C2D-C1D	4.94	133.42	124.73
11	X	101	BCL	C4A-NA-C1A	4.93	108.93	106.68
11	d	101	BCL	CHD-C1D-ND	-4.93	117.87	124.80
11	e	101	BCL	CMD-C2D-C1D	4.92	133.40	124.73
11	P	102	BCL	O2D-CGD-CBD	4.92	119.82	111.23
11	M	403	BCL	C1C-NC-C4C	-4.91	104.44	106.68
11	R	101	BCL	C3D-C2D-C1D	-4.91	99.14	105.83
11	h	102	BCL	O2D-CGD-CBD	4.90	119.79	111.23
11	J	101	BCL	C4A-NA-C1A	4.88	108.90	106.68
11	h	101	BCL	O2D-CGD-CBD	4.87	119.74	111.23
11	i	101	BCL	C3D-C2D-C1D	-4.86	99.19	105.83
11	A	101	BCL	CHD-C1D-ND	-4.86	117.96	124.80
11	J	101	BCL	CHD-C1D-ND	-4.86	117.96	124.80
11	E	102	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
11	b	101	BCL	C1C-NC-C4C	-4.84	104.47	106.68
11	J	102	BCL	C3C-C4C-CHD	-4.84	113.19	123.39
11	T	102	BCL	C3C-C4C-CHD	-4.83	113.21	123.39
11	O	101	BCL	CMD-C2D-C1D	4.80	133.19	124.73
11	Z	101	BCL	C3D-C2D-C1D	-4.79	99.29	105.83
11	A	102	BCL	C3B-C4B-NB	4.79	116.08	109.76
11	E	102	BCL	O2D-CGD-CBD	4.79	119.60	111.23
11	e	101	BCL	C3D-C2D-C1D	-4.78	99.30	105.83
11	h	101	BCL	C4A-NA-C1A	4.77	108.86	106.68
11	N	101	BCL	C4A-NA-C1A	4.77	108.86	106.68
11	d	101	BCL	C1C-NC-C4C	-4.77	104.50	106.68
11	G	102	BCL	C3D-C2D-C1D	-4.77	99.33	105.83
11	P	102	BCL	C3C-C4C-CHD	-4.76	113.35	123.39
11	W	101	BCL	C3D-C2D-C1D	-4.76	99.34	105.83
11	O	101	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
11	W	101	BCL	CMD-C2D-C1D	4.75	133.09	124.73
11	T	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
11	V	101	BCL	C1C-NC-C4C	-4.73	104.52	106.68
11	L	401	BCL	C1C-NC-C4C	-4.73	104.52	106.68
11	U	101	BCL	CMD-C2D-C1D	4.73	133.05	124.73
11	A	101	BCL	C1C-NC-C4C	-4.72	104.53	106.68
11	N	101	BCL	CHD-C1D-ND	-4.71	118.17	124.80
11	Y	101	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
11	j	103	BCL	C3C-C4C-CHD	-4.70	113.47	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	c	101	BCL	C3D-C2D-C1D	-4.70	99.41	105.83
11	G	101	BCL	C4A-NA-C1A	4.70	108.82	106.68
11	h	102	BCL	C3C-C4C-CHD	-4.70	113.48	123.39
11	L	402	BCL	CED-O2D-CGD	4.70	126.57	115.92
11	A	101	BCL	C2D-C1D-ND	4.70	114.78	110.13
11	T	101	BCL	C1C-NC-C4C	-4.70	104.54	106.68
11	b	102	BCL	C3C-C4C-CHD	-4.70	113.49	123.39
11	F	101	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
11	W	101	BCL	O2D-CGD-CBD	4.67	119.40	111.23
11	Q	101	BCL	C3D-C2D-C1D	-4.66	99.48	105.83
11	i	101	BCL	O2D-CGD-CBD	4.66	119.37	111.23
11	b	102	BCL	O2D-CGD-CBD	4.65	119.37	111.23
11	U	101	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
11	G	101	BCL	C2D-C1D-ND	4.63	114.71	110.13
11	A	101	BCL	C4A-NA-C1A	4.63	108.79	106.68
11	h	101	BCL	CHD-C1D-ND	-4.62	118.30	124.80
11	j	103	BCL	O2D-CGD-CBD	4.62	119.30	111.23
11	I	101	BCL	C3D-C2D-C1D	-4.60	99.55	105.83
11	b	101	BCL	CHD-C1D-ND	-4.59	118.34	124.80
11	M	402	BCL	C3D-C2D-C1D	-4.59	99.57	105.83
11	N	102	BCL	C3C-C4C-CHD	-4.58	113.74	123.39
11	E	101	BCL	C2D-C1D-ND	4.58	114.65	110.13
11	N	101	BCL	C2D-C1D-ND	4.57	114.65	110.13
11	T	101	BCL	C2D-C1D-ND	4.57	114.65	110.13
11	h	101	BCL	C2D-C1D-ND	4.56	114.64	110.13
11	j	102	BCL	CHD-C1D-ND	-4.55	118.40	124.80
11	J	102	BCL	O2D-CGD-CBD	4.55	119.18	111.23
11	B	101	BCL	C3D-C2D-C1D	-4.54	99.64	105.83
11	N	101	BCL	O2D-CGD-O1D	-4.53	115.02	123.85
11	Y	101	BCL	O2D-CGD-CBD	4.53	119.16	111.23
11	D	101	BCL	C3D-C2D-C1D	-4.53	99.65	105.83
11	f	102	BCL	C3C-C4C-CHD	-4.52	113.85	123.39
11	e	101	BCL	CHD-C1D-ND	-4.52	118.45	124.80
11	d	101	BCL	C2D-C1D-ND	4.50	114.58	110.13
11	g	101	BCL	C2D-C1D-ND	4.48	114.56	110.13
11	e	101	BCL	O2D-CGD-CBD	4.48	119.06	111.23
11	V	101	BCL	C2D-C1D-ND	4.46	114.54	110.13
11	d	101	BCL	C4A-NA-C1A	4.46	108.71	106.68
11	K	101	BCL	O2D-CGD-CBD	4.45	119.02	111.23
11	a	101	BCL	C3D-C2D-C1D	-4.45	99.76	105.83
11	c	101	BCL	O2D-CGD-CBD	4.45	119.01	111.23
11	I	101	BCL	C2D-C1D-ND	4.43	114.51	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	101	BCL	CHD-C1D-ND	-4.43	118.57	124.80
11	E	101	BCL	O2D-CGD-O1D	-4.42	115.25	123.85
11	V	102	BCL	C3C-C4C-CHD	-4.41	114.10	123.39
11	L	401	BCL	C3D-C2D-C1D	-4.40	99.83	105.83
11	N	102	BCL	C4A-NA-C1A	4.39	108.68	106.68
11	g	101	BCL	CHD-C1D-ND	-4.39	118.63	124.80
11	e	101	BCL	C2D-C1D-ND	4.39	114.47	110.13
11	a	101	BCL	CMD-C2D-C1D	4.38	132.45	124.73
11	c	101	BCL	CHD-C1D-ND	-4.37	118.65	124.80
11	i	101	BCL	C2D-C1D-ND	4.37	114.45	110.13
11	M	402	BCL	C3C-C4C-CHD	-4.37	114.17	123.39
11	J	101	BCL	C2D-C1D-ND	4.36	114.44	110.13
11	L	402	BCL	O2D-CGD-CBD	4.35	118.83	111.23
11	B	101	BCL	C2D-C1D-ND	4.33	114.42	110.13
16	U	102	CRT	C20-C21-C22	4.32	132.35	123.52
11	R	102	BCL	C3C-C4C-CHD	-4.31	114.31	123.39
11	b	102	BCL	O2D-CGD-O1D	-4.31	115.46	123.85
11	Q	101	BCL	CHD-C1D-ND	-4.30	118.75	124.80
11	K	101	BCL	C3D-C2D-C1D	-4.30	99.96	105.83
11	Y	101	BCL	CHD-C1D-ND	-4.30	118.75	124.80
11	Z	101	BCL	C1C-NC-C4C	-4.29	104.72	106.68
9	H	301	PGV	O01-C1-C2	4.28	120.73	111.48
11	I	101	BCL	CHD-C1D-ND	-4.27	118.79	124.80
11	I	101	BCL	CMD-C2D-C1D	4.27	132.25	124.73
11	S	101	BCL	C3D-C2D-C1D	-4.26	100.02	105.83
11	M	402	BCL	O2D-CGD-O1D	-4.25	115.58	123.85
11	G	102	BCL	C3C-C4C-CHD	-4.24	114.46	123.39
11	K	101	BCL	CHD-C1D-ND	-4.23	118.84	124.80
11	D	101	BCL	C2D-C1D-ND	4.22	114.30	110.13
11	g	101	BCL	O2D-CGD-CBD	4.22	118.61	111.23
11	V	101	BCL	C4A-NA-C1A	4.21	108.60	106.68
11	A	102	BCL	O2D-CGD-CBD	4.20	118.57	111.23
11	L	401	BCL	O1D-CGD-CBD	-4.20	116.24	124.52
11	F	101	BCL	C2D-C1D-ND	4.20	114.28	110.13
16	E	103	CRT	C5-C6-C7	4.19	132.23	125.89
11	a	101	BCL	C2D-C1D-ND	4.18	114.26	110.13
9	C	508	PGV	O01-C1-C2	4.17	120.51	111.48
16	I	102	CRT	C6-C7-C9	4.17	125.57	119.01
11	T	101	BCL	O2D-CGD-O1D	-4.17	115.73	123.85
11	X	101	BCL	C1D-ND-C4D	-4.17	103.39	106.31
16	B	102	CRT	C20-C21-C22	4.16	132.03	123.52
11	S	101	BCL	CMD-C2D-C1D	4.16	132.05	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	101	BCL	C2D-C1D-ND	4.15	114.24	110.13
11	Z	101	BCL	C2D-C1D-ND	4.15	114.24	110.13
11	P	101	BCL	C1D-ND-C4D	-4.15	103.40	106.31
11	E	101	BCL	C4A-NA-C1A	4.14	108.57	106.68
11	X	102	BCL	C3C-C4C-CHD	-4.13	114.68	123.39
11	I	101	BCL	C1D-ND-C4D	-4.13	103.42	106.31
11	i	101	BCL	CMD-C2D-C1D	4.13	131.99	124.73
11	R	101	BCL	C2D-C1D-ND	4.11	114.20	110.13
11	f	101	BCL	C2D-C1D-ND	4.11	114.20	110.13
11	O	101	BCL	C2D-C1D-ND	4.11	114.19	110.13
11	W	101	BCL	C2D-C1D-ND	4.10	114.18	110.13
11	g	101	BCL	C1D-ND-C4D	-4.10	103.44	106.31
11	d	102	BCL	C3C-C4C-CHD	-4.09	114.78	123.39
11	T	101	BCL	C4A-NA-C1A	4.09	108.54	106.68
11	Q	101	BCL	CMD-C2D-C1D	4.07	131.90	124.73
11	V	102	BCL	O2D-CGD-O1D	-4.07	115.93	123.85
12	L	403	BPH	C4D-ND-C1D	-4.06	104.00	108.87
9	M	408	PGV	O01-C1-C2	4.06	120.27	111.48
11	F	101	BCL	CMD-C2D-C1D	4.06	131.88	124.73
11	U	101	BCL	O2D-CGD-CBD	4.05	118.31	111.23
11	X	102	BCL	O2D-CGD-O1D	-4.04	115.98	123.85
11	e	101	BCL	C4A-NA-C1A	4.04	108.52	106.68
16	K	102	CRT	C20-C21-C22	4.01	131.72	123.52
9	Z	103	PGV	O01-C1-C2	4.01	120.15	111.48
11	d	102	BCL	O2D-CGD-CBD	3.99	118.21	111.23
11	G	101	BCL	O2D-CGD-O1D	-3.99	116.08	123.85
16	j	101	CRT	C20-C21-C22	3.99	131.67	123.52
11	A	102	BCL	C4A-NA-C1A	3.98	108.50	106.68
12	M	404	BPH	C4D-ND-C1D	-3.98	104.10	108.87
11	U	101	BCL	CHD-C1D-ND	-3.98	119.20	124.80
11	E	102	BCL	C3C-C4C-CHD	-3.97	115.02	123.39
11	M	403	BCL	C2D-C1D-ND	3.96	114.05	110.13
11	c	101	BCL	C2D-C1D-ND	3.96	114.05	110.13
9	H	302	PGV	O01-C1-C2	3.96	120.04	111.48
11	L	402	BCL	O2A-CGA-CBA	3.95	123.89	111.83
16	Z	102	CRT	C21-C20-C19	3.95	131.60	123.52
16	e	102	CRT	C20-C21-C22	3.95	131.60	123.52
11	i	101	BCL	CHD-C1D-ND	-3.95	119.25	124.80
11	a	101	BCL	CHD-C1D-ND	-3.94	119.26	124.80
16	E	103	CRT	C20-C21-C22	3.94	131.57	123.52
11	h	102	BCL	C3B-C4B-NB	3.93	114.94	109.76
11	P	102	BCL	O2D-CGD-O1D	-3.93	116.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	BCL	O2D-CGD-CBD	3.93	118.09	111.23
16	a	102	CRT	C20-C21-C22	3.92	131.54	123.52
11	b	101	BCL	C2D-C1D-ND	3.91	114.00	110.13
11	B	101	BCL	CHD-C1D-ND	-3.91	119.30	124.80
16	Z	102	CRT	C9-C10-C11	3.90	134.51	123.20
11	W	101	BCL	CHD-C1D-ND	-3.89	119.32	124.80
11	M	402	BCL	CHC-C4B-NB	-3.88	118.23	124.05
11	F	101	BCL	O2D-CGD-CBD	3.87	118.00	111.23
11	N	102	BCL	C4-C3-C5	3.87	121.94	115.23
11	b	101	BCL	O2D-CGD-O1D	-3.87	116.32	123.85
11	D	101	BCL	CMD-C2D-C1D	3.86	131.53	124.73
11	U	101	BCL	C2D-C1D-ND	3.86	113.95	110.13
16	A	103	CRT	C20-C21-C22	3.86	131.41	123.52
11	d	101	BCL	C1-C2-C3	-3.85	119.88	126.20
11	R	102	BCL	C3B-C4B-NB	3.84	114.83	109.76
11	M	402	BCL	C1-O2A-CGA	3.84	125.95	116.65
11	G	102	BCL	O2D-CGD-O1D	-3.84	116.37	123.85
11	V	101	BCL	O2D-CGD-O1D	-3.84	116.37	123.85
11	E	101	BCL	C1-C2-C3	-3.83	119.92	126.20
11	G	101	BCL	C1D-ND-C4D	-3.83	103.62	106.31
11	j	103	BCL	O2D-CGD-O1D	-3.83	116.39	123.85
11	L	402	BCL	C2D-C1D-ND	3.83	113.91	110.13
11	h	102	BCL	C2D-C1D-ND	3.83	113.91	110.13
11	A	101	BCL	O2D-CGD-O1D	-3.83	116.40	123.85
11	E	102	BCL	C4-C3-C5	3.82	121.85	115.23
11	P	102	BCL	C1C-NC-C4C	-3.80	104.94	106.68
11	S	101	BCL	C2D-C1D-ND	3.80	113.88	110.13
16	I	102	CRT	C5-C6-C7	3.79	131.62	125.89
11	R	102	BCL	C2D-C1D-ND	3.78	113.87	110.13
16	E	103	CRT	C6-C7-C9	3.78	124.96	119.01
16	R	103	CRT	C20-C21-C22	3.77	131.24	123.52
11	d	101	BCL	O2D-CGD-O1D	-3.77	116.50	123.85
11	A	101	BCL	C1D-ND-C4D	-3.77	103.67	106.31
16	I	102	CRT	C20-C21-C22	3.77	131.23	123.52
7	C	504	HEC	C4D-ND-C1D	3.77	111.96	105.82
11	J	102	BCL	O2D-CGD-O1D	-3.76	116.53	123.85
11	Y	101	BCL	C2D-C1D-ND	3.76	113.85	110.13
11	j	102	BCL	C1D-ND-C4D	-3.76	103.68	106.31
11	S	101	BCL	CHD-C1D-ND	-3.75	119.52	124.80
11	b	101	BCL	C1-C2-C3	-3.75	120.06	126.20
11	I	101	BCL	C1-O2A-CGA	3.74	125.71	116.65
11	i	101	BCL	C1D-ND-C4D	-3.74	103.69	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	101	BCL	C4A-NA-C1A	3.74	108.39	106.68
11	f	102	BCL	C2D-C1D-ND	3.74	113.83	110.13
11	A	102	BCL	C3C-C4C-CHD	-3.73	115.53	123.39
16	W	102	CRT	C20-C21-C22	3.72	131.13	123.52
11	N	101	BCL	C1C-NC-C4C	-3.72	104.98	106.68
16	I	102	CRT	C8-C7-C9	-3.71	116.80	122.82
11	f	101	BCL	C3B-C4B-NB	3.69	114.63	109.76
9	R	104	PGV	O01-C1-C2	3.69	119.46	111.48
11	M	402	BCL	O2A-CGA-CBA	3.68	123.06	111.83
11	E	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
11	a	101	BCL	C1-O2A-CGA	3.67	125.54	116.65
11	A	102	BCL	C2D-C1D-ND	3.67	113.76	110.13
11	N	102	BCL	C3B-C4B-NB	3.65	114.58	109.76
11	D	101	BCL	C4A-NA-C1A	3.65	108.35	106.68
11	J	102	BCL	C2D-C1D-ND	3.65	113.74	110.13
11	e	101	BCL	C1D-ND-C4D	-3.65	103.75	106.31
11	Z	101	BCL	O2D-CGD-O1D	-3.65	116.75	123.85
11	O	101	BCL	O2D-CGD-CBD	3.64	117.60	111.23
11	a	101	BCL	O2D-CGD-CBD	3.64	117.59	111.23
11	B	101	BCL	CMD-C2D-C1D	3.64	131.13	124.73
11	N	102	BCL	C2D-C1D-ND	3.63	113.72	110.13
7	C	503	HEC	C4D-ND-C1D	3.62	111.73	105.82
11	h	101	BCL	C1D-ND-C4D	-3.62	103.77	106.31
11	L	402	BCL	CHC-C4B-NB	-3.62	118.62	124.05
16	Z	102	CRT	C30-C28-C27	3.61	124.69	119.01
11	T	102	BCL	C1-C2-C3	-3.61	120.28	126.20
9	M	407	PGV	O01-C1-C2	3.61	119.28	111.48
11	D	101	BCL	O2D-CGD-CBD	3.60	117.53	111.23
11	V	101	BCL	C1D-ND-C4D	-3.60	103.79	106.31
11	P	101	BCL	C3B-C4B-NB	3.60	114.51	109.76
11	P	102	BCL	C2D-C1D-ND	3.60	113.69	110.13
11	M	402	BCL	C3D-C4D-ND	3.60	115.83	109.99
11	Y	101	BCL	O2A-CGA-CBA	3.60	122.80	111.83
11	f	102	BCL	O2D-CGD-O1D	-3.60	116.85	123.85
11	P	102	BCL	C3B-C4B-NB	3.59	114.50	109.76
11	F	101	BCL	CHD-C1D-ND	-3.59	119.75	124.80
11	R	102	BCL	O2D-CGD-O1D	-3.59	116.86	123.85
11	W	101	BCL	C1D-ND-C4D	-3.59	103.80	106.31
11	b	101	BCL	C3B-C4B-NB	3.58	114.49	109.76
11	R	102	BCL	C1D-ND-C4D	-3.58	103.80	106.31
11	j	102	BCL	C3B-C4B-NB	3.57	114.47	109.76
11	A	102	BCL	CHB-C4A-NA	3.57	129.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	102	CRT	C20-C21-C22	3.57	130.82	123.52
11	Q	101	BCL	O2D-CGD-CBD	3.56	117.45	111.23
11	L	401	BCL	C1-C2-C3	-3.56	120.37	126.20
12	M	404	BPH	C3D-C4D-ND	3.56	112.27	107.71
11	N	102	BCL	C6-C5-C3	-3.55	104.82	113.47
16	Z	102	CRT	C20-C21-C22	3.55	130.77	123.52
11	a	101	BCL	O2A-CGA-CBA	3.54	122.63	111.83
11	L	401	BCL	O2D-CGD-O1D	-3.53	116.97	123.85
11	J	101	BCL	C3B-C4B-NB	3.53	114.42	109.76
11	I	101	BCL	C3B-C4B-NB	3.53	114.42	109.76
16	i	102	CRT	C20-C21-C22	3.53	130.74	123.52
11	A	101	BCL	C3B-C4B-NB	3.53	114.41	109.76
11	S	101	BCL	C1D-ND-C4D	-3.53	103.84	106.31
11	a	101	BCL	C1D-ND-C4D	-3.53	103.84	106.31
11	N	101	BCL	CHC-C4B-NB	-3.52	118.76	124.05
11	D	101	BCL	C1C-NC-C4C	-3.52	105.07	106.68
11	j	102	BCL	CHC-C4B-NB	-3.52	118.77	124.05
11	T	101	BCL	CAC-C3C-C4C	-3.51	104.78	112.58
11	V	102	BCL	C2D-C1D-ND	3.51	113.60	110.13
11	L	401	BCL	C3C-C4C-CHD	-3.51	115.99	123.39
11	N	102	BCL	CHC-C1C-NC	3.51	129.46	124.40
11	J	101	BCL	O2D-CGD-O1D	-3.50	117.03	123.85
11	Y	101	BCL	C3B-C4B-NB	3.50	114.37	109.76
11	Z	101	BCL	C3B-C4B-NB	3.50	114.37	109.76
11	P	101	BCL	C1-C2-C3	-3.49	120.47	126.20
7	C	501	HEC	C4D-ND-C1D	3.49	111.51	105.82
11	J	101	BCL	C1-C2-C3	-3.49	120.48	126.20
11	B	101	BCL	O2D-CGD-CBD	3.49	117.33	111.23
11	h	101	BCL	C1-C2-C3	-3.49	120.49	126.20
11	M	402	BCL	C2D-C1D-ND	3.48	113.57	110.13
11	T	102	BCL	C4-C3-C5	3.47	121.25	115.23
11	j	103	BCL	C2D-C1D-ND	3.46	113.56	110.13
11	b	102	BCL	C2D-C1D-ND	3.46	113.55	110.13
11	E	101	BCL	CHC-C4B-NB	-3.46	118.86	124.05
11	K	101	BCL	C2D-C1D-ND	3.46	113.55	110.13
11	d	102	BCL	C2D-C1D-ND	3.46	113.55	110.13
11	X	101	BCL	O2D-CGD-O1D	-3.45	117.12	123.85
11	E	102	BCL	C3B-C4B-NB	3.45	114.32	109.76
11	i	101	BCL	C1-C2-C3	-3.45	120.54	126.20
11	E	102	BCL	O2D-CGD-O1D	-3.45	117.13	123.85
11	h	101	BCL	C3B-C4B-NB	3.45	114.31	109.76
12	L	403	BPH	C3D-C4D-ND	3.45	112.12	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	101	BCL	C1D-ND-C4D	-3.44	103.89	106.31
11	U	101	BCL	CHC-C4B-NB	-3.44	118.89	124.05
11	d	101	BCL	C1D-ND-C4D	-3.44	103.90	106.31
11	N	102	BCL	O2A-CGA-CBA	3.44	122.32	111.83
16	E	103	CRT	C8-C7-C9	-3.43	117.25	122.82
11	h	102	BCL	O2D-CGD-O1D	-3.43	117.17	123.85
11	N	101	BCL	C1D-ND-C4D	-3.43	103.91	106.31
11	d	101	BCL	C3B-C4B-NB	3.42	114.28	109.76
11	L	402	BCL	C1D-ND-C4D	-3.42	103.91	106.31
11	h	101	BCL	C1D-CHD-C4C	-3.42	118.37	126.62
11	D	101	BCL	C6-C5-C3	-3.42	105.15	113.47
11	c	101	BCL	C1C-NC-C4C	-3.41	105.12	106.68
11	D	101	BCL	CHD-C1D-ND	-3.40	120.02	124.80
11	P	101	BCL	O2D-CGD-O1D	-3.40	117.23	123.85
11	f	102	BCL	C3B-C4B-NB	3.40	114.24	109.76
11	R	102	BCL	C4A-NA-C1A	3.38	108.22	106.68
11	c	101	BCL	O2A-CGA-CBA	3.38	122.13	111.83
11	E	101	BCL	C1C-NC-C4C	-3.38	105.14	106.68
11	J	102	BCL	C4A-NA-C1A	3.38	108.22	106.68
16	P	103	CRT	C20-C21-C22	3.37	130.42	123.52
11	d	102	BCL	C4-C3-C5	3.37	121.08	115.23
11	M	403	BCL	CHC-C4B-NB	-3.37	118.99	124.05
16	N	103	CRT	C20-C21-C22	3.37	130.42	123.52
11	b	102	BCL	C4A-NA-C1A	3.37	108.22	106.68
11	T	102	BCL	C2D-C1D-ND	3.36	113.45	110.13
11	A	101	BCL	C1-C2-C3	-3.36	120.69	126.20
11	f	102	BCL	C1D-ND-C4D	-3.36	103.95	106.31
11	L	402	BCL	C3B-C4B-NB	3.36	114.19	109.76
11	P	101	BCL	CAC-C3C-C4C	-3.36	105.13	112.58
11	V	101	BCL	O2A-CGA-CBA	3.35	122.05	111.83
11	c	101	BCL	C1-O2A-CGA	3.35	124.75	116.65
11	M	402	BCL	C1D-ND-C4D	-3.35	103.97	106.31
11	L	402	BCL	O2A-CGA-O1A	-3.34	115.28	123.63
11	D	101	BCL	CHC-C4B-NB	-3.34	119.04	124.05
11	b	101	BCL	CHC-C4B-NB	-3.33	119.05	124.05
11	O	101	BCL	O2A-CGA-CBA	3.33	121.99	111.83
11	F	101	BCL	C1D-ND-C4D	-3.33	103.98	106.31
16	Z	102	CRT	C16-C17-C19	3.33	124.25	119.01
11	U	101	BCL	C3B-C4B-NB	3.33	114.15	109.76
11	T	101	BCL	C3B-C4B-NB	3.31	114.13	109.76
16	I	102	CRT	C9-C10-C11	3.31	132.78	123.20
11	j	102	BCL	C1D-CHD-C4C	-3.30	118.65	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	BCL	C3D-C4D-ND	3.30	115.34	109.99
11	L	401	BCL	C1-O2A-CGA	3.29	124.62	116.65
11	E	102	BCL	C6-C5-C3	-3.29	105.45	113.47
7	C	502	HEC	C4D-ND-C1D	3.29	111.19	105.82
11	O	101	BCL	C1C-NC-C4C	-3.29	105.18	106.68
11	M	403	BCL	C3B-C4B-NB	3.28	114.09	109.76
11	B	101	BCL	C1-O2A-CGA	3.28	124.59	116.65
11	A	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
11	G	102	BCL	C2D-C1D-ND	3.27	113.36	110.13
11	M	403	BCL	C1-O2A-CGA	3.27	124.57	116.65
11	c	101	BCL	C1D-ND-C4D	-3.26	104.02	106.31
11	X	101	BCL	C1C-NC-C4C	-3.26	105.19	106.68
11	X	102	BCL	C2D-C1D-ND	3.26	113.36	110.13
11	f	101	BCL	C1D-ND-C4D	-3.26	104.03	106.31
11	T	102	BCL	O2D-CGD-O1D	-3.26	117.51	123.85
11	U	101	BCL	C1D-ND-C4D	-3.25	104.03	106.31
11	c	101	BCL	C3B-C4B-NB	3.25	114.05	109.76
11	N	102	BCL	O2D-CGD-O1D	-3.25	117.52	123.85
11	E	101	BCL	C3B-C4B-NB	3.25	114.04	109.76
11	Q	101	BCL	C1-O2A-CGA	3.25	124.51	116.65
11	V	102	BCL	C4-C3-C5	3.24	120.86	115.23
11	T	101	BCL	C1D-CHD-C4C	-3.24	118.80	126.62
11	j	102	BCL	O2D-CGD-O1D	-3.24	117.54	123.85
11	T	101	BCL	C1D-ND-C4D	-3.24	104.04	106.31
16	Z	102	CRT	C25-C23-C22	3.23	124.09	119.01
11	b	102	BCL	C4-C3-C5	3.23	120.83	115.23
11	O	101	BCL	C3B-C4B-NB	3.23	114.02	109.76
11	Z	101	BCL	CHC-C4B-NB	-3.23	119.21	124.05
11	K	101	BCL	CHC-C4B-NB	-3.22	119.21	124.05
11	M	402	BCL	C3B-C4B-NB	3.22	114.01	109.76
11	X	101	BCL	CHC-C4B-NB	-3.22	119.22	124.05
11	f	101	BCL	O2D-CGD-O1D	-3.21	117.59	123.85
11	V	101	BCL	C1-C2-C3	-3.21	120.93	126.20
11	f	101	BCL	C4-C3-C5	3.21	120.80	115.23
12	M	404	BPH	OBD-CAD-CBD	-3.21	121.11	125.82
16	Z	102	CRT	C10-C9-C7	3.21	131.78	127.28
11	T	102	BCL	C1D-ND-C4D	-3.21	104.06	106.31
11	M	403	BCL	C1D-ND-C4D	-3.21	104.06	106.31
11	Y	101	BCL	C1-O2A-CGA	3.20	124.41	116.65
11	E	102	BCL	C2D-C1D-ND	3.20	113.30	110.13
11	Q	101	BCL	C3B-C4B-NB	3.20	113.98	109.76
11	S	101	BCL	C3D-C4D-ND	3.20	115.19	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	h	101	BCL	CHC-C4B-NB	-3.20	119.25	124.05
11	R	101	BCL	C3B-C4B-NB	3.20	113.98	109.76
11	R	102	BCL	CHC-C1C-NC	3.19	129.00	124.40
16	Z	102	CRT	C29-C28-C27	-3.19	117.65	122.82
11	D	101	BCL	C3B-C4B-NB	3.18	113.96	109.76
11	j	103	BCL	CHC-C1C-NC	3.18	128.99	124.40
11	A	101	BCL	CHC-C4B-NB	-3.18	119.28	124.05
11	T	101	BCL	C1-C2-C3	-3.17	121.00	126.20
11	L	401	BCL	C6-C5-C3	-3.17	105.74	113.47
11	F	101	BCL	C4A-NA-C1A	3.17	108.12	106.68
11	P	101	BCL	C4-C3-C5	3.17	120.73	115.23
11	X	102	BCL	C3B-C4B-NB	3.17	113.94	109.76
11	U	101	BCL	O2A-CGA-CBA	3.16	121.48	111.83
11	J	101	BCL	C1D-CHD-C4C	-3.16	118.99	126.62
11	W	101	BCL	O2D-CGD-O1D	-3.16	117.69	123.85
11	W	101	BCL	C3B-C4B-NB	3.16	113.93	109.76
11	b	102	BCL	O2A-CGA-CBA	3.16	121.47	111.83
11	i	101	BCL	C3B-C4B-NB	3.15	113.92	109.76
11	D	101	BCL	C1D-ND-C4D	-3.15	104.10	106.31
11	S	101	BCL	C3B-C4B-NB	3.15	113.92	109.76
11	R	102	BCL	C3D-C4D-ND	3.15	115.11	109.99
11	R	102	BCL	C4-C3-C5	3.15	120.69	115.23
11	h	102	BCL	CHB-C4A-NA	3.15	128.94	124.40
11	Q	101	BCL	C1D-ND-C4D	-3.14	104.11	106.31
11	i	101	BCL	O2A-CGA-CBA	3.14	121.41	111.83
16	I	102	CRT	C11-C12-C14	3.14	123.94	119.01
11	d	102	BCL	CHB-C4A-NA	3.14	128.93	124.40
11	T	102	BCL	C3D-C4D-ND	3.13	115.08	109.99
11	T	102	BCL	C3B-C4B-NB	3.13	113.89	109.76
11	R	101	BCL	C4A-NA-C1A	3.13	108.11	106.68
11	N	101	BCL	C1D-CHD-C4C	-3.13	119.07	126.62
11	R	101	BCL	O2D-CGD-O1D	-3.13	117.75	123.85
11	V	102	BCL	C3B-C4B-NB	3.13	113.89	109.76
11	G	101	BCL	C1-C2-C3	-3.13	121.07	126.20
11	j	102	BCL	C4-C3-C5	3.13	120.65	115.23
11	A	101	BCL	C1D-CHD-C4C	-3.12	119.09	126.62
11	R	101	BCL	O2A-CGA-CBA	3.12	121.35	111.83
11	e	101	BCL	C3B-C4B-NB	3.12	113.88	109.76
9	H	302	PGV	C02-O01-C1	-3.12	110.34	117.80
11	S	101	BCL	O2D-CGD-CBD	3.12	116.68	111.23
11	f	102	BCL	CHB-C4A-NA	3.12	128.90	124.40
11	D	101	BCL	O2A-CGA-CBA	3.11	121.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	102	BCL	C1C-NC-C4C	-3.11	105.26	106.68
11	h	102	BCL	C4A-NA-C1A	3.11	108.10	106.68
11	e	101	BCL	O2A-CGA-CBA	3.11	121.31	111.83
11	V	101	BCL	CHC-C4B-NB	-3.11	119.39	124.05
11	M	403	BCL	C1D-CHD-C4C	-3.11	119.13	126.62
11	W	101	BCL	C3D-C4D-ND	3.10	115.02	109.99
11	K	101	BCL	C1D-ND-C4D	-3.09	104.14	106.31
11	K	101	BCL	O2A-CGA-CBA	3.09	121.27	111.83
11	M	403	BCL	O2A-CGA-CBA	3.09	121.27	111.83
11	d	101	BCL	CHC-C4B-NB	-3.09	119.41	124.05
11	P	101	BCL	O2A-CGA-CBA	3.09	121.25	111.83
16	Z	102	CRT	C5-C6-C7	3.08	130.55	125.89
16	R	103	CRT	C8-C7-C9	-3.08	117.82	122.82
11	Z	101	BCL	C4-C3-C5	3.08	120.58	115.23
11	V	102	BCL	CHC-C1C-NC	3.07	128.83	124.40
11	f	101	BCL	C1-C2-C3	-3.07	121.17	126.20
11	G	102	BCL	C3B-C4B-NB	3.07	113.81	109.76
11	h	102	BCL	CHC-C1C-NC	3.07	128.83	124.40
11	Q	101	BCL	C4A-NA-C1A	3.07	108.08	106.68
11	d	102	BCL	C3B-C4B-NB	3.06	113.80	109.76
11	Q	101	BCL	O2A-CGA-CBA	3.06	121.17	111.83
11	T	102	BCL	C4A-NA-C1A	3.06	108.08	106.68
11	X	101	BCL	C3B-C4B-NB	3.06	113.80	109.76
9	M	408	PGV	O03-C19-C20	3.06	121.16	111.83
11	j	103	BCL	CHB-C1B-C2B	-3.06	118.55	127.43
11	X	101	BCL	C1D-CHD-C4C	-3.06	119.25	126.62
11	T	102	BCL	CHC-C1C-NC	3.06	128.81	124.40
11	b	101	BCL	C1D-CHD-C4C	-3.06	119.25	126.62
9	C	508	PGV	O03-C19-C20	3.05	120.42	111.15
11	J	101	BCL	C1D-ND-C4D	-3.05	104.17	106.31
11	D	101	BCL	C1D-CHD-C4C	-3.05	119.26	126.62
9	L	410	PGV	O03-C19-C20	3.05	121.13	111.83
11	W	101	BCL	C1-C2-C3	-3.05	121.20	126.20
16	I	102	CRT	C13-C12-C14	-3.05	117.88	122.82
11	a	101	BCL	C3D-C4D-ND	3.05	114.94	109.99
16	j	101	CRT	C8-C7-C9	-3.04	117.88	122.82
11	S	101	BCL	C1-O2A-CGA	3.04	124.02	116.65
11	d	102	BCL	O2D-CGD-O1D	-3.04	117.92	123.85
11	A	101	BCL	C4-C3-C5	3.04	120.51	115.23
12	L	403	BPH	OBD-CAD-CBD	-3.04	121.36	125.82
11	E	101	BCL	C1D-CHD-C4C	-3.04	119.29	126.62
11	h	101	BCL	O2D-CGD-O1D	-3.04	117.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	401	BCL	CMB-C2B-C3B	3.04	135.25	125.67
11	j	103	BCL	C4-C3-C5	3.03	120.49	115.23
11	c	101	BCL	C4-C3-C5	3.03	120.48	115.23
11	d	101	BCL	C1D-CHD-C4C	-3.03	119.32	126.62
11	B	101	BCL	C1D-ND-C4D	-3.03	104.19	106.31
16	P	103	CRT	C8-C7-C9	-3.02	117.92	122.82
11	G	101	BCL	C1D-CHD-C4C	-3.02	119.33	126.62
11	S	101	BCL	O2A-CGA-CBA	3.02	121.05	111.83
11	f	101	BCL	C1D-CHD-C4C	-3.02	119.34	126.62
11	N	102	BCL	C1C-NC-C4C	-3.02	105.30	106.68
11	N	101	BCL	C6-C5-C3	-3.01	106.13	113.47
11	K	101	BCL	C3B-C4B-NB	3.01	113.73	109.76
11	Z	101	BCL	C3D-C4D-ND	3.01	114.88	109.99
11	c	101	BCL	C6-C5-C3	-3.01	106.14	113.47
11	G	101	BCL	C3B-C4B-NB	3.01	113.73	109.76
11	D	101	BCL	O2D-CGD-O1D	-3.01	117.99	123.85
11	b	102	BCL	CHB-C4A-NA	3.01	128.74	124.40
11	M	403	BCL	C3D-C4D-ND	3.00	114.87	109.99
11	B	101	BCL	CHC-C4B-NB	-3.00	119.55	124.05
11	I	101	BCL	CHC-C4B-NB	-3.00	119.55	124.05
11	V	102	BCL	CHB-C4A-NA	3.00	128.73	124.40
11	B	101	BCL	CMB-C2B-C3B	3.00	135.13	125.67
11	b	102	BCL	C6-C5-C3	-3.00	106.17	113.47
11	g	101	BCL	C3D-C4D-ND	3.00	114.86	109.99
11	R	101	BCL	CHC-C4B-NB	-3.00	119.56	124.05
16	Y	102	CRT	C21-C20-C19	2.99	129.65	123.52
11	L	401	BCL	C1D-CHD-C4C	-2.99	119.40	126.62
11	P	102	BCL	C4-C3-C5	2.99	120.42	115.23
16	A	103	CRT	C8-C7-C9	-2.99	117.97	122.82
11	c	101	BCL	CHC-C4B-NB	-2.99	119.57	124.05
11	N	101	BCL	CAC-C3C-C4C	-2.98	105.96	112.58
11	j	102	BCL	O2A-CGA-CBA	2.98	120.94	111.83
16	R	103	CRT	C6-C7-C9	2.98	123.70	119.01
11	i	101	BCL	C3D-C4D-ND	2.98	114.83	109.99
9	H	301	PGV	C02-O01-C1	-2.98	110.67	117.80
16	Z	102	CRT	C18-C17-C19	-2.98	117.99	122.82
11	N	101	BCL	C3B-C4B-NB	2.98	113.69	109.76
11	J	102	BCL	C1D-ND-C4D	-2.98	104.22	106.31
11	d	101	BCL	O2A-CGA-CBA	2.97	120.90	111.83
11	J	102	BCL	C4-C3-C5	2.97	120.39	115.23
9	R	104	PGV	O03-C19-C20	2.97	120.90	111.83
11	D	101	BCL	C1-O2A-CGA	2.97	123.83	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	101	BCL	C3D-C4D-ND	2.97	114.81	109.99
11	T	102	BCL	C1C-NC-C4C	-2.96	105.33	106.68
11	h	102	BCL	C1C-NC-C4C	-2.96	105.33	106.68
11	G	102	BCL	CHC-C1C-NC	2.96	128.67	124.40
11	K	101	BCL	C3D-C4D-ND	2.96	114.79	109.99
11	I	101	BCL	O2A-CGA-CBA	2.96	120.85	111.83
11	T	101	BCL	O2A-CGA-CBA	2.96	120.85	111.83
11	h	102	BCL	CHC-C4B-NB	-2.95	119.62	124.05
11	G	101	BCL	C3D-C4D-ND	2.95	114.79	109.99
11	X	101	BCL	C1-C2-C3	-2.95	121.36	126.20
11	e	101	BCL	CHC-C4B-NB	-2.95	119.62	124.05
11	j	103	BCL	C4A-NA-C1A	2.95	108.03	106.68
11	N	102	BCL	C1D-ND-C4D	-2.95	104.24	106.31
11	e	101	BCL	C3D-C4D-ND	2.95	114.78	109.99
9	H	301	PGV	O03-C19-C20	2.95	120.82	111.83
11	E	102	BCL	CHC-C4B-NB	-2.95	119.63	124.05
16	i	102	CRT	C8-C7-C9	-2.95	118.04	122.82
11	E	102	BCL	CHB-C4A-NA	2.94	128.65	124.40
11	b	102	BCL	CHC-C1C-NC	2.94	128.65	124.40
11	V	101	BCL	C1D-CHD-C4C	-2.94	119.53	126.62
11	d	102	BCL	CHC-C1C-NC	2.94	128.64	124.40
11	a	101	BCL	O2D-CGD-O1D	-2.94	118.13	123.85
11	f	102	BCL	C3D-C4D-ND	2.94	114.76	109.99
11	D	101	BCL	CMB-C2B-C3B	2.94	134.94	125.67
11	L	401	BCL	C3D-C4D-ND	2.94	114.76	109.99
11	B	101	BCL	C3B-C4B-NB	2.94	113.63	109.76
11	G	102	BCL	C4-C3-C5	2.94	120.32	115.23
11	f	101	BCL	CHC-C4B-NB	-2.94	119.65	124.05
11	U	101	BCL	C3D-C4D-ND	2.93	114.76	109.99
16	j	101	CRT	C6-C7-C9	2.93	123.62	119.01
11	O	101	BCL	C6-C5-C3	-2.93	106.32	113.47
11	L	401	BCL	O2A-CGA-CBA	2.93	120.78	111.83
11	g	101	BCL	C3B-C4B-NB	2.93	113.63	109.76
11	X	102	BCL	CHC-C1C-NC	2.93	128.63	124.40
16	B	102	CRT	C8-C7-C9	-2.93	118.07	122.82
16	Z	102	CRT	C24-C23-C22	-2.93	118.07	122.82
11	i	101	BCL	C1D-CHD-C4C	-2.93	119.56	126.62
11	G	102	BCL	C3D-C4D-ND	2.93	114.74	109.99
11	i	101	BCL	C4-C3-C5	2.93	120.31	115.23
16	e	102	CRT	C8-C7-C9	-2.92	118.08	122.82
11	V	101	BCL	C3B-C4B-NB	2.92	113.62	109.76
11	f	101	BCL	C1-O2A-CGA	2.92	123.72	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	101	BCL	CHB-C4A-NA	2.92	128.61	124.40
16	N	103	CRT	C8-C7-C9	-2.92	118.09	122.82
11	Z	101	BCL	CAC-C3C-C4C	-2.91	106.12	112.58
11	X	101	BCL	C3D-C4D-ND	2.91	114.72	109.99
11	F	101	BCL	C3B-C4B-NB	2.91	113.60	109.76
11	j	103	BCL	CHC-C4B-NB	-2.91	119.69	124.05
11	V	102	BCL	C1D-ND-C4D	-2.90	104.27	106.31
11	R	101	BCL	CAC-C3C-C4C	-2.90	106.14	112.58
11	K	101	BCL	O2D-CGD-O1D	-2.90	118.20	123.85
11	d	102	BCL	C6-C5-C3	-2.90	106.40	113.47
16	U	102	CRT	C8-C7-C9	-2.90	118.12	122.82
11	A	102	BCL	C4-C3-C5	2.90	120.26	115.23
11	E	101	BCL	O2A-CGA-CBA	2.90	120.67	111.83
11	L	402	BCL	CHC-C1C-NC	2.90	128.58	124.40
11	b	102	BCL	OBB-CAB-C3B	-2.90	115.31	120.43
11	Y	101	BCL	C1C-NC-C4C	-2.89	105.36	106.68
11	R	102	BCL	CHC-C4B-NB	-2.89	119.71	124.05
11	J	102	BCL	C3B-C4B-NB	2.89	113.57	109.76
11	F	101	BCL	C1D-CHD-C4C	-2.89	119.66	126.62
11	c	101	BCL	O2D-CGD-O1D	-2.88	118.23	123.85
11	c	101	BCL	C3D-C4D-ND	2.88	114.67	109.99
11	A	102	BCL	CHC-C1C-NC	2.88	128.56	124.40
11	E	102	BCL	CHC-C1C-NC	2.88	128.56	124.40
11	I	101	BCL	CHC-C1C-NC	2.88	128.56	124.40
11	J	102	BCL	C3D-C4D-ND	2.88	114.67	109.99
11	f	101	BCL	C3D-C4D-ND	2.88	114.67	109.99
11	Q	101	BCL	C3D-C4D-ND	2.87	114.66	109.99
11	h	102	BCL	O2A-CGA-CBA	2.87	120.59	111.83
11	W	101	BCL	O2A-CGA-CBA	2.87	120.58	111.83
11	g	101	BCL	C1-C2-C3	-2.87	121.50	126.20
7	C	504	HEC	C2A-C1A-NA	-2.86	107.56	110.32
11	V	102	BCL	C3D-C4D-ND	2.86	114.64	109.99
11	J	102	BCL	C1C-NC-C4C	-2.86	105.37	106.68
11	e	101	BCL	C1-O2A-CGA	2.86	123.57	116.65
11	j	103	BCL	O2A-CGA-CBA	2.86	120.54	111.83
11	Z	101	BCL	C1D-CHD-C4C	-2.86	119.73	126.62
11	N	102	BCL	C3D-C4D-ND	2.85	114.63	109.99
16	Z	102	CRT	C34-C33-C32	-2.85	118.19	122.82
11	P	101	BCL	C3D-C4D-ND	2.85	114.62	109.99
11	L	402	BCL	C3D-C4D-ND	2.85	114.62	109.99
11	A	102	BCL	C3D-C4D-ND	2.85	114.62	109.99
16	P	103	CRT	C6-C7-C9	2.85	123.49	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	302	PGV	O03-C19-C20	2.85	120.52	111.83
11	F	101	BCL	CHC-C4B-NB	-2.85	119.78	124.05
16	E	103	CRT	C11-C12-C14	2.85	123.49	119.01
11	a	101	BCL	C3B-C4B-NB	2.85	113.52	109.76
11	M	403	BCL	CMB-C2B-C3B	2.85	134.64	125.67
11	L	401	BCL	CHB-C1B-C2B	-2.85	119.17	127.43
11	X	102	BCL	CHB-C4A-NA	2.85	128.51	124.40
16	E	103	CRT	C13-C12-C14	-2.84	118.21	122.82
11	B	101	BCL	O2A-CGA-CBA	2.84	120.51	111.83
11	i	101	BCL	O2D-CGD-O1D	-2.84	118.31	123.85
11	V	101	BCL	C3D-C4D-ND	2.84	114.61	109.99
11	I	101	BCL	O2D-CGD-O1D	-2.84	118.33	123.85
11	T	102	BCL	CHC-C4B-NB	-2.83	119.80	124.05
12	L	403	BPH	C2D-C1D-ND	2.83	111.48	109.43
11	i	101	BCL	C1-O2A-CGA	2.83	123.50	116.65
11	Q	101	BCL	CHC-C4B-NB	-2.83	119.80	124.05
11	F	101	BCL	C1-C2-C3	-2.83	121.56	126.20
11	J	101	BCL	O2A-CGA-CBA	2.83	120.45	111.83
11	a	101	BCL	C1D-CHD-C4C	-2.83	119.81	126.62
16	Z	102	CRT	C35-C33-C32	2.82	123.45	119.01
11	d	101	BCL	CED-O2D-CGD	2.82	122.32	115.92
11	O	101	BCL	CHC-C4B-NB	-2.82	119.81	124.05
11	R	101	BCL	C3D-C4D-ND	2.82	114.57	109.99
11	P	102	BCL	O2A-CGA-CBA	2.82	120.44	111.83
12	M	404	BPH	C2D-C1D-ND	2.82	111.47	109.43
11	b	101	BCL	O2A-CGA-CBA	2.82	120.42	111.83
11	Q	101	BCL	O2D-CGD-O1D	-2.81	118.38	123.85
11	h	101	BCL	C4-C3-C5	2.81	120.10	115.23
16	U	102	CRT	C6-C7-C9	2.81	123.42	119.01
11	X	102	BCL	CHB-C1B-C2B	-2.81	119.28	127.43
11	W	101	BCL	CHC-C4B-NB	-2.80	119.85	124.05
11	X	102	BCL	CHC-C4B-NB	-2.80	119.85	124.05
16	Y	102	CRT	C8-C7-C9	-2.80	118.28	122.82
16	e	102	CRT	C6-C7-C9	2.80	123.41	119.01
11	W	101	BCL	C4-C3-C5	2.79	120.08	115.23
9	L	410	PGV	C02-O01-C1	-2.79	111.12	117.80
11	I	101	BCL	C4-C3-C5	2.79	120.07	115.23
16	A	103	CRT	C13-C12-C14	-2.79	118.30	122.82
11	U	101	BCL	C1D-CHD-C4C	-2.79	119.90	126.62
11	U	101	BCL	C4A-NA-C1A	2.79	107.95	106.68
11	d	101	BCL	C3D-C4D-ND	2.79	114.51	109.99
11	B	101	BCL	O2D-CGD-O1D	-2.78	118.44	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	101	BCL	O2A-CGA-CBA	2.78	120.31	111.83
11	j	103	BCL	C3B-C4B-NB	2.78	113.43	109.76
11	P	102	BCL	CHC-C1C-NC	2.78	128.41	124.40
11	E	102	BCL	CHB-C1B-C2B	-2.77	119.39	127.43
11	O	101	BCL	O2D-CGD-O1D	-2.77	118.46	123.85
11	A	101	BCL	C3D-C4D-ND	2.77	114.48	109.99
11	J	102	BCL	CHC-C1C-NC	2.77	128.39	124.40
16	A	103	CRT	C6-C7-C9	2.76	123.36	119.01
11	J	101	BCL	CHC-C4B-NB	-2.76	119.91	124.05
16	K	102	CRT	C25-C23-C22	2.76	123.35	119.01
11	U	101	BCL	C1-O2A-CGA	2.76	123.33	116.65
11	N	102	BCL	CHC-C4B-NB	-2.76	119.92	124.05
11	Z	101	BCL	O2A-CGA-CBA	2.75	120.23	111.83
11	e	101	BCL	C1-C2-C3	-2.75	121.69	126.20
11	b	102	BCL	C3B-C4B-NB	2.75	113.39	109.76
11	X	101	BCL	O2A-CGA-CBA	2.75	120.22	111.83
11	G	102	BCL	O2A-CGA-CBA	2.75	120.21	111.83
11	O	101	BCL	C1D-ND-C4D	-2.75	104.38	106.31
11	R	101	BCL	C1D-ND-C4D	-2.75	104.38	106.31
11	B	101	BCL	C1C-NC-C4C	-2.75	105.43	106.68
11	E	102	BCL	C3D-C4D-ND	2.75	114.45	109.99
11	P	101	BCL	C1D-CHD-C4C	-2.74	120.00	126.62
9	L	410	PGV	C3-C2-C1	-2.74	103.65	113.69
11	G	101	BCL	CHC-C4B-NB	-2.74	119.94	124.05
11	g	101	BCL	CHC-C4B-NB	-2.74	119.94	124.05
11	J	102	BCL	CHB-C4A-NA	2.74	128.35	124.40
11	P	102	BCL	C1D-ND-C4D	-2.74	104.39	106.31
16	I	102	CRT	C4-C5-C6	2.73	128.75	124.91
11	L	402	BCL	C4-C3-C5	2.73	119.97	115.23
11	F	101	BCL	C1-O2A-CGA	2.73	123.26	116.65
11	G	102	BCL	C1D-ND-C4D	-2.73	104.40	106.31
11	a	101	BCL	CHC-C4B-NB	-2.73	119.95	124.05
11	L	401	BCL	C4-C3-C5	2.73	119.97	115.23
11	e	101	BCL	C1C-NC-C4C	-2.73	105.43	106.68
11	U	101	BCL	CMB-C2B-C3B	2.73	134.28	125.67
16	U	102	CRT	C24-C23-C22	-2.73	118.40	122.82
11	b	102	BCL	C1C-NC-C4C	-2.72	105.44	106.68
11	f	102	BCL	CHC-C4B-NB	-2.72	119.97	124.05
11	R	101	BCL	C1D-CHD-C4C	-2.72	120.06	126.62
11	G	101	BCL	O2A-CGA-CBA	2.72	120.13	111.83
11	b	102	BCL	CHB-C1B-C2B	-2.72	119.53	127.43
16	K	102	CRT	C13-C12-C14	-2.72	118.41	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	101	BCL	C4-C3-C5	2.72	119.95	115.23
11	i	101	BCL	CHC-C4B-NB	-2.72	119.97	124.05
16	W	102	CRT	C8-C7-C9	-2.72	118.42	122.82
11	L	402	BCL	C4A-NA-C1A	2.71	107.92	106.68
16	A	103	CRT	C24-C23-C22	-2.71	118.42	122.82
11	N	102	BCL	CHB-C4A-NA	2.71	128.31	124.40
11	j	102	BCL	C3D-C4D-ND	2.71	114.39	109.99
11	E	102	BCL	C1-C2-C3	-2.71	121.76	126.20
11	G	101	BCL	CAC-C3C-C4C	-2.71	106.58	112.58
11	B	101	BCL	C1D-CHD-C4C	-2.71	120.09	126.62
11	G	101	BCL	C1-O2A-CGA	2.70	123.20	116.65
16	K	102	CRT	C24-C23-C22	-2.70	118.44	122.82
11	E	101	BCL	CAC-C3C-C4C	-2.70	106.59	112.58
11	T	102	BCL	O2A-CGA-CBA	2.70	120.06	111.83
11	E	101	BCL	C3D-C4D-ND	2.70	114.37	109.99
11	T	102	BCL	C1D-CHD-C4C	-2.70	120.11	126.62
11	P	102	BCL	CHC-C4B-NB	-2.70	120.00	124.05
16	B	102	CRT	C6-C7-C9	2.70	123.25	119.01
11	h	101	BCL	C3D-C4D-ND	2.70	114.37	109.99
11	V	102	BCL	O2A-CGA-CBA	2.70	120.06	111.83
11	K	101	BCL	C1-O2A-CGA	2.69	123.17	116.65
11	j	103	BCL	CMB-C2B-C3B	2.69	134.16	125.67
11	P	101	BCL	CHC-C4B-NB	-2.69	120.01	124.05
11	Y	101	BCL	C1D-CHD-C4C	-2.69	120.13	126.62
11	V	102	BCL	C4A-NA-C1A	2.69	107.91	106.68
11	W	101	BCL	CMB-C2B-C3B	2.69	134.15	125.67
16	A	103	CRT	C25-C23-C22	2.69	123.24	119.01
11	f	102	BCL	CHC-C1C-NC	2.69	128.28	124.40
11	J	102	BCL	C6-C5-C3	-2.69	106.92	113.47
11	K	101	BCL	CMB-C2B-C3B	2.69	134.15	125.67
11	E	101	BCL	CAA-C2A-C3A	-2.69	105.74	113.00
11	h	102	BCL	CMB-C2B-C3B	2.69	134.14	125.67
11	h	102	BCL	C1D-ND-C4D	-2.69	104.43	106.31
16	E	103	CRT	C9-C10-C11	2.69	130.98	123.20
16	E	103	CRT	C25-C23-C22	2.68	123.23	119.01
11	O	101	BCL	C3D-C4D-ND	2.68	114.35	109.99
11	d	102	BCL	C1D-ND-C4D	-2.68	104.43	106.31
11	R	102	BCL	C1D-CHD-C4C	-2.68	120.16	126.62
11	Q	101	BCL	C1D-CHD-C4C	-2.67	120.17	126.62
11	e	101	BCL	C1D-CHD-C4C	-2.67	120.17	126.62
11	e	101	BCL	CHB-C4A-NA	2.67	128.25	124.40
11	M	402	BCL	CHB-C1B-C2B	-2.67	119.68	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	j	103	BCL	CHB-C4A-NA	2.67	128.25	124.40
9	M	407	PGV	O03-C19-C20	2.67	119.97	111.83
11	T	101	BCL	C3D-C4D-ND	2.67	114.32	109.99
11	A	102	BCL	O2D-CGD-O1D	-2.67	118.66	123.85
16	N	103	CRT	C6-C7-C9	2.67	123.20	119.01
12	M	404	BPH	C6-C5-C3	2.66	119.96	113.47
16	a	102	CRT	C24-C23-C22	-2.66	118.50	122.82
16	E	103	CRT	C24-C23-C22	-2.66	118.50	122.82
11	G	102	BCL	C6-C5-C3	-2.66	106.98	113.47
9	Z	103	PGV	O03-C19-C20	2.66	119.94	111.83
11	Y	101	BCL	CHC-C4B-NB	-2.66	120.06	124.05
11	d	102	BCL	C3D-C4D-ND	2.66	114.31	109.99
16	U	102	CRT	C25-C23-C22	2.66	123.19	119.01
11	J	101	BCL	C1-O2A-CGA	2.66	123.08	116.65
11	b	101	BCL	C3D-C4D-ND	2.65	114.30	109.99
11	j	102	BCL	CAC-C3C-C4C	-2.65	106.69	112.58
11	h	102	BCL	C4-C3-C5	2.65	119.83	115.23
16	e	102	CRT	C24-C23-C22	-2.65	118.52	122.82
11	L	402	BCL	CMB-C2B-C3B	2.65	134.03	125.67
11	U	101	BCL	O2D-CGD-O1D	-2.65	118.69	123.85
16	M	406	CRT	C8-C7-C9	-2.65	118.53	122.82
11	L	401	BCL	C3B-C4B-NB	2.65	113.25	109.76
11	K	101	BCL	C4-C3-C5	2.64	119.82	115.23
11	g	101	BCL	C1-O2A-CGA	2.64	123.05	116.65
11	P	102	BCL	C3D-C4D-ND	2.64	114.28	109.99
16	W	102	CRT	C24-C23-C22	-2.64	118.53	122.82
16	j	101	CRT	C24-C23-C22	-2.64	118.54	122.82
11	M	403	BCL	CAA-C2A-C3A	-2.64	105.86	113.00
11	d	101	BCL	CHC-C1C-NC	2.64	128.21	124.40
16	R	103	CRT	C13-C12-C14	-2.64	118.54	122.82
11	V	102	BCL	CHC-C4B-NB	-2.64	120.09	124.05
11	N	101	BCL	C3D-C4D-ND	2.63	114.27	109.99
16	B	102	CRT	C13-C12-C14	-2.63	118.55	122.82
11	G	101	BCL	C4-C3-C5	2.63	119.79	115.23
16	Y	102	CRT	C24-C23-C22	-2.63	118.56	122.82
11	b	101	BCL	C4A-NA-C1A	2.63	107.88	106.68
11	B	101	BCL	C4A-NA-C1A	2.63	107.88	106.68
16	B	102	CRT	C24-C23-C22	-2.63	118.56	122.82
11	T	102	BCL	CHB-C1B-C2B	-2.63	119.81	127.43
11	J	102	BCL	O2A-CGA-CBA	2.62	119.83	111.83
11	g	101	BCL	O2A-CGA-CBA	2.62	119.83	111.83
11	B	101	BCL	C3D-C4D-ND	2.62	114.25	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	i	101	BCL	CHB-C4A-NA	2.62	128.18	124.40
11	J	102	BCL	C1D-CHD-C4C	-2.62	120.30	126.62
11	I	101	BCL	C4A-NA-C1A	2.62	107.87	106.68
11	A	102	BCL	C1D-CHD-C4C	-2.61	120.32	126.62
16	e	102	CRT	C25-C23-C22	2.61	123.12	119.01
11	j	103	BCL	C1D-CHD-C4C	-2.61	120.33	126.62
11	N	101	BCL	CMB-C2B-C3B	2.61	133.90	125.67
11	E	102	BCL	CMB-C2B-C3B	2.61	133.90	125.67
11	c	101	BCL	C1D-CHD-C4C	-2.61	120.33	126.62
16	P	103	CRT	C21-C20-C19	2.61	128.85	123.52
16	W	102	CRT	C13-C12-C14	-2.60	118.60	122.82
16	Y	102	CRT	C6-C7-C9	2.60	123.10	119.01
11	T	102	BCL	CHB-C4A-NA	2.60	128.15	124.40
11	j	102	BCL	CHB-C4A-NA	2.60	128.15	124.40
11	I	101	BCL	C1D-CHD-C4C	-2.60	120.36	126.62
16	e	102	CRT	C13-C12-C14	-2.60	118.61	122.82
11	X	101	BCL	CHC-C1C-NC	2.60	128.15	124.40
16	I	102	CRT	C24-C23-C22	-2.59	118.62	122.82
11	Y	101	BCL	C3D-C4D-ND	2.59	114.20	109.99
11	W	101	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
11	b	101	BCL	CAC-C3C-C4C	-2.59	106.84	112.58
11	c	101	BCL	CHC-C1C-NC	2.59	128.13	124.40
11	a	101	BCL	C4-C3-C5	2.59	119.72	115.23
11	R	102	BCL	CHB-C4A-NA	2.59	128.13	124.40
11	D	101	BCL	C3D-C4D-ND	2.59	114.19	109.99
11	d	102	BCL	CHB-C1B-C2B	-2.58	119.92	127.43
11	h	102	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
16	R	103	CRT	C24-C23-C22	-2.58	118.63	122.82
11	f	102	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
16	K	102	CRT	C8-C7-C9	-2.58	118.64	122.82
16	A	103	CRT	C11-C12-C14	2.58	123.06	119.01
11	O	101	BCL	CMB-C2B-C3B	2.58	133.80	125.67
11	b	102	BCL	CHC-C4B-NB	-2.57	120.19	124.05
16	Y	102	CRT	C18-C17-C19	-2.57	118.65	122.82
12	L	403	BPH	OBB-CAB-CBB	-2.57	114.72	120.19
7	C	503	HEC	C2A-C1A-NA	-2.57	107.85	110.32
16	W	102	CRT	C6-C7-C9	2.57	123.04	119.01
11	F	101	BCL	CMB-C2B-C3B	2.56	133.76	125.67
16	a	102	CRT	C8-C7-C9	-2.56	118.66	122.82
11	N	101	BCL	C4-C3-C5	2.56	119.68	115.23
16	Y	102	CRT	C4-C5-C6	2.56	128.51	124.91
11	b	101	BCL	C4-C3-C5	2.56	119.68	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	101	BCL	O2D-CGD-O1D	-2.56	118.87	123.85
11	V	101	BCL	C4-C3-C5	2.56	119.66	115.23
16	N	103	CRT	C21-C20-C19	2.55	128.75	123.52
11	N	101	BCL	CHB-C1B-C2B	-2.55	120.01	127.43
16	K	102	CRT	C31-C32-C33	2.55	130.86	127.28
11	T	101	BCL	CHC-C4B-NB	-2.55	120.22	124.05
11	A	101	BCL	C1-O2A-CGA	2.55	122.83	116.65
16	K	102	CRT	C18-C17-C19	-2.55	118.68	122.82
11	J	102	BCL	CHB-C1B-C2B	-2.55	120.02	127.43
11	R	101	BCL	C1-C2-C3	-2.55	122.02	126.20
16	a	102	CRT	C25-C23-C22	2.55	123.02	119.01
16	Y	102	CRT	C5-C6-C7	2.55	129.74	125.89
16	j	101	CRT	C13-C12-C14	-2.55	118.69	122.82
11	G	102	BCL	C1C-NC-C4C	-2.55	105.52	106.68
11	b	101	BCL	C1D-ND-C4D	-2.55	104.53	106.31
11	G	102	BCL	CHB-C4A-NA	2.55	128.07	124.40
16	P	103	CRT	C13-C12-C14	-2.54	118.69	122.82
16	M	406	CRT	C34-C33-C32	-2.54	118.70	122.82
11	W	101	BCL	C1-O2A-CGA	2.54	122.80	116.65
11	O	101	BCL	C1D-CHD-C4C	-2.54	120.50	126.62
16	Z	102	CRT	C27-C26-C25	2.54	130.55	123.20
16	i	102	CRT	C24-C23-C22	-2.54	118.71	122.82
11	X	102	BCL	C3D-C4D-ND	2.54	114.11	109.99
9	C	508	PGV	C02-O01-C1	-2.53	111.73	117.80
16	P	103	CRT	C24-C23-C22	-2.53	118.71	122.82
16	K	102	CRT	C11-C12-C14	2.53	122.99	119.01
16	K	102	CRT	C36-C35-C33	2.53	129.71	125.89
11	Y	101	BCL	O2D-CGD-O1D	-2.53	118.93	123.85
16	Y	102	CRT	C13-C12-C14	-2.53	118.72	122.82
16	N	103	CRT	C13-C12-C14	-2.53	118.72	122.82
11	h	102	BCL	CHB-C1B-C2B	-2.53	120.09	127.43
11	J	101	BCL	C3D-C4D-ND	2.53	114.09	109.99
16	B	102	CRT	C25-C23-C22	2.53	122.98	119.01
11	i	101	BCL	C1C-NC-C4C	-2.53	105.53	106.68
11	L	402	BCL	C1D-CHD-C4C	-2.52	120.54	126.62
11	P	101	BCL	C6-C5-C3	-2.52	107.33	113.47
11	J	101	BCL	C4-C3-C5	2.52	119.60	115.23
11	M	402	BCL	CAA-CBA-CGA	-2.52	106.06	113.21
16	N	103	CRT	C24-C23-C22	-2.52	118.74	122.82
16	E	103	CRT	C4-C5-C6	2.52	128.45	124.91
11	b	102	BCL	C3D-C4D-ND	2.52	114.08	109.99
11	J	102	BCL	C1-C2-C3	-2.51	122.08	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	102	BCL	C1D-CHD-C4C	-2.51	120.56	126.62
16	i	102	CRT	C6-C7-C9	2.51	122.96	119.01
11	a	101	BCL	CMB-C2B-C3B	2.51	133.59	125.67
11	N	101	BCL	CAA-C2A-C3A	-2.51	106.22	113.00
11	h	101	BCL	O2A-CGA-CBA	2.51	119.49	111.83
11	j	103	BCL	C3D-C4D-ND	2.51	114.06	109.99
11	X	102	BCL	CMB-C2B-C3B	2.51	133.58	125.67
11	J	102	BCL	C16-C15-C13	-2.51	107.63	115.97
11	d	101	BCL	C6-C5-C3	-2.51	107.36	113.47
11	R	101	BCL	C4-C3-C5	2.50	119.58	115.23
16	i	102	CRT	C13-C12-C14	-2.50	118.76	122.82
11	B	101	BCL	CAC-C3C-C4C	-2.50	107.03	112.58
9	Z	103	PGV	C02-O01-C1	-2.50	111.80	117.80
11	g	101	BCL	C1D-CHD-C4C	-2.50	120.59	126.62
11	P	102	BCL	C6-C5-C3	-2.50	107.38	113.47
16	N	103	CRT	C18-C17-C19	-2.50	118.77	122.82
11	R	102	BCL	O2A-CGA-CBA	2.50	119.45	111.83
11	E	102	BCL	C1D-ND-C4D	-2.50	104.56	106.31
11	Q	101	BCL	C4-C3-C5	2.50	119.56	115.23
16	I	102	CRT	C18-C17-C19	-2.49	118.78	122.82
16	j	101	CRT	C18-C17-C19	-2.49	118.78	122.82
11	X	102	BCL	O2A-CGA-CBA	2.49	119.43	111.83
16	W	102	CRT	C25-C23-C22	2.49	122.93	119.01
11	S	101	BCL	C1D-CHD-C4C	-2.49	120.61	126.62
11	J	101	BCL	CAC-C3C-C4C	-2.49	107.06	112.58
11	U	101	BCL	C4-C3-C5	2.49	119.55	115.23
11	N	102	BCL	CHB-C1B-C2B	-2.49	120.20	127.43
11	a	101	BCL	C4A-NA-C1A	2.49	107.81	106.68
16	Z	102	CRT	C13-C12-C14	-2.49	118.79	122.82
11	M	402	BCL	CHD-C1D-C2D	2.49	130.66	125.49
16	E	103	CRT	C18-C17-C19	-2.48	118.80	122.82
11	T	101	BCL	CHC-C1C-NC	2.48	127.98	124.40
16	U	102	CRT	C13-C12-C14	-2.48	118.80	122.82
11	P	102	BCL	C1-C2-C3	-2.48	122.14	126.20
11	Y	101	BCL	C1D-ND-C4D	-2.48	104.57	106.31
16	P	103	CRT	C18-C17-C19	-2.48	118.80	122.82
11	A	102	BCL	O2A-CGA-CBA	2.48	119.38	111.83
16	I	102	CRT	C25-C23-C22	2.47	122.90	119.01
11	I	101	BCL	CHB-C4A-NA	2.47	127.97	124.40
11	M	403	BCL	CED-O2D-CGD	2.47	121.52	115.92
11	F	101	BCL	C4-C3-C5	2.47	119.51	115.23
11	X	101	BCL	CAA-C2A-C3A	-2.47	106.33	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	e	102	CRT	C31-C32-C33	2.47	130.74	127.28
11	K	101	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
11	V	102	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
11	g	101	BCL	C4-C3-C5	2.46	119.50	115.23
11	P	102	BCL	C1D-CHD-C4C	-2.46	120.69	126.62
11	O	101	BCL	C1-O2A-CGA	2.46	122.60	116.65
11	g	101	BCL	CMB-C2B-C3B	2.46	133.42	125.67
11	A	101	BCL	C6-C5-C3	-2.46	107.48	113.47
16	j	101	CRT	C25-C23-C22	2.46	122.87	119.01
11	d	102	BCL	CMB-C2B-C3B	2.46	133.41	125.67
12	L	403	BPH	CMB-C2B-C3B	2.46	129.59	124.68
11	K	101	BCL	C4D-CHA-C1A	-2.45	118.32	121.24
16	U	102	CRT	C36-C35-C33	2.45	129.60	125.89
11	c	101	BCL	C4A-NA-C1A	2.45	107.80	106.68
11	A	102	BCL	CED-O2D-CGD	2.45	121.48	115.92
11	S	101	BCL	CHB-C4A-NA	2.45	127.94	124.40
11	N	102	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
11	M	402	BCL	CHC-C1C-NC	2.45	127.93	124.40
16	R	103	CRT	C4-C5-C6	2.45	128.35	124.91
11	e	101	BCL	C6-C5-C3	-2.45	107.51	113.47
11	j	102	BCL	CAA-C2A-C3A	-2.44	106.40	113.00
16	R	103	CRT	C25-C23-C22	2.44	122.85	119.01
11	U	101	BCL	CHB-C1B-C2B	-2.44	120.34	127.43
11	F	101	BCL	CED-O2D-CGD	2.44	121.45	115.92
16	R	103	CRT	C18-C17-C19	-2.44	118.86	122.82
16	K	102	CRT	C6-C7-C9	2.44	122.84	119.01
12	M	404	BPH	CMD-C2D-C3D	2.44	129.55	124.68
16	Y	102	CRT	C25-C23-C22	2.44	122.84	119.01
16	a	102	CRT	C29-C28-C27	-2.44	118.87	122.82
11	f	102	BCL	C4-C3-C5	2.44	119.45	115.23
11	A	101	BCL	CMB-C2B-C3B	2.43	133.35	125.67
16	i	102	CRT	C21-C20-C19	2.43	128.50	123.52
16	U	102	CRT	C18-C17-C19	-2.43	118.88	122.82
16	M	406	CRT	C24-C23-C22	-2.43	118.88	122.82
16	A	103	CRT	C31-C32-C33	2.43	130.69	127.28
16	a	102	CRT	C4-C5-C6	2.43	128.32	124.91
16	R	103	CRT	C11-C12-C14	2.43	122.83	119.01
11	V	101	BCL	CAA-C2A-C3A	-2.42	106.45	113.00
11	G	101	BCL	CMB-C2B-C3B	2.42	133.32	125.67
11	T	102	BCL	CMB-C2B-C3B	2.42	133.31	125.67
11	Q	101	BCL	CHB-C4A-NA	2.42	127.89	124.40
11	V	102	BCL	CHB-C1B-C2B	-2.42	120.41	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	401	BCL	CHC-C4B-NB	-2.42	120.42	124.05
11	j	103	BCL	CED-O2D-CGD	2.42	121.40	115.92
16	B	102	CRT	C11-C12-C14	2.42	122.81	119.01
11	V	102	BCL	C1-C2-C3	-2.42	122.24	126.20
11	N	102	BCL	C3B-C2B-C1B	-2.42	98.69	106.40
11	E	101	BCL	C4-C3-C5	2.42	119.42	115.23
16	K	102	CRT	C21-C20-C19	2.41	128.46	123.52
11	N	102	BCL	O2A-CGA-O1A	-2.41	117.59	123.63
11	Y	101	BCL	CHC-C1C-NC	2.41	127.88	124.40
11	b	101	BCL	CED-O2D-CGD	2.41	121.39	115.92
11	P	102	BCL	CMB-C2B-C3B	2.41	133.28	125.67
9	L	410	PGV	O03-C19-O04	-2.41	117.60	123.63
11	h	102	BCL	C3D-C4D-ND	2.41	113.91	109.99
16	M	406	CRT	C13-C12-C14	-2.41	118.91	122.82
11	M	402	BCL	CMB-C2B-C3B	2.41	133.27	125.67
11	V	101	BCL	CMB-C2B-C3B	2.41	133.26	125.67
11	B	101	BCL	CHB-C1B-C2B	-2.40	120.45	127.43
11	N	102	BCL	CMB-C2B-C3B	2.40	133.25	125.67
16	a	102	CRT	C18-C17-C19	-2.40	118.92	122.82
11	L	402	BCL	C4D-CHA-C1A	-2.40	118.38	121.24
16	B	102	CRT	C18-C17-C19	-2.40	118.93	122.82
11	d	102	BCL	C1-C2-C3	-2.40	122.27	126.20
16	e	102	CRT	C18-C17-C19	-2.40	118.93	122.82
16	A	103	CRT	C18-C17-C19	-2.40	118.93	122.82
11	U	101	BCL	CHC-C1C-NC	2.40	127.86	124.40
16	i	102	CRT	C18-C17-C19	-2.40	118.93	122.82
16	B	102	CRT	C34-C33-C32	-2.39	118.94	122.82
9	M	408	PGV	C02-O01-C1	-2.39	112.07	117.80
11	A	102	BCL	CHC-C4B-NB	-2.39	120.46	124.05
11	V	101	BCL	CHB-C1B-C2B	-2.39	120.48	127.43
11	c	101	BCL	CMB-C2B-C3B	2.39	133.22	125.67
11	A	102	BCL	CHB-C1B-NB	-2.39	120.46	124.05
11	A	101	BCL	O2A-CGA-CBA	2.39	119.12	111.83
11	d	102	BCL	CMD-C2D-C3D	-2.39	122.21	127.69
16	a	102	CRT	C5-C6-C7	2.39	129.50	125.89
11	N	102	BCL	CAA-C2A-C3A	-2.39	106.55	113.00
11	L	402	BCL	O2D-CGD-O1D	-2.38	119.21	123.85
16	W	102	CRT	C18-C17-C19	-2.38	118.95	122.82
11	P	101	BCL	O2A-CGA-O1A	-2.38	117.67	123.63
11	M	403	BCL	O2A-CGA-O1A	-2.38	117.67	123.63
11	f	101	BCL	CMB-C2B-C3B	2.38	133.18	125.67
11	g	101	BCL	O2D-CGD-O1D	-2.38	119.22	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	102	CRT	C13-C12-C14	-2.38	118.96	122.82
11	S	101	BCL	C11-C12-C13	-2.38	108.06	115.97
16	U	102	CRT	C31-C32-C33	2.38	130.62	127.28
11	b	102	BCL	C1D-ND-C4D	-2.38	104.64	106.31
11	L	401	BCL	C2D-C1D-ND	2.38	112.48	110.13
11	N	101	BCL	O2A-CGA-CBA	2.38	119.08	111.83
16	i	102	CRT	C25-C23-C22	2.38	122.75	119.01
11	X	101	BCL	CAC-C3C-C4C	-2.37	107.31	112.58
11	i	101	BCL	CMB-C2B-C3B	2.37	133.16	125.67
16	M	406	CRT	C6-C7-C9	2.37	122.74	119.01
11	F	101	BCL	CBA-CAA-C2A	-2.37	106.74	113.79
16	P	103	CRT	C25-C23-C22	2.37	122.73	119.01
11	f	102	BCL	O2A-CGA-CBA	2.37	119.06	111.83
16	Y	102	CRT	C29-C28-C27	-2.37	118.98	122.82
11	W	101	BCL	CHB-C4A-NA	2.37	127.81	124.40
11	j	103	BCL	C1D-ND-C4D	-2.37	104.65	106.31
11	G	102	BCL	CHC-C4B-NB	-2.37	120.50	124.05
11	Q	101	BCL	CMB-C2B-C3B	2.36	133.12	125.67
16	I	102	CRT	C36-C35-C33	2.36	129.46	125.89
16	E	103	CRT	C31-C32-C33	2.36	130.59	127.28
16	M	406	CRT	C35-C33-C32	2.36	122.72	119.01
11	b	101	BCL	CHC-C1C-NC	2.36	127.81	124.40
11	S	101	BCL	C1-C2-C3	-2.36	122.33	126.20
16	W	102	CRT	C31-C32-C33	2.36	130.59	127.28
11	T	102	BCL	C6-C5-C3	-2.36	107.73	113.47
11	D	101	BCL	CHB-C1B-C2B	-2.35	120.61	127.43
11	b	102	BCL	CMB-C2B-C3B	2.35	133.07	125.67
11	F	101	BCL	C6-C5-C3	-2.34	107.76	113.47
11	N	101	BCL	CHC-C1C-NC	2.34	127.78	124.40
11	a	101	BCL	C1C-NC-C4C	-2.34	105.61	106.68
16	K	102	CRT	C29-C28-C27	-2.34	119.03	122.82
11	Q	101	BCL	CHC-C1C-NC	2.34	127.77	124.40
11	S	101	BCL	C1C-NC-C4C	-2.33	105.61	106.68
16	R	103	CRT	C31-C32-C33	2.33	130.55	127.28
11	a	101	BCL	CED-O2D-CGD	2.33	121.21	115.92
11	N	102	BCL	C5-C3-C2	-2.33	115.93	121.17
11	Z	101	BCL	C1-C2-C3	-2.33	122.38	126.20
11	J	102	BCL	CMB-C2B-C3B	2.33	133.02	125.67
11	X	101	BCL	CHB-C1B-C2B	-2.33	120.66	127.43
11	S	101	BCL	CMB-C2B-C3B	2.33	133.02	125.67
16	M	406	CRT	C20-C19-C17	2.33	130.54	127.28
16	N	103	CRT	C29-C28-C27	-2.33	119.04	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	101	BCL	C1-C2-C3	-2.33	122.38	126.20
11	j	102	BCL	CHC-C1C-NC	2.33	127.76	124.40
11	j	102	BCL	C1-C2-C3	-2.33	122.39	126.20
16	B	102	CRT	C29-C28-C27	-2.32	119.05	122.82
11	Z	101	BCL	CMB-C2B-C3B	2.32	133.00	125.67
16	j	101	CRT	C31-C32-C33	2.32	130.54	127.28
11	e	101	BCL	C4-C3-C5	2.32	119.26	115.23
11	j	103	BCL	C1C-NC-C4C	-2.32	105.62	106.68
16	N	103	CRT	C25-C23-C22	2.32	122.66	119.01
16	i	102	CRT	C5-C6-C7	2.32	129.40	125.89
16	I	102	CRT	C31-C32-C33	2.32	130.53	127.28
11	Y	101	BCL	C6-C5-C3	-2.32	107.82	113.47
16	I	102	CRT	C29-C28-C27	-2.32	119.06	122.82
11	V	101	BCL	C6-C5-C3	-2.32	107.83	113.47
11	X	101	BCL	C6-C5-C3	-2.32	107.83	113.47
11	G	102	BCL	CHB-C1B-C2B	-2.32	120.70	127.43
16	e	102	CRT	C11-C12-C14	2.32	122.65	119.01
11	X	102	BCL	C1D-CHD-C4C	-2.31	121.04	126.62
11	E	101	BCL	CMB-C2B-C3B	2.31	132.97	125.67
11	e	101	BCL	O2D-CGD-O1D	-2.31	119.35	123.85
16	a	102	CRT	C34-C33-C32	-2.31	119.07	122.82
11	X	101	BCL	CMB-C2B-C3B	2.31	132.96	125.67
11	S	101	BCL	CHC-C4B-NB	-2.31	120.58	124.05
11	e	101	BCL	CMB-C2B-C3B	2.31	132.96	125.67
11	K	101	BCL	CHB-C1B-C2B	-2.31	120.72	127.43
16	j	101	CRT	C21-C20-C19	2.31	128.24	123.52
11	G	102	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
11	f	102	BCL	CHB-C1B-C2B	-2.30	120.74	127.43
11	Z	101	BCL	C1-O2A-CGA	2.30	122.22	116.65
11	g	101	BCL	CHB-C4A-NA	2.30	127.72	124.40
11	f	102	BCL	CMD-C2D-C3D	-2.30	122.42	127.69
12	M	404	BPH	C11-C10-C8	2.30	123.61	115.97
16	Y	102	CRT	C31-C32-C33	2.30	130.50	127.28
11	N	102	BCL	CHB-C1B-NB	-2.30	120.60	124.05
16	Y	102	CRT	C11-C12-C14	2.30	122.62	119.01
11	G	102	BCL	C3B-C2B-C1B	-2.29	99.07	106.40
11	Z	101	BCL	CHC-C1C-NC	2.29	127.71	124.40
16	N	103	CRT	C34-C33-C32	-2.29	119.11	122.82
11	d	102	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
11	A	102	BCL	CMD-C2D-C3D	-2.29	122.44	127.69
11	K	101	BCL	CHC-C1C-NC	2.29	127.70	124.40
11	d	101	BCL	CMB-C2B-C3B	2.29	132.88	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	102	CRT	C29-C28-C27	-2.29	119.11	122.82
11	P	102	BCL	CHB-C1B-C2B	-2.29	120.79	127.43
11	B	101	BCL	C6-C5-C3	-2.28	107.91	113.47
16	Y	102	CRT	C34-C33-C32	-2.28	119.12	122.82
9	M	408	PGV	O14-P-O13	2.28	119.73	110.83
11	U	101	BCL	CAC-C3C-C4C	-2.28	107.52	112.58
16	i	102	CRT	C34-C33-C32	-2.28	119.12	122.82
16	M	406	CRT	C29-C28-C27	-2.28	119.12	122.82
11	J	102	BCL	CHC-C4B-NB	-2.28	120.63	124.05
16	I	102	CRT	C21-C20-C19	2.28	128.19	123.52
16	i	102	CRT	C29-C28-C27	-2.28	119.12	122.82
11	I	101	BCL	CMB-C2B-C3B	2.28	132.86	125.67
16	e	102	CRT	C29-C28-C27	-2.28	119.12	122.82
11	P	101	BCL	CHB-C4A-NA	2.28	127.69	124.40
11	J	102	BCL	C3B-C2B-C1B	-2.28	99.13	106.40
11	b	102	BCL	C3B-C2B-C1B	-2.28	99.13	106.40
11	L	402	BCL	C1-O2A-CGA	2.27	122.16	116.65
12	L	403	BPH	CMD-C2D-C3D	2.27	129.22	124.68
11	X	102	BCL	C1D-ND-C4D	-2.27	104.72	106.31
16	E	103	CRT	C29-C28-C27	-2.27	119.14	122.82
16	W	102	CRT	C11-C12-C14	2.27	122.57	119.01
16	P	103	CRT	C34-C33-C32	-2.27	119.15	122.82
11	Z	101	BCL	CAA-C2A-C3A	-2.26	106.88	113.00
11	Y	101	BCL	CMB-C2B-C3B	2.26	132.81	125.67
7	C	501	HEC	C2A-C1A-NA	-2.26	108.14	110.32
16	R	103	CRT	C34-C33-C32	-2.26	119.15	122.82
11	S	101	BCL	C2A-C3A-C4A	-2.26	98.21	101.87
11	T	102	BCL	CMD-C2D-C3D	-2.26	122.50	127.69
16	K	102	CRT	C4-C5-C6	2.26	128.09	124.91
11	N	102	BCL	OBB-CAB-C3B	-2.26	116.44	120.43
11	f	102	BCL	C6-C5-C3	-2.26	107.96	113.47
16	Y	102	CRT	C36-C35-C33	2.26	129.31	125.89
11	G	102	BCL	CMD-C2D-C3D	-2.26	122.51	127.69
11	J	101	BCL	CAA-C2A-C3A	-2.26	106.90	113.00
16	A	103	CRT	C29-C28-C27	-2.26	119.16	122.82
16	j	101	CRT	C11-C12-C14	2.25	122.56	119.01
11	W	101	BCL	CHB-C1B-C2B	-2.25	120.89	127.43
11	E	101	BCL	CHB-C1B-C2B	-2.25	120.89	127.43
15	M	405	MQ8	C11-C3-C2	-2.25	121.03	124.89
11	G	101	BCL	C7-C6-C5	-2.25	107.26	113.26
16	W	102	CRT	C29-C28-C27	-2.25	119.17	122.82
11	j	103	BCL	C3B-C2B-C1B	-2.25	99.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	401	BCL	CHD-C1D-C2D	2.25	130.16	125.49
16	W	102	CRT	C21-C20-C19	2.25	128.12	123.52
11	T	101	BCL	C1-O2A-CGA	2.25	122.09	116.65
11	Q	101	BCL	C1C-NC-C4C	-2.25	105.65	106.68
11	M	403	BCL	C4-C3-C5	2.25	119.13	115.23
11	E	101	BCL	CHB-C4A-NA	2.25	127.64	124.40
11	d	102	BCL	C3B-C2B-C1B	-2.24	99.23	106.40
16	P	103	CRT	C29-C28-C27	-2.24	119.18	122.82
11	b	101	BCL	C11-C10-C8	-2.24	108.51	115.97
16	Y	102	CRT	C16-C17-C19	2.24	122.54	119.01
11	W	101	BCL	C4D-CHA-C1A	-2.24	118.57	121.24
11	a	101	BCL	CHB-C1B-C2B	-2.24	120.92	127.43
7	C	502	HEC	C2A-C1A-NA	-2.24	108.16	110.32
11	M	403	BCL	C6-C5-C3	-2.24	108.01	113.47
11	M	402	BCL	CHB-C4A-NA	2.24	127.63	124.40
16	j	101	CRT	C34-C33-C32	-2.24	119.19	122.82
16	P	103	CRT	C11-C12-C14	2.23	122.52	119.01
11	B	101	BCL	C4-C3-C5	2.23	119.10	115.23
11	F	101	BCL	C4D-CHA-C1A	-2.23	118.58	121.24
11	E	102	BCL	C1D-CHD-C4C	-2.23	121.24	126.62
11	Q	101	BCL	CHB-C1B-C2B	-2.23	120.96	127.43
16	Z	102	CRT	C11-C12-C14	2.23	122.51	119.01
16	N	103	CRT	C11-C12-C14	2.23	122.51	119.01
11	f	102	BCL	CMB-C2B-C3B	2.22	132.69	125.67
16	U	102	CRT	C34-C33-C32	-2.22	119.21	122.82
11	Q	101	BCL	C6-C5-C3	-2.22	108.05	113.47
11	F	101	BCL	O2D-CGD-O1D	-2.22	119.52	123.85
16	M	406	CRT	C18-C17-C19	-2.22	119.22	122.82
11	j	102	BCL	CMB-C2B-C3B	2.22	132.68	125.67
11	S	101	BCL	C6-C5-C3	-2.22	108.06	113.47
11	Q	101	BCL	C16-C17-C18	-2.22	106.04	115.94
11	f	101	BCL	CHB-C1B-C2B	-2.22	120.99	127.43
11	F	101	BCL	CHC-C1C-NC	2.22	127.60	124.40
11	M	402	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
11	b	101	BCL	CMB-C2B-C3B	2.22	132.66	125.67
11	S	101	BCL	C4D-CHA-C1A	-2.22	118.60	121.24
11	G	102	BCL	CMB-C2B-C1B	2.21	128.79	125.42
11	A	101	BCL	CHB-C1B-C2B	-2.21	121.00	127.43
16	I	102	CRT	C34-C33-C32	-2.21	119.23	122.82
11	U	101	BCL	CHB-C4A-NA	2.21	127.59	124.40
16	W	102	CRT	C34-C33-C32	-2.21	119.23	122.82
11	P	102	BCL	CHB-C4A-NA	2.21	127.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	103	CRT	C31-C32-C33	2.21	130.38	127.28
11	F	101	BCL	CHB-C1B-C2B	-2.21	121.02	127.43
11	X	102	BCL	C11-C10-C8	-2.21	108.63	115.97
11	X	102	BCL	CMD-C2D-C3D	-2.21	122.63	127.69
11	L	402	BCL	CMC-C2C-C3C	-2.20	105.46	113.98
9	H	301	PGV	O03-C19-O04	-2.20	118.11	123.63
11	O	101	BCL	CHB-C1B-C2B	-2.20	121.03	127.43
11	f	101	BCL	O2A-CGA-CBA	2.20	118.55	111.83
11	R	102	BCL	CMB-C2B-C3B	2.20	132.61	125.67
16	E	103	CRT	C34-C33-C32	-2.20	119.25	122.82
7	C	503	HEC	CHB-C4A-NA	2.20	126.85	124.45
16	j	101	CRT	C29-C28-C27	-2.20	119.25	122.82
11	R	101	BCL	CED-O2D-CGD	2.20	120.90	115.92
11	d	102	BCL	O2A-CGA-CBA	2.20	118.53	111.83
11	F	101	BCL	C1C-NC-C4C	-2.20	105.68	106.68
11	J	102	BCL	CMD-C2D-C3D	-2.20	122.65	127.69
11	P	102	BCL	CHB-C1B-NB	-2.20	120.76	124.05
11	h	101	BCL	CMB-C2B-C3B	2.20	132.59	125.67
11	R	102	BCL	CMD-C2D-C3D	-2.19	122.66	127.69
11	R	101	BCL	CMB-C2B-C3B	2.19	132.59	125.67
11	Y	101	BCL	O2A-CGA-O1A	-2.19	118.14	123.63
11	D	101	BCL	CHC-C1C-NC	2.19	127.56	124.40
11	Y	101	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
11	O	101	BCL	C4-C3-C5	2.19	119.03	115.23
16	K	102	CRT	C16-C17-C19	2.19	122.45	119.01
11	L	402	BCL	CHB-C1B-C2B	-2.19	121.07	127.43
11	b	101	BCL	C6-C5-C3	-2.19	108.14	113.47
16	U	102	CRT	C11-C12-C14	2.18	122.44	119.01
11	A	102	BCL	CAC-C3C-C4C	-2.18	107.74	112.58
11	j	103	BCL	C6-C5-C3	-2.18	108.16	113.47
11	P	102	BCL	C3B-C2B-C1B	-2.18	99.44	106.40
16	Z	102	CRT	C32-C31-C30	2.18	129.51	123.20
11	T	102	BCL	C11-C10-C8	-2.18	108.73	115.97
16	e	102	CRT	C34-C33-C32	-2.18	119.29	122.82
11	a	101	BCL	CHB-C4A-NA	2.18	127.54	124.40
7	C	503	HEC	CAA-CBA-CGA	-2.17	107.90	113.67
11	d	101	BCL	CAA-CBA-CGA	-2.17	107.05	113.21
16	i	102	CRT	C11-C12-C14	2.17	122.42	119.01
11	G	101	BCL	CHB-C1B-C2B	-2.17	121.13	127.43
12	L	403	BPH	O2D-CGD-CBD	2.17	113.33	110.95
11	V	101	BCL	CAC-C3C-C4C	-2.17	107.78	112.58
11	R	102	BCL	CHB-C1B-C2B	-2.17	121.14	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	103	CRT	C34-C33-C32	-2.16	119.31	122.82
11	b	102	BCL	CAA-CBA-CGA	-2.16	107.07	113.21
16	M	406	CRT	C25-C23-C22	2.16	122.41	119.01
16	a	102	CRT	C21-C20-C19	2.16	127.94	123.52
16	E	103	CRT	C21-C20-C19	2.16	127.94	123.52
11	X	101	BCL	CED-O2D-CGD	2.16	120.81	115.92
16	R	103	CRT	C29-C28-C27	-2.16	119.32	122.82
11	E	102	BCL	C3B-C2B-C1B	-2.16	99.51	106.40
11	R	101	BCL	CHB-C1B-C2B	-2.16	121.17	127.43
11	Z	101	BCL	CHB-C1B-C2B	-2.16	121.17	127.43
16	P	103	CRT	C31-C32-C33	2.15	130.29	127.28
11	K	101	BCL	CHB-C4A-NA	2.15	127.50	124.40
11	R	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
11	D	101	BCL	C4-C3-C5	2.15	118.96	115.23
16	A	103	CRT	C36-C35-C33	2.15	129.14	125.89
9	M	407	PGV	C02-O01-C1	-2.14	112.67	117.80
11	V	102	BCL	CMB-C2B-C3B	2.14	132.42	125.67
11	X	101	BCL	C4-C3-C5	2.14	118.94	115.23
11	S	101	BCL	CED-O2D-CGD	2.14	120.76	115.92
16	i	102	CRT	C31-C32-C33	2.13	130.27	127.28
11	g	101	BCL	CHB-C1B-C2B	-2.13	121.23	127.43
11	A	102	BCL	CMB-C2B-C3B	2.13	132.39	125.67
16	a	102	CRT	C30-C28-C27	2.13	122.36	119.01
11	T	101	BCL	C6-C5-C3	-2.13	108.28	113.47
11	N	101	BCL	CHB-C4A-NA	2.13	127.47	124.40
11	i	101	BCL	CHC-C1C-NC	2.13	127.47	124.40
11	P	102	BCL	CMD-C2D-C3D	-2.13	122.81	127.69
11	g	101	BCL	CBA-CAA-C2A	-2.13	107.46	113.79
16	K	102	CRT	C34-C33-C32	-2.13	119.37	122.82
11	B	101	BCL	CHB-C4A-NA	2.13	127.47	124.40
11	Y	101	BCL	C11-C12-C13	-2.12	108.90	115.97
11	O	101	BCL	C4A-NA-C1A	2.12	107.65	106.68
11	i	101	BCL	C4A-NA-C1A	2.12	107.65	106.68
11	X	102	BCL	C3B-C2B-C1B	-2.12	99.62	106.40
11	D	101	BCL	CAA-C2A-C3A	-2.12	107.26	113.00
16	M	406	CRT	C30-C28-C27	2.12	122.35	119.01
16	R	103	CRT	C21-C20-C19	2.12	127.86	123.52
11	c	101	BCL	CHB-C4A-NA	2.12	127.46	124.40
9	Z	103	PGV	O01-C1-O02	-2.12	118.75	123.70
11	J	101	BCL	CHC-C1C-NC	2.12	127.45	124.40
11	I	101	BCL	CHB-C1B-C2B	-2.12	121.28	127.43
9	M	408	PGV	O03-C19-O04	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	101	BCL	CHB-C4A-NA	2.12	127.45	124.40
16	e	102	CRT	C21-C20-C19	2.12	127.85	123.52
11	d	102	BCL	CHC-C4B-NB	-2.11	120.88	124.05
9	M	407	PGV	O14-P-O13	2.11	119.07	110.83
11	E	102	BCL	CMD-C2D-C3D	-2.11	122.84	127.69
11	B	101	BCL	C16-C17-C18	-2.11	106.51	115.94
11	e	101	BCL	CHB-C1B-C2B	-2.11	121.30	127.43
11	V	102	BCL	C6-C5-C3	-2.11	108.33	113.47
11	Y	101	BCL	CAA-C2A-C3A	-2.11	107.30	113.00
11	D	101	BCL	CMC-C2C-C3C	-2.11	105.84	113.98
11	d	102	BCL	CED-O2D-CGD	2.11	120.69	115.92
11	R	102	BCL	C1-O2A-CGA	2.10	121.74	116.65
11	f	102	BCL	C1-O2A-CGA	2.10	121.74	116.65
11	Y	101	BCL	C4A-NA-C1A	2.10	107.64	106.68
11	A	101	BCL	OBD-CAD-C3D	-2.10	123.51	128.42
16	a	102	CRT	C6-C7-C9	2.10	122.31	119.01
16	j	101	CRT	C16-C17-C19	2.10	122.31	119.01
11	M	403	BCL	CHB-C1B-NB	-2.10	120.91	124.05
11	A	102	BCL	CHC-C4B-C3B	-2.09	123.41	131.72
11	d	101	BCL	CHB-C1B-C2B	-2.09	121.36	127.43
7	C	504	HEC	CAD-C3D-C4D	2.09	129.01	124.94
11	E	101	BCL	CHC-C1C-NC	2.09	127.41	124.40
11	T	102	BCL	C3B-C2B-C1B	-2.08	99.74	106.40
11	X	101	BCL	CAA-CBA-CGA	-2.08	107.29	113.21
16	I	102	CRT	C16-C17-C19	2.08	122.28	119.01
11	V	101	BCL	C1-O2A-CGA	2.08	121.69	116.65
11	h	101	BCL	CAC-C3C-C4C	-2.08	107.97	112.58
11	V	102	BCL	CED-O2D-CGD	2.08	120.63	115.92
11	R	101	BCL	C1-O2A-CGA	2.08	121.68	116.65
11	E	101	BCL	OBD-CAD-C3D	-2.08	123.56	128.42
11	G	102	BCL	CHB-C1B-NB	-2.08	120.93	124.05
11	N	101	BCL	C3A-C2A-C1A	2.08	104.45	101.34
11	D	101	BCL	C1-C2-C3	-2.08	122.80	126.20
11	U	101	BCL	CBA-CAA-C2A	-2.08	107.62	113.79
11	V	102	BCL	C11-C10-C8	-2.07	109.07	115.97
11	b	101	BCL	CHB-C1B-C2B	-2.07	121.42	127.43
11	A	101	BCL	CAC-C3C-C4C	-2.07	107.99	112.58
11	L	401	BCL	C3B-C2B-C1B	-2.07	99.79	106.40
11	f	101	BCL	CHB-C4A-NA	2.07	127.38	124.40
11	P	101	BCL	CBA-CAA-C2A	-2.07	107.64	113.79
11	Q	101	BCL	C11-C12-C13	-2.06	109.10	115.97
11	h	102	BCL	C3B-C2B-C1B	-2.06	99.81	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	101	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
16	B	102	CRT	C31-C32-C33	2.06	130.17	127.28
16	N	103	CRT	C16-C17-C19	2.06	122.25	119.01
16	R	103	CRT	C16-C17-C19	2.06	122.25	119.01
11	j	102	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
11	c	101	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
16	E	103	CRT	C16-C17-C19	2.06	122.25	119.01
11	T	101	BCL	CHB-C1B-C2B	-2.06	121.45	127.43
16	Z	102	CRT	C4-C5-C6	-2.06	122.03	124.91
11	K	101	BCL	CAC-C3C-C4C	-2.06	108.02	112.58
11	N	102	BCL	CED-O2D-CGD	2.06	120.58	115.92
16	E	103	CRT	C36-C35-C33	2.05	128.99	125.89
11	A	102	BCL	C3B-C2B-C1B	-2.05	99.85	106.40
11	G	102	BCL	CMB-C2B-C3B	2.05	132.14	125.67
11	I	101	BCL	CAA-C2A-C3A	-2.05	107.46	113.00
11	M	403	BCL	CHB-C4A-NA	2.05	127.36	124.40
11	T	101	BCL	C4-C3-C5	2.05	118.78	115.23
11	d	101	BCL	C2A-C3A-C4A	-2.04	98.57	101.87
11	L	402	BCL	CMD-C2D-C3D	-2.04	123.00	127.69
11	V	102	BCL	C3B-C2B-C1B	-2.04	99.88	106.40
11	O	101	BCL	C3B-C2B-C1B	-2.04	99.88	106.40
11	R	102	BCL	C6-C5-C3	-2.04	108.50	113.47
16	P	103	CRT	C16-C17-C19	2.04	122.21	119.01
11	J	101	BCL	C6-C5-C3	-2.04	108.51	113.47
11	Y	101	BCL	CHB-C1B-C2B	-2.03	121.52	127.43
11	h	101	BCL	CAA-C2A-C3A	-2.03	107.50	113.00
11	d	101	BCL	CAC-C3C-C4C	-2.03	108.07	112.58
11	J	102	BCL	CED-O2D-CGD	2.03	120.53	115.92
11	M	403	BCL	CMC-C2C-C3C	-2.03	106.12	113.98
16	i	102	CRT	C4-C5-C6	2.03	127.76	124.91
11	L	401	BCL	CMD-C2D-C3D	-2.03	123.04	127.69
11	Y	101	BCL	C3B-C2B-C1B	-2.02	99.93	106.40
11	a	101	BCL	CHC-C1C-NC	2.02	127.32	124.40
16	Y	102	CRT	C30-C28-C27	2.02	122.19	119.01
11	g	101	BCL	C4D-CHA-C1A	-2.02	118.83	121.24
11	Y	101	BCL	CHB-C4A-NA	2.02	127.32	124.40
11	Z	101	BCL	C2A-C3A-C4A	-2.02	98.61	101.87
11	G	101	BCL	CHC-C1C-NC	2.02	127.31	124.40
11	A	102	BCL	CHD-C1D-C2D	2.02	129.68	125.49
11	O	101	BCL	CBA-CAA-C2A	-2.02	107.80	113.79
11	X	102	BCL	CHD-C1D-C2D	2.01	129.68	125.49
11	a	101	BCL	C6-C5-C3	-2.01	108.56	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	101	BCL	C4-C3-C5	2.01	118.72	115.23
11	G	102	BCL	C1-O2A-CGA	2.01	121.52	116.65
9	C	508	PGV	O01-C1-O02	-2.01	119.00	123.70
11	h	101	BCL	C6-C5-C3	-2.01	108.57	113.47
11	f	101	BCL	CAC-C3C-C4C	-2.01	108.12	112.58
11	J	101	BCL	CED-O2D-CGD	2.01	120.47	115.92
7	C	501	HEC	CAD-CBD-CGD	-2.01	108.34	113.67
11	K	101	BCL	C3B-C2B-C1B	-2.01	99.99	106.40
11	D	101	BCL	C11-C12-C13	-2.01	109.29	115.97
11	f	101	BCL	C6-C5-C3	-2.01	108.58	113.47
11	X	101	BCL	C1-O2A-CGA	2.01	121.51	116.65
11	A	101	BCL	C11-C10-C8	-2.01	109.30	115.97
11	i	101	BCL	CHB-C1B-C2B	-2.01	121.60	127.43
11	j	103	BCL	OBb-CAB-C3B	-2.01	116.89	120.43
11	I	101	BCL	CED-O2D-CGD	2.00	120.46	115.92
11	W	101	BCL	CBA-CAA-C2A	-2.00	107.83	113.79
11	h	101	BCL	CHB-C1B-C2B	-2.00	121.61	127.43
11	b	102	BCL	CMD-C2D-C3D	-2.00	123.10	127.69
11	A	102	BCL	C11-C10-C8	-2.00	109.31	115.97
11	L	402	BCL	C1C-NC-C4C	-2.00	105.77	106.68

There are no chirality outliers.

All (1095) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	HEC	C2B-C3B-CAB-CBB
7	C	501	HEC	C4B-C3B-CAB-CBB
7	C	501	HEC	C2C-C3C-CAC-CBC
7	C	501	HEC	C4C-C3C-CAC-CBC
7	C	502	HEC	C2B-C3B-CAB-CBB
7	C	502	HEC	C4B-C3B-CAB-CBB
7	C	502	HEC	C2C-C3C-CAC-CBC
7	C	502	HEC	C4C-C3C-CAC-CBC
7	C	503	HEC	C2B-C3B-CAB-CBB
7	C	503	HEC	C4B-C3B-CAB-CBB
7	C	503	HEC	C2C-C3C-CAC-CBC
7	C	503	HEC	C4C-C3C-CAC-CBC
7	C	504	HEC	C2B-C3B-CAB-CBB
7	C	504	HEC	C4B-C3B-CAB-CBB
7	C	504	HEC	C2C-C3C-CAC-CBC
9	C	508	PGV	C03-O11-P-O12
9	L	410	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
9	L	410	PGV	O01-C02-C03-O11
9	M	407	PGV	C03-O11-P-O12
9	M	407	PGV	C03-O11-P-O14
9	H	301	PGV	C03-O11-P-O12
9	H	301	PGV	C03-O11-P-O14
9	H	301	PGV	C04-O12-P-O11
9	H	301	PGV	C04-O12-P-O13
9	H	301	PGV	C04-O12-P-O14
9	R	104	PGV	C03-O11-P-O12
9	Z	103	PGV	C04-O12-P-O11
9	Z	103	PGV	C04-O12-P-O13
9	Z	103	PGV	C04-O12-P-O14
9	Z	103	PGV	C2-C1-O01-C02
11	L	401	BCL	C4C-C3C-CAC-CBC
11	M	402	BCL	C1A-C2A-CAA-CBA
11	M	402	BCL	C3A-C2A-CAA-CBA
11	M	403	BCL	CAD-CBD-CGD-O1D
11	M	403	BCL	CAD-CBD-CGD-O2D
11	A	101	BCL	C2C-C3C-CAC-CBC
11	A	101	BCL	C4C-C3C-CAC-CBC
11	A	102	BCL	C1A-C2A-CAA-CBA
11	A	102	BCL	C3A-C2A-CAA-CBA
11	A	102	BCL	CBA-CGA-O2A-C1
11	A	102	BCL	O1A-CGA-O2A-C1
11	A	102	BCL	C2C-C3C-CAC-CBC
11	A	102	BCL	C4C-C3C-CAC-CBC
11	D	101	BCL	C1A-C2A-CAA-CBA
11	D	101	BCL	C3A-C2A-CAA-CBA
11	E	101	BCL	C1A-C2A-CAA-CBA
11	E	101	BCL	C3A-C2A-CAA-CBA
11	E	101	BCL	C4C-C3C-CAC-CBC
11	E	102	BCL	C1A-C2A-CAA-CBA
11	E	102	BCL	C3A-C2A-CAA-CBA
11	E	102	BCL	CBA-CGA-O2A-C1
11	E	102	BCL	O1A-CGA-O2A-C1
11	F	101	BCL	C1A-C2A-CAA-CBA
11	F	101	BCL	C3A-C2A-CAA-CBA
11	F	101	BCL	C2C-C3C-CAC-CBC
11	F	101	BCL	C4C-C3C-CAC-CBC
11	G	101	BCL	C1A-C2A-CAA-CBA
11	G	101	BCL	C2C-C3C-CAC-CBC
11	G	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	G	101	BCL	C14-C13-C15-C16
11	G	102	BCL	C3A-C2A-CAA-CBA
11	G	102	BCL	C2C-C3C-CAC-CBC
11	J	101	BCL	C1A-C2A-CAA-CBA
11	J	101	BCL	C2C-C3C-CAC-CBC
11	J	101	BCL	C4C-C3C-CAC-CBC
11	J	101	BCL	C14-C13-C15-C16
11	J	102	BCL	C3A-C2A-CAA-CBA
11	K	101	BCL	C1A-C2A-CAA-CBA
11	K	101	BCL	C3A-C2A-CAA-CBA
11	N	101	BCL	C3A-C2A-CAA-CBA
11	N	101	BCL	C2C-C3C-CAC-CBC
11	N	101	BCL	C4C-C3C-CAC-CBC
11	N	102	BCL	CBD-CGD-O2D-CED
11	O	101	BCL	C2C-C3C-CAC-CBC
11	O	101	BCL	C4C-C3C-CAC-CBC
11	P	101	BCL	C1A-C2A-CAA-CBA
11	P	101	BCL	C2C-C3C-CAC-CBC
11	P	101	BCL	C4C-C3C-CAC-CBC
11	P	102	BCL	C3A-C2A-CAA-CBA
11	P	102	BCL	CBA-CGA-O2A-C1
11	P	102	BCL	O1A-CGA-O2A-C1
11	Q	101	BCL	C1A-C2A-CAA-CBA
11	Q	101	BCL	C3A-C2A-CAA-CBA
11	Q	101	BCL	C2C-C3C-CAC-CBC
11	Q	101	BCL	C4C-C3C-CAC-CBC
11	R	101	BCL	C3A-C2A-CAA-CBA
11	R	101	BCL	C2C-C3C-CAC-CBC
11	R	101	BCL	C4C-C3C-CAC-CBC
11	R	102	BCL	C3A-C2A-CAA-CBA
11	R	102	BCL	C4C-C3C-CAC-CBC
11	S	101	BCL	C1A-C2A-CAA-CBA
11	T	101	BCL	C2C-C3C-CAC-CBC
11	T	101	BCL	C4C-C3C-CAC-CBC
11	T	102	BCL	C3A-C2A-CAA-CBA
11	T	102	BCL	CBA-CGA-O2A-C1
11	T	102	BCL	O1A-CGA-O2A-C1
11	T	102	BCL	CBD-CGD-O2D-CED
11	U	101	BCL	C1A-C2A-CAA-CBA
11	U	101	BCL	C3A-C2A-CAA-CBA
11	U	101	BCL	C6-C7-C8-C10
11	V	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	V	101	BCL	C4C-C3C-CAC-CBC
11	V	102	BCL	C3A-C2A-CAA-CBA
11	V	102	BCL	CBA-CGA-O2A-C1
11	V	102	BCL	O1A-CGA-O2A-C1
11	V	102	BCL	CBD-CGD-O2D-CED
11	W	101	BCL	C2C-C3C-CAC-CBC
11	W	101	BCL	C4C-C3C-CAC-CBC
11	X	101	BCL	C1A-C2A-CAA-CBA
11	X	101	BCL	C3A-C2A-CAA-CBA
11	X	101	BCL	C2C-C3C-CAC-CBC
11	X	101	BCL	C4C-C3C-CAC-CBC
11	X	101	BCL	C11-C12-C13-C15
11	X	102	BCL	C1A-C2A-CAA-CBA
11	X	102	BCL	C3A-C2A-CAA-CBA
11	X	102	BCL	CBA-CGA-O2A-C1
11	X	102	BCL	O1A-CGA-O2A-C1
11	Y	101	BCL	C1A-C2A-CAA-CBA
11	Y	101	BCL	C2C-C3C-CAC-CBC
11	Y	101	BCL	C4C-C3C-CAC-CBC
11	Z	101	BCL	C1A-C2A-CAA-CBA
11	Z	101	BCL	C2C-C3C-CAC-CBC
11	Z	101	BCL	C4C-C3C-CAC-CBC
11	a	101	BCL	C1A-C2A-CAA-CBA
11	a	101	BCL	C3A-C2A-CAA-CBA
11	a	101	BCL	C2C-C3C-CAC-CBC
11	a	101	BCL	C4C-C3C-CAC-CBC
11	b	101	BCL	C1A-C2A-CAA-CBA
11	b	102	BCL	C1A-C2A-CAA-CBA
11	b	102	BCL	C3A-C2A-CAA-CBA
11	b	102	BCL	CBA-CGA-O2A-C1
11	b	102	BCL	O1A-CGA-O2A-C1
11	c	101	BCL	C1A-C2A-CAA-CBA
11	c	101	BCL	C3A-C2A-CAA-CBA
11	c	101	BCL	C2C-C3C-CAC-CBC
11	c	101	BCL	C4C-C3C-CAC-CBC
11	d	101	BCL	C1A-C2A-CAA-CBA
11	d	101	BCL	C2C-C3C-CAC-CBC
11	d	101	BCL	C4C-C3C-CAC-CBC
11	d	102	BCL	C1A-C2A-CAA-CBA
11	d	102	BCL	C3A-C2A-CAA-CBA
11	d	102	BCL	CBA-CGA-O2A-C1
11	d	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	e	101	BCL	C1A-C2A-CAA-CBA
11	e	101	BCL	C2C-C3C-CAC-CBC
11	e	101	BCL	C4C-C3C-CAC-CBC
11	f	101	BCL	C1A-C2A-CAA-CBA
11	f	101	BCL	C3A-C2A-CAA-CBA
11	f	101	BCL	C2C-C3C-CAC-CBC
11	f	101	BCL	C4C-C3C-CAC-CBC
11	f	102	BCL	C3A-C2A-CAA-CBA
11	g	101	BCL	C1A-C2A-CAA-CBA
11	g	101	BCL	C3A-C2A-CAA-CBA
11	g	101	BCL	C2C-C3C-CAC-CBC
11	g	101	BCL	C4C-C3C-CAC-CBC
11	h	101	BCL	C1A-C2A-CAA-CBA
11	h	101	BCL	C2C-C3C-CAC-CBC
11	h	101	BCL	C4C-C3C-CAC-CBC
11	h	101	BCL	C4-C3-C5-C6
11	h	102	BCL	C1A-C2A-CAA-CBA
11	h	102	BCL	C3A-C2A-CAA-CBA
11	h	102	BCL	CBA-CGA-O2A-C1
11	h	102	BCL	O1A-CGA-O2A-C1
11	h	102	BCL	CBD-CGD-O2D-CED
11	j	102	BCL	C2C-C3C-CAC-CBC
11	j	102	BCL	C4C-C3C-CAC-CBC
11	j	103	BCL	C3A-C2A-CAA-CBA
11	j	103	BCL	CBA-CGA-O2A-C1
11	j	103	BCL	O1A-CGA-O2A-C1
11	j	103	BCL	CBD-CGD-O2D-CED
16	B	102	CRT	C1-C4-C5-C6
16	B	102	CRT	C4-C5-C6-C7
16	B	102	CRT	C5-C6-C7-C8
16	B	102	CRT	C5-C6-C7-C9
16	A	103	CRT	C1-C4-C5-C6
16	A	103	CRT	C4-C5-C6-C7
16	A	103	CRT	C5-C6-C7-C8
16	A	103	CRT	C5-C6-C7-C9
16	E	103	CRT	C4-C5-C6-C7
16	I	102	CRT	C4-C5-C6-C7
16	N	103	CRT	C1-C4-C5-C6
16	N	103	CRT	C4-C5-C6-C7
16	N	103	CRT	C5-C6-C7-C8
16	N	103	CRT	C5-C6-C7-C9
16	P	103	CRT	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
16	P	103	CRT	C4-C5-C6-C7
16	P	103	CRT	C5-C6-C7-C8
16	P	103	CRT	C5-C6-C7-C9
16	R	103	CRT	C1-C4-C5-C6
16	R	103	CRT	C4-C5-C6-C7
16	U	102	CRT	C1-C4-C5-C6
16	U	102	CRT	C4-C5-C6-C7
16	U	102	CRT	C5-C6-C7-C8
16	U	102	CRT	C5-C6-C7-C9
16	W	102	CRT	O1-C1-C4-C5
16	W	102	CRT	C1-C4-C5-C6
16	W	102	CRT	C4-C5-C6-C7
16	Z	102	CRT	C1-C4-C5-C6
16	Z	102	CRT	C35-C36-C37-C38
16	a	102	CRT	C35-C36-C37-C38
16	e	102	CRT	C1-C4-C5-C6
16	e	102	CRT	C4-C5-C6-C7
16	e	102	CRT	C5-C6-C7-C8
16	e	102	CRT	C5-C6-C7-C9
16	i	102	CRT	C1-C4-C5-C6
16	i	102	CRT	C4-C5-C6-C7
16	i	102	CRT	C5-C6-C7-C9
16	j	101	CRT	C1-C4-C5-C6
16	j	101	CRT	C4-C5-C6-C7
16	j	101	CRT	C5-C6-C7-C8
16	j	101	CRT	C5-C6-C7-C9
11	E	102	BCL	O1D-CGD-O2D-CED
11	E	102	BCL	CBD-CGD-O2D-CED
11	G	102	BCL	CBD-CGD-O2D-CED
11	P	102	BCL	CBD-CGD-O2D-CED
11	X	102	BCL	CBD-CGD-O2D-CED
11	b	102	BCL	CBD-CGD-O2D-CED
11	d	102	BCL	CBD-CGD-O2D-CED
11	i	101	BCL	CBD-CGD-O2D-CED
11	P	102	BCL	O1D-CGD-O2D-CED
11	b	102	BCL	O1D-CGD-O2D-CED
11	J	102	BCL	CBD-CGD-O2D-CED
11	U	101	BCL	CBD-CGD-O2D-CED
11	j	103	BCL	O1D-CGD-O2D-CED
11	T	102	BCL	O1D-CGD-O2D-CED
11	V	102	BCL	O1D-CGD-O2D-CED
11	h	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	Z	103	PGV	O02-C1-O01-C02
11	G	101	BCL	C3-C5-C6-C7
11	N	102	BCL	C3-C5-C6-C7
11	R	101	BCL	C3-C5-C6-C7
11	X	101	BCL	C3-C5-C6-C7
11	Z	101	BCL	C3-C5-C6-C7
11	d	102	BCL	C3-C5-C6-C7
11	f	101	BCL	C3-C5-C6-C7
11	D	101	BCL	CBD-CGD-O2D-CED
11	R	102	BCL	CBD-CGD-O2D-CED
11	V	101	BCL	CBD-CGD-O2D-CED
11	d	101	BCL	CBD-CGD-O2D-CED
11	f	101	BCL	CBD-CGD-O2D-CED
11	f	102	BCL	CBD-CGD-O2D-CED
11	N	102	BCL	O1D-CGD-O2D-CED
11	A	101	BCL	C4-C3-C5-C6
11	J	101	BCL	C4-C3-C5-C6
11	V	101	BCL	C4-C3-C5-C6
11	f	101	BCL	C4-C3-C5-C6
11	j	102	BCL	C4-C3-C5-C6
15	M	405	MQ8	C19-C18-C20-C21
11	J	101	BCL	C2-C3-C5-C6
11	f	101	BCL	C2-C3-C5-C6
11	h	101	BCL	C2-C3-C5-C6
11	j	102	BCL	C2-C3-C5-C6
11	X	102	BCL	O1D-CGD-O2D-CED
11	L	401	BCL	C13-C15-C16-C17
11	N	102	BCL	C2A-CAA-CBA-CGA
11	A	101	BCL	C3-C5-C6-C7
11	E	102	BCL	C3-C5-C6-C7
11	X	102	BCL	C3-C5-C6-C7
11	b	102	BCL	C3-C5-C6-C7
11	f	102	BCL	C3-C5-C6-C7
11	M	402	BCL	CBA-CGA-O2A-C1
16	Z	102	CRT	C11-C10-C9-C7
11	P	101	BCL	C3-C5-C6-C7
11	T	102	BCL	C3-C5-C6-C7
11	i	101	BCL	O1D-CGD-O2D-CED
9	H	301	PGV	C20-C19-O03-C01
11	G	102	BCL	CBA-CGA-O2A-C1
11	G	102	BCL	O1D-CGD-O2D-CED
11	d	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	J	101	BCL	C3-C5-C6-C7
11	E	101	BCL	C4-C3-C5-C6
11	G	101	BCL	C4-C3-C5-C6
11	N	101	BCL	C4-C3-C5-C6
11	P	101	BCL	C4-C3-C5-C6
11	X	101	BCL	C4-C3-C5-C6
11	b	101	BCL	C4-C3-C5-C6
11	A	101	BCL	C2-C3-C5-C6
11	E	101	BCL	C2-C3-C5-C6
11	G	101	BCL	C2-C3-C5-C6
11	N	101	BCL	C2-C3-C5-C6
11	P	101	BCL	C2-C3-C5-C6
11	X	101	BCL	C2-C3-C5-C6
11	b	101	BCL	C2-C3-C5-C6
15	M	405	MQ8	C17-C18-C20-C21
15	M	405	MQ8	C13-C15-C16-C17
11	Y	101	BCL	CBD-CGD-O2D-CED
11	G	102	BCL	C2A-CAA-CBA-CGA
11	J	102	BCL	C2A-CAA-CBA-CGA
11	R	102	BCL	C2A-CAA-CBA-CGA
11	J	102	BCL	O1D-CGD-O2D-CED
11	U	101	BCL	O1D-CGD-O2D-CED
9	H	301	PGV	O04-C19-O03-C01
11	M	402	BCL	O1A-CGA-O2A-C1
11	Q	101	BCL	CBA-CGA-O2A-C1
11	A	102	BCL	CBD-CGD-O2D-CED
11	W	101	BCL	CBD-CGD-O2D-CED
11	G	102	BCL	O1A-CGA-O2A-C1
11	J	102	BCL	CBA-CGA-O2A-C1
11	Y	101	BCL	CBA-CGA-O2A-C1
11	X	101	BCL	CBD-CGD-O2D-CED
11	R	101	BCL	C4-C3-C5-C6
11	T	101	BCL	C4-C3-C5-C6
11	Z	101	BCL	C4-C3-C5-C6
15	M	405	MQ8	C45-C43-C44-C46
11	R	101	BCL	C2-C3-C5-C6
11	T	101	BCL	C2-C3-C5-C6
11	V	101	BCL	C2-C3-C5-C6
11	Z	101	BCL	C2-C3-C5-C6
15	M	405	MQ8	C42-C43-C44-C46
11	L	402	BCL	C14-C13-C15-C16
11	M	402	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
11	A	101	BCL	C14-C13-C15-C16
11	O	101	BCL	C11-C12-C13-C14
11	P	101	BCL	C14-C13-C15-C16
11	R	101	BCL	C14-C13-C15-C16
11	T	101	BCL	C11-C12-C13-C14
11	V	101	BCL	C11-C12-C13-C14
11	X	101	BCL	C14-C13-C15-C16
11	X	102	BCL	C14-C13-C15-C16
11	c	101	BCL	C11-C12-C13-C14
11	d	101	BCL	C14-C13-C15-C16
11	j	102	BCL	C14-C13-C15-C16
12	M	404	BPH	C11-C10-C8-C9
11	J	102	BCL	O1A-CGA-O2A-C1
16	W	102	CRT	C5-C6-C7-C8
16	Y	102	CRT	C5-C6-C7-C8
16	Z	102	CRT	C10-C11-C12-C13
16	Z	102	CRT	C34-C33-C35-C36
16	a	102	CRT	C5-C6-C7-C8
16	i	102	CRT	C5-C6-C7-C8
16	W	102	CRT	C5-C6-C7-C9
16	Y	102	CRT	C5-C6-C7-C9
16	Z	102	CRT	C32-C33-C35-C36
11	T	102	BCL	C2A-CAA-CBA-CGA
11	f	101	BCL	O1D-CGD-O2D-CED
11	Y	101	BCL	O1A-CGA-O2A-C1
11	I	101	BCL	CBA-CGA-O2A-C1
11	a	101	BCL	CBA-CGA-O2A-C1
11	Z	101	BCL	C13-C15-C16-C17
11	a	101	BCL	C5-C6-C7-C8
11	G	102	BCL	C2-C1-O2A-CGA
11	d	101	BCL	O1D-CGD-O2D-CED
11	L	401	BCL	C15-C16-C17-C18
11	Y	101	BCL	C5-C6-C7-C8
11	b	102	BCL	C13-C15-C16-C17
11	e	101	BCL	C10-C11-C12-C13
11	A	101	BCL	C11-C12-C13-C15
11	I	101	BCL	C6-C7-C8-C10
11	I	101	BCL	C11-C12-C13-C15
11	J	101	BCL	C11-C12-C13-C15
11	J	102	BCL	C6-C7-C8-C10
11	N	102	BCL	C6-C7-C8-C10
11	P	101	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	P	102	BCL	C6-C7-C8-C10
11	R	101	BCL	C11-C12-C13-C15
11	S	101	BCL	C6-C7-C8-C10
11	T	102	BCL	C6-C7-C8-C10
11	X	102	BCL	C6-C7-C8-C10
11	X	102	BCL	C11-C12-C13-C15
11	b	102	BCL	C6-C7-C8-C10
11	d	102	BCL	C6-C7-C8-C10
11	f	102	BCL	C6-C7-C8-C10
11	R	102	BCL	CBA-CGA-O2A-C1
11	V	101	BCL	O1D-CGD-O2D-CED
11	R	102	BCL	O1D-CGD-O2D-CED
11	f	102	BCL	O1D-CGD-O2D-CED
11	F	101	BCL	C8-C10-C11-C12
11	b	102	BCL	C5-C6-C7-C8
11	Q	101	BCL	O1A-CGA-O2A-C1
11	a	101	BCL	O1A-CGA-O2A-C1
11	I	101	BCL	C5-C6-C7-C8
11	N	101	BCL	C13-C15-C16-C17
11	R	101	BCL	C13-C15-C16-C17
11	c	101	BCL	C10-C11-C12-C13
11	f	102	BCL	C8-C10-C11-C12
11	E	102	BCL	C2A-CAA-CBA-CGA
11	T	101	BCL	C2A-CAA-CBA-CGA
11	V	101	BCL	C2A-CAA-CBA-CGA
11	X	101	BCL	C2A-CAA-CBA-CGA
11	X	102	BCL	C2A-CAA-CBA-CGA
11	Z	101	BCL	C2A-CAA-CBA-CGA
11	b	102	BCL	C2A-CAA-CBA-CGA
11	h	101	BCL	C2A-CAA-CBA-CGA
11	h	102	BCL	C2A-CAA-CBA-CGA
11	j	102	BCL	C2A-CAA-CBA-CGA
11	j	103	BCL	C2A-CAA-CBA-CGA
11	E	101	BCL	C10-C11-C12-C13
11	T	102	BCL	C8-C10-C11-C12
11	Y	101	BCL	C8-C10-C11-C12
11	a	101	BCL	C13-C15-C16-C17
11	b	101	BCL	C10-C11-C12-C13
11	d	101	BCL	C13-C15-C16-C17
9	L	410	PGV	C1-C2-C3-C4
11	I	101	BCL	O1A-CGA-O2A-C1
11	h	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	h	102	BCL	C3-C5-C6-C7
11	j	102	BCL	C3-C5-C6-C7
11	M	402	BCL	C5-C6-C7-C8
11	A	102	BCL	C8-C10-C11-C12
11	E	101	BCL	C5-C6-C7-C8
11	F	101	BCL	C10-C11-C12-C13
11	F	101	BCL	C15-C16-C17-C18
11	J	101	BCL	C10-C11-C12-C13
11	N	101	BCL	C8-C10-C11-C12
11	O	101	BCL	C15-C16-C17-C18
11	P	101	BCL	C10-C11-C12-C13
11	Q	101	BCL	C5-C6-C7-C8
11	Q	101	BCL	C8-C10-C11-C12
11	R	102	BCL	C8-C10-C11-C12
11	R	102	BCL	C15-C16-C17-C18
11	T	101	BCL	C5-C6-C7-C8
11	V	101	BCL	C5-C6-C7-C8
11	V	101	BCL	C8-C10-C11-C12
11	V	101	BCL	C13-C15-C16-C17
11	d	102	BCL	C13-C15-C16-C17
11	i	101	BCL	CBA-CGA-O2A-C1
11	A	101	BCL	C10-C11-C12-C13
11	O	101	BCL	C10-C11-C12-C13
11	P	101	BCL	C5-C6-C7-C8
11	d	102	BCL	C15-C16-C17-C18
11	D	101	BCL	O1D-CGD-O2D-CED
11	T	101	BCL	C15-C16-C17-C18
11	Z	101	BCL	C5-C6-C7-C8
11	c	101	BCL	C15-C16-C17-C18
11	d	102	BCL	C5-C6-C7-C8
11	i	101	BCL	C5-C6-C7-C8
11	N	101	BCL	C5-C6-C7-C8
11	N	102	BCL	CBA-CGA-O2A-C1
11	P	101	BCL	CBA-CGA-O2A-C1
11	j	103	BCL	C8-C10-C11-C12
11	M	402	BCL	C10-C11-C12-C13
11	I	101	BCL	C13-C15-C16-C17
11	a	101	BCL	C8-C10-C11-C12
11	A	101	BCL	C2A-CAA-CBA-CGA
11	E	101	BCL	C2A-CAA-CBA-CGA
11	J	101	BCL	C2A-CAA-CBA-CGA
11	R	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	b	101	BCL	C2A-CAA-CBA-CGA
11	d	101	BCL	C2A-CAA-CBA-CGA
11	d	102	BCL	C2A-CAA-CBA-CGA
11	B	101	BCL	CBA-CGA-O2A-C1
11	G	102	BCL	C15-C16-C17-C18
11	P	102	BCL	C15-C16-C17-C18
11	T	101	BCL	C8-C10-C11-C12
11	V	102	BCL	C13-C15-C16-C17
11	X	102	BCL	C13-C15-C16-C17
11	f	102	BCL	C15-C16-C17-C18
11	h	101	BCL	C13-C15-C16-C17
11	j	103	BCL	C15-C16-C17-C18
11	L	402	BCL	C15-C16-C17-C18
11	D	101	BCL	C15-C16-C17-C18
11	T	101	BCL	C13-C15-C16-C17
11	d	102	BCL	C8-C10-C11-C12
11	A	101	BCL	C5-C6-C7-C8
11	S	101	BCL	C8-C10-C11-C12
11	V	101	BCL	C10-C11-C12-C13
11	i	101	BCL	C13-C15-C16-C17
11	c	101	BCL	CBA-CGA-O2A-C1
11	Y	101	BCL	C13-C15-C16-C17
11	h	102	BCL	C13-C15-C16-C17
11	Z	101	BCL	C14-C13-C15-C16
11	B	101	BCL	O1A-CGA-O2A-C1
11	K	101	BCL	CBA-CGA-O2A-C1
11	f	102	BCL	CBA-CGA-O2A-C1
11	T	101	BCL	C16-C17-C18-C19
11	T	102	BCL	C16-C17-C18-C19
11	a	101	BCL	C16-C17-C18-C20
11	T	102	BCL	C15-C16-C17-C18
11	R	102	BCL	O1A-CGA-O2A-C1
16	Z	102	CRT	C8-C7-C9-C10
11	K	101	BCL	C13-C15-C16-C17
11	h	101	BCL	C15-C16-C17-C18
16	K	102	CRT	C5-C6-C7-C8
16	R	103	CRT	C5-C6-C7-C8
16	a	102	CRT	C34-C33-C35-C36
16	K	102	CRT	C5-C6-C7-C9
16	R	103	CRT	C5-C6-C7-C9
16	Z	102	CRT	C10-C11-C12-C14
16	a	102	CRT	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
11	P	101	BCL	O1A-CGA-O2A-C1
11	i	101	BCL	O1A-CGA-O2A-C1
11	A	102	BCL	C2A-CAA-CBA-CGA
11	G	101	BCL	C2A-CAA-CBA-CGA
11	N	101	BCL	C2A-CAA-CBA-CGA
11	P	102	BCL	C2A-CAA-CBA-CGA
11	V	102	BCL	C2A-CAA-CBA-CGA
11	M	402	BCL	C13-C15-C16-C17
11	B	101	BCL	C16-C17-C18-C19
11	P	102	BCL	C16-C17-C18-C19
11	R	101	BCL	C16-C17-C18-C20
11	V	102	BCL	C16-C17-C18-C19
11	X	101	BCL	C16-C17-C18-C19
11	X	102	BCL	C16-C17-C18-C20
11	b	102	BCL	C16-C17-C18-C19
11	i	101	BCL	C16-C17-C18-C20
11	g	101	BCL	C8-C10-C11-C12
9	R	104	PGV	C2-C1-O01-C02
11	i	101	BCL	C8-C10-C11-C12
11	W	101	BCL	O1D-CGD-O2D-CED
11	O	101	BCL	CBA-CGA-O2A-C1
11	b	101	BCL	C15-C16-C17-C18
11	A	101	BCL	C2-C1-O2A-CGA
11	D	101	BCL	C16-C17-C18-C20
11	I	101	BCL	C16-C17-C18-C20
11	V	102	BCL	C16-C17-C18-C20
11	X	101	BCL	C16-C17-C18-C20
11	X	102	BCL	C16-C17-C18-C19
11	d	102	BCL	C16-C17-C18-C19
11	f	102	BCL	C16-C17-C18-C20
13	L	408	LMT	C1-C2-C3-C4
11	c	101	BCL	O1A-CGA-O2A-C1
11	h	102	BCL	C15-C16-C17-C18
9	R	104	PGV	C7-C8-C9-C10
9	M	407	PGV	C21-C22-C23-C24
9	R	104	PGV	C2-C3-C4-C5
13	L	408	LMT	O5B-C5B-C6B-O6B
9	H	301	PGV	C14-C15-C16-C17
9	R	104	PGV	C13-C14-C15-C16
9	R	104	PGV	O02-C1-O01-C02
9	R	104	PGV	C22-C23-C24-C25
11	D	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	P	101	BCL	C16-C17-C18-C19
11	P	102	BCL	C16-C17-C18-C20
11	R	101	BCL	C16-C17-C18-C19
11	T	101	BCL	C16-C17-C18-C20
11	Y	101	BCL	C16-C17-C18-C19
11	Y	101	BCL	C16-C17-C18-C20
11	Z	101	BCL	C16-C17-C18-C19
11	Z	101	BCL	C16-C17-C18-C20
11	a	101	BCL	C16-C17-C18-C19
11	b	102	BCL	C16-C17-C18-C20
11	f	102	BCL	C16-C17-C18-C19
11	i	101	BCL	C16-C17-C18-C19
11	Y	101	BCL	O1D-CGD-O2D-CED
11	K	101	BCL	O1A-CGA-O2A-C1
11	N	102	BCL	O1A-CGA-O2A-C1
11	J	102	BCL	C15-C16-C17-C18
11	b	101	BCL	CBD-CGD-O2D-CED
11	E	102	BCL	C6-C7-C8-C10
11	N	101	BCL	C11-C10-C8-C7
11	W	101	BCL	C6-C7-C8-C10
11	W	101	BCL	C12-C13-C15-C16
11	g	101	BCL	C6-C7-C8-C10
11	h	102	BCL	C6-C7-C8-C10
11	i	101	BCL	C6-C7-C8-C10
11	E	101	BCL	C15-C16-C17-C18
11	T	102	BCL	C13-C15-C16-C17
11	P	102	BCL	C3-C5-C6-C7
11	B	101	BCL	C3A-C2A-CAA-CBA
11	A	101	BCL	C3A-C2A-CAA-CBA
11	G	101	BCL	C3A-C2A-CAA-CBA
11	I	101	BCL	C3A-C2A-CAA-CBA
11	J	101	BCL	C3A-C2A-CAA-CBA
11	O	101	BCL	C3A-C2A-CAA-CBA
11	P	101	BCL	C3A-C2A-CAA-CBA
11	S	101	BCL	C3A-C2A-CAA-CBA
11	T	101	BCL	C3A-C2A-CAA-CBA
11	V	101	BCL	C3A-C2A-CAA-CBA
11	W	101	BCL	C3A-C2A-CAA-CBA
11	Y	101	BCL	C3A-C2A-CAA-CBA
11	Z	101	BCL	C3A-C2A-CAA-CBA
11	b	101	BCL	C3A-C2A-CAA-CBA
11	d	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	e	101	BCL	C3A-C2A-CAA-CBA
11	h	101	BCL	C3A-C2A-CAA-CBA
11	i	101	BCL	C3A-C2A-CAA-CBA
11	j	102	BCL	C3A-C2A-CAA-CBA
11	D	101	BCL	C10-C11-C12-C13
12	M	404	BPH	C8-C10-C11-C12
11	A	101	BCL	C16-C17-C18-C20
11	I	101	BCL	C16-C17-C18-C19
11	A	102	BCL	O1D-CGD-O2D-CED
11	Z	101	BCL	CBD-CGD-O2D-CED
10	j	104	8K6	C6-C7-C8-C9
11	E	102	BCL	C8-C10-C11-C12
11	b	102	BCL	C8-C10-C11-C12
10	L	407	8K6	C11-C10-C9-C8
11	O	101	BCL	O1A-CGA-O2A-C1
11	f	102	BCL	O1A-CGA-O2A-C1
9	C	508	PGV	C4-C5-C6-C7
11	d	102	BCL	C16-C17-C18-C20
11	h	102	BCL	C16-C17-C18-C19
11	j	102	BCL	C16-C17-C18-C19
11	J	102	BCL	C8-C10-C11-C12
9	H	302	PGV	C14-C15-C16-C17
9	L	410	PGV	C22-C23-C24-C25
11	W	101	BCL	C8-C10-C11-C12
11	D	101	BCL	CBA-CGA-O2A-C1
11	S	101	BCL	CBA-CGA-O2A-C1
11	K	101	BCL	C11-C12-C13-C14
11	V	101	BCL	C15-C16-C17-C18
11	f	102	BCL	C5-C6-C7-C8
9	H	302	PGV	C2-C1-O01-C02
10	P	104	8K6	C13-C14-C15-C16
9	M	407	PGV	C12-C13-C14-C15
11	E	101	BCL	C8-C10-C11-C12
9	H	301	PGV	C6-C7-C8-C9
10	d	103	8K6	C7-C8-C9-C10
11	b	101	BCL	C3-C5-C6-C7
11	d	101	BCL	C3-C5-C6-C7
11	B	101	BCL	C16-C17-C18-C20
11	A	101	BCL	C16-C17-C18-C19
11	G	102	BCL	C16-C17-C18-C19
11	T	102	BCL	C16-C17-C18-C20
11	h	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
11	j	102	BCL	C16-C17-C18-C20
12	L	403	BPH	C4-C3-C5-C6
11	S	101	BCL	O1A-CGA-O2A-C1
11	D	101	BCL	C8-C10-C11-C12
11	F	101	BCL	C5-C6-C7-C8
11	b	101	BCL	C5-C6-C7-C8
11	D	101	BCL	O1A-CGA-O2A-C1
11	T	101	BCL	C10-C11-C12-C13
11	f	102	BCL	C13-C15-C16-C17
11	X	101	BCL	O1D-CGD-O2D-CED
11	M	403	BCL	C3-C5-C6-C7
9	M	408	PGV	O03-C01-C02-O01
9	H	301	PGV	C12-C13-C14-C15
11	J	101	BCL	C13-C15-C16-C17
11	e	101	BCL	C8-C10-C11-C12
10	C	509	8K6	C11-C10-C9-C8
11	V	102	BCL	C10-C11-C12-C13
11	f	102	BCL	C4-C3-C5-C6
12	L	403	BPH	C2-C3-C5-C6
11	f	101	BCL	C2A-CAA-CBA-CGA
11	W	101	BCL	CBA-CGA-O2A-C1
11	E	102	BCL	C5-C6-C7-C8
11	V	101	BCL	C3-C5-C6-C7
11	L	401	BCL	C1A-C2A-CAA-CBA
11	B	101	BCL	C1A-C2A-CAA-CBA
11	A	101	BCL	C1A-C2A-CAA-CBA
11	G	102	BCL	C1A-C2A-CAA-CBA
11	I	101	BCL	C1A-C2A-CAA-CBA
11	J	102	BCL	C1A-C2A-CAA-CBA
11	N	101	BCL	C1A-C2A-CAA-CBA
11	O	101	BCL	C1A-C2A-CAA-CBA
11	P	102	BCL	C1A-C2A-CAA-CBA
11	R	101	BCL	C1A-C2A-CAA-CBA
11	R	102	BCL	C1A-C2A-CAA-CBA
11	T	101	BCL	C1A-C2A-CAA-CBA
11	T	102	BCL	C1A-C2A-CAA-CBA
11	V	102	BCL	C1A-C2A-CAA-CBA
11	W	101	BCL	C1A-C2A-CAA-CBA
11	f	102	BCL	C1A-C2A-CAA-CBA
11	i	101	BCL	C1A-C2A-CAA-CBA
11	j	102	BCL	C1A-C2A-CAA-CBA
11	j	103	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	H	302	PGV	O02-C1-O01-C02
11	M	403	BCL	C6-C7-C8-C10
11	B	101	BCL	C12-C13-C15-C16
11	D	101	BCL	C11-C10-C8-C7
11	E	101	BCL	C6-C7-C8-C10
11	K	101	BCL	C6-C7-C8-C10
11	N	101	BCL	C6-C7-C8-C10
11	N	102	BCL	C11-C12-C13-C15
11	Q	101	BCL	C12-C13-C15-C16
11	S	101	BCL	C12-C13-C15-C16
11	Y	101	BCL	C12-C13-C15-C16
11	Z	101	BCL	C6-C7-C8-C10
11	e	101	BCL	C6-C7-C8-C10
11	f	101	BCL	C11-C10-C8-C7
11	h	102	BCL	C11-C12-C13-C15
11	i	101	BCL	C12-C13-C15-C16
11	G	101	BCL	C16-C17-C18-C19
11	G	102	BCL	C16-C17-C18-C20
11	e	101	BCL	C16-C17-C18-C19
11	B	101	BCL	C2C-C3C-CAC-CBC
11	D	101	BCL	C2C-C3C-CAC-CBC
11	E	101	BCL	C2C-C3C-CAC-CBC
11	I	101	BCL	C2C-C3C-CAC-CBC
11	U	101	BCL	C2C-C3C-CAC-CBC
11	V	101	BCL	C2C-C3C-CAC-CBC
11	b	101	BCL	C2C-C3C-CAC-CBC
11	i	101	BCL	C2C-C3C-CAC-CBC
16	W	102	CRT	C3-C1-C4-C5
11	f	101	BCL	C13-C15-C16-C17
11	X	102	BCL	C4-C3-C5-C6
11	W	101	BCL	O1A-CGA-O2A-C1
11	c	101	BCL	C3-C5-C6-C7
11	M	403	BCL	C6-C7-C8-C9
11	E	101	BCL	C6-C7-C8-C9
11	J	101	BCL	C11-C10-C8-C9
11	N	101	BCL	C6-C7-C8-C9
11	N	101	BCL	C11-C10-C8-C9
11	N	102	BCL	C6-C7-C8-C9
11	P	101	BCL	C11-C12-C13-C14
11	V	102	BCL	C11-C12-C13-C14
11	Y	101	BCL	C14-C13-C15-C16
11	Z	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	a	101	BCL	C14-C13-C15-C16
11	f	101	BCL	C11-C10-C8-C9
11	i	101	BCL	C14-C13-C15-C16
11	K	101	BCL	C16-C17-C18-C19
11	E	101	BCL	C13-C15-C16-C17
11	S	101	BCL	C5-C6-C7-C8
9	M	407	PGV	O03-C01-C02-C03
11	A	102	BCL	C13-C15-C16-C17
11	P	101	BCL	C16-C17-C18-C20
9	H	301	PGV	C1-C2-C3-C4
9	M	407	PGV	C2-C1-O01-C02
11	T	102	BCL	C2-C3-C5-C6
11	X	102	BCL	C2-C3-C5-C6
11	f	102	BCL	C2-C3-C5-C6
11	P	102	BCL	C8-C10-C11-C12
9	H	301	PGV	C29-C30-C31-C32
11	f	102	BCL	C2A-CAA-CBA-CGA
11	b	102	BCL	C15-C16-C17-C18
11	G	102	BCL	C13-C15-C16-C17
11	G	101	BCL	C16-C17-C18-C20
16	I	102	CRT	C6-C7-C9-C10
16	Z	102	CRT	C6-C7-C9-C10
9	H	301	PGV	O01-C02-C03-O11
11	U	101	BCL	CBA-CGA-O2A-C1
11	R	102	BCL	C2-C3-C5-C6
9	H	302	PGV	C2-C3-C4-C5
9	M	407	PGV	O03-C01-C02-O01
11	Q	101	BCL	C13-C15-C16-C17
11	h	102	BCL	C8-C10-C11-C12
11	Q	101	BCL	C16-C17-C18-C19
11	G	102	BCL	C10-C11-C12-C13
9	H	302	PGV	C13-C14-C15-C16
11	F	101	BCL	CBA-CGA-O2A-C1
11	F	101	BCL	C4-C3-C5-C6
11	R	102	BCL	C4-C3-C5-C6
11	T	102	BCL	C4-C3-C5-C6
11	d	102	BCL	C4-C3-C5-C6
10	j	105	8K6	C9-C10-C11-C12
11	B	101	BCL	C14-C13-C15-C16
11	E	101	BCL	C14-C13-C15-C16
11	I	101	BCL	C14-C13-C15-C16
11	J	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	P	101	BCL	C6-C7-C8-C9
11	R	101	BCL	C11-C12-C13-C14
11	X	102	BCL	C6-C7-C8-C9
11	d	102	BCL	C6-C7-C8-C9
11	d	102	BCL	C11-C12-C13-C14
11	e	101	BCL	C14-C13-C15-C16
11	f	102	BCL	C6-C7-C8-C9
11	J	102	BCL	C13-C15-C16-C17
10	H	303	8K6	C13-C14-C15-C16
11	L	401	BCL	C11-C10-C8-C7
11	G	101	BCL	C12-C13-C15-C16
11	J	101	BCL	C12-C13-C15-C16
11	P	101	BCL	C6-C7-C8-C10
11	T	101	BCL	C6-C7-C8-C10
11	V	101	BCL	C6-C7-C8-C10
11	V	102	BCL	C11-C12-C13-C15
11	a	101	BCL	C12-C13-C15-C16
11	b	102	BCL	C12-C13-C15-C16
11	d	101	BCL	C12-C13-C15-C16
11	d	102	BCL	C11-C12-C13-C15
11	e	101	BCL	C12-C13-C15-C16
11	b	102	BCL	C10-C11-C12-C13
11	b	101	BCL	O1D-CGD-O2D-CED
9	L	410	PGV	C3-C4-C5-C6
11	E	102	BCL	C4-C3-C5-C6
11	N	102	BCL	C4-C3-C5-C6
11	P	102	BCL	C4-C3-C5-C6
11	G	102	BCL	C8-C10-C11-C12
11	h	102	BCL	C2-C3-C5-C6
11	U	101	BCL	O1A-CGA-O2A-C1
11	b	101	BCL	C13-C15-C16-C17
11	e	101	BCL	C16-C17-C18-C20
11	L	402	BCL	C5-C6-C7-C8
16	E	103	CRT	C5-C6-C7-C8
11	E	102	BCL	C15-C16-C17-C18
11	V	102	BCL	C15-C16-C17-C18
9	M	408	PGV	O03-C01-C02-C03
9	Z	103	PGV	C4-C5-C6-C7
11	A	102	BCL	C4-C3-C5-C6
11	b	102	BCL	C4-C3-C5-C6
11	h	102	BCL	C4-C3-C5-C6
11	E	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	N	102	BCL	C2-C3-C5-C6
11	P	102	BCL	C2-C3-C5-C6
11	d	102	BCL	C2-C3-C5-C6
11	K	101	BCL	C16-C17-C18-C20
10	X	103	8K6	C11-C10-C9-C8
9	C	508	PGV	C12-C13-C14-C15
11	J	102	BCL	C5-C6-C7-C8
11	N	101	BCL	C15-C16-C17-C18
11	B	101	BCL	C5-C6-C7-C8
7	C	502	HEC	C3D-CAD-CBD-CGD
10	j	105	8K6	C5-C6-C7-C8
11	j	103	BCL	C16-C17-C18-C19
11	F	101	BCL	C3-C5-C6-C7
11	A	102	BCL	C2-C3-C5-C6
11	F	101	BCL	C2-C3-C5-C6
11	b	102	BCL	C2-C3-C5-C6
11	A	101	BCL	C6-C7-C8-C9
11	I	101	BCL	C6-C7-C8-C9
11	J	102	BCL	C6-C7-C8-C9
11	T	101	BCL	C6-C7-C8-C9
11	U	101	BCL	C11-C10-C8-C9
11	b	101	BCL	C6-C7-C8-C9
11	e	101	BCL	C6-C7-C8-C9
11	h	102	BCL	C11-C12-C13-C14
11	J	101	BCL	C16-C17-C18-C20
11	Z	101	BCL	O1D-CGD-O2D-CED
9	L	410	PGV	C20-C19-O03-C01
15	M	405	MQ8	C18-C20-C21-C22
11	B	101	BCL	C4C-C3C-CAC-CBC
11	D	101	BCL	C4C-C3C-CAC-CBC
11	X	102	BCL	C4C-C3C-CAC-CBC
11	b	101	BCL	C4C-C3C-CAC-CBC
16	I	102	CRT	C8-C7-C9-C10
11	N	102	BCL	C13-C15-C16-C17
9	H	301	PGV	C01-C02-C03-O11
7	C	504	HEC	C4D-C3D-CAD-CBD
16	I	102	CRT	C5-C6-C7-C8
11	L	402	BCL	C11-C12-C13-C15
11	L	402	BCL	C12-C13-C15-C16
11	A	101	BCL	C6-C7-C8-C10
11	E	101	BCL	C12-C13-C15-C16
11	G	102	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	I	101	BCL	C12-C13-C15-C16
11	J	101	BCL	C11-C10-C8-C7
11	U	101	BCL	C11-C10-C8-C7
11	V	101	BCL	C11-C12-C13-C15
11	X	101	BCL	C12-C13-C15-C16
11	b	101	BCL	C6-C7-C8-C10
11	b	102	BCL	C11-C12-C13-C15
11	f	101	BCL	C12-C13-C15-C16
11	h	102	BCL	C12-C13-C15-C16
16	E	103	CRT	C5-C6-C7-C9
16	I	102	CRT	C5-C6-C7-C9
16	a	102	CRT	C32-C33-C35-C36
11	J	102	BCL	C4-C3-C5-C6
11	F	101	BCL	O1A-CGA-O2A-C1
9	R	104	PGV	C01-C02-O01-C1
9	L	410	PGV	O04-C19-O03-C01
11	T	101	BCL	C3-C5-C6-C7
9	M	408	PGV	C20-C19-O03-C01
11	g	101	BCL	C13-C15-C16-C17
9	M	407	PGV	O02-C1-O01-C02
9	H	302	PGV	O01-C02-C03-O11
11	Q	101	BCL	C16-C17-C18-C20
11	X	101	BCL	C10-C11-C12-C13
11	c	101	BCL	C8-C10-C11-C12
11	L	402	BCL	C11-C12-C13-C14
11	U	101	BCL	C6-C7-C8-C9
11	b	102	BCL	C11-C12-C13-C14
11	f	101	BCL	C14-C13-C15-C16
11	h	102	BCL	C14-C13-C15-C16
13	L	408	LMT	O5B-C1B-O1B-C4'
16	B	102	CRT	O1-C1-C4-C5
16	N	103	CRT	O1-C1-C4-C5
16	U	102	CRT	O1-C1-C4-C5
16	e	102	CRT	O1-C1-C4-C5
16	j	101	CRT	O1-C1-C4-C5
11	F	101	BCL	C13-C15-C16-C17
11	N	102	BCL	C5-C6-C7-C8
11	g	101	BCL	O1A-CGA-O2A-C1
11	f	101	BCL	C2-C1-O2A-CGA
11	J	101	BCL	C16-C17-C18-C19
11	W	101	BCL	C16-C17-C18-C19
11	h	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	j	103	BCL	C4-C3-C5-C6
12	M	404	BPH	C4-C3-C5-C6
11	g	101	BCL	CBA-CGA-O2A-C1
9	M	407	PGV	C2-C3-C4-C5
15	M	405	MQ8	C24-C23-C25-C26
11	J	102	BCL	C2-C3-C5-C6
11	E	101	BCL	C3-C5-C6-C7
9	H	302	PGV	C01-C02-C03-O11
11	M	402	BCL	C11-C10-C8-C7
11	M	402	BCL	C11-C12-C13-C15
11	M	403	BCL	C11-C10-C8-C7
11	A	101	BCL	C12-C13-C15-C16
11	K	101	BCL	C11-C10-C8-C7
11	P	101	BCL	C12-C13-C15-C16
11	R	101	BCL	C11-C10-C8-C7
11	V	102	BCL	C12-C13-C15-C16
11	Y	101	BCL	C6-C7-C8-C10
11	Z	101	BCL	C11-C10-C8-C7
11	j	102	BCL	C12-C13-C15-C16
11	j	103	BCL	C16-C17-C18-C20
11	e	101	BCL	O1A-CGA-O2A-C1
11	K	101	BCL	C2C-C3C-CAC-CBC
16	U	102	CRT	C3-C1-C4-C5
16	W	102	CRT	C2-C1-C4-C5
11	e	101	BCL	CBA-CGA-O2A-C1
7	C	504	HEC	C4C-C3C-CAC-CBC
11	S	101	BCL	C16-C17-C18-C19
10	C	509	8K6	C9-C10-C11-C12
11	L	401	BCL	C11-C10-C8-C9
11	G	102	BCL	C14-C13-C15-C16
11	P	102	BCL	C6-C7-C8-C9
11	R	101	BCL	C11-C10-C8-C9
11	S	101	BCL	C14-C13-C15-C16
11	b	102	BCL	C14-C13-C15-C16
11	L	402	BCL	C16-C17-C18-C19
11	W	101	BCL	C13-C15-C16-C17
9	R	104	PGV	C3-C4-C5-C6
9	M	408	PGV	O04-C19-O03-C01
11	e	101	BCL	C4-C3-C5-C6
13	L	408	LMT	C2B-C1B-O1B-C4'
11	L	402	BCL	C2A-CAA-CBA-CGA
9	C	508	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
9	C	508	PGV	C04-O12-P-O13
9	H	301	PGV	C03-O11-P-O13
9	R	104	PGV	C03-O11-P-O13
9	R	104	PGV	C04-O12-P-O13
16	Y	102	CRT	C4-C5-C6-C7
11	M	403	BCL	C4-C3-C5-C6
11	h	102	BCL	C10-C11-C12-C13
9	H	301	PGV	C30-C31-C32-C33
10	L	406	8K6	C10-C11-C12-C13
11	j	103	BCL	C2-C3-C5-C6
11	A	101	BCL	C11-C12-C13-C14
11	K	101	BCL	C11-C10-C8-C9
11	N	101	BCL	C14-C13-C15-C16
11	Q	101	BCL	C14-C13-C15-C16
11	T	102	BCL	C6-C7-C8-C9
11	V	101	BCL	C6-C7-C8-C9
11	W	101	BCL	C14-C13-C15-C16
11	R	102	BCL	C6-C7-C8-C10
11	b	101	BCL	C12-C13-C15-C16
11	b	101	BCL	C16-C17-C18-C20
10	H	303	8K6	C5-C6-C7-C8
11	f	101	BCL	C16-C17-C18-C19
11	h	101	BCL	C16-C17-C18-C20
9	M	408	PGV	C28-C29-C30-C31
9	H	302	PGV	O12-C04-C05-O05
11	e	101	BCL	C13-C15-C16-C17
11	J	101	BCL	C2-C1-O2A-CGA
11	V	102	BCL	C4-C3-C5-C6
10	V	103	8K6	C5-C6-C7-C8
13	L	408	LMT	C5'-C4'-O1B-C1B
10	L	405	8K6	C10-C11-C12-C13
13	L	408	LMT	C3'-C4'-O1B-C1B
11	g	101	BCL	C4-C3-C5-C6
15	M	405	MQ8	C34-C33-C35-C36
11	M	402	BCL	C11-C12-C13-C14
11	M	403	BCL	C11-C10-C8-C9
11	V	102	BCL	C14-C13-C15-C16
11	W	101	BCL	C6-C7-C8-C9
9	Z	103	PGV	C05-C04-O12-P
11	f	101	BCL	C8-C10-C11-C12
11	V	102	BCL	C2-C3-C5-C6
11	g	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	G	101	BCL	C11-C12-C13-C15
11	T	101	BCL	C11-C12-C13-C15
11	U	101	BCL	C12-C13-C15-C16
11	V	101	BCL	C12-C13-C15-C16
11	e	101	BCL	C11-C10-C8-C7
11	g	101	BCL	C12-C13-C15-C16
11	W	101	BCL	C16-C17-C18-C20
9	H	301	PGV	C5-C6-C7-C8
16	Z	102	CRT	C21-C22-C23-C24
11	R	102	BCL	C2-C1-O2A-CGA
11	X	101	BCL	C2-C1-O2A-CGA
9	H	301	PGV	C02-C03-O11-P
9	H	302	PGV	C6-C7-C8-C9
11	e	101	BCL	C2-C3-C5-C6
15	M	405	MQ8	C22-C23-C25-C26
11	U	101	BCL	C16-C17-C18-C19
11	f	101	BCL	C16-C17-C18-C20
11	j	103	BCL	C13-C15-C16-C17
11	D	101	BCL	C3-C5-C6-C7
11	L	401	BCL	C14-C13-C15-C16
11	N	102	BCL	C14-C13-C15-C16
11	U	101	BCL	C14-C13-C15-C16
11	Y	101	BCL	C11-C12-C13-C14
11	b	102	BCL	C11-C10-C8-C9
11	d	102	BCL	C11-C10-C8-C9
13	L	408	LMT	C2-C3-C4-C5
16	Z	102	CRT	C21-C22-C23-C25
11	V	102	BCL	C8-C10-C11-C12
11	E	102	BCL	C16-C17-C18-C20
15	M	405	MQ8	C32-C33-C35-C36
11	M	403	BCL	C11-C12-C13-C15
11	B	101	BCL	C11-C10-C8-C7
11	A	102	BCL	C11-C10-C8-C7
16	U	102	CRT	C2-C1-C4-C5
9	R	104	PGV	C12-C13-C14-C15
12	L	403	BPH	C16-C17-C18-C20
9	M	407	PGV	O03-C19-C20-C21
11	A	101	BCL	O1D-CGD-O2D-CED
9	H	301	PGV	C20-C21-C22-C23
11	e	101	BCL	C11-C10-C8-C9
11	f	101	BCL	C11-C12-C13-C14
11	S	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	M	405	MQ8	C30-C31-C32-C33
11	M	403	BCL	C2-C3-C5-C6
12	M	404	BPH	C2-C3-C5-C6
11	O	101	BCL	C13-C15-C16-C17
11	J	102	BCL	C3-C5-C6-C7
9	H	301	PGV	C2-C3-C4-C5
9	Z	103	PGV	C3-C4-C5-C6
11	U	101	BCL	C4C-C3C-CAC-CBC
10	J	104	8K6	C5-C6-C7-C8
9	M	407	PGV	O01-C02-C03-O11
9	R	104	PGV	O01-C02-C03-O11
11	F	101	BCL	C16-C17-C18-C19
11	S	101	BCL	C13-C15-C16-C17
11	G	102	BCL	C11-C10-C8-C7
9	M	408	PGV	C25-C26-C27-C28
12	M	404	BPH	C3-C5-C6-C7
9	M	408	PGV	C30-C31-C32-C33
11	M	403	BCL	C11-C12-C13-C14
11	B	101	BCL	C11-C10-C8-C9
11	E	101	BCL	C11-C10-C8-C9
11	P	102	BCL	C11-C12-C13-C14
11	Q	101	BCL	C11-C12-C13-C14
11	S	101	BCL	C6-C7-C8-C9
11	X	101	BCL	C11-C12-C13-C14
11	Z	101	BCL	C11-C10-C8-C9
11	g	101	BCL	C14-C13-C15-C16
11	i	101	BCL	C6-C7-C8-C9
10	d	103	8K6	C10-C11-C12-C13
11	G	101	BCL	C2-C1-O2A-CGA
11	M	403	BCL	C15-C16-C17-C18
11	Z	101	BCL	C8-C10-C11-C12
11	M	403	BCL	C3A-C2A-CAA-CBA
11	B	101	BCL	C13-C15-C16-C17
11	E	101	BCL	C16-C17-C18-C20
11	M	402	BCL	O2A-C1-C2-C3
9	H	302	PGV	C11-C12-C13-C14
16	K	102	CRT	C9-C10-C11-C12
9	M	407	PGV	C22-C23-C24-C25
7	C	504	HEC	C2D-C3D-CAD-CBD
9	R	104	PGV	C11-C12-C13-C14
9	M	408	PGV	C24-C25-C26-C27
10	f	103	8K6	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	A	102	BCL	C11-C10-C8-C9
11	I	101	BCL	C11-C12-C13-C14
11	b	101	BCL	C14-C13-C15-C16
9	M	407	PGV	C01-C02-C03-O11
9	Z	103	PGV	C1-C2-C3-C4
16	P	103	CRT	O1-C1-C4-C5
11	L	401	BCL	C12-C13-C15-C16
11	B	101	BCL	C6-C7-C8-C10
11	E	101	BCL	C11-C10-C8-C7
11	K	101	BCL	C12-C13-C15-C16
11	O	101	BCL	C11-C12-C13-C15
11	P	102	BCL	C11-C12-C13-C15
11	a	101	BCL	C11-C12-C13-C15
11	c	101	BCL	C11-C12-C13-C15
11	f	101	BCL	C11-C12-C13-C15
12	M	404	BPH	C11-C10-C8-C7
10	L	406	8K6	C11-C12-C13-C14
9	Z	103	PGV	C9-C10-C11-C12
11	Z	101	BCL	C2-C1-O2A-CGA
11	g	101	BCL	C2-C1-O2A-CGA
12	M	404	BPH	C2C-C3C-CAC-CBC
11	M	402	BCL	O1D-CGD-O2D-CED
11	Q	101	BCL	C3-C5-C6-C7
11	U	101	BCL	C13-C15-C16-C17
11	U	101	BCL	C16-C17-C18-C20
9	C	508	PGV	C13-C14-C15-C16
10	j	104	8K6	C7-C8-C9-C10
7	C	504	HEC	CAA-CBA-CGA-O2A
11	b	102	BCL	C6-C7-C8-C9
11	h	102	BCL	C6-C7-C8-C9
11	M	403	BCL	C1A-C2A-CAA-CBA
10	d	103	8K6	C11-C10-C9-C8
9	L	410	PGV	O03-C19-C20-C21
15	M	405	MQ8	C25-C26-C27-C28
11	E	102	BCL	C13-C15-C16-C17
11	e	101	BCL	C2-C1-O2A-CGA
11	D	101	BCL	C12-C13-C15-C16
11	R	101	BCL	C12-C13-C15-C16
11	X	102	BCL	C12-C13-C15-C16
9	H	301	PGV	O12-C04-C05-O05
11	R	102	BCL	C2C-C3C-CAC-CBC
16	e	102	CRT	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
11	W	101	BCL	C5-C6-C7-C8
11	E	101	BCL	C16-C17-C18-C19
9	M	408	PGV	C23-C24-C25-C26
11	A	101	BCL	CAA-CBA-CGA-O2A
11	c	101	BCL	C16-C17-C18-C19
11	N	102	BCL	C8-C10-C11-C12
11	D	101	BCL	C14-C13-C15-C16
11	G	102	BCL	C11-C10-C8-C9
11	K	101	BCL	C14-C13-C15-C16
11	d	101	BCL	C10-C11-C12-C13
7	C	504	HEC	CAA-CBA-CGA-O1A
11	M	403	BCL	C13-C15-C16-C17
11	O	101	BCL	C8-C10-C11-C12
11	j	102	BCL	O1D-CGD-O2D-CED
11	b	101	BCL	C8-C10-C11-C12
11	Q	101	BCL	CAA-CBA-CGA-O2A
11	I	101	BCL	C3-C5-C6-C7
9	M	408	PGV	O02-C1-O01-C02
11	L	401	BCL	O1D-CGD-O2D-CED
9	L	410	PGV	O04-C19-C20-C21
11	F	101	BCL	C2-C1-O2A-CGA
11	A	101	BCL	CAA-CBA-CGA-O1A
11	X	102	BCL	C5-C6-C7-C8
9	H	302	PGV	C20-C21-C22-C23
9	H	302	PGV	O03-C19-C20-C21
11	G	101	BCL	CAA-CBA-CGA-O2A
11	K	101	BCL	CAA-CBA-CGA-O2A
9	M	408	PGV	C19-C20-C21-C22

There are no ring outliers.

98 monomers are involved in 393 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	406	CRT	3	0
11	E	102	BCL	3	0
16	a	102	CRT	5	0
9	M	407	PGV	4	0
11	U	101	BCL	5	0
11	Q	101	BCL	4	0
11	R	101	BCL	3	0
9	H	301	PGV	7	0
16	E	103	CRT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	409	8K6	5	0
11	P	102	BCL	3	0
16	U	102	CRT	8	0
11	A	102	BCL	4	0
10	J	103	8K6	1	0
10	N	104	8K6	4	0
16	i	102	CRT	8	0
10	P	104	8K6	2	0
9	R	104	PGV	2	0
9	Z	103	PGV	3	0
10	H	304	8K6	2	0
11	X	101	BCL	4	0
11	h	102	BCL	3	0
16	W	102	CRT	5	0
11	d	102	BCL	3	0
11	R	102	BCL	2	0
9	M	408	PGV	7	0
10	d	103	8K6	1	0
16	j	101	CRT	8	0
7	C	502	HEC	8	0
12	L	403	BPH	4	0
9	L	410	PGV	40	0
11	P	101	BCL	3	0
16	I	102	CRT	10	0
10	X	103	8K6	1	0
11	M	402	BCL	2	0
11	g	101	BCL	5	0
11	Y	101	BCL	4	0
11	D	101	BCL	4	0
16	Y	102	CRT	7	0
11	N	101	BCL	4	0
16	A	103	CRT	6	0
16	P	103	CRT	7	0
10	V	104	8K6	1	0
11	I	101	BCL	5	0
11	Z	101	BCL	3	0
11	G	101	BCL	4	0
11	i	101	BCL	7	0
11	J	101	BCL	3	0
11	K	101	BCL	5	0
11	A	101	BCL	3	0
11	h	101	BCL	5	0

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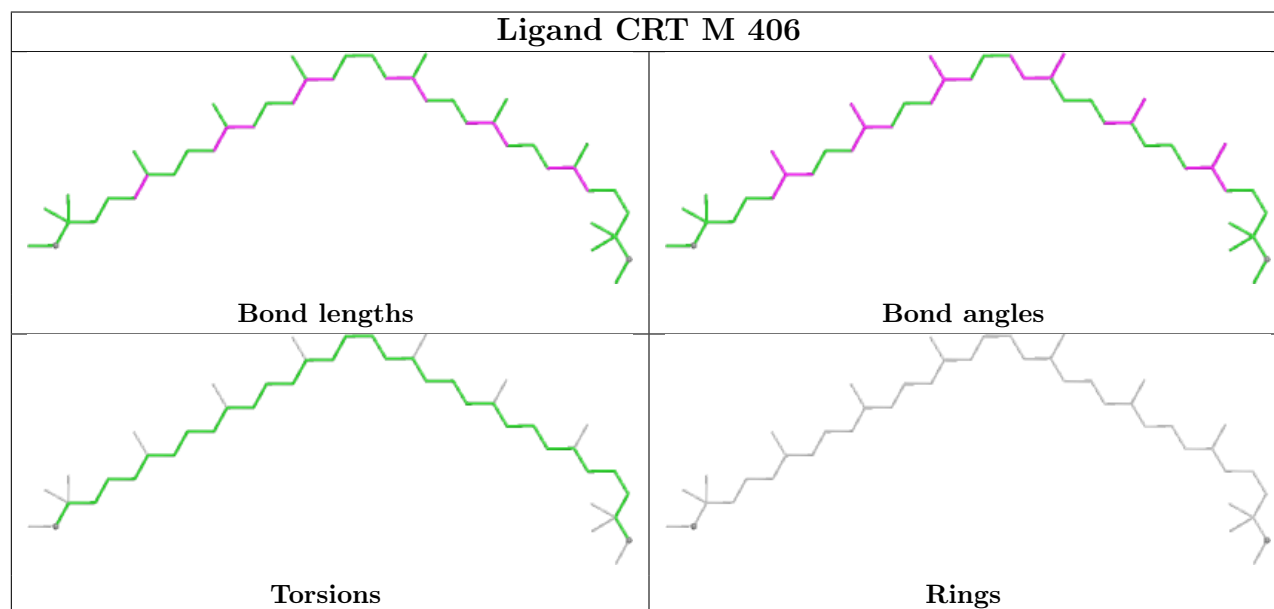
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	303	8K6	2	0
11	d	101	BCL	4	0
11	G	102	BCL	2	0
11	X	102	BCL	4	0
11	a	101	BCL	4	0
11	T	101	BCL	5	0
16	K	102	CRT	8	0
10	j	105	8K6	1	0
10	C	509	8K6	2	0
16	R	103	CRT	8	0
11	S	101	BCL	2	0
11	c	101	BCL	7	0
10	L	404	8K6	2	0
12	M	404	BPH	3	0
11	b	102	BCL	3	0
11	F	101	BCL	3	0
10	L	406	8K6	1	0
11	e	101	BCL	1	0
7	C	501	HEC	1	0
10	J	104	8K6	2	0
11	W	101	BCL	3	0
9	H	302	PGV	5	0
11	j	103	BCL	2	0
11	J	102	BCL	2	0
11	j	102	BCL	4	0
15	M	405	MQ8	7	0
10	j	104	8K6	1	0
10	L	405	8K6	2	0
7	C	504	HEC	1	0
16	Z	102	CRT	15	0
11	L	402	BCL	4	0
16	N	103	CRT	6	0
10	f	103	8K6	3	0
16	e	102	CRT	5	0
11	T	102	BCL	2	0
10	V	103	8K6	1	0
11	f	101	BCL	6	0
11	f	102	BCL	5	0
7	C	503	HEC	6	0
10	L	407	8K6	2	0
11	V	101	BCL	3	0
11	B	101	BCL	2	0

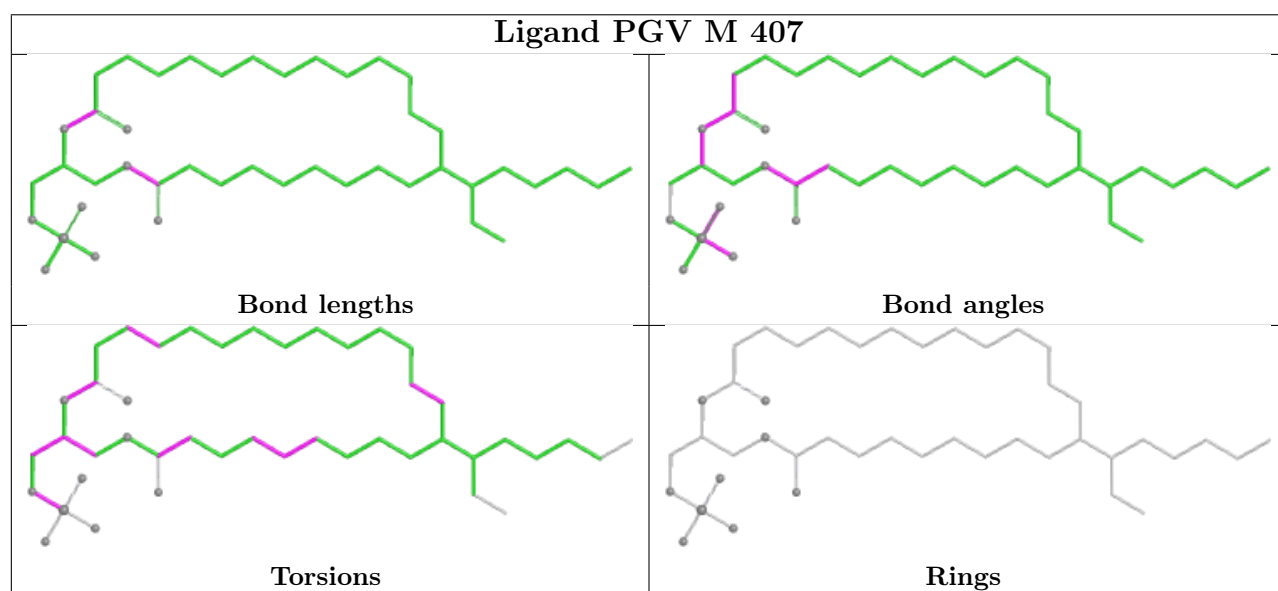
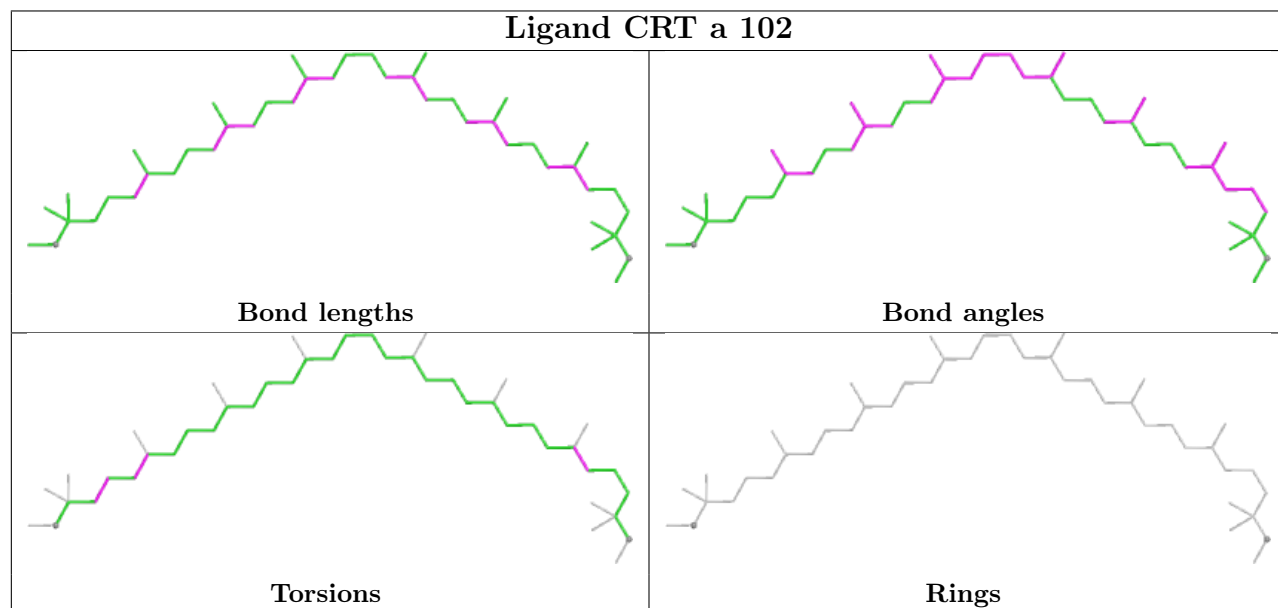
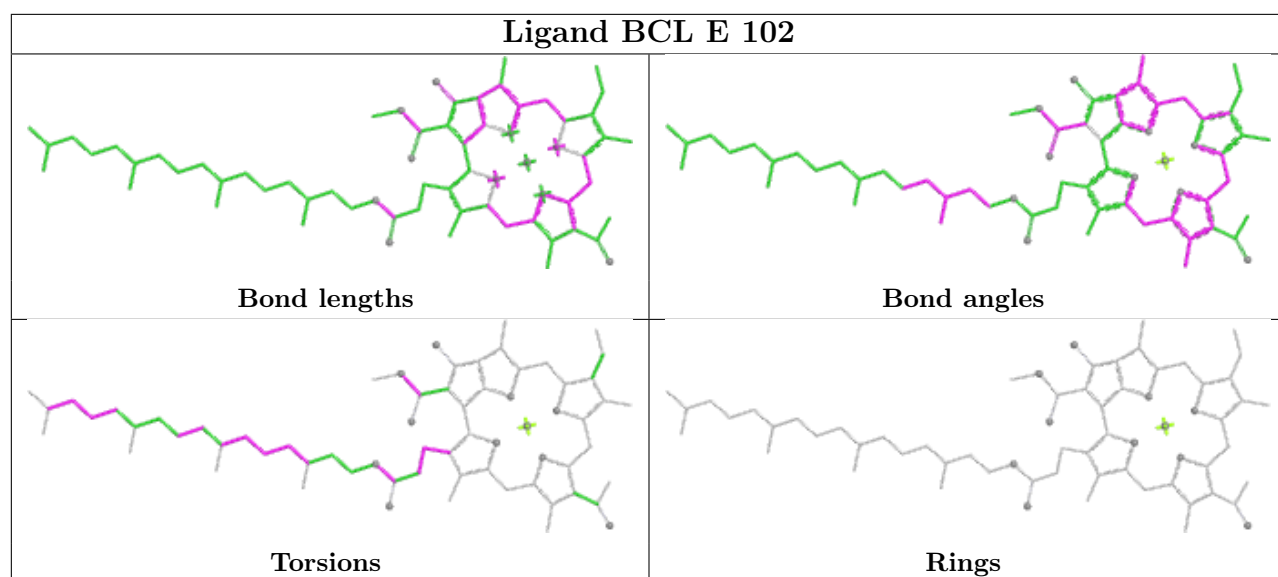
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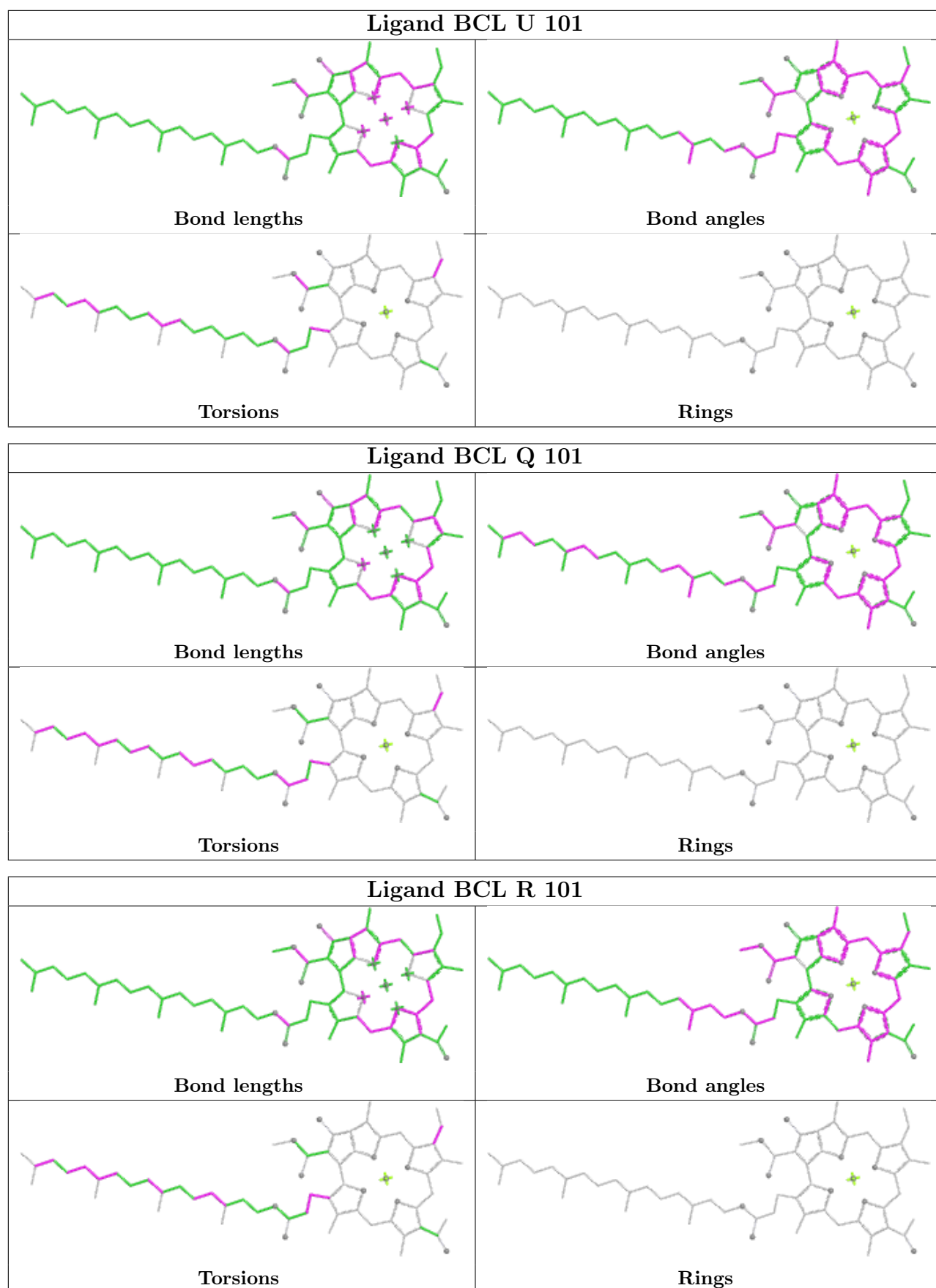
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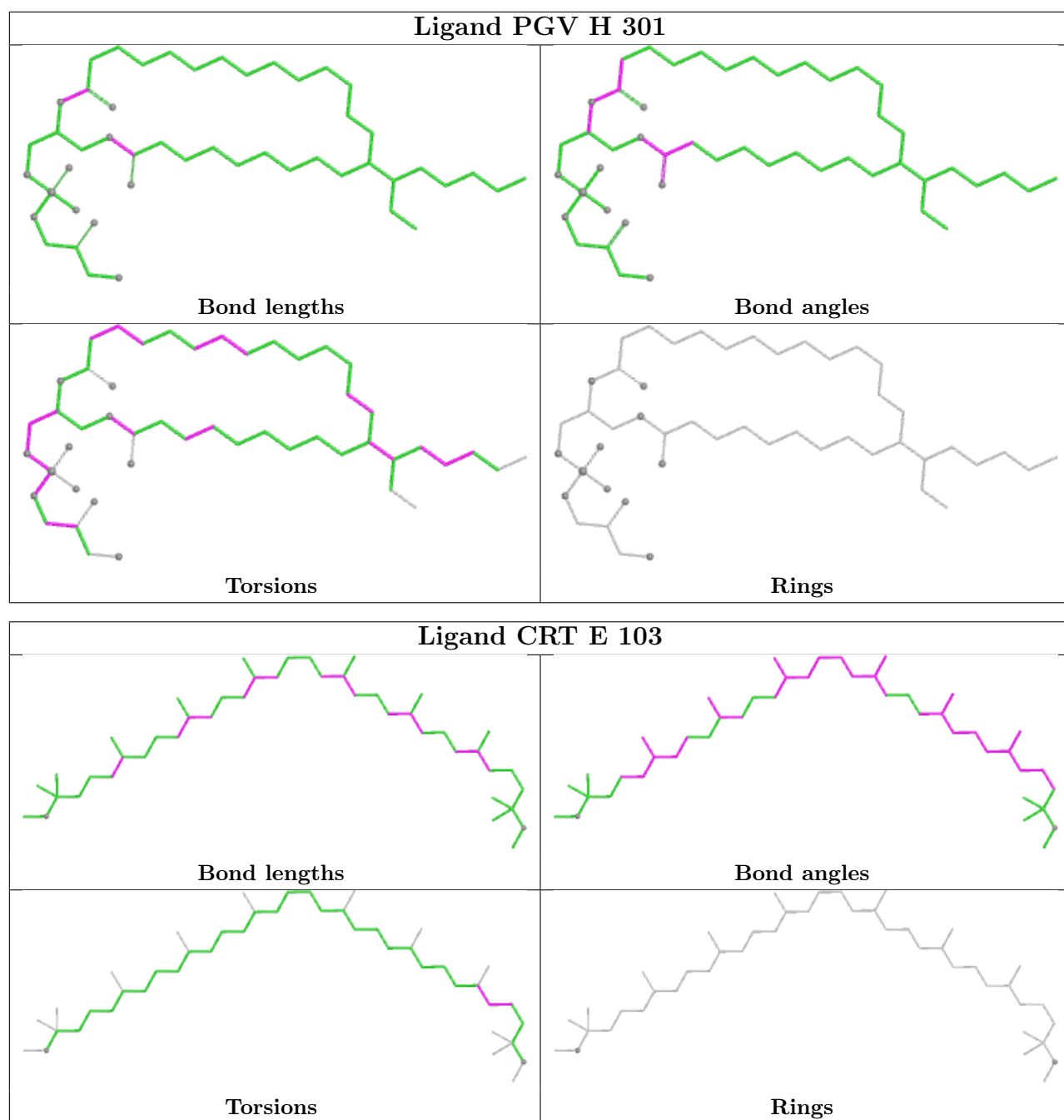
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	401	BCL	8	0
11	O	101	BCL	6	0
16	B	102	CRT	4	0
11	E	101	BCL	1	0
11	b	101	BCL	4	0

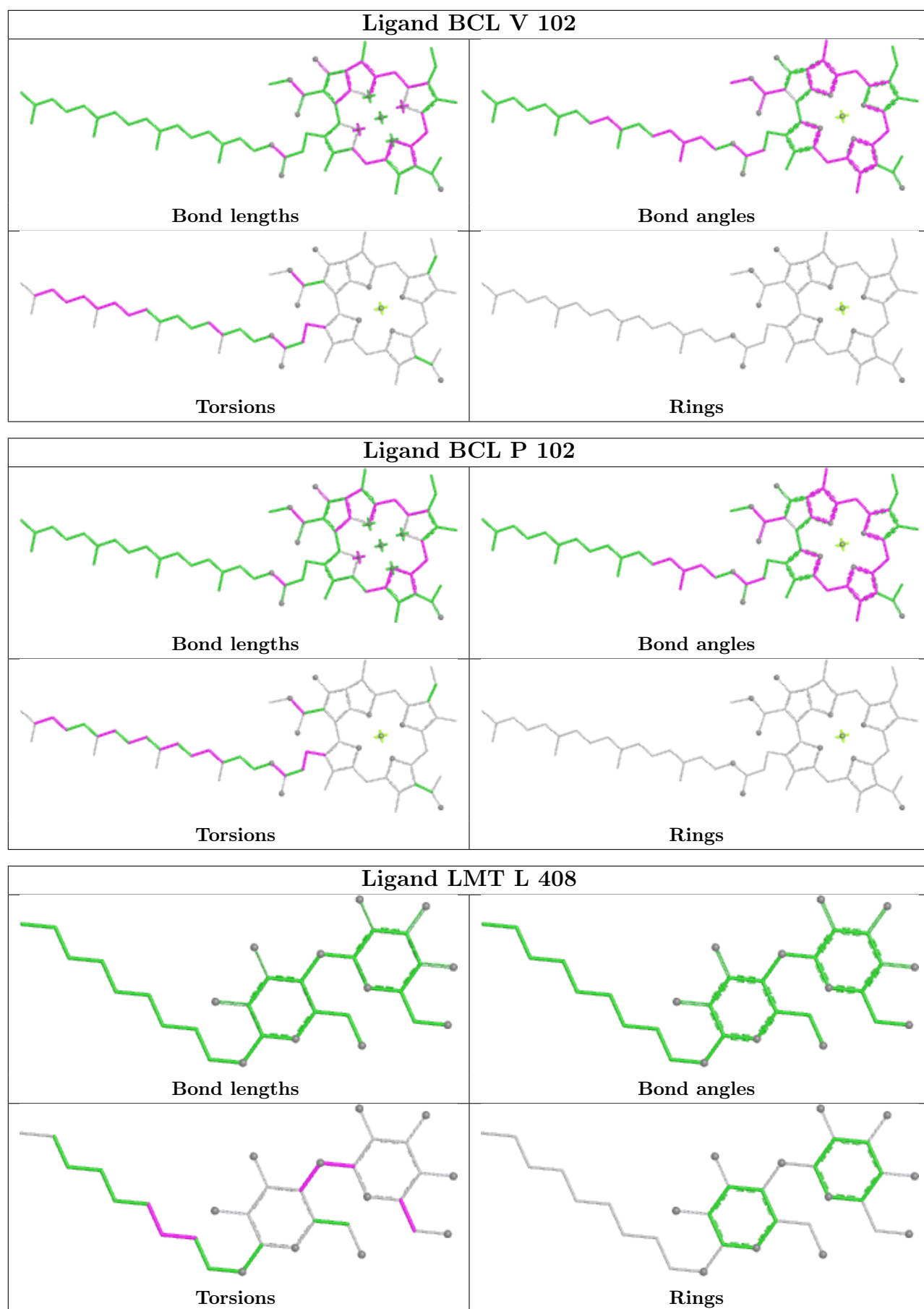
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

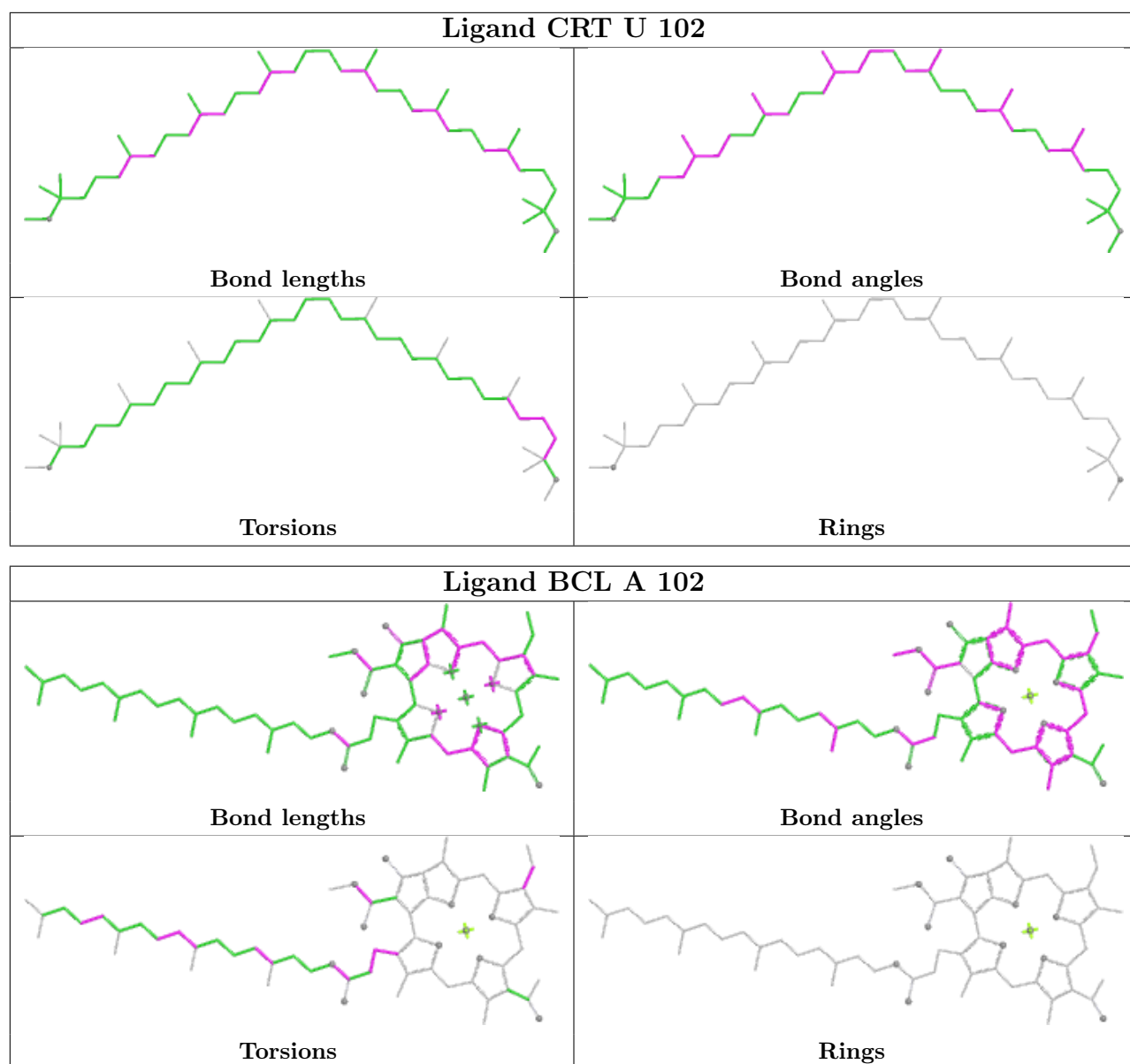


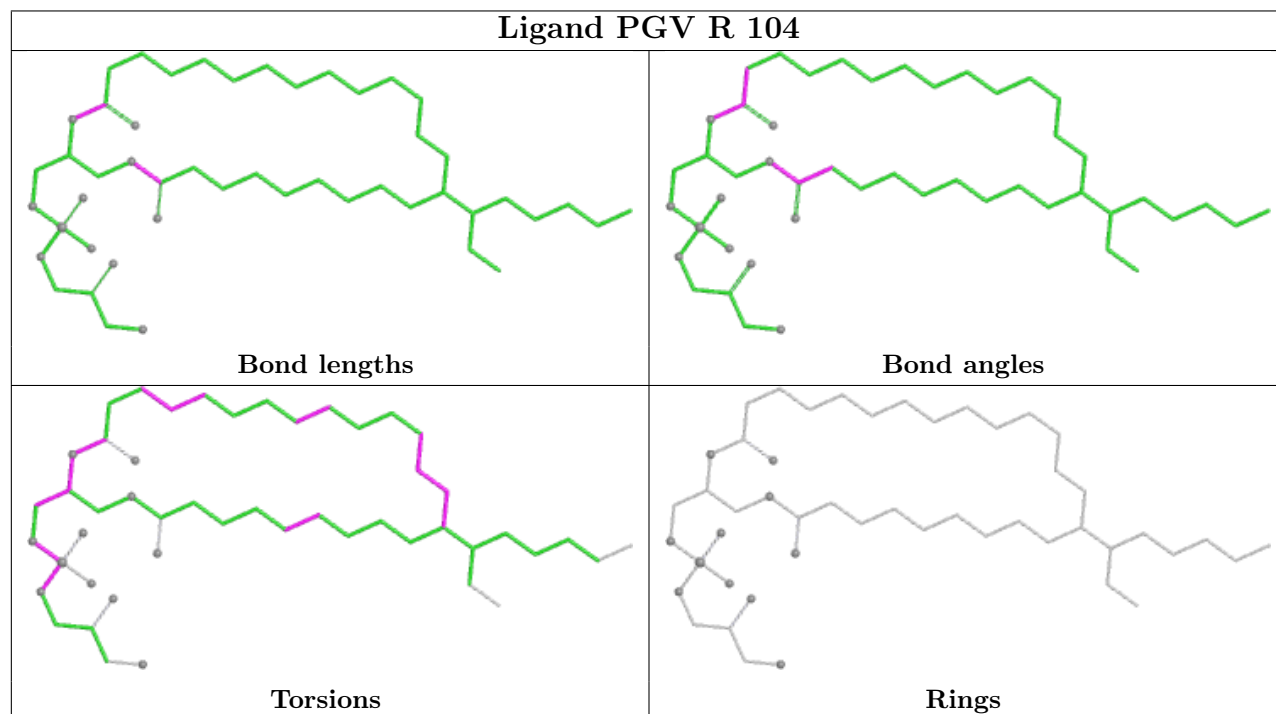
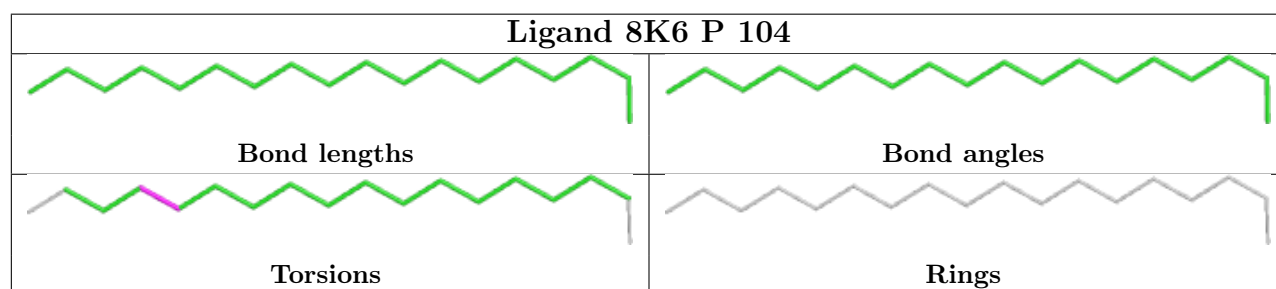
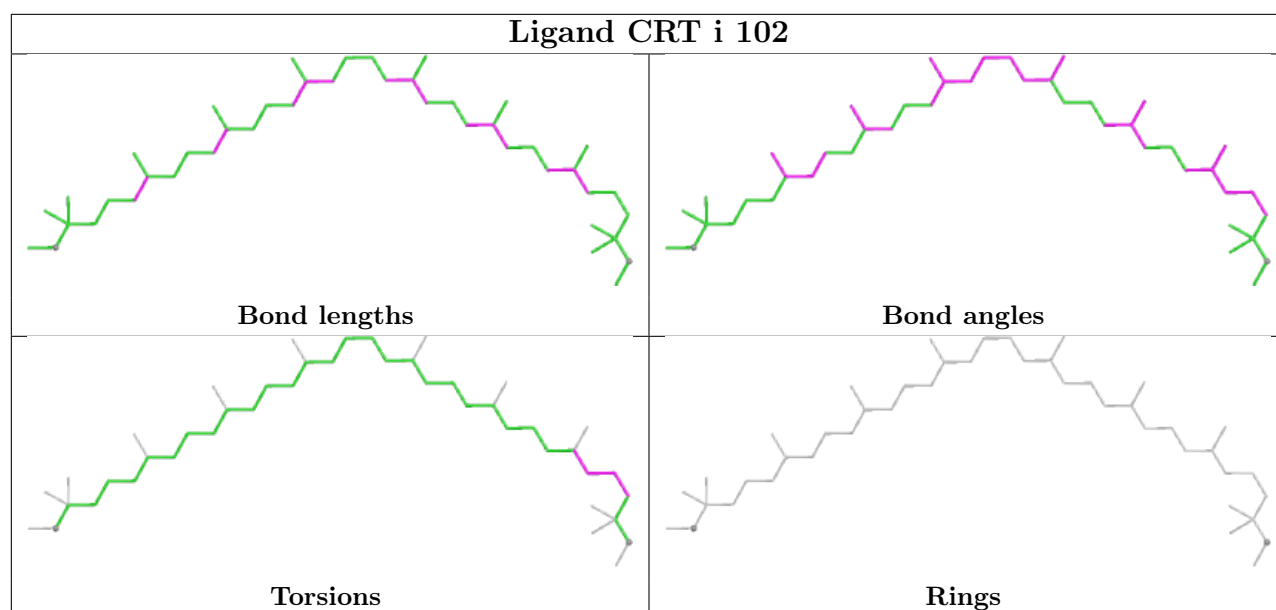




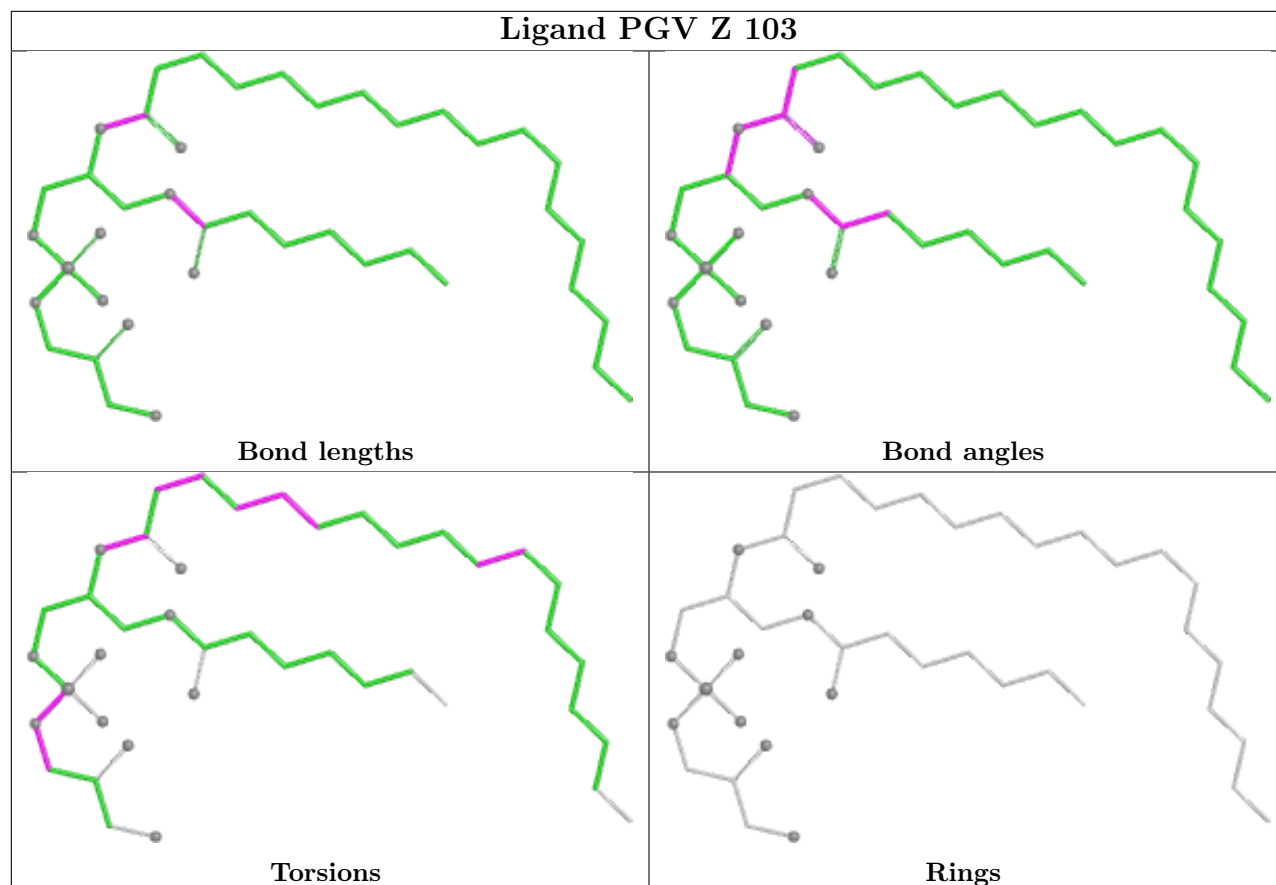




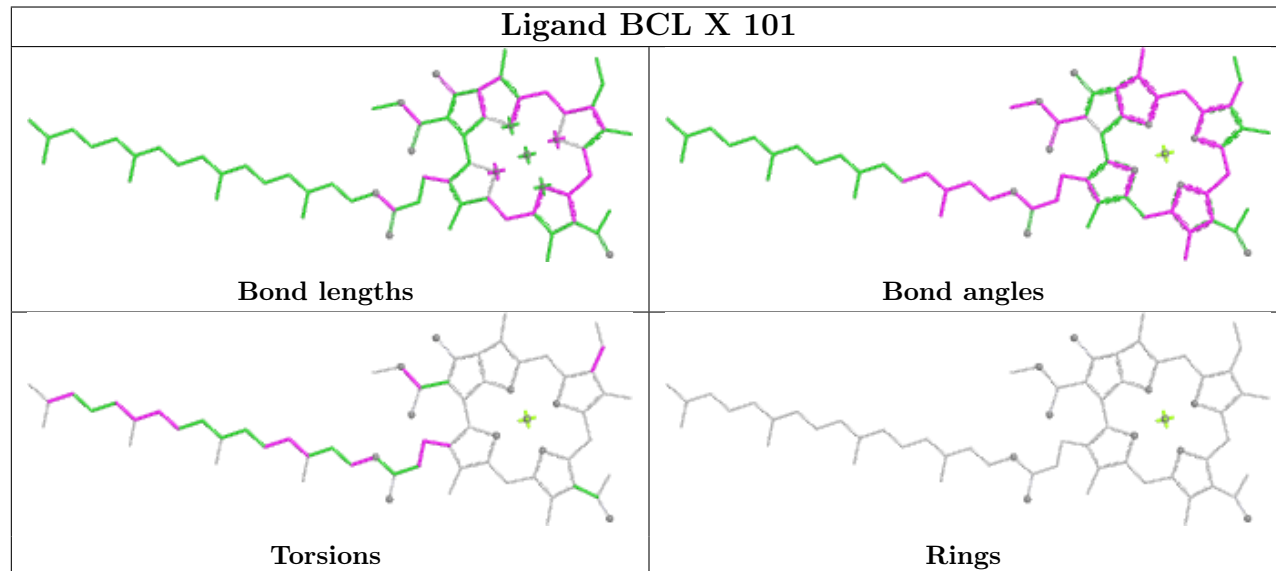


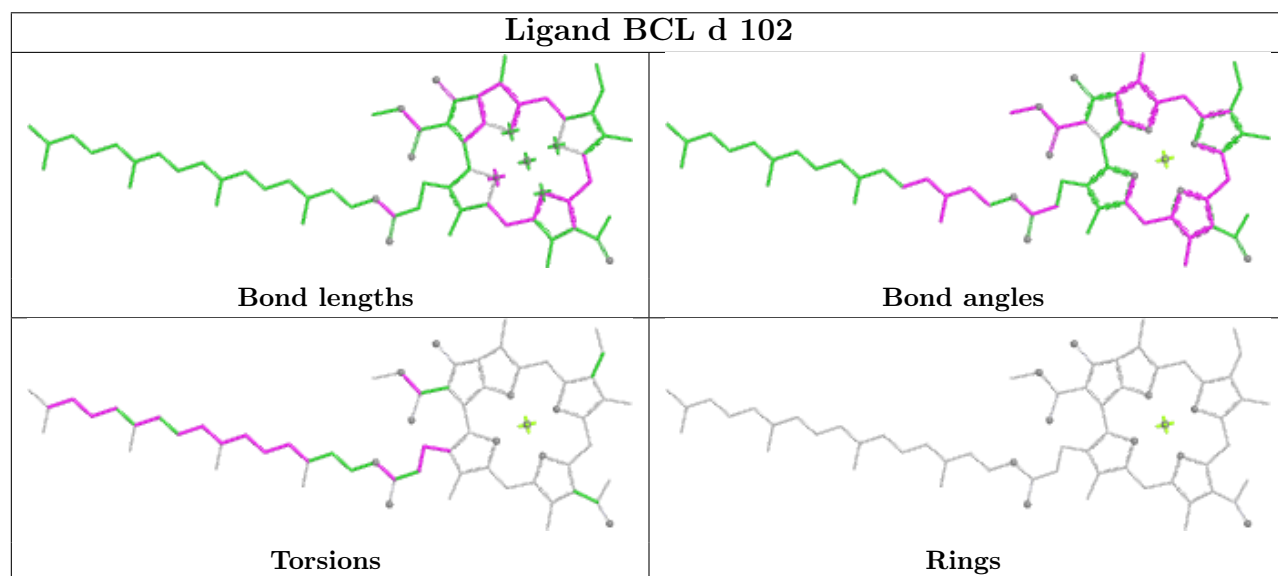
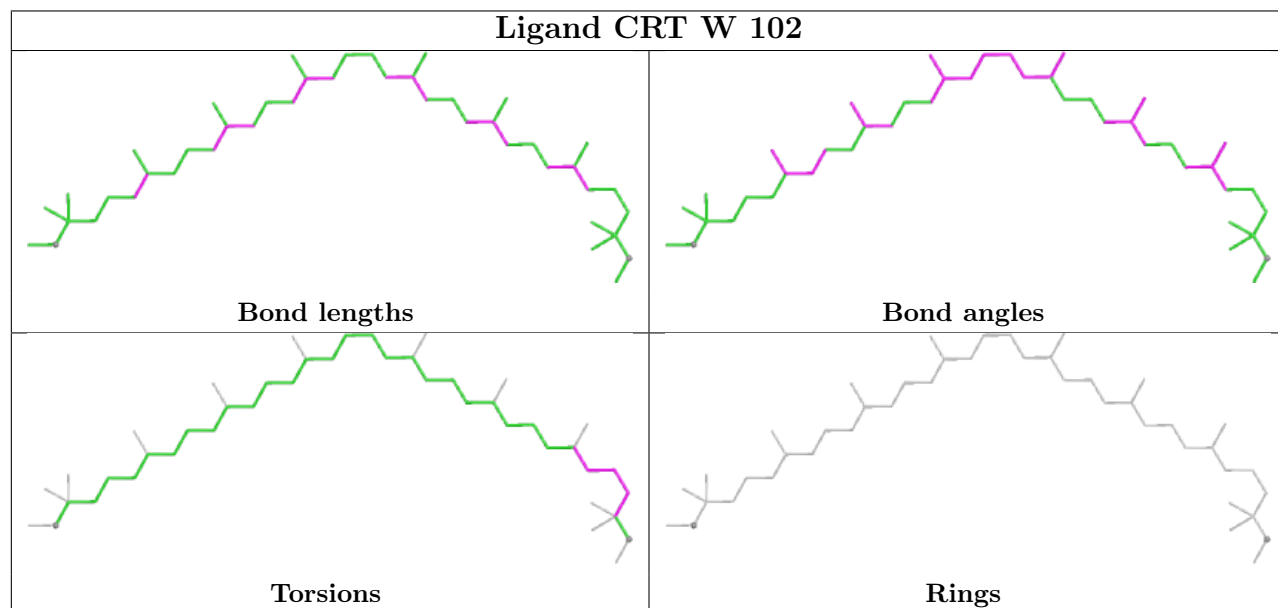
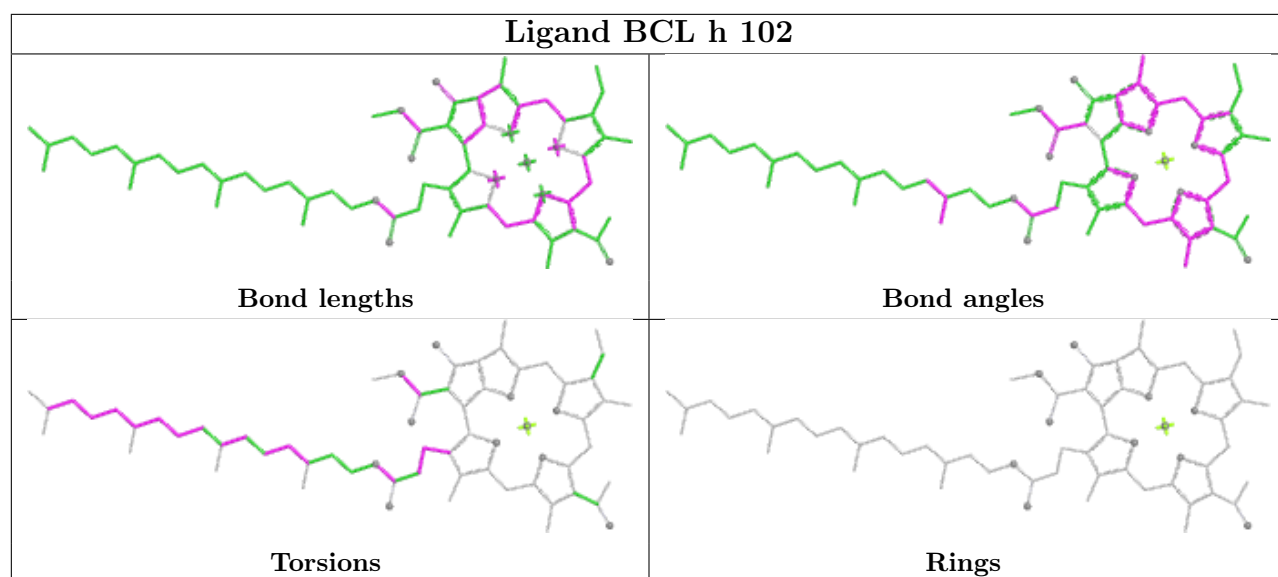


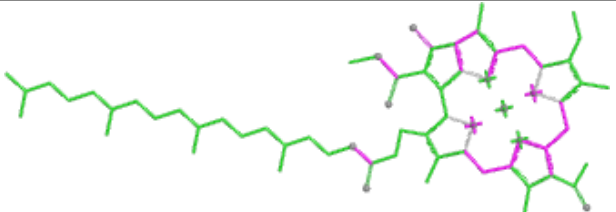
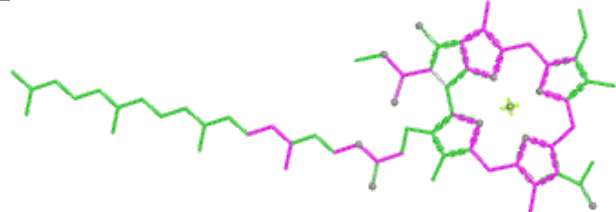
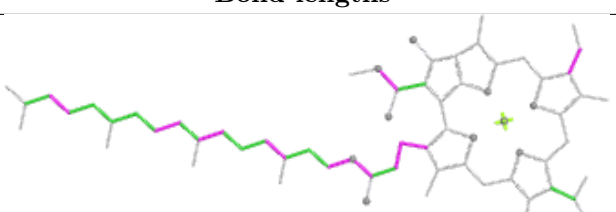
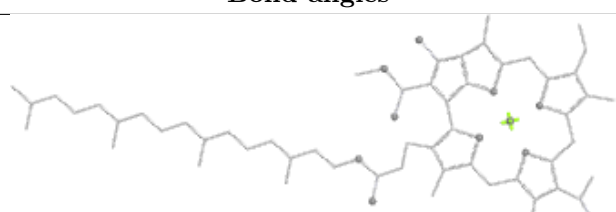
Ligand PGV Z 103

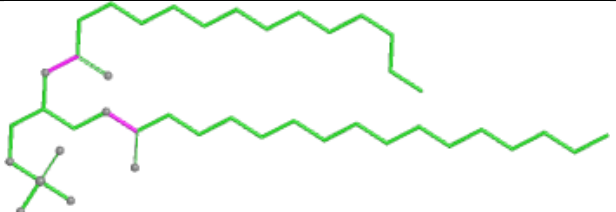
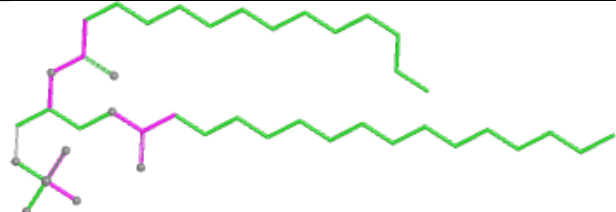
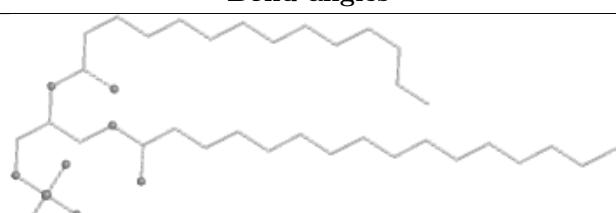


Ligand BCL X 101

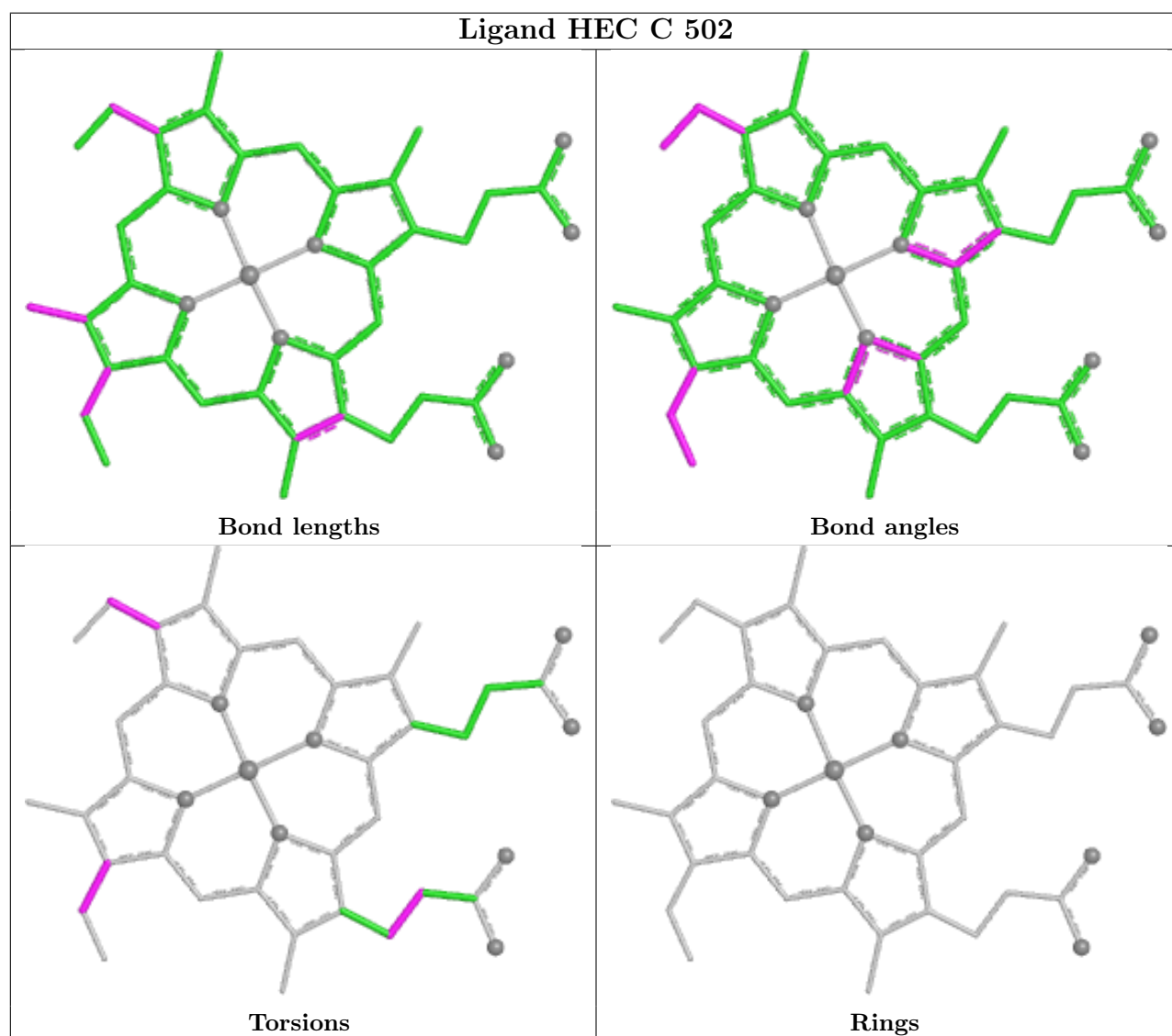
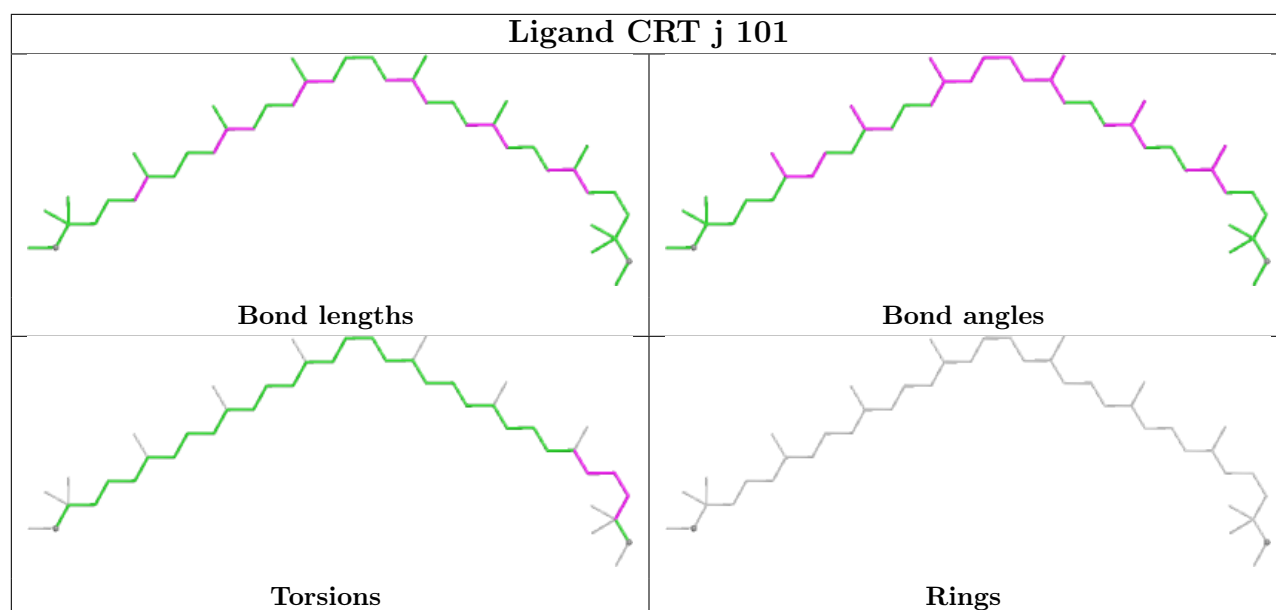




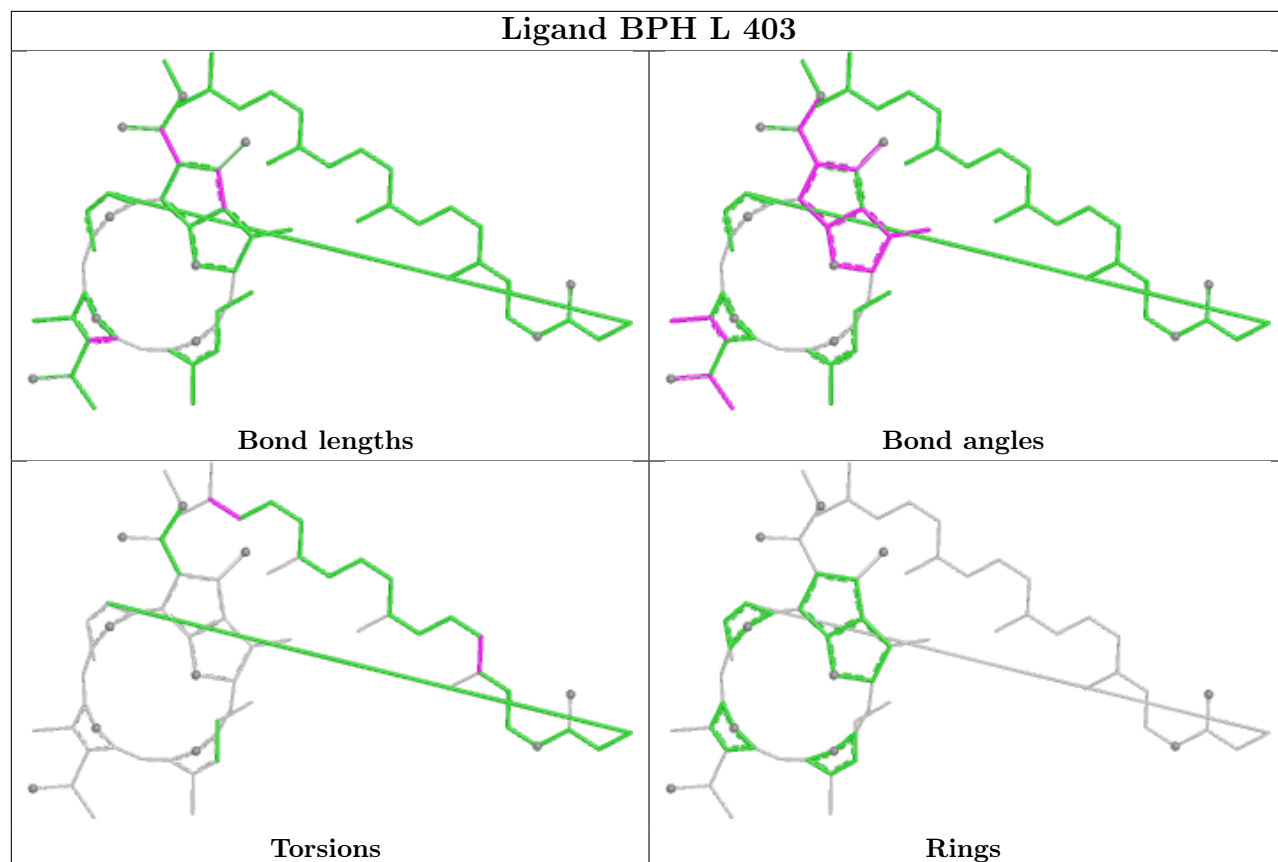
Ligand BCL R 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PGV M 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

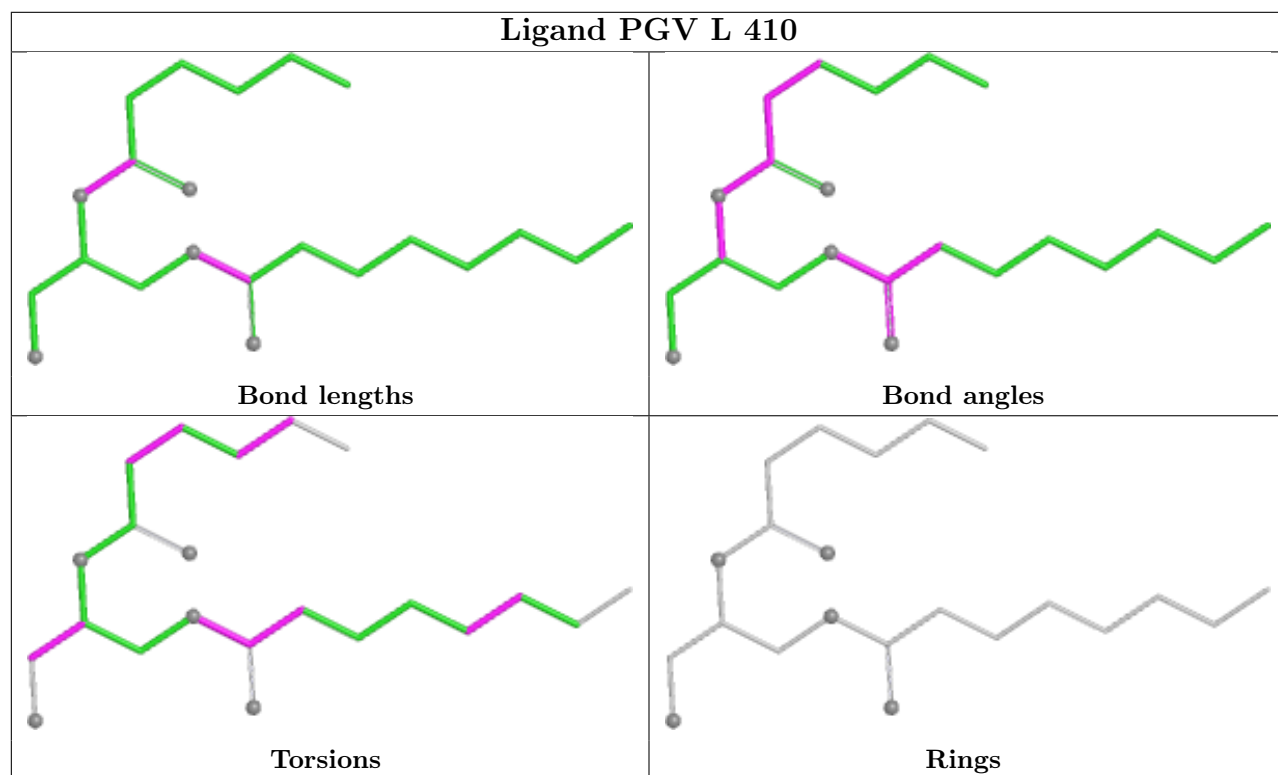
Ligand 8K6 d 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

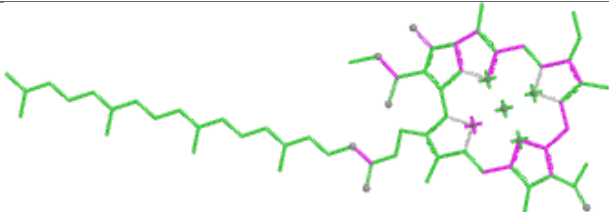
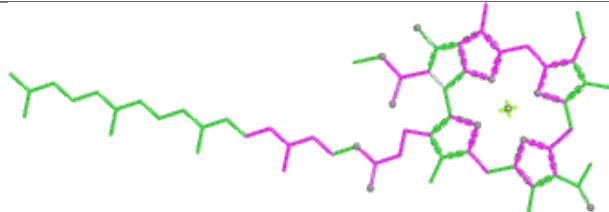
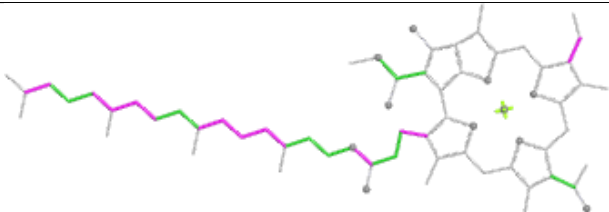
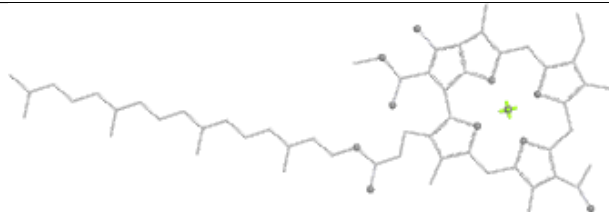


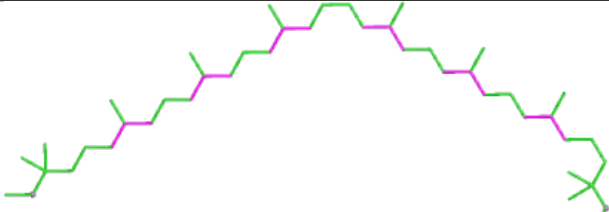
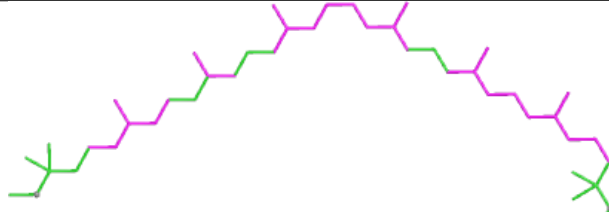
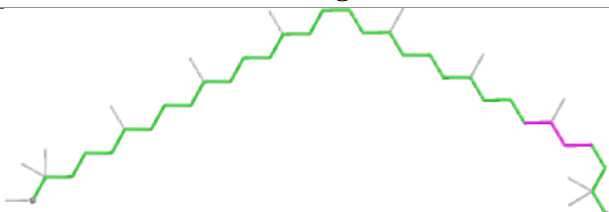
Ligand BPH L 403

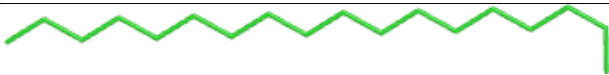
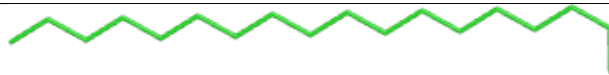
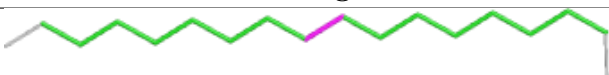


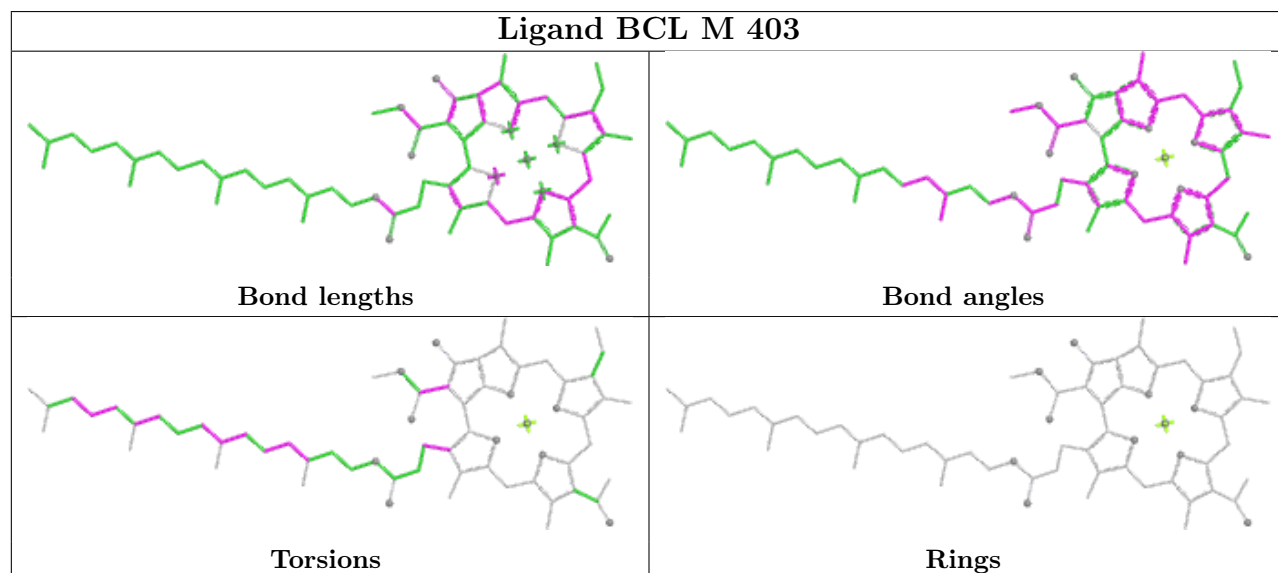
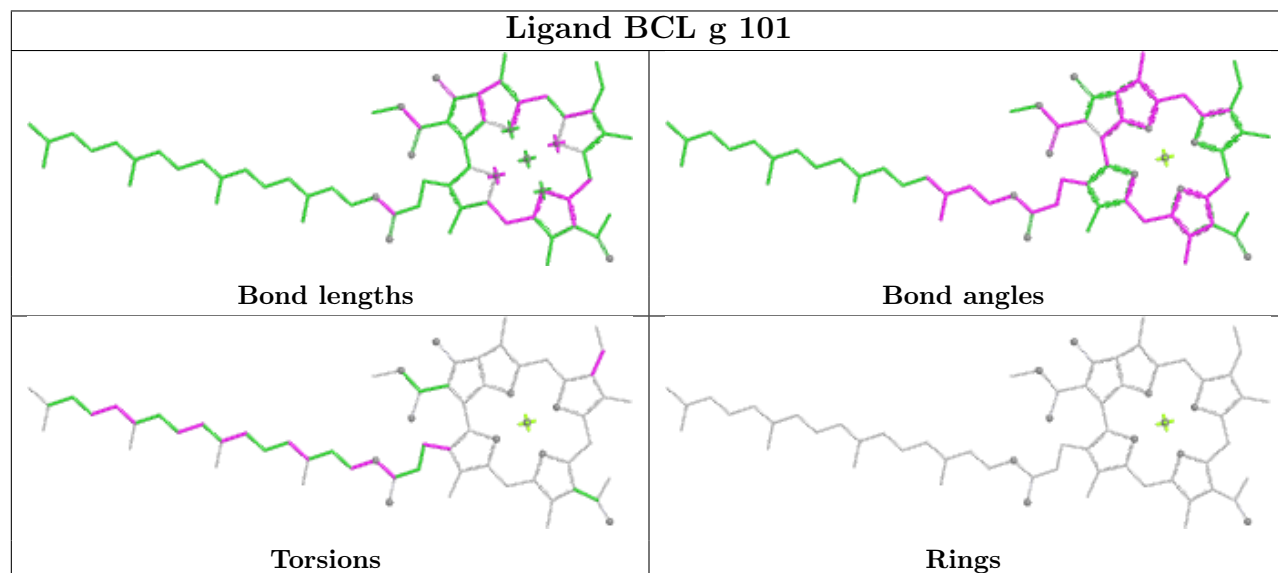
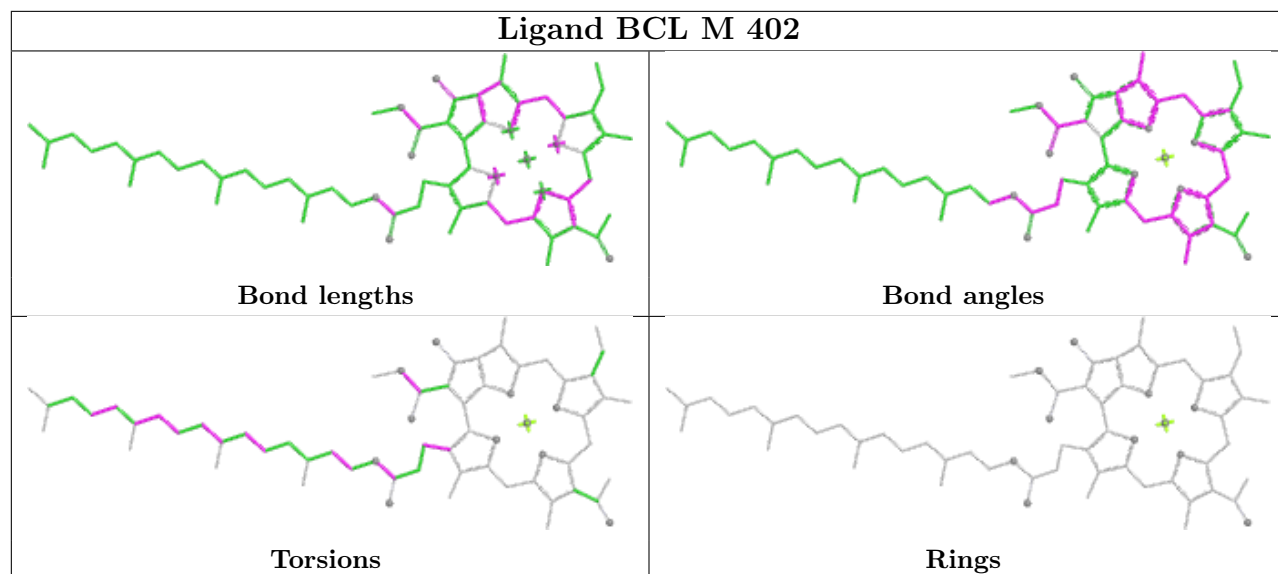
Ligand PGV L 410

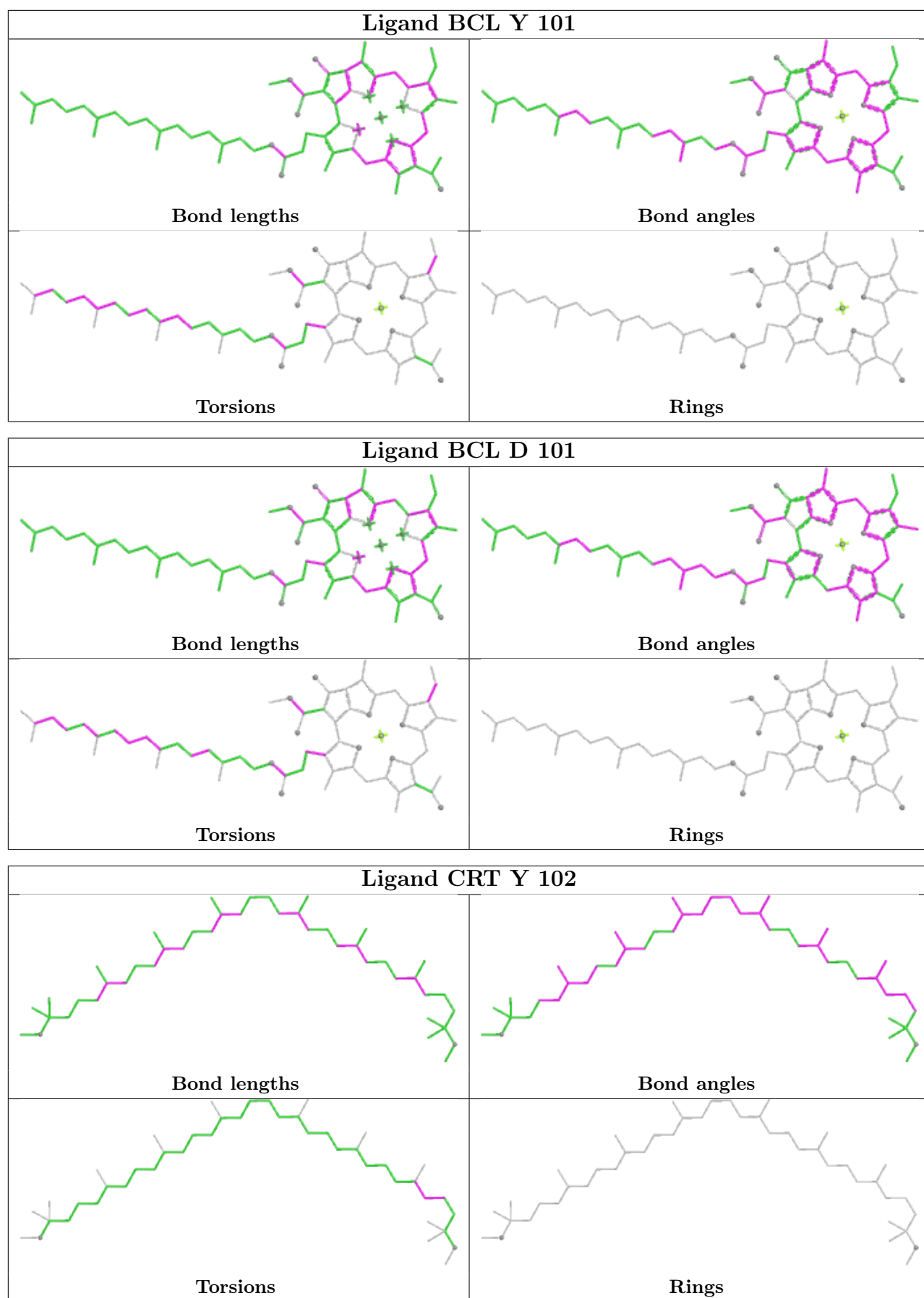


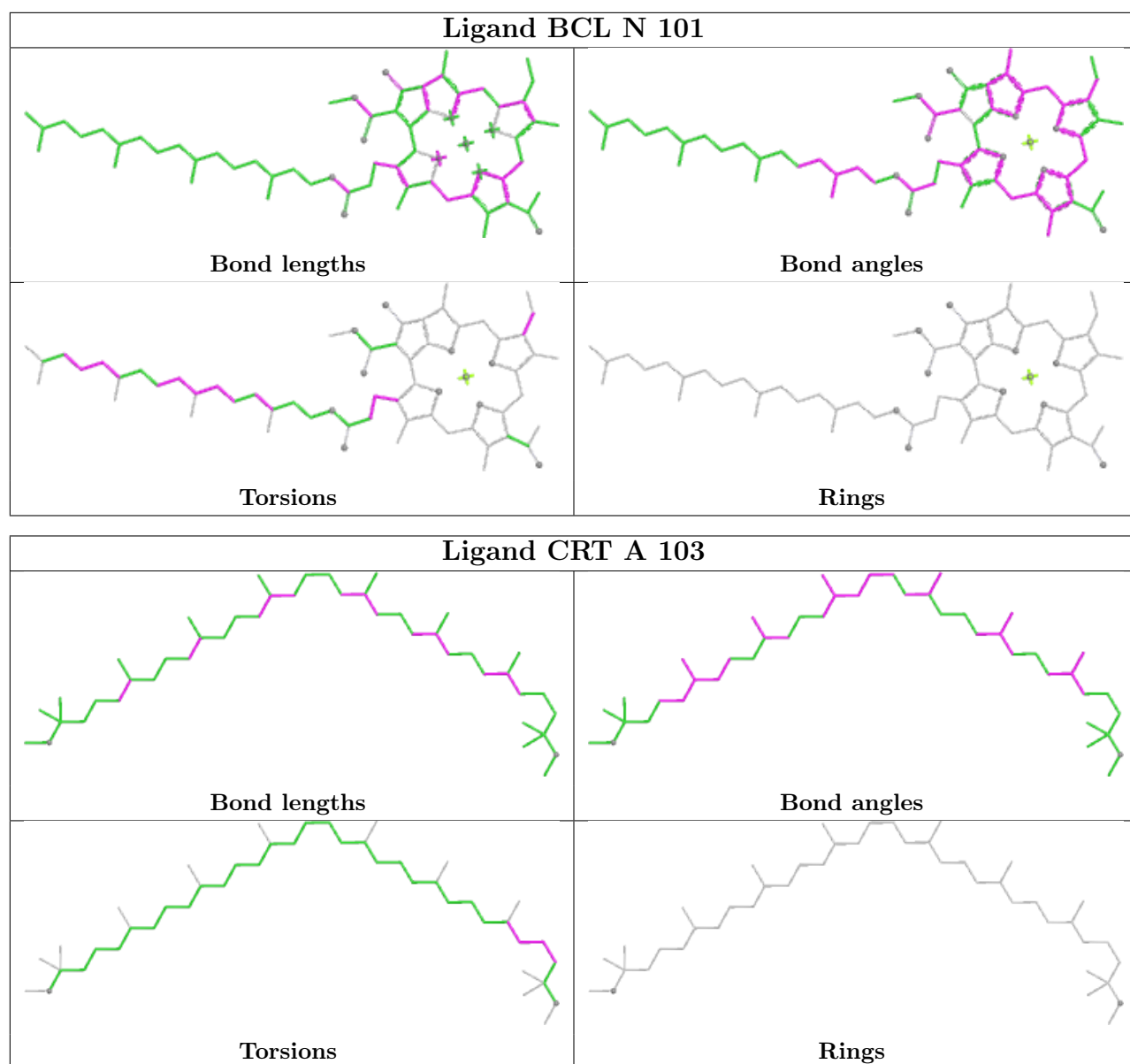
Ligand BCL P 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

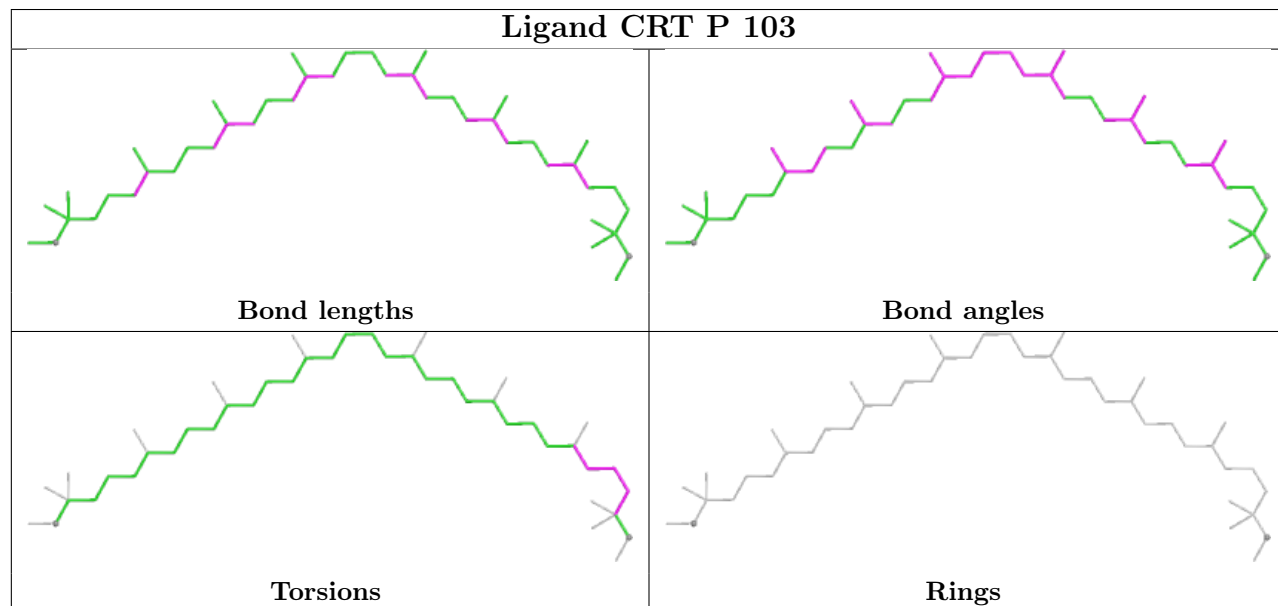
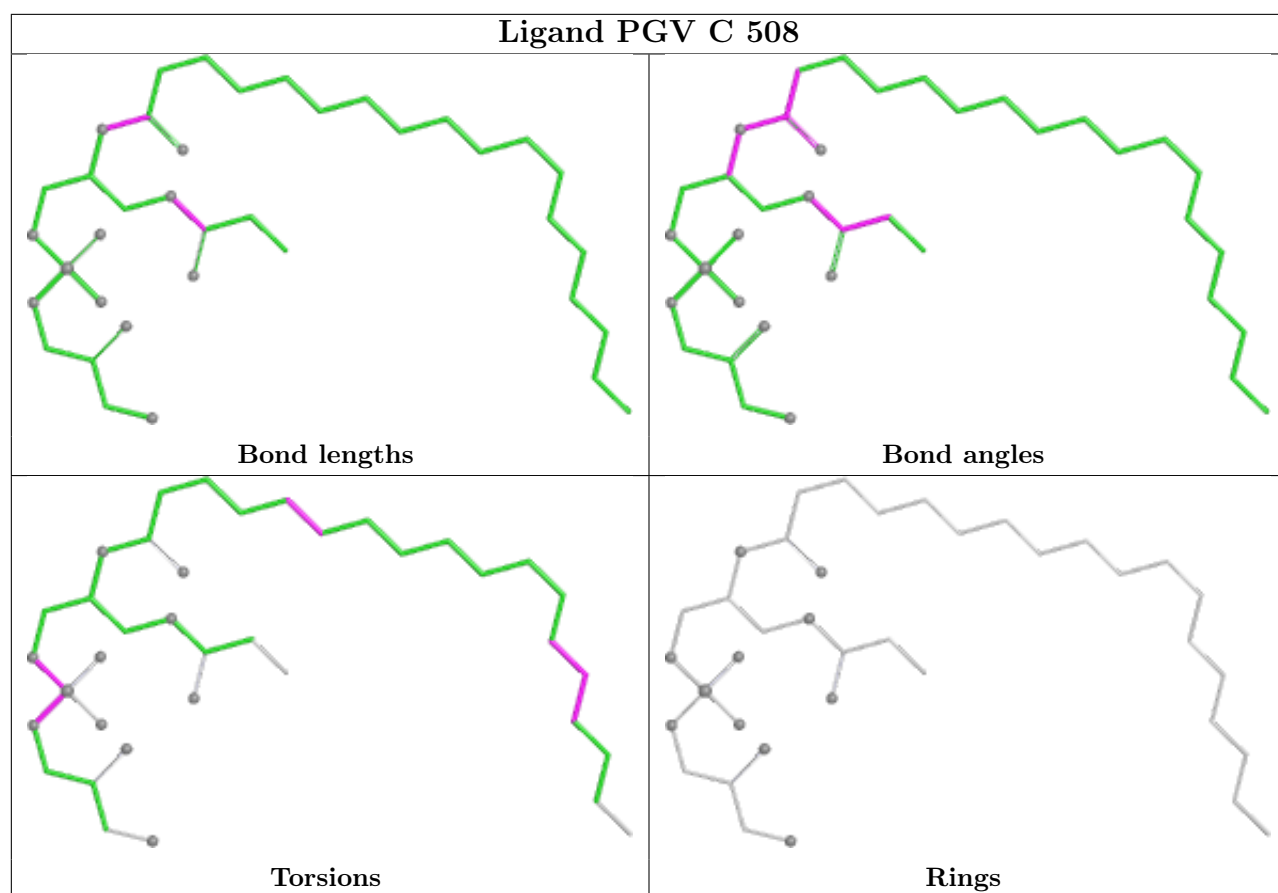
Ligand CRT I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

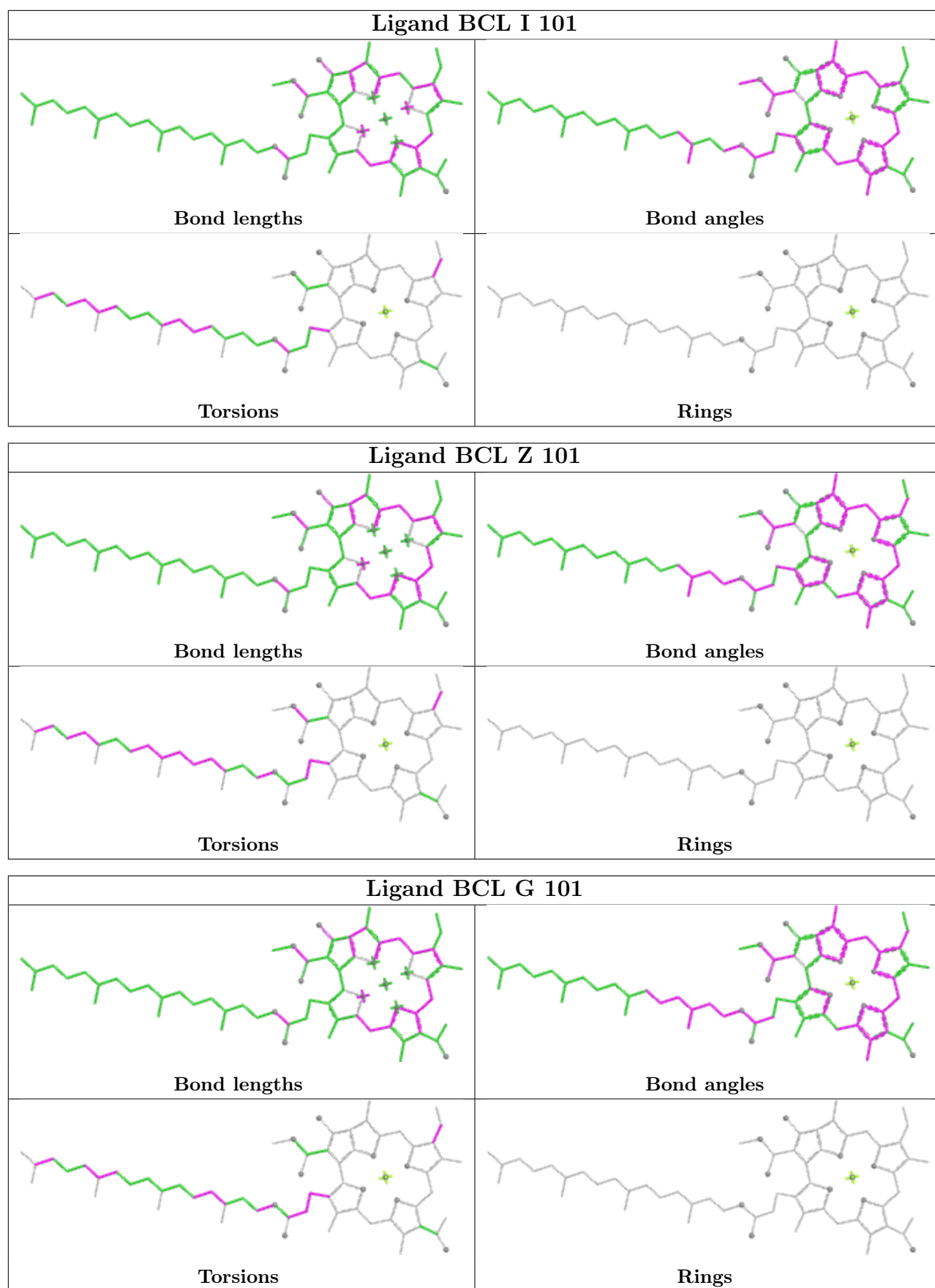
Ligand 8K6 X 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

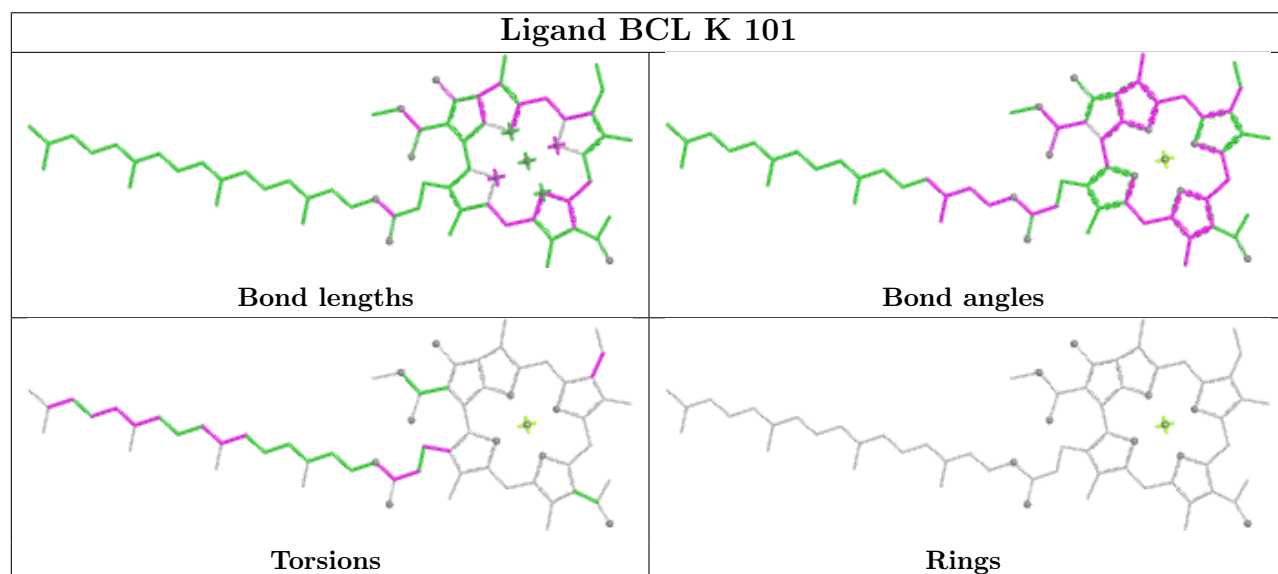
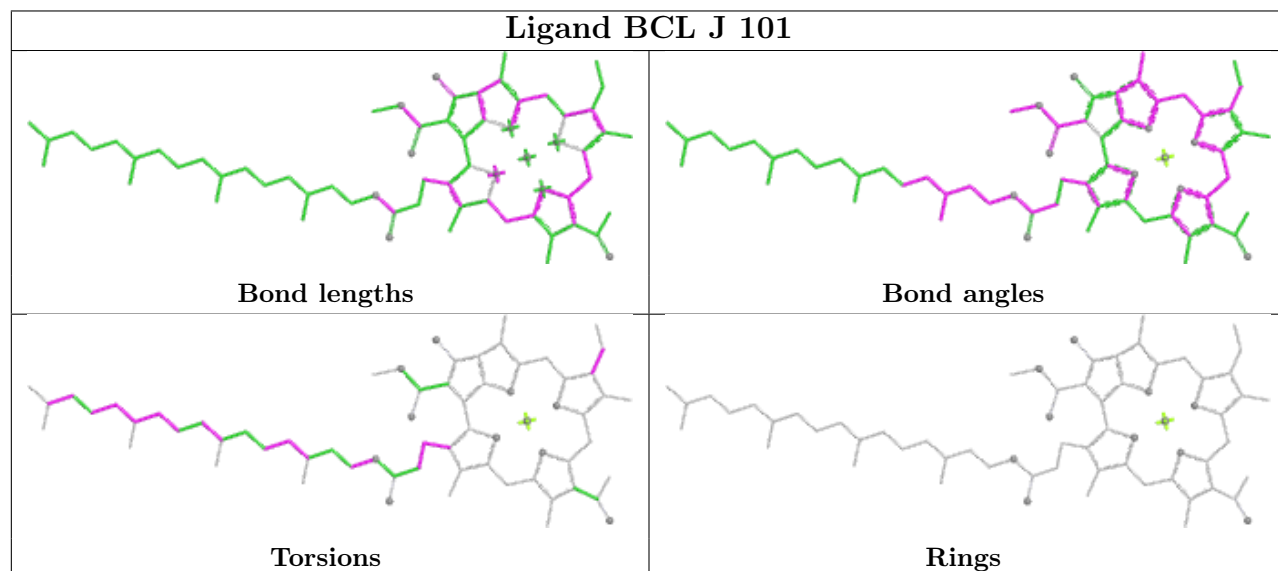
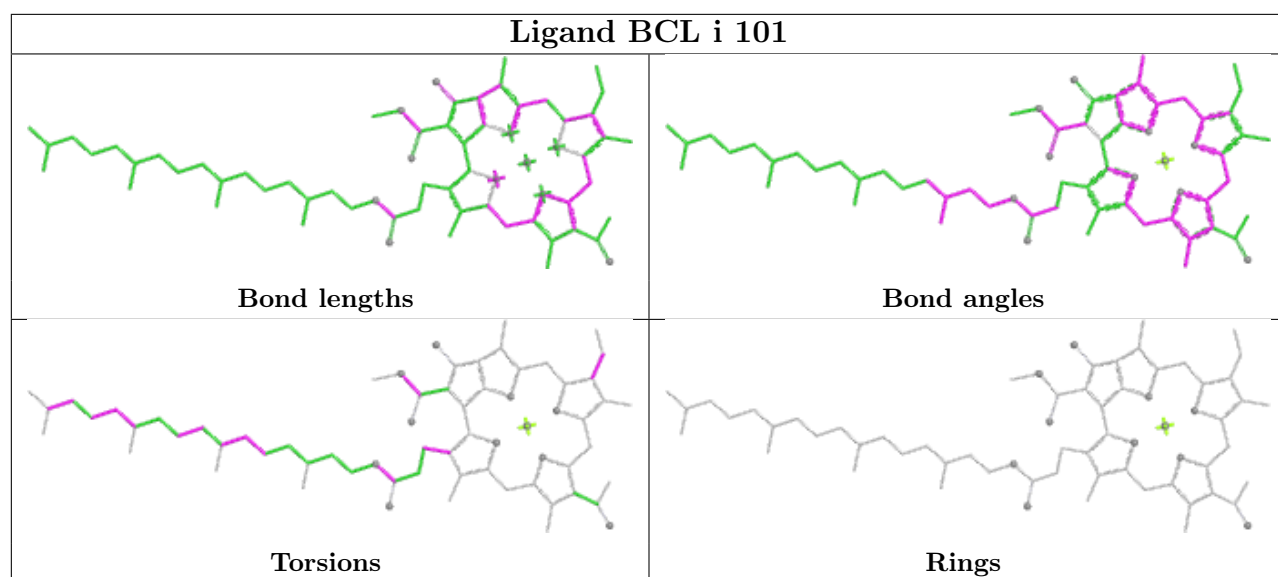


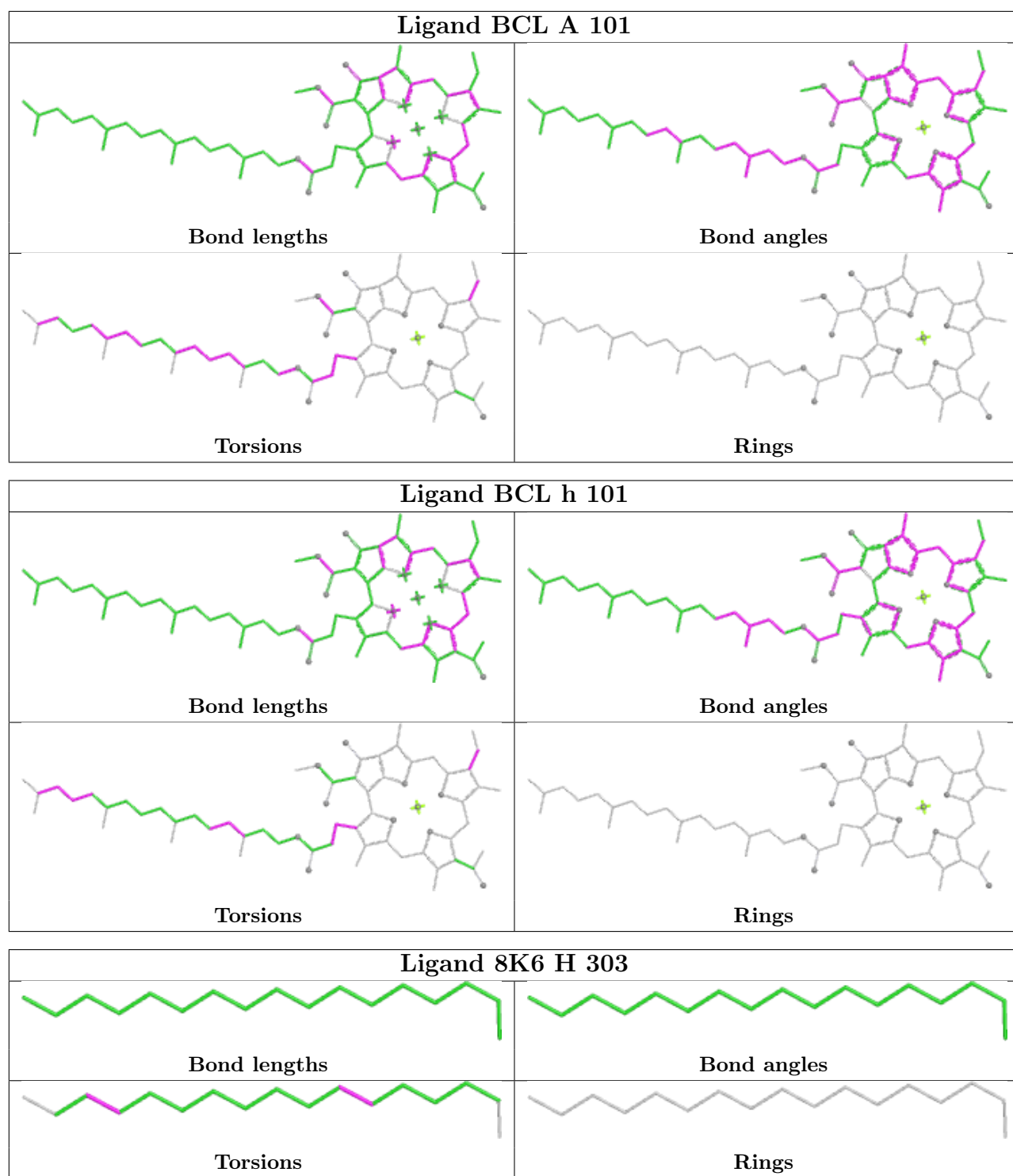


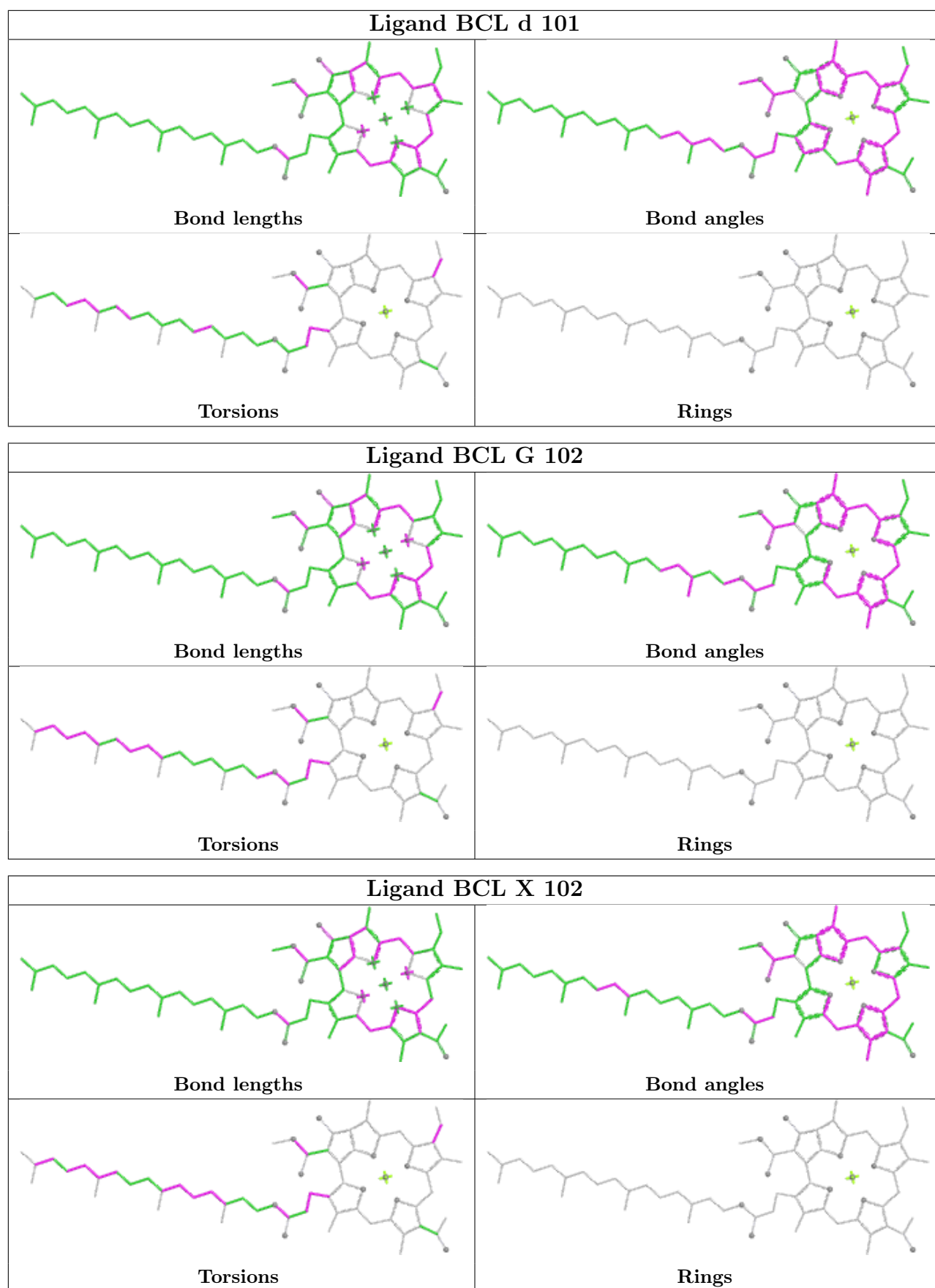


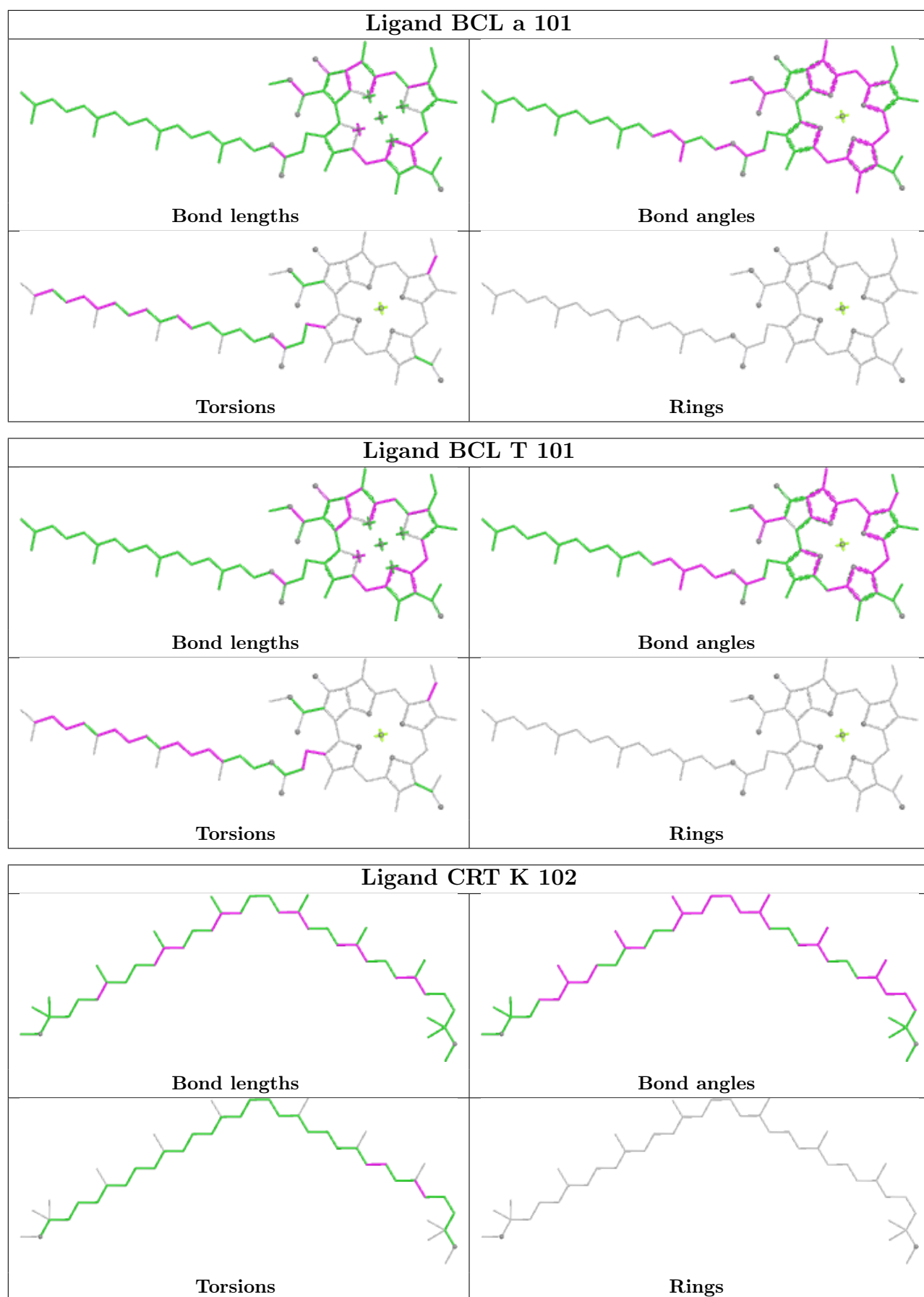


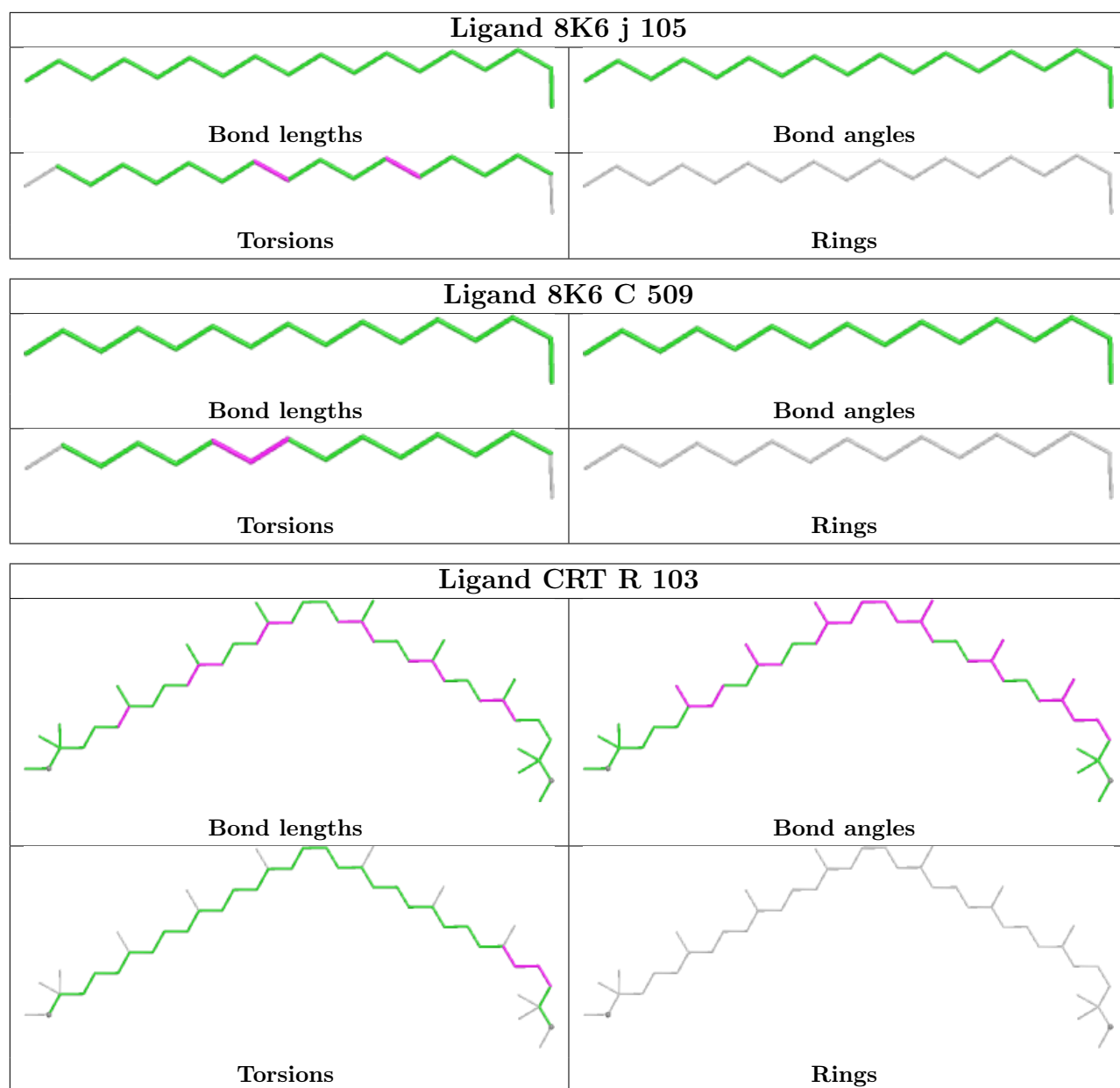


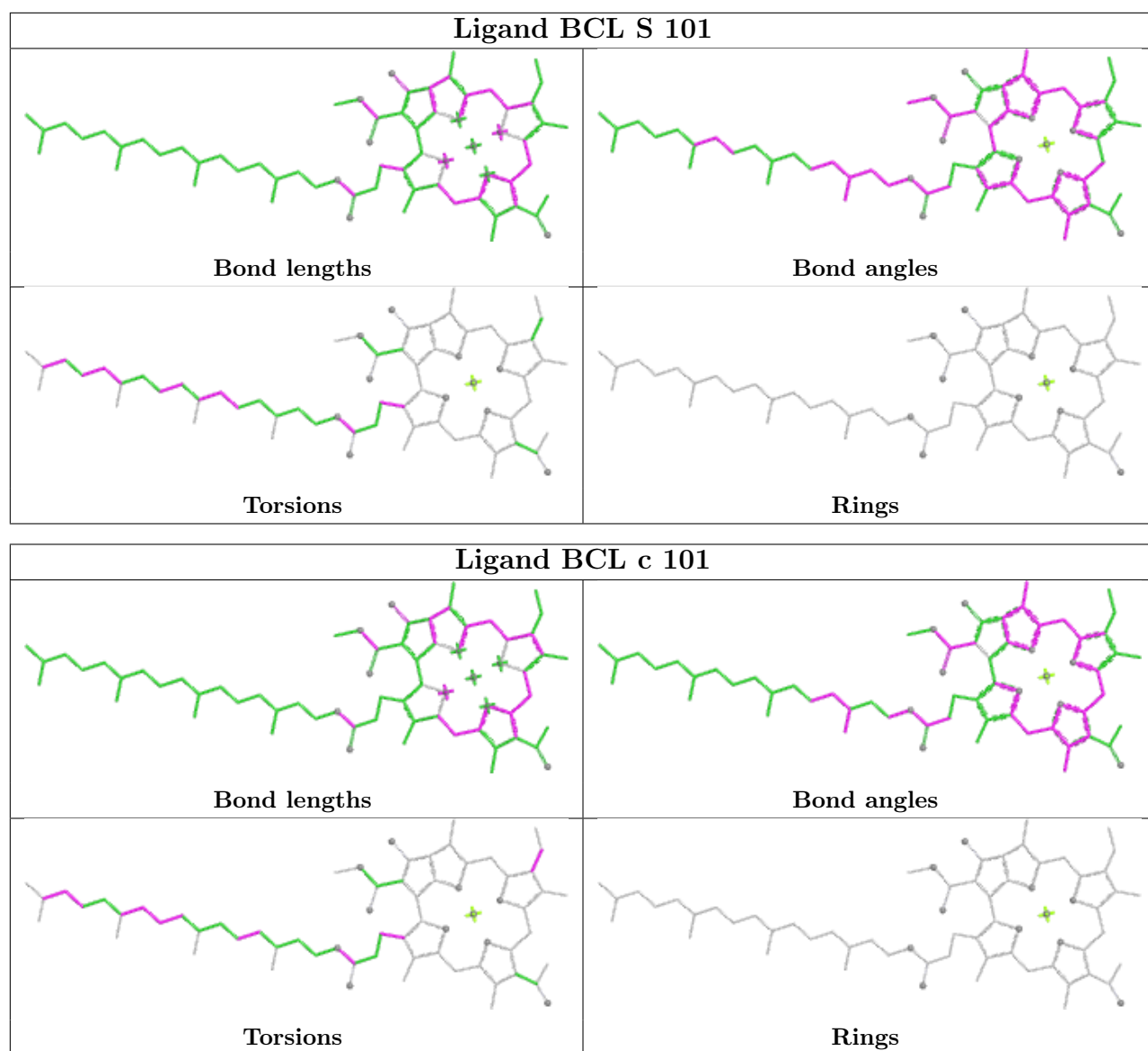


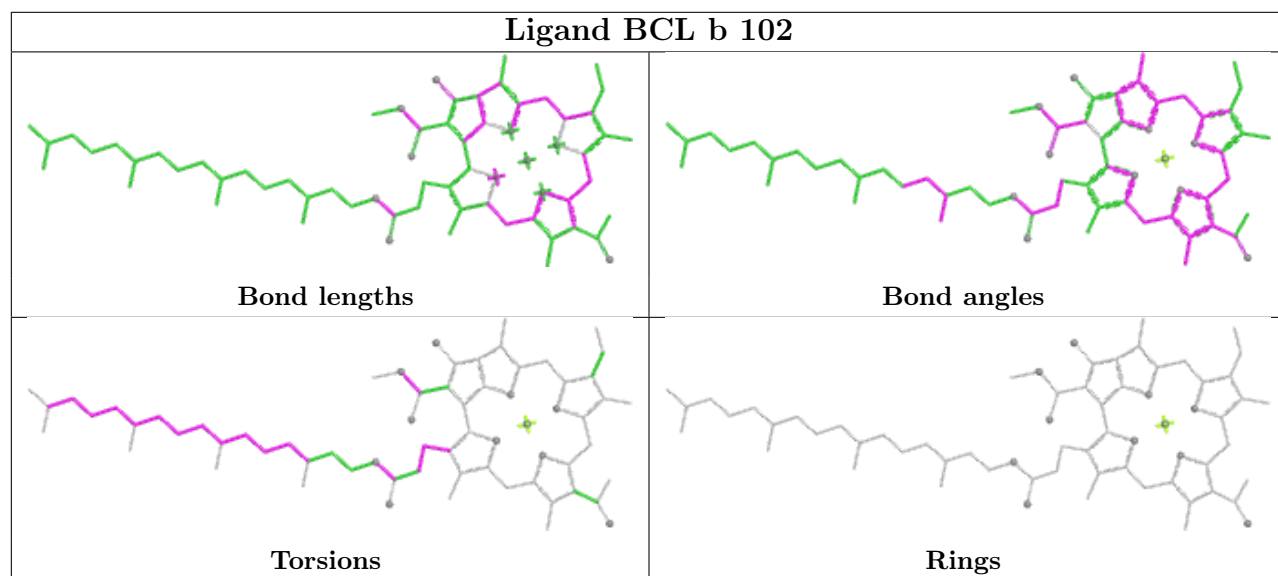
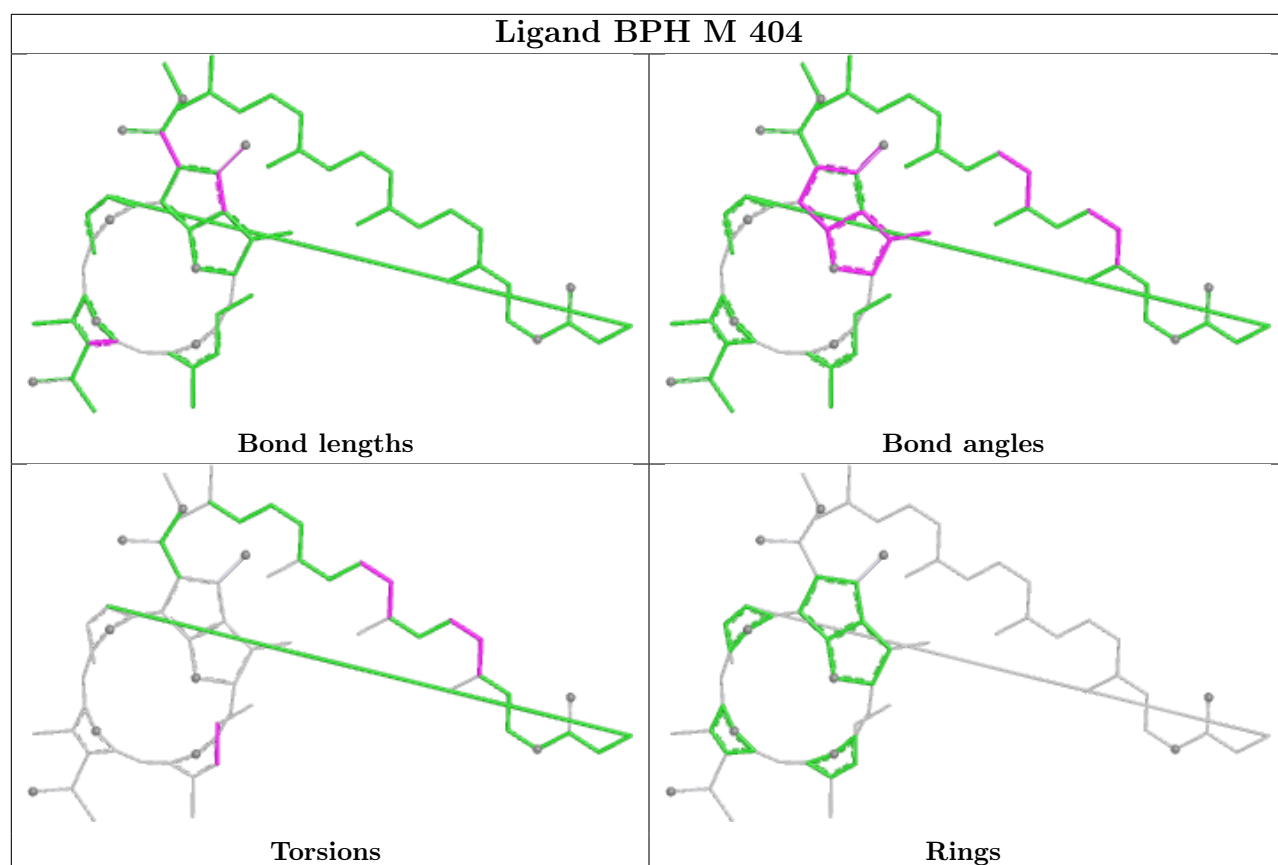


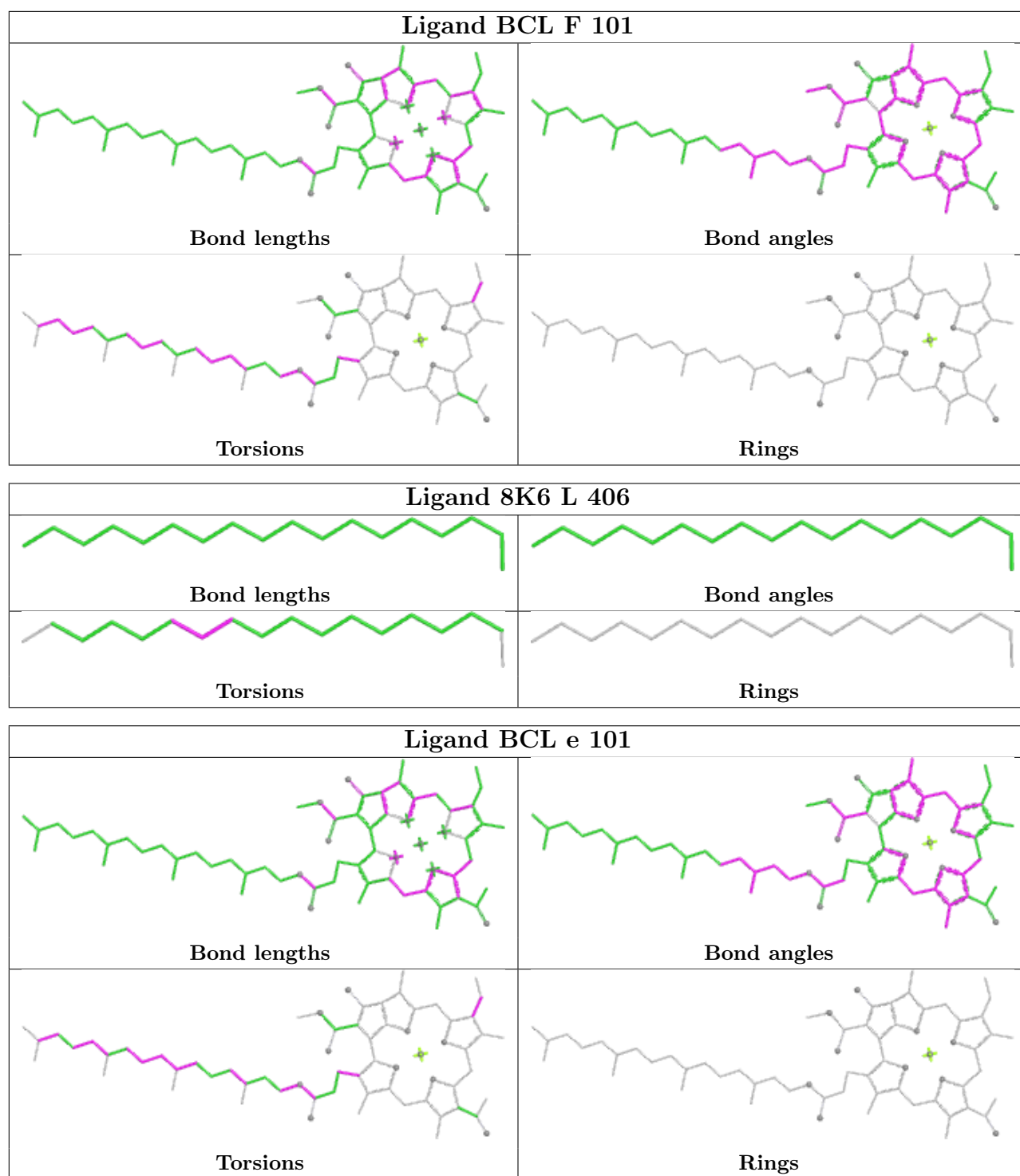


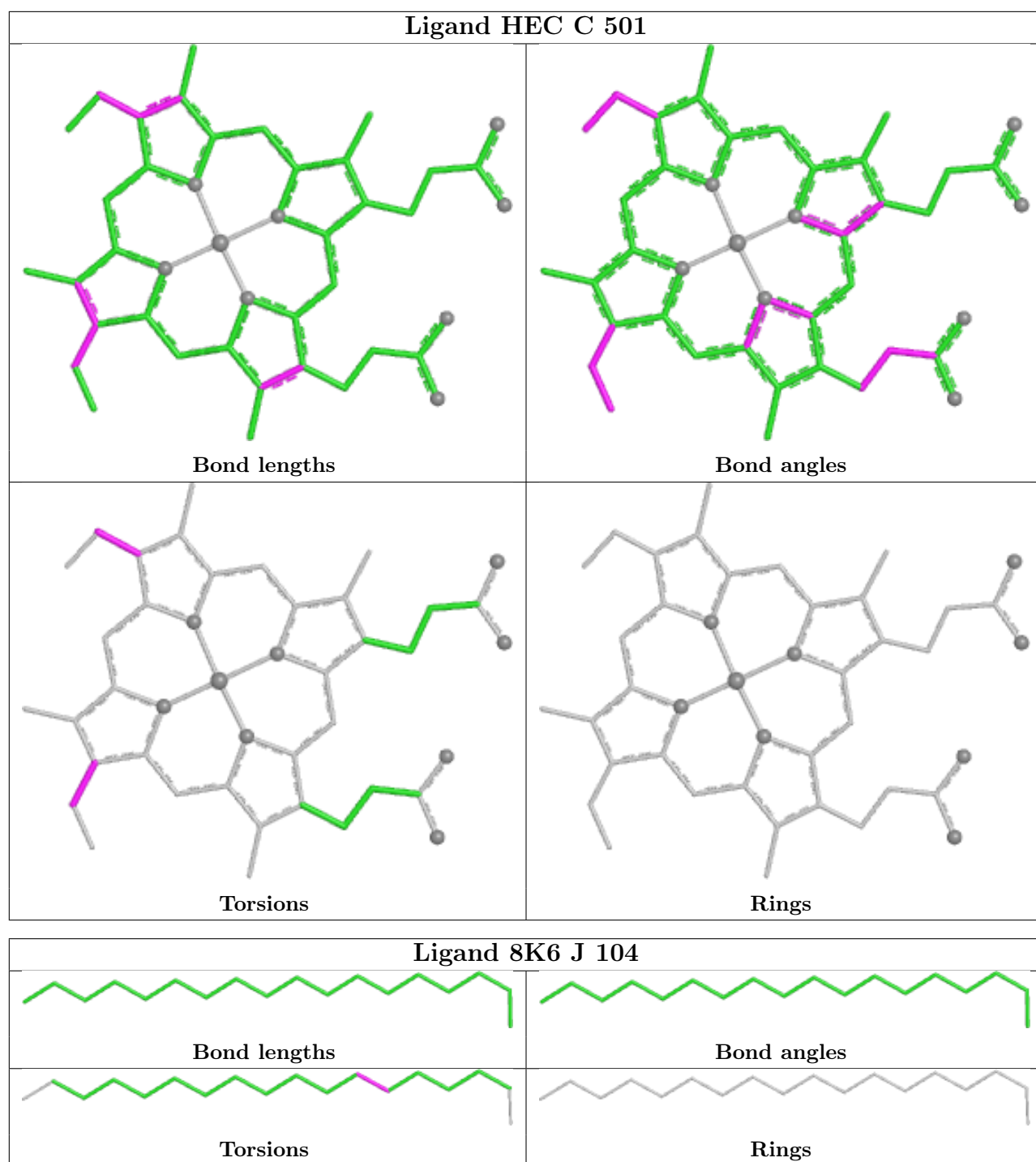


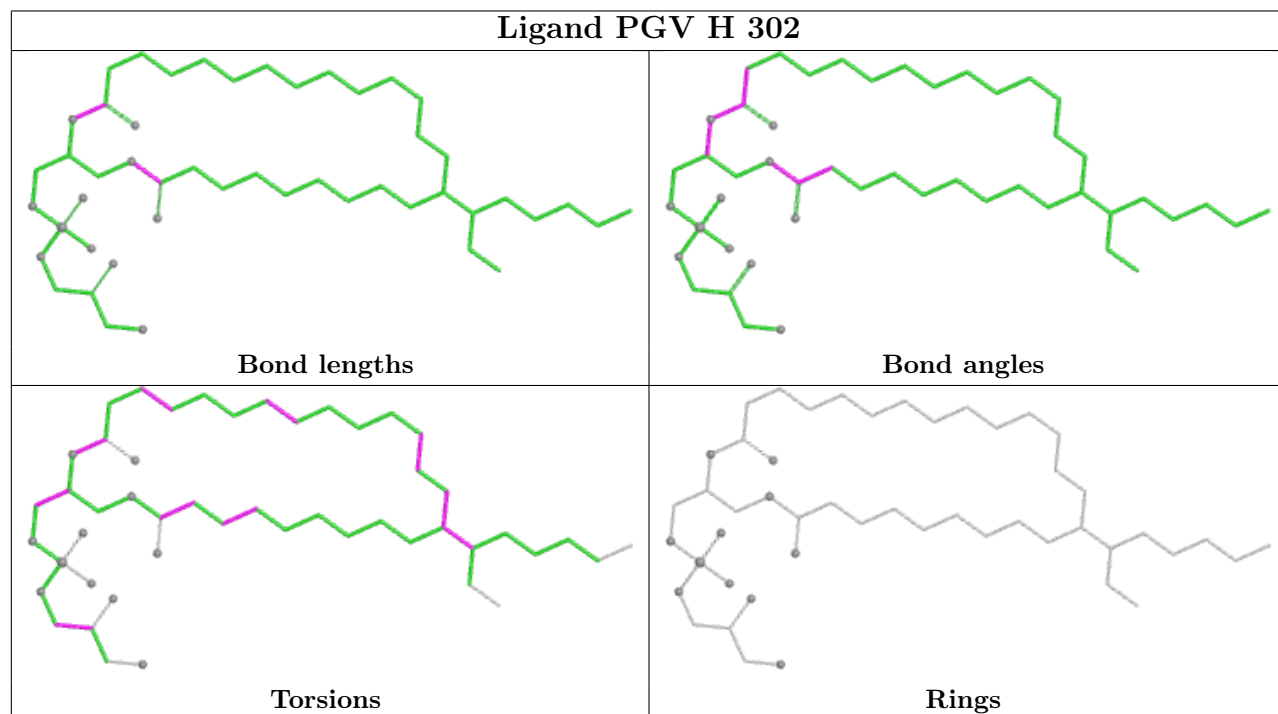
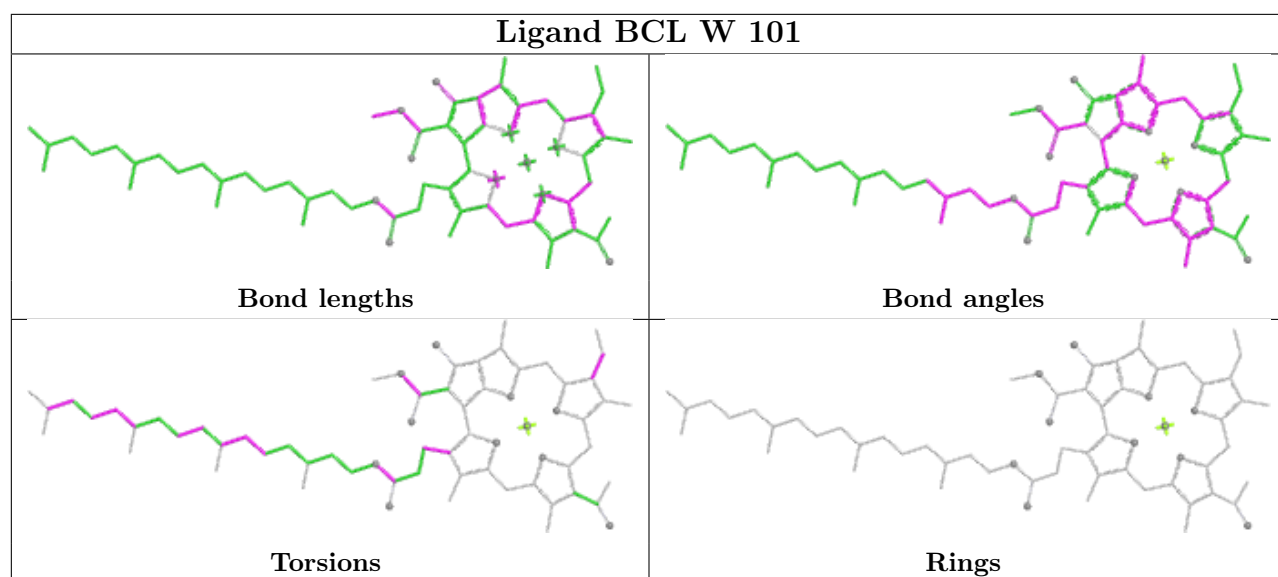


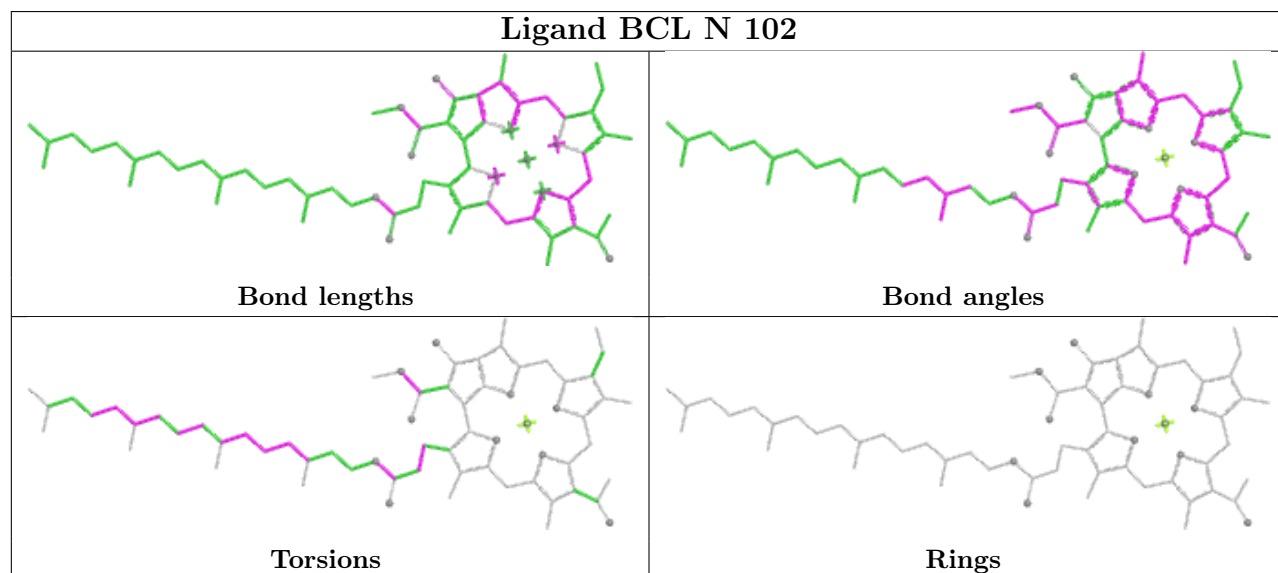
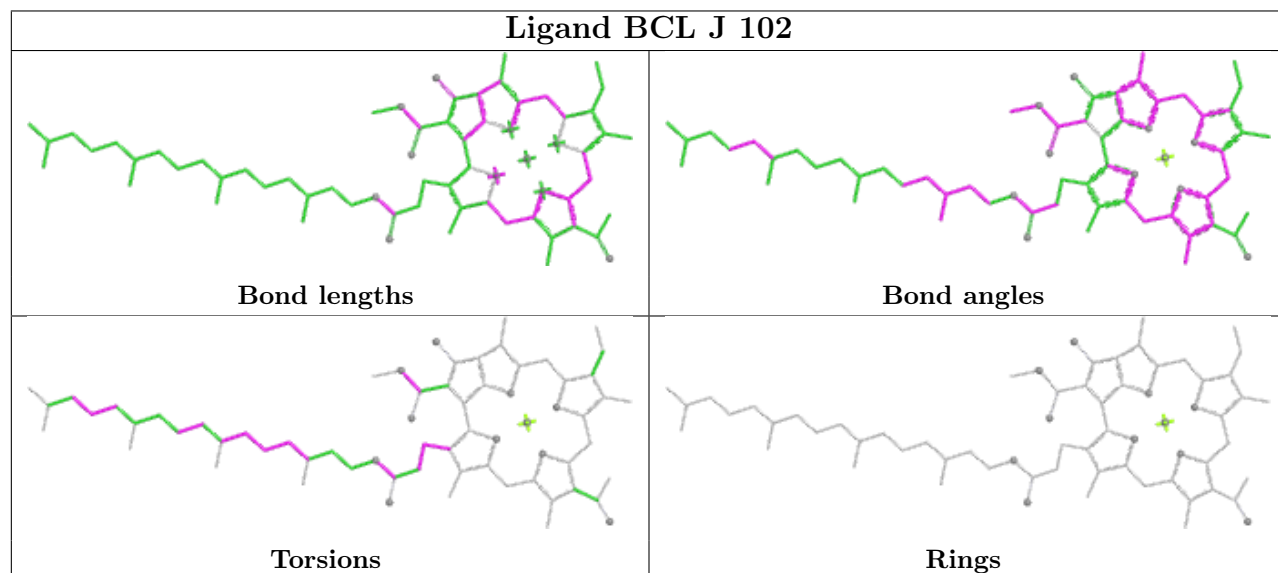
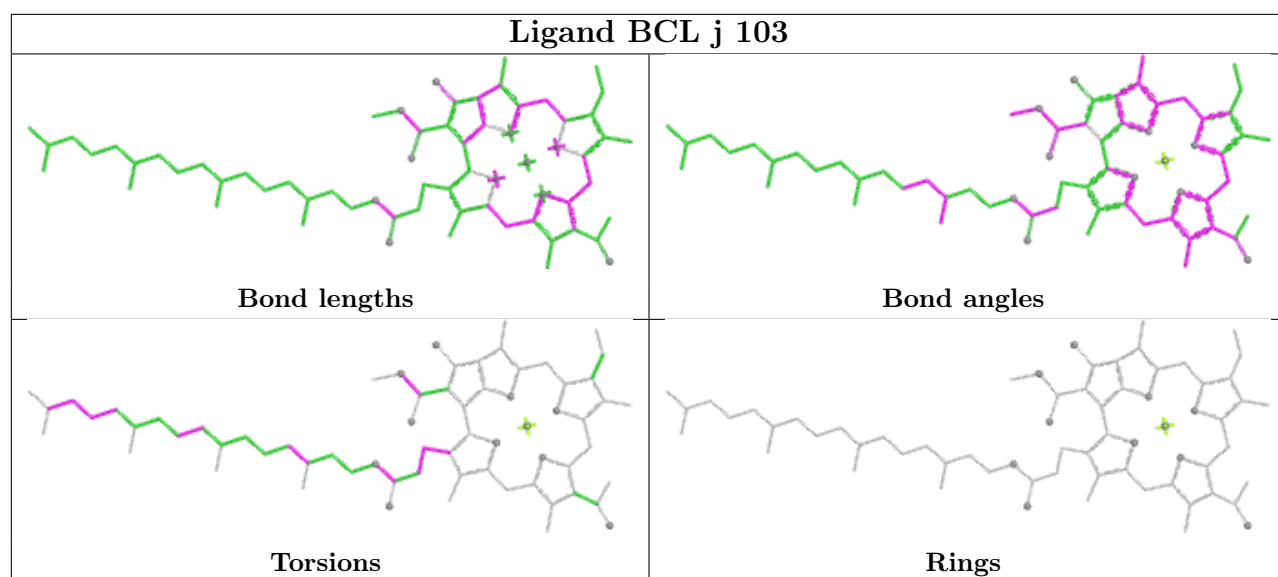


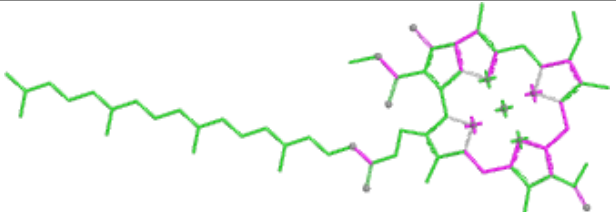
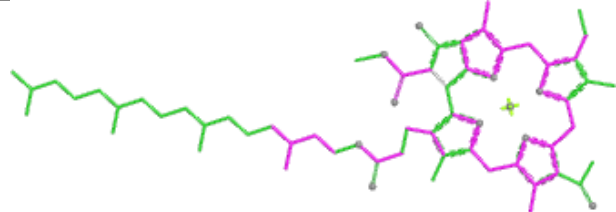
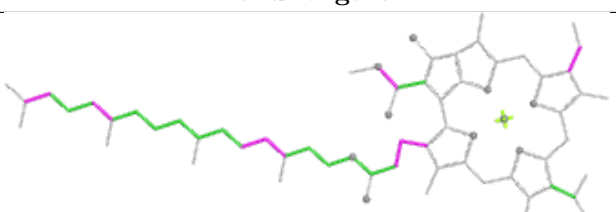
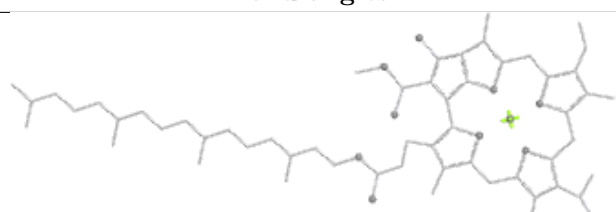


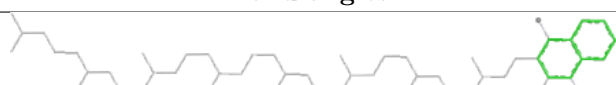


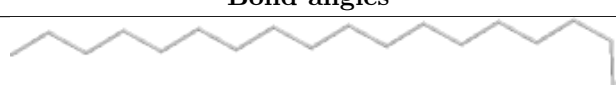




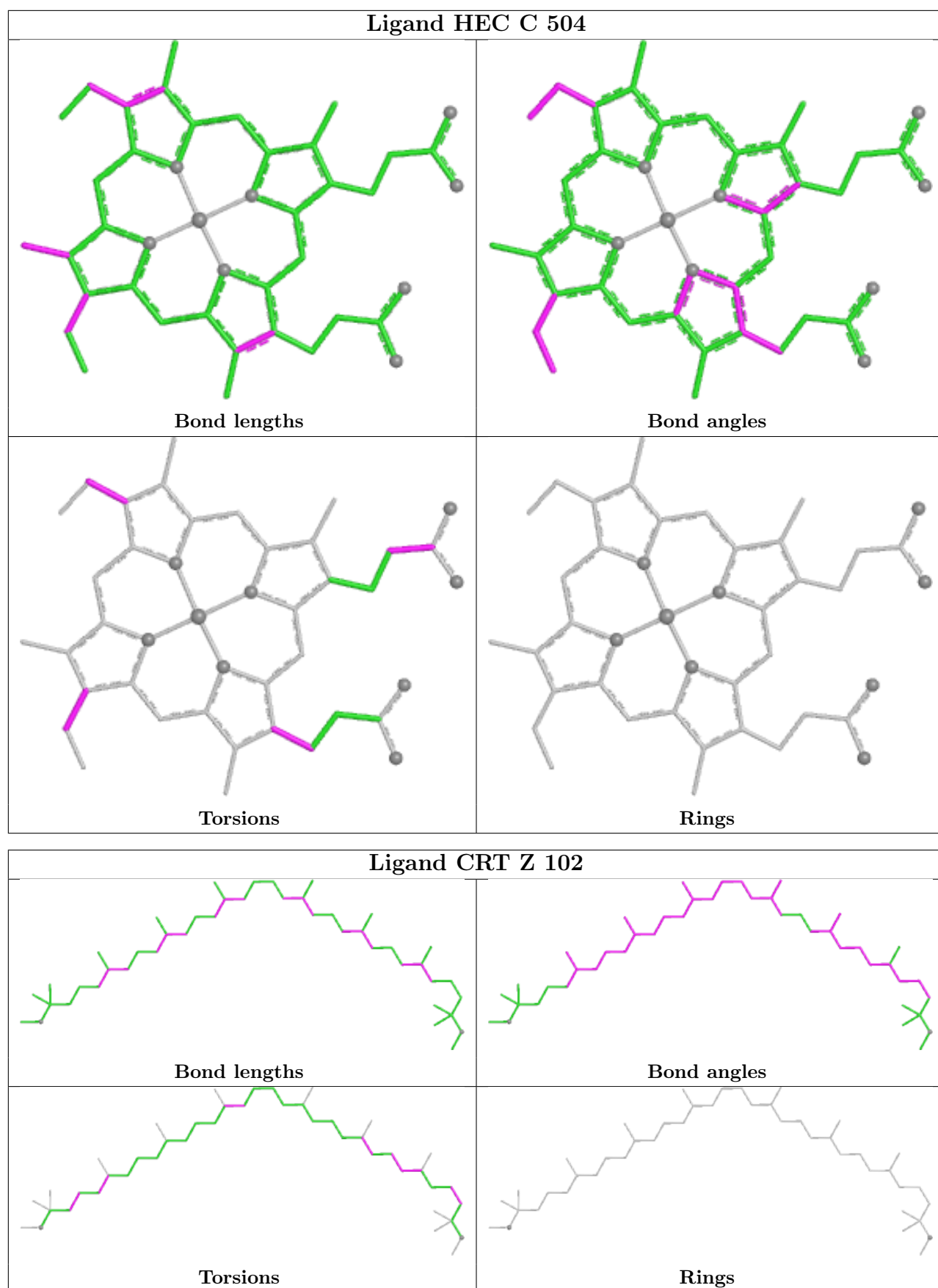


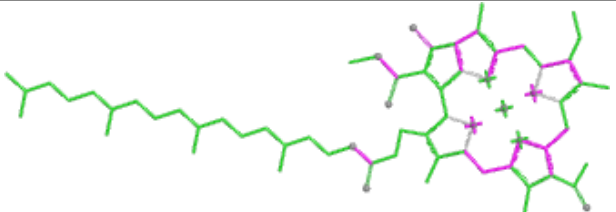
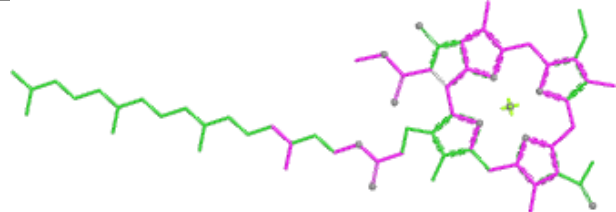
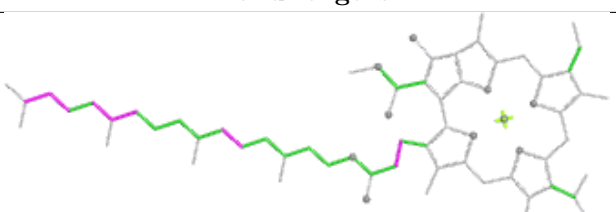
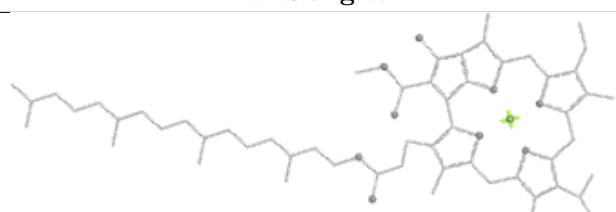
Ligand BCL j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

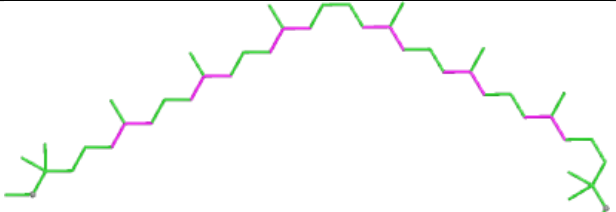
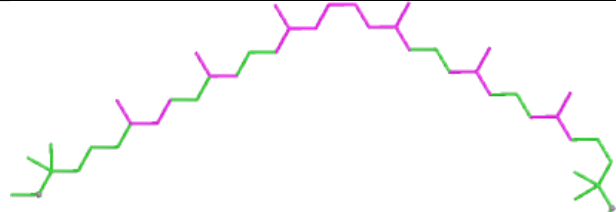
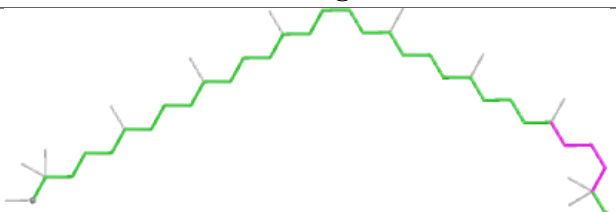
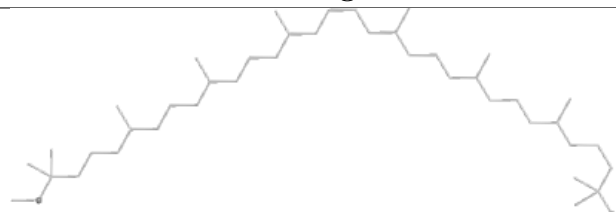
Ligand MQ8 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8K6 j 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

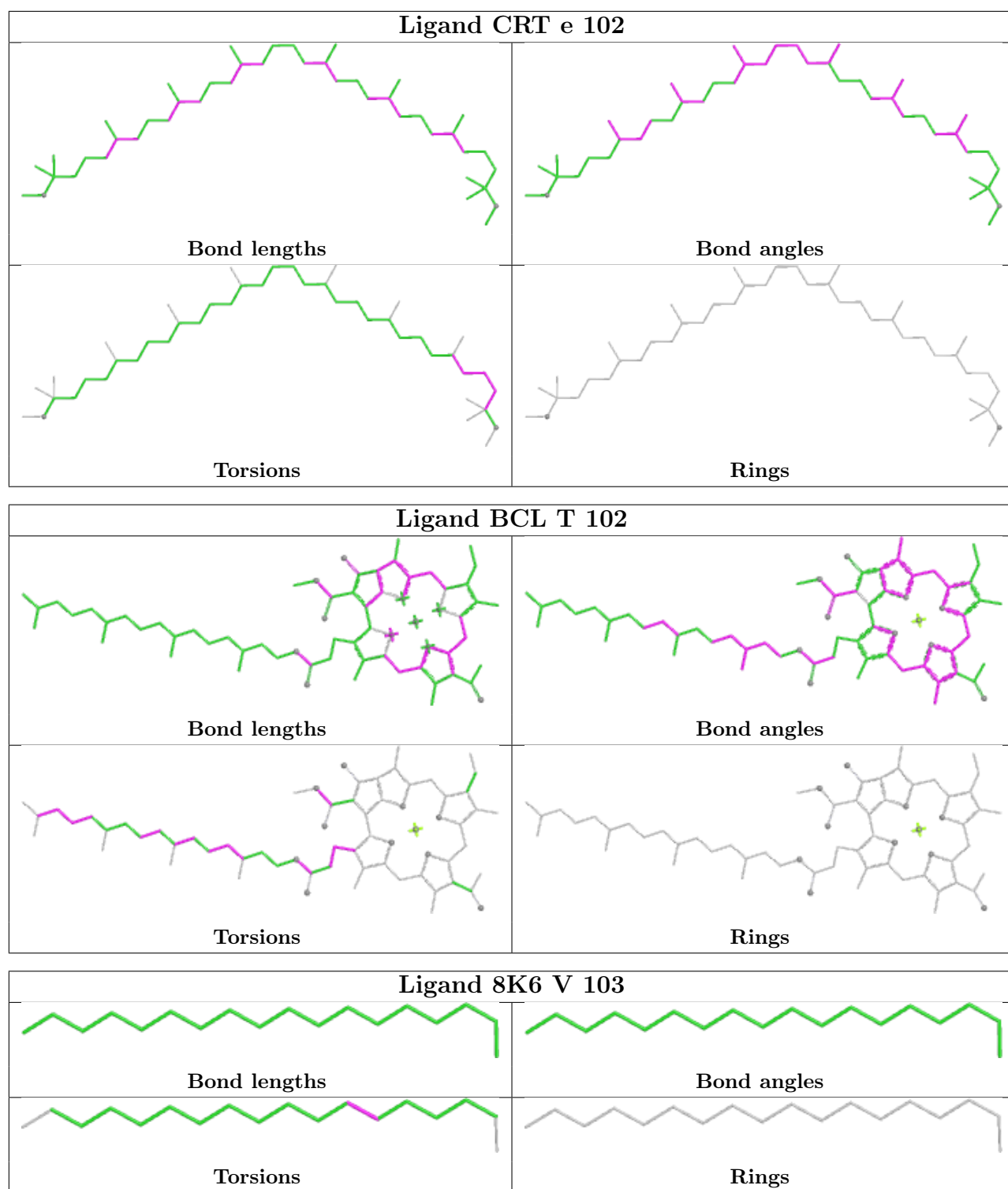
Ligand 8K6 L 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

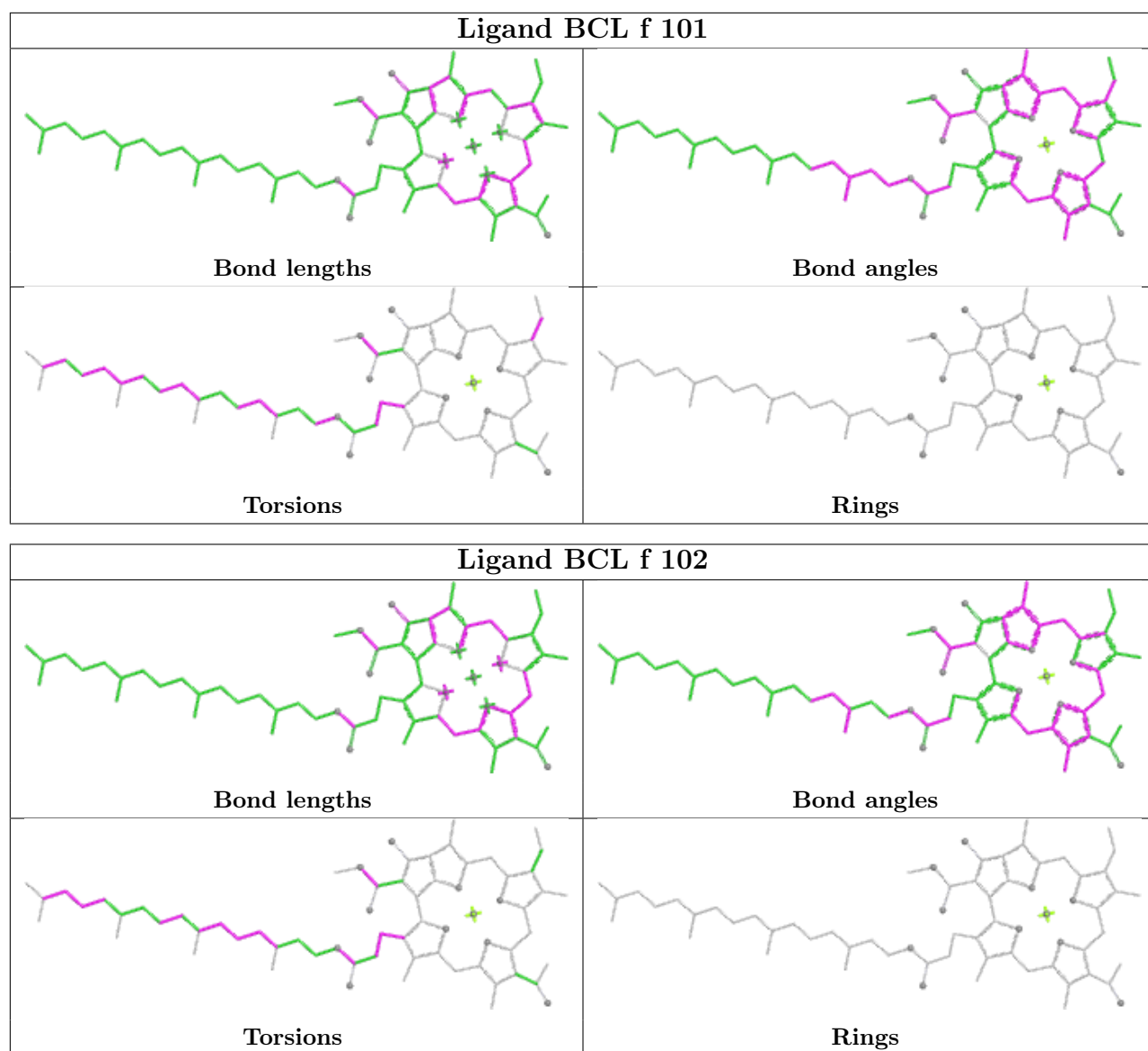


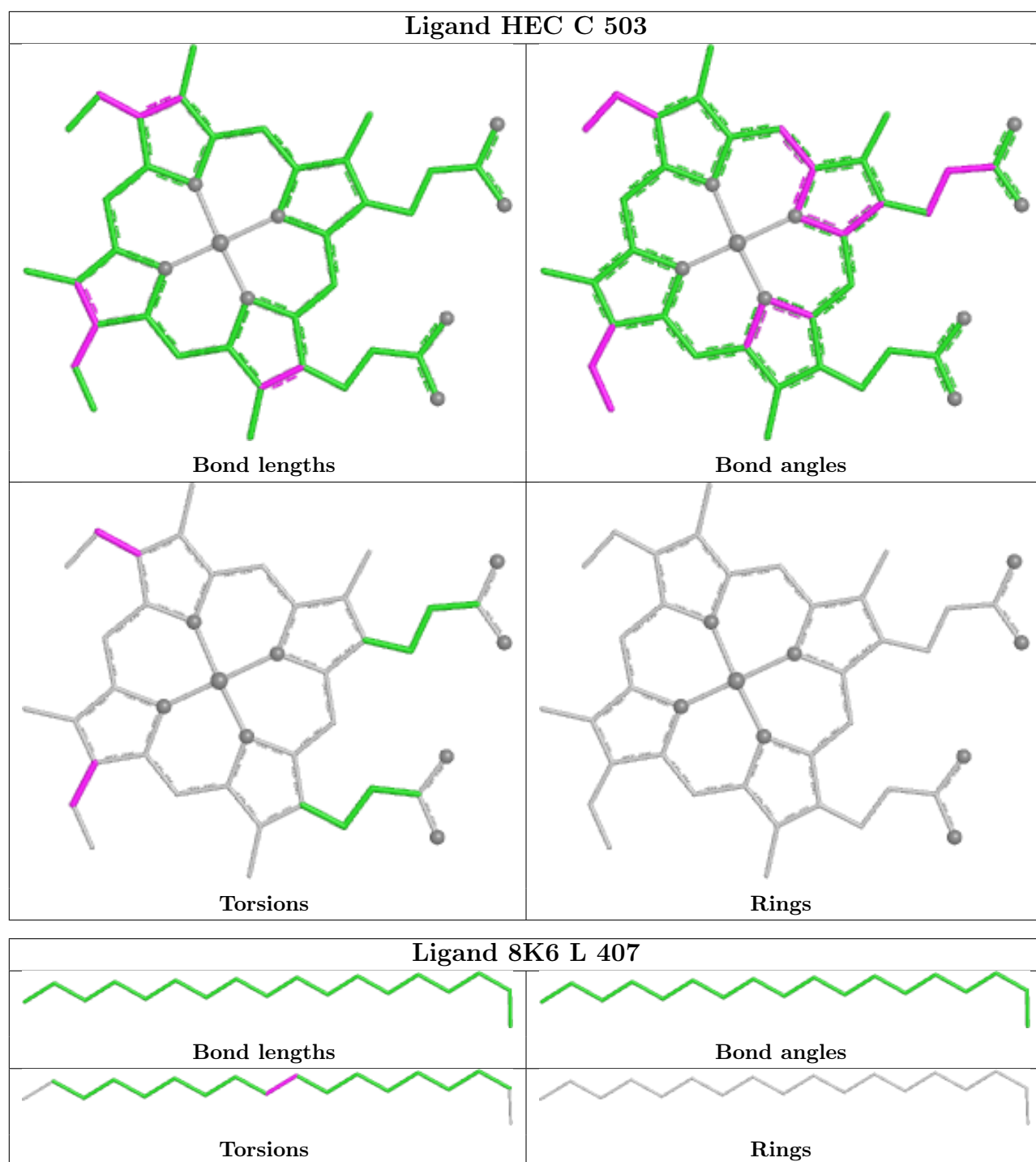
Ligand BCL L 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

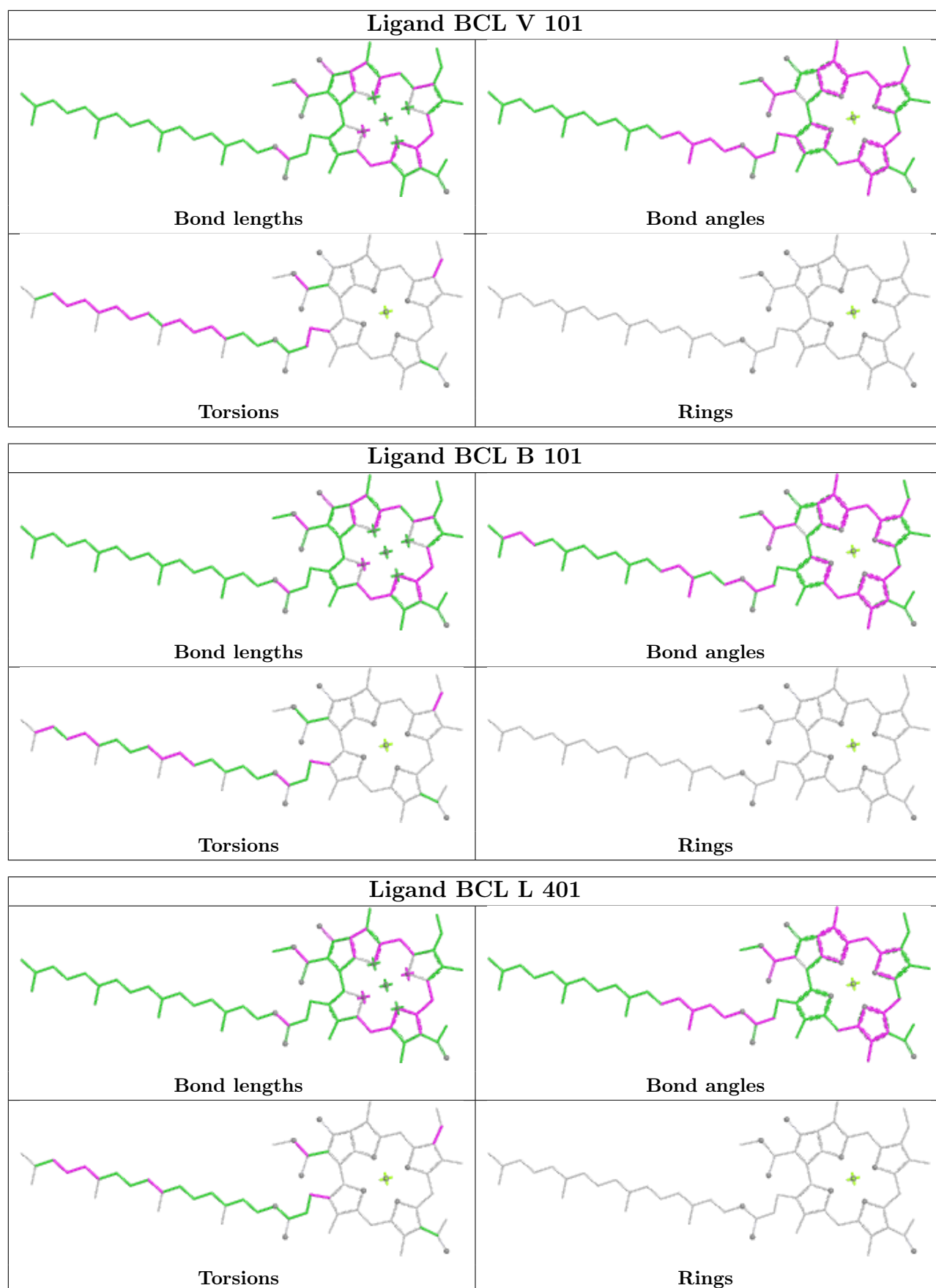
Ligand CRT N 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

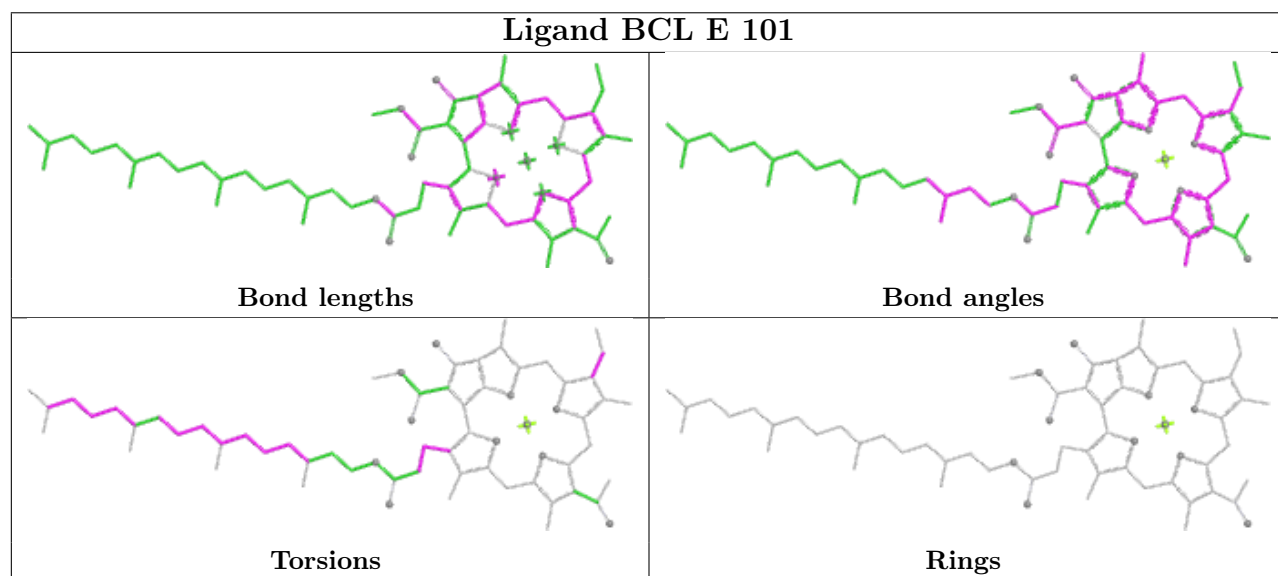
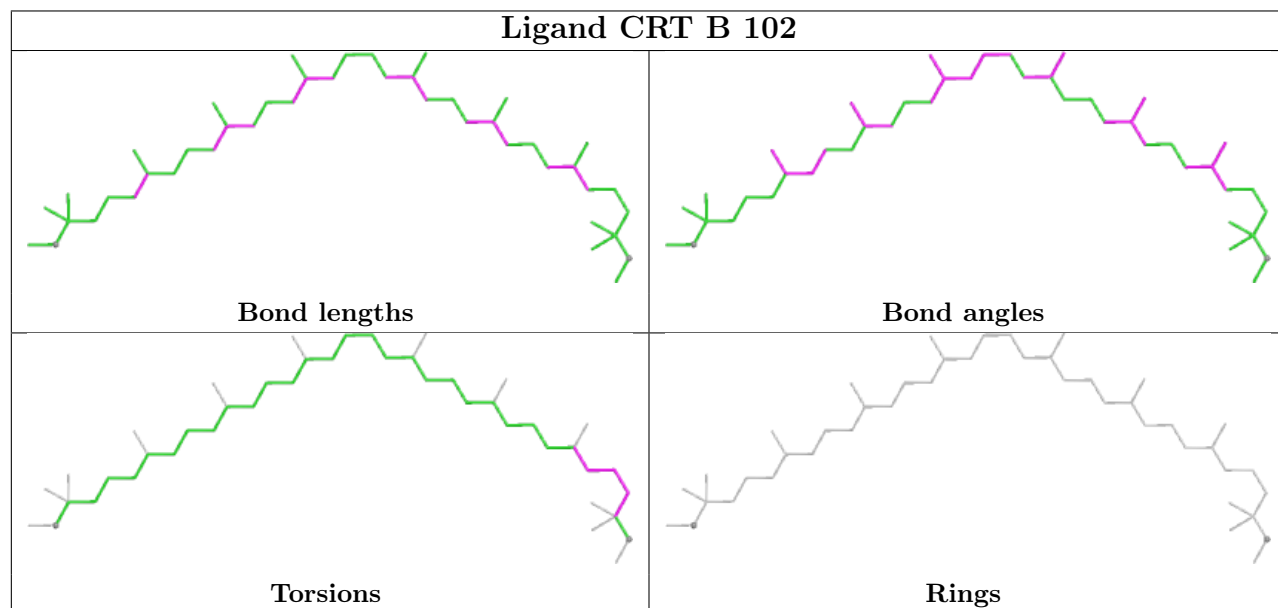
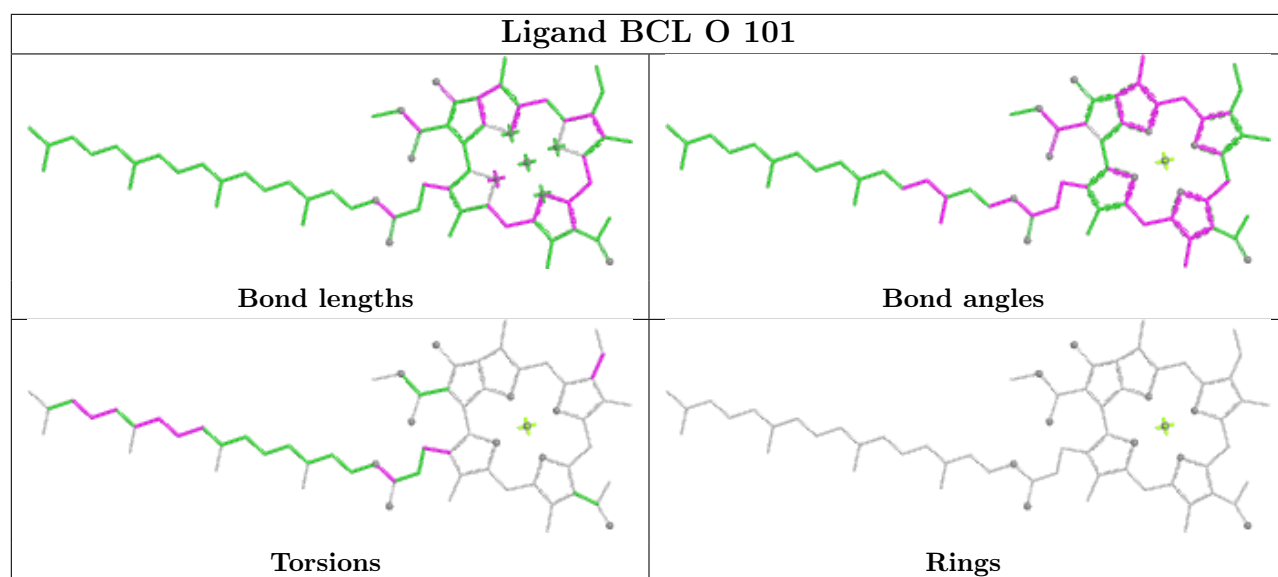
Ligand 8K6 f 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

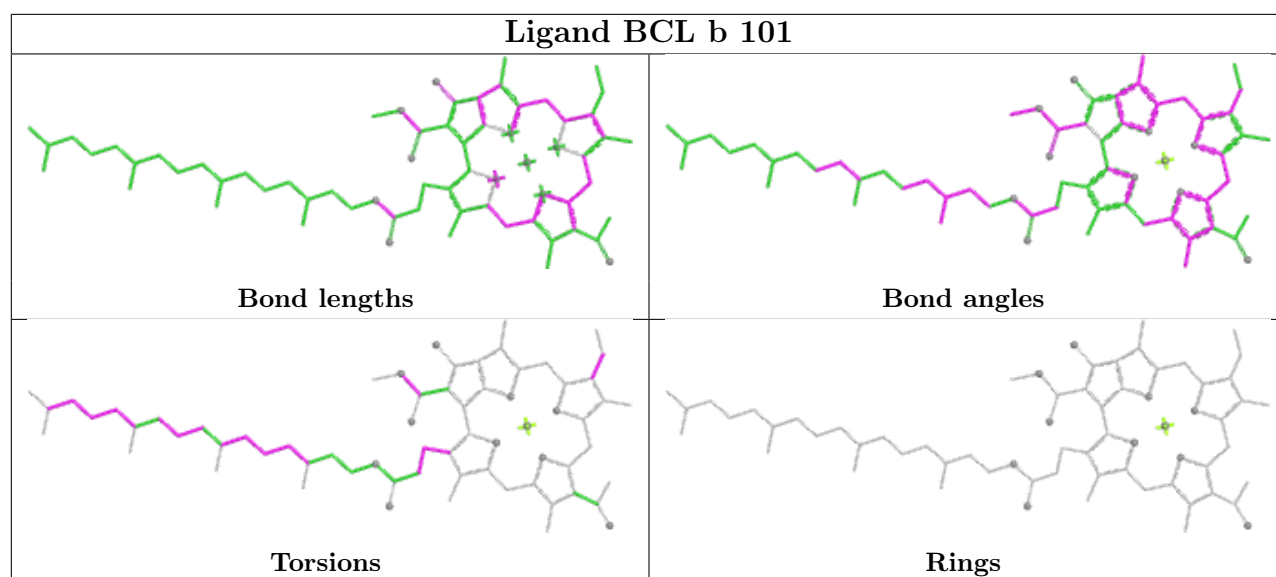












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

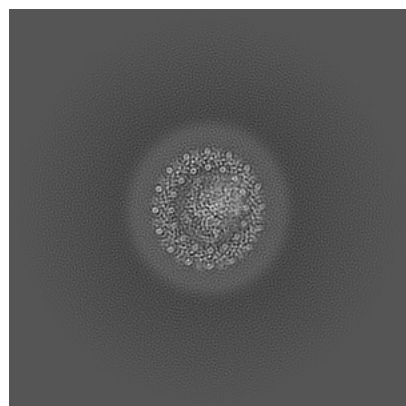
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60165. These allow visual inspection of the internal detail of the map and identification of artifacts.

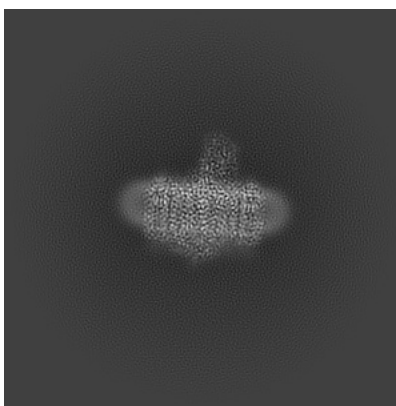
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

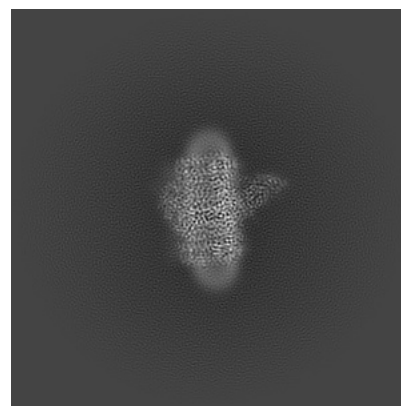
6.1.1 Primary map



X

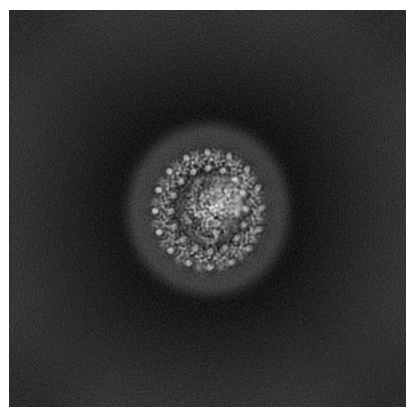


Y

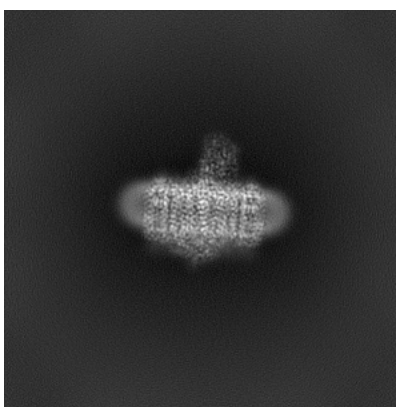


Z

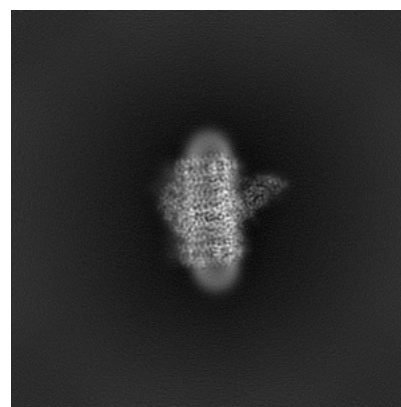
6.1.2 Raw map



X



Y

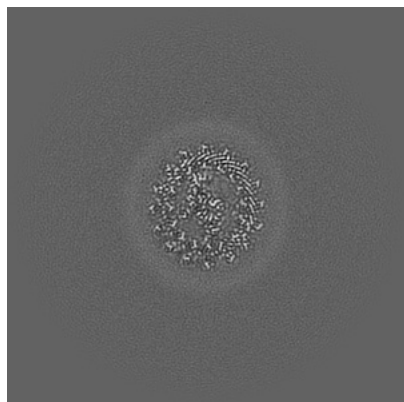


Z

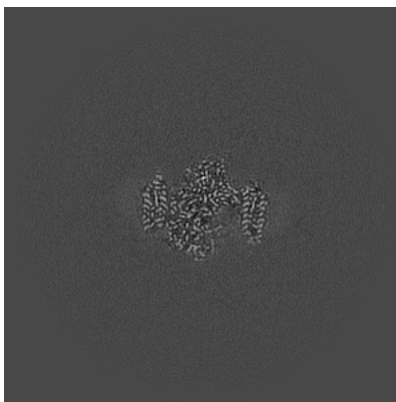
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

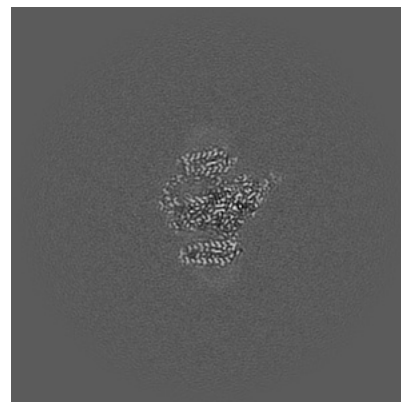
6.2.1 Primary map



X Index: 180

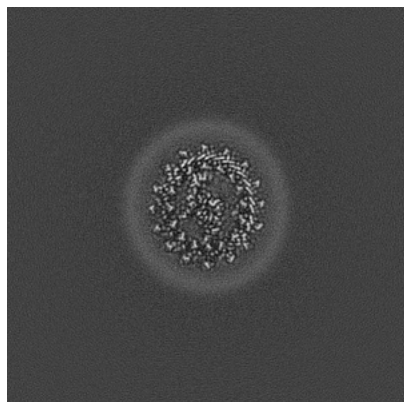


Y Index: 180

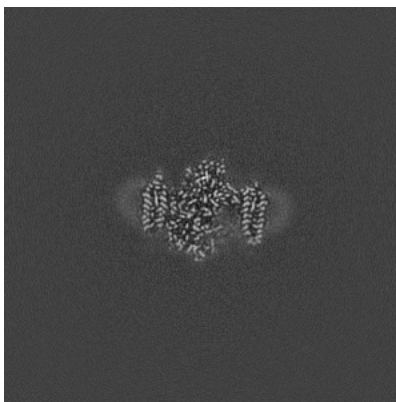


Z Index: 180

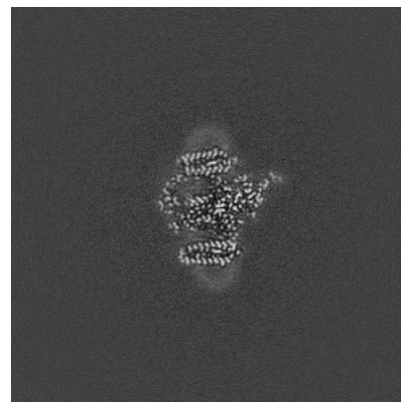
6.2.2 Raw map



X Index: 180



Y Index: 180

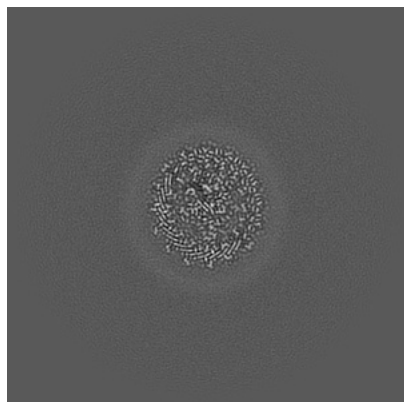


Z Index: 180

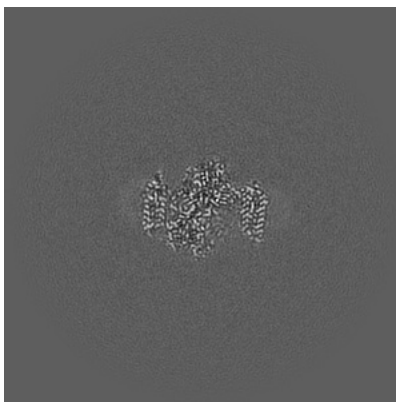
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

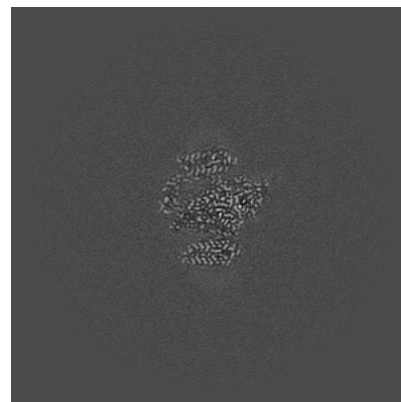
6.3.1 Primary map



X Index: 187

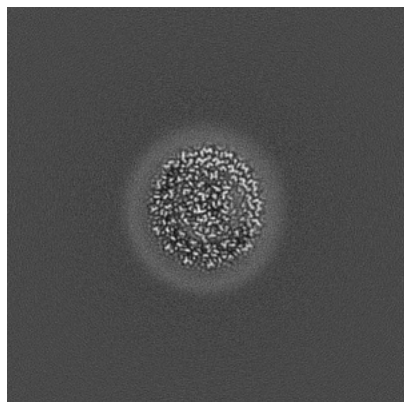


Y Index: 179

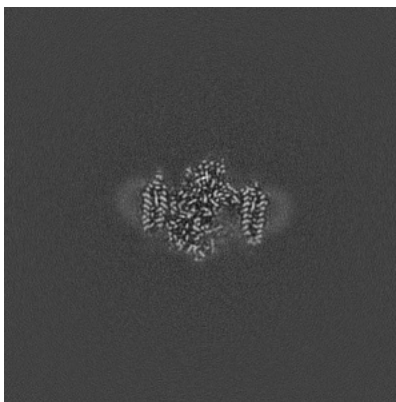


Z Index: 179

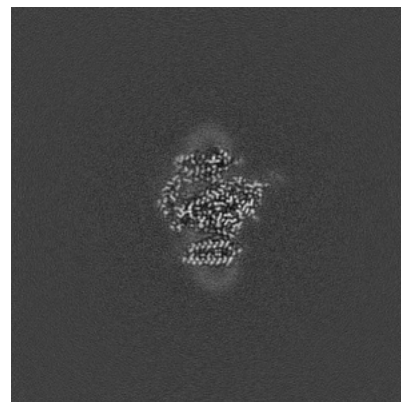
6.3.2 Raw map



X Index: 192



Y Index: 180

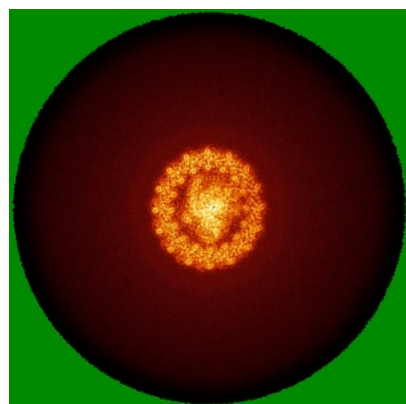


Z Index: 178

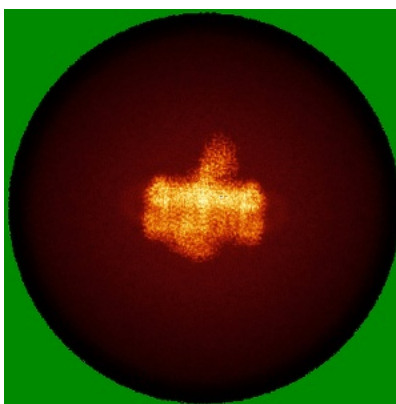
The images above show the largest variance slices of the map in three orthogonal directions.

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

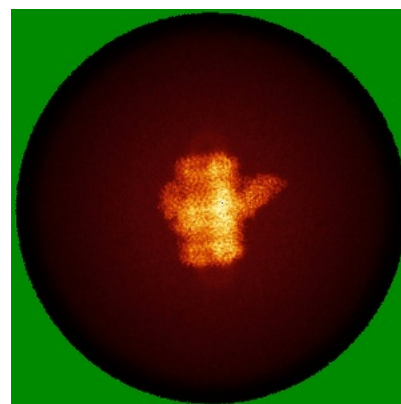
6.4.1 Primary map



X

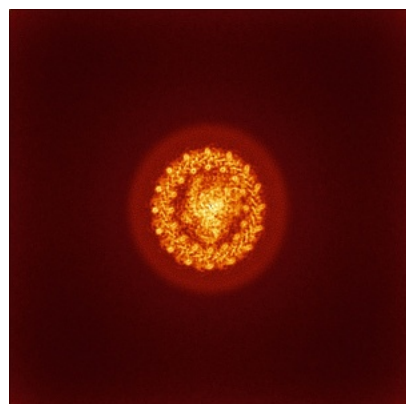


Y

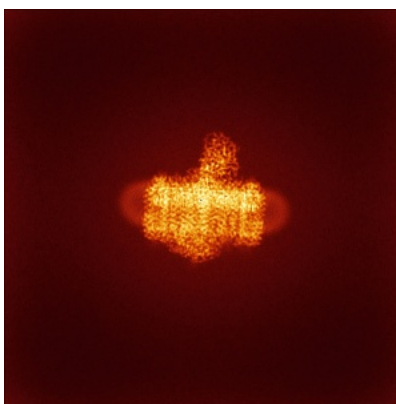


Z

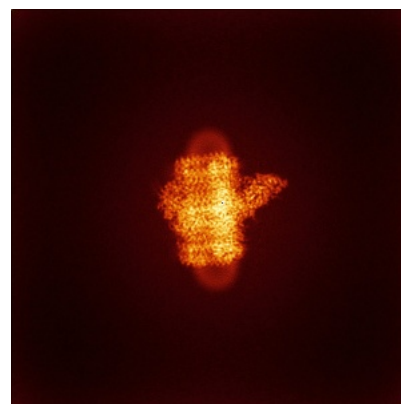
6.4.2 Raw map



X



Y

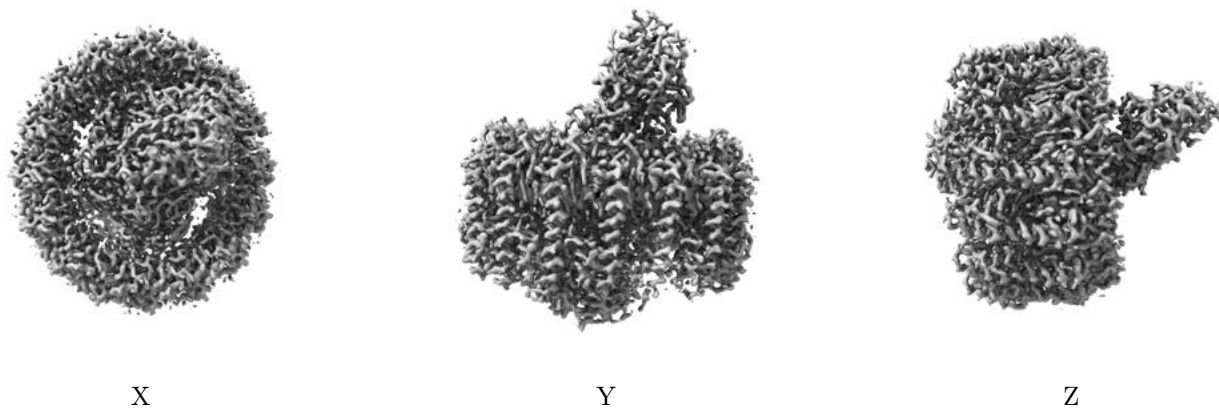


Z

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.

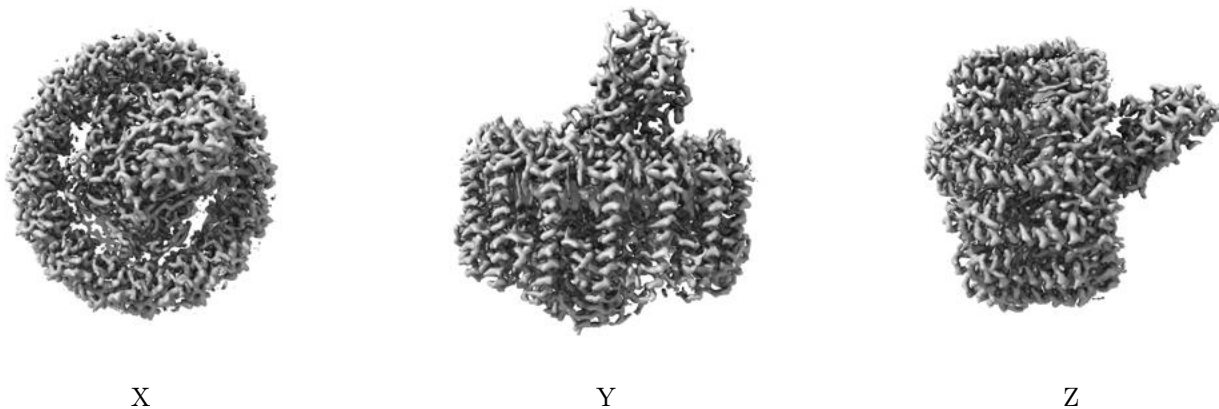
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.562. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

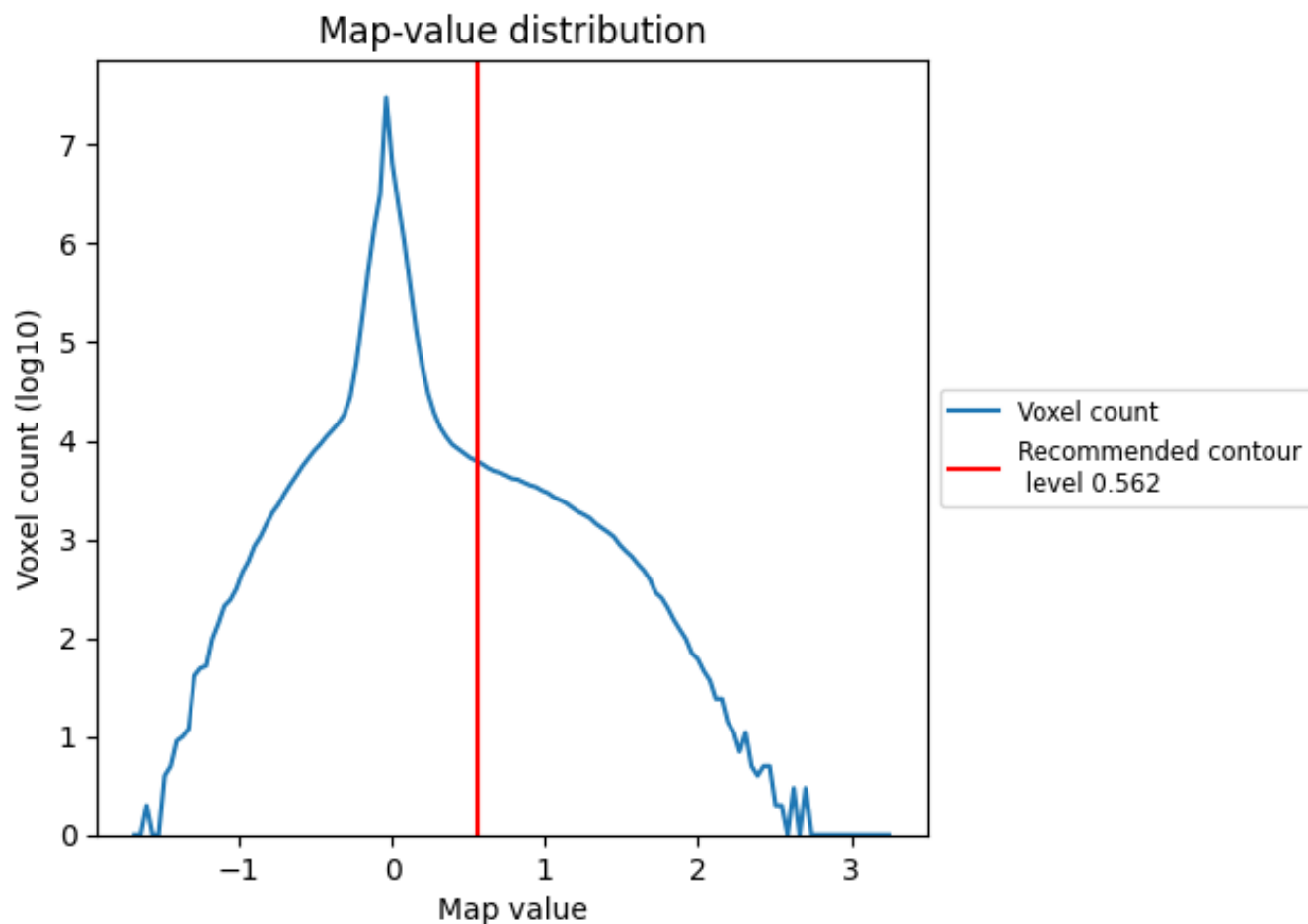
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

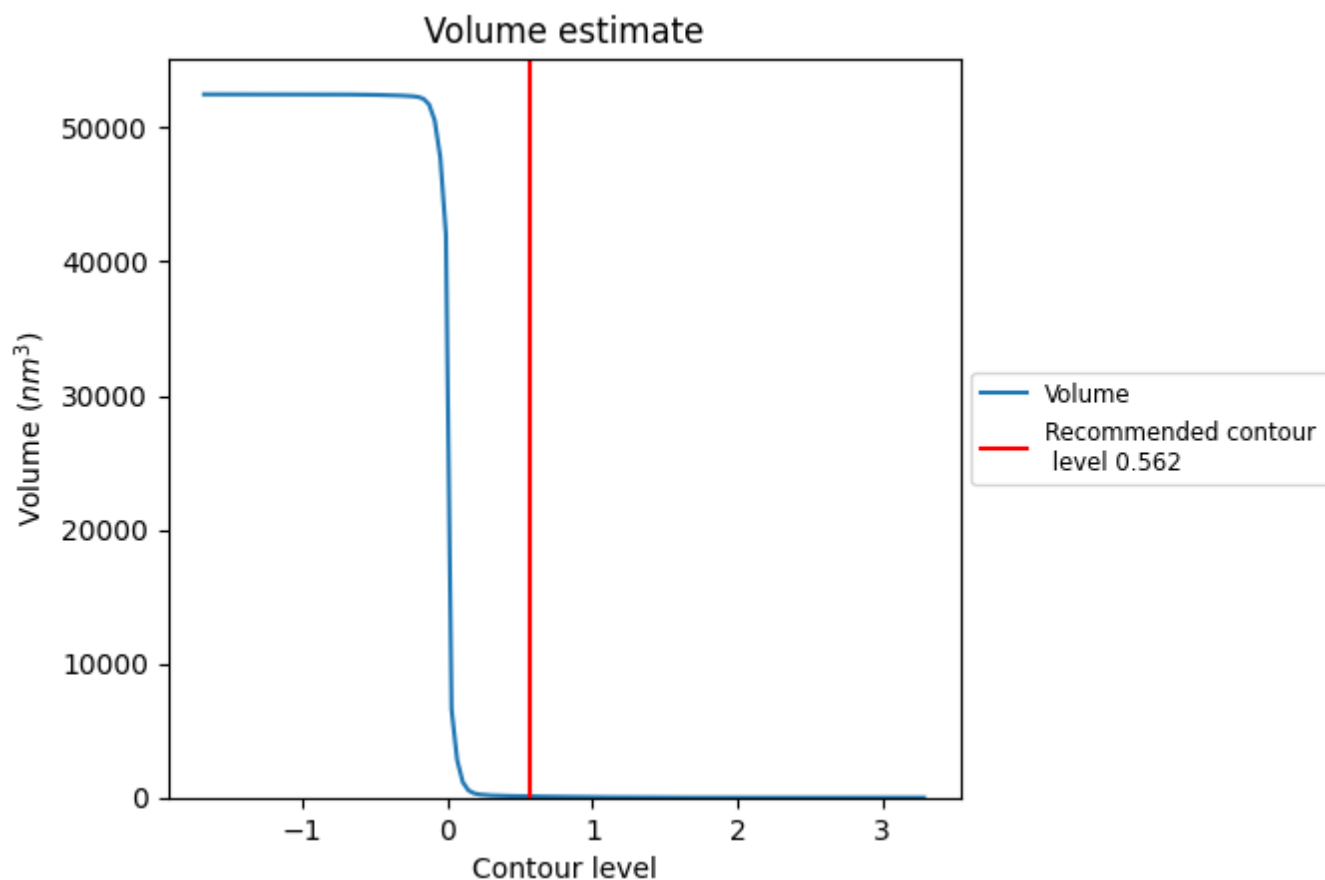
This section contains the results of statistical analysis of the map.

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.

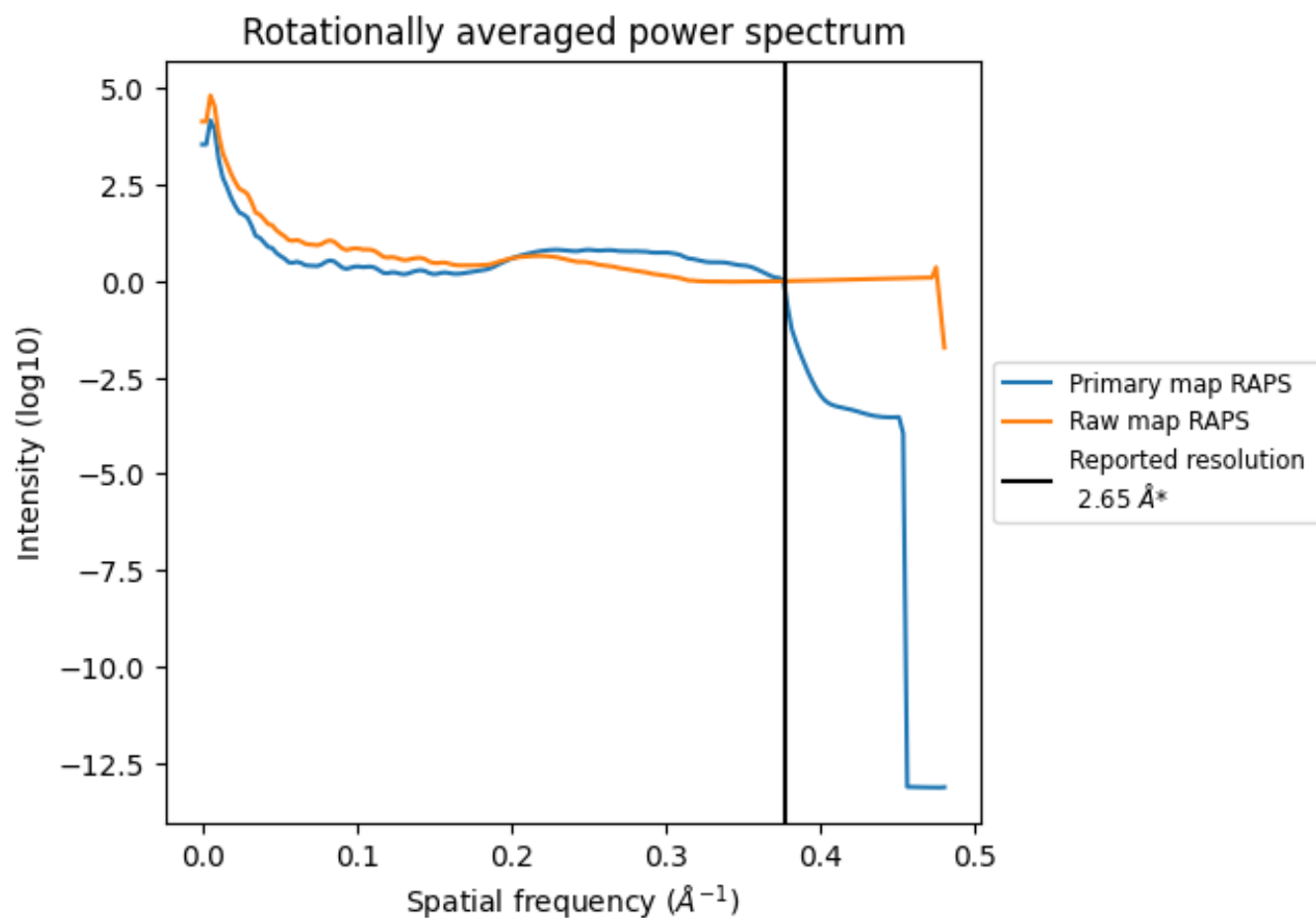
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

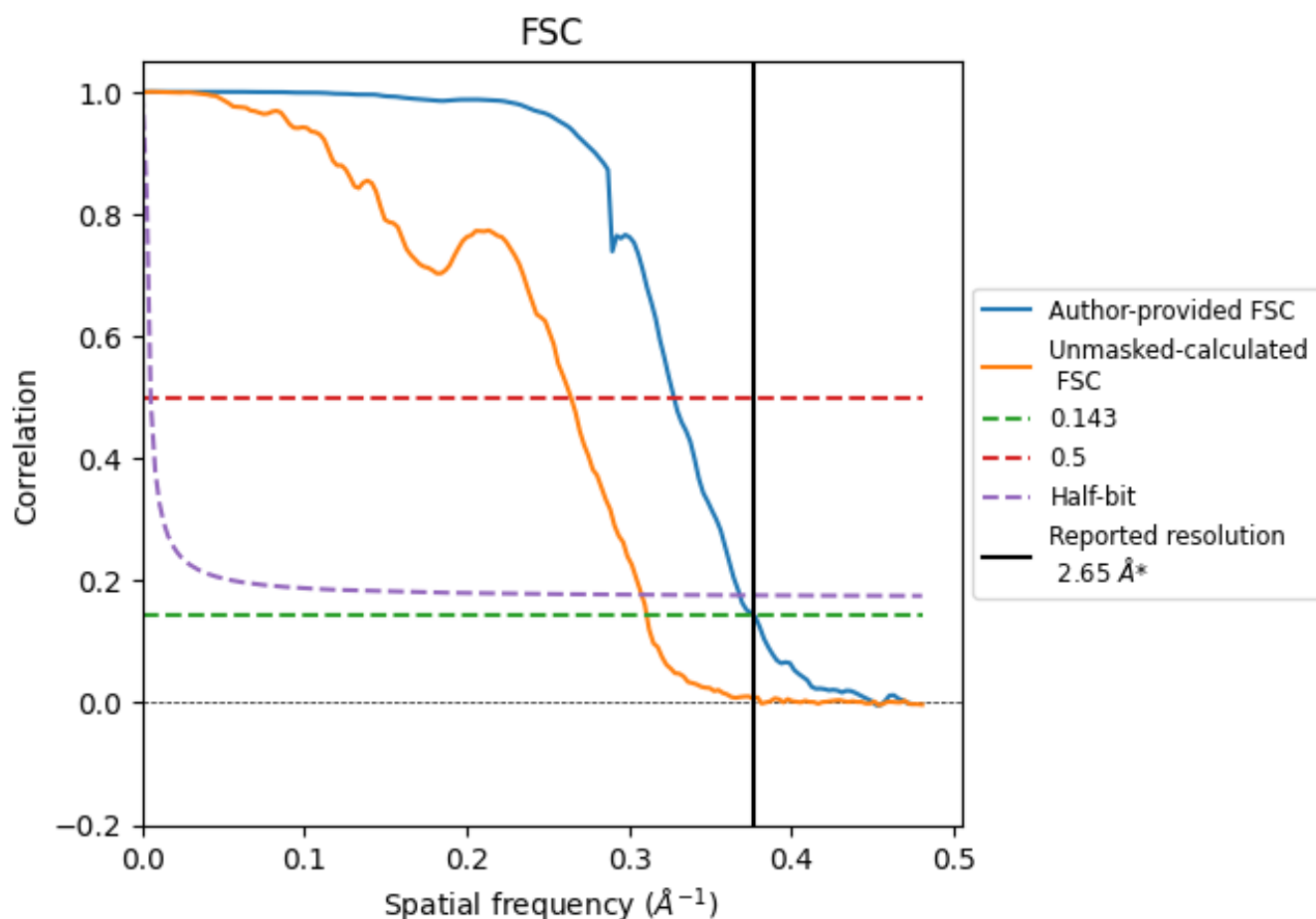


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

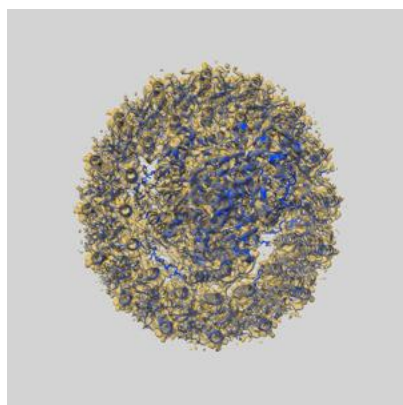
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.05	2.71
Unmasked-calculated*	3.22	3.79	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.65 by more than 10 %

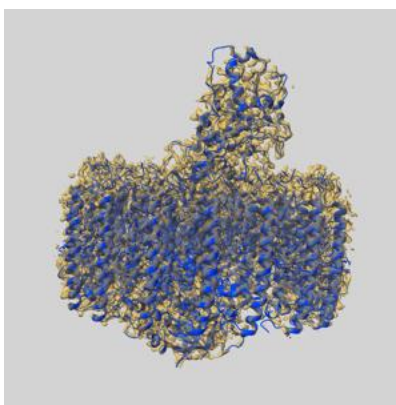
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60165 and PDB model 8ZK2. Per-residue inclusion information can be found in section 3 on page 18.

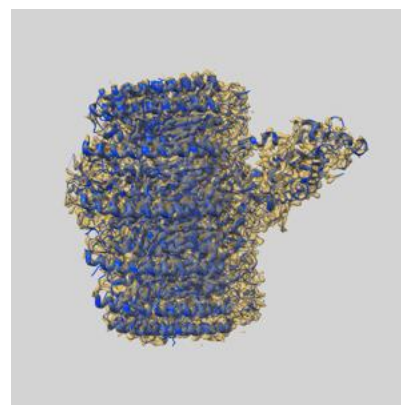
9.1 Map-model overlay [i](#)



X



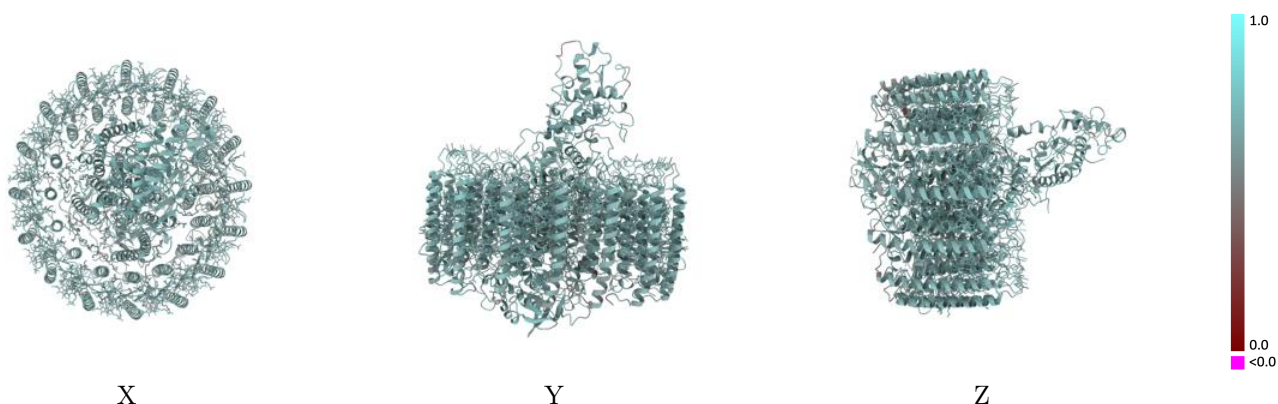
Y



Z

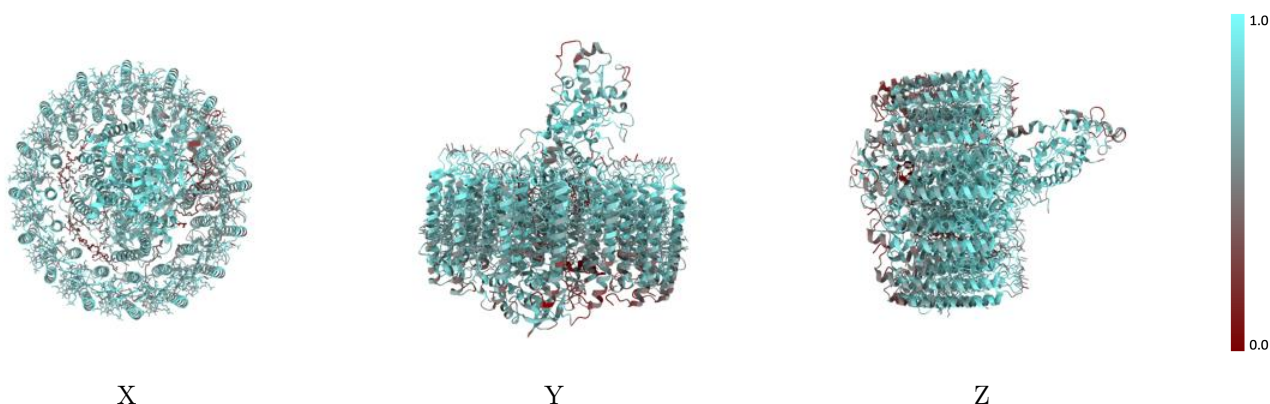
The images above show the 3D surface view of the map at the recommended contour level 0.562 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



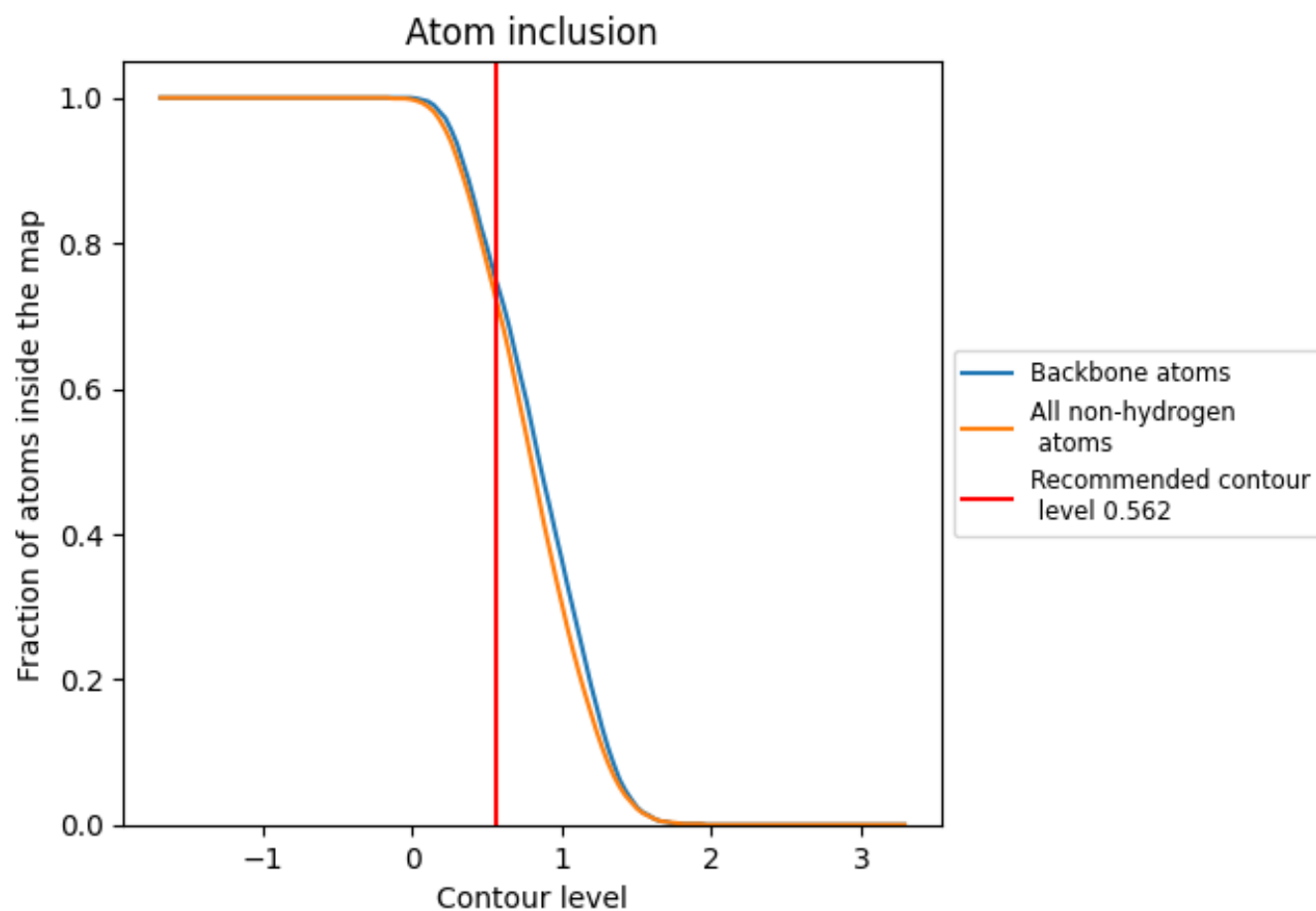
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.562).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.562) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.6360
A	 0.6740	 0.6380
B	 0.6430	 0.6190
C	 0.7380	 0.6320
D	 0.6850	 0.6350
E	 0.7510	 0.6440
F	 0.7150	 0.6240
G	 0.7620	 0.6460
H	 0.6530	 0.6250
I	 0.7250	 0.6320
J	 0.7380	 0.6410
K	 0.7160	 0.6300
L	 0.7920	 0.6510
M	 0.7740	 0.6520
N	 0.7220	 0.6390
O	 0.6990	 0.6220
P	 0.6970	 0.6340
Q	 0.7180	 0.6290
R	 0.7320	 0.6390
S	 0.7200	 0.6370
T	 0.7490	 0.6480
U	 0.7290	 0.6330
V	 0.7020	 0.6410
W	 0.7650	 0.6340
X	 0.7700	 0.6490
Y	 0.6090	 0.6110
Z	 0.5700	 0.5990
a	 0.7580	 0.6360
b	 0.7640	 0.6480
c	 0.6410	 0.6220
d	 0.6320	 0.6290
e	 0.7080	 0.6340
f	 0.7020	 0.6390
g	 0.7010	 0.6400
h	 0.7140	 0.6350



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Chain	Atom inclusion	Q-score
i	 0.7580	 0.6340
j	 0.7150	 0.6350