



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 08:45 PM JST

PDB ID : 8HJV  
EMDB ID : EMD-34839  
Title : Cryo-EM structure of carotenoid-depleted RC-LH complex from *Roseiflexus castenholzii* at 10,000 lux  
Authors : Xu, X.; Xin, J.  
Deposited on : 2022-11-23  
Resolution : 3.10 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

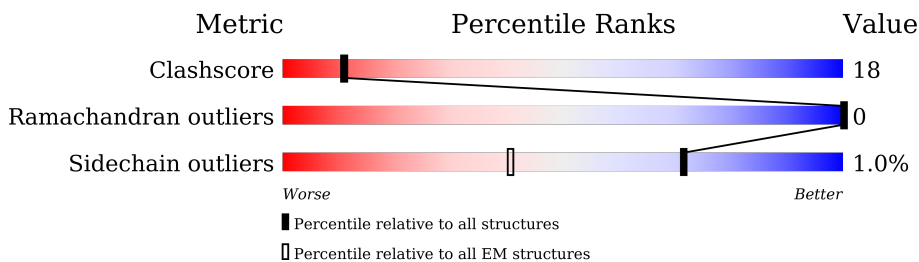
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	0	55	 38% 62% 27% 11%
1	2	55	 11% 67% 22% 11%
1	4	55	 5% 60% 29% 11%
1	6	55	 5% 60% 29% 11%
1	8	55	 5% 58% 31% 11%
1	B	55	 5% 65% 24% 11%
1	E	55	 5% 58% 31% 11%
1	G	55	 5% 60% 29% 11%

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Mol	Chain	Length	Quality of chain
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	1	42	
2	3	42	
2	5	42	
2	7	42	
2	9	42	
2	A	42	
2	D	42	
2	F	42	
2	H	42	
2	J	42	
2	N	42	
2	P	42	
2	R	42	
2	T	42	
2	V	42	
3	L	315	
4	M	307	
5	Y	39	

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Mol	Chain	Length	Quality of chain
6	C	320	<div><div></div><div>8%</div><div>64%</div><div>27%</div><div>9%</div></div>
7	Z	63	<div><div></div><div>43%</div><div>32%</div><div>25%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22193 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 Beta subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	2	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	4	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	6	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	8	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	B	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	E	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	G	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	I	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	K	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	O	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	Q	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	S	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	U	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	W	49	Total	C	N	O	S	0	0
			407	275	68	63	1		

- Molecule 2 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	35	Total	C	N	O	S	0	0
			271	181	45	44	1		
2	3	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	5	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	7	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	J	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	N	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	P	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	R	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	31	Total	C	N	O	S	0	0
			232	156	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	294	Total	C	N	O	S	0	0
			2337	1565	377	387	8		

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		

- Molecule 5 is a protein called SUBUNIT Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

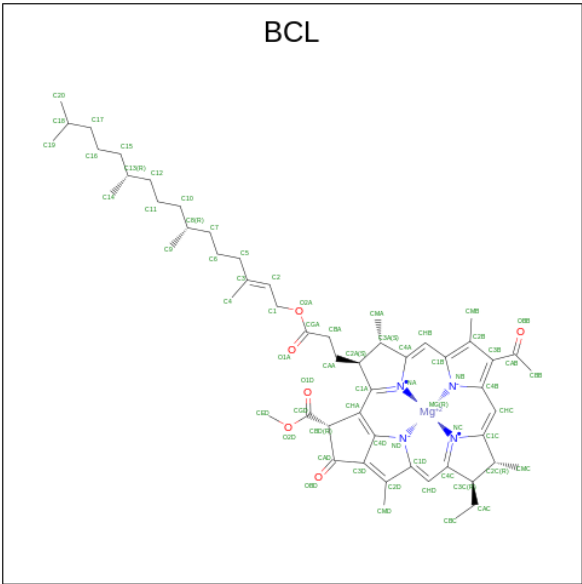
- Molecule 6 is a protein called MULTIHEME\_CYTC DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	291	Total	C	N	O	S	0	0
			2216	1407	376	411	22		

- Molecule 7 is a protein called SUBUNIT Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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Mol	Chain	Residues	Atoms					AltConf
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0

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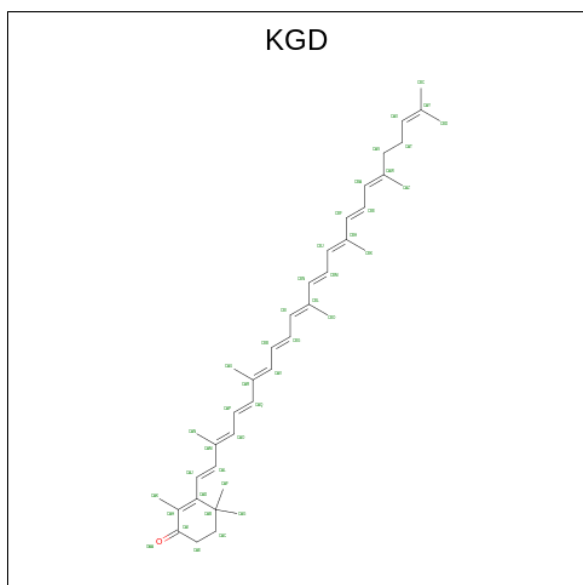
Mol	Chain	Residues	Atoms					AltConf
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0

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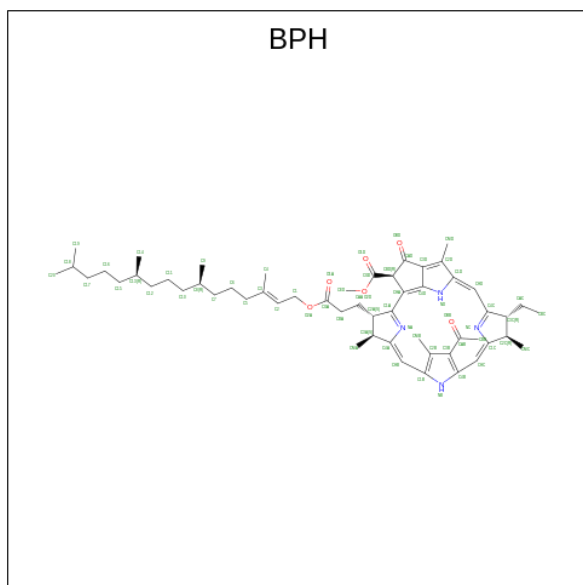
Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is beta,psi-caroten-4-one (three-letter code: KGD) (formula:  $C_{40}H_{54}O$ ).



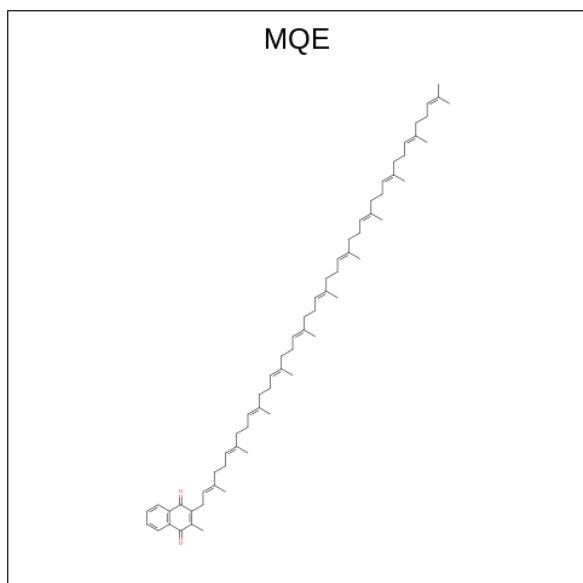
Mol	Chain	Residues	Atoms			AltConf
9	9	1	Total	C	O	0
			41	40	1	
9	D	1	Total	C	O	0
			41	40	1	
9	I	1	Total	C	O	0
			41	40	1	
9	J	1	Total	C	O	0
			41	40	1	
9	N	1	Total	C	O	0
			41	40	1	

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



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

- Molecule 11 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (three-letter code: MQE) (formula: C<sub>66</sub>H<sub>96</sub>O<sub>2</sub>).

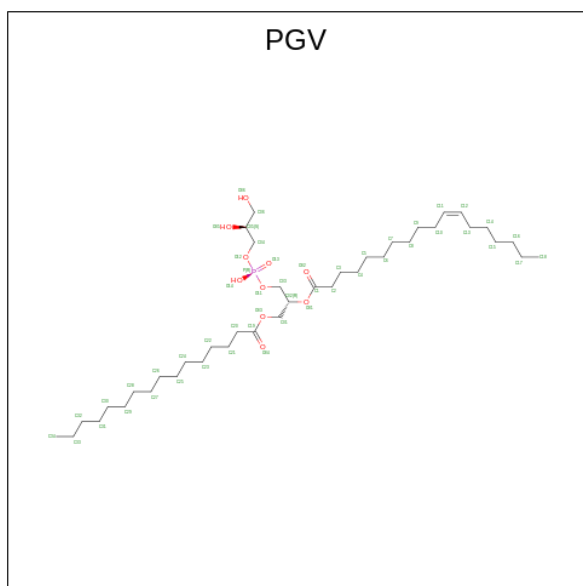


Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			68	66	2	
11	M	1	Total	C	O	0
			68	66	2	
11	M	1	Total	C	O	0
			25	23	2	

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

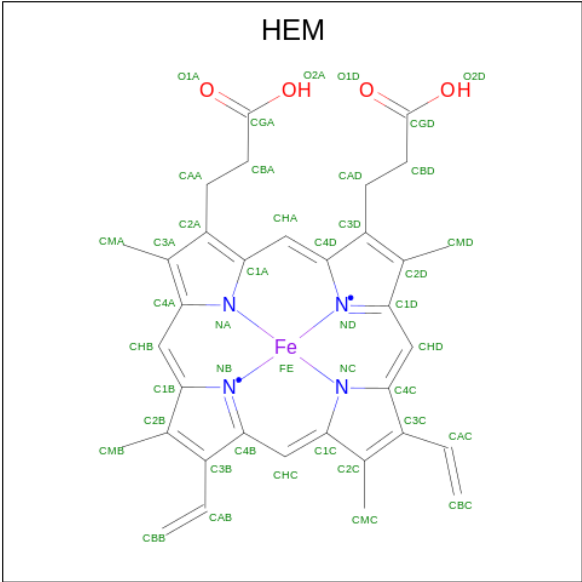
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

- Molecule 13 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	O	P	0
			45	34	10	1	
13	M	1	Total	C	O	P	0
			42	31	10	1	
13	M	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).

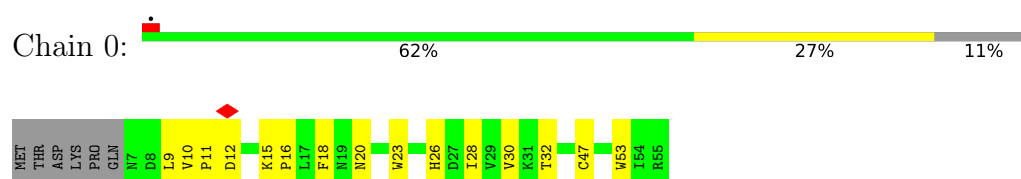


Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

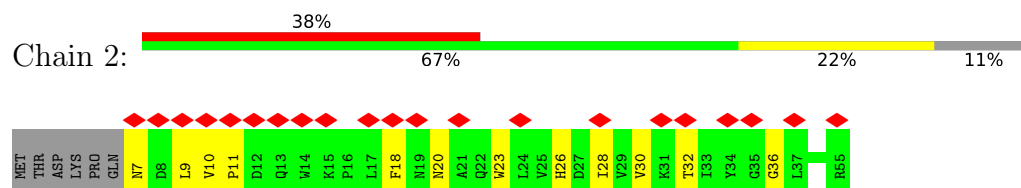
### 3 Residue-property plots [i](#)

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

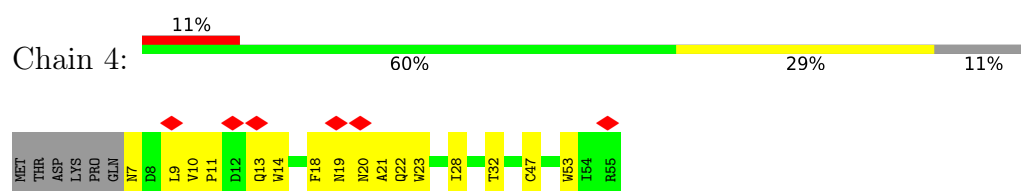
- Molecule 1: Beta subunit of light-harvesting 1



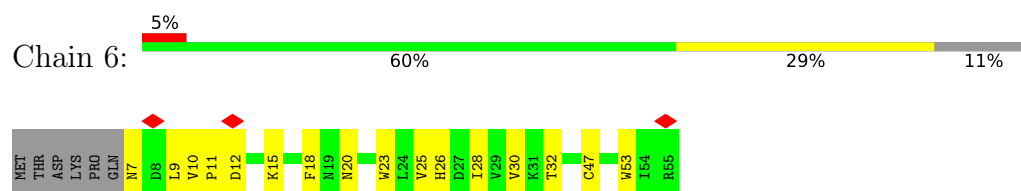
- Molecule 1: Beta subunit of light-harvesting 1



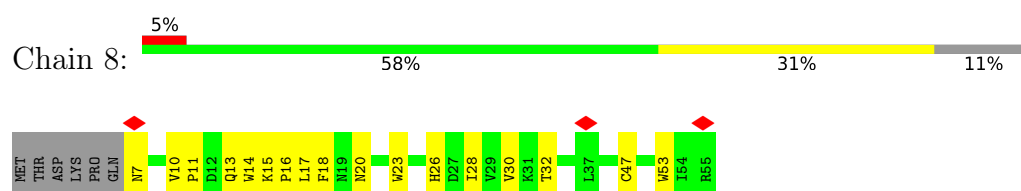
- Molecule 1: Beta subunit of light-harvesting 1



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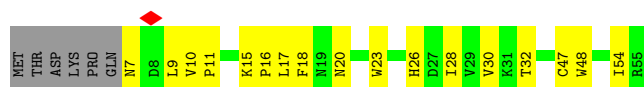
- Molecule 1: Beta subunit of light-harvesting 1



## ● Molecule 1: Beta subunit of light-harvesting 1



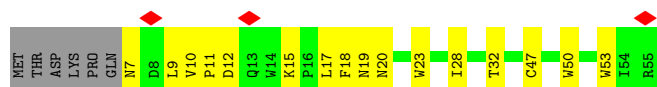
## ● Molecule 1: Beta subunit of light-harvesting 1



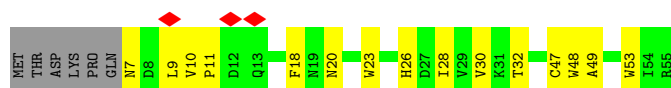
## ● Molecule 1: Beta subunit of light-harvesting 1



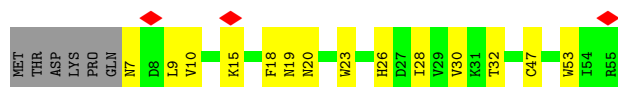
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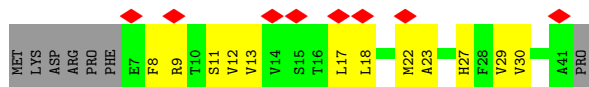
- Molecule 1: Beta subunit of light-harvesting 1



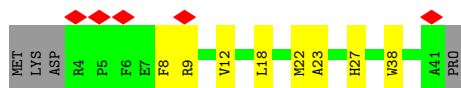
- Molecule 1: Beta subunit of light-harvesting 1



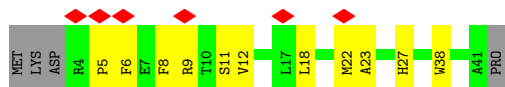
- Molecule 2: Alpha subunit of light-harvesting 1



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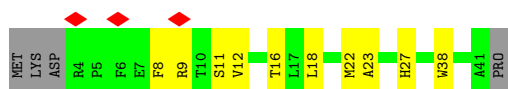


- Molecule 2: Alpha subunit of light-harvesting 1

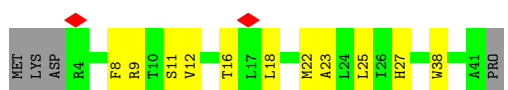


- Molecule 2: Alpha subunit of light-harvesting 1

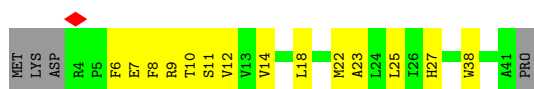




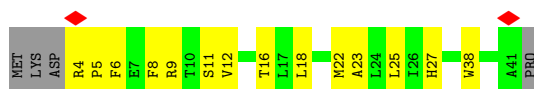
- Molecule 2: Alpha subunit of light-harvesting 1



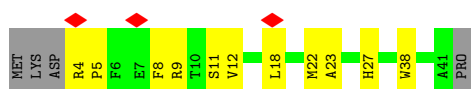
- Molecule 2: Alpha subunit of light-harvesting 1



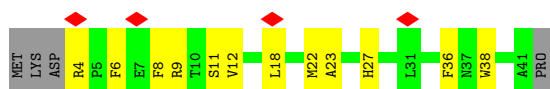
- Molecule 2: Alpha subunit of light-harvesting 1



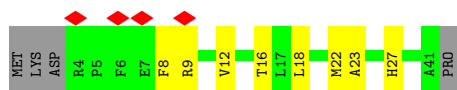
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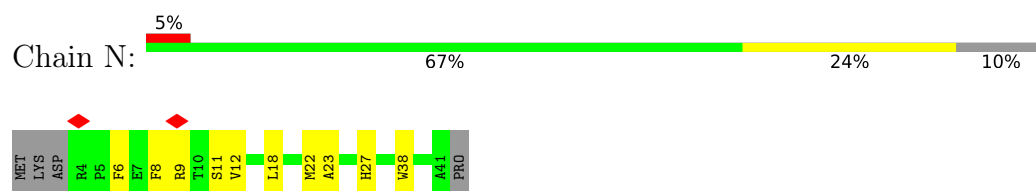
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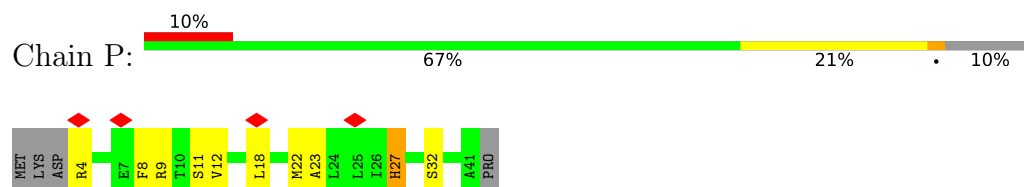
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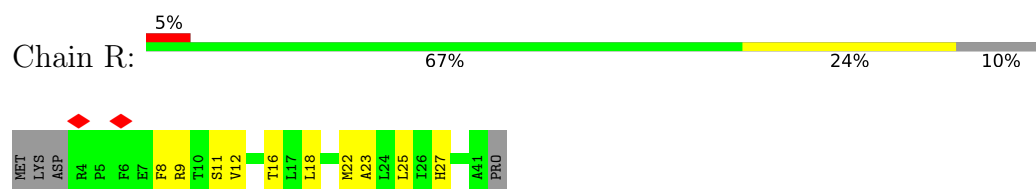
- Molecule 2: Alpha subunit of light-harvesting 1



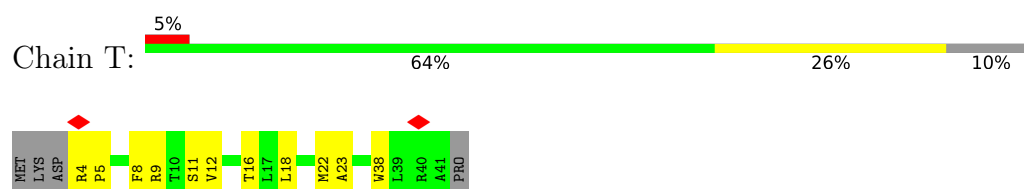
- Molecule 2: Alpha subunit of light-harvesting 1



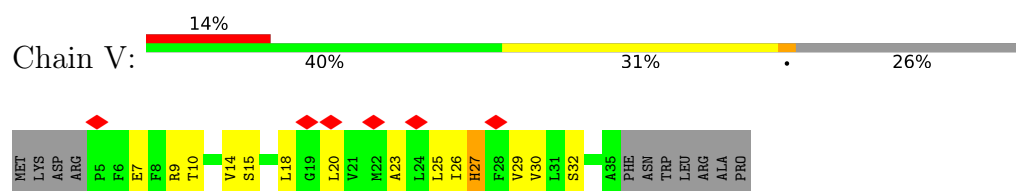
- Molecule 2: Alpha subunit of light-harvesting 1



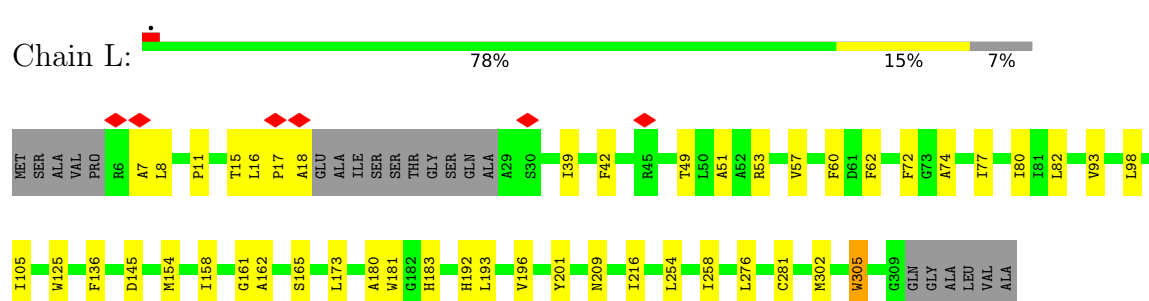
- Molecule 2: Alpha subunit of light-harvesting 1




- Molecule 2: Alpha subunit of light-harvesting 1

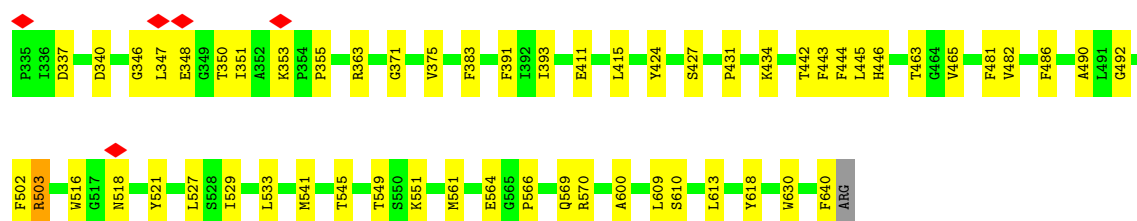


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain

Chain M: 



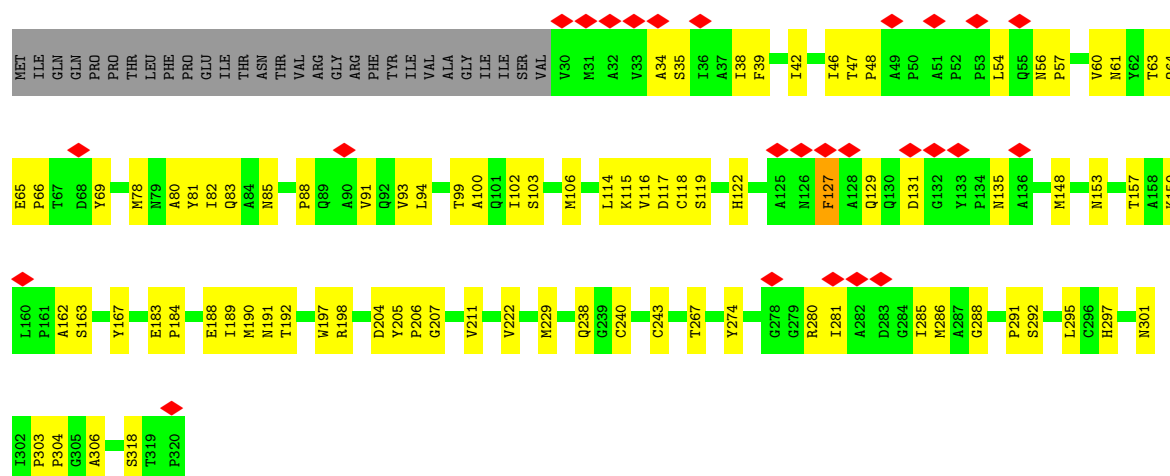
• Molecule 5: SUBUNIT Y

Chain Y: 



• Molecule 6: MULTHEME\_CYTC DOMAIN-CONTAINING PROTEIN

Chain C: 



• Molecule 7: SUBUNIT Z

Chain Z: 



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Property	Value	Source
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	235.752, 235.752, 235.752	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.893, 0.893, 0.893	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQE, KGD, BPH, BCL, HEM, FE, PGV

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	0	0.50	0/423	0.48	0/585
1	2	0.35	0/423	0.46	0/585
1	4	0.37	0/423	0.45	0/585
1	6	0.44	0/423	0.52	0/585
1	8	0.43	0/423	0.50	0/585
1	B	0.46	0/423	0.51	0/585
1	E	0.49	0/423	0.54	0/585
1	G	0.39	0/423	0.51	0/585
1	I	0.45	0/423	0.49	0/585
1	K	0.41	0/423	0.49	0/585
1	O	0.45	0/423	0.50	0/585
1	Q	0.51	0/423	0.52	0/585
1	S	0.43	0/423	0.50	0/585
1	U	0.43	0/423	0.46	0/585
1	W	0.53	0/423	0.54	0/585
2	1	0.51	0/276	0.55	0/375
2	3	0.47	0/307	0.54	0/417
2	5	0.44	0/307	0.54	0/417
2	7	0.39	0/307	0.53	0/417
2	9	0.40	0/307	0.53	0/417
2	A	0.44	0/307	0.53	0/417
2	D	0.40	0/307	0.51	0/417
2	F	0.41	0/307	0.55	0/417
2	H	0.40	0/307	0.54	0/417
2	J	0.46	0/307	0.52	0/417
2	N	0.43	0/307	0.50	0/417
2	P	0.46	0/307	0.52	0/417
2	R	0.44	0/307	0.51	0/417
2	T	0.38	0/307	0.69	0/417
2	V	0.36	0/236	0.50	0/320
3	L	0.38	0/2421	0.50	0/3304
4	M	0.40	0/2597	0.46	0/3566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Y	0.38	0/268	0.55	0/370
6	C	0.39	0/2276	0.52	0/3107
7	Z	0.36	0/374	0.47	0/513
All	All	0.42	0/18784	0.51	0/25751

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	407	0	407	15	0
1	2	407	0	407	9	0
1	4	407	0	407	23	0
1	6	407	0	407	19	0
1	8	407	0	407	13	0
1	B	407	0	407	14	0
1	E	407	0	407	16	0
1	G	407	0	407	23	0
1	I	407	0	407	19	0
1	K	407	0	407	16	0
1	O	407	0	407	16	0
1	Q	407	0	407	18	0
1	S	407	0	407	15	0
1	U	407	0	407	21	0
1	W	407	0	407	14	0
2	1	271	0	287	13	0
2	3	300	0	316	9	0
2	5	300	0	316	11	0
2	7	300	0	316	11	0
2	9	300	0	316	14	0
2	A	300	0	316	23	0
2	D	300	0	316	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	300	0	316	12	0
2	H	300	0	316	18	0
2	J	300	0	316	15	0
2	N	300	0	316	12	0
2	P	300	0	316	11	0
2	R	300	0	316	18	0
2	T	300	0	316	12	0
2	V	232	0	250	19	0
3	L	2337	0	2296	49	0
4	M	2488	0	2373	97	0
5	Y	259	0	272	8	0
6	C	2216	0	2163	85	0
7	Z	362	0	366	41	0
8	0	132	0	148	13	0
8	1	66	0	74	3	0
8	2	132	0	144	6	0
8	3	66	0	74	4	0
8	4	132	0	148	15	0
8	5	66	0	74	4	0
8	6	132	0	148	17	0
8	7	66	0	74	5	0
8	8	132	0	148	12	0
8	9	66	0	74	7	0
8	A	66	0	74	5	0
8	B	132	0	148	16	0
8	D	66	0	74	7	0
8	E	132	0	148	14	0
8	F	66	0	74	4	0
8	G	132	0	148	20	0
8	H	66	0	74	3	0
8	I	132	0	148	16	0
8	J	66	0	74	9	0
8	K	132	0	148	16	0
8	L	66	0	74	12	0
8	M	132	0	148	11	0
8	N	66	0	74	4	0
8	O	132	0	148	15	0
8	P	66	0	74	3	0
8	Q	132	0	148	17	0
8	R	66	0	74	8	0
8	S	132	0	148	14	0
8	T	66	0	74	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	132	0	148	14	0
8	V	66	0	74	9	0
8	W	132	0	144	14	0
9	9	41	0	0	3	0
9	D	41	0	0	3	0
9	I	41	0	0	1	0
9	J	41	0	0	1	0
9	N	41	0	0	0	0
10	L	195	0	228	22	0
11	L	68	0	0	1	0
11	M	93	0	0	11	0
12	M	1	0	0	0	0
13	M	121	0	153	17	0
14	C	172	0	120	12	0
All	All	22193	0	22265	803	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 18.

All (803) 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)
6:C:240:CYS:SG	14:C:503:HEM:HAB	1.33	1.68
7:Z:39:ARG:HH12	7:Z:43:LYS:CG	1.14	1.60
7:Z:39:ARG:NH1	7:Z:43:LYS:HG3	1.20	1.46
6:C:240:CYS:SG	14:C:503:HEM:CAB	2.19	1.30
6:C:243:CYS:SG	14:C:503:HEM:HAC	1.74	1.28
1:W:8:ASP:OD1	1:W:15:LYS:HE3	1.35	1.25
6:C:243:CYS:SG	14:C:503:HEM:CAC	2.25	1.24
4:M:518:ASN:ND2	4:M:521:TYR:CE2	2.05	1.23
4:M:570:ARG:HH21	7:Z:58:ASN:ND2	1.38	1.22
4:M:518:ASN:ND2	4:M:521:TYR:CD2	2.13	1.17
2:R:23:ALA:HB2	8:S:101:BCL:HED1	1.34	1.10
2:R:16:THR:OG1	8:R:101:BCL:H203	1.53	1.09
6:C:61:ASN:HB3	6:C:304:PRO:HB3	1.27	1.09
2:5:23:ALA:HB2	8:6:101:BCL:HED1	1.32	1.09
2:F:23:ALA:HB2	8:G:101:BCL:HED1	1.27	1.09
2:J:16:THR:OG1	8:J:101:BCL:H203	1.51	1.08
2:A:23:ALA:HB2	8:B:101:BCL:CED	1.83	1.07
7:Z:39:ARG:NH1	7:Z:43:LYS:CD	2.16	1.07
2:H:23:ALA:HB2	8:I:101:BCL:CED	1.82	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:23:ALA:HB2	8:Q:101:BCL:CED	1.85	1.07
2:H:23:ALA:HB2	8:I:101:BCL:HED1	1.20	1.06
3:L:16:LEU:CD1	3:L:17:PRO:HD2	1.84	1.05
4:M:518:ASN:CG	4:M:521:TYR:HD2	1.59	1.05
4:M:570:ARG:NH2	7:Z:58:ASN:HD21	1.52	1.05
10:L:404:BPH:H193	11:M:1003:MQE:CCA	1.86	1.05
2:A:23:ALA:HB2	8:B:101:BCL:HED1	1.38	1.04
1:U:47:CYS:CB	8:U:101:BCL:HBC1	1.88	1.03
7:Z:39:ARG:NH1	7:Z:43:LYS:CG	1.90	1.03
2:F:23:ALA:HB2	8:G:101:BCL:CED	1.87	1.02
4:M:518:ASN:OD1	4:M:521:TYR:HD2	1.40	1.02
4:M:551:LYS:HE2	13:M:1007:PGV:O06	1.57	1.01
4:M:570:ARG:NH2	7:Z:58:ASN:ND2	2.07	1.01
2:J:23:ALA:HB2	8:K:101:BCL:CED	1.91	1.01
6:C:88:PRO:HG3	6:C:102:ILE:HD12	1.35	1.01
2:3:23:ALA:HB2	8:4:101:BCL:HED1	1.44	1.00
2:R:23:ALA:HB2	8:S:101:BCL:CED	1.90	1.00
2:J:23:ALA:HB2	8:K:101:BCL:HED1	1.38	1.00
2:7:23:ALA:HB2	8:8:101:BCL:CED	1.91	0.99
3:L:16:LEU:HD12	3:L:17:PRO:HD2	0.99	0.99
2:P:23:ALA:HB2	8:Q:101:BCL:HED1	1.44	0.99
4:M:570:ARG:HH21	7:Z:58:ASN:CG	1.65	0.98
3:L:16:LEU:HD12	3:L:17:PRO:CD	1.93	0.98
2:N:23:ALA:HB2	8:O:101:BCL:HED1	1.43	0.97
4:M:518:ASN:CG	4:M:521:TYR:CD2	2.36	0.97
1:6:47:CYS:CB	8:6:101:BCL:HBC1	1.95	0.97
1:G:12:ASP:HA	1:G:15:LYS:HG2	1.46	0.96
4:M:527:LEU:HD21	7:Z:26:PRO:HB3	1.50	0.94
1:W:8:ASP:OD1	1:W:15:LYS:CE	2.16	0.93
4:M:551:LYS:NZ	13:M:1007:PGV:O05	2.01	0.93
1:G:12:ASP:HA	1:G:15:LYS:CG	1.99	0.93
2:D:23:ALA:HB2	8:E:101:BCL:CED	1.99	0.92
1:U:47:CYS:HB3	8:U:101:BCL:HBC1	1.49	0.92
1:4:47:CYS:CB	8:4:101:BCL:HBC1	2.00	0.91
4:M:570:ARG:CZ	7:Z:58:ASN:HD21	1.82	0.91
6:C:56:ASN:OD1	6:C:57:PRO:HD2	1.71	0.91
1:E:47:CYS:HB2	8:E:101:BCL:HBC1	1.53	0.90
2:7:23:ALA:HB2	8:8:101:BCL:HED1	1.52	0.90
2:5:23:ALA:HB2	8:6:101:BCL:CED	2.01	0.90
2:A:7:GLU:O	2:A:10:THR:HG22	1.71	0.89
4:M:518:ASN:HD21	4:M:521:TYR:HE2	0.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:518:ASN:OD1	4:M:521:TYR:CD2	2.26	0.89
1:6:47:CYS:HB3	8:6:101:BCL:HBC1	1.54	0.88
1:G:53:TRP:HE1	8:G:101:BCL:HBB2	1.40	0.87
2:N:23:ALA:HB2	8:O:101:BCL:CED	2.05	0.86
2:7:16:THR:OG1	8:7:101:BCL:H203	1.76	0.86
1:B:47:CYS:HB2	8:B:101:BCL:HBC1	1.56	0.86
6:C:189:ILE:HG13	6:C:190:MET:HG3	1.58	0.85
2:T:23:ALA:HB2	8:U:101:BCL:HED1	1.59	0.84
2:3:23:ALA:HB2	8:4:101:BCL:CED	2.07	0.83
3:L:216:ILE:HG12	8:L:401:BCL:HMB3	1.59	0.83
2:D:23:ALA:HB2	8:E:101:BCL:HED1	1.60	0.83
1:4:47:CYS:HB3	8:4:101:BCL:HBC1	1.59	0.83
2:D:16:THR:OG1	8:D:101:BCL:H203	1.79	0.82
7:Z:39:ARG:HH12	7:Z:43:LYS:CD	1.85	0.82
3:L:49:THR:HG23	3:L:145:ASP:OD2	1.80	0.81
1:O:47:CYS:HB2	8:O:101:BCL:HBC1	1.60	0.81
4:M:570:ARG:NE	7:Z:58:ASN:HD21	1.77	0.81
6:C:88:PRO:HG3	6:C:102:ILE:CD1	2.11	0.81
1:G:47:CYS:HB2	8:G:101:BCL:HBC1	1.62	0.81
4:M:393:ILE:HG21	11:M:1003:MQE:CCE	2.11	0.81
3:L:82:LEU:HD23	2:R:25:LEU:HD21	1.60	0.80
4:M:527:LEU:HD11	7:Z:26:PRO:HG3	1.62	0.80
8:0:102:BCL:HED1	2:9:23:ALA:HB2	1.62	0.79
4:M:518:ASN:HB3	4:M:618:TYR:HB2	1.64	0.79
4:M:351:ILE:HD12	4:M:375:VAL:HG21	1.63	0.79
4:M:492:GLY:HA3	13:M:1008:PGV:H32	1.63	0.79
2:A:9:ARG:HG3	4:M:347:LEU:HD22	1.65	0.78
1:G:12:ASP:CA	1:G:15:LYS:HG2	2.12	0.78
1:S:53:TRP:HE1	8:S:101:BCL:HBB2	1.47	0.78
1:I:47:CYS:CB	8:I:101:BCL:HBC1	2.14	0.77
6:C:81:TYR:CD2	6:C:127:PHE:CZ	2.72	0.77
3:L:82:LEU:CD2	2:R:25:LEU:HD21	2.15	0.77
6:C:243:CYS:SG	14:C:503:HEM:C3C	2.77	0.77
1:S:47:CYS:HB2	8:S:101:BCL:HBC1	1.65	0.76
7:Z:28:ALA:O	7:Z:32:LEU:HD13	1.85	0.76
3:L:7:ALA:HB1	3:L:15:THR:HG22	1.66	0.76
1:K:47:CYS:HB2	8:K:101:BCL:HBC1	1.67	0.76
2:V:23:ALA:HA	8:W:101:BCL:CED	2.16	0.75
6:C:297:HIS:HA	6:C:303:PRO:HB3	1.69	0.75
6:C:69:TYR:CE2	6:C:115:LYS:HA	2.22	0.75
1:4:13:GLN:HE21	1:4:14:TRP:HE1	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:351:ILE:CD1	4:M:375:VAL:HG21	2.16	0.75
1:O:9:LEU:HD12	1:O:20:ASN:OD1	1.86	0.75
2:D:25:LEU:HD11	4:M:443:PHE:CE1	2.22	0.74
6:C:60:VAL:HG23	6:C:306:ALA:O	1.86	0.74
2:T:23:ALA:HB2	8:U:101:BCL:CED	2.16	0.74
1:6:53:TRP:HE1	8:6:101:BCL:HBB2	1.52	0.74
3:L:49:THR:HG23	3:L:145:ASP:CG	2.08	0.74
2:A:25:LEU:HD21	4:M:444:PHE:CE2	2.23	0.74
1:4:7:ASN:HA	1:4:20:ASN:HB2	1.70	0.73
3:L:42:PHE:CD2	7:Z:54:PRO:HB2	2.22	0.73
2:D:25:LEU:HD11	4:M:443:PHE:CZ	2.23	0.73
1:6:9:LEU:HD12	1:6:20:ASN:OD1	1.86	0.73
4:M:551:LYS:CE	13:M:1007:PGV:O06	2.34	0.73
1:4:53:TRP:HE1	8:4:101:BCL:HBB2	1.53	0.72
2:V:23:ALA:HA	8:W:101:BCL:HED3	1.70	0.72
4:M:570:ARG:HE	7:Z:58:ASN:HD21	1.36	0.72
1:2:7:ASN:HA	1:2:20:ASN:HB2	1.69	0.72
1:8:47:CYS:HB2	8:8:101:BCL:HBC1	1.70	0.72
1:I:53:TRP:HE1	8:I:101:BCL:HBB2	1.52	0.72
4:M:570:ARG:HH21	7:Z:58:ASN:HD21	1.06	0.72
8:0:102:BCL:CED	2:9:23:ALA:HB2	2.20	0.71
6:C:88:PRO:CG	6:C:102:ILE:CD1	2.68	0.71
11:M:1002:MQE:CAG	7:Z:34:PHE:HZ	2.03	0.71
6:C:88:PRO:CG	6:C:102:ILE:HD12	2.16	0.71
1:W:8:ASP:HA	1:W:15:LYS:NZ	2.06	0.71
6:C:114:LEU:HB3	6:C:116:VAL:HG13	1.72	0.71
4:M:549:THR:HG22	4:M:549:THR:O	1.89	0.70
8:9:102:BCL:H161	2:A:14:VAL:HG21	1.72	0.70
1:U:47:CYS:HB3	8:U:101:BCL:CBC	2.21	0.70
6:C:56:ASN:OD1	6:C:57:PRO:CD	2.40	0.70
1:O:47:CYS:CB	8:O:101:BCL:HBC1	2.22	0.70
6:C:157:THR:O	6:C:157:THR:HG22	1.90	0.70
2:P:4:ARG:NH2	1:Q:17:LEU:O	2.24	0.70
1:U:47:CYS:HB2	8:U:101:BCL:HBC1	1.71	0.70
1:2:9:LEU:HD12	1:2:20:ASN:OD1	1.92	0.69
2:1:30:VAL:HG22	6:C:46:ILE:HD13	1.74	0.69
7:Z:39:ARG:NH1	7:Z:43:LYS:HD3	2.07	0.69
6:C:153:ASN:OD1	6:C:318:SER:HB3	1.92	0.69
6:C:81:TYR:CD2	6:C:127:PHE:HZ	2.09	0.68
1:0:47:CYS:CB	8:0:102:BCL:HBC1	2.24	0.68
10:L:404:BPH:H1C1	10:L:405:BPH:HBB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:CYS:HB2	8:I:101:BCL:HBC1	1.73	0.68
2:D:23:ALA:HB2	8:E:101:BCL:O2D	1.94	0.67
6:C:81:TYR:CG	6:C:127:PHE:HZ	2.12	0.67
4:M:516:TRP:CD1	4:M:610:SER:HB3	2.30	0.67
2:J:16:THR:OG1	8:J:101:BCL:C20	2.38	0.67
1:Q:53:TRP:HE1	8:Q:101:BCL:HBB2	1.60	0.67
10:L:404:BPH:C19	11:M:1003:MQE:CCA	2.69	0.66
1:U:9:LEU:HD12	1:U:20:ASN:OD1	1.96	0.66
1:4:13:GLN:NE2	1:4:14:TRP:NE1	2.43	0.66
1:U:53:TRP:HE1	8:U:101:BCL:HBB2	1.60	0.66
2:D:23:ALA:CB	8:E:101:BCL:O2D	2.43	0.66
2:1:13:VAL:O	2:1:17:LEU:HD13	1.96	0.66
6:C:240:CYS:SG	14:C:503:HEM:C3B	2.89	0.66
7:Z:39:ARG:HH12	7:Z:43:LYS:HG3	0.49	0.66
2:R:9:ARG:HD3	2:T:5:PRO:HB2	1.78	0.65
8:B:101:BCL:H18	9:D:102:KGD:CBO	2.26	0.65
6:C:122:HIS:HD2	14:C:501:HEM:C4B	2.14	0.65
1:B:9:LEU:HD12	1:B:20:ASN:OD1	1.96	0.65
1:K:7:ASN:HA	1:K:20:ASN:HB2	1.79	0.65
1:S:9:LEU:HD12	1:S:20:ASN:OD1	1.96	0.65
4:M:442:THR:O	4:M:446:HIS:ND1	2.29	0.65
2:P:23:ALA:HB2	8:Q:101:BCL:O2D	1.97	0.65
1:8:10:VAL:HG13	1:8:11:PRO:HD2	1.79	0.65
1:I:10:VAL:HG13	1:I:11:PRO:HD2	1.79	0.65
1:K:47:CYS:CB	8:K:101:BCL:HBC1	2.27	0.65
1:Q:10:VAL:HG13	1:Q:11:PRO:HD2	1.79	0.64
6:C:122:HIS:HD2	14:C:501:HEM:NB	1.94	0.64
2:R:16:THR:OG1	8:R:101:BCL:C20	2.39	0.64
1:6:10:VAL:HG13	1:6:11:PRO:HD2	1.80	0.64
1:0:47:CYS:HB2	8:0:102:BCL:HBC1	1.78	0.64
2:H:38:TRP:CZ2	8:H:101:BCL:HHC	2.33	0.64
1:E:9:LEU:HD12	1:E:20:ASN:OD1	1.96	0.64
7:Z:39:ARG:CZ	7:Z:43:LYS:CD	2.75	0.64
8:W:101:BCL:HED2	8:W:101:BCL:OBD	1.97	0.64
1:4:10:VAL:HG13	1:4:11:PRO:HD2	1.79	0.64
2:7:23:ALA:HB2	8:8:101:BCL:O2D	1.97	0.63
1:G:9:LEU:HD12	1:G:20:ASN:OD1	1.97	0.63
3:L:216:ILE:HD11	8:L:401:BCL:C1B	2.28	0.63
1:6:26:HIS:O	1:6:30:VAL:HG23	1.98	0.63
1:G:10:VAL:O	1:G:15:LYS:HD3	1.98	0.63
1:W:8:ASP:HA	1:W:15:LYS:HZ2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:10:VAL:HG13	1:0:11:PRO:HD2	1.80	0.63
1:E:10:VAL:HG13	1:E:11:PRO:HD2	1.80	0.63
1:O:7:ASN:HA	1:O:20:ASN:HB2	1.78	0.63
1:U:10:VAL:HG13	1:U:11:PRO:HD2	1.80	0.63
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.79	0.63
1:O:53:TRP:HE1	8:O:101:BCL:HBB2	1.63	0.63
14:C:504:HEM:HHD	14:C:504:HEM:HBC2	1.80	0.63
1:S:10:VAL:HG13	1:S:11:PRO:HD2	1.80	0.63
6:C:81:TYR:CE2	6:C:127:PHE:CZ	2.86	0.63
2:7:23:ALA:CB	8:8:101:BCL:O2D	2.46	0.63
1:0:9:LEU:HD12	1:0:20:ASN:OD1	1.99	0.63
3:L:57:VAL:HB	2:T:9:ARG:CZ	2.29	0.63
1:4:13:GLN:NE2	1:4:14:TRP:HE1	1.97	0.62
2:A:25:LEU:HD21	4:M:444:PHE:HE2	1.62	0.62
1:K:10:VAL:HG13	1:K:11:PRO:HD2	1.80	0.62
1:G:10:VAL:HG13	1:G:11:PRO:HD2	1.80	0.62
1:G:8:ASP:HA	1:G:15:LYS:HZ3	1.64	0.62
4:M:518:ASN:CB	4:M:618:TYR:HB2	2.29	0.62
3:L:93:VAL:HG22	2:P:32:SER:HB3	1.82	0.62
1:Q:47:CYS:CB	8:Q:101:BCL:HBC1	2.30	0.62
1:2:10:VAL:HG13	1:2:11:PRO:HD2	1.79	0.62
3:L:193:LEU:HD11	8:M:1001:BCL:HED3	1.82	0.62
2:D:4:ARG:NH1	1:E:17:LEU:O	2.34	0.61
1:Q:9:LEU:HD12	1:Q:20:ASN:OD1	1.99	0.61
6:C:184:PRO:HB3	6:C:295:LEU:HD23	1.81	0.61
1:4:9:LEU:HD12	1:4:20:ASN:OD1	2.00	0.61
1:8:47:CYS:CB	8:8:101:BCL:HBC1	2.30	0.61
1:I:12:ASP:HA	1:I:15:LYS:HG3	1.81	0.61
7:Z:39:ARG:CZ	7:Z:43:LYS:HD2	2.29	0.61
3:L:49:THR:HG22	3:L:51:ALA:H	1.64	0.61
6:C:82:ILE:HG23	6:C:100:ALA:HA	1.81	0.61
2:1:30:VAL:HA	6:C:46:ILE:HD12	1.83	0.61
4:M:516:TRP:CE3	4:M:516:TRP:HA	2.36	0.61
4:M:551:LYS:NZ	13:M:1007:PGV:C05	2.64	0.60
6:C:60:VAL:HG22	6:C:167:TYR:CE2	2.36	0.60
8:1:101:BCL:H12	8:2:101:BCL:H101	1.83	0.60
10:L:405:BPH:H13	11:M:1003:MQE:CBG	2.31	0.60
2:A:23:ALA:CB	8:B:101:BCL:O2D	2.50	0.60
8:L:401:BCL:HBA1	8:M:1001:BCL:HBC1	1.82	0.60
2:T:38:TRP:CZ2	8:T:101:BCL:HHC	2.36	0.60
1:K:53:TRP:HE1	8:K:101:BCL:HBB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:158:ILE:HG12	13:M:1007:PGV:H22	1.84	0.60
1:G:8:ASP:HA	1:G:15:LYS:NZ	2.17	0.60
4:M:570:ARG:HE	7:Z:58:ASN:ND2	2.00	0.59
1:Q:12:ASP:HA	1:Q:15:LYS:HE2	1.84	0.59
2:A:23:ALA:HB2	8:B:101:BCL:O2D	2.01	0.59
2:D:25:LEU:CD1	4:M:443:PHE:CZ	2.85	0.59
1:8:26:HIS:O	1:8:30:VAL:HG23	2.01	0.59
2:H:4:ARG:HH12	1:I:19:ASN:HB2	1.67	0.59
1:E:7:ASN:N	1:E:20:ASN:HB2	2.18	0.59
2:J:8:PHE:HD1	8:K:102:BCL:HBB3	1.65	0.59
2:P:23:ALA:CB	8:Q:101:BCL:O2D	2.51	0.59
1:Q:26:HIS:O	1:Q:30:VAL:HG23	2.03	0.59
1:E:9:LEU:HB2	1:E:20:ASN:OD1	2.03	0.58
2:J:9:ARG:HB3	2:N:6:PHE:HE1	1.68	0.58
1:8:14:TRP:HE3	1:8:17:LEU:HD12	1.69	0.58
2:D:8:PHE:HD1	8:E:102:BCL:HBB3	1.68	0.58
2:T:4:ARG:HB3	2:T:5:PRO:HD3	1.85	0.58
1:6:53:TRP:NE1	8:6:101:BCL:HBB2	2.19	0.58
3:L:216:ILE:CD1	8:L:401:BCL:C2B	2.82	0.58
6:C:102:ILE:O	6:C:106:MET:HG3	2.04	0.58
1:4:53:TRP:NE1	8:4:101:BCL:HBB2	2.19	0.58
2:J:23:ALA:HB2	8:K:101:BCL:O2D	2.02	0.58
1:K:26:HIS:O	1:K:30:VAL:HG23	2.04	0.58
1:B:26:HIS:O	1:B:30:VAL:HG23	2.04	0.58
1:S:47:CYS:CB	8:S:101:BCL:HBC1	2.34	0.58
1:0:28:ILE:HG22	9:9:101:KGD:CAF	2.33	0.58
1:4:21:ALA:HB1	2:5:5:PRO:HD3	1.86	0.58
2:V:25:LEU:O	2:V:29:VAL:HG23	2.04	0.58
6:C:281:ILE:HD12	6:C:281:ILE:H	1.68	0.58
1:G:26:HIS:O	1:G:30:VAL:HG23	2.03	0.58
4:M:350:THR:O	4:M:353:LYS:HE3	2.04	0.57
2:N:23:ALA:CB	8:N:101:BCL:O1A	2.53	0.57
1:Q:9:LEU:HB2	1:Q:20:ASN:OD1	2.04	0.57
8:W:101:BCL:HED2	8:W:101:BCL:CAD	2.34	0.57
2:D:38:TRP:CZ2	8:D:101:BCL:HHC	2.40	0.57
1:0:26:HIS:O	1:0:30:VAL:HG23	2.04	0.57
1:W:19:ASN:HB2	1:W:22:GLN:NE2	2.20	0.57
1:6:47:CYS:HB3	8:6:101:BCL:CBC	2.31	0.56
4:M:518:ASN:HD22	4:M:618:TYR:HD1	1.54	0.56
1:2:26:HIS:O	1:2:30:VAL:HG23	2.05	0.56
6:C:93:VAL:HG22	6:C:94:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:183:GLU:OE2	6:C:183:GLU:N	2.38	0.56
1:G:11:PRO:O	1:G:15:LYS:CD	2.53	0.56
2:7:16:THR:OG1	8:7:101:BCL:C20	2.52	0.56
1:E:26:HIS:O	1:E:30:VAL:HG23	2.06	0.56
1:Q:47:CYS:HB2	8:Q:101:BCL:HBC1	1.86	0.56
2:F:8:PHE:HD1	8:G:102:BCL:HBB3	1.71	0.56
8:A:101:BCL:HHB	9:D:102:KGD:CAZ	2.35	0.55
1:I:9:LEU:HG	1:I:20:ASN:HD21	1.72	0.55
4:M:516:TRP:HA	4:M:516:TRP:HE3	1.69	0.55
4:M:551:LYS:HE2	13:M:1007:PGV:H06	1.67	0.55
11:M:1002:MQE:CBG	7:Z:34:PHE:HZ	2.19	0.55
1:O:26:HIS:O	1:O:30:VAL:HG23	2.05	0.55
6:C:34:ALA:O	6:C:38:ILE:HG12	2.05	0.55
3:L:209:ASN:HD21	3:L:281:CYS:HB2	1.72	0.55
11:M:1002:MQE:CAG	7:Z:34:PHE:CZ	2.88	0.55
1:K:9:LEU:HB2	1:K:20:ASN:OD1	2.07	0.55
6:C:60:VAL:HG22	6:C:167:TYR:HE2	1.71	0.55
2:H:23:ALA:CB	8:H:101:BCL:O1A	2.55	0.55
1:U:47:CYS:CB	8:U:101:BCL:CBC	2.76	0.55
6:C:47:THR:HG23	6:C:48:PRO:HD2	1.88	0.55
2:T:8:PHE:O	2:T:11:SER:OG	2.15	0.55
1:B:47:CYS:CB	8:B:101:BCL:HBC1	2.32	0.54
3:L:258:ILE:HG22	11:L:403:MQE:CBQ	2.37	0.54
1:W:26:HIS:O	1:W:30:VAL:HG23	2.07	0.54
6:C:69:TYR:CZ	6:C:115:LYS:HD3	2.41	0.54
4:M:363:ARG:HD3	5:Y:28:TRP:NE1	2.22	0.54
4:M:569:GLN:HE21	7:Z:51:ARG:HB3	1.71	0.54
6:C:229:MET:HB3	14:C:503:HEM:C4B	2.42	0.54
1:I:47:CYS:HB3	8:I:101:BCL:HBC1	1.90	0.54
1:Q:53:TRP:NE1	8:Q:101:BCL:HBB2	2.22	0.54
1:S:53:TRP:NE1	8:S:101:BCL:HBB2	2.21	0.54
1:G:12:ASP:HA	1:G:15:LYS:HG3	1.84	0.54
8:J:101:BCL:H13	9:J:102:KGD:CAJ	2.37	0.54
2:V:23:ALA:HA	8:W:101:BCL:HED1	1.88	0.54
2:D:23:ALA:CB	8:D:101:BCL:O1A	2.56	0.54
1:E:47:CYS:CB	8:E:101:BCL:HBC1	2.31	0.54
2:H:18:LEU:O	2:H:22:MET:HG2	2.08	0.54
4:M:570:ARG:NH2	7:Z:58:ASN:CG	2.48	0.54
6:C:65:GLU:HB3	6:C:66:PRO:HD3	1.90	0.54
2:F:18:LEU:O	2:F:22:MET:HG2	2.08	0.54
1:6:47:CYS:HB2	8:6:101:BCL:HBC1	1.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:10:THR:HB	4:M:347:LEU:CD1	2.38	0.53
2:H:23:ALA:CB	8:I:101:BCL:CED	2.72	0.53
2:N:18:LEU:O	2:N:22:MET:HG2	2.08	0.53
2:1:18:LEU:O	2:1:22:MET:HG2	2.08	0.53
2:5:18:LEU:O	2:5:22:MET:HG2	2.08	0.53
2:J:18:LEU:O	2:J:22:MET:HG2	2.08	0.53
2:R:18:LEU:O	2:R:22:MET:HG2	2.08	0.53
2:A:18:LEU:O	2:A:22:MET:HG2	2.08	0.53
4:M:431:PRO:HG2	4:M:434:LYS:HB2	1.89	0.53
6:C:54:LEU:HD21	6:C:63:THR:HB	1.90	0.53
2:3:18:LEU:O	2:3:22:MET:HG2	2.08	0.53
4:M:570:ARG:NH2	7:Z:58:ASN:OD1	2.39	0.53
6:C:291:PRO:O	6:C:292:SER:OG	2.22	0.53
1:G:47:CYS:CB	8:G:101:BCL:HBC1	2.36	0.53
2:V:10:THR:O	2:V:14:VAL:HG12	2.09	0.53
2:9:18:LEU:O	2:9:22:MET:HG2	2.08	0.53
3:L:51:ALA:HB2	3:L:72:PHE:CZ	2.44	0.53
4:M:490:ALA:HB2	13:M:1008:PGV:H042	1.89	0.53
2:1:29:VAL:HG12	6:C:46:ILE:HD11	1.91	0.53
2:T:16:THR:OG1	8:T:101:BCL:H203	2.08	0.53
1:U:53:TRP:NE1	8:U:101:BCL:HBB2	2.23	0.53
2:J:23:ALA:CB	8:K:101:BCL:O2D	2.57	0.53
2:D:18:LEU:O	2:D:22:MET:HG2	2.08	0.53
4:M:503:ARG:HH22	6:C:192:THR:HG23	1.74	0.53
2:T:18:LEU:O	2:T:22:MET:HG2	2.08	0.53
2:P:18:LEU:O	2:P:22:MET:HG2	2.08	0.52
1:8:15:LYS:N	1:8:16:PRO:HD2	2.24	0.52
2:J:23:ALA:CB	8:J:101:BCL:O1A	2.57	0.52
2:R:23:ALA:CB	8:R:101:BCL:O1A	2.57	0.52
7:Z:39:ARG:NH2	7:Z:43:LYS:HD2	2.24	0.52
2:A:10:THR:CB	4:M:347:LEU:HD11	2.39	0.52
1:I:7:ASN:OD1	1:I:19:ASN:OD1	2.28	0.52
2:P:23:ALA:CB	8:P:101:BCL:O1A	2.57	0.52
2:V:27:HIS:HE1	8:V:101:BCL:CHC	2.21	0.52
2:3:38:TRP:CZ2	8:3:101:BCL:HHC	2.44	0.52
1:4:13:GLN:HG3	1:4:14:TRP:CD1	2.44	0.52
2:7:18:LEU:O	2:7:22:MET:HG2	2.08	0.52
1:I:53:TRP:NE1	8:I:101:BCL:HBB2	2.22	0.52
8:T:101:BCL:C20	2:V:18:LEU:HD11	2.39	0.52
1:U:19:ASN:H	1:U:22:GLN:CD	2.13	0.52
2:9:9:ARG:HA	2:9:12:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:393:ILE:CG2	11:M:1003:MQE:CCE	2.86	0.52
2:N:9:ARG:HA	2:N:12:VAL:HG22	1.92	0.52
2:9:25:LEU:CD2	4:M:391:PHE:CZ	2.93	0.52
9:9:101:KGD:CAU	8:9:102:BCL:H41	2.40	0.52
8:D:101:BCL:O1A	8:E:101:BCL:HED1	2.09	0.52
1:I:7:ASN:HA	1:I:20:ASN:HB2	1.92	0.52
1:O:53:TRP:NE1	8:O:101:BCL:HBB2	2.25	0.52
2:P:9:ARG:HA	2:P:12:VAL:HG22	1.92	0.52
7:Z:20:TYR:HA	7:Z:24:PHE:CD2	2.44	0.52
2:T:9:ARG:HA	2:T:12:VAL:HG22	1.92	0.52
1:O:12:ASP:HA	1:O:15:LYS:HE2	1.90	0.52
3:L:158:ILE:CG1	13:M:1007:PGV:H22	2.39	0.52
3:L:180:ALA:HB3	3:L:183:HIS:CD2	2.45	0.52
2:R:9:ARG:HA	2:R:12:VAL:HG22	1.92	0.52
2:3:9:ARG:HA	2:3:12:VAL:HG22	1.92	0.51
1:B:53:TRP:HE1	8:B:101:BCL:HBB2	1.76	0.51
5:Y:18:LEU:HB3	5:Y:19:PRO:HD3	1.92	0.51
6:C:78:MET:HG2	6:C:82:ILE:HD11	1.92	0.51
2:5:9:ARG:HA	2:5:12:VAL:HG22	1.92	0.51
2:H:9:ARG:HA	2:H:12:VAL:HG22	1.92	0.51
2:A:25:LEU:CD2	4:M:444:PHE:HE2	2.23	0.51
3:L:82:LEU:CD2	2:R:25:LEU:CD2	2.85	0.51
1:O:9:LEU:HG	1:O:20:ASN:HD21	1.75	0.51
2:D:9:ARG:HA	2:D:12:VAL:HG22	1.92	0.51
2:H:8:PHE:O	2:H:11:SER:OG	2.22	0.51
5:Y:5:VAL:O	5:Y:9:MET:HG2	2.11	0.51
2:3:8:PHE:HB2	1:4:22:GLN:HE21	1.76	0.51
2:7:9:ARG:HA	2:7:12:VAL:HG22	1.92	0.51
2:9:38:TRP:CZ2	8:9:102:BCL:HHC	2.46	0.51
4:M:541:MET:O	4:M:545:THR:HG22	2.11	0.51
2:9:8:PHE:HD2	2:A:6:PHE:HZ	1.57	0.51
2:J:16:THR:CB	8:J:101:BCL:C20	2.89	0.51
2:D:16:THR:OG1	8:D:101:BCL:C20	2.56	0.51
2:P:27:HIS:CE1	8:Q:101:BCL:HMD1	2.46	0.51
2:R:8:PHE:O	2:R:11:SER:OG	2.22	0.51
2:V:27:HIS:CE1	8:V:101:BCL:CHC	2.94	0.51
1:W:7:ASN:HA	1:W:20:ASN:HB2	1.93	0.51
5:Y:11:MET:O	5:Y:15:VAL:HG23	2.10	0.51
2:9:25:LEU:HD21	4:M:391:PHE:CE2	2.46	0.51
2:J:9:ARG:HA	2:J:12:VAL:HG22	1.92	0.51
1:S:7:ASN:HA	1:S:20:ASN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:53:TRP:HE1	8:Q:101:BCL:CBB	2.23	0.50
2:1:9:ARG:HA	2:1:12:VAL:HG22	1.92	0.50
2:A:9:ARG:HA	2:A:12:VAL:HG22	1.92	0.50
2:D:8:PHE:O	2:D:11:SER:OG	2.22	0.50
3:L:216:ILE:CG1	8:L:401:BCL:HMB3	2.36	0.50
1:6:53:TRP:HE1	8:6:101:BCL:CBB	2.24	0.50
2:R:23:ALA:HB2	8:S:101:BCL:O2D	2.11	0.50
2:1:23:ALA:CB	8:1:101:BCL:O1A	2.60	0.50
1:6:7:ASN:N	1:6:20:ASN:HD22	2.10	0.50
2:F:4:ARG:N	2:F:5:PRO:HD2	2.27	0.50
2:F:9:ARG:HA	2:F:12:VAL:HG22	1.92	0.50
1:W:36:GLY:HA3	8:W:101:BCL:H52	1.93	0.50
2:5:8:PHE:O	2:5:11:SER:OG	2.22	0.50
4:M:350:THR:HG23	4:M:353:LYS:HD3	1.92	0.50
2:V:32:SER:O	2:V:32:SER:OG	2.26	0.50
6:C:80:ALA:HA	6:C:83:GLN:HE21	1.77	0.50
1:4:19:ASN:HB2	1:4:22:GLN:OE1	2.12	0.50
2:F:23:ALA:CB	8:F:101:BCL:O1A	2.60	0.50
1:4:53:TRP:HE1	8:4:101:BCL:CBB	2.23	0.50
1:6:12:ASP:HA	1:6:15:LYS:HD2	1.93	0.50
8:M:1005:BCL:HBD	8:M:1005:BCL:HAA2	1.94	0.50
1:4:47:CYS:HB3	8:4:101:BCL:CBC	2.36	0.50
1:G:7:ASN:HA	1:G:20:ASN:HB2	1.93	0.50
3:L:60:PHE:HB3	3:L:62:PHE:CE2	2.47	0.50
4:M:518:ASN:ND2	4:M:521:TYR:HE2	1.72	0.50
1:Q:47:CYS:HB3	8:Q:101:BCL:HBC1	1.93	0.50
2:T:23:ALA:CB	8:T:101:BCL:O1A	2.60	0.50
2:1:29:VAL:HG21	6:C:39:PHE:HE1	1.77	0.49
2:R:16:THR:CB	8:R:101:BCL:H203	2.40	0.49
1:U:26:HIS:O	1:U:30:VAL:HG23	2.12	0.49
1:I:53:TRP:HE1	8:I:101:BCL:CBB	2.23	0.49
3:L:8:LEU:HD13	3:L:18:ALA:HA	1.94	0.49
11:M:1002:MQE:CBG	7:Z:34:PHE:CZ	2.95	0.49
2:9:8:PHE:O	2:9:11:SER:OG	2.22	0.49
6:C:117:ASP:OD1	6:C:118:CYS:N	2.45	0.49
2:A:8:PHE:O	2:A:11:SER:OG	2.22	0.49
1:6:9:LEU:HG	1:6:20:ASN:HD21	1.76	0.49
2:J:16:THR:CB	8:J:101:BCL:H203	2.39	0.49
6:C:204:ASP:C	6:C:206:PRO:HD3	2.33	0.49
10:L:405:BPH:HHC	10:L:405:BPH:HBB3	1.95	0.49
4:M:551:LYS:H	4:M:551:LYS:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:16:THR:CB	8:R:101:BCL:C20	2.90	0.49
6:C:60:VAL:CG2	6:C:167:TYR:CE2	2.96	0.49
7:Z:47:SER:OG	7:Z:48:ALA:N	2.46	0.49
2:H:4:ARG:NH1	1:I:19:ASN:HB2	2.28	0.49
4:M:549:THR:O	4:M:549:THR:CG2	2.59	0.49
8:T:101:BCL:HMB3	8:W:101:BCL:CHB	2.42	0.48
6:C:82:ILE:CG2	6:C:100:ALA:HA	2.43	0.48
2:3:23:ALA:CB	8:3:101:BCL:O1A	2.61	0.48
2:9:25:LEU:HD23	4:M:391:PHE:CZ	2.47	0.48
2:J:16:THR:HB	8:J:101:BCL:H202	1.95	0.48
2:9:23:ALA:CB	8:9:102:BCL:O1A	2.61	0.48
3:L:254:LEU:HD11	10:L:405:BPH:HED3	1.95	0.48
10:L:405:BPH:H7C2	4:M:383:PHE:CD1	2.49	0.48
4:M:527:LEU:HD11	7:Z:26:PRO:CG	2.38	0.48
6:C:85:ASN:O	6:C:99:THR:HG21	2.13	0.48
2:7:8:PHE:O	2:7:11:SER:OG	2.22	0.48
2:H:23:ALA:CB	8:I:101:BCL:O2D	2.61	0.48
6:C:157:THR:O	6:C:157:THR:CG2	2.58	0.48
1:G:12:ASP:C	1:G:15:LYS:HG2	2.33	0.48
8:I:102:BCL:HBC3	8:I:102:BCL:H2C	1.60	0.48
3:L:136:PHE:CZ	8:L:401:BCL:H112	2.49	0.48
1:Q:46:LEU:C	1:Q:48:TRP:H	2.17	0.48
1:S:10:VAL:CG1	1:S:11:PRO:HD2	2.44	0.48
1:0:53:TRP:HE1	8:0:102:BCL:HBB2	1.79	0.48
1:4:10:VAL:CG1	1:4:11:PRO:HD2	2.44	0.48
2:5:23:ALA:CB	8:5:101:BCL:O1A	2.61	0.48
2:F:23:ALA:CB	8:G:101:BCL:CED	2.78	0.48
1:K:53:TRP:NE1	8:K:101:BCL:HBB2	2.27	0.48
6:C:82:ILE:HG23	6:C:100:ALA:CA	2.44	0.48
1:8:10:VAL:CG1	1:8:11:PRO:HD2	2.44	0.48
2:H:4:ARG:HG3	2:H:6:PHE:O	2.14	0.48
10:L:402:BPH:H111	8:M:1001:BCL:H192	1.96	0.48
4:M:566:PRO:HD3	7:Z:57:ALA:HB1	1.95	0.48
1:U:7:ASN:HA	1:U:20:ASN:HB2	1.96	0.48
1:U:10:VAL:CG1	1:U:11:PRO:HD2	2.44	0.48
2:V:26:ILE:O	2:V:30:VAL:HG23	2.13	0.48
2:7:23:ALA:CB	8:7:101:BCL:O1A	2.61	0.48
1:G:10:VAL:CG1	1:G:11:PRO:HD2	2.44	0.48
4:M:355:PRO:HB3	4:M:371:GLY:HA2	1.94	0.48
2:R:23:ALA:CB	8:S:101:BCL:O2D	2.62	0.48
2:V:27:HIS:CE1	8:V:101:BCL:C4B	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:VAL:CG1	1:E:11:PRO:HD2	2.44	0.47
4:M:424:TYR:HB2	4:M:427:SER:HB3	1.96	0.47
1:U:18:PHE:HA	1:U:22:GLN:OE1	2.14	0.47
1:6:10:VAL:CG1	1:6:11:PRO:HD2	2.44	0.47
1:0:10:VAL:CG1	1:0:11:PRO:HD2	2.44	0.47
1:B:32:THR:HG22	8:E:102:BCL:H61	1.95	0.47
2:F:23:ALA:HB2	8:G:101:BCL:O2D	2.14	0.47
1:K:10:VAL:CG1	1:K:11:PRO:HD2	2.44	0.47
8:9:102:BCL:C16	2:A:14:VAL:HG21	2.42	0.47
8:M:1005:BCL:HMB1	8:M:1005:BCL:HBB3	1.97	0.47
8:Q:102:BCL:H2C	8:Q:102:BCL:HBC3	1.59	0.47
8:0:101:BCL:H2C	8:0:101:BCL:HBC3	1.59	0.47
8:E:102:BCL:H2C	8:E:102:BCL:HBC3	1.60	0.47
3:L:161:GLY:O	13:M:1007:PGV:H11	2.14	0.47
8:U:101:BCL:H41	8:U:101:BCL:H62	1.50	0.47
6:C:88:PRO:HG2	6:C:102:ILE:CD1	2.45	0.47
8:0:102:BCL:H41	8:0:102:BCL:H62	1.50	0.47
8:2:101:BCL:H91	8:2:101:BCL:H111	1.54	0.47
2:A:10:THR:HB	4:M:347:LEU:HD13	1.95	0.47
1:W:19:ASN:H	1:W:22:GLN:CD	2.18	0.47
2:1:22:MET:CE	6:C:35:SER:HB2	2.45	0.47
8:V:101:BCL:H151	8:V:101:BCL:H18	1.54	0.47
8:W:102:BCL:HBC3	8:W:102:BCL:H2C	1.60	0.47
4:M:518:ASN:ND2	4:M:618:TYR:HD1	2.13	0.47
10:L:405:BPH:H13	11:M:1003:MQE:CAM	2.44	0.46
4:M:570:ARG:NE	7:Z:58:ASN:ND2	2.55	0.46
8:M:1001:BCL:H161	8:M:1001:BCL:H141	1.65	0.46
2:N:8:PHE:HD1	8:O:102:BCL:HBB3	1.80	0.46
2:1:8:PHE:O	2:1:11:SER:OG	2.22	0.46
1:K:53:TRP:HE1	8:K:101:BCL:CBB	2.28	0.46
4:M:482:VAL:HA	4:M:486:PHE:HB2	1.97	0.46
8:T:101:BCL:H142	2:V:15:SER:HB2	1.97	0.46
1:E:32:THR:HA	8:G:102:BCL:H61	1.97	0.46
8:F:101:BCL:H2C	8:F:101:BCL:HBC3	1.67	0.46
1:I:10:VAL:CG1	1:I:11:PRO:HD2	2.44	0.46
1:Q:10:VAL:CG1	1:Q:11:PRO:HD2	2.44	0.46
2:R:16:THR:HB	8:R:101:BCL:H202	1.96	0.46
6:C:82:ILE:HG12	6:C:103:SER:OG	2.15	0.46
8:A:101:BCL:HBC3	8:A:101:BCL:H2C	1.67	0.46
8:A:101:BCL:H3A	9:D:102:KGD:CAZ	2.45	0.46
8:L:401:BCL:H161	8:L:401:BCL:H203	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:8:PHE:O	2:P:11:SER:OG	2.22	0.46
6:C:267:THR:HG23	6:C:291:PRO:HB2	1.98	0.46
3:L:98:LEU:HD12	3:L:98:LEU:HA	1.84	0.46
3:L:302:MET:HB2	3:L:305:TRP:NE1	2.30	0.46
4:M:363:ARG:HD3	5:Y:28:TRP:HE1	1.78	0.46
4:M:551:LYS:HZ1	13:M:1007:PGV:C05	2.15	0.46
2:N:8:PHE:O	2:N:11:SER:OG	2.22	0.46
1:6:25:VAL:HG23	1:6:26:HIS:N	2.30	0.46
8:B:102:BCL:HBC3	8:B:102:BCL:H2C	1.59	0.46
2:D:5:PRO:HB2	2:D:6:PHE:CD1	2.51	0.46
2:F:8:PHE:O	2:F:11:SER:OG	2.22	0.46
8:K:102:BCL:H112	8:K:102:BCL:H93	1.67	0.46
13:M:1008:PGV:H22	13:M:1008:PGV:H261	1.98	0.46
1:Q:7:ASN:N	1:Q:20:ASN:HB2	2.30	0.46
8:3:101:BCL:HBC3	8:3:101:BCL:H2C	1.67	0.46
8:E:101:BCL:H41	8:E:101:BCL:H62	1.50	0.46
8:T:101:BCL:H121	8:T:101:BCL:H162	1.60	0.46
8:W:101:BCL:H142	8:W:101:BCL:H111	1.52	0.46
8:6:102:BCL:H2C	8:6:102:BCL:HBC3	1.59	0.46
8:W:101:BCL:H93	8:W:101:BCL:H61	1.78	0.46
6:C:280:ARG:HD2	6:C:288:GLY:HA3	1.98	0.46
1:G:11:PRO:O	1:G:15:LYS:HG2	2.16	0.45
8:M:1005:BCL:H143	8:M:1005:BCL:H161	1.78	0.45
1:S:12:ASP:HA	1:S:15:LYS:HE2	1.96	0.45
1:B:10:VAL:CG1	1:B:11:PRO:HD2	2.44	0.45
2:D:25:LEU:CD1	4:M:443:PHE:CE1	2.95	0.45
8:K:102:BCL:H2C	8:K:102:BCL:HBC3	1.59	0.45
4:M:609:LEU:HD22	4:M:613:LEU:HD12	1.98	0.45
8:O:102:BCL:H112	8:O:102:BCL:H93	1.67	0.45
1:U:53:TRP:HE1	8:U:101:BCL:CBB	2.28	0.45
8:4:102:BCL:H112	8:4:102:BCL:H93	1.67	0.45
3:L:42:PHE:CE2	7:Z:54:PRO:HB2	2.52	0.45
2:7:38:TRP:CZ2	8:7:101:BCL:HHC	2.52	0.45
2:A:25:LEU:CD2	4:M:444:PHE:CE2	2.97	0.45
1:B:53:TRP:NE1	8:B:101:BCL:HBB2	2.30	0.45
1:O:10:VAL:HG12	1:O:23:TRP:CG	2.52	0.45
8:T:101:BCL:H2C	8:T:101:BCL:HBC3	1.67	0.45
8:V:101:BCL:H93	8:V:101:BCL:H111	1.55	0.45
6:C:42:ILE:O	6:C:46:ILE:HG12	2.17	0.45
8:8:102:BCL:H2C	8:8:102:BCL:HBC3	1.59	0.45
2:F:23:ALA:CB	8:G:101:BCL:O2D	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:101:BCL:H62	8:Q:101:BCL:H41	1.50	0.45
8:W:101:BCL:H203	8:W:101:BCL:H162	1.75	0.45
1:2:10:VAL:CG1	1:2:11:PRO:HD2	2.44	0.45
8:Q:102:BCL:H93	8:Q:102:BCL:H112	1.67	0.45
6:C:93:VAL:O	6:C:94:LEU:HB2	2.17	0.45
1:4:47:CYS:HB2	8:4:101:BCL:HBC1	1.90	0.45
1:8:7:ASN:HA	1:8:20:ASN:HB3	1.98	0.45
8:4:102:BCL:HBC3	8:4:102:BCL:H2C	1.59	0.45
2:H:8:PHE:HD1	8:I:102:BCL:HBB3	1.82	0.45
8:Q:101:BCL:H93	8:Q:101:BCL:H61	1.85	0.45
2:9:8:PHE:HD2	2:A:6:PHE:CZ	2.34	0.45
8:8:101:BCL:H62	8:8:101:BCL:H41	1.50	0.44
2:A:10:THR:HG23	2:A:11:SER:N	2.32	0.44
4:M:640:PHE:N	6:C:238:GLN:OE1	2.49	0.44
1:O:7:ASN:OD1	1:O:19:ASN:OD1	2.34	0.44
8:T:101:BCL:H161	2:V:14:VAL:CG1	2.47	0.44
2:5:38:TRP:CZ2	8:5:101:BCL:HHC	2.52	0.44
10:L:405:BPH:H192	10:L:405:BPH:H162	1.63	0.44
8:S:102:BCL:H2C	8:S:102:BCL:HBC3	1.60	0.44
8:V:101:BCL:H2C	8:V:101:BCL:HBC3	1.49	0.44
1:8:53:TRP:CZ3	8:8:101:BCL:HAC2	2.53	0.44
1:B:7:ASN:HA	1:B:20:ASN:HB2	1.99	0.44
2:H:23:ALA:HB2	8:I:101:BCL:O2D	2.14	0.44
3:L:105:ILE:HG22	3:L:125:TRP:HD1	1.82	0.44
1:S:15:LYS:HE2	1:S:15:LYS:HB2	1.83	0.44
3:L:216:ILE:HG12	8:L:401:BCL:CHB	2.48	0.44
4:M:411:GLU:O	4:M:415:LEU:HG	2.17	0.44
4:M:502:PHE:HE1	13:M:1006:PGV:H61	1.82	0.44
8:T:101:BCL:H143	2:V:14:VAL:HG13	1.99	0.44
6:C:162:ALA:O	6:C:163:SER:OG	2.34	0.44
8:G:101:BCL:H93	8:G:101:BCL:H61	1.85	0.44
10:L:405:BPH:H7C2	4:M:383:PHE:HD1	1.83	0.44
8:M:1005:BCL:H91	8:M:1005:BCL:H112	1.77	0.44
1:E:48:TRP:HH2	1:E:54:ILE:HD11	1.83	0.44
3:L:49:THR:O	3:L:53:ARG:HG2	2.17	0.44
6:C:197:TRP:O	6:C:198:ARG:NH1	2.50	0.44
7:Z:27:LEU:HD23	7:Z:27:LEU:HA	1.80	0.44
10:L:405:BPH:H112	10:L:405:BPH:H142	1.59	0.44
8:O:101:BCL:H62	8:O:101:BCL:H41	1.49	0.44
8:R:101:BCL:HBC3	8:R:101:BCL:H2C	1.67	0.44
1:K:9:LEU:HD12	1:K:20:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:346:GLY:C	4:M:348:GLU:H	2.21	0.44
4:M:446:HIS:HD2	4:M:481:PHE:CE1	2.36	0.44
8:V:101:BCL:H143	8:V:101:BCL:H162	1.70	0.44
6:C:285:ILE:HG13	6:C:286:MET:HG3	1.99	0.44
8:9:102:BCL:H2C	8:9:102:BCL:HBC3	1.67	0.44
1:O:15:LYS:HB2	1:O:15:LYS:HE3	1.63	0.44
2:T:8:PHE:HE2	1:U:25:VAL:CG1	2.31	0.44
8:W:101:BCL:H3A	8:W:101:BCL:HBA1	1.62	0.43
1:O:15:LYS:N	1:O:16:PRO:HD2	2.33	0.43
8:S:102:BCL:H112	8:S:102:BCL:H93	1.67	0.43
1:U:19:ASN:HB3	1:U:22:GLN:HG3	2.00	0.43
6:C:188:GLU:OE2	6:C:188:GLU:N	2.45	0.43
6:C:207:GLY:HA2	14:C:503:HEM:O2D	2.18	0.43
14:C:504:HEM:HBC2	14:C:504:HEM:CHD	2.47	0.43
8:1:101:BCL:H121	8:1:101:BCL:H162	1.85	0.43
8:2:102:BCL:H112	8:2:102:BCL:H93	1.67	0.43
10:L:405:BPH:O1D	10:L:405:BPH:H2A	2.18	0.43
8:P:101:BCL:H2C	8:P:101:BCL:HBC3	1.67	0.43
8:3:101:BCL:H121	8:3:101:BCL:H162	1.85	0.43
8:6:101:BCL:H41	8:6:101:BCL:H62	1.50	0.43
1:B:53:TRP:HE1	8:B:101:BCL:CBB	2.31	0.43
8:B:101:BCL:H41	8:B:101:BCL:H62	1.50	0.43
2:J:16:THR:HB	8:J:101:BCL:C20	2.49	0.43
4:M:541:MET:HE1	11:M:1002:MQE:CBY	2.48	0.43
6:C:205:TYR:N	6:C:206:PRO:HD3	2.33	0.43
8:D:101:BCL:HBC3	8:D:101:BCL:H2C	1.67	0.43
8:G:101:BCL:H151	9:I:103:KGD:CBJ	2.48	0.43
10:L:404:BPH:HBC3	8:M:1005:BCL:H43	2.01	0.43
8:4:101:BCL:H62	8:4:101:BCL:H41	1.49	0.43
2:H:23:ALA:HA	8:I:101:BCL:O2D	2.18	0.43
1:I:10:VAL:HG22	1:I:23:TRP:CG	2.54	0.43
3:L:77:ILE:HA	3:L:80:ILE:HD12	1.99	0.43
4:M:463:THR:OG1	4:M:465:VAL:HG22	2.18	0.43
6:C:184:PRO:HB2	6:C:292:SER:OG	2.18	0.43
10:L:404:BPH:H9C1	10:L:404:BPH:H112	1.67	0.43
8:4:101:BCL:H93	8:4:101:BCL:H61	1.85	0.43
8:9:102:BCL:H121	8:9:102:BCL:H162	1.85	0.43
1:G:53:TRP:CE2	8:G:101:BCL:H2C	2.54	0.43
3:L:74:ALA:O	3:L:77:ILE:HG22	2.19	0.43
3:L:165:SER:HB3	13:M:1007:PGV:H101	2.01	0.43
4:M:492:GLY:CA	13:M:1008:PGV:H32	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:551:LYS:CE	13:M:1007:PGV:O05	2.67	0.43
1:W:7:ASN:CA	1:W:20:ASN:HB2	2.49	0.43
7:Z:17:TRP:CG	7:Z:18:SER:N	2.87	0.43
8:8:102:BCL:H93	8:8:102:BCL:H112	1.67	0.43
1:S:46:LEU:C	1:S:48:TRP:H	2.22	0.43
1:2:10:VAL:HG22	1:2:23:TRP:CG	2.54	0.42
2:A:38:TRP:CZ2	8:A:101:BCL:HHC	2.54	0.42
1:E:10:VAL:HG22	1:E:23:TRP:CG	2.54	0.42
8:E:102:BCL:H112	8:E:102:BCL:H93	1.67	0.42
1:O:18:PHE:HE2	8:O:102:BCL:HMA1	1.84	0.42
1:W:9:LEU:HA	1:W:9:LEU:HD12	1.59	0.42
2:3:8:PHE:CB	1:4:22:GLN:HE21	2.32	0.42
1:4:18:PHE:HE2	8:4:102:BCL:HMA1	1.84	0.42
1:8:18:PHE:HE2	8:8:102:BCL:HMA1	1.84	0.42
10:L:402:BPH:HBA1	10:L:402:BPH:H3A	1.50	0.42
10:L:405:BPH:HBC1	4:M:600:ALA:HB2	2.01	0.42
4:M:503:ARG:O	4:M:503:ARG:HG2	2.19	0.42
1:S:18:PHE:HE2	8:S:102:BCL:HMA1	1.84	0.42
6:C:88:PRO:HB2	6:C:91:VAL:HG13	2.00	0.42
8:6:101:BCL:O1D	8:6:101:BCL:H2A	2.19	0.42
1:8:28:ILE:O	1:8:32:THR:HG23	2.20	0.42
1:E:15:LYS:N	1:E:16:PRO:HD2	2.34	0.42
1:G:10:VAL:HG22	1:G:23:TRP:CG	2.54	0.42
4:M:564:GLU:OE1	7:Z:49:TYR:HE1	2.02	0.42
8:U:102:BCL:HBC3	8:U:102:BCL:H2C	1.60	0.42
2:1:30:VAL:HA	6:C:46:ILE:CD1	2.48	0.42
1:2:28:ILE:O	1:2:32:THR:HG23	2.20	0.42
1:6:10:VAL:HG22	1:6:23:TRP:CG	2.54	0.42
1:8:10:VAL:HG22	1:8:23:TRP:CG	2.54	0.42
1:G:18:PHE:HE2	8:G:102:BCL:HMA1	1.84	0.42
8:K:101:BCL:H2A	8:K:101:BCL:O1D	2.20	0.42
3:L:11:PRO:HD2	4:M:561:MET:O	2.20	0.42
3:L:192:HIS:O	3:L:196:VAL:HG23	2.19	0.42
1:4:28:ILE:O	1:4:32:THR:HG23	2.20	0.42
8:E:101:BCL:O1D	8:E:101:BCL:H2A	2.19	0.42
1:G:10:VAL:O	1:G:15:LYS:CD	2.68	0.42
8:K:101:BCL:H41	8:K:101:BCL:H62	1.49	0.42
3:L:49:THR:HG23	3:L:145:ASP:OD1	2.19	0.42
2:N:38:TRP:CZ2	8:N:101:BCL:HHC	2.54	0.42
8:T:101:BCL:H202	2:V:18:LEU:HD11	2.01	0.42
6:C:93:VAL:HG22	6:C:94:LEU:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:148:MET:HG3	6:C:274:TYR:CZ	2.54	0.42
6:C:159:LYS:HD3	6:C:159:LYS:HA	1.81	0.42
8:5:101:BCL:H2C	8:5:101:BCL:HBC3	1.67	0.42
8:7:101:BCL:H2C	8:7:101:BCL:HBC3	1.67	0.42
8:G:101:BCL:O1D	8:G:101:BCL:H2A	2.19	0.42
1:I:28:ILE:O	1:I:32:THR:HG23	2.20	0.42
8:P:101:BCL:H121	8:P:101:BCL:H162	1.85	0.42
1:O:15:LYS:HE2	1:O:15:LYS:HB2	1.73	0.42
1:O:28:ILE:O	1:O:32:THR:HG23	2.20	0.42
1:6:53:TRP:CZ3	8:6:101:BCL:HAC2	2.54	0.42
4:M:337:ASP:OD2	4:M:340:ASP:HB2	2.20	0.42
1:S:10:VAL:HG22	1:S:23:TRP:CG	2.54	0.42
1:U:7:ASN:O	1:U:9:LEU:N	2.53	0.42
1:B:18:PHE:HE2	8:B:102:BCL:HMA1	1.84	0.42
2:F:38:TRP:CZ2	8:F:101:BCL:HHC	2.54	0.42
1:K:28:ILE:O	1:K:32:THR:HG23	2.20	0.42
2:N:23:ALA:HB1	8:N:101:BCL:O1A	2.20	0.42
8:Q:101:BCL:O1D	8:Q:101:BCL:H2A	2.20	0.42
2:V:27:HIS:HE1	8:V:101:BCL:C1C	2.32	0.42
2:V:27:HIS:NE2	8:V:101:BCL:NB	2.67	0.42
8:O:101:BCL:H93	8:O:101:BCL:H112	1.67	0.42
1:B:28:ILE:O	1:B:32:THR:HG23	2.20	0.42
1:E:18:PHE:HE2	8:E:102:BCL:HMA1	1.84	0.42
10:L:402:BPH:H9C2	10:L:402:BPH:H6C2	1.81	0.42
2:R:16:THR:HB	8:R:101:BCL:C20	2.50	0.42
1:O:18:PHE:HE2	8:O:101:BCL:HMA1	1.84	0.42
8:A:101:BCL:H121	8:A:101:BCL:H162	1.85	0.42
1:E:28:ILE:O	1:E:32:THR:HG23	2.20	0.42
1:E:32:THR:HG22	8:G:102:BCL:H61	2.02	0.42
8:I:101:BCL:O1D	8:I:101:BCL:H2A	2.19	0.42
1:K:10:VAL:HG22	1:K:23:TRP:CG	2.54	0.42
1:K:18:PHE:HE2	8:K:102:BCL:HMA1	1.84	0.42
2:N:23:ALA:CB	8:O:101:BCL:CED	2.89	0.42
1:Q:28:ILE:O	1:Q:32:THR:HG23	2.20	0.42
8:S:101:BCL:H41	8:S:101:BCL:H62	1.50	0.42
8:O:102:BCL:H93	8:O:102:BCL:H61	1.85	0.41
1:4:10:VAL:HG22	1:4:23:TRP:CG	2.54	0.41
8:4:101:BCL:O1D	8:4:101:BCL:H2A	2.19	0.41
1:8:11:PRO:HB2	1:8:13:GLN:OE1	2.20	0.41
2:A:10:THR:HB	4:M:347:LEU:HD11	2.02	0.41
2:H:4:ARG:NE	1:I:17:LEU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:351:ILE:HD11	4:M:375:VAL:HG21	2.00	0.41
1:O:10:VAL:HG12	1:O:23:TRP:CD2	2.54	0.41
1:O:19:ASN:CG	1:O:20:ASN:H	2.23	0.41
1:Q:10:VAL:HG22	1:Q:23:TRP:CG	2.54	0.41
8:W:101:BCL:CED	8:W:101:BCL:CAD	2.98	0.41
8:O:102:BCL:HMD1	2:9:27:HIS:CE1	2.56	0.41
2:H:36:PHE:O	1:I:50:TRP:CH2	2.74	0.41
3:L:201:TYR:O	6:C:240:CYS:HB3	2.21	0.41
13:M:1008:PGV:H211	13:M:1008:PGV:C1	2.49	0.41
8:N:101:BCL:H121	8:N:101:BCL:H162	1.85	0.41
1:O:28:ILE:O	1:O:32:THR:HG23	2.20	0.41
1:U:10:VAL:HG22	1:U:23:TRP:CG	2.54	0.41
1:W:28:ILE:O	1:W:32:THR:HG23	2.20	0.41
2:1:22:MET:HE2	6:C:35:SER:HB2	2.02	0.41
1:4:21:ALA:CB	2:5:5:PRO:HD3	2.49	0.41
1:K:53:TRP:CZ3	8:K:101:BCL:HAC2	2.56	0.41
1:S:28:ILE:O	1:S:32:THR:HG23	2.20	0.41
1:S:53:TRP:HE1	8:S:101:BCL:CBB	2.27	0.41
8:S:101:BCL:O1D	8:S:101:BCL:H2A	2.20	0.41
8:U:101:BCL:H2A	8:U:101:BCL:O1D	2.19	0.41
1:2:36:GLY:HA3	8:2:101:BCL:H61	2.03	0.41
1:G:28:ILE:O	1:G:32:THR:HG23	2.20	0.41
3:L:216:ILE:CD1	8:L:401:BCL:C1B	2.96	0.41
10:L:405:BPH:HHB	10:L:405:BPH:HMB1	1.91	0.41
1:Q:18:PHE:HE2	8:Q:102:BCL:HMA1	1.85	0.41
6:C:129:GLN:NE2	6:C:131:ASP:OD1	2.53	0.41
8:6:101:BCL:H93	8:6:101:BCL:H61	1.85	0.41
1:B:10:VAL:HG22	1:B:23:TRP:CG	2.55	0.41
1:I:18:PHE:HE2	8:I:102:BCL:HMA1	1.84	0.41
8:J:101:BCL:H121	8:J:101:BCL:H162	1.85	0.41
1:U:28:ILE:O	1:U:32:THR:HG23	2.20	0.41
1:W:8:ASP:OD1	1:W:15:LYS:NZ	2.52	0.41
1:W:18:PHE:HE2	8:W:102:BCL:HMA1	1.84	0.41
5:Y:3:TRP:HA	5:Y:3:TRP:CE3	2.55	0.41
8:O:102:BCL:O1D	8:O:102:BCL:H2A	2.19	0.41
1:6:18:PHE:HE2	8:6:102:BCL:HMA1	1.84	0.41
8:8:101:BCL:O1D	8:8:101:BCL:H2A	2.20	0.41
3:L:276:LEU:HB3	5:Y:17:PHE:CE1	2.55	0.41
8:L:401:BCL:HBA2	8:L:401:BCL:HBD	2.02	0.41
4:M:445:LEU:HD11	8:M:1005:BCL:H141	2.02	0.41
2:N:23:ALA:CB	8:O:101:BCL:HED1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:101:BCL:O1D	8:O:101:BCL:H2A	2.20	0.41
6:C:64:GLN:OE1	6:C:64:GLN:N	2.43	0.41
6:C:301:ASN:OD1	6:C:301:ASN:N	2.53	0.41
1:O:10:VAL:HG22	1:O:23:TRP:CG	2.54	0.41
8:F:101:BCL:H121	8:F:101:BCL:H162	1.85	0.41
2:H:23:ALA:HB1	8:H:101:BCL:O1A	2.20	0.41
1:O:53:TRP:HE1	8:O:101:BCL:CBB	2.31	0.41
8:G:101:BCL:H41	8:G:101:BCL:H62	1.50	0.41
3:L:154:MET:O	3:L:158:ILE:HG13	2.21	0.41
1:U:18:PHE:HE2	8:U:102:BCL:HMA1	1.84	0.41
6:C:60:VAL:CG2	6:C:167:TYR:CD2	3.03	0.41
6:C:191:ASN:N	6:C:191:ASN:OD1	2.54	0.41
6:C:211:VAL:HG21	6:C:222:VAL:HG22	2.01	0.41
2:5:23:ALA:HA	8:6:101:BCL:O2D	2.20	0.41
1:6:28:ILE:O	1:6:32:THR:HG23	2.20	0.41
8:B:101:BCL:O1D	8:B:101:BCL:H2A	2.19	0.41
8:D:101:BCL:H121	8:D:101:BCL:H162	1.85	0.41
3:L:162:ALA:O	3:L:165:SER:OG	2.31	0.41
4:M:529:ILE:HG12	8:M:1005:BCL:HMB3	2.03	0.41
4:M:564:GLU:OE1	7:Z:49:TYR:CE1	2.74	0.41
1:2:18:PHE:HE2	8:2:102:BCL:HMA1	1.84	0.41
2:3:12:VAL:HG21	2:5:6:PHE:HZ	1.86	0.41
8:5:101:BCL:H92	8:5:101:BCL:H61	1.90	0.41
8:G:102:BCL:H112	8:G:102:BCL:H93	1.67	0.41
8:G:102:BCL:HBC3	8:G:102:BCL:H2C	1.59	0.41
3:L:216:ILE:HG12	8:L:401:BCL:CMB	2.40	0.41
2:V:7:GLU:HB3	2:V:9:ARG:HG2	2.02	0.41
6:C:148:MET:HG3	6:C:274:TYR:CE1	2.56	0.41
7:Z:25:VAL:O	7:Z:29:ALA:HB3	2.21	0.41
8:6:102:BCL:H93	8:6:102:BCL:H112	1.67	0.40
2:9:16:THR:HG22	9:9:101:KGD:CAN	2.51	0.40
1:K:48:TRP:O	1:K:49:ALA:C	2.58	0.40
4:M:613:LEU:HD23	4:M:613:LEU:HA	1.88	0.40
3:L:173:LEU:HD22	5:Y:9:MET:SD	2.62	0.40
10:L:402:BPH:HBB1	4:M:533:LEU:HD13	2.04	0.40
10:L:402:BPH:HHD	10:L:402:BPH:HAC1	1.83	0.40
10:L:404:BPH:H142	10:L:404:BPH:H111	1.83	0.40
8:O:101:BCL:H93	8:O:101:BCL:H61	1.85	0.40
1:O:53:TRP:NE1	8:O:102:BCL:HBB2	2.36	0.40
8:G:101:BCL:HBB2	8:G:101:BCL:HHC	2.04	0.40
2:V:20:LEU:HD23	2:V:20:LEU:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:119:SER:O	6:C:135:ASN:OD1	2.39	0.40
2:1:8:PHE:HD1	8:2:102:BCL:HBB3	1.85	0.40
8:B:101:BCL:HBB2	8:B:101:BCL:HHC	2.04	0.40
3:L:216:ILE:HD11	8:L:401:BCL:C2B	2.47	0.40
8:B:101:BCL:HBA1	8:B:101:BCL:H3A	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	2	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	4	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	6	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	8	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	B	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	E	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	G	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	I	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	K	47/55 (86%)	43 (92%)	4 (8%)	0	100	100
1	O	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	Q	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	S	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	U	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	W	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
2	1	33/42 (79%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	5	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	7	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	9	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	A	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	D	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	H	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	J	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	N	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	P	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	R	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	T	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	V	29/42 (69%)	26 (90%)	3 (10%)	0	100	100
3	L	290/315 (92%)	282 (97%)	8 (3%)	0	100	100
4	M	304/307 (99%)	291 (96%)	13 (4%)	0	100	100
5	Y	30/39 (77%)	30 (100%)	0	0	100	100
6	C	289/320 (90%)	260 (90%)	29 (10%)	0	100	100
7	Z	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
All	All	2193/2499 (88%)	2068 (94%)	125 (6%)	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	0	43/49 (88%)	43 (100%)	0	100	100
1	2	43/49 (88%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	43/49 (88%)	43 (100%)	0	100	100
1	6	43/49 (88%)	43 (100%)	0	100	100
1	8	43/49 (88%)	43 (100%)	0	100	100
1	B	43/49 (88%)	43 (100%)	0	100	100
1	E	43/49 (88%)	43 (100%)	0	100	100
1	G	43/49 (88%)	43 (100%)	0	100	100
1	I	43/49 (88%)	43 (100%)	0	100	100
1	K	43/49 (88%)	43 (100%)	0	100	100
1	O	43/49 (88%)	43 (100%)	0	100	100
1	Q	43/49 (88%)	43 (100%)	0	100	100
1	S	43/49 (88%)	43 (100%)	0	100	100
1	U	43/49 (88%)	43 (100%)	0	100	100
1	W	43/49 (88%)	43 (100%)	0	100	100
2	1	30/37 (81%)	29 (97%)	1 (3%)	33	62
2	3	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	5	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	7	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	D	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	F	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	H	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	J	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	N	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	P	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	R	33/37 (89%)	32 (97%)	1 (3%)	36	64
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	27/37 (73%)	26 (96%)	1 (4%)	29	59
3	L	239/253 (94%)	236 (99%)	3 (1%)	65	82
4	M	244/245 (100%)	242 (99%)	2 (1%)	79	89
5	Y	29/36 (81%)	28 (97%)	1 (3%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	236/262 (90%)	235 (100%)	1 (0%)	89	94
7	Z	36/50 (72%)	36 (100%)	0	100	100
All	All	1915/2136 (90%)	1895 (99%)	20 (1%)	71	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	27	HIS
2	3	27	HIS
2	5	27	HIS
2	7	27	HIS
2	A	27	HIS
2	D	27	HIS
2	F	27	HIS
2	H	27	HIS
2	J	27	HIS
3	L	39	ILE
3	L	181	TRP
3	L	305	TRP
4	M	503	ARG
4	M	630	TRP
2	N	27	HIS
2	P	27	HIS
2	R	27	HIS
2	V	27	HIS
5	Y	17	PHE
6	C	127	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	13	GLN
6	C	83	GLN
7	Z	58	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 1 is monoatomic - leaving 66 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	$\# Z  > 2$
8	BCL	8	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.22	27 (34%)
8	BCL	I	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.20	27 (34%)
8	BCL	J	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	S	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.21	27 (34%)
14	HEM	C	503	6	41,50,50	1.38	3 (7%)	45,82,82	2.22	11 (24%)
8	BCL	B	101	-	64,74,74	1.79	14 (21%)	78,115,115	2.21	27 (34%)
8	BCL	M	1001	-	64,74,74	1.76	14 (21%)	78,115,115	2.27	27 (34%)
13	PGV	M	1006	-	44,44,50	0.72	0	47,50,56	1.00	3 (6%)
8	BCL	D	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.25	31 (39%)
8	BCL	F	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.27	31 (39%)
8	BCL	K	101	-	64,74,74	1.78	12 (18%)	78,115,115	2.22	27 (34%)
9	KGD	J	102	-	41,41,41	0.98	3 (7%)	49,53,53	2.20	16 (32%)
14	HEM	C	501	6	41,50,50	1.24	3 (7%)	45,82,82	1.80	9 (20%)
8	BCL	I	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.22	27 (34%)
8	BCL	N	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
11	MQE	M	1002	-	69,69,69	0.82	1 (1%)	84,87,87	1.53	14 (16%)
8	BCL	5	101	-	64,74,74	1.77	13 (20%)	78,115,115	2.27	31 (39%)
8	BCL	0	102	-	64,74,74	1.78	13 (20%)	78,115,115	2.21	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	E	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.21	27 (34%)
9	KGD	N	102	-	41,41,41	0.92	1 (2%)	49,53,53	2.48	14 (28%)
8	BCL	3	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.25	31 (39%)
13	PGV	M	1008	-	33,33,50	1.16	3 (9%)	36,39,56	1.02	2 (5%)
11	MQE	L	403	-	69,69,69	0.58	0	84,87,87	1.31	12 (14%)
8	BCL	U	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.21	26 (33%)
8	BCL	A	101	-	64,74,74	1.79	13 (20%)	78,115,115	2.35	31 (39%)
8	BCL	Q	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.21	26 (33%)
8	BCL	Q	101	-	64,74,74	1.78	12 (18%)	78,115,115	2.22	27 (34%)
8	BCL	E	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.20	27 (34%)
9	KGD	I	103	-	41,41,41	1.09	3 (7%)	49,53,53	2.44	15 (30%)
8	BCL	6	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.20	26 (33%)
8	BCL	G	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.20	27 (34%)
8	BCL	6	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.21	27 (34%)
11	MQE	M	1003	-	26,26,69	1.21	4 (15%)	32,35,87	1.52	3 (9%)
8	BCL	2	101	-	64,74,74	1.79	13 (20%)	78,115,115	2.38	33 (42%)
8	BCL	4	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.20	26 (33%)
8	BCL	G	101	-	64,74,74	1.79	14 (21%)	78,115,115	2.21	27 (34%)
8	BCL	2	102	-	64,74,74	1.74	14 (21%)	78,115,115	2.21	26 (33%)
8	BCL	4	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.22	27 (34%)
8	BCL	7	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	S	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.22	27 (34%)
9	KGD	D	102	-	41,41,41	1.26	5 (12%)	49,53,53	2.47	16 (32%)
10	BPH	L	402	-	51,70,70	1.22	7 (13%)	52,101,101	1.59	11 (21%)
10	BPH	L	405	-	51,70,70	1.26	6 (11%)	52,101,101	1.47	6 (11%)
8	BCL	M	1005	-	64,74,74	1.71	13 (20%)	78,115,115	2.30	27 (34%)
8	BCL	8	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.22	27 (34%)
8	BCL	B	102	-	64,74,74	1.74	14 (21%)	78,115,115	2.20	27 (34%)
13	PGV	M	1007	-	41,41,50	0.80	1 (2%)	44,47,56	1.04	3 (6%)
14	HEM	C	502	6	41,50,50	1.27	3 (7%)	45,82,82	1.89	9 (20%)
8	BCL	V	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.37	30 (38%)
8	BCL	K	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.21	27 (34%)
8	BCL	O	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.21	27 (34%)
10	BPH	L	404	-	51,70,70	1.26	6 (11%)	52,101,101	1.46	9 (17%)
8	BCL	W	102	-	64,74,74	1.74	14 (21%)	78,115,115	2.20	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	HEM	C	504	6	41,50,50	1.31	3 (7%)	45,82,82	1.96	10 (22%)
8	BCL	0	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.20	27 (34%)
8	BCL	W	101	-	64,74,74	1.77	11 (17%)	78,115,115	2.44	31 (39%)
8	BCL	U	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.21	27 (34%)
8	BCL	O	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.20	26 (33%)
8	BCL	1	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	P	101	-	64,74,74	1.79	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	R	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	9	102	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
9	KGD	9	101	-	41,41,41	1.08	2 (4%)	49,53,53	2.37	13 (26%)
8	BCL	H	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.26	31 (39%)
8	BCL	T	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.32	32 (41%)
8	BCL	L	401	-	64,74,74	1.74	13 (20%)	78,115,115	2.37	30 (38%)

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
8	BCL	8	101	-	-	16/37/137/137	-
8	BCL	I	102	-	-	16/37/137/137	-
8	BCL	J	101	-	-	19/37/137/137	-
8	BCL	S	102	-	-	16/37/137/137	-
14	HEM	C	503	6	-	4/12/54/54	-
8	BCL	B	101	-	-	16/37/137/137	-
8	BCL	M	1001	-	-	18/37/137/137	-
13	PGV	M	1006	-	-	11/49/49/55	-
8	BCL	D	101	-	-	19/37/137/137	-
8	BCL	F	101	-	-	18/37/137/137	-
8	BCL	K	101	-	-	16/37/137/137	-
9	KGD	J	102	-	-	13/36/56/56	0/1/1/1
14	HEM	C	501	6	-	6/12/54/54	-
8	BCL	I	101	-	-	16/37/137/137	-
8	BCL	N	101	-	-	18/37/137/137	-
11	MQE	M	1002	-	-	21/65/85/85	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	5	101	-	-	19/37/137/137	-
8	BCL	0	102	-	-	16/37/137/137	-
8	BCL	E	101	-	-	16/37/137/137	-
9	KGD	N	102	-	-	10/36/56/56	0/1/1/1
8	BCL	3	101	-	-	18/37/137/137	-
13	PGV	M	1008	-	-	12/38/38/55	-
11	MQE	L	403	-	-	16/65/85/85	0/2/2/2
8	BCL	U	102	-	-	17/37/137/137	-
8	BCL	A	101	-	-	18/37/137/137	-
8	BCL	Q	102	-	-	16/37/137/137	-
8	BCL	Q	101	-	-	16/37/137/137	-
8	BCL	E	102	-	-	16/37/137/137	-
9	KGD	I	103	-	-	14/36/56/56	0/1/1/1
8	BCL	6	102	-	-	16/37/137/137	-
8	BCL	G	102	-	-	16/37/137/137	-
8	BCL	6	101	-	-	16/37/137/137	-
11	MQE	M	1003	-	-	7/14/34/85	0/2/2/2
8	BCL	2	101	-	-	27/37/137/137	-
8	BCL	4	102	-	-	17/37/137/137	-
8	BCL	G	101	-	-	16/37/137/137	-
8	BCL	2	102	-	-	16/37/137/137	-
8	BCL	4	101	-	-	16/37/137/137	-
8	BCL	7	101	-	-	19/37/137/137	-
8	BCL	S	101	-	-	16/37/137/137	-
9	KGD	D	102	-	-	17/36/56/56	0/1/1/1
10	BPH	L	402	-	-	17/37/105/105	0/5/6/6
10	BPH	L	405	-	-	14/37/105/105	0/5/6/6
8	BCL	M	1005	-	-	15/37/137/137	-
8	BCL	8	102	-	-	16/37/137/137	-
8	BCL	B	102	-	-	16/37/137/137	-
13	PGV	M	1007	-	-	14/46/46/55	-
14	HEM	C	502	6	-	1/12/54/54	-
8	BCL	V	101	-	-	20/37/137/137	-
8	BCL	K	102	-	-	16/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	O	101	-	-	16/37/137/137	-
10	BPH	L	404	-	-	15/37/105/105	0/5/6/6
8	BCL	W	102	-	-	16/37/137/137	-
14	HEM	C	504	6	-	4/12/54/54	-
8	BCL	0	101	-	-	16/37/137/137	-
8	BCL	W	101	-	-	27/37/137/137	-
8	BCL	U	101	-	-	16/37/137/137	-
8	BCL	O	102	-	-	16/37/137/137	-
8	BCL	1	101	-	-	18/37/137/137	-
8	BCL	P	101	-	-	17/37/137/137	-
8	BCL	R	101	-	-	19/37/137/137	-
8	BCL	9	102	-	-	16/37/137/137	-
9	KGD	9	101	-	-	15/36/56/56	0/1/1/1
8	BCL	H	101	-	-	16/37/137/137	-
8	BCL	T	101	-	-	18/37/137/137	-
8	BCL	L	401	-	-	18/37/137/137	-

All (682) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	101	BCL	MG-ND	-6.67	1.92	2.05
8	2	101	BCL	MG-ND	-6.64	1.92	2.05
8	V	101	BCL	MG-ND	-6.02	1.93	2.05
8	4	101	BCL	MG-ND	-6.01	1.93	2.05
8	6	101	BCL	MG-ND	-6.01	1.93	2.05
8	8	101	BCL	MG-ND	-5.99	1.93	2.05
8	B	101	BCL	MG-ND	-5.98	1.93	2.05
8	O	101	BCL	MG-ND	-5.97	1.94	2.05
8	S	101	BCL	MG-ND	-5.97	1.94	2.05
8	Q	101	BCL	MG-ND	-5.96	1.94	2.05
8	F	101	BCL	MG-ND	-5.96	1.94	2.05
8	U	101	BCL	MG-ND	-5.96	1.94	2.05
8	0	102	BCL	MG-ND	-5.95	1.94	2.05
8	N	101	BCL	MG-ND	-5.95	1.94	2.05
8	T	101	BCL	MG-ND	-5.95	1.94	2.05
8	G	101	BCL	MG-ND	-5.95	1.94	2.05
8	I	101	BCL	MG-ND	-5.95	1.94	2.05
8	3	101	BCL	MG-ND	-5.95	1.94	2.05
8	L	401	BCL	MG-ND	-5.95	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	101	BCL	MG-ND	-5.94	1.94	2.05
8	K	101	BCL	MG-ND	-5.94	1.94	2.05
8	E	101	BCL	MG-ND	-5.93	1.94	2.05
8	P	101	BCL	MG-ND	-5.93	1.94	2.05
8	H	101	BCL	MG-ND	-5.93	1.94	2.05
8	D	101	BCL	MG-ND	-5.92	1.94	2.05
8	1	101	BCL	MG-ND	-5.92	1.94	2.05
8	7	101	BCL	MG-ND	-5.92	1.94	2.05
8	R	101	BCL	MG-ND	-5.90	1.94	2.05
8	5	101	BCL	MG-ND	-5.90	1.94	2.05
8	9	102	BCL	MG-ND	-5.90	1.94	2.05
8	A	101	BCL	MG-ND	-5.89	1.94	2.05
8	M	1001	BCL	MG-ND	-5.88	1.94	2.05
8	G	102	BCL	MG-ND	-5.86	1.94	2.05
8	M	1005	BCL	MG-ND	-5.86	1.94	2.05
8	6	102	BCL	MG-ND	-5.86	1.94	2.05
8	4	102	BCL	MG-ND	-5.85	1.94	2.05
8	U	102	BCL	MG-ND	-5.84	1.94	2.05
8	O	102	BCL	MG-ND	-5.84	1.94	2.05
8	Q	102	BCL	MG-ND	-5.83	1.94	2.05
8	I	102	BCL	MG-ND	-5.83	1.94	2.05
8	S	102	BCL	MG-ND	-5.82	1.94	2.05
8	K	102	BCL	MG-ND	-5.82	1.94	2.05
8	8	102	BCL	MG-ND	-5.81	1.94	2.05
8	W	102	BCL	MG-ND	-5.79	1.94	2.05
8	E	102	BCL	MG-ND	-5.79	1.94	2.05
8	2	102	BCL	MG-ND	-5.77	1.94	2.05
8	0	101	BCL	MG-ND	-5.77	1.94	2.05
8	B	102	BCL	MG-ND	-5.76	1.94	2.05
8	9	102	BCL	C4D-ND	-4.83	1.31	1.37
8	R	101	BCL	C4D-ND	-4.78	1.31	1.37
8	D	101	BCL	C4D-ND	-4.78	1.31	1.37
8	A	101	BCL	C4D-ND	-4.77	1.31	1.37
8	J	101	BCL	C4D-ND	-4.77	1.31	1.37
8	7	101	BCL	C4D-ND	-4.76	1.31	1.37
8	1	101	BCL	C4D-ND	-4.75	1.31	1.37
8	N	101	BCL	C4D-ND	-4.74	1.31	1.37
8	3	101	BCL	C4D-ND	-4.73	1.31	1.37
8	P	101	BCL	C4D-ND	-4.73	1.31	1.37
8	5	101	BCL	C4D-ND	-4.72	1.31	1.37
8	H	101	BCL	C4D-ND	-4.72	1.31	1.37
8	4	102	BCL	OBD-CAD	4.71	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	C4D-ND	-4.71	1.31	1.37
8	F	101	BCL	C4D-ND	-4.71	1.31	1.37
8	6	102	BCL	OBD-CAD	4.69	1.30	1.22
8	8	102	BCL	OBD-CAD	4.66	1.30	1.22
8	S	102	BCL	OBD-CAD	4.65	1.30	1.22
8	0	101	BCL	OBD-CAD	4.65	1.30	1.22
8	G	102	BCL	OBD-CAD	4.64	1.30	1.22
8	K	102	BCL	OBD-CAD	4.64	1.30	1.22
8	E	102	BCL	OBD-CAD	4.64	1.30	1.22
8	O	102	BCL	OBD-CAD	4.64	1.30	1.22
8	I	102	BCL	OBD-CAD	4.63	1.30	1.22
8	W	102	BCL	OBD-CAD	4.63	1.30	1.22
8	B	102	BCL	OBD-CAD	4.63	1.30	1.22
8	Q	102	BCL	OBD-CAD	4.63	1.30	1.22
8	V	101	BCL	OBD-CAD	4.63	1.30	1.22
8	2	101	BCL	OBD-CAD	4.62	1.30	1.22
8	U	102	BCL	OBD-CAD	4.62	1.30	1.22
14	C	503	HEM	C4D-ND	-4.60	1.32	1.40
8	S	101	BCL	OBD-CAD	4.60	1.30	1.22
8	2	102	BCL	OBD-CAD	4.59	1.30	1.22
8	8	101	BCL	OBD-CAD	4.59	1.30	1.22
8	0	102	BCL	OBD-CAD	4.59	1.30	1.22
8	6	101	BCL	OBD-CAD	4.59	1.30	1.22
8	G	101	BCL	OBD-CAD	4.59	1.30	1.22
8	O	101	BCL	OBD-CAD	4.57	1.30	1.22
8	W	101	BCL	OBD-CAD	4.57	1.30	1.22
8	I	101	BCL	OBD-CAD	4.57	1.30	1.22
8	Q	101	BCL	OBD-CAD	4.57	1.30	1.22
8	E	101	BCL	OBD-CAD	4.55	1.30	1.22
8	U	101	BCL	OBD-CAD	4.54	1.30	1.22
8	4	101	BCL	OBD-CAD	4.53	1.30	1.22
8	B	101	BCL	OBD-CAD	4.53	1.30	1.22
8	L	401	BCL	OBD-CAD	4.51	1.30	1.22
8	K	101	BCL	OBD-CAD	4.51	1.30	1.22
8	P	101	BCL	OBD-CAD	4.50	1.30	1.22
8	1	101	BCL	OBD-CAD	4.45	1.30	1.22
8	3	101	BCL	OBD-CAD	4.45	1.30	1.22
8	D	101	BCL	OBD-CAD	4.45	1.30	1.22
8	N	101	BCL	OBD-CAD	4.44	1.30	1.22
8	A	101	BCL	OBD-CAD	4.44	1.30	1.22
8	J	101	BCL	OBD-CAD	4.43	1.30	1.22
8	T	101	BCL	OBD-CAD	4.43	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	101	BCL	C4D-ND	-4.43	1.31	1.37
8	O	102	BCL	C4D-ND	-4.43	1.31	1.37
8	5	101	BCL	OBD-CAD	4.42	1.30	1.22
8	G	102	BCL	C4D-ND	-4.42	1.31	1.37
8	U	102	BCL	C4D-ND	-4.42	1.31	1.37
8	H	101	BCL	OBD-CAD	4.42	1.30	1.22
8	0	101	BCL	C4D-ND	-4.42	1.31	1.37
8	F	101	BCL	OBD-CAD	4.41	1.30	1.22
8	7	101	BCL	OBD-CAD	4.41	1.30	1.22
8	9	102	BCL	OBD-CAD	4.41	1.30	1.22
8	6	102	BCL	C4D-ND	-4.40	1.31	1.37
8	8	102	BCL	C4D-ND	-4.40	1.31	1.37
8	W	101	BCL	C4D-ND	-4.40	1.31	1.37
8	B	102	BCL	C4D-ND	-4.39	1.31	1.37
8	2	102	BCL	C4D-ND	-4.39	1.31	1.37
8	2	101	BCL	C4D-ND	-4.39	1.31	1.37
8	R	101	BCL	OBD-CAD	4.39	1.30	1.22
8	M	1001	BCL	OBD-CAD	4.38	1.30	1.22
8	L	401	BCL	C4D-ND	-4.38	1.31	1.37
8	K	101	BCL	C4D-ND	-4.38	1.31	1.37
8	E	102	BCL	C4D-ND	-4.38	1.31	1.37
8	4	102	BCL	C4D-ND	-4.37	1.31	1.37
8	I	102	BCL	C4D-ND	-4.36	1.31	1.37
8	M	1001	BCL	O1D-CGD	-4.36	1.10	1.21
8	B	101	BCL	C4D-ND	-4.35	1.31	1.37
8	S	102	BCL	C4D-ND	-4.34	1.31	1.37
8	4	101	BCL	C4D-ND	-4.34	1.31	1.37
8	W	102	BCL	C4D-ND	-4.34	1.31	1.37
8	G	101	BCL	C4D-ND	-4.34	1.31	1.37
8	0	102	BCL	C4D-ND	-4.33	1.31	1.37
8	Q	101	BCL	C4D-ND	-4.33	1.31	1.37
8	Q	102	BCL	C4D-ND	-4.33	1.31	1.37
8	K	102	BCL	C4D-ND	-4.33	1.31	1.37
8	M	1001	BCL	C4D-ND	-4.33	1.31	1.37
8	8	101	BCL	C4D-ND	-4.32	1.31	1.37
8	S	101	BCL	C4D-ND	-4.31	1.31	1.37
8	6	101	BCL	C4D-ND	-4.31	1.31	1.37
8	L	401	BCL	O1D-CGD	-4.29	1.10	1.21
8	I	101	BCL	C4D-ND	-4.29	1.31	1.37
8	E	101	BCL	C4D-ND	-4.27	1.31	1.37
8	O	101	BCL	C4D-ND	-4.27	1.31	1.37
8	1	101	BCL	O1D-CGD	-4.25	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	101	BCL	O1D-CGD	-4.24	1.10	1.21
8	B	101	BCL	O1D-CGD	-4.24	1.10	1.21
8	O	101	BCL	O1D-CGD	-4.24	1.10	1.21
8	R	101	BCL	O1D-CGD	-4.23	1.10	1.21
8	A	101	BCL	O1D-CGD	-4.23	1.10	1.21
8	3	101	BCL	O1D-CGD	-4.23	1.10	1.21
8	F	101	BCL	O1D-CGD	-4.22	1.10	1.21
8	M	1005	BCL	C4D-ND	-4.22	1.31	1.37
8	5	101	BCL	O1D-CGD	-4.22	1.10	1.21
8	8	101	BCL	O1D-CGD	-4.22	1.10	1.21
8	N	101	BCL	O1D-CGD	-4.21	1.10	1.21
8	7	101	BCL	O1D-CGD	-4.21	1.10	1.21
8	K	101	BCL	O1D-CGD	-4.21	1.10	1.21
8	U	101	BCL	O1D-CGD	-4.21	1.10	1.21
8	H	101	BCL	O1D-CGD	-4.20	1.10	1.21
8	T	101	BCL	O1D-CGD	-4.20	1.10	1.21
8	9	102	BCL	O1D-CGD	-4.20	1.10	1.21
8	Q	101	BCL	O1D-CGD	-4.20	1.10	1.21
8	E	101	BCL	O1D-CGD	-4.19	1.10	1.21
8	4	101	BCL	O1D-CGD	-4.19	1.10	1.21
8	M	1005	BCL	O1D-CGD	-4.19	1.10	1.21
8	0	102	BCL	O1D-CGD	-4.18	1.10	1.21
8	D	101	BCL	O1D-CGD	-4.18	1.10	1.21
8	J	101	BCL	O1D-CGD	-4.18	1.10	1.21
8	W	101	BCL	O1D-CGD	-4.18	1.10	1.21
8	I	101	BCL	O1D-CGD	-4.17	1.10	1.21
8	6	101	BCL	O1D-CGD	-4.17	1.10	1.21
8	G	101	BCL	O1D-CGD	-4.17	1.10	1.21
8	S	101	BCL	O1D-CGD	-4.16	1.10	1.21
8	M	1005	BCL	OBD-CAD	4.14	1.29	1.22
8	B	102	BCL	O1D-CGD	-4.13	1.10	1.21
8	S	102	BCL	O1D-CGD	-4.13	1.10	1.21
8	W	102	BCL	O1D-CGD	-4.12	1.10	1.21
8	K	102	BCL	O1D-CGD	-4.11	1.10	1.21
8	6	102	BCL	O1D-CGD	-4.10	1.10	1.21
8	Q	102	BCL	O1D-CGD	-4.09	1.11	1.21
8	0	101	BCL	O1D-CGD	-4.08	1.11	1.21
14	C	504	HEM	C4D-ND	-4.08	1.33	1.40
8	U	102	BCL	O1D-CGD	-4.08	1.11	1.21
8	O	102	BCL	O1D-CGD	-4.07	1.11	1.21
8	8	102	BCL	O1D-CGD	-4.07	1.11	1.21
8	G	102	BCL	O1D-CGD	-4.07	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	102	BCL	O1D-CGD	-4.06	1.11	1.21
8	2	101	BCL	O1D-CGD	-4.06	1.11	1.21
8	2	102	BCL	O1D-CGD	-4.06	1.11	1.21
8	I	102	BCL	O1D-CGD	-4.05	1.11	1.21
8	E	102	BCL	O1D-CGD	-4.05	1.11	1.21
8	V	101	BCL	O1D-CGD	-4.04	1.11	1.21
14	C	502	HEM	C4D-ND	-4.03	1.33	1.40
8	V	101	BCL	C4D-ND	-4.00	1.32	1.37
8	G	101	BCL	O2D-CED	3.99	1.54	1.45
8	E	101	BCL	O2D-CED	3.96	1.54	1.45
8	Q	101	BCL	O2D-CED	3.95	1.54	1.45
8	U	101	BCL	O2D-CED	3.95	1.54	1.45
8	O	101	BCL	O2D-CED	3.95	1.54	1.45
8	K	101	BCL	O2D-CED	3.94	1.54	1.45
8	I	101	BCL	O2D-CED	3.93	1.54	1.45
8	0	102	BCL	O2D-CED	3.93	1.54	1.45
8	8	101	BCL	O2D-CED	3.92	1.54	1.45
8	S	101	BCL	O2D-CED	3.91	1.54	1.45
8	6	101	BCL	O2D-CED	3.90	1.54	1.45
8	4	101	BCL	O2D-CED	3.90	1.54	1.45
8	B	101	BCL	O2D-CED	3.89	1.54	1.45
10	L	405	BPH	CBD-CGD	-3.74	1.47	1.52
14	C	501	HEM	C4D-ND	-3.62	1.34	1.40
8	W	101	BCL	O2D-CED	3.51	1.53	1.45
8	2	101	BCL	O2D-CGD	-3.48	1.24	1.33
8	A	101	BCL	O1A-CGA	-3.41	1.12	1.22
10	L	404	BPH	CBD-CGD	-3.38	1.47	1.52
8	S	102	BCL	O2D-CED	3.37	1.53	1.45
8	V	101	BCL	O2D-CED	3.37	1.53	1.45
8	8	102	BCL	O2D-CED	3.36	1.53	1.45
8	E	102	BCL	O2D-CED	3.36	1.53	1.45
8	I	102	BCL	O2D-CED	3.36	1.53	1.45
8	1	101	BCL	O2A-CGA	-3.35	1.23	1.33
8	6	102	BCL	O2D-CED	3.35	1.53	1.45
8	U	102	BCL	O2D-CED	3.35	1.53	1.45
8	K	102	BCL	O2D-CED	3.35	1.53	1.45
8	B	102	BCL	O2D-CED	3.35	1.53	1.45
8	F	101	BCL	O2A-CGA	-3.34	1.23	1.33
8	O	102	BCL	O2D-CED	3.34	1.53	1.45
8	A	101	BCL	O2A-CGA	-3.33	1.23	1.33
8	T	101	BCL	O2A-CGA	-3.33	1.23	1.33
8	G	102	BCL	O2D-CED	3.33	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	101	BCL	O2A-CGA	-3.32	1.23	1.33
8	R	101	BCL	O2A-CGA	-3.32	1.23	1.33
8	P	101	BCL	O2A-CGA	-3.32	1.23	1.33
8	0	101	BCL	O2D-CED	3.32	1.53	1.45
8	7	101	BCL	O2A-CGA	-3.32	1.23	1.33
8	5	101	BCL	O2A-CGA	-3.31	1.23	1.33
8	2	101	BCL	O2D-CED	3.31	1.53	1.45
8	9	102	BCL	O2A-CGA	-3.31	1.23	1.33
8	Q	102	BCL	O2D-CED	3.31	1.53	1.45
8	3	101	BCL	O2A-CGA	-3.31	1.23	1.33
8	4	102	BCL	O2D-CED	3.31	1.53	1.45
8	1	101	BCL	O2D-CGD	-3.30	1.25	1.33
8	N	101	BCL	O2A-CGA	-3.30	1.23	1.33
8	2	102	BCL	O2D-CED	3.30	1.53	1.45
8	D	101	BCL	O2D-CGD	-3.30	1.25	1.33
8	W	102	BCL	O2D-CED	3.29	1.53	1.45
8	H	101	BCL	O2A-CGA	-3.29	1.23	1.33
8	N	101	BCL	O2D-CGD	-3.29	1.25	1.33
8	J	101	BCL	O2A-CGA	-3.29	1.23	1.33
8	D	101	BCL	O2D-CED	3.28	1.53	1.45
8	P	101	BCL	O2D-CGD	-3.28	1.25	1.33
8	R	101	BCL	O2D-CED	3.28	1.53	1.45
8	1	101	BCL	O2D-CED	3.27	1.53	1.45
8	7	101	BCL	O2D-CGD	-3.27	1.25	1.33
8	3	101	BCL	O2D-CED	3.27	1.53	1.45
8	A	101	BCL	O2D-CGD	-3.27	1.25	1.33
8	3	101	BCL	O2D-CGD	-3.26	1.25	1.33
8	5	101	BCL	O2D-CGD	-3.26	1.25	1.33
8	N	101	BCL	O2D-CED	3.26	1.53	1.45
8	J	101	BCL	O2D-CED	3.26	1.53	1.45
8	5	101	BCL	O2D-CED	3.26	1.53	1.45
8	R	101	BCL	O2D-CGD	-3.26	1.25	1.33
8	T	101	BCL	O2D-CGD	-3.26	1.25	1.33
8	J	101	BCL	O2D-CGD	-3.25	1.25	1.33
8	7	101	BCL	O2D-CED	3.25	1.53	1.45
8	P	101	BCL	O2D-CED	3.25	1.53	1.45
8	9	102	BCL	O2D-CED	3.25	1.53	1.45
8	H	101	BCL	O2D-CGD	-3.25	1.25	1.33
14	C	503	HEM	C1D-ND	-3.25	1.32	1.38
8	9	102	BCL	O2D-CGD	-3.25	1.25	1.33
8	H	101	BCL	O2D-CED	3.25	1.53	1.45
8	T	101	BCL	O2D-CED	3.25	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	BCL	O2D-CGD	-3.24	1.25	1.33
8	F	101	BCL	O2D-CED	3.24	1.52	1.45
8	A	101	BCL	O2D-CED	3.22	1.52	1.45
8	M	1005	BCL	O2D-CED	3.19	1.52	1.45
8	M	1001	BCL	O2D-CED	3.19	1.52	1.45
8	L	401	BCL	O2D-CED	3.19	1.52	1.45
8	M	1005	BCL	O2D-CGD	-3.17	1.25	1.33
8	M	1001	BCL	O2D-CGD	-3.17	1.25	1.33
10	L	402	BPH	CBD-CGD	-3.17	1.48	1.52
8	B	101	BCL	O2A-CGA	-3.12	1.24	1.33
8	2	102	BCL	O2D-CGD	-3.11	1.25	1.33
8	U	101	BCL	O2A-CGA	-3.10	1.24	1.33
8	I	102	BCL	O2D-CGD	-3.10	1.25	1.33
8	0	101	BCL	O2D-CGD	-3.10	1.25	1.33
8	E	102	BCL	O2D-CGD	-3.10	1.25	1.33
8	G	102	BCL	O2D-CGD	-3.10	1.25	1.33
8	M	1005	BCL	O2A-CGA	-3.10	1.24	1.33
8	O	101	BCL	O2A-CGA	-3.10	1.24	1.33
8	Q	101	BCL	O2A-CGA	-3.10	1.24	1.33
8	O	102	BCL	O2D-CGD	-3.09	1.25	1.33
8	Q	102	BCL	O2D-CGD	-3.09	1.25	1.33
8	U	102	BCL	O2D-CGD	-3.09	1.25	1.33
8	L	401	BCL	O2D-CGD	-3.09	1.25	1.33
8	4	102	BCL	O2D-CGD	-3.09	1.25	1.33
8	I	101	BCL	O2A-CGA	-3.08	1.24	1.33
8	4	101	BCL	O2A-CGA	-3.08	1.24	1.33
8	G	101	BCL	O2A-CGA	-3.08	1.24	1.33
10	L	405	BPH	C3D-C2D	-3.08	1.33	1.39
8	0	102	BCL	O2A-CGA	-3.08	1.24	1.33
8	K	101	BCL	O2A-CGA	-3.08	1.24	1.33
10	L	404	BPH	C2C-C3C	-3.08	1.51	1.54
8	W	101	BCL	O2A-CGA	-3.07	1.24	1.33
8	6	101	BCL	O2A-CGA	-3.07	1.24	1.33
8	E	101	BCL	O2A-CGA	-3.07	1.24	1.33
13	M	1008	PGV	C03-C02	3.07	1.60	1.50
8	8	101	BCL	O2A-CGA	-3.07	1.24	1.33
8	K	102	BCL	O2D-CGD	-3.06	1.25	1.33
8	W	102	BCL	O2D-CGD	-3.06	1.25	1.33
8	S	101	BCL	O2A-CGA	-3.06	1.24	1.33
8	M	1001	BCL	O1A-CGA	-3.05	1.13	1.22
8	6	102	BCL	O2D-CGD	-3.05	1.25	1.33
8	8	102	BCL	O2D-CGD	-3.04	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1001	BCL	O2A-CGA	-3.04	1.24	1.33
14	C	504	HEM	C1D-ND	-3.04	1.32	1.38
9	9	101	KGD	CAB-CAD	-3.04	1.49	1.53
8	B	102	BCL	O2D-CGD	-3.03	1.25	1.33
10	L	405	BPH	CMD-C2D	-3.03	1.44	1.51
8	S	102	BCL	O2D-CGD	-3.03	1.25	1.33
8	V	101	BCL	O2A-CGA	-3.01	1.24	1.33
10	L	404	BPH	C3D-C2D	-3.00	1.34	1.39
14	C	502	HEM	C1D-ND	-3.00	1.32	1.38
8	9	102	BCL	O1A-CGA	-2.99	1.13	1.22
8	L	401	BCL	O2A-CGA	-2.99	1.24	1.33
8	7	101	BCL	O1A-CGA	-2.99	1.13	1.22
8	1	101	BCL	O1A-CGA	-2.98	1.13	1.22
8	3	101	BCL	O1A-CGA	-2.98	1.13	1.22
14	C	503	HEM	C1B-NB	-2.98	1.35	1.40
8	D	101	BCL	O1A-CGA	-2.97	1.13	1.22
8	M	1005	BCL	O1A-CGA	-2.97	1.13	1.22
8	V	101	BCL	O2D-CGD	-2.97	1.26	1.33
8	J	101	BCL	O1A-CGA	-2.97	1.13	1.22
8	L	401	BCL	O1A-CGA	-2.97	1.13	1.22
8	D	101	BCL	C3B-C2B	-2.97	1.34	1.39
8	T	101	BCL	C3B-C2B	-2.97	1.34	1.39
8	P	101	BCL	O1A-CGA	-2.97	1.13	1.22
8	T	101	BCL	O1A-CGA	-2.96	1.13	1.22
8	H	101	BCL	O1A-CGA	-2.96	1.13	1.22
8	A	101	BCL	C3B-C2B	-2.96	1.34	1.39
8	E	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	O	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	F	101	BCL	O1A-CGA	-2.95	1.13	1.22
8	S	102	BCL	O2A-CGA	-2.95	1.24	1.33
8	F	101	BCL	C3B-C2B	-2.95	1.34	1.39
8	Q	102	BCL	O2A-CGA	-2.95	1.24	1.33
8	R	101	BCL	O1A-CGA	-2.94	1.13	1.22
8	N	101	BCL	C3B-C2B	-2.94	1.34	1.39
8	7	101	BCL	C3B-C2B	-2.94	1.34	1.39
8	0	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	N	101	BCL	O1A-CGA	-2.94	1.13	1.22
8	U	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	6	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	G	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	4	102	BCL	O2A-CGA	-2.94	1.24	1.33
8	5	101	BCL	O1A-CGA	-2.94	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	102	BCL	O2A-CGA	-2.93	1.24	1.33
8	3	101	BCL	C3B-C2B	-2.93	1.34	1.39
8	R	101	BCL	C3B-C2B	-2.93	1.34	1.39
10	L	402	BPH	C3D-C2D	-2.92	1.34	1.39
8	P	101	BCL	C3B-C2B	-2.92	1.34	1.39
8	I	102	BCL	O2A-CGA	-2.92	1.24	1.33
8	B	102	BCL	O2A-CGA	-2.92	1.24	1.33
8	8	102	BCL	O2A-CGA	-2.91	1.24	1.33
8	K	102	BCL	O2A-CGA	-2.91	1.24	1.33
8	H	101	BCL	C3B-C2B	-2.91	1.34	1.39
8	W	102	BCL	O2A-CGA	-2.91	1.24	1.33
8	1	101	BCL	C3B-C2B	-2.91	1.34	1.39
10	L	404	BPH	CMD-C2D	-2.90	1.44	1.51
8	J	101	BCL	C3B-C2B	-2.90	1.34	1.39
8	9	102	BCL	C3B-C2B	-2.90	1.34	1.39
9	9	101	KGD	CAZ-CAW	-2.89	1.43	1.50
8	5	101	BCL	C3B-C2B	-2.88	1.34	1.39
10	L	404	BPH	CHA-CBD	-2.86	1.49	1.52
10	L	405	BPH	CHA-CBD	-2.86	1.49	1.52
8	M	1001	BCL	C1D-C2D	-2.86	1.39	1.45
8	S	101	BCL	C3B-C2B	-2.85	1.34	1.39
8	2	102	BCL	C3B-C2B	-2.85	1.34	1.39
8	B	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	S	101	BCL	O1A-CGA	-2.85	1.14	1.22
8	B	101	BCL	C3B-C2B	-2.85	1.34	1.39
8	E	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	U	101	BCL	C3B-C2B	-2.84	1.34	1.39
8	6	101	BCL	C3B-C2B	-2.84	1.34	1.39
8	8	101	BCL	C3B-C2B	-2.84	1.34	1.39
8	K	101	BCL	C3B-C2B	-2.84	1.34	1.39
8	I	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	4	101	BCL	C3B-C2B	-2.84	1.34	1.39
8	W	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	4	102	BCL	C3B-C2B	-2.83	1.34	1.39
8	Q	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	0	102	BCL	O1A-CGA	-2.83	1.14	1.22
8	6	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	O	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	2	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	G	101	BCL	O1A-CGA	-2.83	1.14	1.22
8	G	101	BCL	C3B-C2B	-2.83	1.34	1.39
8	Q	102	BCL	C3B-C2B	-2.82	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	E	101	BCL	C3B-C2B	-2.82	1.34	1.39
8	U	102	BCL	C3B-C2B	-2.82	1.34	1.39
8	2	101	BCL	O2A-CGA	-2.82	1.25	1.33
8	U	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	B	102	BCL	C3B-C2B	-2.82	1.34	1.39
8	4	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	8	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	O	101	BCL	C3B-C2B	-2.81	1.34	1.39
8	S	102	BCL	C3B-C2B	-2.81	1.34	1.39
8	K	102	BCL	C3B-C2B	-2.80	1.34	1.39
8	E	102	BCL	C3B-C2B	-2.80	1.34	1.39
8	0	102	BCL	C3B-C2B	-2.80	1.34	1.39
8	8	102	BCL	C3B-C2B	-2.80	1.34	1.39
8	Q	101	BCL	C3B-C2B	-2.80	1.34	1.39
14	C	502	HEM	C1B-NB	-2.80	1.35	1.40
8	G	102	BCL	C3B-C2B	-2.80	1.34	1.39
8	W	102	BCL	O1A-CGA	-2.80	1.14	1.22
8	2	102	BCL	O1A-CGA	-2.79	1.14	1.22
14	C	504	HEM	C1B-NB	-2.79	1.35	1.40
8	8	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	U	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	W	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	W	102	BCL	C3B-C2B	-2.79	1.34	1.39
8	E	101	BCL	O2D-CGD	-2.79	1.26	1.33
8	K	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	Q	101	BCL	O2D-CGD	-2.78	1.26	1.33
8	0	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	B	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	G	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	V	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	I	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	I	101	BCL	C3B-C2B	-2.78	1.34	1.39
8	6	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	E	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	6	102	BCL	C3B-C2B	-2.78	1.34	1.39
8	S	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	I	102	BCL	C3B-C2B	-2.78	1.34	1.39
14	C	501	HEM	C1D-ND	-2.77	1.33	1.38
8	0	101	BCL	C3B-C2B	-2.77	1.34	1.39
8	0	102	BCL	O2D-CGD	-2.77	1.26	1.33
8	4	102	BCL	O1A-CGA	-2.77	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	BCL	C1D-C2D	-2.77	1.39	1.45
13	M	1008	PGV	P-O11	2.77	1.70	1.59
8	6	101	BCL	C1D-C2D	-2.77	1.39	1.45
8	G	101	BCL	O2D-CGD	-2.77	1.26	1.33
8	O	102	BCL	O1A-CGA	-2.76	1.14	1.22
8	Q	102	BCL	O1A-CGA	-2.76	1.14	1.22
8	U	101	BCL	C1D-C2D	-2.76	1.39	1.45
8	O	102	BCL	C3B-C2B	-2.76	1.34	1.39
8	B	101	BCL	O2D-CGD	-2.76	1.26	1.33
8	O	101	BCL	C1D-C2D	-2.75	1.39	1.45
8	4	101	BCL	O2D-CGD	-2.74	1.26	1.33
8	I	101	BCL	O2D-CGD	-2.74	1.26	1.33
8	O	101	BCL	O2D-CGD	-2.74	1.26	1.33
10	L	402	BPH	CMD-C2D	-2.73	1.45	1.51
8	U	101	BCL	O2D-CGD	-2.73	1.26	1.33
8	S	101	BCL	O2D-CGD	-2.73	1.26	1.33
8	8	101	BCL	C1D-C2D	-2.73	1.39	1.45
8	Q	101	BCL	C1D-C2D	-2.72	1.39	1.45
8	2	101	BCL	C1D-C2D	-2.72	1.40	1.45
8	B	101	BCL	C1D-C2D	-2.72	1.40	1.45
8	M	1001	BCL	C3B-C2B	-2.71	1.34	1.39
8	I	101	BCL	C1D-C2D	-2.71	1.40	1.45
8	4	101	BCL	C1D-C2D	-2.71	1.40	1.45
8	6	101	BCL	O2D-CGD	-2.71	1.26	1.33
8	K	101	BCL	O2D-CGD	-2.70	1.26	1.33
8	8	101	BCL	O2D-CGD	-2.70	1.26	1.33
8	S	101	BCL	C1D-C2D	-2.70	1.40	1.45
8	0	102	BCL	C1D-C2D	-2.70	1.40	1.45
8	W	101	BCL	C1D-C2D	-2.69	1.40	1.45
10	L	405	BPH	CMB-C2B	-2.69	1.45	1.51
8	K	101	BCL	C1D-C2D	-2.69	1.40	1.45
8	E	101	BCL	C1D-C2D	-2.68	1.40	1.45
14	C	501	HEM	C1B-NB	-2.68	1.35	1.40
11	M	1003	MQE	CAY-CBL	2.65	1.54	1.50
13	M	1008	PGV	P-O12	2.64	1.70	1.59
9	D	102	KGD	CAI-CAH	-2.64	1.42	1.47
9	J	102	KGD	CAI-CAH	-2.60	1.42	1.47
8	V	101	BCL	C1D-C2D	-2.60	1.40	1.45
10	L	402	BPH	CMB-C2B	-2.59	1.45	1.51
8	S	102	BCL	C1D-C2D	-2.56	1.40	1.45
8	L	401	BCL	C1D-C2D	-2.55	1.40	1.45
8	P	101	BCL	C1D-C2D	-2.55	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	101	BCL	C1D-C2D	-2.55	1.40	1.45
9	D	102	KGD	CAO-CAM	-2.54	1.32	1.35
9	I	103	KGD	CAE-CAI	-2.54	1.47	1.50
8	2	102	BCL	C1D-C2D	-2.53	1.40	1.45
9	N	102	KGD	CAF-CAB	-2.53	1.48	1.53
8	9	102	BCL	C1D-C2D	-2.53	1.40	1.45
9	D	102	KGD	CAZ-CAW	-2.53	1.44	1.50
8	W	102	BCL	C1D-C2D	-2.53	1.40	1.45
8	J	101	BCL	C1D-C2D	-2.53	1.40	1.45
11	M	1003	MQE	CAY-CAX	-2.53	1.47	1.51
8	F	101	BCL	C1D-C2D	-2.53	1.40	1.45
8	K	102	BCL	C1D-C2D	-2.51	1.40	1.45
8	R	101	BCL	C1D-C2D	-2.51	1.40	1.45
8	G	102	BCL	C1D-C2D	-2.51	1.40	1.45
8	8	102	BCL	C1D-C2D	-2.50	1.40	1.45
8	N	101	BCL	C1D-C2D	-2.50	1.40	1.45
8	T	101	BCL	C1D-C2D	-2.50	1.40	1.45
8	A	101	BCL	C1D-C2D	-2.50	1.40	1.45
8	1	101	BCL	C1D-C2D	-2.49	1.40	1.45
8	H	101	BCL	C1D-C2D	-2.49	1.40	1.45
8	U	102	BCL	C1D-C2D	-2.49	1.40	1.45
8	4	102	BCL	C1D-C2D	-2.49	1.40	1.45
8	D	101	BCL	C1D-C2D	-2.48	1.40	1.45
8	B	102	BCL	C1D-C2D	-2.48	1.40	1.45
8	Q	102	BCL	C1D-C2D	-2.48	1.40	1.45
8	V	101	BCL	C3B-C2B	-2.48	1.35	1.39
8	5	101	BCL	C1D-C2D	-2.48	1.40	1.45
8	I	102	BCL	C1D-C2D	-2.47	1.40	1.45
8	S	101	BCL	C3D-C4D	-2.47	1.38	1.44
8	U	101	BCL	C3D-C4D	-2.47	1.38	1.44
8	B	101	BCL	C3D-C4D	-2.47	1.38	1.44
8	O	101	BCL	C3D-C4D	-2.47	1.38	1.44
8	Q	101	BCL	C3D-C4D	-2.47	1.38	1.44
8	6	102	BCL	C1D-C2D	-2.47	1.40	1.45
8	M	1005	BCL	C1D-C2D	-2.47	1.40	1.45
8	O	102	BCL	C1D-C2D	-2.46	1.40	1.45
8	0	102	BCL	C3D-C4D	-2.46	1.38	1.44
8	E	102	BCL	C1D-C2D	-2.46	1.40	1.45
8	0	101	BCL	C1D-C2D	-2.46	1.40	1.45
8	I	101	BCL	C3D-C4D	-2.46	1.38	1.44
8	3	101	BCL	C1D-C2D	-2.45	1.40	1.45
8	T	101	BCL	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	BCL	C3D-C4D	-2.45	1.38	1.44
8	H	101	BCL	C3D-C4D	-2.44	1.38	1.44
8	7	101	BCL	C3D-C4D	-2.44	1.38	1.44
8	E	101	BCL	C3D-C4D	-2.44	1.38	1.44
8	8	101	BCL	C3D-C4D	-2.44	1.38	1.44
8	2	101	BCL	C3D-C4D	-2.43	1.38	1.44
8	6	101	BCL	C3D-C4D	-2.43	1.38	1.44
8	R	101	BCL	C3D-C4D	-2.43	1.38	1.44
10	L	404	BPH	CMB-C2B	-2.43	1.45	1.51
8	K	101	BCL	C3D-C4D	-2.43	1.38	1.44
8	N	101	BCL	C3D-C4D	-2.42	1.38	1.44
8	F	101	BCL	C3D-C4D	-2.42	1.38	1.44
8	J	101	BCL	C3D-C4D	-2.41	1.38	1.44
8	1	101	BCL	C3D-C4D	-2.41	1.38	1.44
8	4	101	BCL	C3D-C4D	-2.41	1.38	1.44
10	L	402	BPH	C4A-C3A	-2.40	1.47	1.51
8	9	102	BCL	C3D-C4D	-2.40	1.38	1.44
8	D	101	BCL	C3D-C4D	-2.39	1.38	1.44
8	W	101	BCL	C3D-C4D	-2.39	1.38	1.44
8	P	101	BCL	C3D-C4D	-2.38	1.38	1.44
8	A	101	BCL	C3D-C4D	-2.37	1.38	1.44
8	5	101	BCL	C3D-C4D	-2.37	1.38	1.44
8	8	101	BCL	C3D-C2D	-2.36	1.32	1.39
8	6	101	BCL	C3D-C2D	-2.36	1.32	1.39
8	0	102	BCL	C3D-C2D	-2.34	1.32	1.39
8	E	101	BCL	C3D-C2D	-2.33	1.32	1.39
8	U	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	4	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	B	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	G	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	3	101	BCL	C3D-C4D	-2.32	1.38	1.44
8	S	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	O	101	BCL	C3D-C2D	-2.32	1.32	1.39
8	I	101	BCL	C3D-C2D	-2.31	1.32	1.39
8	K	101	BCL	C3D-C2D	-2.30	1.32	1.39
8	L	401	BCL	C3D-C4D	-2.30	1.39	1.44
8	Q	101	BCL	C3D-C2D	-2.30	1.32	1.39
8	M	1005	BCL	C3B-C2B	-2.29	1.35	1.39
11	M	1003	MQE	CAN-CBB	-2.28	1.46	1.51
8	E	102	BCL	C3D-C4D	-2.27	1.39	1.44
8	S	102	BCL	C3D-C4D	-2.26	1.39	1.44
8	M	1005	BCL	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	102	KGD	CAV-CAR	-2.25	1.32	1.35
8	W	102	BCL	C3D-C4D	-2.25	1.39	1.44
11	M	1002	MQE	CAY-CAX	-2.24	1.47	1.51
8	B	102	BCL	C3D-C4D	-2.23	1.39	1.44
8	P	101	BCL	C3D-C2D	-2.23	1.33	1.39
8	0	101	BCL	C3D-C4D	-2.22	1.39	1.44
8	O	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	Q	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	4	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	K	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	3	101	BCL	C3D-C2D	-2.22	1.33	1.39
8	8	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	2	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	L	401	BCL	C3D-C2D	-2.21	1.33	1.39
8	U	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	G	102	BCL	C3D-C4D	-2.21	1.39	1.44
8	6	102	BCL	C3D-C4D	-2.20	1.39	1.44
8	5	101	BCL	C2C-C3C	-2.20	1.48	1.54
8	J	101	BCL	C3D-C2D	-2.20	1.33	1.39
8	7	101	BCL	C3D-C2D	-2.19	1.33	1.39
8	M	1001	BCL	C3D-C4D	-2.19	1.39	1.44
8	A	101	BCL	C3D-C2D	-2.19	1.33	1.39
8	3	101	BCL	C2C-C3C	-2.18	1.48	1.54
8	9	102	BCL	C3D-C2D	-2.18	1.33	1.39
8	I	102	BCL	C3D-C4D	-2.18	1.39	1.44
8	7	101	BCL	C2C-C3C	-2.17	1.48	1.54
8	F	101	BCL	C2C-C3C	-2.17	1.48	1.54
8	5	101	BCL	C3D-C2D	-2.17	1.33	1.39
8	R	101	BCL	C3D-C2D	-2.17	1.33	1.39
8	F	101	BCL	C3D-C2D	-2.17	1.33	1.39
8	N	101	BCL	C2C-C3C	-2.16	1.48	1.54
10	L	402	BPH	CHA-CBD	-2.16	1.49	1.52
8	2	101	BCL	C4B-NB	2.16	1.37	1.35
8	D	101	BCL	C3D-C2D	-2.16	1.33	1.39
8	H	101	BCL	C3D-C2D	-2.16	1.33	1.39
8	J	101	BCL	C2C-C3C	-2.16	1.48	1.54
8	H	101	BCL	C2C-C3C	-2.16	1.48	1.54
8	T	101	BCL	C2C-C3C	-2.16	1.48	1.54
8	T	101	BCL	C3D-C2D	-2.16	1.33	1.39
8	R	101	BCL	C2C-C3C	-2.15	1.48	1.54
8	M	1005	BCL	C2C-C3C	-2.15	1.48	1.54
8	1	101	BCL	C3D-C2D	-2.15	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	101	BCL	C3D-C2D	-2.15	1.33	1.39
8	M	1001	BCL	C4B-NB	2.14	1.37	1.35
8	1	101	BCL	C2C-C3C	-2.14	1.48	1.54
8	D	101	BCL	C2C-C3C	-2.14	1.48	1.54
8	A	101	BCL	C2C-C3C	-2.14	1.48	1.54
8	P	101	BCL	C2C-C3C	-2.14	1.48	1.54
9	I	103	KGD	CAS-CAW	-2.14	1.46	1.51
8	9	102	BCL	C2C-C3C	-2.14	1.48	1.54
8	V	101	BCL	C4B-NB	2.14	1.37	1.35
8	L	401	BCL	C3B-C2B	-2.13	1.35	1.39
9	I	103	KGD	CBJ-CBH	-2.13	1.33	1.35
8	6	102	BCL	C4B-NB	2.13	1.37	1.35
8	M	1001	BCL	C2C-C3C	-2.13	1.48	1.54
8	B	102	BCL	C4B-NB	2.13	1.37	1.35
8	4	102	BCL	C3D-C2D	-2.13	1.33	1.39
10	L	405	BPH	C5-C3	-2.12	1.46	1.51
11	M	1003	MQE	CAG-CAW	-2.12	1.46	1.51
8	Q	102	BCL	C3D-C2D	-2.11	1.33	1.39
8	I	102	BCL	C3D-C2D	-2.11	1.33	1.39
9	J	102	KGD	CAD-CAH	-2.11	1.33	1.35
8	Q	102	BCL	C4B-NB	2.10	1.37	1.35
8	G	102	BCL	C3D-C2D	-2.10	1.33	1.39
8	W	102	BCL	C3D-C2D	-2.10	1.33	1.39
8	6	102	BCL	C3D-C2D	-2.10	1.33	1.39
8	M	1005	BCL	C3D-C2D	-2.10	1.33	1.39
8	0	101	BCL	C3D-C2D	-2.09	1.33	1.39
8	B	102	BCL	C3D-C2D	-2.09	1.33	1.39
8	K	102	BCL	C3D-C2D	-2.09	1.33	1.39
8	V	101	BCL	C3D-C4D	-2.09	1.39	1.44
8	2	101	BCL	C3D-C2D	-2.09	1.33	1.39
8	M	1001	BCL	C3D-C2D	-2.09	1.33	1.39
8	S	102	BCL	C3D-C2D	-2.08	1.33	1.39
8	O	102	BCL	C3D-C2D	-2.08	1.33	1.39
8	K	102	BCL	C4B-NB	2.08	1.37	1.35
8	2	102	BCL	C3D-C2D	-2.07	1.33	1.39
8	S	102	BCL	C4B-NB	2.07	1.37	1.35
8	U	101	BCL	C2C-C3C	-2.06	1.48	1.54
8	U	102	BCL	C3D-C2D	-2.06	1.33	1.39
13	M	1007	PGV	P-O11	2.06	1.67	1.59
8	8	102	BCL	C3D-C2D	-2.06	1.33	1.39
8	E	101	BCL	C2C-C3C	-2.06	1.48	1.54
8	E	102	BCL	C3D-C2D	-2.06	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	BCL	C2C-C3C	-2.05	1.48	1.54
8	B	101	BCL	C4B-NB	2.05	1.37	1.35
9	J	102	KGD	CAE-CAI	-2.05	1.48	1.50
10	L	402	BPH	O2D-CED	-2.05	1.40	1.45
8	W	101	BCL	C3D-C2D	-2.04	1.33	1.39
8	8	101	BCL	C4B-NB	2.04	1.37	1.35
8	S	101	BCL	C2C-C3C	-2.04	1.48	1.54
8	2	101	BCL	C5-C3	2.04	1.55	1.51
8	0	102	BCL	C2C-C3C	-2.03	1.48	1.54
8	4	102	BCL	C2C-C3C	-2.03	1.48	1.54
8	W	102	BCL	C4B-NB	2.03	1.37	1.35
8	2	102	BCL	C2C-C3C	-2.03	1.48	1.54
8	G	102	BCL	C2C-C3C	-2.03	1.48	1.54
8	4	101	BCL	C2C-C3C	-2.03	1.48	1.54
8	U	102	BCL	C4B-NB	2.02	1.37	1.35
8	I	101	BCL	C2C-C3C	-2.02	1.48	1.54
8	G	101	BCL	C2C-C3C	-2.02	1.48	1.54
8	G	101	BCL	C4B-NB	2.02	1.37	1.35
8	I	102	BCL	C2C-C3C	-2.02	1.48	1.54
8	6	101	BCL	C2C-C3C	-2.02	1.48	1.54
8	2	102	BCL	C4B-NB	2.02	1.37	1.35
8	L	401	BCL	C2C-C3C	-2.02	1.48	1.54
8	O	102	BCL	C2C-C3C	-2.02	1.48	1.54
8	6	102	BCL	C2C-C3C	-2.02	1.48	1.54
8	Q	102	BCL	C2C-C3C	-2.01	1.48	1.54
8	4	102	BCL	C4B-NB	2.01	1.37	1.35
8	B	102	BCL	C2C-C3C	-2.01	1.48	1.54
8	U	102	BCL	C2C-C3C	-2.01	1.48	1.54
8	8	102	BCL	C2C-C3C	-2.01	1.48	1.54
8	E	102	BCL	C2C-C3C	-2.01	1.48	1.54
9	D	102	KGD	CAQ-CAR	-2.00	1.41	1.45
8	O	101	BCL	C2C-C3C	-2.00	1.48	1.54
8	W	102	BCL	C2C-C3C	-2.00	1.48	1.54

All (1539) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	103	KGD	CBG-CBI-CBL	-8.14	115.69	127.31
8	W	101	BCL	C1C-NC-C4C	-7.99	103.11	106.71
9	I	103	KGD	CAP-CAO-CAM	-7.88	116.06	127.31
9	N	102	KGD	CAP-CAO-CAM	-7.58	116.49	127.31
8	2	101	BCL	C1C-NC-C4C	-7.49	103.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	KGD	CAP-CAO-CAM	-7.23	117.00	127.31
9	9	101	KGD	CBB-CAV-CAR	-7.10	117.17	127.31
9	N	102	KGD	CBM-CBJ-CBH	-7.10	117.18	127.31
14	C	503	HEM	CHC-C4B-NB	6.73	131.74	124.43
9	D	102	KGD	CAJ-CAL-CAM	-6.71	116.10	126.23
9	N	102	KGD	CBG-CBI-CBL	-6.64	117.84	127.31
8	L	401	BCL	CMB-C2B-C1B	-6.45	118.54	128.46
9	9	101	KGD	CAP-CAO-CAM	-6.45	118.11	127.31
8	A	101	BCL	O2A-CGA-O1A	-6.28	107.73	123.59
8	S	101	BCL	O2D-CGD-O1D	-6.21	111.69	123.84
8	6	101	BCL	O2D-CGD-O1D	-6.21	111.70	123.84
8	O	101	BCL	O2D-CGD-O1D	-6.20	111.72	123.84
8	0	102	BCL	O2D-CGD-O1D	-6.19	111.73	123.84
8	K	101	BCL	O2D-CGD-O1D	-6.19	111.74	123.84
8	I	101	BCL	O2D-CGD-O1D	-6.19	111.74	123.84
8	Q	101	BCL	O2D-CGD-O1D	-6.18	111.76	123.84
8	8	101	BCL	O2D-CGD-O1D	-6.17	111.78	123.84
8	U	101	BCL	O2D-CGD-O1D	-6.16	111.79	123.84
11	M	1002	MQE	CAY-CBL-CBB	-6.16	116.53	126.79
8	4	101	BCL	O2D-CGD-O1D	-6.16	111.80	123.84
8	G	101	BCL	O2D-CGD-O1D	-6.15	111.81	123.84
8	S	102	BCL	C1D-ND-C4D	-6.14	101.97	106.33
8	E	101	BCL	O2D-CGD-O1D	-6.13	111.85	123.84
8	P	101	BCL	C1D-ND-C4D	-6.13	101.98	106.33
8	B	101	BCL	O2D-CGD-O1D	-6.13	111.86	123.84
8	9	102	BCL	C1D-ND-C4D	-6.10	102.00	106.33
8	F	101	BCL	C1D-ND-C4D	-6.10	102.00	106.33
8	T	101	BCL	C1D-ND-C4D	-6.09	102.01	106.33
8	J	101	BCL	C1D-ND-C4D	-6.09	102.01	106.33
8	R	101	BCL	C1D-ND-C4D	-6.09	102.01	106.33
8	7	101	BCL	C1D-ND-C4D	-6.09	102.01	106.33
8	5	101	BCL	C1D-ND-C4D	-6.07	102.02	106.33
8	N	101	BCL	C1D-ND-C4D	-6.07	102.02	106.33
8	Q	102	BCL	C1D-ND-C4D	-6.07	102.02	106.33
8	3	101	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	H	101	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	8	102	BCL	C1D-ND-C4D	-6.05	102.04	106.33
8	1	101	BCL	C1D-ND-C4D	-6.03	102.05	106.33
8	W	102	BCL	C1D-ND-C4D	-6.03	102.05	106.33
8	K	102	BCL	C1D-ND-C4D	-6.03	102.05	106.33
8	6	102	BCL	C1D-ND-C4D	-6.02	102.06	106.33
8	4	102	BCL	C1D-ND-C4D	-6.02	102.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	C1D-ND-C4D	-6.02	102.06	106.33
8	G	102	BCL	C1D-ND-C4D	-6.02	102.06	106.33
8	U	102	BCL	C1D-ND-C4D	-6.00	102.07	106.33
8	I	102	BCL	C1D-ND-C4D	-5.98	102.09	106.33
8	2	102	BCL	C1D-ND-C4D	-5.97	102.09	106.33
8	D	101	BCL	C1D-ND-C4D	-5.97	102.10	106.33
8	0	101	BCL	C1D-ND-C4D	-5.96	102.10	106.33
8	B	102	BCL	C1D-ND-C4D	-5.95	102.11	106.33
8	E	102	BCL	C1D-ND-C4D	-5.94	102.11	106.33
8	O	102	BCL	C1D-ND-C4D	-5.93	102.12	106.33
8	W	101	BCL	O2D-CGD-O1D	-5.88	112.33	123.84
8	M	1001	BCL	C1D-ND-C4D	-5.85	102.18	106.33
8	4	101	BCL	C1D-ND-C4D	-5.84	102.19	106.33
8	B	101	BCL	C1D-ND-C4D	-5.83	102.19	106.33
9	9	101	KGD	CBM-CBJ-CBH	-5.81	119.02	127.31
8	O	101	BCL	C1D-ND-C4D	-5.81	102.21	106.33
9	D	102	KGD	CAE-CAI-CAH	-5.81	113.29	118.65
8	Q	101	BCL	C1D-ND-C4D	-5.79	102.22	106.33
8	S	101	BCL	C1D-ND-C4D	-5.79	102.22	106.33
8	I	101	BCL	C1D-ND-C4D	-5.79	102.22	106.33
8	8	101	BCL	C1D-ND-C4D	-5.79	102.22	106.33
8	6	101	BCL	C1D-ND-C4D	-5.77	102.23	106.33
8	0	102	BCL	C1D-ND-C4D	-5.76	102.24	106.33
8	M	1001	BCL	O2D-CGD-O1D	-5.75	112.59	123.84
8	G	101	BCL	C1D-ND-C4D	-5.75	102.25	106.33
8	M	1001	BCL	C2D-C1D-ND	5.74	114.34	110.10
8	M	1005	BCL	O2D-CGD-O1D	-5.74	112.61	123.84
8	E	101	BCL	C1D-ND-C4D	-5.74	102.26	106.33
8	U	101	BCL	C1D-ND-C4D	-5.73	102.27	106.33
8	M	1005	BCL	C1D-ND-C4D	-5.71	102.28	106.33
8	K	101	BCL	C1D-ND-C4D	-5.69	102.29	106.33
8	M	1005	BCL	CMB-C2B-C1B	-5.55	119.93	128.46
8	J	101	BCL	O2D-CGD-O1D	-5.50	113.09	123.84
9	J	102	KGD	CAE-CAI-CAH	-5.47	113.61	118.65
8	R	101	BCL	O2D-CGD-O1D	-5.46	113.16	123.84
8	A	101	BCL	O2D-CGD-O1D	-5.46	113.16	123.84
8	T	101	BCL	O2D-CGD-O1D	-5.46	113.17	123.84
8	H	101	BCL	O2D-CGD-O1D	-5.45	113.17	123.84
8	9	102	BCL	O2D-CGD-O1D	-5.45	113.19	123.84
8	F	101	BCL	O2D-CGD-O1D	-5.45	113.19	123.84
8	1	101	BCL	O2D-CGD-O1D	-5.44	113.20	123.84
8	5	101	BCL	O2D-CGD-O1D	-5.43	113.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	101	BCL	O2D-CGD-O1D	-5.43	113.22	123.84
8	P	101	BCL	O2D-CGD-O1D	-5.43	113.22	123.84
8	N	101	BCL	O2D-CGD-O1D	-5.41	113.26	123.84
8	3	101	BCL	O2D-CGD-O1D	-5.39	113.30	123.84
8	D	101	BCL	O2D-CGD-O1D	-5.38	113.32	123.84
14	C	503	HEM	C4D-ND-C1D	5.38	110.63	105.07
8	8	102	BCL	C2D-C1D-ND	5.37	114.06	110.10
9	9	101	KGD	CAJ-CAL-CAM	-5.37	118.11	126.23
14	C	504	HEM	C4D-ND-C1D	5.36	110.61	105.07
8	V	101	BCL	C1C-NC-C4C	-5.35	104.30	106.71
8	I	102	BCL	C2D-C1D-ND	5.32	114.02	110.10
8	2	101	BCL	CMB-C2B-C1B	-5.32	120.29	128.46
8	L	401	BCL	C1D-ND-C4D	-5.32	102.56	106.33
8	V	101	BCL	O2D-CGD-O1D	-5.31	113.46	123.84
8	S	102	BCL	C2D-C1D-ND	5.31	114.02	110.10
8	K	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
8	U	102	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	6	102	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	V	101	BCL	C4A-NA-C1A	-5.29	104.33	106.71
8	M	1005	BCL	C2D-C1D-ND	5.29	114.00	110.10
8	6	102	BCL	O2D-CGD-O1D	-5.29	113.50	123.84
9	D	102	KGD	CBG-CBI-CBL	-5.28	119.77	127.31
8	2	102	BCL	C2D-C1D-ND	5.28	114.00	110.10
8	U	102	BCL	O2D-CGD-O1D	-5.27	113.53	123.84
8	W	102	BCL	C2D-C1D-ND	5.27	113.98	110.10
8	8	102	BCL	O2D-CGD-O1D	-5.26	113.55	123.84
8	Q	102	BCL	O2D-CGD-O1D	-5.26	113.55	123.84
8	2	102	BCL	O2D-CGD-O1D	-5.26	113.55	123.84
14	C	502	HEM	CHB-C1B-NB	5.26	130.88	124.38
8	Q	102	BCL	C2D-C1D-ND	5.25	113.97	110.10
8	F	101	BCL	C2D-C1D-ND	5.25	113.97	110.10
8	O	102	BCL	O2D-CGD-O1D	-5.25	113.58	123.84
8	W	102	BCL	O2D-CGD-O1D	-5.24	113.59	123.84
8	W	101	BCL	CMB-C2B-C1B	-5.24	120.41	128.46
8	E	102	BCL	C2D-C1D-ND	5.24	113.97	110.10
8	5	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
8	P	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
8	B	102	BCL	O2D-CGD-O1D	-5.24	113.59	123.84
8	4	102	BCL	O2D-CGD-O1D	-5.23	113.61	123.84
8	K	102	BCL	O2D-CGD-O1D	-5.23	113.62	123.84
8	O	102	BCL	C2D-C1D-ND	5.23	113.96	110.10
8	I	102	BCL	O2D-CGD-O1D	-5.23	113.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	102	BCL	O2D-CGD-O1D	-5.23	113.62	123.84
8	E	102	BCL	O2D-CGD-O1D	-5.22	113.63	123.84
8	G	102	BCL	C2D-C1D-ND	5.22	113.95	110.10
8	G	102	BCL	O2D-CGD-O1D	-5.21	113.64	123.84
8	0	101	BCL	O2D-CGD-O1D	-5.21	113.66	123.84
8	0	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
8	4	101	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	B	102	BCL	C2D-C1D-ND	5.18	113.92	110.10
8	4	102	BCL	C2D-C1D-ND	5.18	113.92	110.10
11	M	1003	MQE	CAM-CAG-CAW	-5.17	106.16	114.62
8	T	101	BCL	C2D-C1D-ND	5.17	113.91	110.10
8	I	101	BCL	C2D-C1D-ND	5.17	113.91	110.10
8	R	101	BCL	C2D-C1D-ND	5.16	113.91	110.10
8	K	101	BCL	C2D-C1D-ND	5.14	113.89	110.10
8	N	101	BCL	C2D-C1D-ND	5.14	113.89	110.10
8	3	101	BCL	C2D-C1D-ND	5.14	113.89	110.10
8	I	101	BCL	CAC-C3C-C2C	-5.14	101.43	114.26
8	1	101	BCL	C2D-C1D-ND	5.13	113.89	110.10
8	Q	101	BCL	C2D-C1D-ND	5.13	113.89	110.10
8	9	102	BCL	C2D-C1D-ND	5.13	113.88	110.10
8	J	101	BCL	C2D-C1D-ND	5.13	113.88	110.10
8	8	101	BCL	CAC-C3C-C2C	-5.13	101.44	114.26
8	G	101	BCL	CAC-C3C-C2C	-5.13	101.45	114.26
8	V	101	BCL	CAC-C3C-C2C	-5.13	101.45	114.26
8	7	101	BCL	C2D-C1D-ND	5.13	113.88	110.10
8	Q	101	BCL	CAC-C3C-C2C	-5.13	101.45	114.26
8	O	101	BCL	CAC-C3C-C2C	-5.13	101.45	114.26
8	H	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
8	K	101	BCL	CAC-C3C-C2C	-5.12	101.46	114.26
8	B	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
8	S	101	BCL	CAC-C3C-C2C	-5.11	101.49	114.26
8	B	101	BCL	CAC-C3C-C2C	-5.11	101.49	114.26
8	6	101	BCL	CAC-C3C-C2C	-5.11	101.50	114.26
14	C	503	HEM	CHB-C1B-NB	5.11	130.69	124.38
8	D	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
8	0	102	BCL	CAC-C3C-C2C	-5.11	101.50	114.26
8	2	101	BCL	O2D-CGD-O1D	-5.11	113.86	123.84
8	L	401	BCL	O2D-CGD-CBD	5.10	120.34	111.27
8	U	101	BCL	CAC-C3C-C2C	-5.10	101.51	114.26
8	4	101	BCL	CAC-C3C-C2C	-5.10	101.51	114.26
8	E	101	BCL	CAC-C3C-C2C	-5.10	101.52	114.26
8	A	101	BCL	C2D-C1D-ND	5.10	113.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	101	BCL	C2D-C1D-ND	5.10	113.86	110.10
8	G	101	BCL	C2D-C1D-ND	5.09	113.86	110.10
8	8	101	BCL	C2D-C1D-ND	5.07	113.84	110.10
8	6	101	BCL	C2D-C1D-ND	5.07	113.84	110.10
8	E	101	BCL	C2D-C1D-ND	5.06	113.84	110.10
8	U	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
8	M	1001	BCL	CAC-C3C-C2C	-5.05	101.63	114.26
8	0	102	BCL	C2D-C1D-ND	5.05	113.83	110.10
8	S	101	BCL	C2D-C1D-ND	5.04	113.82	110.10
8	8	101	BCL	C1C-NC-C4C	-5.03	104.44	106.71
8	G	101	BCL	C1C-NC-C4C	-5.03	104.44	106.71
8	4	101	BCL	C1C-NC-C4C	-5.02	104.45	106.71
8	S	101	BCL	C1C-NC-C4C	-5.00	104.46	106.71
9	9	101	KGD	CAP-CAQ-CAR	-4.99	112.40	126.42
8	U	101	BCL	C1C-NC-C4C	-4.98	104.47	106.71
8	6	101	BCL	C1C-NC-C4C	-4.98	104.47	106.71
8	M	1001	BCL	CMB-C2B-C1B	-4.97	120.82	128.46
14	C	504	HEM	CHC-C4B-NB	4.97	129.83	124.43
8	K	101	BCL	C1C-NC-C4C	-4.96	104.47	106.71
9	J	102	KGD	CBG-CBI-CBL	-4.96	120.23	127.31
8	0	102	BCL	C1C-NC-C4C	-4.96	104.48	106.71
8	O	101	BCL	C1C-NC-C4C	-4.95	104.48	106.71
14	C	504	HEM	CHB-C1B-NB	4.93	130.47	124.38
8	I	101	BCL	C1C-NC-C4C	-4.93	104.49	106.71
8	B	101	BCL	C1C-NC-C4C	-4.93	104.49	106.71
8	E	101	BCL	C1C-NC-C4C	-4.93	104.49	106.71
14	C	501	HEM	CHB-C1B-NB	4.92	130.46	124.38
8	L	401	BCL	C2D-C1D-ND	4.86	113.69	110.10
9	J	102	KGD	CAJ-CAL-CAM	-4.86	118.89	126.23
8	Q	101	BCL	C1C-NC-C4C	-4.84	104.53	106.71
8	B	102	BCL	CAC-C3C-C2C	-4.83	102.20	114.26
8	K	102	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
8	E	102	BCL	CAC-C3C-C2C	-4.82	102.21	114.26
8	G	102	BCL	CAC-C3C-C2C	-4.82	102.22	114.26
8	M	1005	BCL	CAC-C3C-C2C	-4.82	102.23	114.26
8	0	101	BCL	CAC-C3C-C2C	-4.81	102.24	114.26
8	8	102	BCL	CAC-C3C-C2C	-4.81	102.24	114.26
8	W	102	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
8	2	102	BCL	CAC-C3C-C2C	-4.81	102.25	114.26
8	Q	102	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
8	S	102	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
8	L	401	BCL	O2D-CGD-O1D	-4.80	114.45	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	102	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
8	4	102	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	6	102	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	O	102	BCL	CAC-C3C-C2C	-4.79	102.28	114.26
8	I	102	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	A	101	BCL	CAC-C3C-C2C	-4.78	102.32	114.26
8	J	101	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
8	V	101	BCL	C1D-ND-C4D	-4.77	102.95	106.33
8	9	102	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
8	N	101	BCL	CAC-C3C-C2C	-4.77	102.35	114.26
9	I	103	KGD	CAJ-CAL-CAM	-4.76	119.04	126.23
8	1	101	BCL	CAC-C3C-C2C	-4.76	102.36	114.26
8	T	101	BCL	CAC-C3C-C2C	-4.76	102.36	114.26
8	7	101	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	R	101	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	D	101	BCL	CAC-C3C-C2C	-4.76	102.37	114.26
8	F	101	BCL	CAC-C3C-C2C	-4.75	102.38	114.26
8	3	101	BCL	CAC-C3C-C2C	-4.75	102.39	114.26
8	5	101	BCL	CAC-C3C-C2C	-4.75	102.40	114.26
8	H	101	BCL	CAC-C3C-C2C	-4.75	102.40	114.26
8	2	101	BCL	CAC-C3C-C2C	-4.75	102.40	114.26
8	P	101	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
8	W	101	BCL	CAC-C3C-C2C	-4.72	102.45	114.26
8	L	401	BCL	CAC-C3C-C2C	-4.70	102.50	114.26
8	V	101	BCL	C2D-C1D-ND	4.68	113.56	110.10
8	M	1005	BCL	C1C-NC-C4C	-4.68	104.60	106.71
8	2	101	BCL	O2D-CGD-CBD	4.68	119.59	111.27
8	W	101	BCL	CHD-C1D-ND	-4.67	120.16	124.45
14	C	502	HEM	C4D-ND-C1D	4.65	109.87	105.07
14	C	502	HEM	CHC-C4B-NB	4.61	129.44	124.43
8	2	101	BCL	C2C-C3C-C4C	-4.61	94.44	101.34
8	R	101	BCL	CMB-C2B-C1B	-4.55	121.46	128.46
9	D	102	KGD	CBM-CBN-CBL	-4.55	113.63	126.42
8	M	1001	BCL	O2D-CGD-CBD	4.55	119.35	111.27
8	D	101	BCL	CMB-C2B-C1B	-4.55	121.47	128.46
8	1	101	BCL	CMB-C2B-C1B	-4.55	121.47	128.46
8	J	101	BCL	CMB-C2B-C1B	-4.54	121.48	128.46
8	7	101	BCL	CMB-C2B-C1B	-4.54	121.49	128.46
8	3	101	BCL	CMB-C2B-C1B	-4.53	121.50	128.46
8	T	101	BCL	CMB-C2B-C1B	-4.53	121.51	128.46
8	A	101	BCL	CMB-C2B-C1B	-4.53	121.51	128.46
8	N	101	BCL	CMB-C2B-C1B	-4.52	121.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	402	BPH	O2D-CGD-CBD	4.52	116.72	111.00
8	F	101	BCL	CMB-C2B-C1B	-4.52	121.52	128.46
8	5	101	BCL	CMB-C2B-C1B	-4.51	121.53	128.46
8	T	101	BCL	C16-C15-C13	-4.51	101.35	115.92
8	P	101	BCL	CMB-C2B-C1B	-4.50	121.54	128.46
8	V	101	BCL	CMB-C2B-C1B	-4.50	121.54	128.46
8	9	102	BCL	CMB-C2B-C1B	-4.48	121.57	128.46
9	N	102	KGD	CBB-CAV-CAR	-4.48	120.92	127.31
8	H	101	BCL	CMB-C2B-C1B	-4.48	121.58	128.46
14	C	501	HEM	CHC-C4B-NB	4.48	129.29	124.43
8	2	102	BCL	C1C-NC-C4C	-4.47	104.70	106.71
8	W	101	BCL	C2C-C3C-C4C	-4.46	94.66	101.34
8	8	102	BCL	C1C-NC-C4C	-4.46	104.70	106.71
8	2	101	BCL	CHD-C1D-ND	-4.45	120.36	124.45
8	S	102	BCL	C1C-NC-C4C	-4.44	104.71	106.71
8	6	102	BCL	C1C-NC-C4C	-4.43	104.71	106.71
8	W	101	BCL	O2D-CGD-CBD	4.42	119.13	111.27
8	T	101	BCL	O2D-CGD-CBD	4.42	119.13	111.27
9	I	103	KGD	CAE-CAI-CAH	-4.42	114.57	118.65
8	2	102	BCL	O2D-CGD-CBD	4.42	119.12	111.27
8	Q	102	BCL	C1C-NC-C4C	-4.42	104.72	106.71
8	O	102	BCL	O2D-CGD-CBD	4.42	119.12	111.27
8	H	101	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	O	102	BCL	C1C-NC-C4C	-4.41	104.72	106.71
8	Q	102	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	U	102	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	J	101	BCL	O2D-CGD-CBD	4.41	119.10	111.27
8	9	102	BCL	O2D-CGD-CBD	4.40	119.09	111.27
8	4	102	BCL	O2D-CGD-CBD	4.40	119.09	111.27
8	N	101	BCL	O2D-CGD-CBD	4.40	119.08	111.27
8	B	102	BCL	C1C-NC-C4C	-4.40	104.73	106.71
8	0	101	BCL	O2D-CGD-CBD	4.39	119.07	111.27
8	8	102	BCL	O2D-CGD-CBD	4.39	119.07	111.27
8	W	102	BCL	O2D-CGD-CBD	4.39	119.07	111.27
14	C	503	HEM	CBA-CAA-C2A	-4.39	105.13	112.62
8	P	101	BCL	O2D-CGD-CBD	4.39	119.07	111.27
8	F	101	BCL	O2D-CGD-CBD	4.39	119.07	111.27
8	A	101	BCL	O2D-CGD-CBD	4.39	119.07	111.27
8	I	102	BCL	O2D-CGD-CBD	4.39	119.06	111.27
8	7	101	BCL	O2D-CGD-CBD	4.39	119.06	111.27
8	U	101	BCL	CMB-C2B-C1B	-4.38	121.73	128.46
8	G	102	BCL	O2D-CGD-CBD	4.38	119.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	101	BCL	O2D-CGD-CBD	4.38	119.05	111.27
8	U	102	BCL	C1C-NC-C4C	-4.38	104.74	106.71
8	D	101	BCL	O2D-CGD-CBD	4.38	119.05	111.27
8	5	101	BCL	O2D-CGD-CBD	4.37	119.04	111.27
8	6	102	BCL	O2D-CGD-CBD	4.37	119.04	111.27
8	K	102	BCL	O2D-CGD-CBD	4.37	119.03	111.27
8	Q	101	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
8	R	101	BCL	O2D-CGD-CBD	4.37	119.03	111.27
8	6	101	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
8	E	102	BCL	O2D-CGD-CBD	4.37	119.03	111.27
8	3	101	BCL	O2D-CGD-CBD	4.37	119.03	111.27
8	0	102	BCL	CMB-C2B-C1B	-4.37	121.75	128.46
8	0	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	Q	102	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	8	101	BCL	CMB-C2B-C1B	-4.36	121.77	128.46
8	S	102	BCL	O2D-CGD-CBD	4.36	119.01	111.27
8	G	101	BCL	CMB-C2B-C1B	-4.36	121.77	128.46
8	S	101	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
8	K	101	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
8	O	101	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
8	K	102	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
8	B	102	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
8	B	102	BCL	O2D-CGD-CBD	4.35	118.99	111.27
8	E	102	BCL	CMB-C2B-C1B	-4.34	121.79	128.46
8	B	101	BCL	CMB-C2B-C1B	-4.34	121.79	128.46
8	8	102	BCL	CMB-C2B-C1B	-4.34	121.79	128.46
8	E	101	BCL	CMB-C2B-C1B	-4.33	121.80	128.46
8	4	102	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
8	4	101	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
8	2	102	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
8	S	102	BCL	CMB-C2B-C1B	-4.33	121.82	128.46
8	I	101	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
8	W	102	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
8	W	102	BCL	C1C-NC-C4C	-4.32	104.76	106.71
8	U	102	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
8	O	102	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
8	I	102	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
8	K	102	BCL	C1C-NC-C4C	-4.31	104.77	106.71
8	6	102	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	G	102	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	4	102	BCL	C1C-NC-C4C	-4.31	104.77	106.71
8	M	1005	BCL	OBB-CAB-CBB	-4.29	110.50	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	102	BCL	C1C-NC-C4C	-4.27	104.79	106.71
8	I	102	BCL	C1C-NC-C4C	-4.26	104.79	106.71
8	G	102	BCL	C1C-NC-C4C	-4.26	104.79	106.71
9	J	102	KGD	CBF-CBH-CBJ	-4.25	112.43	118.94
9	J	102	KGD	CBB-CAV-CAR	-4.25	121.25	127.31
9	D	102	KGD	CBF-CBH-CBJ	-4.25	112.43	118.94
9	J	102	KGD	CAP-CAO-CAM	-4.22	121.29	127.31
8	M	1005	BCL	CHD-C1D-ND	-4.16	120.63	124.45
8	0	101	BCL	C1C-NC-C4C	-4.16	104.84	106.71
8	5	101	BCL	C1C-NC-C4C	-4.15	104.84	106.71
8	V	101	BCL	O2D-CGD-CBD	4.15	118.64	111.27
8	V	101	BCL	C2A-C3A-C4A	-4.13	95.20	101.87
8	L	401	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	9	102	BCL	C1C-NC-C4C	-4.11	104.86	106.71
8	L	401	BCL	CHD-C1D-ND	-4.11	120.67	124.45
8	A	101	BCL	C1C-NC-C4C	-4.10	104.86	106.71
8	V	101	BCL	CHA-C1A-NA	-4.10	117.01	126.40
8	1	101	BCL	C1C-NC-C4C	-4.10	104.86	106.71
8	3	101	BCL	C1C-NC-C4C	-4.10	104.86	106.71
8	0	102	BCL	O2D-CGD-CBD	4.10	118.55	111.27
8	P	101	BCL	C1C-NC-C4C	-4.09	104.87	106.71
8	N	101	BCL	C1C-NC-C4C	-4.09	104.87	106.71
9	I	103	KGD	CBM-CBJ-CBH	-4.08	121.48	127.31
8	I	101	BCL	O2D-CGD-CBD	4.07	118.50	111.27
8	S	101	BCL	O2D-CGD-CBD	4.07	118.49	111.27
8	4	101	BCL	O2D-CGD-CBD	4.06	118.49	111.27
8	6	101	BCL	O2D-CGD-CBD	4.06	118.49	111.27
9	D	102	KGD	CAP-CAQ-CAR	-4.05	115.03	126.42
8	E	101	BCL	O2D-CGD-CBD	4.05	118.47	111.27
8	Q	101	BCL	O2D-CGD-CBD	4.04	118.44	111.27
14	C	501	HEM	C4D-ND-C1D	4.03	109.24	105.07
8	U	101	BCL	O2D-CGD-CBD	4.03	118.44	111.27
8	G	101	BCL	O2D-CGD-CBD	4.03	118.44	111.27
8	L	401	BCL	OBb-CAB-CBB	-4.03	111.10	120.17
11	M	1003	MQE	CAY-CBL-CBB	4.03	133.50	126.79
8	O	101	BCL	O2D-CGD-CBD	4.03	118.43	111.27
8	B	101	BCL	O2D-CGD-CBD	4.02	118.42	111.27
8	J	101	BCL	OBb-CAB-CBB	-4.02	111.13	120.17
8	T	101	BCL	OBb-CAB-CBB	-4.02	111.13	120.17
8	H	101	BCL	C1C-NC-C4C	-4.01	104.90	106.71
8	K	101	BCL	O2D-CGD-CBD	4.01	118.40	111.27
8	D	101	BCL	C1C-NC-C4C	-4.01	104.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	102	BCL	OBB-CAB-CBB	-4.01	111.15	120.17
8	P	101	BCL	CHD-C1D-ND	-4.01	120.77	124.45
8	7	101	BCL	C1C-NC-C4C	-4.00	104.91	106.71
8	5	101	BCL	OBB-CAB-CBB	-4.00	111.16	120.17
8	J	101	BCL	C1C-NC-C4C	-4.00	104.91	106.71
8	8	101	BCL	O2D-CGD-CBD	4.00	118.37	111.27
8	M	1005	BCL	O2D-CGD-CBD	4.00	118.37	111.27
8	1	101	BCL	OBB-CAB-CBB	-3.99	111.18	120.17
8	A	101	BCL	OBB-CAB-CBB	-3.99	111.18	120.17
8	F	101	BCL	OBB-CAB-CBB	-3.99	111.18	120.17
8	N	101	BCL	OBB-CAB-CBB	-3.99	111.19	120.17
8	D	101	BCL	OBB-CAB-CBB	-3.99	111.19	120.17
8	3	101	BCL	OBB-CAB-CBB	-3.98	111.20	120.17
8	R	101	BCL	OBB-CAB-CBB	-3.98	111.20	120.17
8	P	101	BCL	OBB-CAB-CBB	-3.98	111.22	120.17
9	J	102	KGD	CBK-CBH-CBF	3.97	124.34	118.08
8	H	101	BCL	OBB-CAB-CBB	-3.97	111.23	120.17
8	F	101	BCL	CHD-C1D-ND	-3.97	120.81	124.45
8	7	101	BCL	OBB-CAB-CBB	-3.96	111.26	120.17
8	7	101	BCL	CHD-C1D-ND	-3.96	120.82	124.45
8	R	101	BCL	C1C-NC-C4C	-3.95	104.93	106.71
8	F	101	BCL	C1C-NC-C4C	-3.95	104.93	106.71
8	5	101	BCL	CHD-C1D-ND	-3.95	120.83	124.45
8	J	101	BCL	CHD-C1D-ND	-3.94	120.83	124.45
10	L	405	BPH	O2D-CGD-CBD	3.94	115.99	111.00
8	R	101	BCL	CHD-C1D-ND	-3.93	120.84	124.45
8	A	101	BCL	CHD-C1D-ND	-3.93	120.84	124.45
10	L	404	BPH	O2D-CGD-CBD	3.92	115.96	111.00
8	1	101	BCL	CHD-C1D-ND	-3.92	120.85	124.45
8	N	101	BCL	CHD-C1D-ND	-3.92	120.86	124.45
8	9	102	BCL	CHD-C1D-ND	-3.91	120.86	124.45
8	H	101	BCL	CHD-C1D-ND	-3.90	120.87	124.45
8	3	101	BCL	CHD-C1D-ND	-3.89	120.88	124.45
9	N	102	KGD	CAE-CAI-CAH	-3.87	115.08	118.65
8	T	101	BCL	CHD-C1D-ND	-3.87	120.90	124.45
8	W	101	BCL	C2D-C1D-ND	3.86	112.95	110.10
8	T	101	BCL	C1C-NC-C4C	-3.84	104.98	106.71
8	D	101	BCL	CHD-C1D-ND	-3.83	120.93	124.45
8	M	1001	BCL	OBB-CAB-CBB	-3.83	111.54	120.17
8	2	101	BCL	C2D-C1D-ND	3.83	112.92	110.10
9	9	101	KGD	CBG-CBB-CAV	-3.82	115.64	123.47
9	N	102	KGD	CBE-CBF-CBH	-3.80	115.74	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	103	KGD	CBE-CBF-CBH	-3.79	115.76	126.42
8	V	101	BCL	C2A-C1A-CHA	3.77	130.46	123.86
8	8	102	BCL	CHD-C1D-ND	-3.70	121.06	124.45
8	Q	102	BCL	CHD-C1D-ND	-3.69	121.06	124.45
8	S	102	BCL	CHD-C1D-ND	-3.69	121.06	124.45
8	M	1001	BCL	CHD-C1D-ND	-3.68	121.07	124.45
8	6	102	BCL	CHD-C1D-ND	-3.68	121.08	124.45
8	W	102	BCL	CHD-C1D-ND	-3.67	121.08	124.45
10	L	405	BPH	CMD-C2D-C3D	3.67	131.54	124.68
8	W	101	BCL	C4B-CHC-C1C	-3.66	122.86	130.12
9	N	102	KGD	CBM-CBN-CBL	-3.66	116.13	126.42
8	K	102	BCL	CHD-C1D-ND	-3.66	121.09	124.45
8	2	102	BCL	CHD-C1D-ND	-3.65	121.10	124.45
8	4	102	BCL	CHD-C1D-ND	-3.64	121.11	124.45
8	L	401	BCL	C2A-C3A-C4A	-3.64	95.99	101.87
8	B	102	BCL	CHD-C1D-ND	-3.63	121.11	124.45
8	2	101	BCL	C4B-CHC-C1C	-3.63	122.93	130.12
8	G	102	BCL	CHD-C1D-ND	-3.62	121.12	124.45
8	I	102	BCL	CHD-C1D-ND	-3.61	121.13	124.45
8	U	102	BCL	CHD-C1D-ND	-3.61	121.13	124.45
10	L	402	BPH	CMD-C2D-C3D	3.59	131.39	124.68
8	2	101	BCL	C1D-ND-C4D	-3.59	103.79	106.33
8	E	102	BCL	CHD-C1D-ND	-3.58	121.16	124.45
8	0	101	BCL	CHD-C1D-ND	-3.56	121.18	124.45
11	L	403	MQE	CAY-CAX-CBQ	-3.55	114.70	118.50
8	W	101	BCL	C1D-ND-C4D	-3.55	103.81	106.33
8	O	102	BCL	CHD-C1D-ND	-3.54	121.20	124.45
10	L	402	BPH	C1-C2-C3	-3.54	119.92	126.04
10	L	404	BPH	CMD-C2D-C3D	3.53	131.29	124.68
9	N	102	KGD	CAJ-CAL-CAM	-3.53	120.91	126.23
8	M	1005	BCL	CMB-C2B-C3B	3.51	131.25	124.68
8	T	101	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
8	7	101	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
14	C	503	HEM	C4B-CHC-C1C	-3.50	117.94	122.56
8	J	101	BCL	C4B-CHC-C1C	-3.50	123.19	130.12
8	F	101	BCL	C4B-CHC-C1C	-3.50	123.19	130.12
8	R	101	BCL	C4B-CHC-C1C	-3.50	123.19	130.12
8	9	102	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
8	H	101	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
8	0	101	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
8	L	401	BCL	C4A-NA-C1A	-3.49	105.14	106.71
9	N	102	KGD	CAP-CAQ-CAR	-3.48	116.63	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	101	BCL	C4B-CHC-C1C	-3.48	123.22	130.12
8	M	1001	BCL	O2A-CGA-O1A	-3.48	114.82	123.59
8	3	101	BCL	C4B-CHC-C1C	-3.48	123.23	130.12
8	8	102	BCL	C4B-CHC-C1C	-3.47	123.24	130.12
8	4	102	BCL	C4B-CHC-C1C	-3.47	123.25	130.12
8	P	101	BCL	C4B-CHC-C1C	-3.46	123.26	130.12
8	S	102	BCL	C4B-CHC-C1C	-3.46	123.26	130.12
8	O	102	BCL	C4B-CHC-C1C	-3.46	123.27	130.12
8	2	102	BCL	C4B-CHC-C1C	-3.46	123.27	130.12
8	I	102	BCL	C4B-CHC-C1C	-3.46	123.27	130.12
8	U	102	BCL	C4B-CHC-C1C	-3.46	123.27	130.12
8	B	102	BCL	C4B-CHC-C1C	-3.46	123.27	130.12
8	A	101	BCL	C4B-CHC-C1C	-3.45	123.28	130.12
8	Q	102	BCL	C4B-CHC-C1C	-3.45	123.28	130.12
8	5	101	BCL	C4B-CHC-C1C	-3.45	123.29	130.12
8	E	102	BCL	C4B-CHC-C1C	-3.45	123.29	130.12
8	N	101	BCL	C4B-CHC-C1C	-3.45	123.29	130.12
8	1	101	BCL	C4B-CHC-C1C	-3.44	123.30	130.12
8	K	102	BCL	C4B-CHC-C1C	-3.44	123.30	130.12
8	O	102	BCL	OBB-CAB-CBB	-3.44	112.43	120.17
8	E	102	BCL	OBB-CAB-CBB	-3.44	112.44	120.17
14	C	502	HEM	CHB-C1B-C2B	-3.44	117.22	126.72
8	K	102	BCL	OBB-CAB-CBB	-3.43	112.44	120.17
8	G	102	BCL	C4B-CHC-C1C	-3.43	123.32	130.12
8	6	102	BCL	C4B-CHC-C1C	-3.43	123.33	130.12
8	0	101	BCL	OBB-CAB-CBB	-3.42	112.47	120.17
8	W	102	BCL	C4B-CHC-C1C	-3.42	123.34	130.12
8	N	101	BCL	CHA-C1A-NA	-3.42	118.58	126.40
8	D	101	BCL	CHA-C1A-NA	-3.41	118.58	126.40
8	W	102	BCL	OBB-CAB-CBB	-3.41	112.49	120.17
8	W	101	BCL	CBC-CAC-C3C	3.41	121.06	113.47
8	2	101	BCL	CBC-CAC-C3C	3.41	121.06	113.47
8	B	102	BCL	OBB-CAB-CBB	-3.40	112.51	120.17
8	S	102	BCL	OBB-CAB-CBB	-3.40	112.51	120.17
8	G	102	BCL	OBB-CAB-CBB	-3.40	112.52	120.17
8	1	101	BCL	CHA-C1A-NA	-3.40	118.62	126.40
8	H	101	BCL	CHA-C1A-NA	-3.40	118.62	126.40
8	M	1001	BCL	CHA-C1A-NA	-3.40	118.62	126.40
8	I	102	BCL	OBB-CAB-CBB	-3.40	112.53	120.17
8	V	101	BCL	O2A-CGA-O1A	-3.39	115.02	123.59
8	7	101	BCL	CHA-C1A-NA	-3.39	118.63	126.40
8	4	102	BCL	OBB-CAB-CBB	-3.39	112.53	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5	101	BCL	CHA-C1A-NA	-3.39	118.64	126.40
8	9	102	BCL	CHA-C1A-NA	-3.39	118.64	126.40
8	8	102	BCL	OBB-CAB-CBB	-3.39	112.55	120.17
8	R	101	BCL	CHA-C1A-NA	-3.39	118.64	126.40
8	P	101	BCL	CHA-C1A-NA	-3.38	118.65	126.40
8	Q	102	BCL	OBB-CAB-CBB	-3.38	112.56	120.17
8	U	102	BCL	OBB-CAB-CBB	-3.38	112.56	120.17
8	T	101	BCL	CHA-C1A-NA	-3.38	118.66	126.40
8	2	102	BCL	OBB-CAB-CBB	-3.38	112.57	120.17
8	F	101	BCL	CHA-C1A-NA	-3.38	118.66	126.40
8	6	102	BCL	OBB-CAB-CBB	-3.37	112.58	120.17
8	3	101	BCL	CHA-C1A-NA	-3.37	118.68	126.40
8	A	101	BCL	CHA-C1A-NA	-3.37	118.68	126.40
8	J	101	BCL	CHA-C1A-NA	-3.37	118.69	126.40
8	V	101	BCL	OBB-CAB-CBB	-3.36	112.61	120.17
8	L	401	BCL	C7-C6-C5	-3.36	104.24	113.36
8	W	101	BCL	C16-C15-C13	-3.33	105.14	115.92
8	4	101	BCL	C16-C15-C13	-3.33	105.16	115.92
8	U	101	BCL	C16-C15-C13	-3.32	105.19	115.92
9	J	102	KGD	CAU-CAR-CAQ	3.32	123.30	118.08
14	C	501	HEM	CHB-C1B-C2B	-3.32	117.55	126.72
8	6	101	BCL	C16-C15-C13	-3.32	105.20	115.92
8	E	101	BCL	C16-C15-C13	-3.32	105.20	115.92
8	Q	101	BCL	C16-C15-C13	-3.31	105.22	115.92
8	V	101	BCL	CHD-C1D-ND	-3.31	121.41	124.45
14	C	504	HEM	CBA-CAA-C2A	-3.31	106.97	112.62
8	B	101	BCL	C16-C15-C13	-3.31	105.23	115.92
8	O	101	BCL	C16-C15-C13	-3.31	105.23	115.92
8	K	101	BCL	C16-C15-C13	-3.30	105.24	115.92
8	0	102	BCL	C16-C15-C13	-3.30	105.24	115.92
8	S	101	BCL	C16-C15-C13	-3.30	105.25	115.92
8	I	102	BCL	C16-C15-C13	-3.30	105.25	115.92
8	8	101	BCL	C16-C15-C13	-3.30	105.26	115.92
8	G	101	BCL	C16-C15-C13	-3.30	105.26	115.92
8	0	101	BCL	C16-C15-C13	-3.30	105.26	115.92
8	U	102	BCL	C16-C15-C13	-3.30	105.26	115.92
8	6	102	BCL	C16-C15-C13	-3.30	105.26	115.92
8	Q	102	BCL	C16-C15-C13	-3.30	105.26	115.92
8	O	102	BCL	C16-C15-C13	-3.29	105.27	115.92
8	G	102	BCL	C16-C15-C13	-3.29	105.27	115.92
8	E	102	BCL	C16-C15-C13	-3.29	105.28	115.92
9	I	103	KGD	CBG-CBB-CAV	-3.29	116.73	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	102	BCL	C16-C15-C13	-3.29	105.28	115.92
8	4	101	BCL	O2A-CGA-O1A	-3.29	115.29	123.59
8	4	102	BCL	C16-C15-C13	-3.29	105.29	115.92
8	I	101	BCL	C16-C15-C13	-3.29	105.29	115.92
8	8	102	BCL	C16-C15-C13	-3.29	105.29	115.92
8	S	102	BCL	C16-C15-C13	-3.29	105.30	115.92
8	8	101	BCL	O2A-CGA-O1A	-3.29	115.30	123.59
8	0	102	BCL	O2A-CGA-O1A	-3.28	115.31	123.59
14	C	504	HEM	CHB-C1B-C2B	-3.28	117.64	126.72
8	K	102	BCL	C16-C15-C13	-3.28	105.31	115.92
8	B	102	BCL	C16-C15-C13	-3.28	105.32	115.92
8	S	101	BCL	O2A-CGA-O1A	-3.27	115.33	123.59
8	E	101	BCL	O2A-CGA-O1A	-3.27	115.34	123.59
8	W	102	BCL	C16-C15-C13	-3.27	105.35	115.92
8	Q	101	BCL	O2A-CGA-O1A	-3.26	115.36	123.59
8	G	101	BCL	O2A-CGA-O1A	-3.26	115.37	123.59
8	B	101	BCL	O2A-CGA-O1A	-3.26	115.37	123.59
8	6	101	BCL	O2A-CGA-O1A	-3.25	115.38	123.59
8	V	101	BCL	C4B-CHC-C1C	-3.25	123.67	130.12
10	L	404	BPH	C1-C2-C3	-3.25	120.42	126.04
8	K	101	BCL	O2A-CGA-O1A	-3.25	115.38	123.59
8	I	101	BCL	O2A-CGA-O1A	-3.25	115.39	123.59
8	U	101	BCL	O2A-CGA-O1A	-3.24	115.41	123.59
8	O	101	BCL	O2A-CGA-O1A	-3.22	115.46	123.59
10	L	405	BPH	C1-C2-C3	-3.22	120.48	126.04
8	2	101	BCL	O2A-CGA-O1A	-3.21	115.48	123.59
8	M	1005	BCL	C7-C6-C5	-3.20	104.66	113.36
8	J	101	BCL	C16-C15-C13	-3.20	105.58	115.92
8	5	101	BCL	C16-C15-C13	-3.19	105.59	115.92
8	2	101	BCL	CED-O2D-CGD	-3.19	108.71	115.94
8	R	101	BCL	C16-C15-C13	-3.19	105.61	115.92
8	A	101	BCL	C16-C15-C13	-3.19	105.62	115.92
8	M	1001	BCL	CMC-C2C-C3C	-3.18	100.98	113.83
8	F	101	BCL	C16-C15-C13	-3.18	105.63	115.92
8	N	101	BCL	C16-C15-C13	-3.18	105.64	115.92
8	D	101	BCL	C16-C15-C13	-3.18	105.64	115.92
8	P	101	BCL	C16-C15-C13	-3.18	105.64	115.92
8	7	101	BCL	C16-C15-C13	-3.18	105.65	115.92
11	M	1002	MQE	CAM-CBG-CAT	-3.18	120.01	127.66
8	3	101	BCL	C16-C15-C13	-3.18	105.66	115.92
8	V	101	BCL	C3A-C2A-C1A	-3.17	96.58	101.34
8	1	101	BCL	C16-C15-C13	-3.17	105.66	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	102	BCL	C16-C15-C13	-3.17	105.68	115.92
8	H	101	BCL	C16-C15-C13	-3.17	105.69	115.92
8	K	101	BCL	C4B-CHC-C1C	-3.16	123.85	130.12
8	L	401	BCL	C11-C12-C13	-3.16	105.72	115.92
9	N	102	KGD	CAL-CAJ-CAD	-3.16	118.34	127.20
11	M	1002	MQE	CAJ-CBC-CAP	-3.15	120.06	127.66
8	L	401	BCL	C4D-CHA-C1A	3.15	125.08	121.25
14	C	503	HEM	CHC-C4B-C3B	-3.14	119.76	124.57
8	U	101	BCL	C4B-CHC-C1C	-3.14	123.90	130.12
8	M	1001	BCL	C11-C10-C8	-3.14	105.77	115.92
10	L	405	BPH	C1A-C2A-C3A	-3.14	99.85	102.84
8	2	101	BCL	C4A-NA-C1A	3.13	108.11	106.71
10	L	402	BPH	O2D-CGD-O1D	-3.12	117.74	123.84
8	E	101	BCL	C4B-CHC-C1C	-3.12	123.94	130.12
8	B	101	BCL	C4B-CHC-C1C	-3.12	123.95	130.12
8	N	101	BCL	O2A-CGA-O1A	-3.11	115.74	123.59
8	O	101	BCL	C4B-CHC-C1C	-3.11	123.95	130.12
8	T	101	BCL	O2A-CGA-O1A	-3.11	115.74	123.59
8	M	1005	BCL	C4D-CHA-C1A	3.11	125.03	121.25
8	0	102	BCL	C4B-CHC-C1C	-3.11	123.97	130.12
8	Q	101	BCL	C4B-CHC-C1C	-3.11	123.97	130.12
8	R	101	BCL	O2A-CGA-O1A	-3.10	115.76	123.59
8	B	102	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	6	101	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
8	4	101	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
8	V	101	BCL	C16-C15-C13	-3.10	105.91	115.92
8	F	101	BCL	O2A-CGA-O1A	-3.10	115.78	123.59
8	4	102	BCL	CHA-C1A-NA	-3.09	119.32	126.40
11	M	1002	MQE	CAO-CBI-CAZ	-3.09	120.22	127.66
8	T	101	BCL	C11-C10-C8	-3.09	105.93	115.92
8	S	101	BCL	C4B-CHC-C1C	-3.09	124.00	130.12
11	L	403	MQE	CAY-CBL-CBB	-3.09	121.65	126.79
8	8	101	BCL	C4B-CHC-C1C	-3.09	124.00	130.12
8	I	102	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	5	101	BCL	O2A-CGA-O1A	-3.09	115.80	123.59
8	P	101	BCL	C11-C10-C8	-3.09	105.94	115.92
8	H	101	BCL	O2A-CGA-O1A	-3.09	115.80	123.59
8	I	101	BCL	C4B-CHC-C1C	-3.09	124.00	130.12
8	G	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
8	2	101	BCL	OBB-CAB-CBB	-3.08	113.23	120.17
8	L	401	BCL	O2A-CGA-O1A	-3.08	115.81	123.59
8	L	401	BCL	CHA-C1A-NA	-3.08	119.34	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	BCL	C4B-CHC-C1C	-3.08	124.01	130.12
8	J	101	BCL	O2A-CGA-O1A	-3.08	115.81	123.59
8	0	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	N	101	BCL	C11-C10-C8	-3.08	105.96	115.92
8	9	102	BCL	O2A-CGA-O1A	-3.08	115.82	123.59
8	8	102	BCL	CHA-C1A-NA	-3.08	119.35	126.40
8	K	102	BCL	CHA-C1A-NA	-3.08	119.35	126.40
8	S	102	BCL	CHA-C1A-NA	-3.07	119.36	126.40
8	1	101	BCL	C11-C10-C8	-3.07	105.99	115.92
8	M	1005	BCL	CMA-C3A-C4A	-3.07	103.52	111.77
8	V	101	BCL	CMA-C3A-C4A	-3.07	103.52	111.77
8	M	1001	BCL	CMB-C2B-C3B	3.07	130.43	124.68
8	R	101	BCL	C11-C10-C8	-3.07	105.99	115.92
8	W	102	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	G	101	BCL	CHD-C1D-ND	-3.07	121.63	124.45
8	F	101	BCL	C11-C10-C8	-3.07	106.00	115.92
9	D	102	KGD	CAL-CAJ-CAD	-3.07	118.58	127.20
8	O	102	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	Q	102	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	A	101	BCL	C11-C10-C8	-3.06	106.01	115.92
8	D	101	BCL	O2A-CGA-O1A	-3.06	115.86	123.59
8	7	101	BCL	C11-C10-C8	-3.06	106.02	115.92
8	D	101	BCL	C11-C10-C8	-3.06	106.02	115.92
8	J	101	BCL	C11-C10-C8	-3.06	106.02	115.92
8	9	102	BCL	C11-C10-C8	-3.06	106.03	115.92
8	W	101	BCL	C1-C2-C3	-3.06	120.75	126.04
8	H	101	BCL	C11-C10-C8	-3.06	106.03	115.92
8	W	101	BCL	OBB-CAB-CBB	-3.06	113.29	120.17
8	2	102	BCL	CHA-C1A-NA	-3.06	119.40	126.40
8	5	101	BCL	C11-C10-C8	-3.06	106.04	115.92
8	3	101	BCL	O2A-CGA-O1A	-3.06	115.88	123.59
8	7	101	BCL	O2A-CGA-O1A	-3.06	115.88	123.59
8	L	401	BCL	C16-C15-C13	-3.05	106.05	115.92
8	W	101	BCL	C4A-NA-C1A	3.05	108.08	106.71
8	E	102	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	P	101	BCL	O2A-CGA-O1A	-3.05	115.89	123.59
8	W	101	BCL	C11-C10-C8	-3.05	106.06	115.92
8	6	102	BCL	O2A-CGA-O1A	-3.05	115.90	123.59
8	3	101	BCL	C11-C10-C8	-3.05	106.07	115.92
8	4	102	BCL	O2A-CGA-O1A	-3.05	115.91	123.59
8	0	101	BCL	O2A-CGA-O1A	-3.04	115.91	123.59
8	1	101	BCL	O2A-CGA-O1A	-3.04	115.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	503	HEM	CHB-C1B-C2B	-3.04	118.31	126.72
8	U	102	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	O	101	BCL	CHD-C1D-ND	-3.04	121.66	124.45
8	6	102	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	I	102	BCL	O2A-CGA-O1A	-3.04	115.92	123.59
8	M	1001	BCL	C4B-CHC-C1C	-3.04	124.11	130.12
10	L	402	BPH	CMA-C3A-C4A	-3.03	107.73	114.38
8	8	102	BCL	O2A-CGA-O1A	-3.03	115.94	123.59
8	Q	102	BCL	O2A-CGA-O1A	-3.03	115.95	123.59
8	8	101	BCL	CHD-C1D-ND	-3.03	121.67	124.45
8	S	102	BCL	O2A-CGA-O1A	-3.02	115.96	123.59
8	W	102	BCL	O2A-CGA-O1A	-3.02	115.97	123.59
8	B	101	BCL	CHD-C1D-ND	-3.02	121.68	124.45
8	E	102	BCL	O2A-CGA-O1A	-3.02	115.97	123.59
8	L	401	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	V	101	BCL	C11-C10-C8	-3.02	106.16	115.92
8	Q	101	BCL	CHD-C1D-ND	-3.01	121.68	124.45
8	M	1001	BCL	C16-C15-C13	-3.01	106.19	115.92
8	8	101	BCL	OBB-CAB-CBB	-3.01	113.41	120.17
8	G	102	BCL	O2A-CGA-O1A	-3.00	116.01	123.59
8	6	101	BCL	CHD-C1D-ND	-3.00	121.70	124.45
8	2	102	BCL	O2A-CGA-O1A	-3.00	116.02	123.59
8	K	102	BCL	O2A-CGA-O1A	-3.00	116.02	123.59
8	0	102	BCL	OBB-CAB-CBB	-3.00	113.42	120.17
8	S	101	BCL	CHD-C1D-ND	-3.00	121.70	124.45
8	W	102	BCL	C4D-CHA-C1A	3.00	124.90	121.25
8	U	102	BCL	O2A-CGA-O1A	-2.99	116.03	123.59
8	4	101	BCL	CHD-C1D-ND	-2.99	121.70	124.45
8	0	101	BCL	C4D-CHA-C1A	2.99	124.89	121.25
8	K	101	BCL	OBB-CAB-CBB	-2.99	113.44	120.17
8	O	101	BCL	OBB-CAB-CBB	-2.99	113.44	120.17
8	I	101	BCL	CHD-C1D-ND	-2.99	121.71	124.45
8	B	102	BCL	O2A-CGA-O1A	-2.98	116.06	123.59
8	I	101	BCL	OBB-CAB-CBB	-2.98	113.45	120.17
8	U	101	BCL	OBB-CAB-CBB	-2.98	113.46	120.17
8	S	102	BCL	C4D-CHA-C1A	2.98	124.88	121.25
8	B	102	BCL	C4D-CHA-C1A	2.98	124.88	121.25
8	O	102	BCL	O2A-CGA-O1A	-2.98	116.08	123.59
8	4	102	BCL	C4D-CHA-C1A	2.97	124.87	121.25
9	J	102	KGD	CAL-CAJ-CAD	-2.97	118.86	127.20
8	4	101	BCL	OBB-CAB-CBB	-2.97	113.48	120.17
8	B	101	BCL	OBB-CAB-CBB	-2.97	113.48	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1001	BCL	C2A-C3A-C4A	-2.97	97.08	101.87
9	I	103	KGD	CAL-CAJ-CAD	-2.97	118.87	127.20
8	6	101	BCL	OBG-CAB-CBB	-2.96	113.50	120.17
8	K	102	BCL	C4D-CHA-C1A	2.96	124.86	121.25
8	2	101	BCL	CMB-C2B-C3B	2.96	130.22	124.68
8	0	102	BCL	CHD-C1D-ND	-2.96	121.73	124.45
8	6	102	BCL	CMA-C3A-C4A	-2.96	103.81	111.77
8	U	101	BCL	CHD-C1D-ND	-2.96	121.73	124.45
8	G	101	BCL	OBG-CAB-CBB	-2.96	113.51	120.17
8	E	101	BCL	C11-C10-C8	-2.96	106.36	115.92
8	I	102	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
8	4	102	BCL	CMA-C3A-C4A	-2.95	103.83	111.77
8	K	102	BCL	CMA-C3A-C4A	-2.95	103.84	111.77
8	Q	102	BCL	CMA-C3A-C4A	-2.95	103.84	111.77
8	E	102	BCL	CMA-C3A-C4A	-2.95	103.84	111.77
14	C	503	HEM	CBD-CAD-C3D	-2.95	104.43	112.63
8	W	101	BCL	CMB-C2B-C3B	2.95	130.20	124.68
8	S	101	BCL	OBG-CAB-CBB	-2.95	113.53	120.17
8	L	401	BCL	C11-C10-C8	-2.95	106.38	115.92
8	E	101	BCL	OBG-CAB-CBB	-2.95	113.53	120.17
8	B	102	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	O	102	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	S	102	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	W	102	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	0	101	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	G	102	BCL	CMA-C3A-C4A	-2.95	103.85	111.77
8	Q	102	BCL	C4D-CHA-C1A	2.95	124.83	121.25
8	W	101	BCL	C1D-CHD-C4C	-2.94	119.52	126.62
8	8	102	BCL	CMA-C3A-C4A	-2.94	103.86	111.77
8	U	102	BCL	CMA-C3A-C4A	-2.94	103.87	111.77
8	K	101	BCL	CHD-C1D-ND	-2.94	121.75	124.45
8	4	101	BCL	C11-C10-C8	-2.94	106.42	115.92
8	2	102	BCL	C4D-CHA-C1A	2.94	124.83	121.25
8	V	101	BCL	C7-C6-C5	-2.94	105.38	113.36
8	2	102	BCL	CMA-C3A-C4A	-2.94	103.88	111.77
8	I	101	BCL	C11-C10-C8	-2.94	106.42	115.92
8	L	401	BCL	CMA-C3A-C4A	-2.94	103.88	111.77
10	L	405	BPH	O2D-CGD-O1D	-2.93	118.10	123.84
8	O	101	BCL	C11-C10-C8	-2.93	106.44	115.92
8	S	101	BCL	C11-C10-C8	-2.93	106.44	115.92
8	I	101	BCL	CGD-CBD-CAD	-2.93	101.23	110.73
9	9	101	KGD	CAE-CAI-CAH	-2.93	115.95	118.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	101	BCL	OBB-CAB-CBB	-2.93	113.57	120.17
8	Q	101	BCL	C11-C10-C8	-2.93	106.45	115.92
8	8	102	BCL	C4D-CHA-C1A	2.93	124.81	121.25
8	6	101	BCL	C11-C10-C8	-2.93	106.45	115.92
8	E	101	BCL	CHD-C1D-ND	-2.93	121.76	124.45
8	G	102	BCL	C4D-CHA-C1A	2.93	124.81	121.25
8	8	101	BCL	C11-C10-C8	-2.93	106.46	115.92
8	K	101	BCL	C11-C10-C8	-2.93	106.46	115.92
8	B	101	BCL	C11-C10-C8	-2.93	106.46	115.92
8	0	102	BCL	C11-C10-C8	-2.92	106.47	115.92
8	E	102	BCL	C4D-CHA-C1A	2.92	124.81	121.25
8	S	101	BCL	CGD-CBD-CAD	-2.92	101.27	110.73
8	U	101	BCL	C11-C10-C8	-2.92	106.48	115.92
8	I	102	BCL	C4D-CHA-C1A	2.92	124.80	121.25
8	4	101	BCL	CGD-CBD-CAD	-2.92	101.28	110.73
8	2	101	BCL	C1D-CHD-C4C	-2.92	119.59	126.62
8	U	101	BCL	CGD-CBD-CAD	-2.92	101.29	110.73
8	6	101	BCL	CGD-CBD-CAD	-2.91	101.31	110.73
8	K	101	BCL	CGD-CBD-CAD	-2.91	101.31	110.73
8	G	101	BCL	C11-C10-C8	-2.91	106.52	115.92
8	G	101	BCL	CGD-CBD-CAD	-2.91	101.31	110.73
8	O	102	BCL	C4D-CHA-C1A	2.91	124.79	121.25
8	V	101	BCL	C1B-CHB-C4A	-2.91	124.36	130.12
8	E	101	BCL	CGD-CBD-CAD	-2.91	101.32	110.73
8	O	101	BCL	CGD-CBD-CAD	-2.90	101.33	110.73
8	G	101	BCL	C7-C6-C5	-2.90	105.48	113.36
8	B	102	BCL	C7-C6-C5	-2.90	105.48	113.36
8	Q	101	BCL	C7-C6-C5	-2.90	105.48	113.36
8	K	101	BCL	C7-C6-C5	-2.90	105.48	113.36
8	0	102	BCL	CGD-CBD-CAD	-2.90	101.34	110.73
8	6	102	BCL	C4D-CHA-C1A	2.90	124.78	121.25
8	E	101	BCL	C7-C6-C5	-2.90	105.49	113.36
8	N	101	BCL	C7-C6-C5	-2.90	105.49	113.36
8	H	101	BCL	C7-C6-C5	-2.90	105.49	113.36
8	7	101	BCL	C7-C6-C5	-2.90	105.49	113.36
8	8	101	BCL	C7-C6-C5	-2.89	105.50	113.36
8	3	101	BCL	C7-C6-C5	-2.89	105.50	113.36
8	Q	101	BCL	CGD-CBD-CAD	-2.89	101.37	110.73
8	9	102	BCL	C7-C6-C5	-2.89	105.51	113.36
8	T	101	BCL	C7-C6-C5	-2.89	105.51	113.36
8	8	101	BCL	CGD-CBD-CAD	-2.89	101.38	110.73
8	D	101	BCL	C7-C6-C5	-2.89	105.52	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	101	BCL	CGD-CBD-CAD	-2.89	101.38	110.73
8	P	101	BCL	C7-C6-C5	-2.89	105.52	113.36
8	U	101	BCL	C7-C6-C5	-2.89	105.52	113.36
8	U	102	BCL	C4D-CHA-C1A	2.88	124.76	121.25
8	J	101	BCL	C7-C6-C5	-2.88	105.52	113.36
8	1	101	BCL	C7-C6-C5	-2.88	105.53	113.36
9	D	102	KGD	CBB-CAV-CAR	-2.88	123.19	127.31
8	B	101	BCL	C7-C6-C5	-2.88	105.53	113.36
8	W	101	BCL	CHA-C1A-NA	-2.88	119.80	126.40
8	A	101	BCL	C7-C6-C5	-2.88	105.54	113.36
8	2	101	BCL	CHA-C1A-NA	-2.88	119.80	126.40
8	I	101	BCL	C7-C6-C5	-2.88	105.54	113.36
8	0	102	BCL	C7-C6-C5	-2.88	105.54	113.36
8	2	102	BCL	C7-C6-C5	-2.88	105.54	113.36
8	F	101	BCL	C7-C6-C5	-2.88	105.54	113.36
8	5	101	BCL	C7-C6-C5	-2.88	105.55	113.36
8	T	101	BCL	CMC-C2C-C3C	-2.88	102.22	113.83
14	C	502	HEM	CAD-CBD-CGD	-2.88	107.41	113.60
8	8	102	BCL	C7-C6-C5	-2.88	105.55	113.36
8	R	101	BCL	C7-C6-C5	-2.88	105.55	113.36
8	E	102	BCL	C7-C6-C5	-2.88	105.55	113.36
8	O	102	BCL	C7-C6-C5	-2.88	105.55	113.36
8	U	102	BCL	C7-C6-C5	-2.88	105.55	113.36
8	D	101	BCL	CMC-C2C-C3C	-2.87	102.24	113.83
8	6	102	BCL	C7-C6-C5	-2.87	105.56	113.36
8	O	101	BCL	C7-C6-C5	-2.87	105.56	113.36
8	2	101	BCL	C4D-CHA-C1A	2.87	124.74	121.25
8	F	101	BCL	CMC-C2C-C3C	-2.87	102.25	113.83
8	4	101	BCL	C7-C6-C5	-2.87	105.56	113.36
8	6	101	BCL	C7-C6-C5	-2.87	105.57	113.36
8	0	101	BCL	C7-C6-C5	-2.87	105.57	113.36
8	R	101	BCL	CMC-C2C-C3C	-2.87	102.26	113.83
8	G	102	BCL	C7-C6-C5	-2.87	105.58	113.36
8	I	102	BCL	C7-C6-C5	-2.87	105.58	113.36
8	S	101	BCL	C7-C6-C5	-2.86	105.58	113.36
8	M	1001	BCL	C3D-C2D-C1D	-2.86	101.92	105.83
8	W	102	BCL	C7-C6-C5	-2.86	105.58	113.36
8	1	101	BCL	CMC-C2C-C3C	-2.86	102.28	113.83
8	3	101	BCL	CMC-C2C-C3C	-2.86	102.29	113.83
8	5	101	BCL	CMC-C2C-C3C	-2.86	102.30	113.83
8	4	102	BCL	C7-C6-C5	-2.86	105.60	113.36
8	K	102	BCL	C7-C6-C5	-2.86	105.60	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	102	BCL	C7-C6-C5	-2.86	105.60	113.36
8	H	101	BCL	CMC-C2C-C3C	-2.86	102.31	113.83
8	9	102	BCL	CMC-C2C-C3C	-2.85	102.31	113.83
8	M	1005	BCL	C16-C15-C13	-2.85	106.70	115.92
8	A	101	BCL	CMC-C2C-C3C	-2.85	102.32	113.83
8	N	101	BCL	CMC-C2C-C3C	-2.85	102.33	113.83
8	J	101	BCL	CMC-C2C-C3C	-2.85	102.33	113.83
8	M	1005	BCL	C4B-CHC-C1C	-2.85	124.48	130.12
8	P	101	BCL	CMC-C2C-C3C	-2.85	102.35	113.83
8	7	101	BCL	CMC-C2C-C3C	-2.84	102.36	113.83
8	S	102	BCL	C7-C6-C5	-2.84	105.64	113.36
8	W	101	BCL	C4D-CHA-C1A	2.83	124.69	121.25
8	K	101	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
10	L	404	BPH	O2D-CGD-O1D	-2.82	118.32	123.84
11	M	1002	MQE	CAL-CBF-CAV	-2.82	120.88	127.66
8	M	1005	BCL	CHA-C1A-NA	-2.81	119.97	126.40
14	C	502	HEM	CHA-C4D-ND	2.81	127.85	124.38
8	M	1005	BCL	CMC-C2C-C3C	-2.81	102.50	113.83
8	M	1005	BCL	O2A-CGA-O1A	-2.81	116.51	123.59
8	I	101	BCL	C3D-C2D-C1D	-2.80	102.00	105.83
8	W	101	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
8	4	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
8	G	101	BCL	CMA-C3A-C4A	-2.80	104.25	111.77
8	2	101	BCL	C2A-C1A-CHA	2.80	128.75	123.86
8	8	101	BCL	CMA-C3A-C4A	-2.79	104.26	111.77
8	4	101	BCL	CHA-C1A-NA	-2.79	120.00	126.40
8	M	1005	BCL	CGD-CBD-CAD	-2.79	101.69	110.73
8	Q	101	BCL	CMA-C3A-C4A	-2.79	104.27	111.77
8	4	101	BCL	CMA-C3A-C4A	-2.79	104.27	111.77
8	B	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	O	101	BCL	CMA-C3A-C4A	-2.79	104.29	111.77
8	8	101	BCL	CHA-C1A-NA	-2.79	120.02	126.40
8	Q	101	BCL	CHA-C1A-NA	-2.78	120.03	126.40
8	U	101	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
8	E	101	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
8	K	101	BCL	CHA-C1A-NA	-2.78	120.03	126.40
11	M	1002	MQE	CAL-CBD-CAR	-2.78	120.97	127.66
8	S	101	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
8	W	101	BCL	C2A-C1A-CHA	2.78	128.71	123.86
8	0	102	BCL	CMA-C3A-C4A	-2.77	104.32	111.77
8	B	101	BCL	CMA-C3A-C4A	-2.77	104.32	111.77
8	Q	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CMA-C3A-C4A	-2.77	104.33	111.77
8	6	101	BCL	CMA-C3A-C4A	-2.77	104.33	111.77
8	E	102	BCL	CMC-C2C-C3C	-2.77	102.66	113.83
8	0	102	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	0	102	BCL	CHA-C1A-NA	-2.76	120.07	126.40
8	U	101	BCL	CHA-C1A-NA	-2.76	120.07	126.40
8	5	101	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	Q	102	BCL	CMC-C2C-C3C	-2.76	102.69	113.83
8	8	102	BCL	CMC-C2C-C3C	-2.76	102.70	113.83
8	0	101	BCL	CMC-C2C-C3C	-2.76	102.70	113.83
8	I	101	BCL	CMA-C3A-C4A	-2.76	104.36	111.77
8	S	101	BCL	CHA-C1A-NA	-2.76	120.09	126.40
8	I	101	BCL	CHA-C1A-NA	-2.75	120.09	126.40
8	R	101	BCL	C11-C12-C13	-2.75	107.02	115.92
8	6	102	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	F	101	BCL	C3D-C2D-C1D	-2.75	102.07	105.83
8	O	102	BCL	CMC-C2C-C3C	-2.75	102.72	113.83
8	K	102	BCL	CMC-C2C-C3C	-2.75	102.72	113.83
8	G	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	M	1005	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	2	102	BCL	CMC-C2C-C3C	-2.75	102.73	113.83
8	U	102	BCL	CMC-C2C-C3C	-2.75	102.73	113.83
8	S	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	U	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	H	101	BCL	C11-C12-C13	-2.75	107.03	115.92
8	E	101	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	I	102	BCL	CMC-C2C-C3C	-2.75	102.74	113.83
8	8	102	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
8	G	101	BCL	CHA-C1A-NA	-2.75	120.11	126.40
8	D	101	BCL	C11-C12-C13	-2.75	107.05	115.92
8	4	102	BCL	CMC-C2C-C3C	-2.74	102.75	113.83
8	B	101	BCL	CHA-C1A-NA	-2.74	120.11	126.40
8	W	102	BCL	CMC-C2C-C3C	-2.74	102.76	113.83
8	6	101	BCL	CHA-C1A-NA	-2.74	120.12	126.40
8	S	102	BCL	CMC-C2C-C3C	-2.74	102.76	113.83
8	T	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	E	102	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	5	101	BCL	C11-C12-C13	-2.74	107.06	115.92
8	8	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	A	101	BCL	C11-C12-C13	-2.74	107.06	115.92
8	E	101	BCL	CHA-C1A-NA	-2.74	120.12	126.40
8	3	101	BCL	C11-C12-C13	-2.74	107.06	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
9	I	103	KGD	CAQ-CAR-CAV	-2.74	114.74	118.94
8	O	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	9	102	BCL	CGD-CBD-CAD	-2.74	101.87	110.73
8	O	101	BCL	CHA-C1A-NA	-2.74	120.13	126.40
8	B	102	BCL	CMC-C2C-C3C	-2.74	102.79	113.83
8	J	101	BCL	C11-C12-C13	-2.73	107.08	115.92
8	P	101	BCL	C11-C12-C13	-2.73	107.08	115.92
8	6	102	BCL	CMC-C2C-C3C	-2.73	102.80	113.83
8	T	101	BCL	C11-C12-C13	-2.73	107.08	115.92
8	I	102	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
8	Q	101	BCL	C11-C12-C13	-2.73	107.09	115.92
8	6	101	BCL	C11-C12-C13	-2.73	107.09	115.92
8	1	101	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	N	101	BCL	C11-C12-C13	-2.73	107.09	115.92
8	G	102	BCL	CMC-C2C-C3C	-2.73	102.82	113.83
8	H	101	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	O	102	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	1	101	BCL	C11-C12-C13	-2.73	107.10	115.92
8	L	401	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	D	101	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	U	102	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	F	101	BCL	C11-C12-C13	-2.73	107.11	115.92
8	N	101	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
8	5	101	BCL	CGD-CBD-CAD	-2.72	101.91	110.73
8	1	101	BCL	CGD-CBD-CAD	-2.72	101.91	110.73
8	7	101	BCL	C11-C12-C13	-2.72	107.12	115.92
8	K	101	BCL	CMC-C2C-C3C	-2.72	102.84	113.83
8	Q	101	BCL	CMC-C2C-C3C	-2.72	102.84	113.83
8	E	101	BCL	C11-C12-C13	-2.72	107.12	115.92
8	M	1001	BCL	C3C-C2C-C1C	2.72	106.27	101.87
8	P	101	BCL	CGD-CBD-CAD	-2.72	101.92	110.73
10	L	402	BPH	CBC-CAC-C3C	-2.72	108.28	113.77
8	B	101	BCL	C11-C12-C13	-2.72	107.12	115.92
8	N	101	BCL	CGD-CBD-CAD	-2.72	101.92	110.73
8	I	101	BCL	CMC-C2C-C3C	-2.72	102.85	113.83
8	D	101	BCL	CGD-CBD-CAD	-2.72	101.92	110.73
8	P	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	O	101	BCL	CMC-C2C-C3C	-2.72	102.86	113.83
8	F	101	BCL	CGD-CBD-CAD	-2.72	101.93	110.73
8	R	101	BCL	CGD-CBD-CAD	-2.72	101.93	110.73
8	2	102	BCL	C3D-C2D-C1D	-2.72	102.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	CMC-C2C-C3C	-2.72	102.87	113.83
8	M	1005	BCL	C11-C10-C8	-2.72	107.14	115.92
8	B	101	BCL	CMC-C2C-C3C	-2.72	102.87	113.83
8	4	101	BCL	C11-C12-C13	-2.71	107.15	115.92
8	I	101	BCL	C11-C12-C13	-2.71	107.15	115.92
8	4	101	BCL	CMC-C2C-C3C	-2.71	102.89	113.83
8	0	102	BCL	CMC-C2C-C3C	-2.71	102.89	113.83
8	9	102	BCL	C11-C12-C13	-2.71	107.16	115.92
8	T	101	BCL	CGD-CBD-CAD	-2.71	101.95	110.73
8	2	101	BCL	C7-C6-C5	-2.71	106.00	113.36
8	G	101	BCL	CMC-C2C-C3C	-2.71	102.89	113.83
8	6	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
8	A	101	BCL	CGD-CBD-CAD	-2.71	101.96	110.73
8	O	101	BCL	C11-C12-C13	-2.71	107.17	115.92
8	3	101	BCL	CGD-CBD-CAD	-2.71	101.96	110.73
8	H	101	BCL	CMB-C2B-C3B	2.71	129.74	124.68
8	T	101	BCL	CMB-C2B-C3B	2.71	129.74	124.68
8	7	101	BCL	C3D-C2D-C1D	-2.71	102.14	105.83
8	U	101	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	6	101	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	2	101	BCL	CMC-C2C-C3C	-2.71	102.91	113.83
8	U	101	BCL	C11-C12-C13	-2.71	107.17	115.92
8	K	101	BCL	C11-C12-C13	-2.70	107.18	115.92
8	G	101	BCL	C11-C12-C13	-2.70	107.18	115.92
8	K	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
8	E	101	BCL	CMC-C2C-C3C	-2.70	102.92	113.83
8	H	101	BCL	CGD-CBD-CAD	-2.70	101.98	110.73
8	9	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
8	J	101	BCL	CGD-CBD-CAD	-2.70	101.98	110.73
8	S	101	BCL	C11-C12-C13	-2.70	107.19	115.92
8	7	101	BCL	CGD-CBD-CAD	-2.70	101.98	110.73
8	8	101	BCL	C11-C12-C13	-2.70	107.19	115.92
8	Q	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
8	S	101	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
8	B	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
8	0	102	BCL	C11-C12-C13	-2.70	107.19	115.92
8	J	101	BCL	CMB-C2B-C3B	2.70	129.73	124.68
8	W	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
8	1	101	BCL	CMB-C2B-C3B	2.70	129.72	124.68
8	D	101	BCL	CMB-C2B-C3B	2.70	129.72	124.68
8	A	101	BCL	C3D-C2D-C1D	-2.69	102.15	105.83
8	J	101	BCL	C3D-C2D-C1D	-2.69	102.15	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	102	BCL	C3D-C2D-C1D	-2.69	102.15	105.83
8	R	101	BCL	CMB-C2B-C3B	2.69	129.71	124.68
8	5	101	BCL	CMB-C2B-C3B	2.69	129.71	124.68
8	N	101	BCL	CMB-C2B-C3B	2.68	129.70	124.68
8	G	102	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
8	I	101	BCL	C2C-C3C-C4C	-2.68	97.32	101.34
8	F	101	BCL	CMB-C2B-C3B	2.68	129.69	124.68
8	0	101	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
8	3	101	BCL	C3D-C2D-C1D	-2.68	102.18	105.83
8	9	102	BCL	CMB-C2B-C3B	2.67	129.68	124.68
8	4	102	BCL	C3D-C2D-C1D	-2.67	102.18	105.83
8	7	101	BCL	CMB-C2B-C3B	2.67	129.68	124.68
8	3	101	BCL	CMB-C2B-C3B	2.67	129.67	124.68
8	W	101	BCL	CMC-C2C-C3C	-2.67	103.06	113.83
8	P	101	BCL	CMB-C2B-C3B	2.67	129.67	124.68
8	K	101	BCL	C2C-C3C-C4C	-2.66	97.35	101.34
8	A	101	BCL	CMB-C2B-C3B	2.66	129.66	124.68
9	D	102	KGD	CBG-CBB-CAV	-2.66	118.03	123.47
8	V	101	BCL	CMB-C2B-C3B	2.66	129.65	124.68
8	S	101	BCL	C2C-C3C-C4C	-2.65	97.37	101.34
8	U	101	BCL	C2C-C3C-C4C	-2.64	97.38	101.34
14	C	501	HEM	C4B-C3B-C2B	-2.64	105.02	107.11
8	V	101	BCL	C11-C12-C13	-2.64	107.38	115.92
8	4	101	BCL	C2C-C3C-C4C	-2.64	97.38	101.34
8	G	101	BCL	C2C-C3C-C4C	-2.64	97.39	101.34
8	8	101	BCL	C2C-C3C-C4C	-2.64	97.39	101.34
8	B	101	BCL	C2C-C3C-C4C	-2.64	97.39	101.34
9	D	102	KGD	CAT-CAX-CAY	-2.63	118.75	127.75
8	V	101	BCL	CMC-C2C-C3C	-2.63	103.20	113.83
8	O	101	BCL	C2C-C3C-C4C	-2.63	97.40	101.34
8	Q	101	BCL	C2C-C3C-C4C	-2.62	97.41	101.34
8	L	401	BCL	C2A-C1A-CHA	2.62	128.44	123.86
8	P	101	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
8	W	101	BCL	CGD-CBD-CAD	-2.62	102.26	110.73
8	1	101	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
8	W	101	BCL	C7-C6-C5	-2.61	106.26	113.36
8	W	101	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
8	D	101	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
8	0	102	BCL	C2C-C3C-C4C	-2.61	97.43	101.34
8	R	101	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
11	L	403	MQE	CAK-CBE-CAQ	-2.61	121.39	127.66
8	6	101	BCL	C2C-C3C-C4C	-2.60	97.44	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	102	BCL	CMA-C3A-C4A	-2.60	104.77	111.77
8	J	101	BCL	CMA-C3A-C4A	-2.60	104.77	111.77
8	V	101	BCL	C3D-C2D-C1D	-2.60	102.28	105.83
8	N	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
8	5	101	BCL	CMA-C3A-C4A	-2.60	104.80	111.77
8	A	101	BCL	CMA-C3A-C4A	-2.60	104.80	111.77
8	E	101	BCL	C2C-C3C-C4C	-2.60	97.45	101.34
8	H	101	BCL	CMA-C3A-C4A	-2.60	104.80	111.77
8	M	1001	BCL	C11-C12-C13	-2.59	107.53	115.92
8	4	102	BCL	C4A-NA-C1A	-2.59	105.54	106.71
8	T	101	BCL	CMA-C3A-C4A	-2.59	104.82	111.77
8	3	101	BCL	CMA-C3A-C4A	-2.59	104.82	111.77
8	F	101	BCL	CMA-C3A-C4A	-2.59	104.83	111.77
11	L	403	MQE	CAJ-CBC-CAP	-2.58	121.44	127.66
9	N	102	KGD	CAE-CAC-CAB	-2.58	109.03	113.18
8	B	102	BCL	C4A-NA-C1A	-2.58	105.55	106.71
8	K	102	BCL	CMB-C2B-C3B	2.58	129.50	124.68
8	Q	102	BCL	CMB-C2B-C3B	2.58	129.50	124.68
8	4	102	BCL	CMB-C2B-C3B	2.57	129.49	124.68
8	7	101	BCL	CMA-C3A-C4A	-2.57	104.86	111.77
8	2	101	BCL	C3D-C2D-C1D	-2.57	102.32	105.83
13	M	1006	PGV	O14-P-O13	2.57	124.95	112.24
8	4	101	BCL	CMD-C2D-C1D	2.57	129.24	124.71
8	K	101	BCL	CMD-C2D-C1D	2.56	129.23	124.71
8	L	401	BCL	CGD-CBD-CAD	-2.56	102.44	110.73
8	W	101	BCL	C11-C12-C13	-2.56	107.64	115.92
8	E	102	BCL	CMB-C2B-C3B	2.56	129.47	124.68
13	M	1007	PGV	O14-P-O13	2.56	124.89	112.24
8	G	102	BCL	CMB-C2B-C3B	2.56	129.46	124.68
8	0	101	BCL	CMB-C2B-C3B	2.56	129.46	124.68
8	2	101	BCL	CMA-C3A-C4A	-2.55	104.91	111.77
8	L	401	BCL	CMC-C2C-C3C	-2.55	103.55	113.83
13	M	1007	PGV	P-O12-C04	-2.55	106.74	121.68
8	B	102	BCL	CMB-C2B-C3B	2.55	129.44	124.68
8	U	102	BCL	CMB-C2B-C3B	2.55	129.44	124.68
8	W	101	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
8	I	102	BCL	CMB-C2B-C3B	2.54	129.43	124.68
8	I	102	BCL	C4A-NA-C1A	-2.54	105.56	106.71
8	B	101	BCL	CMB-C2B-C3B	2.54	129.43	124.68
8	0	102	BCL	CMB-C2B-C3B	2.54	129.43	124.68
8	Q	101	BCL	CMD-C2D-C1D	2.54	129.18	124.71
8	2	102	BCL	CMB-C2B-C3B	2.54	129.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CMB-C2B-C3B	2.54	129.42	124.68
8	O	101	BCL	CMB-C2B-C3B	2.53	129.42	124.68
8	U	101	BCL	CMB-C2B-C3B	2.53	129.42	124.68
8	O	102	BCL	CMB-C2B-C3B	2.53	129.42	124.68
14	C	502	HEM	CAA-CBA-CGA	-2.53	106.67	113.76
8	8	102	BCL	CMB-C2B-C3B	2.53	129.41	124.68
8	W	102	BCL	CMB-C2B-C3B	2.53	129.41	124.68
8	Q	101	BCL	CMB-C2B-C3B	2.53	129.41	124.68
11	L	403	MQE	CAI-CBD-CAR	-2.53	121.58	127.66
8	S	101	BCL	CMB-C2B-C3B	2.53	129.40	124.68
8	6	101	BCL	CMB-C2B-C3B	2.52	129.40	124.68
8	L	401	BCL	CMD-C2D-C1D	2.52	129.16	124.71
8	6	102	BCL	CMB-C2B-C3B	2.52	129.40	124.68
8	S	102	BCL	CMB-C2B-C3B	2.52	129.40	124.68
8	I	101	BCL	CMD-C2D-C1D	2.52	129.16	124.71
8	8	101	BCL	CMB-C2B-C3B	2.52	129.40	124.68
8	E	101	BCL	CMD-C2D-C1D	2.52	129.16	124.71
9	9	101	KGD	CAC-CAB-CAD	-2.52	106.60	110.48
8	O	101	BCL	CMD-C2D-C1D	2.52	129.15	124.71
8	8	102	BCL	C4A-NA-C1A	-2.52	105.58	106.71
8	B	101	BCL	CMD-C2D-C1D	2.52	129.15	124.71
8	I	101	BCL	CMB-C2B-C3B	2.51	129.38	124.68
13	M	1008	PGV	O14-P-O13	2.51	124.66	112.24
8	6	101	BCL	CMD-C2D-C1D	2.51	129.14	124.71
8	G	102	BCL	C4A-NA-C1A	-2.51	105.58	106.71
8	U	101	BCL	CMD-C2D-C1D	2.51	129.14	124.71
9	I	103	KGD	CAE-CAC-CAB	-2.51	109.15	113.18
8	G	101	BCL	CMD-C2D-C1D	2.51	129.13	124.71
8	S	101	BCL	CMD-C2D-C1D	2.51	129.13	124.71
8	4	101	BCL	CMB-C2B-C3B	2.51	129.37	124.68
8	0	102	BCL	CMD-C2D-C1D	2.50	129.13	124.71
8	E	101	BCL	CMB-C2B-C3B	2.50	129.36	124.68
8	2	101	BCL	C16-C15-C13	-2.50	107.85	115.92
8	G	101	BCL	CMB-C2B-C3B	2.50	129.35	124.68
9	I	103	KGD	CAP-CAQ-CAR	-2.49	119.43	126.42
9	9	101	KGD	CAL-CAJ-CAD	-2.49	120.22	127.20
9	N	102	KGD	CBG-CBB-CAV	-2.49	118.38	123.47
8	5	101	BCL	CMD-C2D-C1D	2.48	129.09	124.71
8	8	101	BCL	CMD-C2D-C1D	2.48	129.09	124.71
11	L	403	MQE	CAO-CBI-CAZ	-2.48	121.69	127.66
8	2	101	BCL	CGD-CBD-CAD	-2.48	102.71	110.73
8	T	101	BCL	CMD-C2D-C1D	2.48	129.08	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	102	KGD	CAN-CAM-CAL	-2.47	114.18	118.08
8	O	102	BCL	C4A-NA-C1A	-2.47	105.59	106.71
11	M	1002	MQE	CAK-CBE-CAQ	-2.47	121.71	127.66
11	L	403	MQE	CAM-CBG-CAT	-2.47	121.72	127.66
8	M	1005	BCL	CHC-C1C-NC	2.46	127.92	124.51
8	K	102	BCL	C4A-NA-C1A	-2.46	105.60	106.71
8	N	101	BCL	CMD-C2D-C1D	2.46	129.05	124.71
14	C	501	HEM	CHA-C4D-ND	2.46	127.42	124.38
8	F	101	BCL	CMD-C2D-C1D	2.46	129.05	124.71
8	M	1001	BCL	C7-C6-C5	-2.46	106.69	113.36
14	C	504	HEM	CHC-C4B-C3B	-2.45	120.81	124.57
8	3	101	BCL	CMD-C2D-C1D	2.45	129.04	124.71
14	C	504	HEM	C4B-CHC-C1C	-2.45	119.32	122.56
11	M	1002	MQE	CAS-CBH-CAW	-2.45	121.77	127.66
8	D	101	BCL	CMD-C2D-C1D	2.45	129.02	124.71
9	D	102	KGD	OAA-CAI-CAH	2.44	123.13	120.96
8	L	401	BCL	CBB-CAB-C3B	2.44	127.59	120.34
8	H	101	BCL	CMD-C2D-C1D	2.44	129.02	124.71
8	Q	102	BCL	C4A-NA-C1A	-2.44	105.61	106.71
11	L	403	MQE	CBA-CBN-CBM	-2.44	121.78	127.66
10	L	402	BPH	C11-C12-C13	-2.44	108.03	115.92
8	1	101	BCL	CMD-C2D-C1D	2.44	129.01	124.71
8	U	102	BCL	C4A-NA-C1A	-2.44	105.61	106.71
8	P	101	BCL	CMD-C2D-C1D	2.44	129.01	124.71
8	9	102	BCL	CMD-C2D-C1D	2.43	129.00	124.71
14	C	501	HEM	CHC-C4B-C3B	-2.43	120.84	124.57
8	R	101	BCL	CMD-C2D-C1D	2.43	128.99	124.71
11	M	1002	MQE	CBO-CCB-CCC	-2.43	121.82	127.66
8	M	1005	BCL	C11-C12-C13	-2.43	108.08	115.92
8	A	101	BCL	CMD-C2D-C1D	2.42	128.99	124.71
8	L	401	BCL	C1C-NC-C4C	-2.42	105.62	106.71
8	M	1001	BCL	C1C-NC-C4C	-2.42	105.62	106.71
13	M	1007	PGV	P-O11-C03	-2.42	107.47	121.68
8	E	102	BCL	C4A-NA-C1A	-2.42	105.62	106.71
8	7	101	BCL	CMD-C2D-C1D	2.42	128.98	124.71
8	S	102	BCL	C4A-NA-C1A	-2.42	105.62	106.71
11	L	403	MQE	CBO-CCB-CCC	-2.42	121.83	127.66
8	3	101	BCL	CED-O2D-CGD	-2.42	110.47	115.94
9	J	102	KGD	CAQ-CAR-CAV	-2.42	115.23	118.94
8	R	101	BCL	C2A-C3A-C4A	-2.42	97.97	101.87
8	J	101	BCL	C2A-C3A-C4A	-2.41	97.97	101.87
8	N	101	BCL	C4D-CHA-C1A	2.41	124.18	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	C2A-C3A-C4A	-2.41	97.98	101.87
8	J	101	BCL	CMD-C2D-C1D	2.41	128.95	124.71
8	7	101	BCL	CED-O2D-CGD	-2.41	110.50	115.94
8	5	101	BCL	C2A-C3A-C4A	-2.40	97.99	101.87
8	M	1001	BCL	C2A-C1A-CHA	2.40	128.06	123.86
8	H	101	BCL	C2A-C3A-C4A	-2.40	97.99	101.87
8	F	101	BCL	C2A-C3A-C4A	-2.40	97.99	101.87
8	D	101	BCL	CED-O2D-CGD	-2.40	110.51	115.94
8	9	102	BCL	CED-O2D-CGD	-2.40	110.52	115.94
8	H	101	BCL	CED-O2D-CGD	-2.39	110.52	115.94
8	D	101	BCL	C2A-C3A-C4A	-2.39	98.00	101.87
14	C	502	HEM	C4B-C3B-C2B	-2.39	105.22	107.11
8	E	102	BCL	C2C-C3C-C4C	-2.39	97.76	101.34
8	1	101	BCL	CED-O2D-CGD	-2.39	110.53	115.94
8	7	101	BCL	C4D-CHA-C1A	2.39	124.16	121.25
8	9	102	BCL	C2A-C3A-C4A	-2.39	98.01	101.87
8	N	101	BCL	CED-O2D-CGD	-2.39	110.54	115.94
8	A	101	BCL	CED-O2D-CGD	-2.39	110.54	115.94
8	8	102	BCL	C2C-C3C-C4C	-2.38	97.77	101.34
8	R	101	BCL	CED-O2D-CGD	-2.38	110.55	115.94
11	L	403	MQE	CAL-CBF-CAV	-2.38	121.92	127.66
8	J	101	BCL	CED-O2D-CGD	-2.38	110.55	115.94
8	H	101	BCL	C4D-CHA-C1A	2.38	124.15	121.25
8	U	102	BCL	C2C-C3C-C4C	-2.38	97.78	101.34
8	T	101	BCL	C2A-C3A-C4A	-2.38	98.03	101.87
8	P	101	BCL	C2A-C3A-C4A	-2.38	98.03	101.87
8	8	102	BCL	CMD-C2D-C1D	2.38	128.91	124.71
8	U	102	BCL	CMD-C2D-C1D	2.38	128.91	124.71
8	T	101	BCL	CED-O2D-CGD	-2.38	110.56	115.94
8	3	101	BCL	C2A-C3A-C4A	-2.38	98.03	101.87
9	9	101	KGD	CBG-CBI-CBL	-2.38	123.92	127.31
8	K	102	BCL	C2C-C3C-C4C	-2.38	97.78	101.34
8	A	101	BCL	C2A-C3A-C4A	-2.37	98.03	101.87
8	2	102	BCL	CMD-C2D-C1D	2.37	128.90	124.71
8	5	101	BCL	CED-O2D-CGD	-2.37	110.57	115.94
8	V	101	BCL	CHC-C1C-NC	2.37	127.79	124.51
8	F	101	BCL	CED-O2D-CGD	-2.37	110.58	115.94
8	2	101	BCL	C11-C10-C8	-2.37	108.26	115.92
8	4	102	BCL	C2C-C3C-C4C	-2.37	97.79	101.34
8	Q	102	BCL	C2C-C3C-C4C	-2.37	97.79	101.34
8	6	102	BCL	CMD-C2D-C1D	2.37	128.89	124.71
8	2	102	BCL	C2C-C3C-C4C	-2.37	97.79	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	101	BCL	C2A-C3A-C4A	-2.37	98.04	101.87
8	0	101	BCL	C2C-C3C-C4C	-2.37	97.79	101.34
8	O	102	BCL	C2C-C3C-C4C	-2.37	97.80	101.34
8	S	102	BCL	C2C-C3C-C4C	-2.37	97.80	101.34
8	7	101	BCL	C2A-C3A-C4A	-2.37	98.05	101.87
8	9	102	BCL	C4D-CHA-C1A	2.36	124.13	121.25
8	W	102	BCL	C4A-NA-C1A	-2.36	105.64	106.71
8	W	102	BCL	C2C-C3C-C4C	-2.36	97.80	101.34
8	T	101	BCL	C4D-CHA-C1A	2.36	124.12	121.25
8	P	101	BCL	CED-O2D-CGD	-2.36	110.59	115.94
8	S	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	W	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	K	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	O	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
8	M	1001	BCL	CMA-C3A-C4A	-2.36	105.44	111.77
8	I	102	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	G	102	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	6	102	BCL	C2C-C3C-C4C	-2.35	97.82	101.34
8	0	101	BCL	C4A-NA-C1A	-2.35	105.65	106.71
8	R	101	BCL	C4D-CHA-C1A	2.35	124.11	121.25
8	0	101	BCL	CMD-C2D-C1D	2.35	128.85	124.71
8	D	101	BCL	C4D-CHA-C1A	2.35	124.10	121.25
8	1	101	BCL	C4D-CHA-C1A	2.35	124.10	121.25
8	E	102	BCL	CMD-C2D-C1D	2.34	128.84	124.71
9	J	102	KGD	OAA-CAI-CAH	2.34	123.04	120.96
8	3	101	BCL	C4D-CHA-C1A	2.34	124.10	121.25
8	I	102	BCL	C2C-C3C-C4C	-2.34	97.83	101.34
14	C	503	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
8	B	102	BCL	C2C-C3C-C4C	-2.34	97.84	101.34
9	9	101	KGD	CAZ-CAW-CAS	2.33	119.20	115.27
8	B	102	BCL	CMD-C2D-C1D	2.33	128.83	124.71
9	J	102	KGD	CBG-CBB-CAV	-2.33	118.70	123.47
8	5	101	BCL	C4D-CHA-C1A	2.33	124.09	121.25
8	2	102	BCL	C4A-NA-C1A	-2.33	105.66	106.71
8	M	1005	BCL	CMD-C2D-C1D	2.33	128.82	124.71
11	M	1002	MQE	CAJ-CAD-CAQ	-2.33	105.33	112.98
8	J	101	BCL	C4D-CHA-C1A	2.32	124.08	121.25
9	N	102	KGD	CAZ-CAW-CAS	2.32	119.18	115.27
9	D	102	KGD	CBK-CBH-CBF	2.32	121.73	118.08
8	G	102	BCL	C2C-C3C-C4C	-2.32	97.87	101.34
14	C	504	HEM	CHA-C4D-ND	2.31	127.23	124.38
11	M	1002	MQE	CAY-CAX-CBQ	-2.31	116.03	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	BCL	C4D-CHA-C1A	2.30	124.05	121.25
8	L	401	BCL	CHC-C1C-NC	2.30	127.69	124.51
8	4	102	BCL	CMD-C2D-C1D	2.29	128.76	124.71
8	Q	102	BCL	CMD-C2D-C1D	2.29	128.76	124.71
8	P	101	BCL	C4D-CHA-C1A	2.29	124.03	121.25
8	M	1001	BCL	C12-C11-C10	-2.29	102.74	113.24
8	T	101	BCL	C4-C3-C2	-2.29	117.82	123.68
8	A	101	BCL	C4D-CHA-C1A	2.28	124.03	121.25
8	6	102	BCL	C4A-NA-C1A	-2.28	105.68	106.71
13	M	1006	PGV	P-O12-C04	-2.28	108.32	121.68
10	L	404	BPH	CMC-C2C-C1C	-2.28	109.39	114.38
11	M	1002	MQE	CAS-CAN-CBB	-2.27	105.49	112.98
8	Q	102	BCL	C11-C10-C8	-2.27	108.57	115.92
9	J	102	KGD	CAZ-CAW-CAS	2.27	119.10	115.27
8	K	102	BCL	C11-C10-C8	-2.27	108.59	115.92
8	I	102	BCL	C11-C10-C8	-2.27	108.60	115.92
8	0	101	BCL	CHC-C1C-NC	2.26	127.64	124.51
8	S	102	BCL	C11-C10-C8	-2.26	108.60	115.92
11	L	403	MQE	CCA-CBB-CAN	2.26	119.08	115.27
8	6	102	BCL	C11-C10-C8	-2.26	108.61	115.92
13	M	1006	PGV	P-O11-C03	-2.26	108.43	121.68
8	O	102	BCL	C11-C10-C8	-2.26	108.62	115.92
9	I	103	KGD	CAT-CAS-CAW	-2.25	105.56	112.98
10	L	404	BPH	CMA-C3A-C4A	-2.25	109.44	114.38
8	G	102	BCL	C11-C10-C8	-2.25	108.64	115.92
8	W	102	BCL	C11-C10-C8	-2.25	108.64	115.92
11	M	1002	MQE	CBA-CBN-CBM	-2.25	122.24	127.66
8	B	102	BCL	C11-C10-C8	-2.25	108.65	115.92
8	2	101	BCL	CMD-C2D-C1D	2.25	128.67	124.71
14	C	503	HEM	CHA-C4D-ND	2.25	127.16	124.38
14	C	501	HEM	C4B-CHC-C1C	-2.25	119.59	122.56
8	0	101	BCL	C11-C10-C8	-2.25	108.66	115.92
8	E	102	BCL	C11-C10-C8	-2.24	108.66	115.92
8	U	102	BCL	C11-C10-C8	-2.24	108.67	115.92
8	8	102	BCL	C11-C10-C8	-2.24	108.67	115.92
8	4	102	BCL	C11-C10-C8	-2.24	108.67	115.92
10	L	404	BPH	C11-C12-C13	-2.24	108.68	115.92
9	I	103	KGD	OAA-CAI-CAH	2.24	122.94	120.96
8	Q	101	BCL	C4D-CHA-C1A	2.24	123.97	121.25
8	2	102	BCL	C11-C10-C8	-2.23	108.70	115.92
8	V	101	BCL	CGD-CBD-CAD	-2.23	103.50	110.73
8	4	101	BCL	C4D-CHA-C1A	2.23	123.97	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	101	BCL	C4D-CHA-C1A	2.23	123.97	121.25
8	W	101	BCL	CMD-C2D-C1D	2.23	128.65	124.71
9	N	102	KGD	CAC-CAB-CAD	-2.23	107.05	110.48
8	S	101	BCL	C4D-CHA-C1A	2.23	123.96	121.25
8	R	101	BCL	C2C-C3C-C4C	-2.22	98.01	101.34
8	V	101	BCL	CHB-C4A-NA	-2.22	121.44	124.51
14	C	502	HEM	CHC-C4B-C3B	-2.22	121.17	124.57
10	L	402	BPH	C16-C15-C13	-2.22	108.75	115.92
8	4	102	BCL	CHC-C1C-NC	2.22	127.58	124.51
8	8	101	BCL	C4D-CHA-C1A	2.22	123.94	121.25
9	J	102	KGD	CAL-CAM-CAO	2.21	122.34	118.94
8	0	102	BCL	C4D-CHA-C1A	2.21	123.94	121.25
8	U	101	BCL	C4D-CHA-C1A	2.21	123.94	121.25
8	2	101	BCL	C1-O2A-CGA	2.21	122.24	116.44
8	6	101	BCL	C4D-CHA-C1A	2.21	123.94	121.25
8	L	401	BCL	C3C-C2C-C1C	2.20	105.42	101.87
8	N	101	BCL	C2C-C3C-C4C	-2.19	98.05	101.34
8	I	102	BCL	CHC-C1C-NC	2.19	127.55	124.51
8	G	101	BCL	C4D-CHA-C1A	2.19	123.92	121.25
8	E	102	BCL	CHC-C1C-NC	2.19	127.55	124.51
8	U	102	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	D	101	BCL	C2C-C3C-C4C	-2.19	98.06	101.34
11	M	1003	MQE	CCE-CBK-CAX	-2.19	120.83	124.40
8	E	101	BCL	C4D-CHA-C1A	2.19	123.92	121.25
8	3	101	BCL	C2C-C3C-C4C	-2.19	98.06	101.34
8	S	102	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	T	101	BCL	CHC-C1C-NC	2.19	127.53	124.51
8	B	102	BCL	CHC-C1C-NC	2.18	127.53	124.51
8	B	101	BCL	C4D-CHA-C1A	2.18	123.90	121.25
8	2	102	BCL	CHC-C1C-NC	2.18	127.53	124.51
8	J	101	BCL	C2C-C3C-C4C	-2.18	98.08	101.34
8	8	102	BCL	CHC-C1C-NC	2.18	127.52	124.51
8	5	101	BCL	C2C-C3C-C4C	-2.18	98.08	101.34
8	G	102	BCL	CHC-C1C-NC	2.18	127.52	124.51
8	1	101	BCL	C2C-C3C-C4C	-2.18	98.08	101.34
8	9	102	BCL	C2C-C3C-C4C	-2.18	98.08	101.34
8	H	101	BCL	C1B-CHB-C4A	-2.18	125.81	130.12
8	F	101	BCL	C2C-C3C-C4C	-2.17	98.08	101.34
8	K	101	BCL	C4D-CHA-C1A	2.17	123.89	121.25
8	A	101	BCL	C2C-C3C-C4C	-2.17	98.09	101.34
8	O	101	BCL	C4D-CHA-C1A	2.17	123.89	121.25
8	F	101	BCL	CHC-C1C-NC	2.17	127.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	102	BCL	CHC-C1C-NC	2.17	127.51	124.51
8	2	101	BCL	O2A-C1-C2	2.17	114.33	108.64
8	Q	101	BCL	C2A-C1A-CHA	2.17	127.65	123.86
8	T	101	BCL	C2C-C3C-C4C	-2.17	98.10	101.34
8	T	101	BCL	C1B-CHB-C4A	-2.17	125.83	130.12
8	H	101	BCL	C2C-C3C-C4C	-2.16	98.10	101.34
8	3	101	BCL	C1B-CHB-C4A	-2.16	125.83	130.12
8	6	102	BCL	CHC-C1C-NC	2.16	127.50	124.51
8	Q	102	BCL	CHC-C1C-NC	2.16	127.50	124.51
10	L	405	BPH	CMC-C2C-C1C	-2.16	109.66	114.38
8	7	101	BCL	C2C-C3C-C4C	-2.16	98.11	101.34
8	9	102	BCL	C1B-CHB-C4A	-2.15	125.85	130.12
8	P	101	BCL	C1B-CHB-C4A	-2.15	125.85	130.12
8	2	101	BCL	C12-C11-C10	-2.15	103.34	113.24
8	4	101	BCL	C2A-C1A-CHA	2.15	127.62	123.86
10	L	402	BPH	CAA-CBA-CGA	-2.15	106.97	113.25
8	M	1001	BCL	CHC-C1C-NC	2.15	127.49	124.51
8	K	101	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	8	101	BCL	C2A-C1A-CHA	2.15	127.62	123.86
14	C	501	HEM	CBB-CAB-C3B	-2.15	116.93	127.62
8	P	101	BCL	C2C-C3C-C4C	-2.15	98.12	101.34
8	7	101	BCL	C1B-CHB-C4A	-2.15	125.86	130.12
8	R	101	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	W	102	BCL	CHC-C1C-NC	2.15	127.48	124.51
10	L	402	BPH	C4C-C3C-C2C	-2.15	100.80	102.84
8	1	101	BCL	C1B-CHB-C4A	-2.15	125.87	130.12
8	A	101	BCL	C1B-CHB-C4A	-2.15	125.87	130.12
8	O	102	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	7	101	BCL	CHC-C1C-NC	2.14	127.47	124.51
8	D	101	BCL	C1B-CHB-C4A	-2.14	125.88	130.12
8	U	101	BCL	C2A-C1A-CHA	2.14	127.60	123.86
8	5	101	BCL	C1B-CHB-C4A	-2.14	125.88	130.12
8	F	101	BCL	C1B-CHB-C4A	-2.14	125.88	130.12
8	D	101	BCL	CHC-C1C-NC	2.14	127.47	124.51
8	U	102	BCL	C11-C12-C13	-2.14	109.01	115.92
8	R	101	BCL	C1B-CHB-C4A	-2.14	125.89	130.12
8	E	102	BCL	C11-C12-C13	-2.13	109.02	115.92
8	J	101	BCL	CHC-C1C-NC	2.13	127.46	124.51
8	2	102	BCL	C11-C12-C13	-2.13	109.03	115.92
8	I	101	BCL	C2A-C1A-CHA	2.13	127.59	123.86
9	J	102	KGD	CBJ-CBM-CBN	-2.13	116.56	123.22
8	K	101	BCL	C2A-C1A-CHA	2.13	127.59	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	102	BCL	C11-C12-C13	-2.13	109.03	115.92
8	W	102	BCL	C11-C12-C13	-2.13	109.04	115.92
8	Q	101	BCL	CHC-C1C-NC	2.13	127.45	124.51
8	Q	102	BCL	C11-C12-C13	-2.13	109.05	115.92
8	B	101	BCL	CHC-C1C-NC	2.13	127.45	124.51
8	B	102	BCL	C11-C12-C13	-2.13	109.05	115.92
8	I	102	BCL	C11-C12-C13	-2.13	109.05	115.92
8	E	101	BCL	CHC-C1C-NC	2.12	127.45	124.51
8	M	1001	BCL	C4A-NA-C1A	-2.12	105.75	106.71
8	0	102	BCL	CHC-C1C-NC	2.12	127.45	124.51
8	D	101	BCL	C12-C11-C10	-2.12	103.48	113.24
8	8	102	BCL	C11-C12-C13	-2.12	109.06	115.92
8	H	101	BCL	C12-C11-C10	-2.12	103.48	113.24
9	I	103	KGD	CBN-CBL-CBI	2.12	122.20	118.94
8	U	101	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	R	101	BCL	C12-C11-C10	-2.12	103.50	113.24
8	B	101	BCL	C2A-C1A-CHA	2.12	127.57	123.86
8	N	101	BCL	C1B-CHB-C4A	-2.12	125.92	130.12
8	A	101	BCL	C12-C11-C10	-2.12	103.50	113.24
8	3	101	BCL	C12-C11-C10	-2.12	103.50	113.24
8	5	101	BCL	C12-C11-C10	-2.12	103.50	113.24
8	S	102	BCL	C11-C12-C13	-2.12	109.07	115.92
8	J	101	BCL	C12-C11-C10	-2.12	103.51	113.24
8	O	102	BCL	C11-C12-C13	-2.12	109.07	115.92
8	F	101	BCL	C12-C11-C10	-2.12	103.51	113.24
8	P	101	BCL	C12-C11-C10	-2.12	103.51	113.24
8	6	102	BCL	C11-C12-C13	-2.12	109.08	115.92
8	K	102	BCL	C11-C12-C13	-2.12	109.08	115.92
8	J	101	BCL	C1B-CHB-C4A	-2.11	125.93	130.12
8	6	101	BCL	C2A-C1A-CHA	2.11	127.56	123.86
8	G	102	BCL	C11-C12-C13	-2.11	109.09	115.92
8	0	101	BCL	C11-C12-C13	-2.11	109.09	115.92
8	T	101	BCL	C12-C11-C10	-2.11	103.53	113.24
8	4	101	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	6	101	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	S	101	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	9	102	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	I	101	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	S	101	BCL	CHC-C1C-NC	2.11	127.43	124.51
8	N	101	BCL	C12-C11-C10	-2.11	103.56	113.24
8	O	101	BCL	CHC-C1C-NC	2.11	127.42	124.51
8	0	102	BCL	C2A-C1A-CHA	2.11	127.54	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	BCL	C2A-C1A-CHA	2.11	127.54	123.86
9	D	102	KGD	CAT-CAS-CAW	-2.11	106.05	112.98
8	V	101	BCL	C3C-C2C-C1C	2.10	105.27	101.87
8	1	101	BCL	C12-C11-C10	-2.10	103.57	113.24
8	7	101	BCL	C12-C11-C10	-2.10	103.57	113.24
8	W	101	BCL	C12-C11-C10	-2.10	103.58	113.24
8	3	101	BCL	CHC-C1C-NC	2.10	127.42	124.51
8	E	101	BCL	C2A-C1A-CHA	2.10	127.53	123.86
11	L	403	MQE	CBY-CAW-CAG	2.10	118.80	115.27
8	9	102	BCL	C12-C11-C10	-2.10	103.59	113.24
14	C	504	HEM	CBB-CAB-C3B	-2.10	117.18	127.62
8	B	102	BCL	CGD-CBD-CAD	-2.10	103.94	110.73
8	O	101	BCL	C2A-C1A-CHA	2.09	127.51	123.86
8	E	101	BCL	C12-C11-C10	-2.09	103.64	113.24
10	L	404	BPH	C16-C15-C13	-2.09	109.17	115.92
8	R	101	BCL	C1-C2-C3	-2.09	122.43	126.04
8	H	101	BCL	CHC-C1C-NC	2.09	127.40	124.51
8	2	102	BCL	CGD-CBD-CAD	-2.09	103.98	110.73
14	C	504	HEM	C4B-C3B-C2B	-2.09	105.46	107.11
9	9	101	KGD	CBM-CBN-CBL	-2.08	120.56	126.42
8	8	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
8	I	101	BCL	C12-C11-C10	-2.08	103.67	113.24
8	6	101	BCL	C12-C11-C10	-2.08	103.68	113.24
8	E	102	BCL	CGD-CBD-CAD	-2.08	104.00	110.73
8	K	102	BCL	CGD-CBD-CAD	-2.08	104.00	110.73
8	N	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
8	S	102	BCL	CGD-CBD-CAD	-2.08	104.00	110.73
8	A	101	BCL	CAA-CBA-CGA	-2.08	107.18	113.25
8	B	101	BCL	C12-C11-C10	-2.08	103.69	113.24
8	J	101	BCL	C1-C2-C3	-2.08	122.45	126.04
8	Q	101	BCL	C12-C11-C10	-2.08	103.69	113.24
8	5	101	BCL	CAA-CBA-CGA	-2.08	107.18	113.25
8	3	101	BCL	C1-C2-C3	-2.08	122.45	126.04
8	Q	102	BCL	CGD-CBD-CAD	-2.08	104.01	110.73
8	O	101	BCL	C12-C11-C10	-2.08	103.70	113.24
8	H	101	BCL	CAA-CBA-CGA	-2.08	107.19	113.25
8	0	101	BCL	CGD-CBD-CAD	-2.08	104.01	110.73
8	D	101	BCL	CAA-CBA-CGA	-2.07	107.19	113.25
8	R	101	BCL	CAA-CBA-CGA	-2.07	107.19	113.25
8	8	102	BCL	CGD-CBD-CAD	-2.07	104.02	110.73
8	U	102	BCL	CGD-CBD-CAD	-2.07	104.02	110.73
8	S	101	BCL	C12-C11-C10	-2.07	103.71	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	CHC-C1C-NC	2.07	127.38	124.51
8	G	101	BCL	CHC-C1C-NC	2.07	127.38	124.51
8	4	101	BCL	C12-C11-C10	-2.07	103.72	113.24
8	6	102	BCL	CGD-CBD-CAD	-2.07	104.03	110.73
8	M	1001	BCL	CGD-CBD-CAD	-2.07	104.03	110.73
8	W	102	BCL	CGD-CBD-CAD	-2.07	104.03	110.73
8	K	101	BCL	C12-C11-C10	-2.07	103.73	113.24
8	I	102	BCL	CGD-CBD-CAD	-2.07	104.03	110.73
8	V	101	BCL	C12-C11-C10	-2.07	103.74	113.24
8	L	401	BCL	C1-O2A-CGA	2.07	121.87	116.44
8	8	101	BCL	C12-C11-C10	-2.07	103.74	113.24
11	M	1002	MQE	CBZ-CAZ-CAU	2.07	118.75	115.27
8	G	102	BCL	CGD-CBD-CAD	-2.07	104.04	110.73
8	5	101	BCL	C1-C2-C3	-2.07	122.47	126.04
8	G	101	BCL	C12-C11-C10	-2.07	103.75	113.24
8	U	101	BCL	C12-C11-C10	-2.06	103.75	113.24
8	4	102	BCL	CGD-CBD-CAD	-2.06	104.05	110.73
8	P	101	BCL	CAA-CBA-CGA	-2.06	107.22	113.25
8	7	101	BCL	CAA-CBA-CGA	-2.06	107.23	113.25
13	M	1008	PGV	P-O12-C04	-2.06	109.59	121.68
8	J	101	BCL	CAA-CBA-CGA	-2.06	107.23	113.25
8	7	101	BCL	C1-C2-C3	-2.06	122.48	126.04
8	O	102	BCL	CGD-CBD-CAD	-2.06	104.07	110.73
8	0	102	BCL	C12-C11-C10	-2.06	103.78	113.24
8	1	101	BCL	CHC-C1C-NC	2.06	127.36	124.51
8	D	101	BCL	C1-C2-C3	-2.06	122.49	126.04
8	3	101	BCL	CAA-CBA-CGA	-2.06	107.24	113.25
8	A	101	BCL	CHC-C1C-NC	2.06	127.36	124.51
8	T	101	BCL	CAA-CBA-CGA	-2.06	107.25	113.25
8	M	1005	BCL	C2A-C1A-CHA	2.05	127.45	123.86
8	N	101	BCL	C1-C2-C3	-2.05	122.49	126.04
8	F	101	BCL	CAA-CBA-CGA	-2.05	107.25	113.25
8	9	102	BCL	CAA-CBA-CGA	-2.05	107.26	113.25
8	1	101	BCL	CAA-CBA-CGA	-2.05	107.26	113.25
9	I	103	KGD	CAU-CAR-CAV	2.05	125.80	122.92
8	M	1005	BCL	C12-C11-C10	-2.05	103.84	113.24
8	1	101	BCL	C1-C2-C3	-2.05	122.51	126.04
8	N	101	BCL	CAA-CBA-CGA	-2.04	107.28	113.25
8	5	101	BCL	CHC-C1C-NC	2.04	127.33	124.51
8	W	101	BCL	C4-C3-C2	-2.04	118.45	123.68
8	9	102	BCL	C1-C2-C3	-2.04	122.52	126.04
10	L	402	BPH	C6-C7-C8	-2.04	109.34	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	C1-C2-C3	-2.04	122.52	126.04
8	T	101	BCL	C1-C2-C3	-2.03	122.53	126.04
10	L	404	BPH	C6-C7-C8	-2.03	109.35	115.92
8	F	101	BCL	C1-C2-C3	-2.03	122.54	126.04
8	M	1005	BCL	CED-O2D-CGD	-2.02	111.36	115.94
8	H	101	BCL	C1-C2-C3	-2.02	122.54	126.04
8	S	102	BCL	CED-O2D-CGD	-2.02	111.36	115.94
14	C	503	HEM	C3D-C4D-ND	-2.02	107.91	110.17
8	A	101	BCL	C1-C2-C3	-2.02	122.54	126.04
9	D	102	KGD	CBM-CBJ-CBH	2.02	130.19	127.31
8	B	102	BCL	CED-O2D-CGD	-2.02	111.38	115.94
8	E	102	BCL	CED-O2D-CGD	-2.01	111.38	115.94
8	2	101	BCL	C11-C12-C13	-2.01	109.42	115.92
8	2	101	BCL	CHD-C4C-NC	-2.01	122.84	125.08
9	D	102	KGD	CBK-CBH-CBJ	2.01	125.74	122.92
8	8	102	BCL	CED-O2D-CGD	-2.01	111.39	115.94
8	G	102	BCL	CED-O2D-CGD	-2.01	111.40	115.94
8	W	102	BCL	CED-O2D-CGD	-2.01	111.40	115.94
8	I	102	BCL	CED-O2D-CGD	-2.01	111.40	115.94
8	0	101	BCL	CED-O2D-CGD	-2.01	111.40	115.94
9	9	101	KGD	CAE-CAC-CAB	-2.00	109.97	113.18
8	K	102	BCL	CED-O2D-CGD	-2.00	111.41	115.94

There are no chirality outliers.

All (1038) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	0	101	BCL	CHA-CBD-CGD-O1D
8	0	101	BCL	C1-C2-C3-C5
8	0	102	BCL	C1A-C2A-CAA-CBA
8	0	102	BCL	C3A-C2A-CAA-CBA
8	0	102	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	C2-C3-C5-C6
8	1	101	BCL	C1-C2-C3-C5
8	2	101	BCL	C2C-C3C-CAC-CBC
8	2	101	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	C1-C2-C3-C4
8	2	101	BCL	C1-C2-C3-C5
8	2	102	BCL	CHA-CBD-CGD-O1D
8	2	102	BCL	C1-C2-C3-C5
8	3	101	BCL	C1-C2-C3-C5
8	4	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	4	101	BCL	C3A-C2A-CAA-CBA
8	4	101	BCL	C4C-C3C-CAC-CBC
8	4	101	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	C2-C3-C5-C6
8	4	102	BCL	CHA-CBD-CGD-O1D
8	4	102	BCL	C1-C2-C3-C5
8	5	101	BCL	C1-C2-C3-C5
8	6	101	BCL	C1A-C2A-CAA-CBA
8	6	101	BCL	C3A-C2A-CAA-CBA
8	6	101	BCL	C4C-C3C-CAC-CBC
8	6	101	BCL	CBD-CGD-O2D-CED
8	6	101	BCL	C2-C3-C5-C6
8	6	102	BCL	CHA-CBD-CGD-O1D
8	6	102	BCL	C1-C2-C3-C5
8	7	101	BCL	C1-C2-C3-C5
8	8	101	BCL	C1A-C2A-CAA-CBA
8	8	101	BCL	C3A-C2A-CAA-CBA
8	8	101	BCL	C4C-C3C-CAC-CBC
8	8	101	BCL	C2-C3-C5-C6
8	8	102	BCL	CHA-CBD-CGD-O1D
8	8	102	BCL	C1-C2-C3-C5
8	9	102	BCL	C1-C2-C3-C5
8	A	101	BCL	C1-C2-C3-C5
8	B	101	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C4C-C3C-CAC-CBC
8	B	101	BCL	CBD-CGD-O2D-CED
8	B	101	BCL	C2-C3-C5-C6
8	B	102	BCL	CHA-CBD-CGD-O1D
8	B	102	BCL	C1-C2-C3-C5
8	D	101	BCL	C1-C2-C3-C5
8	E	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C3A-C2A-CAA-CBA
8	E	101	BCL	C4C-C3C-CAC-CBC
8	E	101	BCL	C2-C3-C5-C6
8	E	102	BCL	CHA-CBD-CGD-O1D
8	E	102	BCL	C1-C2-C3-C5
8	F	101	BCL	C1-C2-C3-C5
8	G	101	BCL	C1A-C2A-CAA-CBA
8	G	101	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C4C-C3C-CAC-CBC
8	G	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	G	101	BCL	C2-C3-C5-C6
8	G	102	BCL	CHA-CBD-CGD-O1D
8	G	102	BCL	C1-C2-C3-C5
8	H	101	BCL	C1-C2-C3-C5
8	I	101	BCL	C1A-C2A-CAA-CBA
8	I	101	BCL	C3A-C2A-CAA-CBA
8	I	101	BCL	C4C-C3C-CAC-CBC
8	I	101	BCL	CBD-CGD-O2D-CED
8	I	101	BCL	C2-C3-C5-C6
8	I	102	BCL	CHA-CBD-CGD-O1D
8	I	102	BCL	C1-C2-C3-C5
8	J	101	BCL	C1-C2-C3-C5
8	K	101	BCL	C1A-C2A-CAA-CBA
8	K	101	BCL	C3A-C2A-CAA-CBA
8	K	101	BCL	C4C-C3C-CAC-CBC
8	K	101	BCL	CBD-CGD-O2D-CED
8	K	101	BCL	C2-C3-C5-C6
8	K	102	BCL	CHA-CBD-CGD-O1D
8	K	102	BCL	C1-C2-C3-C5
8	L	401	BCL	C1A-C2A-CAA-CBA
8	L	401	BCL	CBD-CGD-O2D-CED
8	L	401	BCL	C1-C2-C3-C4
8	M	1001	BCL	C1A-C2A-CAA-CBA
8	M	1001	BCL	C3A-C2A-CAA-CBA
8	M	1001	BCL	C2A-CAA-CBA-CGA
8	M	1001	BCL	C4C-C3C-CAC-CBC
8	M	1001	BCL	C1-C2-C3-C5
8	M	1005	BCL	CHA-CBD-CGD-O2D
8	N	101	BCL	C1-C2-C3-C5
8	O	101	BCL	C1A-C2A-CAA-CBA
8	O	101	BCL	C3A-C2A-CAA-CBA
8	O	101	BCL	C4C-C3C-CAC-CBC
8	O	101	BCL	C2-C3-C5-C6
8	O	102	BCL	CHA-CBD-CGD-O1D
8	O	102	BCL	C1-C2-C3-C5
8	P	101	BCL	C1-C2-C3-C5
8	Q	101	BCL	C1A-C2A-CAA-CBA
8	Q	101	BCL	C3A-C2A-CAA-CBA
8	Q	101	BCL	C4C-C3C-CAC-CBC
8	Q	101	BCL	CBD-CGD-O2D-CED
8	Q	101	BCL	C2-C3-C5-C6
8	Q	102	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	Q	102	BCL	C1-C2-C3-C5
8	R	101	BCL	C1-C2-C3-C5
8	S	101	BCL	C1A-C2A-CAA-CBA
8	S	101	BCL	C3A-C2A-CAA-CBA
8	S	101	BCL	C4C-C3C-CAC-CBC
8	S	101	BCL	CBD-CGD-O2D-CED
8	S	101	BCL	C2-C3-C5-C6
8	S	102	BCL	CHA-CBD-CGD-O1D
8	S	102	BCL	C1-C2-C3-C5
8	T	101	BCL	C1-C2-C3-C5
8	U	101	BCL	C1A-C2A-CAA-CBA
8	U	101	BCL	C3A-C2A-CAA-CBA
8	U	101	BCL	C4C-C3C-CAC-CBC
8	U	101	BCL	C2-C3-C5-C6
8	U	102	BCL	CHA-CBD-CGD-O1D
8	U	102	BCL	C1-C2-C3-C5
8	V	101	BCL	O1A-CGA-O2A-C1
8	V	101	BCL	C2C-C3C-CAC-CBC
8	V	101	BCL	C1-C2-C3-C5
8	W	101	BCL	C3A-C2A-CAA-CBA
8	W	101	BCL	C2A-CAA-CBA-CGA
8	W	101	BCL	C2C-C3C-CAC-CBC
8	W	101	BCL	C4C-C3C-CAC-CBC
8	W	101	BCL	CBD-CGD-O2D-CED
8	W	102	BCL	CHA-CBD-CGD-O1D
8	W	102	BCL	C1-C2-C3-C5
9	9	101	KGD	CAB-CAD-CAJ-CAL
9	9	101	KGD	CAH-CAD-CAJ-CAL
9	9	101	KGD	CBB-CBG-CBI-CBL
9	D	102	KGD	CBE-CBF-CBH-CBJ
9	D	102	KGD	CBE-CBF-CBH-CBK
9	D	102	KGD	CBH-CBJ-CBM-CBN
9	D	102	KGD	CBI-CBL-CBN-CBM
9	D	102	KGD	CBO-CBL-CBN-CBM
9	I	103	KGD	CBE-CBF-CBH-CBJ
9	I	103	KGD	CBE-CBF-CBH-CBK
9	I	103	KGD	CBI-CBL-CBN-CBM
9	I	103	KGD	CBO-CBL-CBN-CBM
9	J	102	KGD	CAW-CAS-CAT-CAX
9	N	102	KGD	CAB-CAD-CAJ-CAL
9	N	102	KGD	CAH-CAD-CAJ-CAL
9	N	102	KGD	CAJ-CAL-CAM-CAN

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Mol	Chain	Res	Type	Atoms
9	N	102	KGD	CAJ-CAL-CAM-CAO
9	N	102	KGD	CAP-CAQ-CAR-CAU
9	N	102	KGD	CAP-CAQ-CAR-CAV
10	L	402	BPH	C3A-C2A-CAA-CBA
10	L	402	BPH	C2A-CAA-CBA-CGA
10	L	404	BPH	C4C-C3C-CAC-CBC
10	L	405	BPH	C4C-C3C-CAC-CBC
10	L	405	BPH	C2C-C3C-CAC-CBC
11	L	403	MQE	CAS-CAN-CBB-CCA
11	L	403	MQE	CBM-CBJ-CBO-CCB
11	M	1002	MQE	CAR-CAE-CAL-CBF
11	M	1002	MQE	CAT-CAF-CAK-CBE
11	M	1002	MQE	CAM-CAG-CAW-CBY
11	M	1002	MQE	CAV-CAH-CAO-CBI
11	M	1003	MQE	CAX-CAY-CBL-CBB
13	M	1006	PGV	C2-C1-O01-C02
14	C	501	HEM	C2B-C3B-CAB-CBB
14	C	501	HEM	C4B-C3B-CAB-CBB
14	C	503	HEM	C2B-C3B-CAB-CBB
14	C	503	HEM	C4B-C3B-CAB-CBB
14	C	504	HEM	C2B-C3B-CAB-CBB
8	W	101	BCL	O1D-CGD-O2D-CED
8	0	102	BCL	CBD-CGD-O2D-CED
8	8	101	BCL	CBD-CGD-O2D-CED
8	E	101	BCL	CBD-CGD-O2D-CED
8	O	101	BCL	CBD-CGD-O2D-CED
8	U	101	BCL	CBD-CGD-O2D-CED
8	V	101	BCL	CBD-CGD-O2D-CED
8	L	401	BCL	O1A-CGA-O2A-C1
8	M	1005	BCL	O1D-CGD-O2D-CED
8	0	101	BCL	O1D-CGD-O2D-CED
8	2	102	BCL	O1D-CGD-O2D-CED
8	4	102	BCL	O1D-CGD-O2D-CED
8	5	101	BCL	O1D-CGD-O2D-CED
8	6	102	BCL	O1D-CGD-O2D-CED
8	8	102	BCL	O1D-CGD-O2D-CED
8	B	102	BCL	O1D-CGD-O2D-CED
8	E	101	BCL	O1D-CGD-O2D-CED
8	E	102	BCL	O1D-CGD-O2D-CED
8	G	102	BCL	O1D-CGD-O2D-CED
8	I	102	BCL	O1D-CGD-O2D-CED
8	K	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	O	102	BCL	O1D-CGD-O2D-CED
8	P	101	BCL	O1D-CGD-O2D-CED
8	Q	102	BCL	O1D-CGD-O2D-CED
8	S	102	BCL	O1D-CGD-O2D-CED
8	U	102	BCL	O1D-CGD-O2D-CED
8	V	101	BCL	O1D-CGD-O2D-CED
8	W	102	BCL	O1D-CGD-O2D-CED
8	0	101	BCL	CBD-CGD-O2D-CED
8	1	101	BCL	CBD-CGD-O2D-CED
8	2	101	BCL	CBD-CGD-O2D-CED
8	2	102	BCL	CBD-CGD-O2D-CED
8	3	101	BCL	CBD-CGD-O2D-CED
8	4	102	BCL	CBD-CGD-O2D-CED
8	5	101	BCL	CBD-CGD-O2D-CED
8	6	102	BCL	CBD-CGD-O2D-CED
8	7	101	BCL	CBD-CGD-O2D-CED
8	8	102	BCL	CBD-CGD-O2D-CED
8	9	102	BCL	CBD-CGD-O2D-CED
8	A	101	BCL	CBD-CGD-O2D-CED
8	B	102	BCL	CBD-CGD-O2D-CED
8	D	101	BCL	CBD-CGD-O2D-CED
8	E	102	BCL	CBD-CGD-O2D-CED
8	F	101	BCL	CBD-CGD-O2D-CED
8	G	102	BCL	CBD-CGD-O2D-CED
8	H	101	BCL	CBD-CGD-O2D-CED
8	I	102	BCL	CBD-CGD-O2D-CED
8	J	101	BCL	CBD-CGD-O2D-CED
8	K	102	BCL	CBD-CGD-O2D-CED
8	N	101	BCL	CBD-CGD-O2D-CED
8	O	102	BCL	CBD-CGD-O2D-CED
8	P	101	BCL	CBD-CGD-O2D-CED
8	Q	102	BCL	CBD-CGD-O2D-CED
8	R	101	BCL	CBD-CGD-O2D-CED
8	S	102	BCL	CBD-CGD-O2D-CED
8	T	101	BCL	CBD-CGD-O2D-CED
8	U	102	BCL	CBD-CGD-O2D-CED
8	W	102	BCL	CBD-CGD-O2D-CED
8	0	101	BCL	O1A-CGA-O2A-C1
8	2	101	BCL	O1A-CGA-O2A-C1
8	2	102	BCL	O1A-CGA-O2A-C1
8	4	102	BCL	O1A-CGA-O2A-C1
8	6	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	8	102	BCL	O1A-CGA-O2A-C1
8	A	101	BCL	O1A-CGA-O2A-C1
8	B	102	BCL	O1A-CGA-O2A-C1
8	E	102	BCL	O1A-CGA-O2A-C1
8	G	102	BCL	O1A-CGA-O2A-C1
8	I	102	BCL	O1A-CGA-O2A-C1
8	K	102	BCL	O1A-CGA-O2A-C1
8	O	102	BCL	O1A-CGA-O2A-C1
8	Q	102	BCL	O1A-CGA-O2A-C1
8	S	102	BCL	O1A-CGA-O2A-C1
8	U	102	BCL	O1A-CGA-O2A-C1
8	W	102	BCL	O1A-CGA-O2A-C1
8	1	101	BCL	O1D-CGD-O2D-CED
8	3	101	BCL	O1D-CGD-O2D-CED
8	7	101	BCL	O1D-CGD-O2D-CED
8	9	102	BCL	O1D-CGD-O2D-CED
8	A	101	BCL	O1D-CGD-O2D-CED
8	D	101	BCL	O1D-CGD-O2D-CED
8	F	101	BCL	O1D-CGD-O2D-CED
8	H	101	BCL	O1D-CGD-O2D-CED
8	J	101	BCL	O1D-CGD-O2D-CED
8	N	101	BCL	O1D-CGD-O2D-CED
8	R	101	BCL	O1D-CGD-O2D-CED
8	T	101	BCL	O1D-CGD-O2D-CED
8	M	1001	BCL	O1D-CGD-O2D-CED
10	L	404	BPH	C3-C5-C6-C7
8	L	401	BCL	CBA-CGA-O2A-C1
8	V	101	BCL	CBA-CGA-O2A-C1
8	W	101	BCL	CBA-CGA-O2A-C1
10	L	404	BPH	CBA-CGA-O2A-C1
11	M	1002	MQE	CAO-CAH-CAV-CBX
11	M	1002	MQE	CCL-CCC-CCD-CCI
11	L	403	MQE	CAS-CAN-CBB-CBL
11	M	1002	MQE	CAO-CAH-CAV-CBF
8	2	101	BCL	C2A-CAA-CBA-CGA
8	L	401	BCL	C2A-CAA-CBA-CGA
8	0	101	BCL	C3-C5-C6-C7
8	2	102	BCL	C3-C5-C6-C7
8	4	102	BCL	C3-C5-C6-C7
8	6	102	BCL	C3-C5-C6-C7
8	8	102	BCL	C3-C5-C6-C7
8	B	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	E	102	BCL	C3-C5-C6-C7
8	G	102	BCL	C3-C5-C6-C7
8	I	102	BCL	C3-C5-C6-C7
8	K	102	BCL	C3-C5-C6-C7
8	O	102	BCL	C3-C5-C6-C7
8	Q	102	BCL	C3-C5-C6-C7
8	S	102	BCL	C3-C5-C6-C7
8	U	102	BCL	C3-C5-C6-C7
8	W	102	BCL	C3-C5-C6-C7
8	0	101	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	CBA-CGA-O2A-C1
8	2	102	BCL	CBA-CGA-O2A-C1
8	4	102	BCL	CBA-CGA-O2A-C1
8	6	102	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	CBA-CGA-O2A-C1
8	B	102	BCL	CBA-CGA-O2A-C1
8	E	102	BCL	CBA-CGA-O2A-C1
8	G	102	BCL	CBA-CGA-O2A-C1
8	I	102	BCL	CBA-CGA-O2A-C1
8	K	102	BCL	CBA-CGA-O2A-C1
8	O	102	BCL	CBA-CGA-O2A-C1
8	Q	102	BCL	CBA-CGA-O2A-C1
8	S	102	BCL	CBA-CGA-O2A-C1
8	U	102	BCL	CBA-CGA-O2A-C1
8	W	102	BCL	CBA-CGA-O2A-C1
8	L	401	BCL	O1D-CGD-O2D-CED
8	L	401	BCL	C1-C2-C3-C5
13	M	1006	PGV	O02-C1-O01-C02
8	0	102	BCL	O1A-CGA-O2A-C1
8	1	101	BCL	O1A-CGA-O2A-C1
8	3	101	BCL	O1A-CGA-O2A-C1
8	4	101	BCL	O1A-CGA-O2A-C1
8	5	101	BCL	O1A-CGA-O2A-C1
8	6	101	BCL	O1A-CGA-O2A-C1
8	7	101	BCL	O1A-CGA-O2A-C1
8	8	101	BCL	O1A-CGA-O2A-C1
8	9	102	BCL	O1A-CGA-O2A-C1
8	B	101	BCL	O1A-CGA-O2A-C1
8	D	101	BCL	O1A-CGA-O2A-C1
8	E	101	BCL	O1A-CGA-O2A-C1
8	F	101	BCL	O1A-CGA-O2A-C1
8	G	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	H	101	BCL	O1A-CGA-O2A-C1
8	I	101	BCL	O1A-CGA-O2A-C1
8	J	101	BCL	O1A-CGA-O2A-C1
8	K	101	BCL	O1A-CGA-O2A-C1
8	N	101	BCL	O1A-CGA-O2A-C1
8	O	101	BCL	O1A-CGA-O2A-C1
8	P	101	BCL	O1A-CGA-O2A-C1
8	Q	101	BCL	O1A-CGA-O2A-C1
8	R	101	BCL	O1A-CGA-O2A-C1
8	S	101	BCL	O1A-CGA-O2A-C1
8	T	101	BCL	O1A-CGA-O2A-C1
8	U	101	BCL	O1A-CGA-O2A-C1
8	W	101	BCL	O1A-CGA-O2A-C1
13	M	1007	PGV	O04-C19-O03-C01
9	9	101	KGD	CAR-CAV-CBB-CBG
8	M	1001	BCL	CBD-CGD-O2D-CED
8	M	1005	BCL	CBD-CGD-O2D-CED
10	L	405	BPH	CBD-CGD-O2D-CED
8	O	101	BCL	O1D-CGD-O2D-CED
8	U	101	BCL	O1D-CGD-O2D-CED
13	M	1008	PGV	O12-C04-C05-O05
10	L	405	BPH	C3-C5-C6-C7
13	M	1007	PGV	C20-C19-O03-C01
10	L	404	BPH	O1A-CGA-O2A-C1
8	2	101	BCL	C3-C5-C6-C7
9	9	101	KGD	CAT-CAS-CAW-CAZ
9	N	102	KGD	CAT-CAS-CAW-CAZ
11	L	403	MQE	CAM-CAG-CAW-CBY
11	L	403	MQE	CCL-CCC-CCD-CCI
11	M	1002	MQE	CBA-CAU-CAZ-CBZ
11	M	1002	MQE	CBO-CBJ-CBM-CCF
9	9	101	KGD	CAT-CAS-CAW-CBA
9	N	102	KGD	CAT-CAS-CAW-CBA
11	L	403	MQE	CAM-CAG-CAW-CBH
11	L	403	MQE	CCB-CCC-CCD-CCI
11	M	1002	MQE	CAM-CAG-CAW-CBH
11	M	1002	MQE	CBA-CAU-CAZ-CBI
11	M	1002	MQE	CBO-CBJ-CBM-CBN
8	8	101	BCL	O1D-CGD-O2D-CED
8	0	102	BCL	O1D-CGD-O2D-CED
9	I	103	KGD	CAW-CAS-CAT-CAX
11	L	403	MQE	CAP-CAC-CAI-CBD

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Mol	Chain	Res	Type	Atoms
11	L	403	MQE	CAQ-CAD-CAJ-CBC
11	L	403	MQE	CAZ-CAU-CBA-CBN
11	M	1002	MQE	CAW-CAG-CAM-CBG
11	M	1002	MQE	CAZ-CAU-CBA-CBN
11	M	1002	MQE	CCC-CCD-CCI-CCM
11	M	1003	MQE	CBB-CAN-CAS-CBH
8	0	102	BCL	CBA-CGA-O2A-C1
8	1	101	BCL	CBA-CGA-O2A-C1
8	3	101	BCL	CBA-CGA-O2A-C1
8	4	101	BCL	CBA-CGA-O2A-C1
8	5	101	BCL	CBA-CGA-O2A-C1
8	6	101	BCL	CBA-CGA-O2A-C1
8	7	101	BCL	CBA-CGA-O2A-C1
8	8	101	BCL	CBA-CGA-O2A-C1
8	9	102	BCL	CBA-CGA-O2A-C1
8	A	101	BCL	CBA-CGA-O2A-C1
8	B	101	BCL	CBA-CGA-O2A-C1
8	D	101	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	CBA-CGA-O2A-C1
8	F	101	BCL	CBA-CGA-O2A-C1
8	G	101	BCL	CBA-CGA-O2A-C1
8	H	101	BCL	CBA-CGA-O2A-C1
8	I	101	BCL	CBA-CGA-O2A-C1
8	J	101	BCL	CBA-CGA-O2A-C1
8	K	101	BCL	CBA-CGA-O2A-C1
8	N	101	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	CBA-CGA-O2A-C1
8	P	101	BCL	CBA-CGA-O2A-C1
8	Q	101	BCL	CBA-CGA-O2A-C1
8	R	101	BCL	CBA-CGA-O2A-C1
8	S	101	BCL	CBA-CGA-O2A-C1
8	T	101	BCL	CBA-CGA-O2A-C1
8	U	101	BCL	CBA-CGA-O2A-C1
9	I	103	KGD	CBB-CBG-CBI-CBL
8	L	401	BCL	C10-C11-C12-C13
10	L	405	BPH	C10-C11-C12-C13
8	6	101	BCL	C4-C3-C5-C6
8	B	101	BCL	C4-C3-C5-C6
8	E	101	BCL	C4-C3-C5-C6
8	Q	101	BCL	C4-C3-C5-C6
11	M	1002	MQE	CCB-CCC-CCD-CCI
8	2	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	2	101	BCL	C11-C10-C8-C9
8	V	101	BCL	C14-C13-C15-C16
8	W	101	BCL	C6-C7-C8-C9
8	W	101	BCL	C11-C10-C8-C9
10	L	405	BPH	C11-C12-C13-C14
8	B	101	BCL	O1D-CGD-O2D-CED
9	9	101	KGD	CAP-CAQ-CAR-CAU
9	D	102	KGD	CAJ-CAL-CAM-CAN
9	D	102	KGD	CAP-CAQ-CAR-CAU
9	I	103	KGD	CAJ-CAL-CAM-CAN
9	I	103	KGD	CAP-CAQ-CAR-CAU
9	J	102	KGD	CBE-CBF-CBH-CBK
9	D	102	KGD	CAJ-CAL-CAM-CAO
9	D	102	KGD	CAP-CAQ-CAR-CAV
9	I	103	KGD	CAJ-CAL-CAM-CAO
9	I	103	KGD	CAP-CAQ-CAR-CAV
9	J	102	KGD	CAJ-CAL-CAM-CAO
8	W	101	BCL	C10-C11-C12-C13
10	L	405	BPH	C15-C16-C17-C18
8	W	101	BCL	C1-C2-C3-C5
8	M	1005	BCL	C5-C6-C7-C8
11	M	1003	MQE	CAW-CAG-CAM-CBG
8	L	401	BCL	C15-C16-C17-C18
8	G	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C4-C3-C5-C6
8	O	101	BCL	C4-C3-C5-C6
9	9	101	KGD	CAM-CAO-CAP-CAQ
9	D	102	KGD	CAR-CAV-CBB-CBG
8	6	101	BCL	O1D-CGD-O2D-CED
8	0	101	BCL	C8-C10-C11-C12
8	2	101	BCL	C8-C10-C11-C12
8	2	102	BCL	C8-C10-C11-C12
8	4	102	BCL	C8-C10-C11-C12
8	6	102	BCL	C8-C10-C11-C12
8	8	102	BCL	C8-C10-C11-C12
8	B	102	BCL	C8-C10-C11-C12
8	E	102	BCL	C8-C10-C11-C12
8	G	102	BCL	C8-C10-C11-C12
8	I	102	BCL	C8-C10-C11-C12
8	K	102	BCL	C8-C10-C11-C12
8	O	102	BCL	C8-C10-C11-C12
8	Q	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	S	102	BCL	C8-C10-C11-C12
8	U	102	BCL	C8-C10-C11-C12
8	W	102	BCL	C8-C10-C11-C12
11	L	403	MQE	CAV-CAH-CAO-CBI
11	M	1002	MQE	CBB-CAN-CAS-CBH
8	M	1001	BCL	C3-C5-C6-C7
8	W	101	BCL	C13-C15-C16-C17
8	V	101	BCL	C15-C16-C17-C18
8	W	101	BCL	C15-C16-C17-C18
10	L	404	BPH	C10-C11-C12-C13
13	M	1008	PGV	C03-O11-P-O12
13	M	1008	PGV	C04-O12-P-O11
8	0	102	BCL	C4-C3-C5-C6
8	4	101	BCL	C4-C3-C5-C6
8	8	101	BCL	C4-C3-C5-C6
8	I	101	BCL	C4-C3-C5-C6
8	S	101	BCL	C4-C3-C5-C6
8	U	101	BCL	C4-C3-C5-C6
8	W	101	BCL	C4-C3-C5-C6
8	0	101	BCL	C16-C17-C18-C19
8	2	102	BCL	C16-C17-C18-C19
8	4	102	BCL	C16-C17-C18-C19
8	6	102	BCL	C16-C17-C18-C19
8	8	102	BCL	C16-C17-C18-C19
8	B	102	BCL	C16-C17-C18-C19
8	E	102	BCL	C16-C17-C18-C19
8	G	102	BCL	C16-C17-C18-C19
8	I	102	BCL	C16-C17-C18-C19
8	K	102	BCL	C16-C17-C18-C19
8	O	102	BCL	C16-C17-C18-C19
8	Q	102	BCL	C16-C17-C18-C19
8	S	102	BCL	C16-C17-C18-C19
8	U	102	BCL	C16-C17-C18-C19
8	W	102	BCL	C16-C17-C18-C19
10	L	405	BPH	CBA-CGA-O2A-C1
8	1	101	BCL	C5-C6-C7-C8
8	5	101	BCL	C5-C6-C7-C8
8	9	102	BCL	C5-C6-C7-C8
8	H	101	BCL	C5-C6-C7-C8
8	M	1005	BCL	C15-C16-C17-C18
8	N	101	BCL	C5-C6-C7-C8
8	R	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	T	101	BCL	C5-C6-C7-C8
9	D	102	KGD	CAM-CAO-CAP-CAQ
8	3	101	BCL	C5-C6-C7-C8
8	7	101	BCL	C5-C6-C7-C8
8	A	101	BCL	C5-C6-C7-C8
8	D	101	BCL	C5-C6-C7-C8
8	F	101	BCL	C5-C6-C7-C8
8	J	101	BCL	C5-C6-C7-C8
8	P	101	BCL	C5-C6-C7-C8
10	L	404	BPH	C15-C16-C17-C18
8	5	101	BCL	C16-C17-C18-C20
8	7	101	BCL	C16-C17-C18-C20
8	D	101	BCL	C16-C17-C18-C20
8	J	101	BCL	C16-C17-C18-C20
8	R	101	BCL	C16-C17-C18-C20
13	M	1007	PGV	C7-C8-C9-C10
8	S	101	BCL	O1D-CGD-O2D-CED
8	Q	101	BCL	O1D-CGD-O2D-CED
8	M	1005	BCL	C10-C11-C12-C13
10	L	405	BPH	O1A-CGA-O2A-C1
8	A	101	BCL	C16-C17-C18-C19
8	1	101	BCL	C2-C3-C5-C6
8	3	101	BCL	C2-C3-C5-C6
8	5	101	BCL	C2-C3-C5-C6
8	7	101	BCL	C2-C3-C5-C6
8	9	102	BCL	C2-C3-C5-C6
8	A	101	BCL	C2-C3-C5-C6
8	D	101	BCL	C2-C3-C5-C6
8	F	101	BCL	C2-C3-C5-C6
8	H	101	BCL	C2-C3-C5-C6
8	J	101	BCL	C2-C3-C5-C6
8	N	101	BCL	C2-C3-C5-C6
8	P	101	BCL	C2-C3-C5-C6
8	R	101	BCL	C2-C3-C5-C6
8	T	101	BCL	C2-C3-C5-C6
9	9	101	KGD	CBE-CBF-CBH-CBK
9	J	102	KGD	CAJ-CAL-CAM-CAN
13	M	1007	PGV	C5-C6-C7-C8
9	9	101	KGD	CAP-CAQ-CAR-CAV
9	9	101	KGD	CBE-CBF-CBH-CBJ
8	2	101	BCL	C15-C16-C17-C18
8	0	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
8	2	102	BCL	C16-C17-C18-C20
8	3	101	BCL	C16-C17-C18-C19
8	3	101	BCL	C16-C17-C18-C20
8	4	102	BCL	C16-C17-C18-C20
8	5	101	BCL	C16-C17-C18-C19
8	6	102	BCL	C16-C17-C18-C20
8	7	101	BCL	C16-C17-C18-C19
8	8	102	BCL	C16-C17-C18-C20
8	A	101	BCL	C16-C17-C18-C20
8	B	102	BCL	C16-C17-C18-C20
8	D	101	BCL	C16-C17-C18-C19
8	E	102	BCL	C16-C17-C18-C20
8	G	102	BCL	C16-C17-C18-C20
8	I	102	BCL	C16-C17-C18-C20
8	J	101	BCL	C16-C17-C18-C19
8	K	102	BCL	C16-C17-C18-C20
8	O	102	BCL	C16-C17-C18-C20
8	Q	102	BCL	C16-C17-C18-C20
8	R	101	BCL	C16-C17-C18-C19
8	S	102	BCL	C16-C17-C18-C20
8	U	102	BCL	C16-C17-C18-C20
8	W	102	BCL	C16-C17-C18-C20
8	K	101	BCL	O1D-CGD-O2D-CED
10	L	405	BPH	O1D-CGD-O2D-CED
8	V	101	BCL	C3A-C2A-CAA-CBA
8	0	102	BCL	O2A-C1-C2-C3
8	4	101	BCL	O2A-C1-C2-C3
8	6	101	BCL	O2A-C1-C2-C3
8	8	101	BCL	O2A-C1-C2-C3
8	B	101	BCL	O2A-C1-C2-C3
8	E	101	BCL	O2A-C1-C2-C3
8	G	101	BCL	O2A-C1-C2-C3
8	I	101	BCL	O2A-C1-C2-C3
8	K	101	BCL	O2A-C1-C2-C3
8	O	101	BCL	O2A-C1-C2-C3
8	Q	101	BCL	O2A-C1-C2-C3
8	S	101	BCL	O2A-C1-C2-C3
8	U	101	BCL	O2A-C1-C2-C3
13	M	1006	PGV	C19-C20-C21-C22
10	L	402	BPH	C2-C3-C5-C6
8	W	101	BCL	C5-C6-C7-C8
8	2	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	D	102	KGD	CAH-CAD-CAJ-CAL
9	I	103	KGD	CAH-CAD-CAJ-CAL
9	J	102	KGD	CAB-CAD-CAJ-CAL
9	J	102	KGD	CAH-CAD-CAJ-CAL
10	L	402	BPH	C10-C11-C12-C13
8	M	1005	BCL	C6-C7-C8-C10
8	V	101	BCL	C2-C3-C5-C6
8	V	101	BCL	C6-C7-C8-C10
8	W	101	BCL	C6-C7-C8-C10
10	L	402	BPH	C11-C12-C13-C15
8	M	1001	BCL	C16-C17-C18-C20
13	M	1008	PGV	C20-C19-O03-C01
8	U	101	BCL	C15-C16-C17-C18
8	0	102	BCL	C15-C16-C17-C18
8	4	101	BCL	C15-C16-C17-C18
8	6	101	BCL	C15-C16-C17-C18
8	8	101	BCL	C15-C16-C17-C18
8	B	101	BCL	C15-C16-C17-C18
8	E	101	BCL	C15-C16-C17-C18
8	G	101	BCL	C15-C16-C17-C18
8	I	101	BCL	C15-C16-C17-C18
8	K	101	BCL	C15-C16-C17-C18
8	O	101	BCL	C15-C16-C17-C18
8	Q	101	BCL	C15-C16-C17-C18
8	S	101	BCL	C15-C16-C17-C18
14	C	504	HEM	C4B-C3B-CAB-CBB
8	1	101	BCL	C13-C15-C16-C17
8	3	101	BCL	C13-C15-C16-C17
8	5	101	BCL	C13-C15-C16-C17
8	7	101	BCL	C13-C15-C16-C17
8	9	102	BCL	C13-C15-C16-C17
8	A	101	BCL	C13-C15-C16-C17
8	D	101	BCL	C13-C15-C16-C17
8	F	101	BCL	C13-C15-C16-C17
8	H	101	BCL	C13-C15-C16-C17
8	J	101	BCL	C13-C15-C16-C17
8	N	101	BCL	C13-C15-C16-C17
8	P	101	BCL	C13-C15-C16-C17
8	R	101	BCL	C13-C15-C16-C17
8	I	101	BCL	O1D-CGD-O2D-CED
10	L	402	BPH	C4-C3-C5-C6
8	W	101	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	L	402	BPH	C11-C12-C13-C14
13	M	1006	PGV	C22-C23-C24-C25
8	0	101	BCL	C1A-C2A-CAA-CBA
8	2	102	BCL	C1A-C2A-CAA-CBA
8	4	102	BCL	C1A-C2A-CAA-CBA
8	6	102	BCL	C1A-C2A-CAA-CBA
8	8	102	BCL	C1A-C2A-CAA-CBA
8	B	102	BCL	C1A-C2A-CAA-CBA
8	E	102	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	K	102	BCL	C1A-C2A-CAA-CBA
8	O	102	BCL	C1A-C2A-CAA-CBA
8	Q	102	BCL	C1A-C2A-CAA-CBA
8	S	102	BCL	C1A-C2A-CAA-CBA
8	U	102	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C1A-C2A-CAA-CBA
8	W	102	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C16-C17-C18-C20
10	L	402	BPH	C16-C17-C18-C20
10	L	405	BPH	C16-C17-C18-C20
8	1	101	BCL	C16-C17-C18-C20
8	0	102	BCL	C2C-C3C-CAC-CBC
8	4	101	BCL	C2C-C3C-CAC-CBC
8	6	101	BCL	C2C-C3C-CAC-CBC
8	8	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C2C-C3C-CAC-CBC
8	E	101	BCL	C2C-C3C-CAC-CBC
8	G	101	BCL	C2C-C3C-CAC-CBC
8	I	101	BCL	C2C-C3C-CAC-CBC
8	K	101	BCL	C2C-C3C-CAC-CBC
8	O	101	BCL	C2C-C3C-CAC-CBC
8	Q	101	BCL	C2C-C3C-CAC-CBC
8	S	101	BCL	C2C-C3C-CAC-CBC
8	U	101	BCL	C2C-C3C-CAC-CBC
13	M	1008	PGV	O04-C19-O03-C01
8	1	101	BCL	C16-C17-C18-C19
8	M	1001	BCL	C16-C17-C18-C19
10	L	402	BPH	C16-C17-C18-C19
13	M	1008	PGV	C25-C26-C27-C28
8	4	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	0	101	BCL	C5-C6-C7-C8
8	2	102	BCL	C5-C6-C7-C8
8	8	102	BCL	C5-C6-C7-C8
8	K	102	BCL	C5-C6-C7-C8
8	O	102	BCL	C5-C6-C7-C8
8	Q	102	BCL	C5-C6-C7-C8
8	S	102	BCL	C5-C6-C7-C8
8	U	102	BCL	C5-C6-C7-C8
8	4	102	BCL	C5-C6-C7-C8
8	6	102	BCL	C5-C6-C7-C8
8	B	102	BCL	C5-C6-C7-C8
8	E	102	BCL	C5-C6-C7-C8
8	G	102	BCL	C5-C6-C7-C8
8	I	102	BCL	C5-C6-C7-C8
8	W	102	BCL	C5-C6-C7-C8
8	G	101	BCL	O1D-CGD-O2D-CED
8	8	102	BCL	C10-C11-C12-C13
8	G	102	BCL	C10-C11-C12-C13
8	I	102	BCL	C10-C11-C12-C13
8	K	102	BCL	C10-C11-C12-C13
8	O	102	BCL	C10-C11-C12-C13
8	Q	102	BCL	C10-C11-C12-C13
8	S	102	BCL	C10-C11-C12-C13
8	2	101	BCL	C16-C17-C18-C20
8	0	101	BCL	C10-C11-C12-C13
8	2	102	BCL	C10-C11-C12-C13
8	E	102	BCL	C10-C11-C12-C13
8	M	1001	BCL	C13-C15-C16-C17
8	4	102	BCL	C10-C11-C12-C13
8	6	102	BCL	C10-C11-C12-C13
8	B	102	BCL	C10-C11-C12-C13
8	M	1001	BCL	C15-C16-C17-C18
8	U	102	BCL	C10-C11-C12-C13
8	W	102	BCL	C10-C11-C12-C13
8	0	101	BCL	C13-C15-C16-C17
8	2	102	BCL	C13-C15-C16-C17
8	4	102	BCL	C13-C15-C16-C17
8	6	102	BCL	C13-C15-C16-C17
8	8	102	BCL	C13-C15-C16-C17
8	E	102	BCL	C13-C15-C16-C17
8	G	102	BCL	C13-C15-C16-C17
8	I	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	K	102	BCL	C13-C15-C16-C17
8	O	102	BCL	C13-C15-C16-C17
8	Q	102	BCL	C13-C15-C16-C17
8	S	102	BCL	C13-C15-C16-C17
8	U	102	BCL	C13-C15-C16-C17
8	W	102	BCL	C13-C15-C16-C17
13	M	1007	PGV	C14-C15-C16-C17
11	M	1002	MQE	CAS-CAN-CBB-CCA
8	B	102	BCL	C13-C15-C16-C17
8	0	102	BCL	C11-C12-C13-C15
8	4	101	BCL	C11-C12-C13-C15
8	6	101	BCL	C11-C12-C13-C15
8	8	101	BCL	C11-C12-C13-C15
8	B	101	BCL	C11-C12-C13-C15
8	E	101	BCL	C11-C12-C13-C15
8	G	101	BCL	C11-C12-C13-C15
8	I	101	BCL	C11-C12-C13-C15
8	K	101	BCL	C11-C12-C13-C15
8	L	401	BCL	C11-C10-C8-C7
8	O	101	BCL	C11-C12-C13-C15
8	Q	101	BCL	C11-C12-C13-C15
8	S	101	BCL	C11-C12-C13-C15
8	U	101	BCL	C11-C12-C13-C15
8	V	101	BCL	C12-C13-C15-C16
8	W	101	BCL	C12-C13-C15-C16
8	0	102	BCL	C11-C12-C13-C14
8	4	101	BCL	C11-C12-C13-C14
8	6	101	BCL	C11-C12-C13-C14
8	8	101	BCL	C11-C12-C13-C14
8	B	101	BCL	C11-C12-C13-C14
8	E	101	BCL	C11-C12-C13-C14
8	G	101	BCL	C11-C12-C13-C14
8	I	101	BCL	C11-C12-C13-C14
8	K	101	BCL	C11-C12-C13-C14
8	L	401	BCL	C11-C10-C8-C9
8	M	1005	BCL	C6-C7-C8-C9
8	O	101	BCL	C11-C12-C13-C14
8	Q	101	BCL	C11-C12-C13-C14
8	S	101	BCL	C11-C12-C13-C14
8	U	101	BCL	C11-C12-C13-C14
9	J	102	KGD	CAR-CAV-CBB-CBG
8	5	101	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	7	101	BCL	C15-C16-C17-C18
8	D	101	BCL	C15-C16-C17-C18
8	J	101	BCL	C15-C16-C17-C18
8	N	101	BCL	C15-C16-C17-C18
8	R	101	BCL	C15-C16-C17-C18
8	F	101	BCL	C16-C17-C18-C19
8	V	101	BCL	C16-C17-C18-C20
9	D	102	KGD	CAT-CAS-CAW-CAZ
8	2	101	BCL	C3A-C2A-CAA-CBA
10	L	404	BPH	C3A-C2A-CAA-CBA
13	M	1007	PGV	O03-C01-C02-O01
10	L	405	BPH	C16-C17-C18-C19
9	D	102	KGD	CAW-CAS-CAT-CAX
13	M	1008	PGV	O12-C04-C05-C06
8	V	101	BCL	C6-C7-C8-C9
13	M	1008	PGV	C02-C03-O11-P
8	M	1001	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	C6-C7-C8-C10
8	2	101	BCL	C11-C10-C8-C7
8	W	101	BCL	C11-C10-C8-C7
9	I	103	KGD	CAW-CBA-CBE-CBF
10	L	404	BPH	C2A-CAA-CBA-CGA
8	0	101	BCL	CAD-CBD-CGD-O2D
8	1	101	BCL	CAD-CBD-CGD-O2D
8	2	102	BCL	CAD-CBD-CGD-O2D
8	3	101	BCL	CAD-CBD-CGD-O2D
8	4	102	BCL	CAD-CBD-CGD-O2D
8	5	101	BCL	CAD-CBD-CGD-O2D
8	6	102	BCL	CAD-CBD-CGD-O2D
8	7	101	BCL	CAD-CBD-CGD-O2D
8	8	102	BCL	CAD-CBD-CGD-O2D
8	9	102	BCL	CAD-CBD-CGD-O2D
8	A	101	BCL	CAD-CBD-CGD-O2D
8	B	102	BCL	CAD-CBD-CGD-O2D
8	D	101	BCL	CAD-CBD-CGD-O2D
8	E	102	BCL	CAD-CBD-CGD-O2D
8	F	101	BCL	CAD-CBD-CGD-O2D
8	G	102	BCL	CAD-CBD-CGD-O2D
8	H	101	BCL	CAD-CBD-CGD-O2D
8	I	102	BCL	CAD-CBD-CGD-O2D
8	J	101	BCL	CAD-CBD-CGD-O2D
8	K	102	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	M	1005	BCL	CAD-CBD-CGD-O2D
8	N	101	BCL	CAD-CBD-CGD-O2D
8	O	102	BCL	CAD-CBD-CGD-O2D
8	P	101	BCL	CAD-CBD-CGD-O2D
8	Q	102	BCL	CAD-CBD-CGD-O2D
8	R	101	BCL	CAD-CBD-CGD-O2D
8	S	102	BCL	CAD-CBD-CGD-O2D
8	T	101	BCL	CAD-CBD-CGD-O2D
8	U	102	BCL	CAD-CBD-CGD-O2D
8	W	102	BCL	CAD-CBD-CGD-O2D
14	C	502	HEM	C2B-C3B-CAB-CBB
11	M	1003	MQE	CAS-CAN-CBB-CCA
8	M	1005	BCL	C2A-CAA-CBA-CGA
8	M	1001	BCL	CHA-CBD-CGD-O1D
8	M	1001	BCL	CHA-CBD-CGD-O2D
13	M	1007	PGV	O05-C05-C06-O06
11	M	1002	MQE	CAI-CAC-CAP-CBT
8	T	101	BCL	C16-C17-C18-C20
9	9	101	KGD	CAJ-CAL-CAM-CAN
10	L	402	BPH	C2C-C3C-CAC-CBC
9	9	101	KGD	CAJ-CAL-CAM-CAO
13	M	1007	PGV	C03-O11-P-O12
11	L	403	MQE	CAJ-CAD-CAQ-CBU
11	M	1003	MQE	CAM-CAG-CAW-CBY
8	2	101	BCL	C10-C11-C12-C13
13	M	1006	PGV	C02-C03-O11-P
11	M	1003	MQE	CAS-CAN-CBB-CBL
13	M	1008	PGV	C03-O11-P-O13
13	M	1008	PGV	C04-O12-P-O13
13	M	1008	PGV	C04-O12-P-O14
8	2	101	BCL	C16-C17-C18-C19
8	0	102	BCL	CAD-CBD-CGD-O1D
8	4	101	BCL	CAD-CBD-CGD-O1D
8	6	101	BCL	CAD-CBD-CGD-O1D
8	8	101	BCL	CAD-CBD-CGD-O1D
8	B	101	BCL	CAD-CBD-CGD-O1D
8	E	101	BCL	CAD-CBD-CGD-O1D
8	G	101	BCL	CAD-CBD-CGD-O1D
8	I	101	BCL	CAD-CBD-CGD-O1D
8	K	101	BCL	CAD-CBD-CGD-O1D
8	O	101	BCL	CAD-CBD-CGD-O1D
8	Q	101	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	S	101	BCL	CAD-CBD-CGD-O1D
8	U	101	BCL	CAD-CBD-CGD-O1D
8	W	101	BCL	CAD-CBD-CGD-O1D
8	1	101	BCL	C11-C10-C8-C7
8	3	101	BCL	C11-C10-C8-C7
8	5	101	BCL	C11-C10-C8-C7
8	7	101	BCL	C11-C10-C8-C7
8	9	102	BCL	C11-C10-C8-C7
8	A	101	BCL	C11-C10-C8-C7
8	D	101	BCL	C11-C10-C8-C7
8	F	101	BCL	C11-C10-C8-C7
8	H	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C11-C10-C8-C7
8	M	1005	BCL	C2C-C3C-CAC-CBC
8	N	101	BCL	C11-C10-C8-C7
8	P	101	BCL	C11-C10-C8-C7
8	R	101	BCL	C11-C10-C8-C7
8	T	101	BCL	C11-C10-C8-C7
14	C	504	HEM	C2A-CAA-CBA-CGA
10	L	402	BPH	C4C-C3C-CAC-CBC
10	L	402	BPH	C8-C10-C11-C12
8	2	101	BCL	C4-C3-C5-C6
11	L	403	MQE	CAL-CAE-CAR-CBV
8	1	101	BCL	C6-C7-C8-C9
8	1	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C6-C7-C8-C9
8	3	101	BCL	C11-C10-C8-C9
8	5	101	BCL	C6-C7-C8-C9
8	5	101	BCL	C11-C10-C8-C9
8	7	101	BCL	C6-C7-C8-C9
8	7	101	BCL	C11-C10-C8-C9
8	9	102	BCL	C6-C7-C8-C9
8	9	102	BCL	C11-C10-C8-C9
8	A	101	BCL	C6-C7-C8-C9
8	A	101	BCL	C11-C10-C8-C9
8	D	101	BCL	C6-C7-C8-C9
8	D	101	BCL	C11-C10-C8-C9
8	F	101	BCL	C6-C7-C8-C9
8	F	101	BCL	C11-C10-C8-C9
8	H	101	BCL	C6-C7-C8-C9
8	H	101	BCL	C11-C10-C8-C9
8	J	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	J	101	BCL	C11-C10-C8-C9
8	N	101	BCL	C6-C7-C8-C9
8	N	101	BCL	C11-C10-C8-C9
8	P	101	BCL	C6-C7-C8-C9
8	P	101	BCL	C11-C10-C8-C9
8	R	101	BCL	C6-C7-C8-C9
8	R	101	BCL	C11-C10-C8-C9
8	T	101	BCL	C6-C7-C8-C9
8	T	101	BCL	C11-C10-C8-C9
9	9	101	KGD	CBA-CBE-CBF-CBH
9	D	102	KGD	CBA-CBE-CBF-CBH
9	J	102	KGD	CAO-CAP-CAQ-CAR
9	J	102	KGD	CBA-CBE-CBF-CBH
8	V	101	BCL	C16-C17-C18-C19
8	V	101	BCL	C4-C3-C5-C6
11	L	403	MQE	CAJ-CAD-CAQ-CBE
11	M	1003	MQE	CAM-CAG-CAW-CBH
13	M	1006	PGV	C01-C02-O01-C1
8	M	1001	BCL	C2-C1-O2A-CGA
13	M	1008	PGV	C2-C3-C4-C5
11	M	1002	MQE	CAI-CAC-CAP-CBC
13	M	1006	PGV	C03-O11-P-O12
13	M	1007	PGV	C04-O12-P-O11
8	1	101	BCL	C4-C3-C5-C6
8	3	101	BCL	C4-C3-C5-C6
8	5	101	BCL	C4-C3-C5-C6
8	7	101	BCL	C4-C3-C5-C6
8	9	102	BCL	C4-C3-C5-C6
8	A	101	BCL	C4-C3-C5-C6
8	D	101	BCL	C4-C3-C5-C6
8	F	101	BCL	C4-C3-C5-C6
8	H	101	BCL	C4-C3-C5-C6
8	J	101	BCL	C4-C3-C5-C6
8	N	101	BCL	C4-C3-C5-C6
8	P	101	BCL	C4-C3-C5-C6
8	R	101	BCL	C4-C3-C5-C6
10	L	402	BPH	C11-C10-C8-C7
10	L	404	BPH	C12-C13-C15-C16
11	M	1002	MQE	CAS-CAN-CBB-CBL
9	I	103	KGD	CAM-CAO-CAP-CAQ
8	M	1005	BCL	C16-C17-C18-C20
9	I	103	KGD	CBH-CBJ-CBM-CBN

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Mol	Chain	Res	Type	Atoms
13	M	1006	PGV	C11-C12-C13-C14
8	T	101	BCL	C13-C15-C16-C17
8	F	101	BCL	C8-C10-C11-C12
8	J	101	BCL	C8-C10-C11-C12
8	P	101	BCL	C8-C10-C11-C12
9	D	102	KGD	CAW-CBA-CBE-CBF
8	1	101	BCL	C8-C10-C11-C12
8	W	101	BCL	C11-C12-C13-C14
10	L	404	BPH	C14-C13-C15-C16
10	L	405	BPH	C6-C7-C8-C9
8	P	101	BCL	C16-C17-C18-C20
8	3	101	BCL	C8-C10-C11-C12
8	5	101	BCL	C8-C10-C11-C12
8	7	101	BCL	C8-C10-C11-C12
8	9	102	BCL	C8-C10-C11-C12
8	A	101	BCL	C8-C10-C11-C12
8	D	101	BCL	C8-C10-C11-C12
8	H	101	BCL	C8-C10-C11-C12
8	N	101	BCL	C8-C10-C11-C12
8	R	101	BCL	C8-C10-C11-C12
8	T	101	BCL	C8-C10-C11-C12
9	J	102	KGD	CAN-CAM-CAO-CAP
13	M	1007	PGV	O03-C01-C02-C03
14	C	503	HEM	CAA-CBA-CGA-O1A
8	2	101	BCL	O2A-C1-C2-C3
9	N	102	KGD	CAW-CAS-CAT-CAX
8	1	101	BCL	C1A-C2A-CAA-CBA
8	2	101	BCL	C1A-C2A-CAA-CBA
8	3	101	BCL	C1A-C2A-CAA-CBA
8	5	101	BCL	C1A-C2A-CAA-CBA
8	7	101	BCL	C1A-C2A-CAA-CBA
8	9	102	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C1A-C2A-CAA-CBA
8	D	101	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C1A-C2A-CAA-CBA
8	H	101	BCL	C1A-C2A-CAA-CBA
8	J	101	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C1A-C2A-CAA-CBA
8	R	101	BCL	C1A-C2A-CAA-CBA
8	T	101	BCL	C1A-C2A-CAA-CBA
10	L	405	BPH	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	C	501	HEM	CAA-CBA-CGA-O2A
13	M	1007	PGV	C6-C7-C8-C9
11	L	403	MQE	CAL-CAE-CAR-CBD
14	C	501	HEM	C3D-CAD-CBD-CGD
13	M	1006	PGV	C2-C3-C4-C5
9	J	102	KGD	CAL-CAM-CAO-CAP
14	C	501	HEM	CAA-CBA-CGA-O1A
10	L	404	BPH	C4-C3-C5-C6
8	V	101	BCL	C2-C1-O2A-CGA
8	W	101	BCL	C2-C1-O2A-CGA
8	T	101	BCL	C4-C3-C5-C6
9	D	102	KGD	CAT-CAS-CAW-CBA
14	C	503	HEM	CAA-CBA-CGA-O2A
13	M	1006	PGV	C9-C10-C11-C12
8	V	101	BCL	C10-C11-C12-C13
9	J	102	KGD	CAT-CAS-CAW-CAZ
8	L	401	BCL	C11-C12-C13-C15
8	M	1001	BCL	C2-C3-C5-C6
8	0	101	BCL	C1-C2-C3-C4
8	2	102	BCL	C1-C2-C3-C4
8	4	102	BCL	C1-C2-C3-C4
8	6	102	BCL	C1-C2-C3-C4
8	8	102	BCL	C1-C2-C3-C4
8	B	102	BCL	C1-C2-C3-C4
8	E	102	BCL	C1-C2-C3-C4
8	G	102	BCL	C1-C2-C3-C4
8	I	102	BCL	C1-C2-C3-C4
8	K	102	BCL	C1-C2-C3-C4
8	M	1001	BCL	C1-C2-C3-C4
8	O	102	BCL	C1-C2-C3-C4
8	Q	102	BCL	C1-C2-C3-C4
8	S	102	BCL	C1-C2-C3-C4
8	U	102	BCL	C1-C2-C3-C4
8	W	102	BCL	C1-C2-C3-C4
8	L	401	BCL	C2-C3-C5-C6
8	M	1005	BCL	C2-C3-C5-C6
10	L	404	BPH	C2-C3-C5-C6
8	N	101	BCL	C16-C17-C18-C19
8	0	102	BCL	C6-C7-C8-C9
8	4	101	BCL	C6-C7-C8-C9
8	6	101	BCL	C6-C7-C8-C9
8	8	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	B	101	BCL	C6-C7-C8-C9
8	E	101	BCL	C6-C7-C8-C9
8	G	101	BCL	C6-C7-C8-C9
8	I	101	BCL	C6-C7-C8-C9
8	K	101	BCL	C6-C7-C8-C9
8	O	101	BCL	C6-C7-C8-C9
8	Q	101	BCL	C6-C7-C8-C9
8	S	101	BCL	C6-C7-C8-C9
8	U	101	BCL	C6-C7-C8-C9
10	L	402	BPH	C14-C13-C15-C16
8	A	101	BCL	C3A-C2A-CAA-CBA
8	2	101	BCL	CAD-CBD-CGD-O2D
8	V	101	BCL	CAD-CBD-CGD-O2D
10	L	404	BPH	CAD-CBD-CGD-O2D
8	L	401	BCL	C2-C1-O2A-CGA
9	J	102	KGD	CBE-CBF-CBH-CBJ
9	9	101	KGD	CAW-CAS-CAT-CAX
11	L	403	MQE	CAT-CAF-CAK-CBE
13	M	1007	PGV	C11-C12-C13-C14
8	2	101	BCL	CHA-CBD-CGD-O2D
8	L	401	BCL	C16-C17-C18-C20
8	W	101	BCL	C16-C17-C18-C20
8	W	101	BCL	CAA-CBA-CGA-O2A
10	L	404	BPH	CHA-CBD-CGD-O1D
8	L	401	BCL	C11-C12-C13-C14
10	L	402	BPH	C11-C10-C8-C9
13	M	1007	PGV	C11-C10-C9-C8
8	M	1005	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	CAA-CBA-CGA-O1A
13	M	1006	PGV	C04-O12-P-O13
13	M	1007	PGV	C04-O12-P-O13
8	2	101	BCL	CAA-CBA-CGA-O1A
8	2	101	BCL	C2-C3-C5-C6
8	L	401	BCL	CAD-CBD-CGD-O1D
8	M	1005	BCL	CAD-CBD-CGD-O1D
8	4	102	BCL	C11-C10-C8-C9
8	U	102	BCL	C11-C10-C8-C9
10	L	402	BPH	CAA-CBA-CGA-O2A
8	T	101	BCL	C15-C16-C17-C18
14	C	504	HEM	CAA-CBA-CGA-O1A
10	L	404	BPH	CAA-CBA-CGA-O2A
14	C	501	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	1	101	BCL	C3A-C2A-CAA-CBA
8	3	101	BCL	C3A-C2A-CAA-CBA
8	5	101	BCL	C3A-C2A-CAA-CBA
8	7	101	BCL	C3A-C2A-CAA-CBA
8	9	102	BCL	C3A-C2A-CAA-CBA
8	D	101	BCL	C3A-C2A-CAA-CBA
8	F	101	BCL	C3A-C2A-CAA-CBA
8	H	101	BCL	C3A-C2A-CAA-CBA
8	J	101	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	R	101	BCL	C3A-C2A-CAA-CBA
8	T	101	BCL	C3A-C2A-CAA-CBA
10	L	402	BPH	C12-C13-C15-C16
9	N	102	KGD	CBE-CBF-CBH-CBJ

There are no ring outliers.

64 monomers are involved in 383 short contacts:

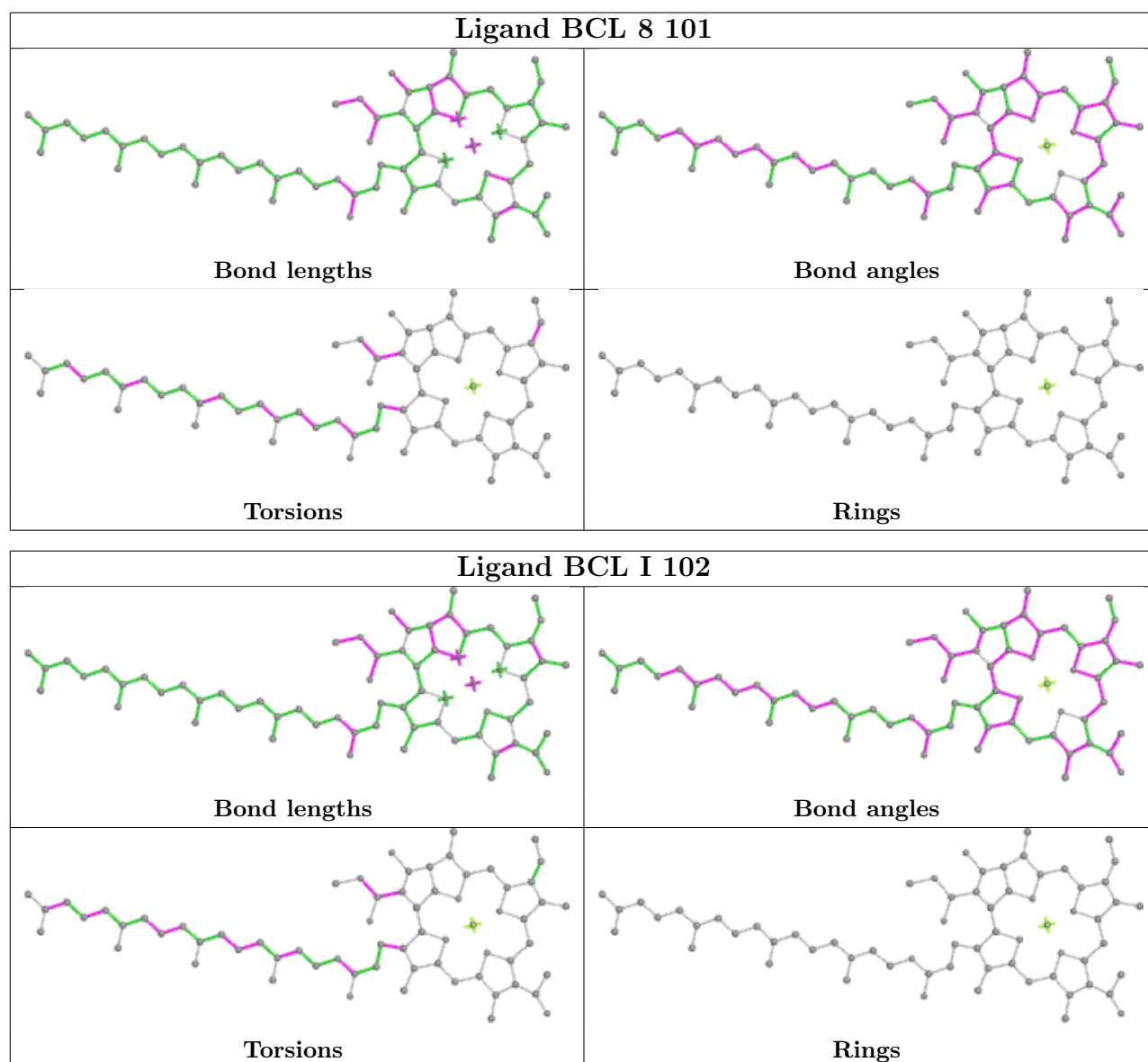
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	8	101	BCL	9	0
8	I	102	BCL	3	0
8	J	101	BCL	9	0
8	S	102	BCL	3	0
14	C	503	HEM	8	0
8	B	101	BCL	14	0
8	M	1001	BCL	4	0
13	M	1006	PGV	1	0
8	D	101	BCL	7	0
8	F	101	BCL	4	0
8	K	101	BCL	12	0
9	J	102	KGD	1	0
14	C	501	HEM	2	0
8	I	101	BCL	13	0
8	N	101	BCL	4	0
11	M	1002	MQE	5	0
8	5	101	BCL	4	0
8	0	102	BCL	10	0
8	E	101	BCL	9	0
8	3	101	BCL	4	0
13	M	1008	PGV	5	0
11	L	403	MQE	1	0

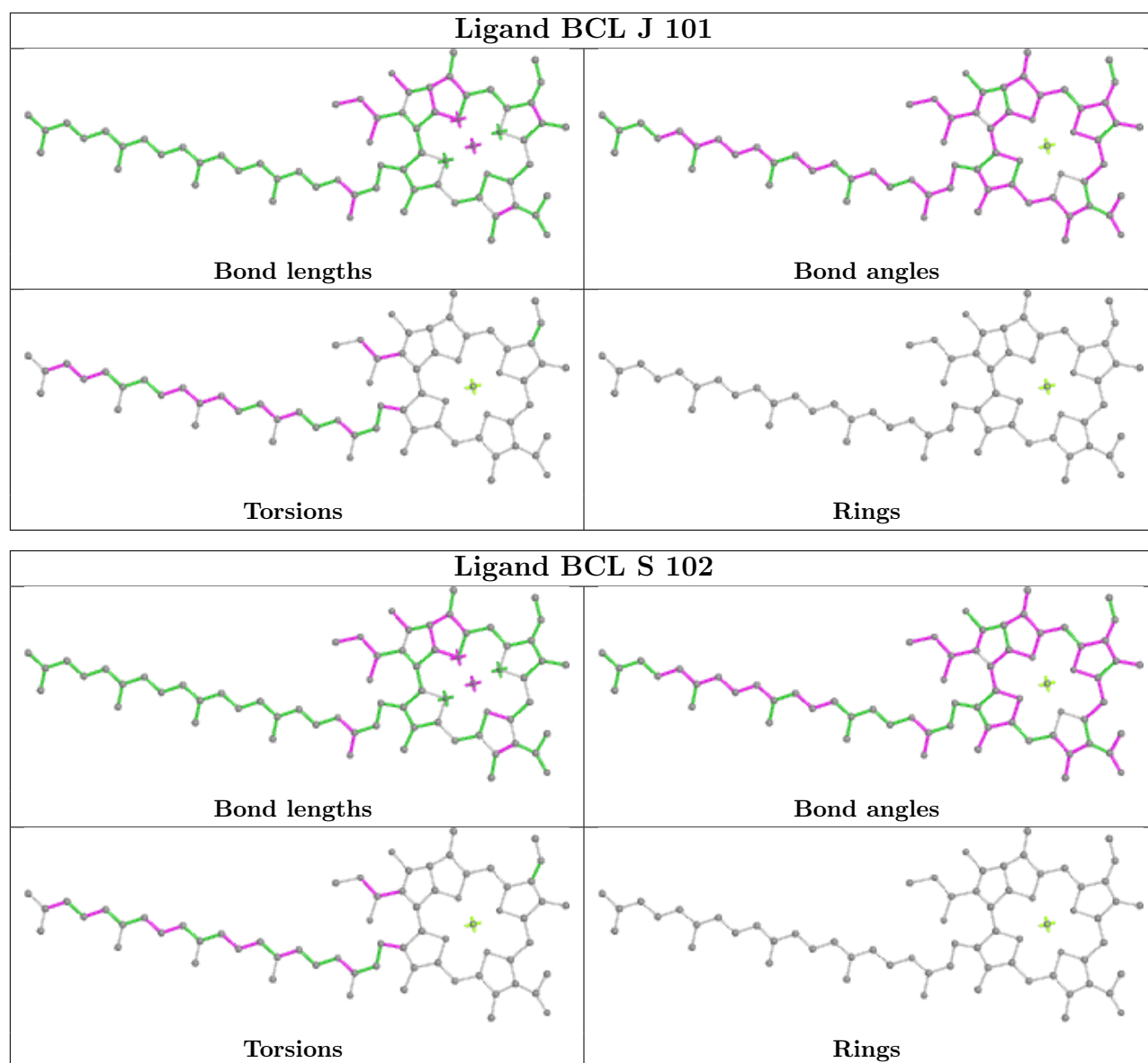
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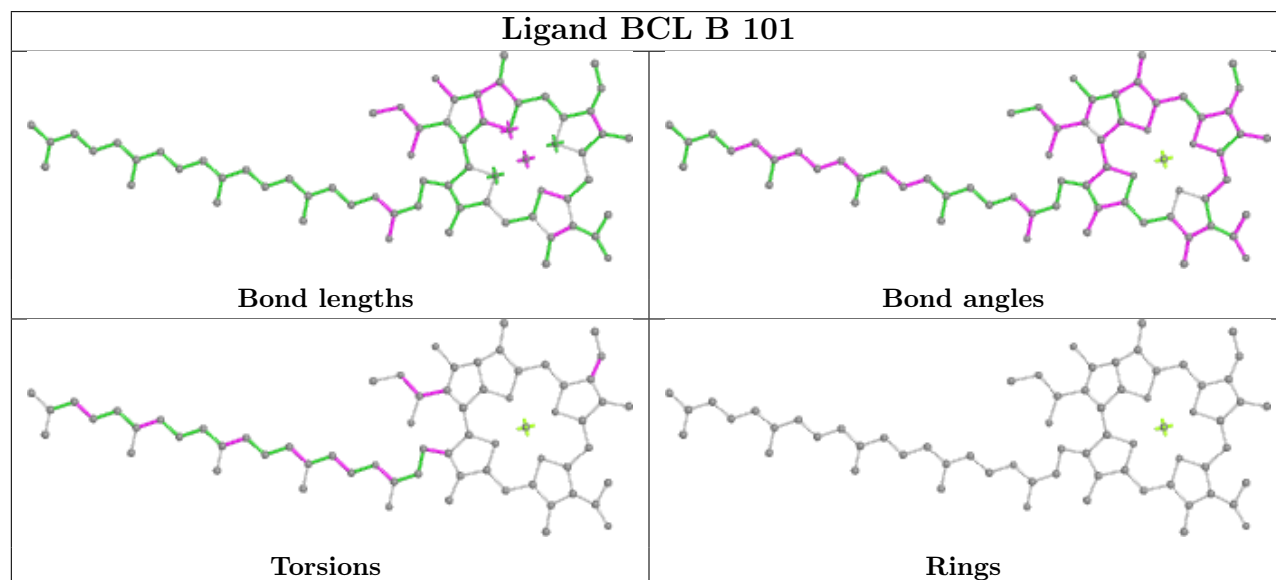
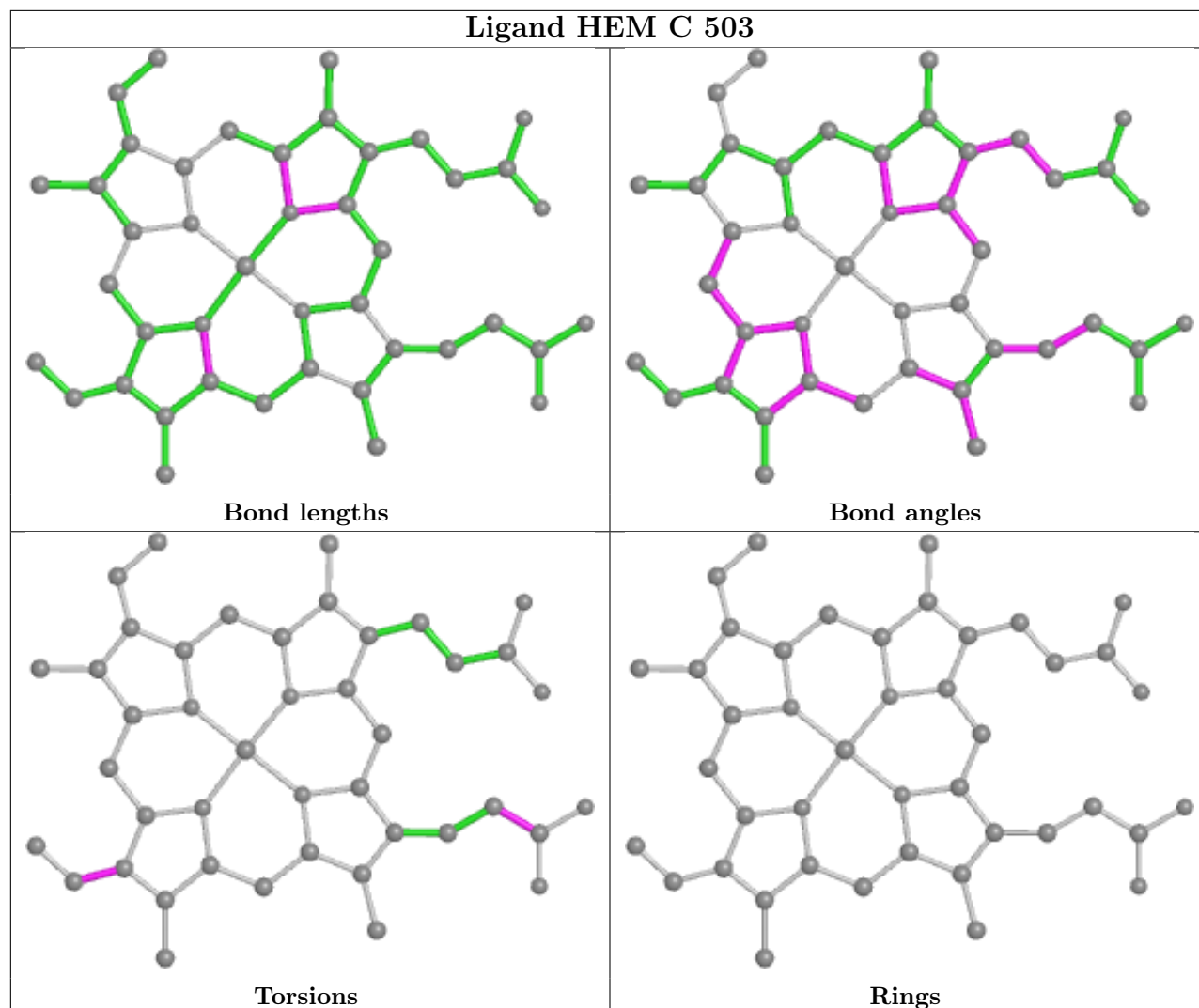
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	102	BCL	2	0
8	A	101	BCL	5	0
8	Q	102	BCL	3	0
8	Q	101	BCL	14	0
8	E	102	BCL	5	0
9	I	103	KGD	1	0
8	6	102	BCL	3	0
8	G	102	BCL	6	0
8	6	101	BCL	14	0
11	M	1003	MQE	6	0
8	2	101	BCL	3	0
8	4	102	BCL	3	0
8	G	101	BCL	14	0
8	2	102	BCL	3	0
8	4	101	BCL	12	0
8	7	101	BCL	5	0
8	S	101	BCL	11	0
9	D	102	KGD	3	0
10	L	402	BPH	5	0
10	L	405	BPH	12	0
8	M	1005	BCL	7	0
8	8	102	BCL	3	0
8	B	102	BCL	2	0
13	M	1007	PGV	11	0
8	V	101	BCL	9	0
8	K	102	BCL	4	0
8	O	101	BCL	12	0
10	L	404	BPH	6	0
8	W	102	BCL	2	0
14	C	504	HEM	2	0
8	0	101	BCL	3	0
8	W	101	BCL	12	0
8	U	101	BCL	12	0
8	O	102	BCL	3	0
8	1	101	BCL	3	0
8	P	101	BCL	3	0
8	R	101	BCL	8	0
8	9	102	BCL	7	0
9	9	101	KGD	3	0
8	H	101	BCL	3	0
8	T	101	BCL	11	0
8	L	401	BCL	12	0

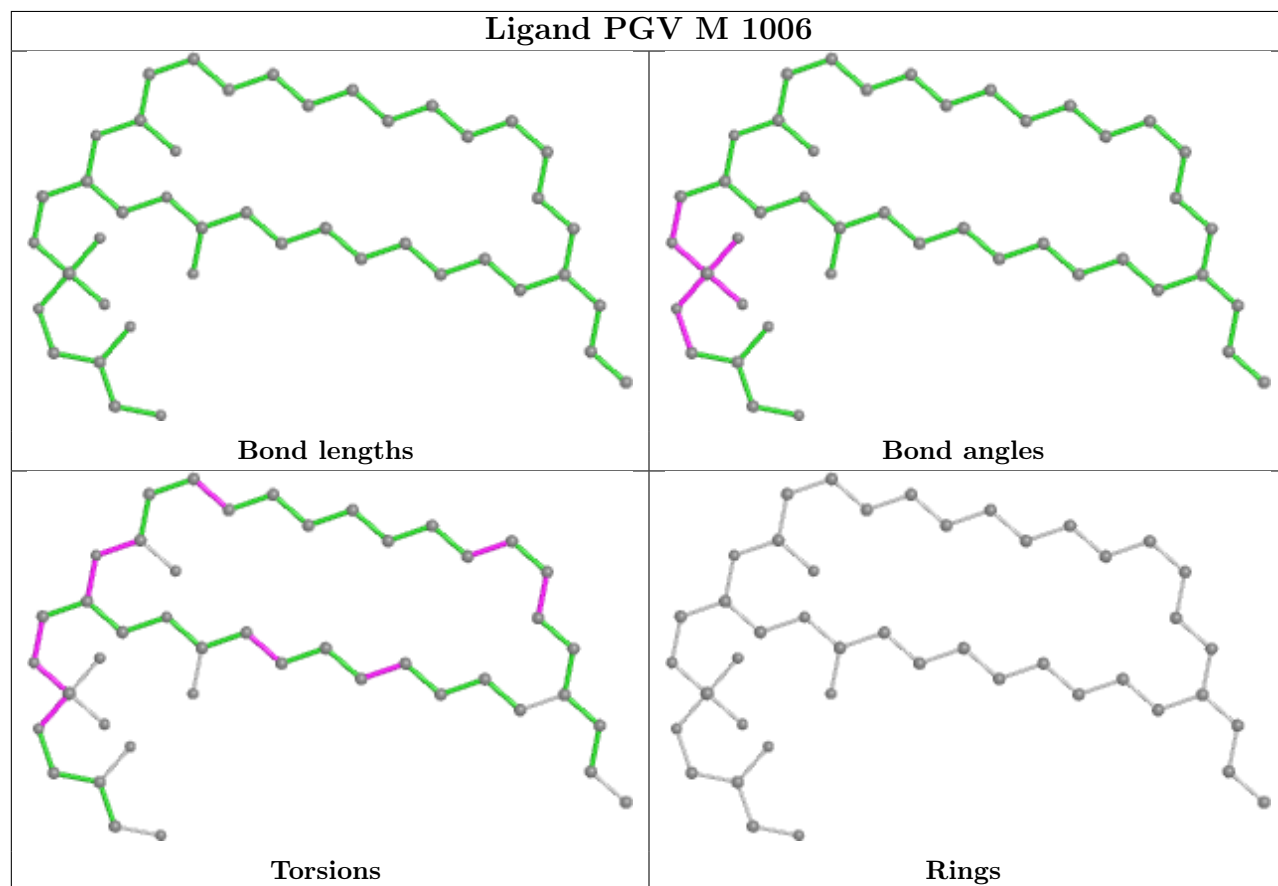
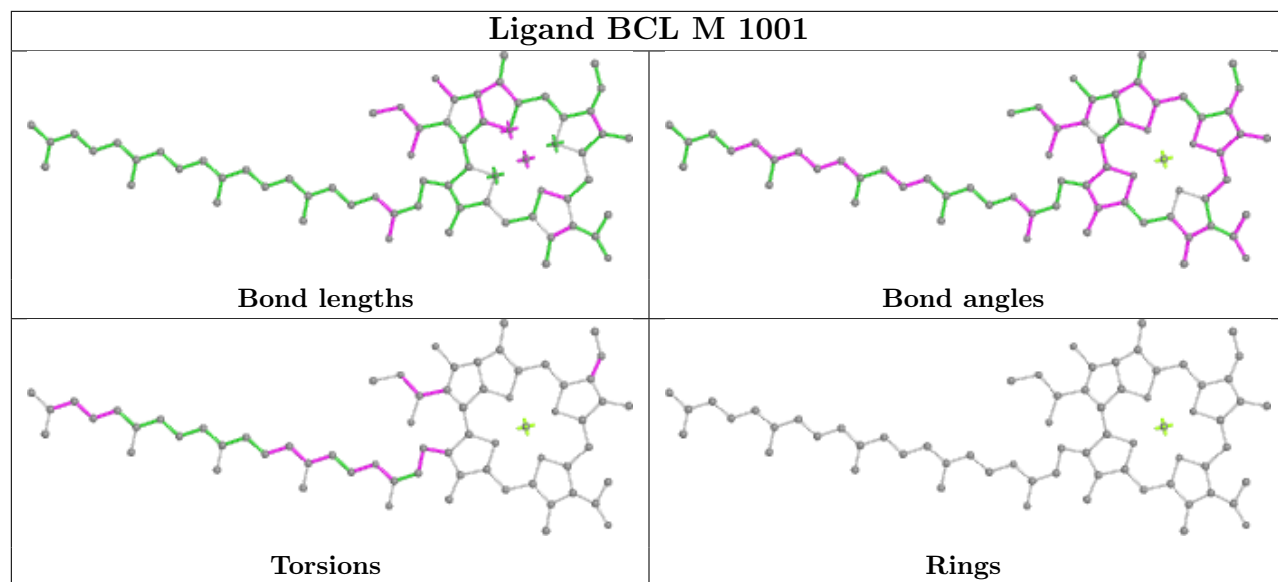
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

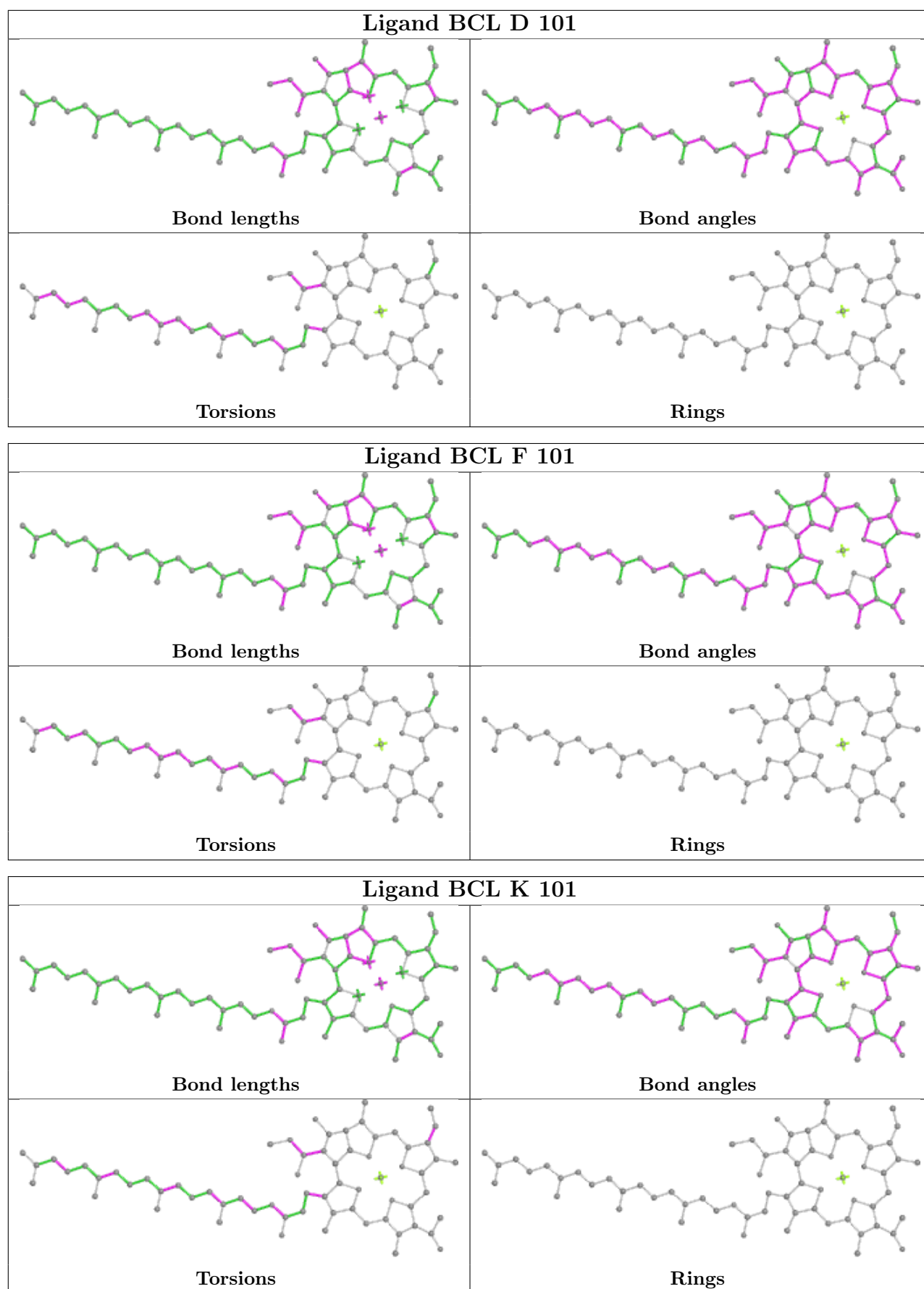


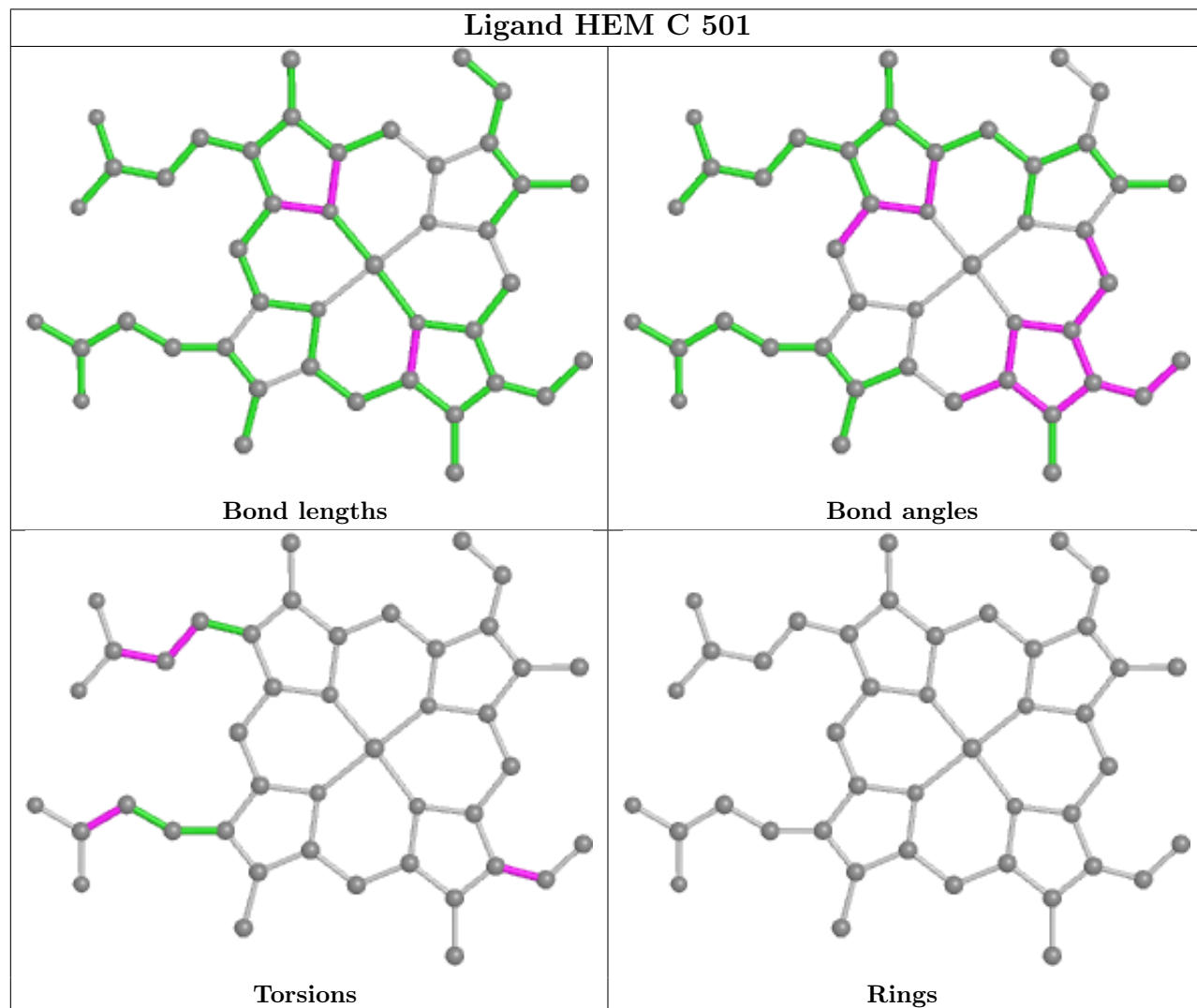
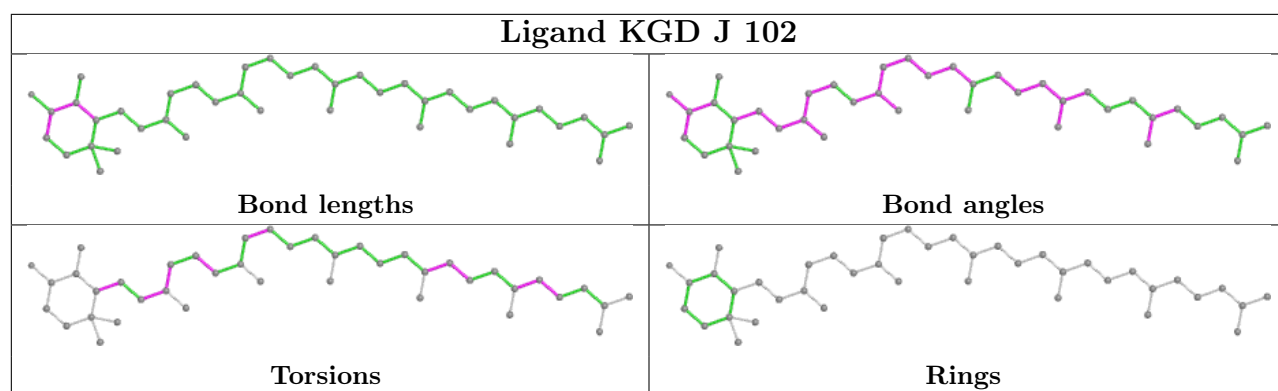


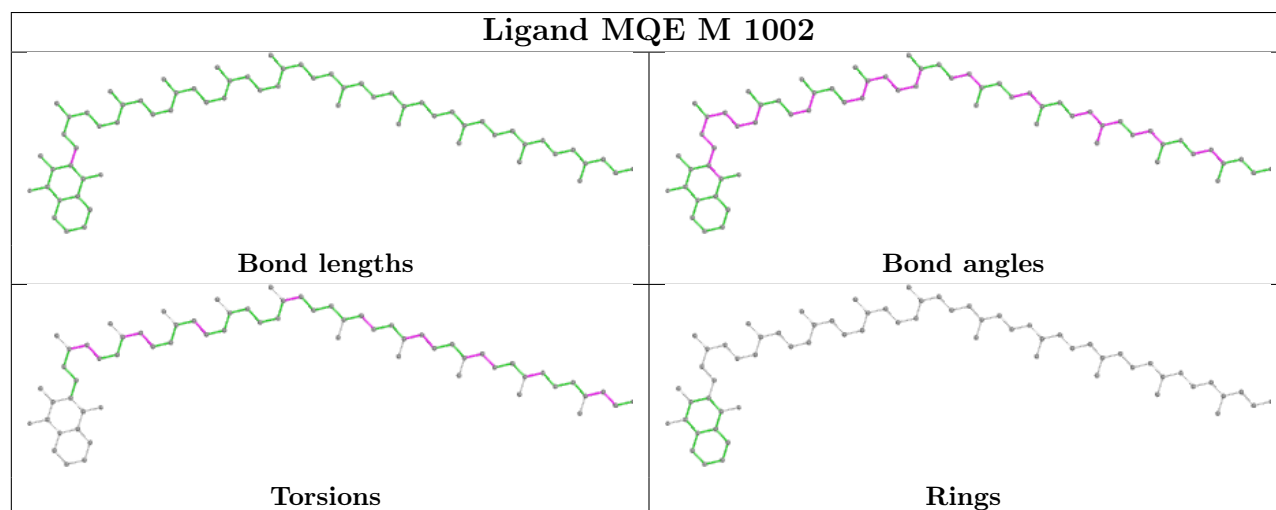
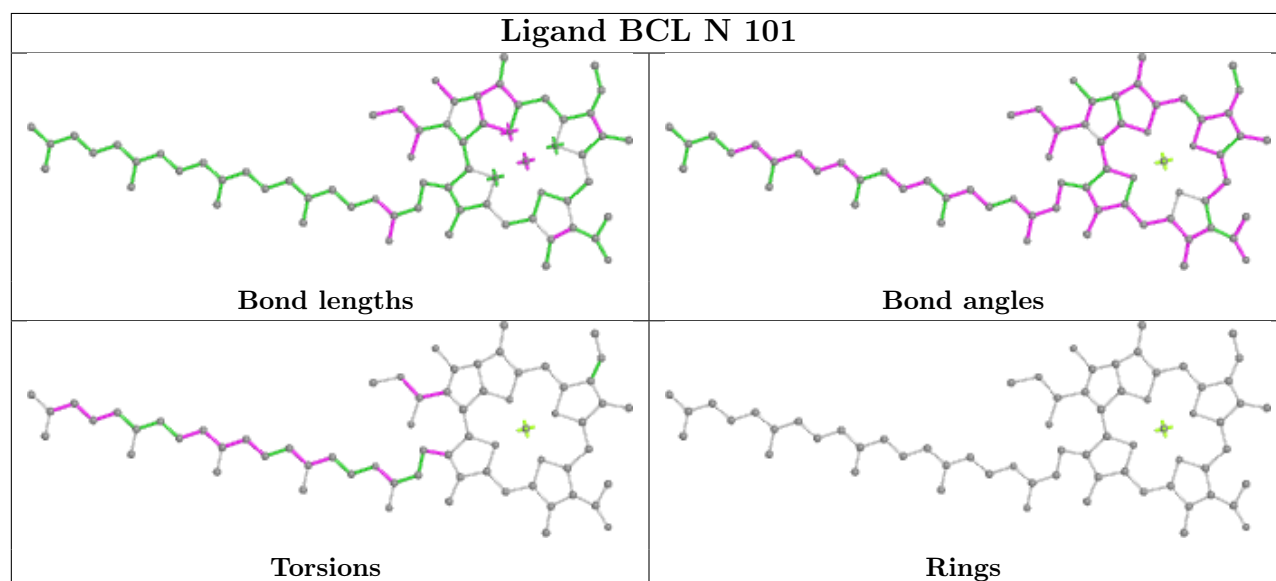
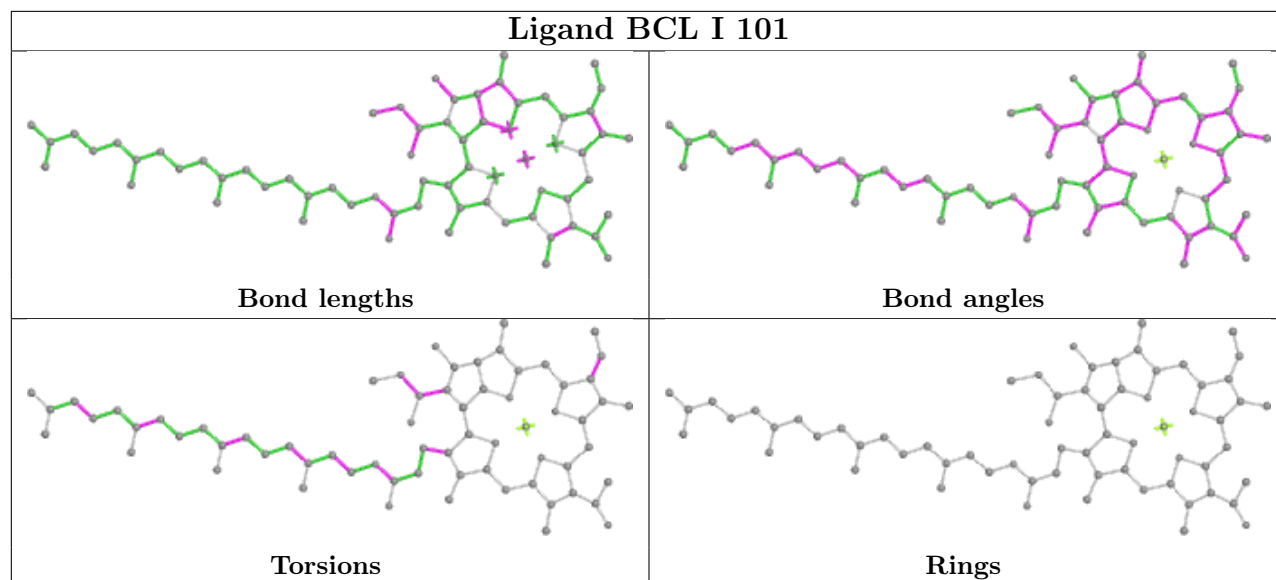


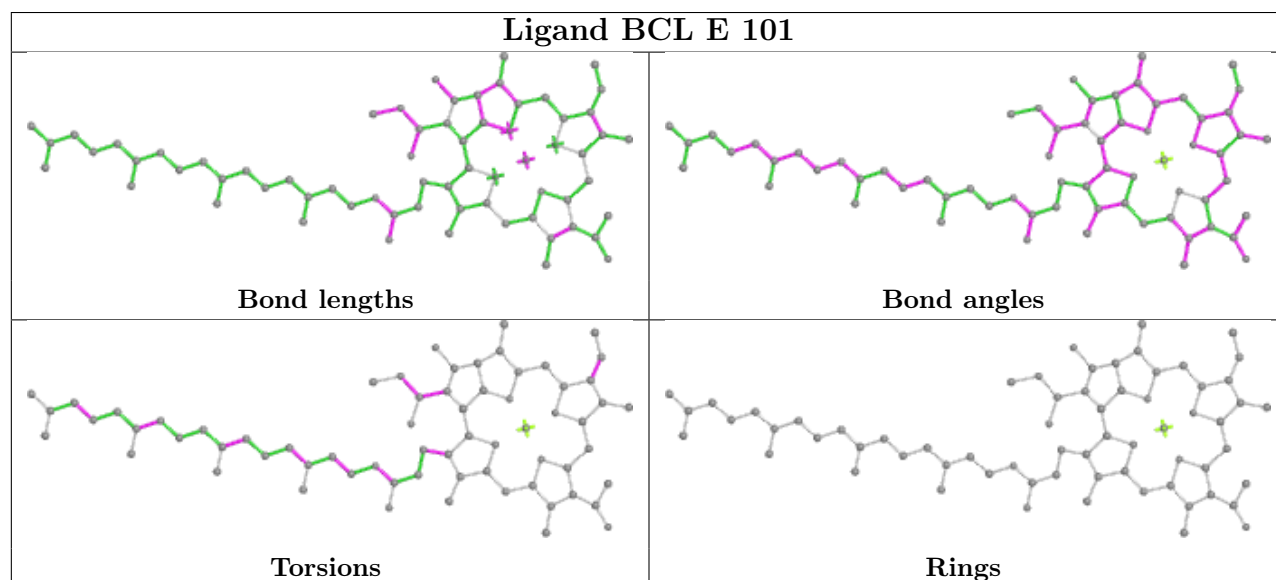
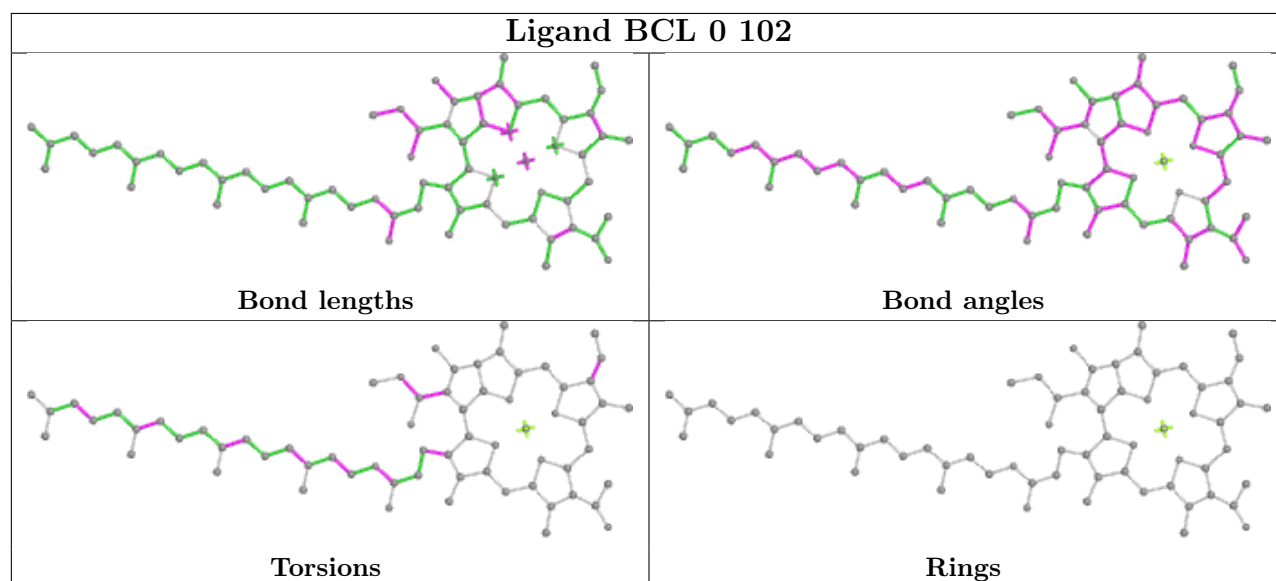
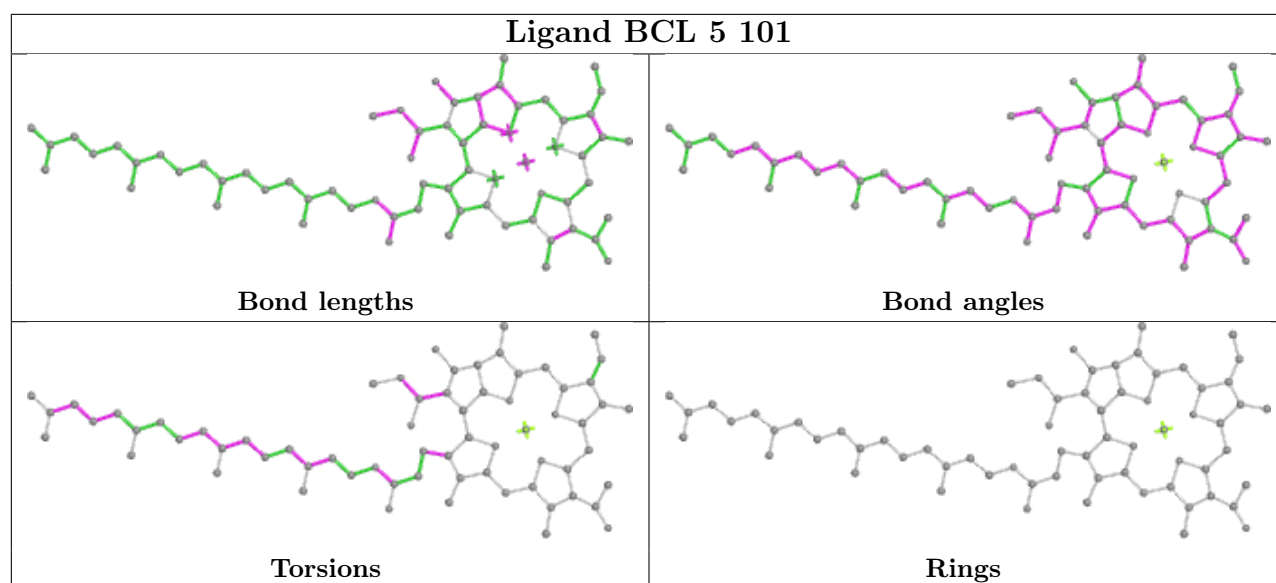


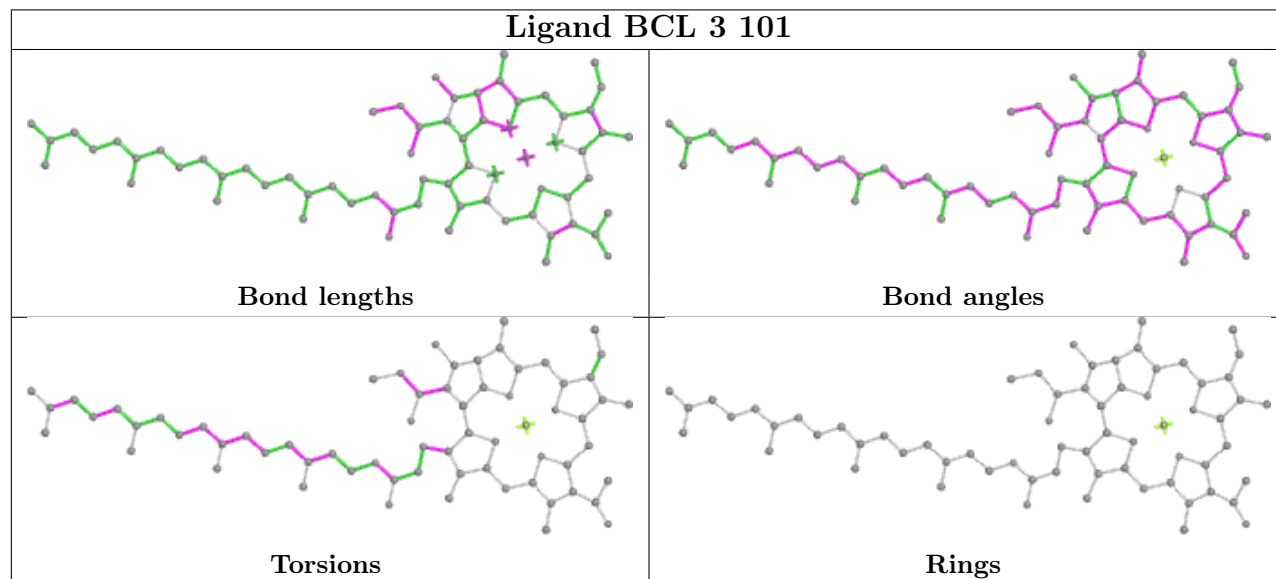
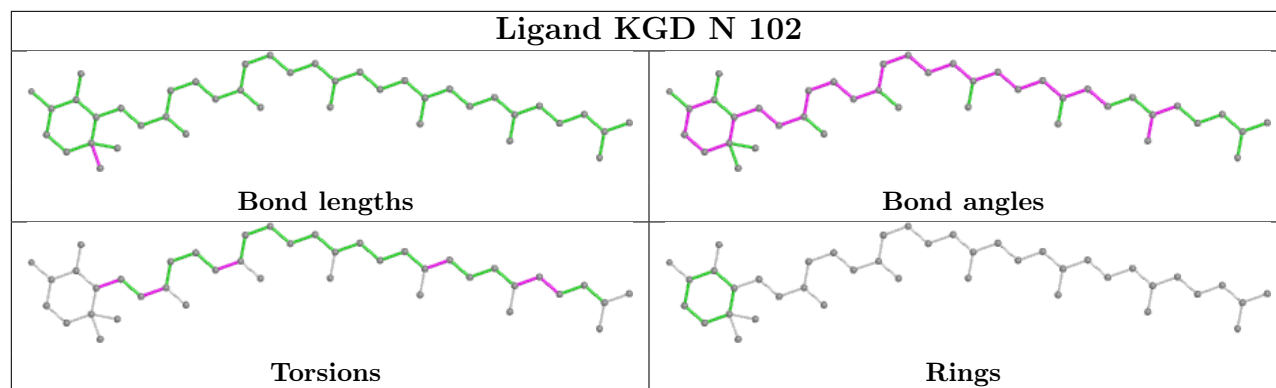


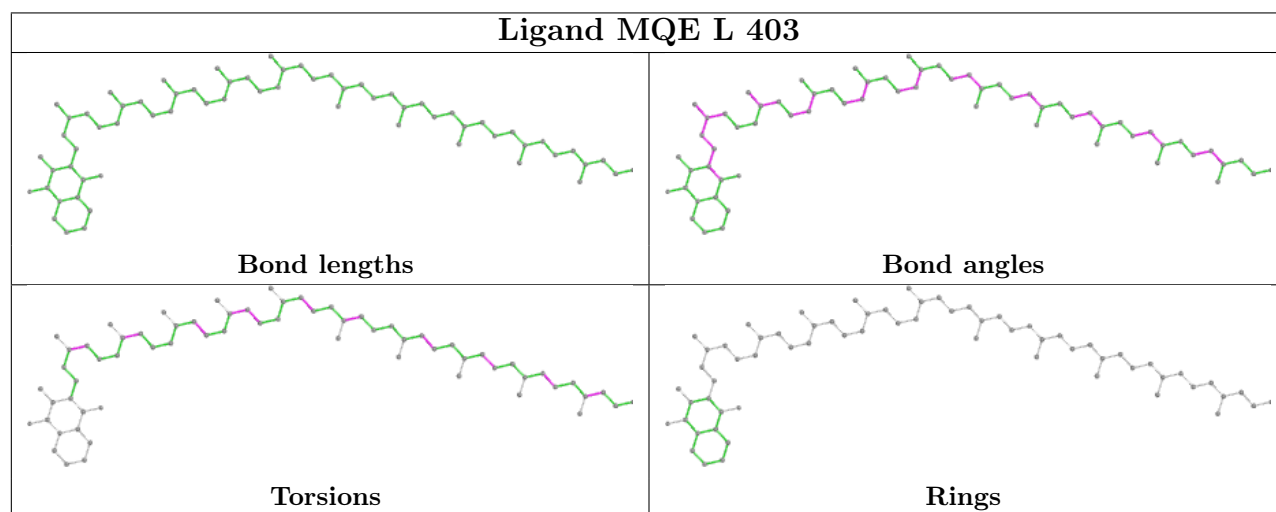
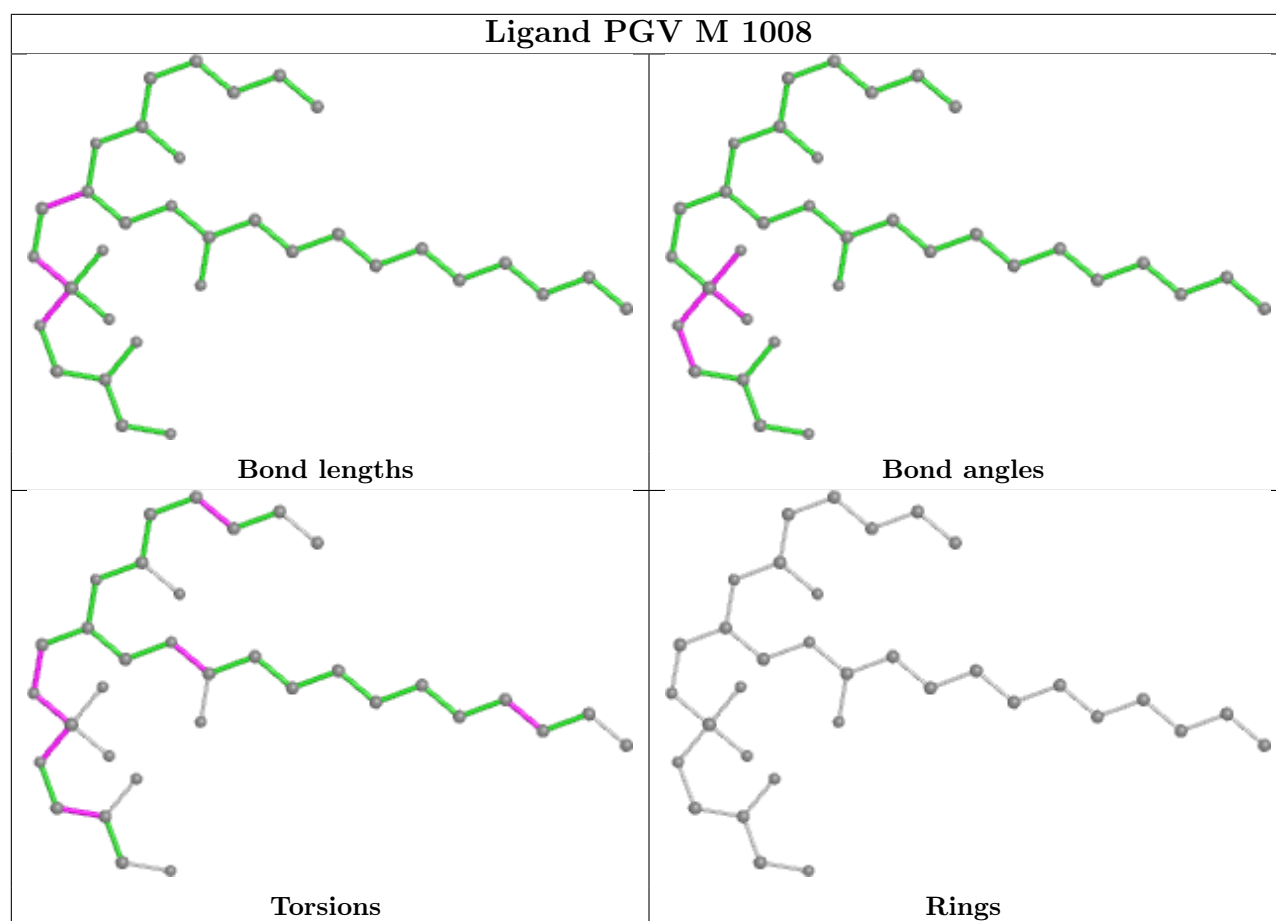


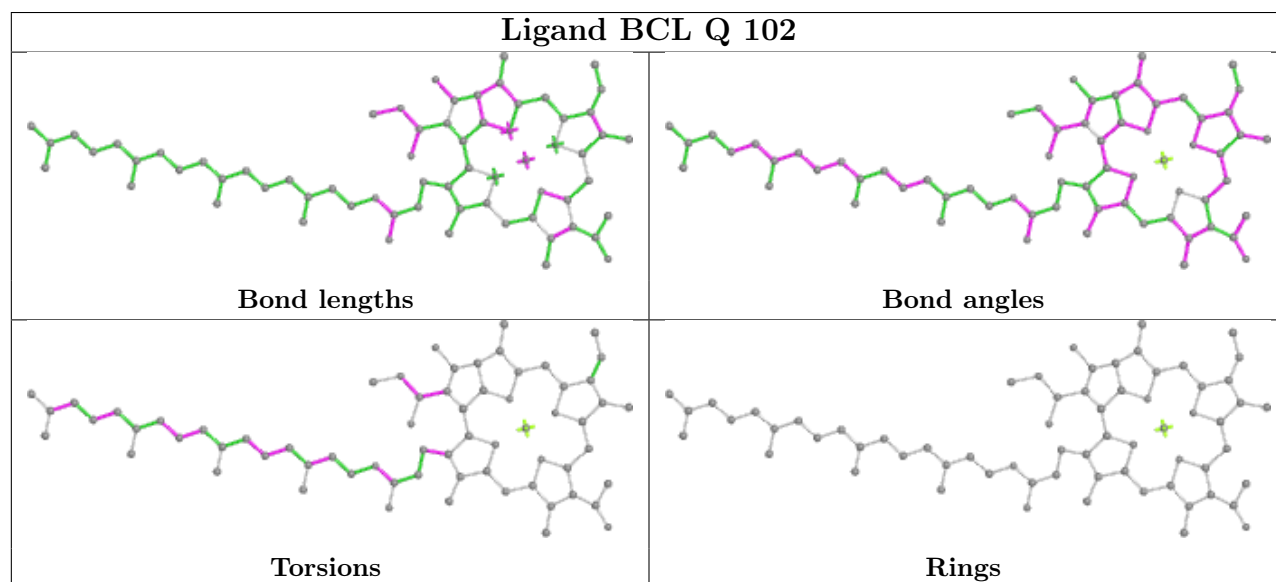
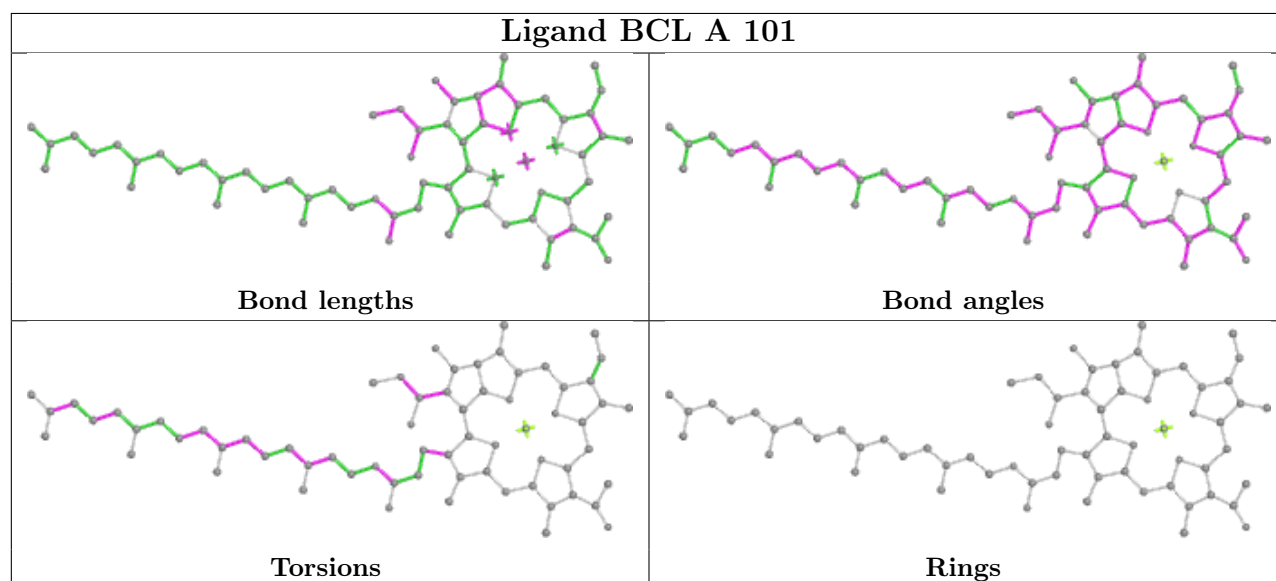
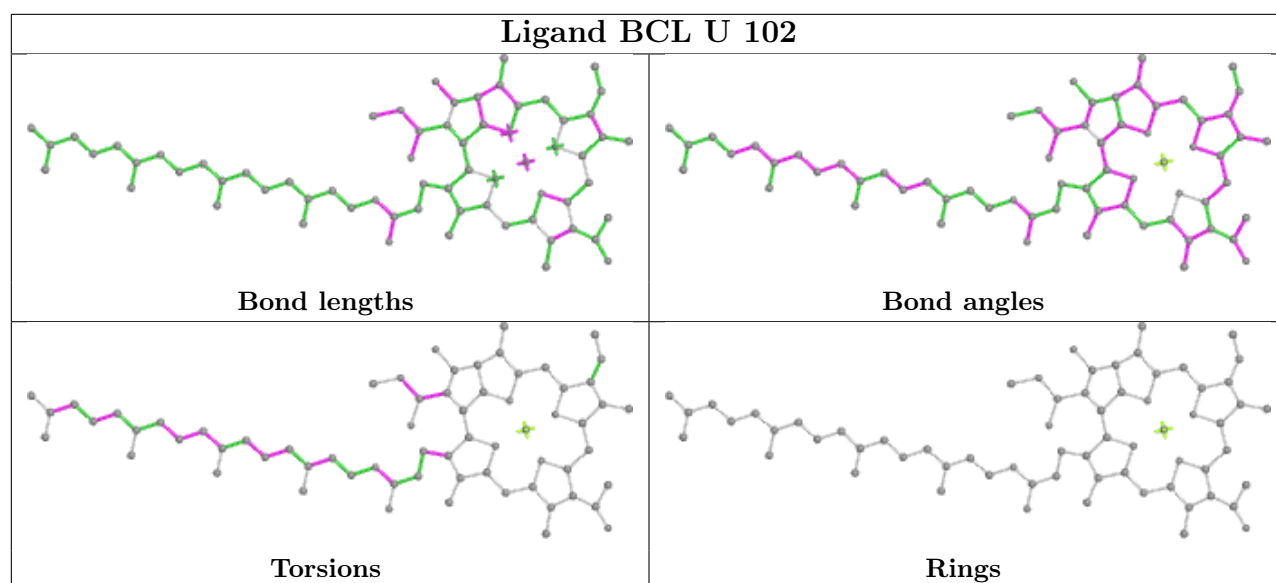




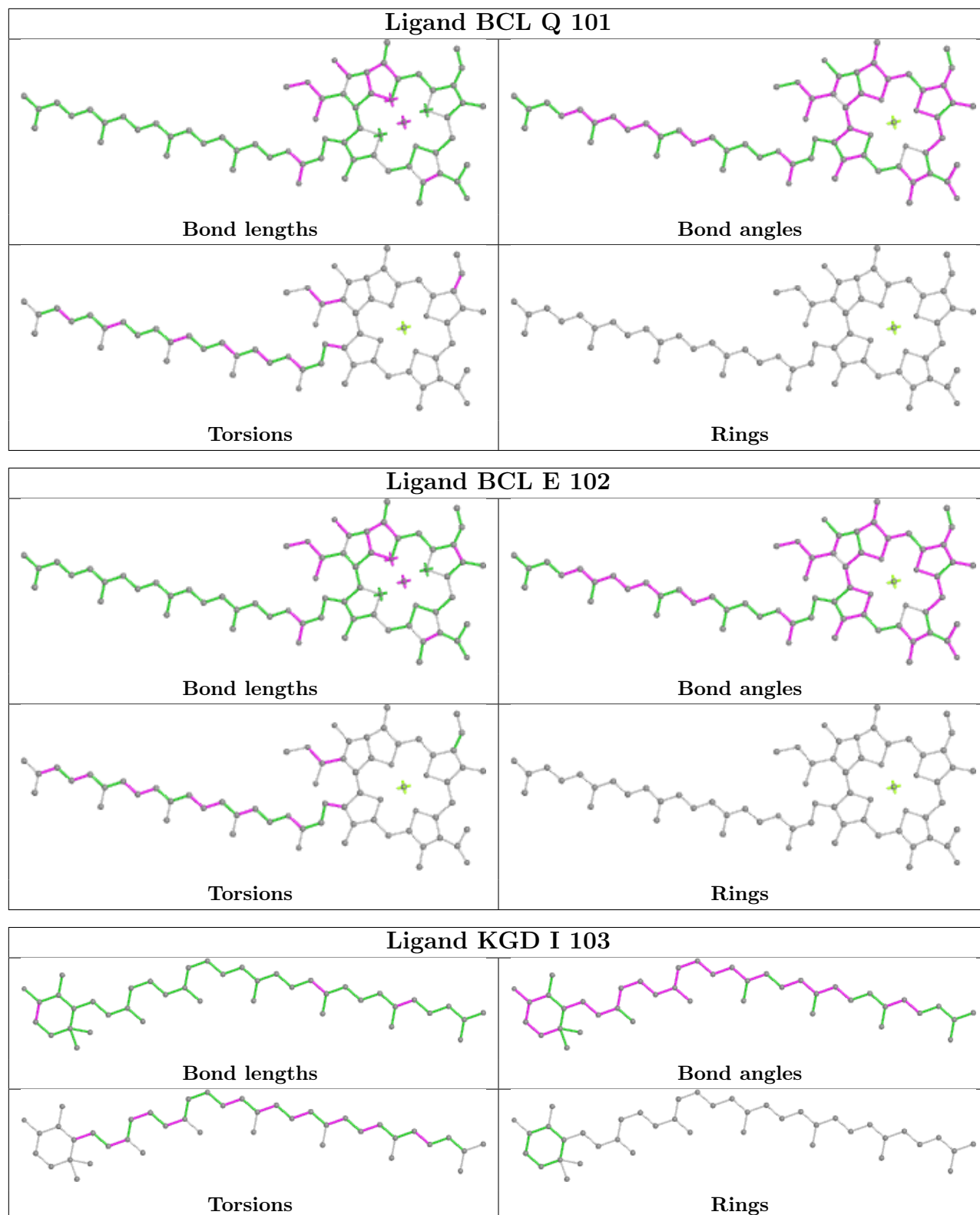


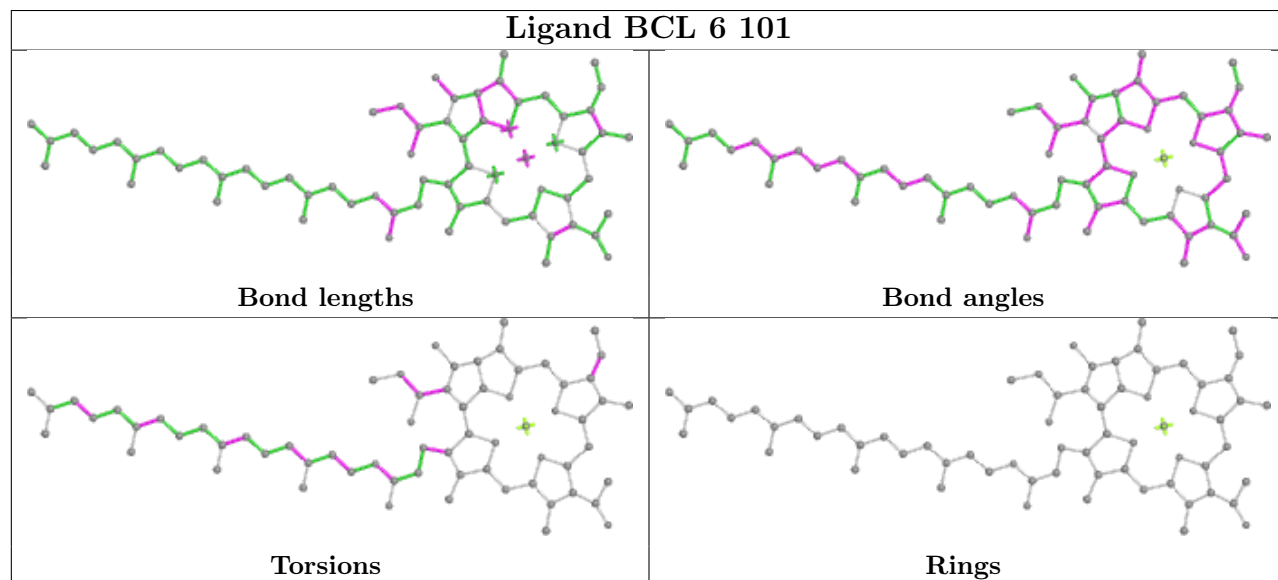
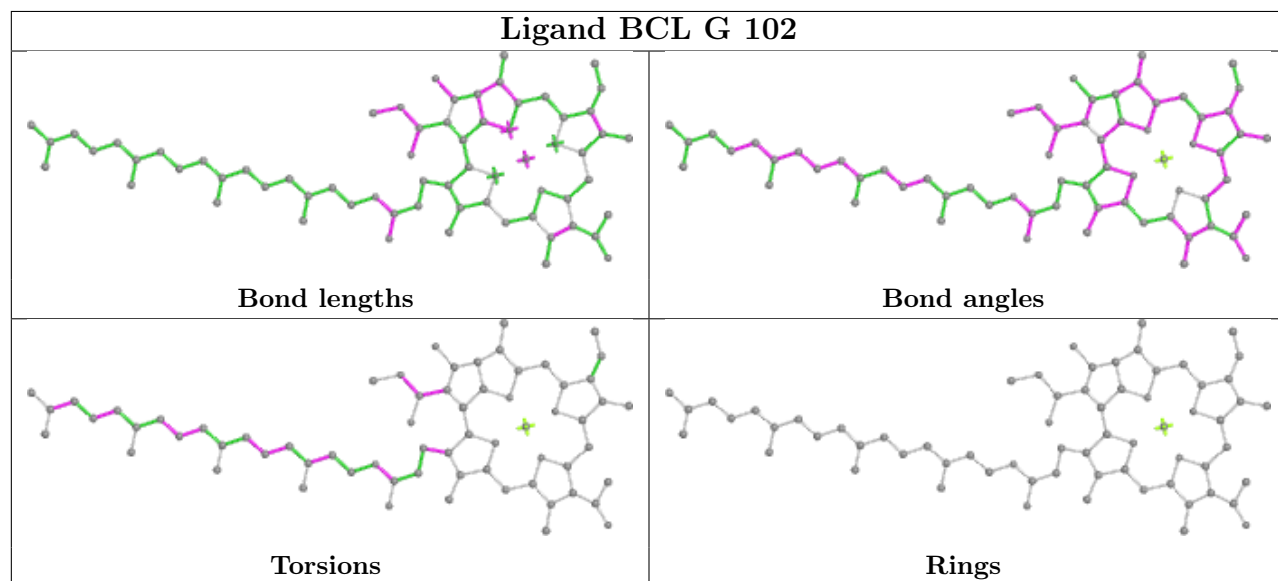
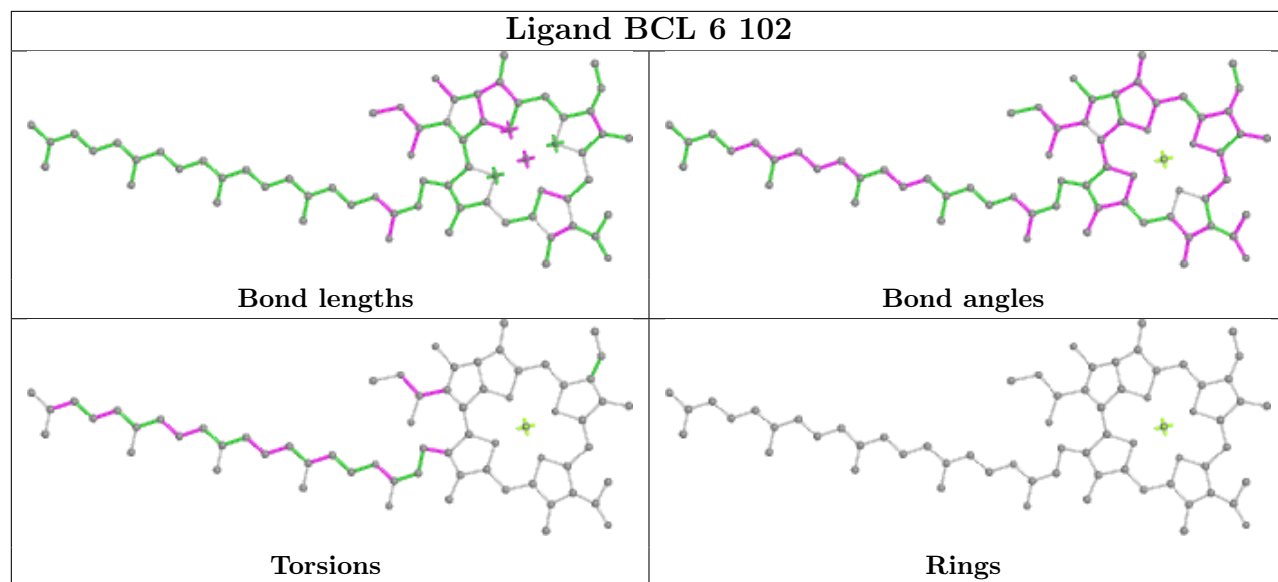




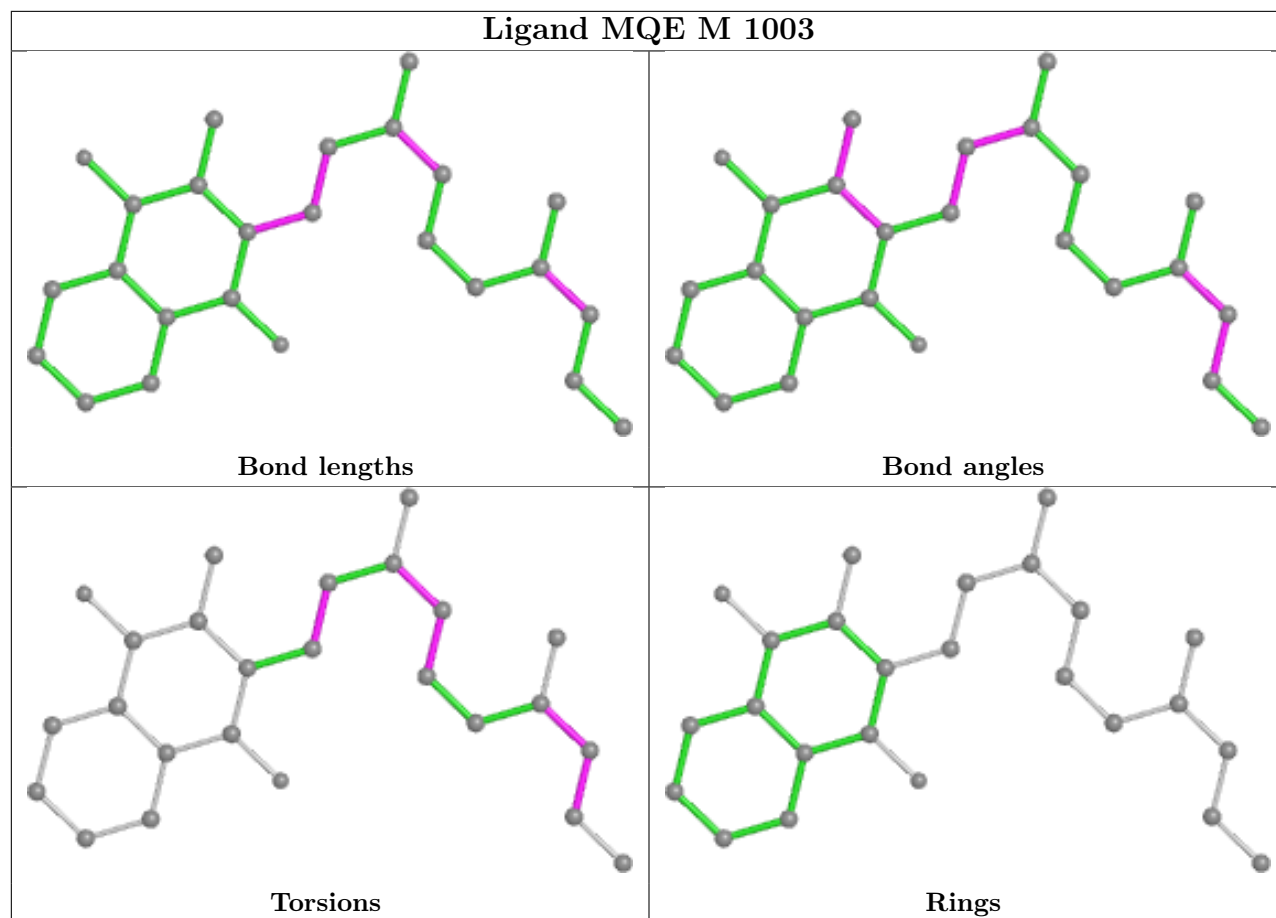




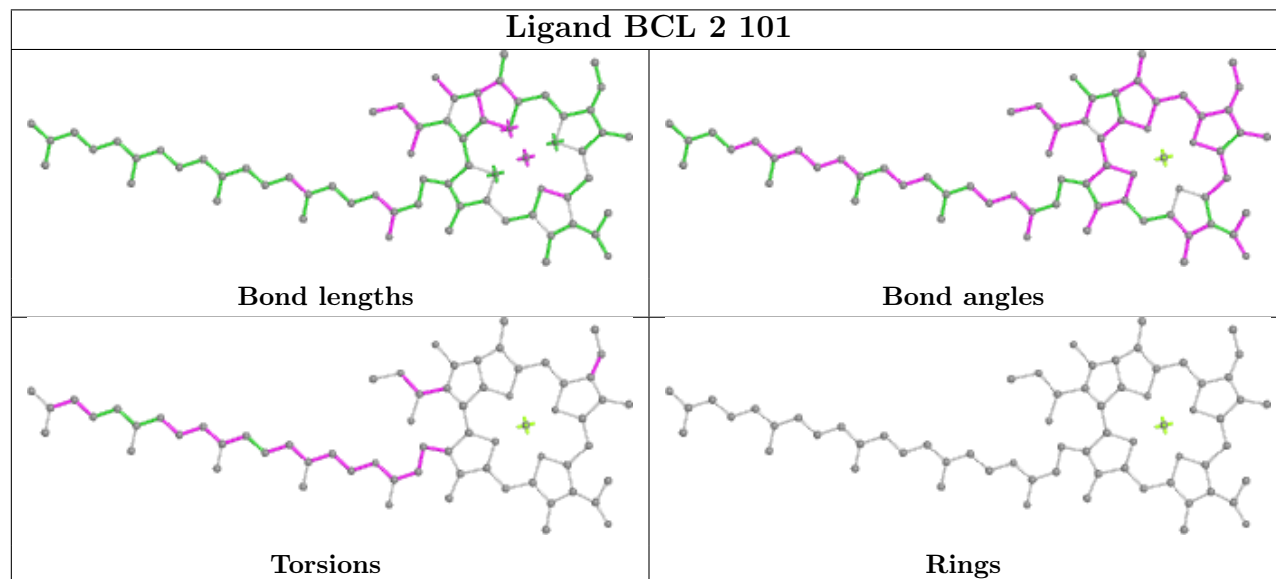


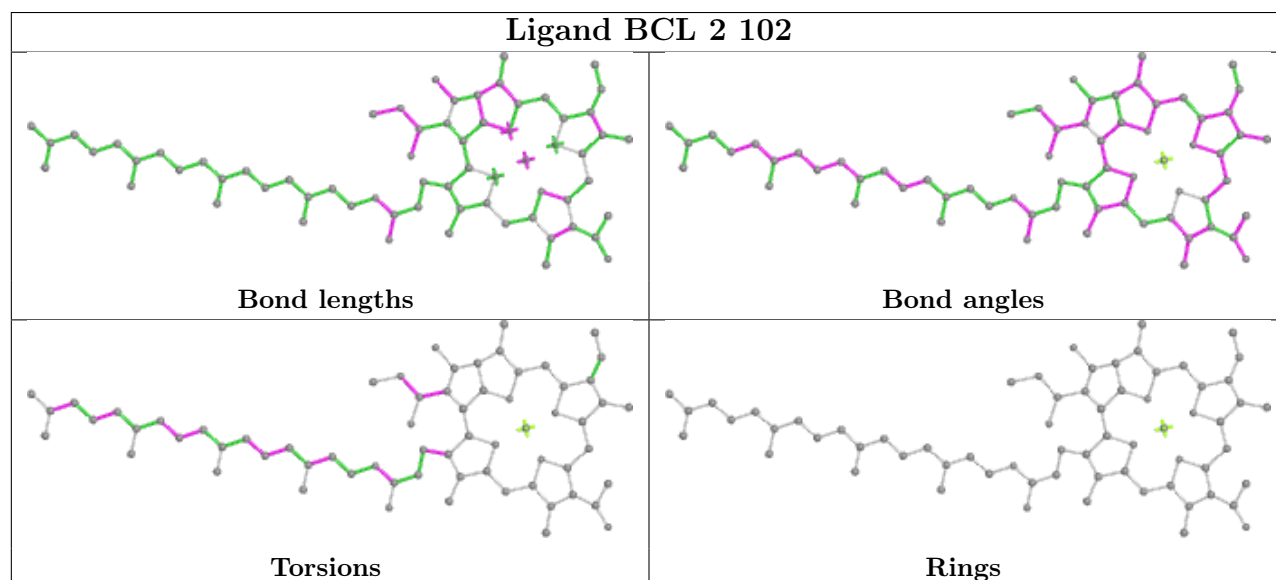
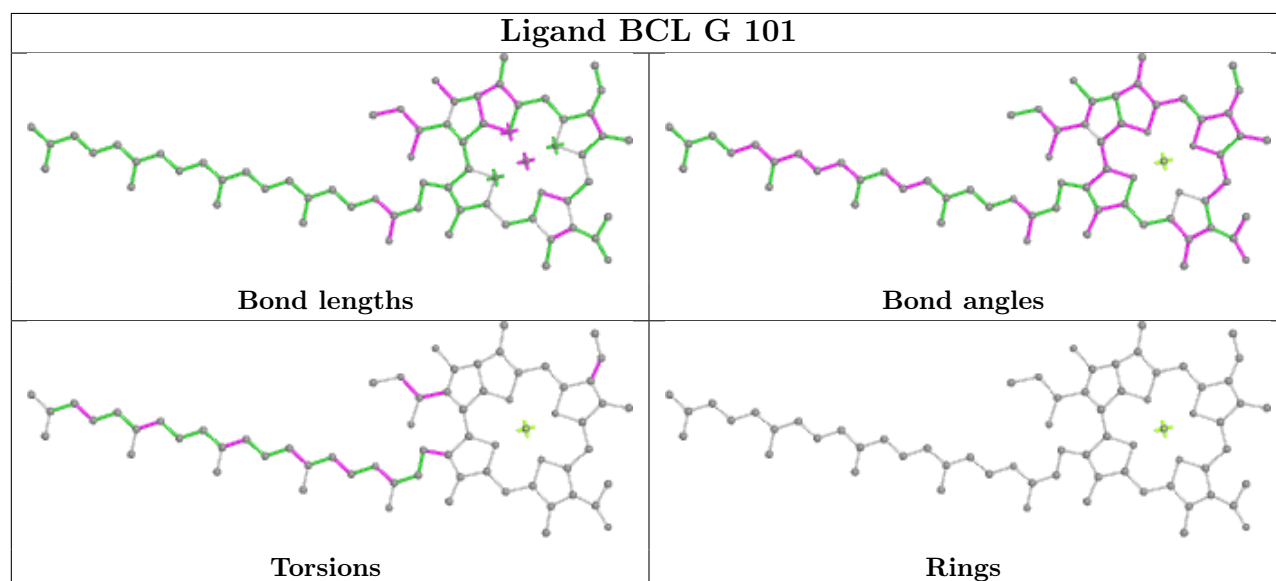
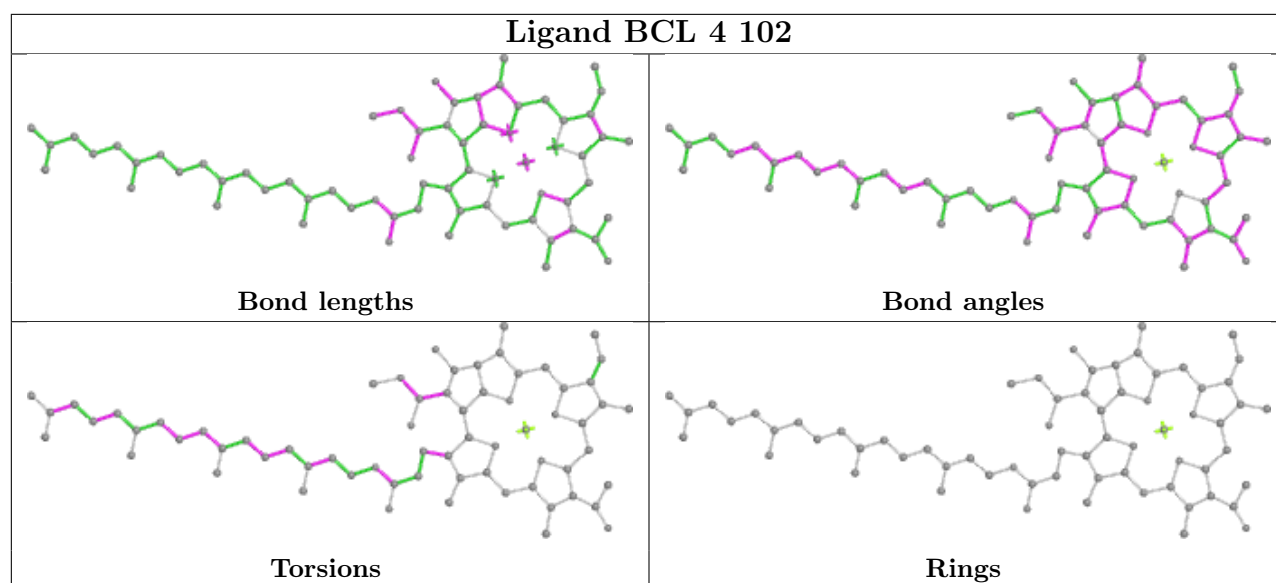


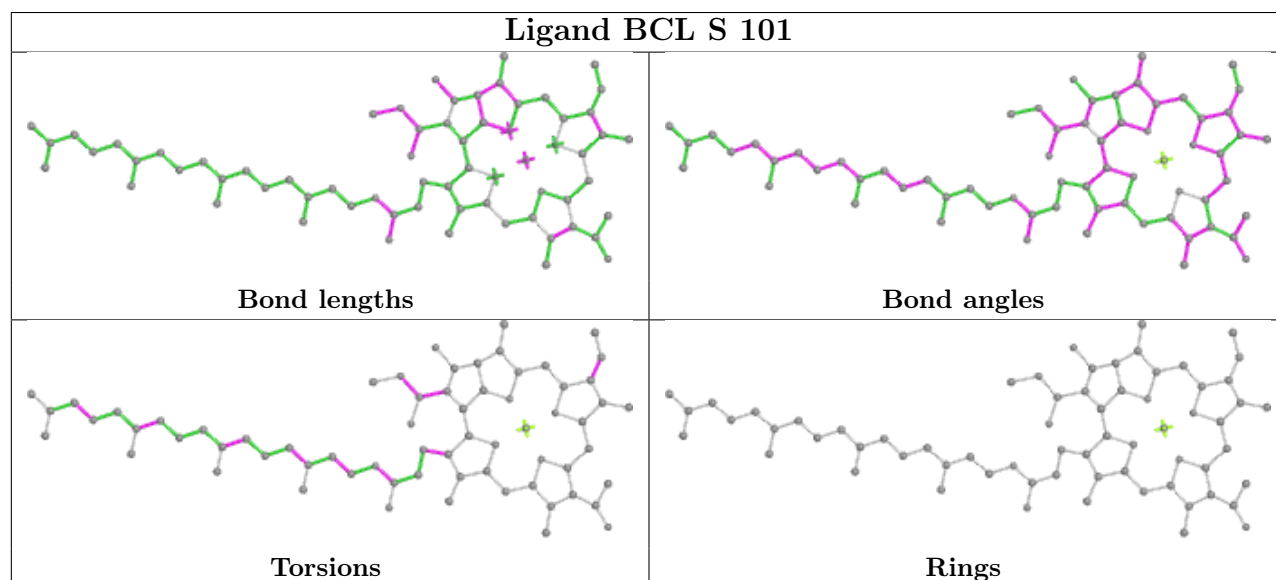
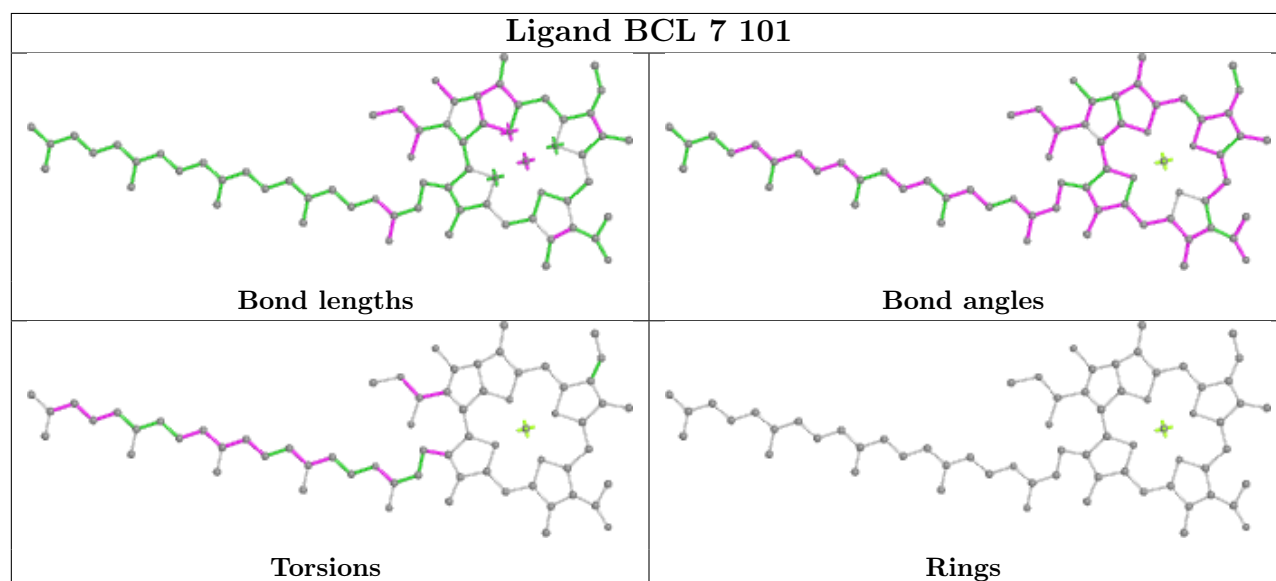
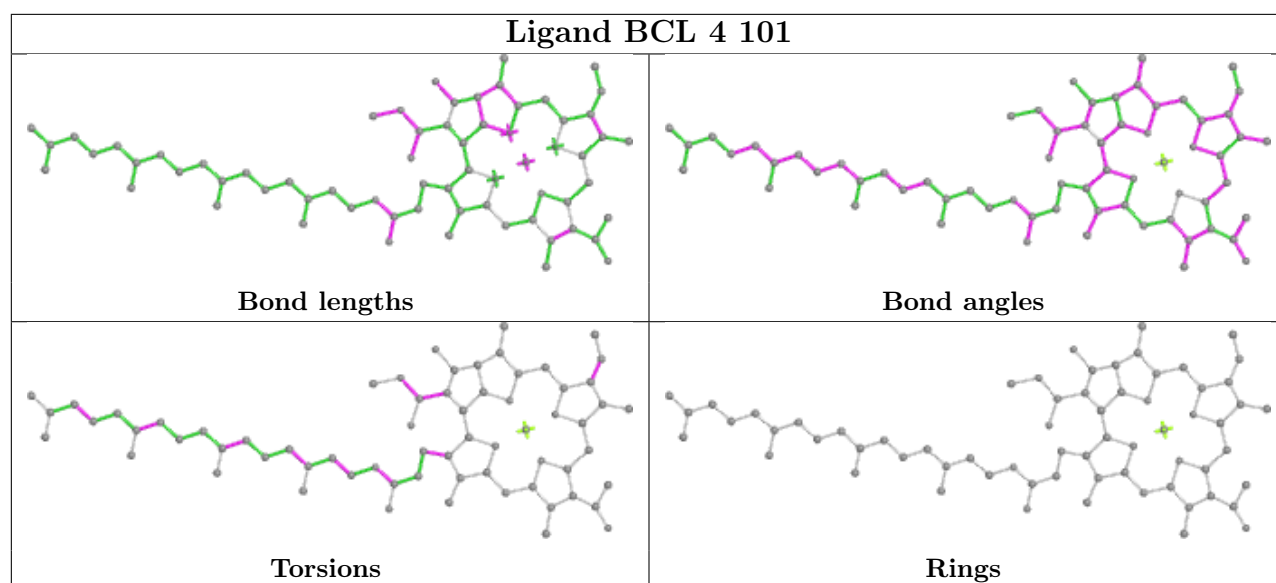
## Ligand MQE M 1003

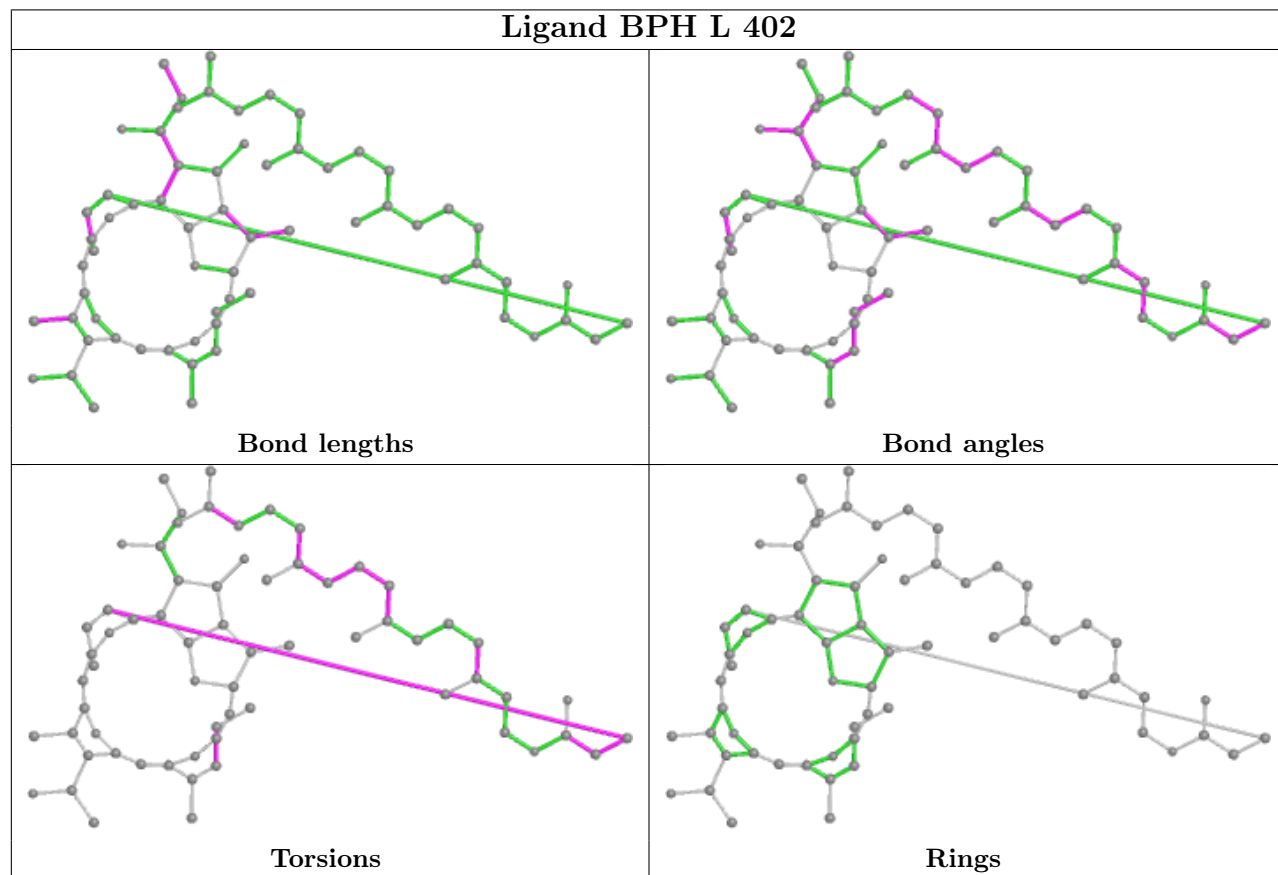
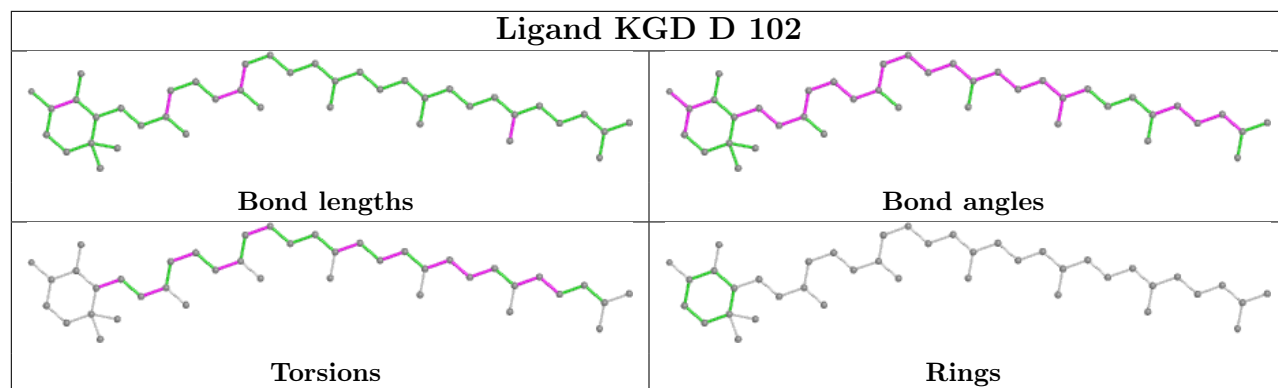


## Ligand BCL 2 101

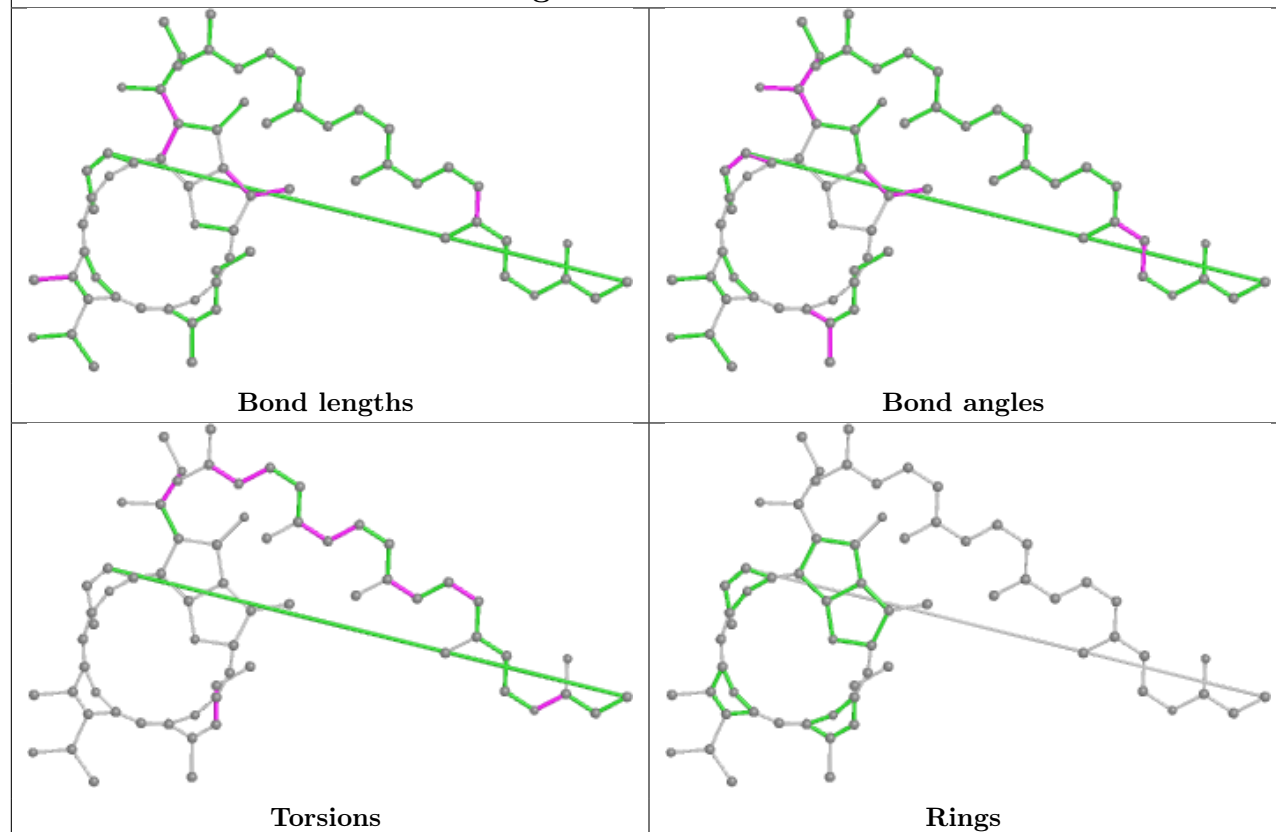




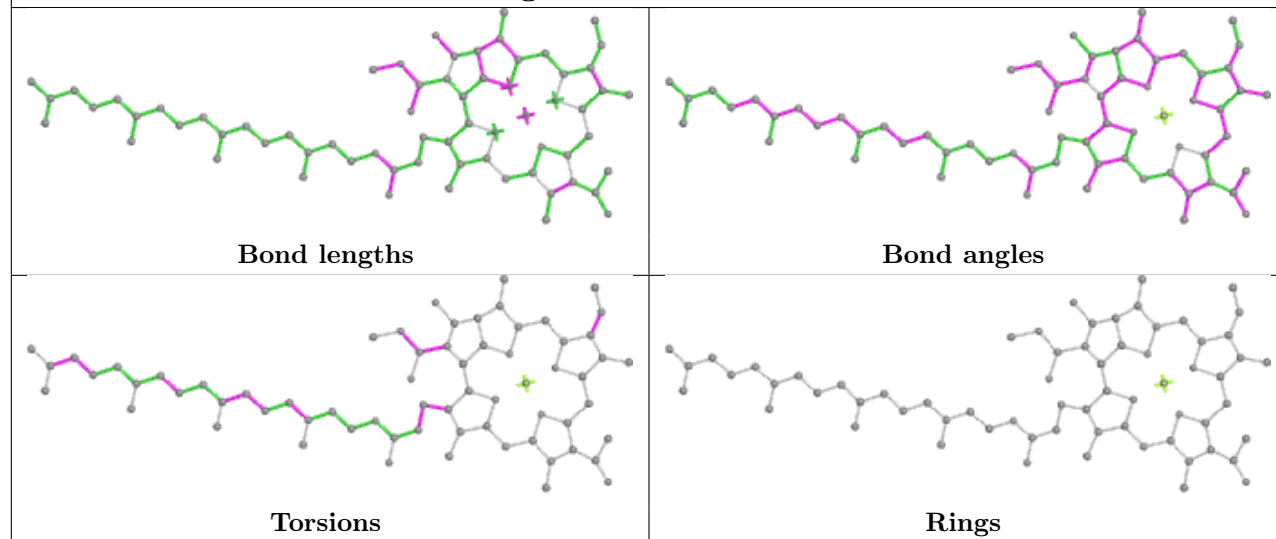


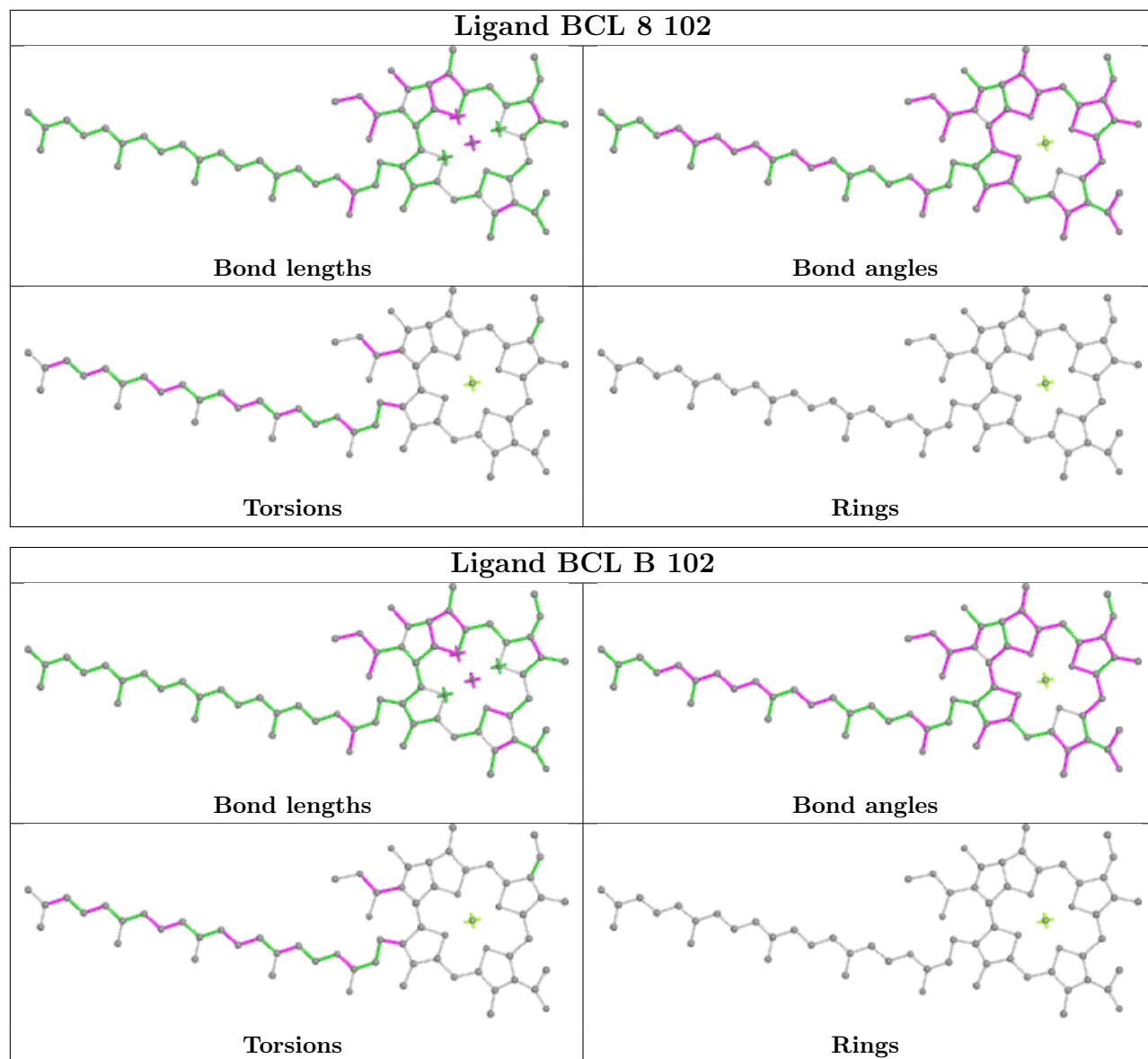


## Ligand BPH L 405

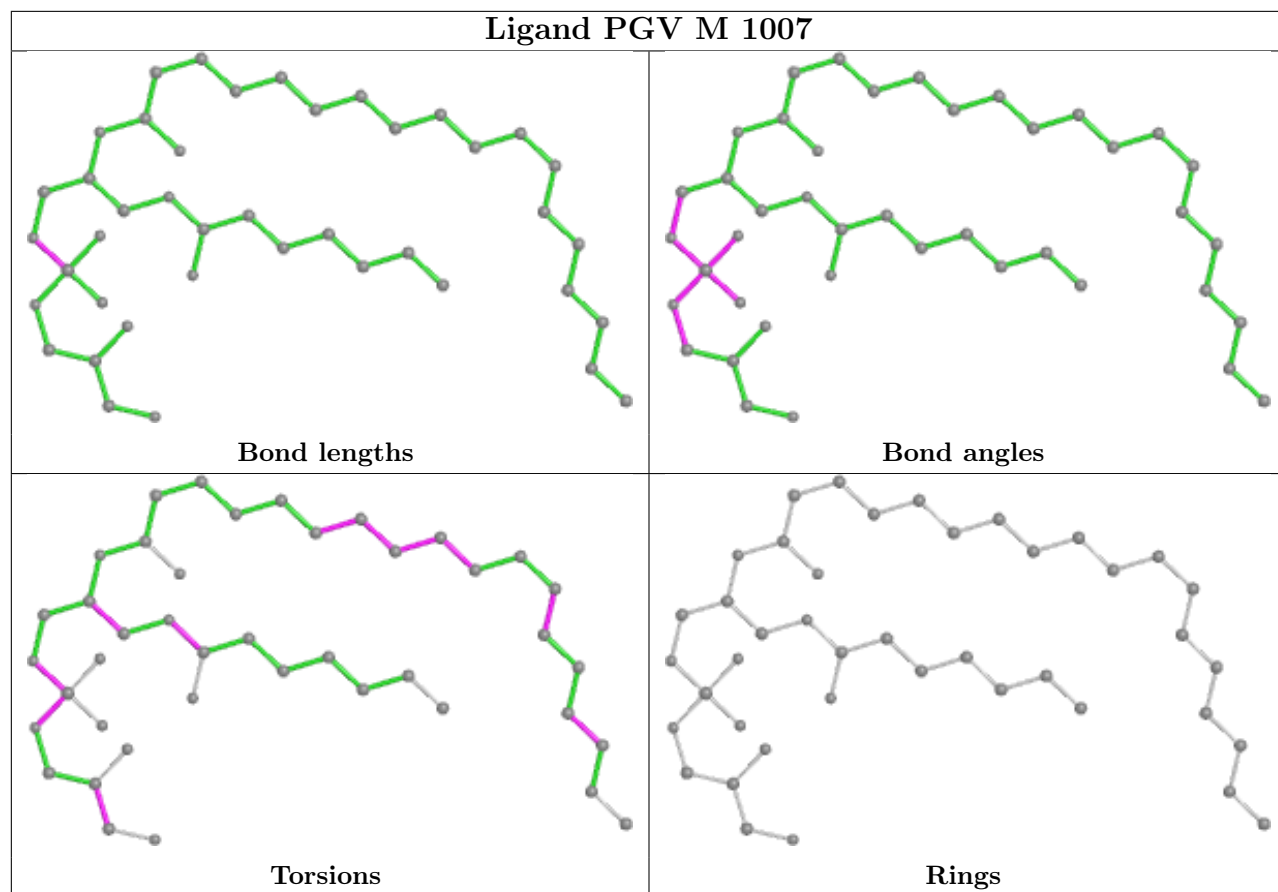


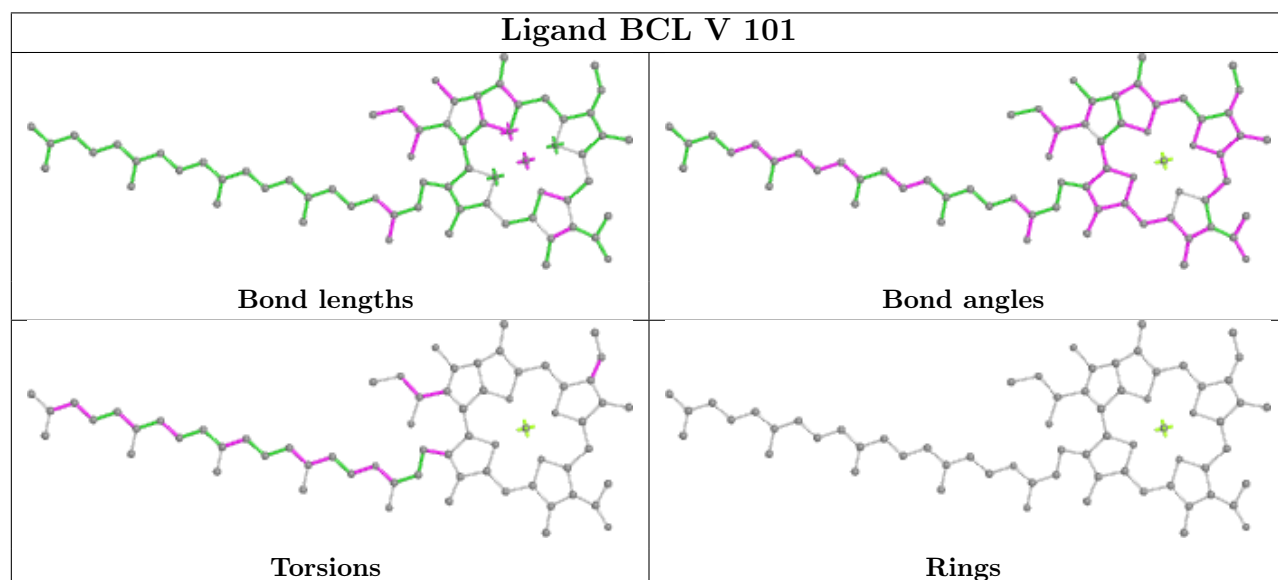
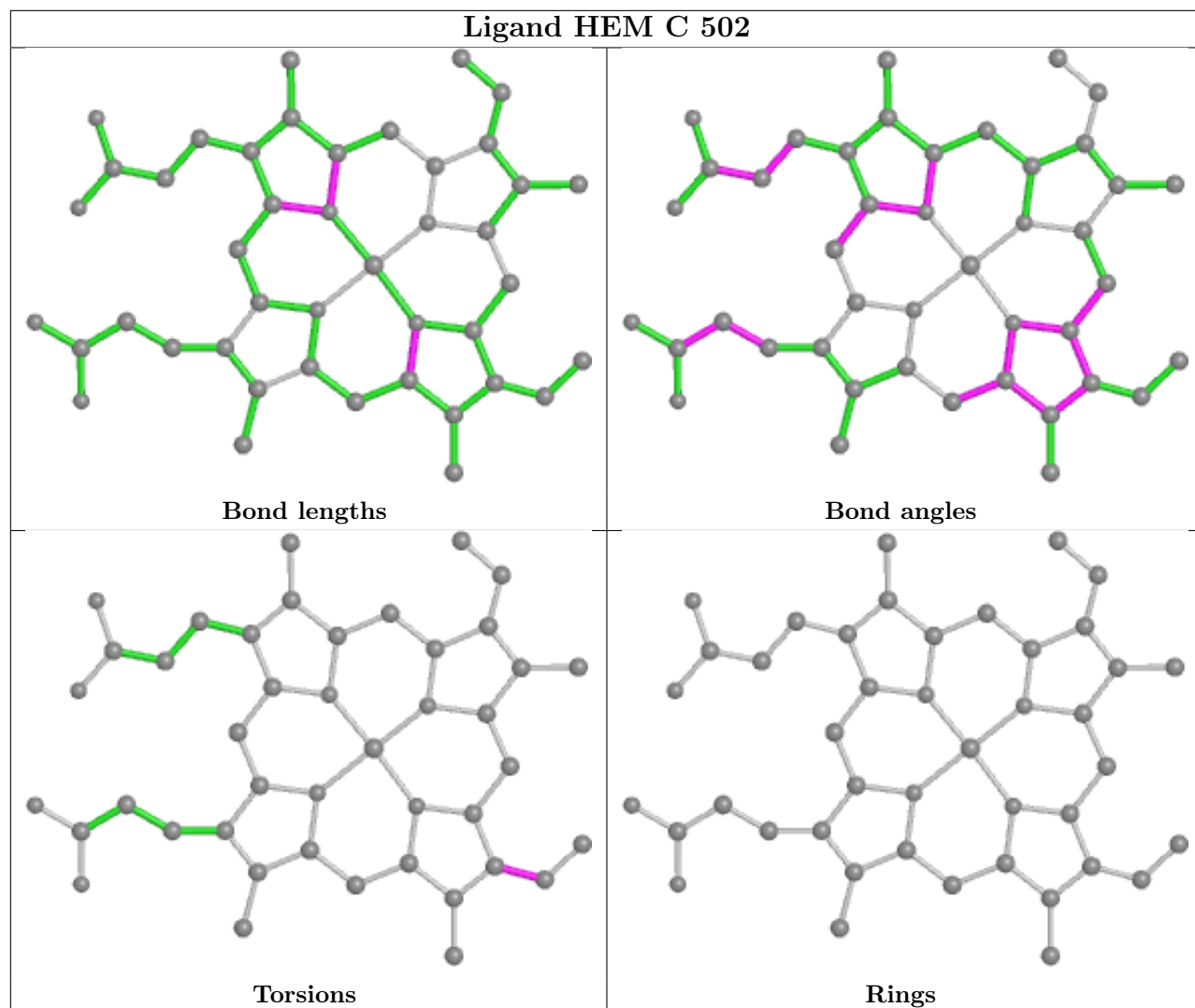
## Ligand BCL M 1005

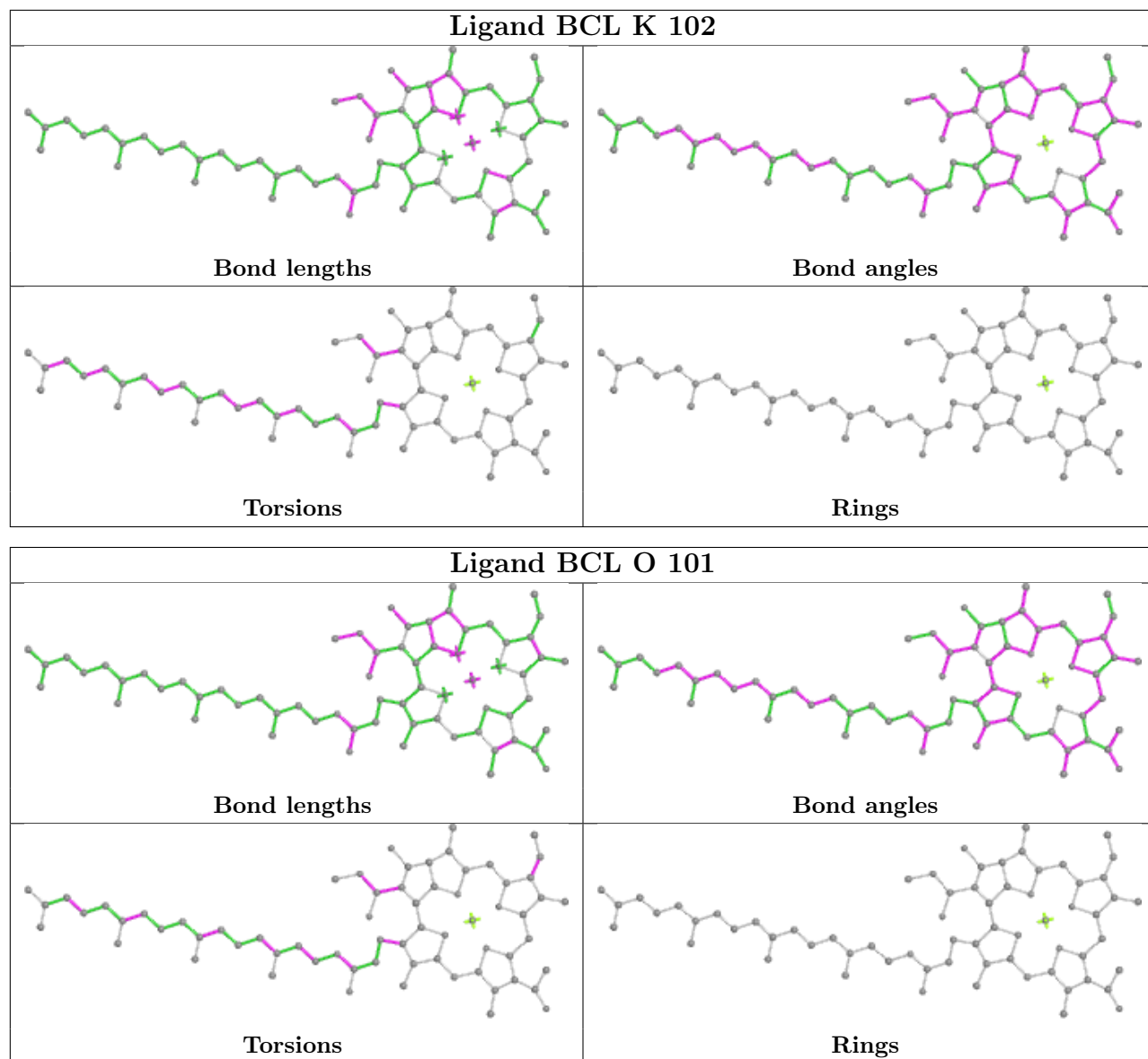




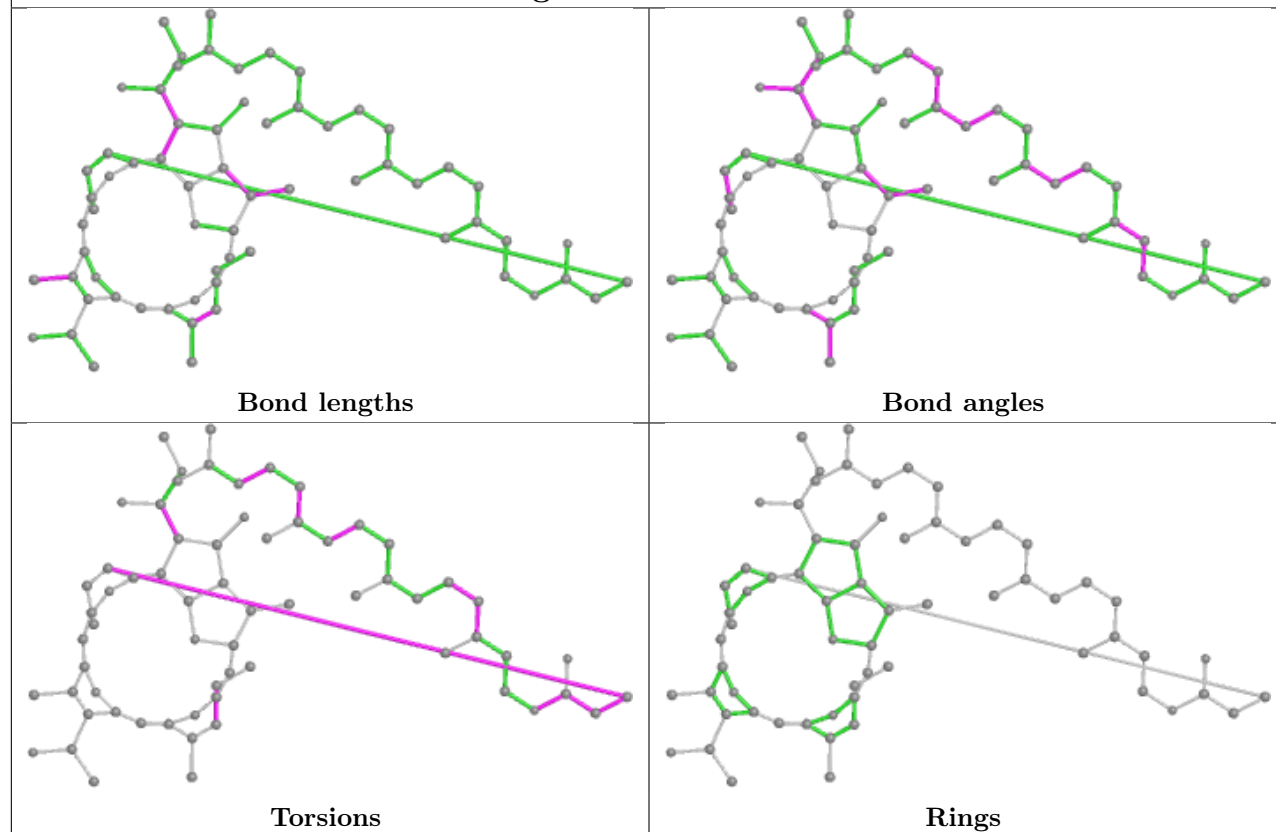




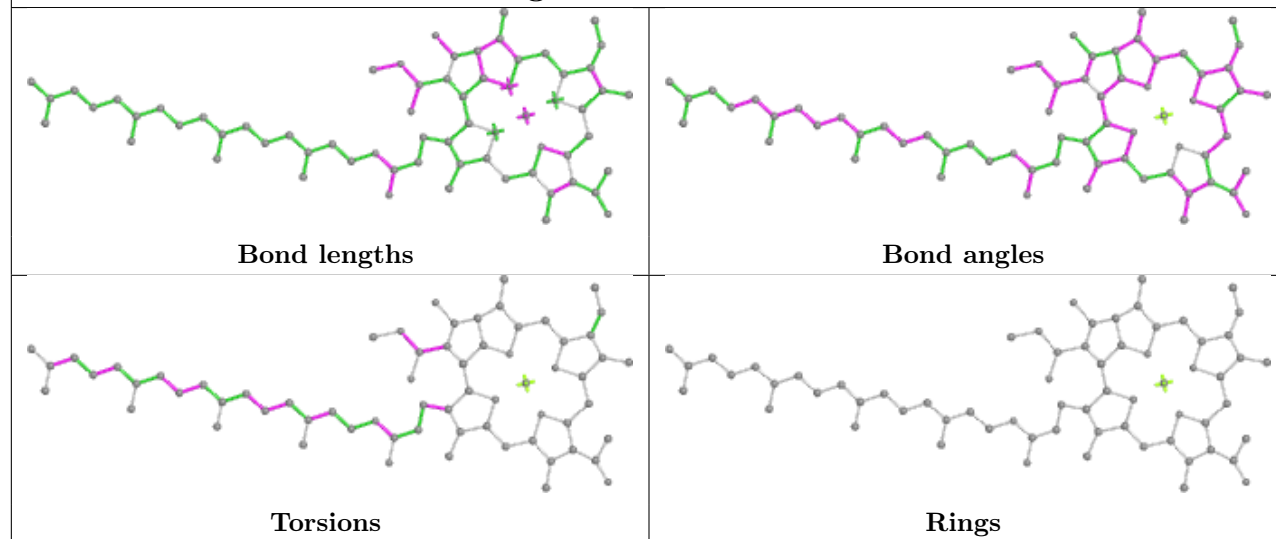


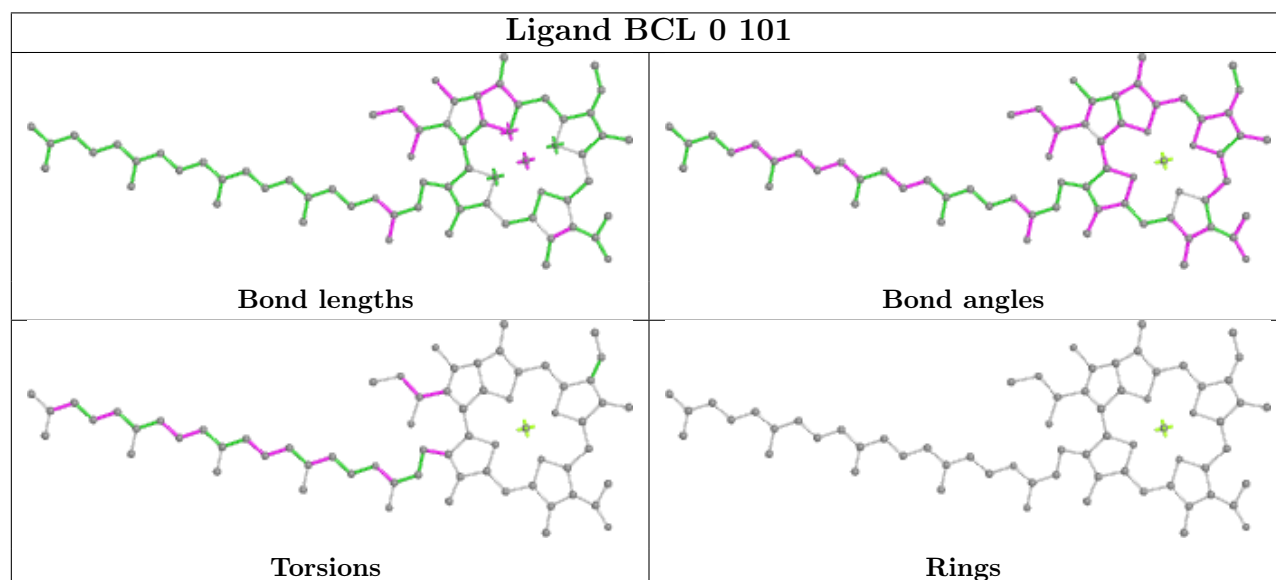
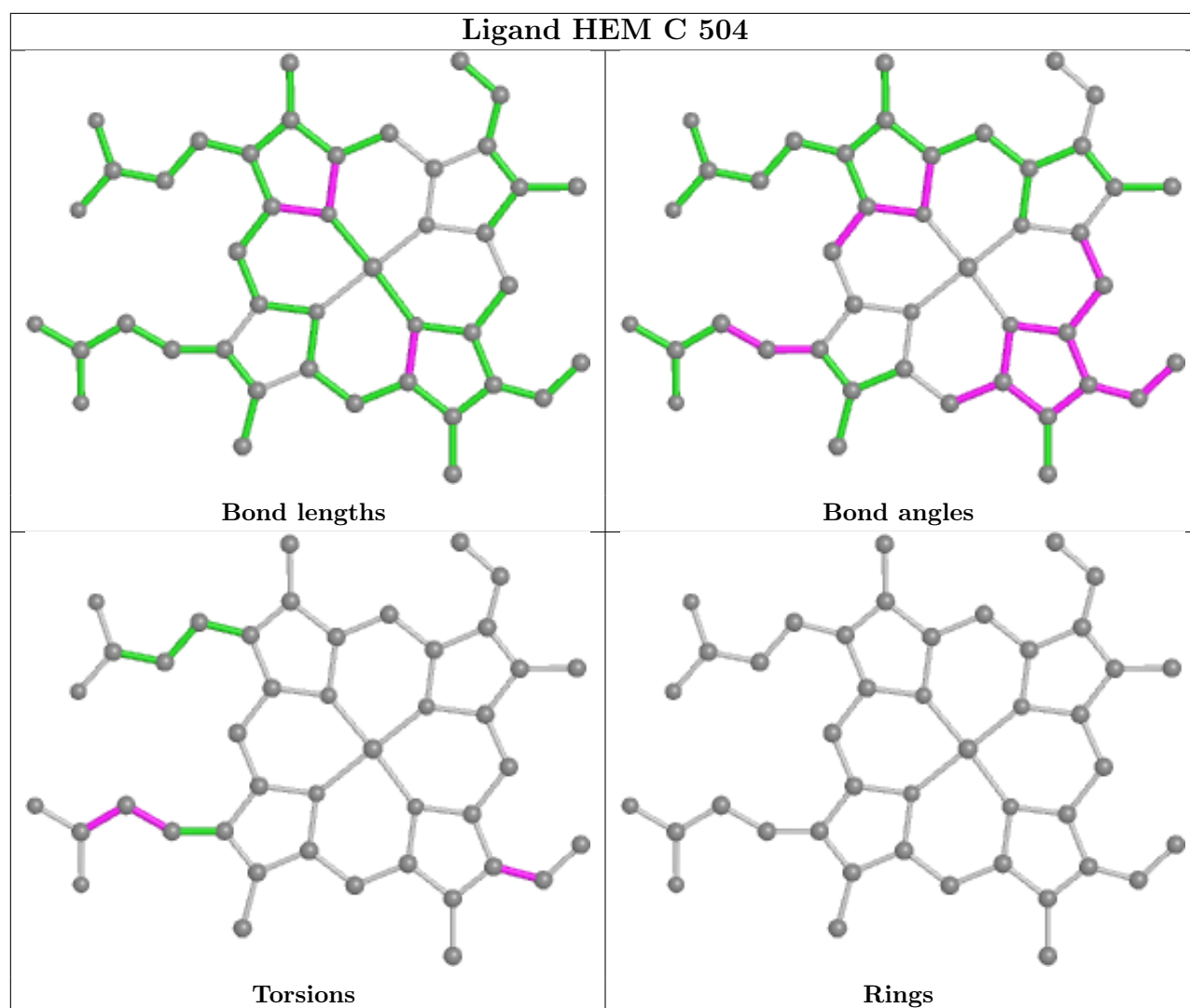


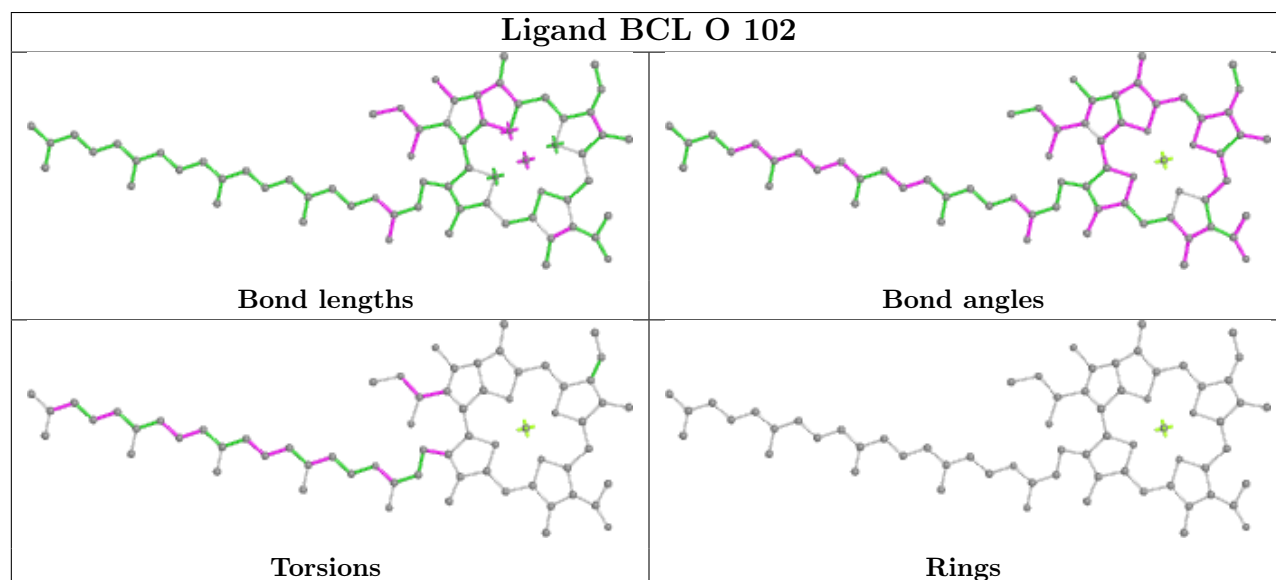
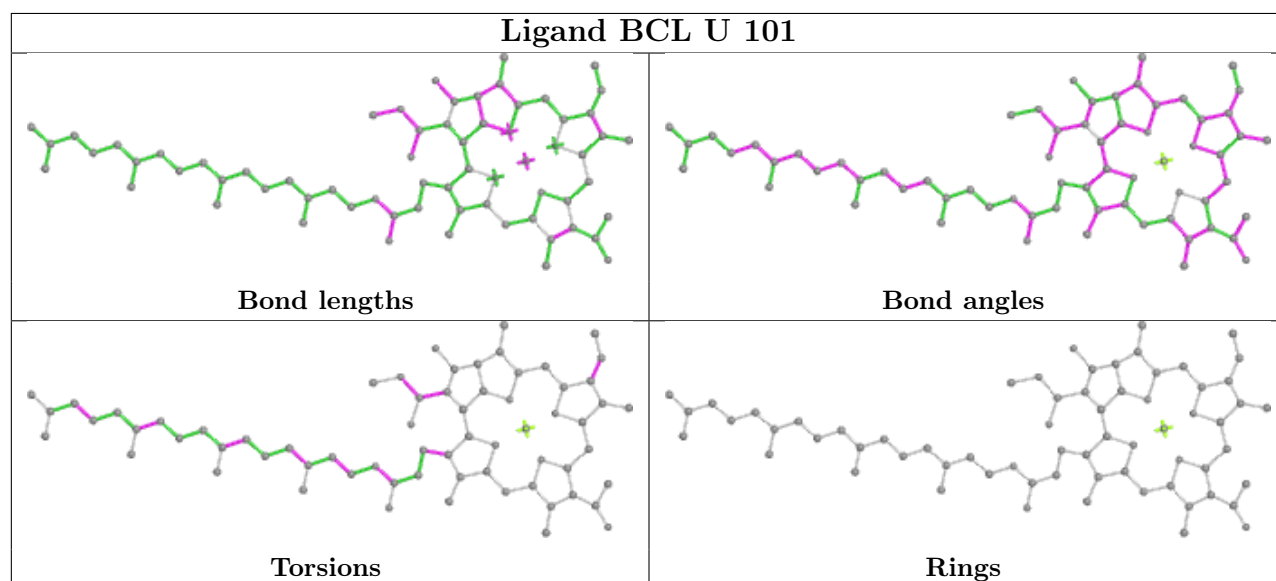
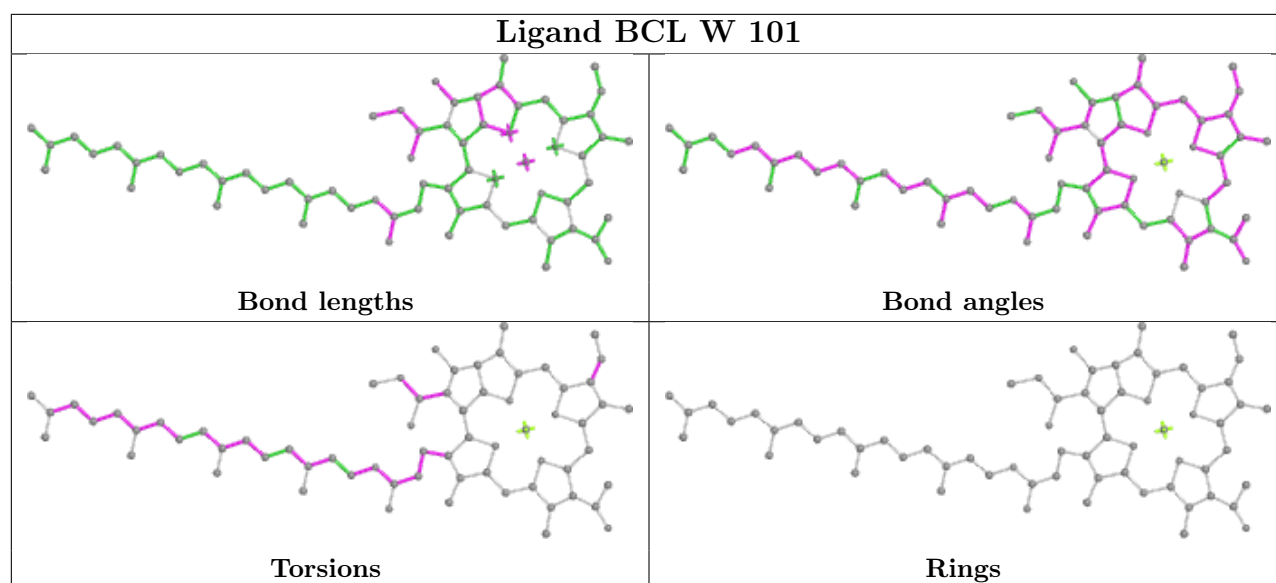
## Ligand BPH L 404

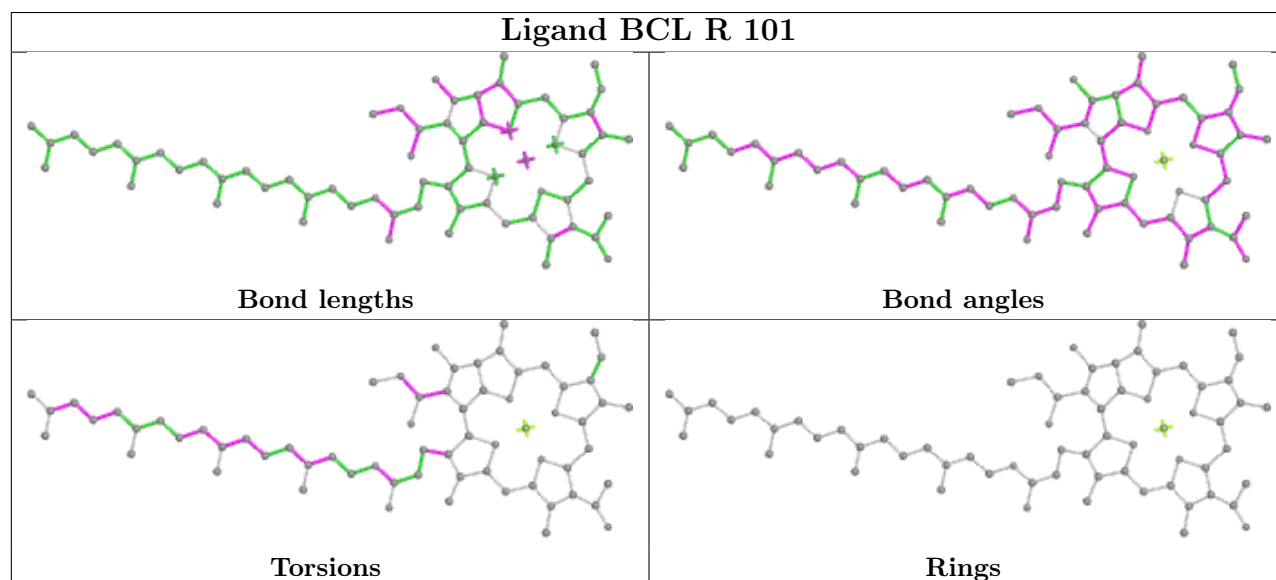
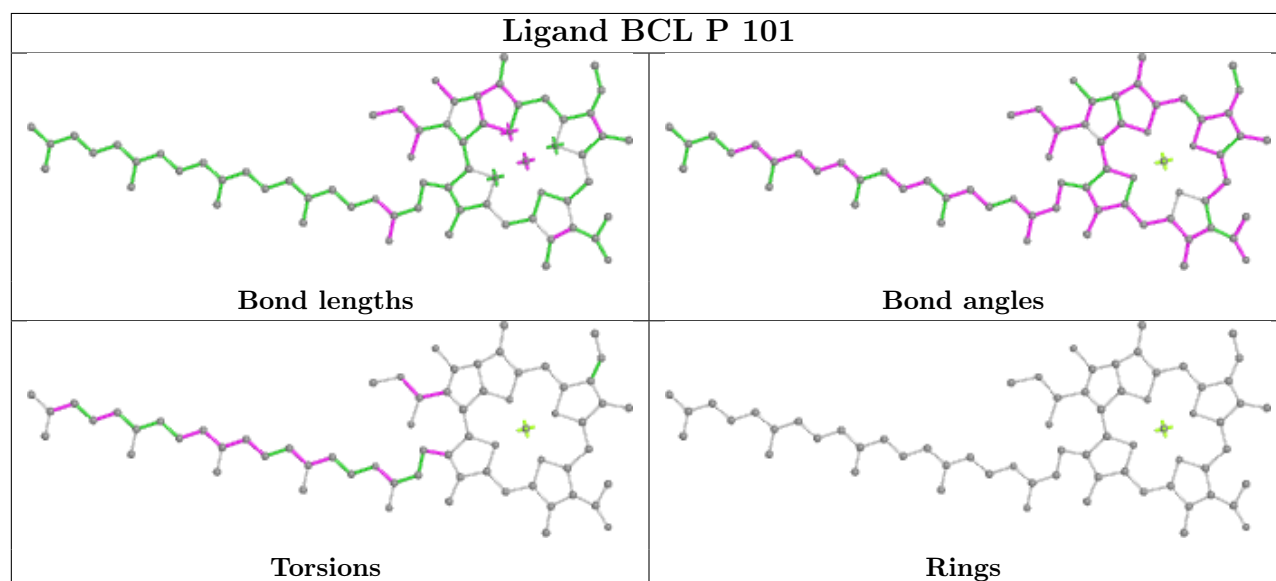
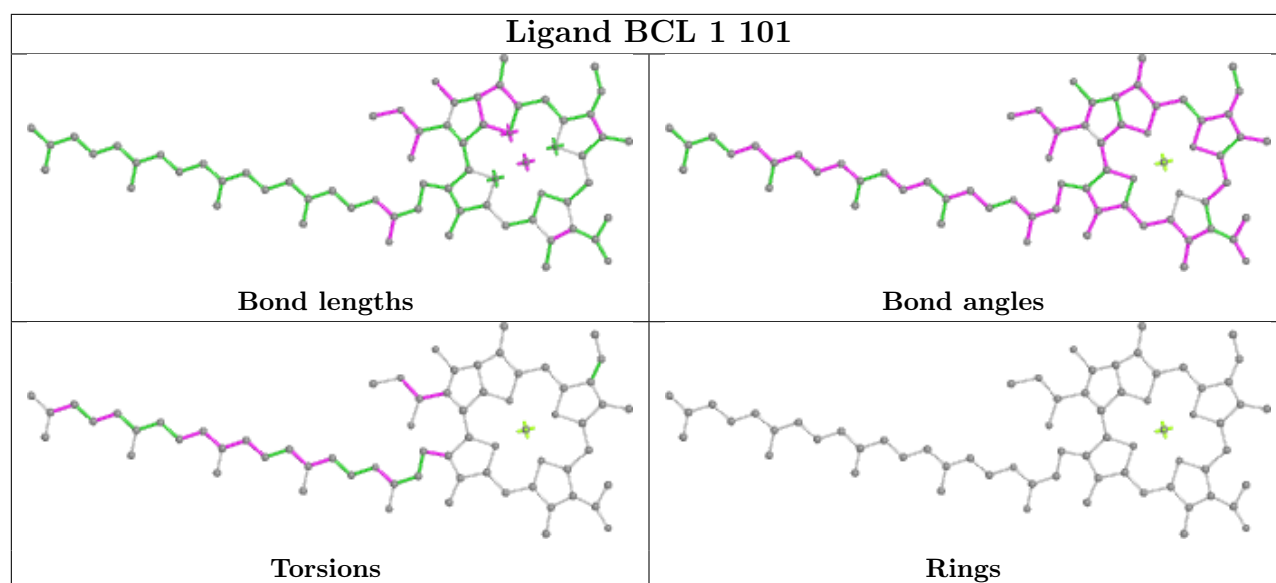


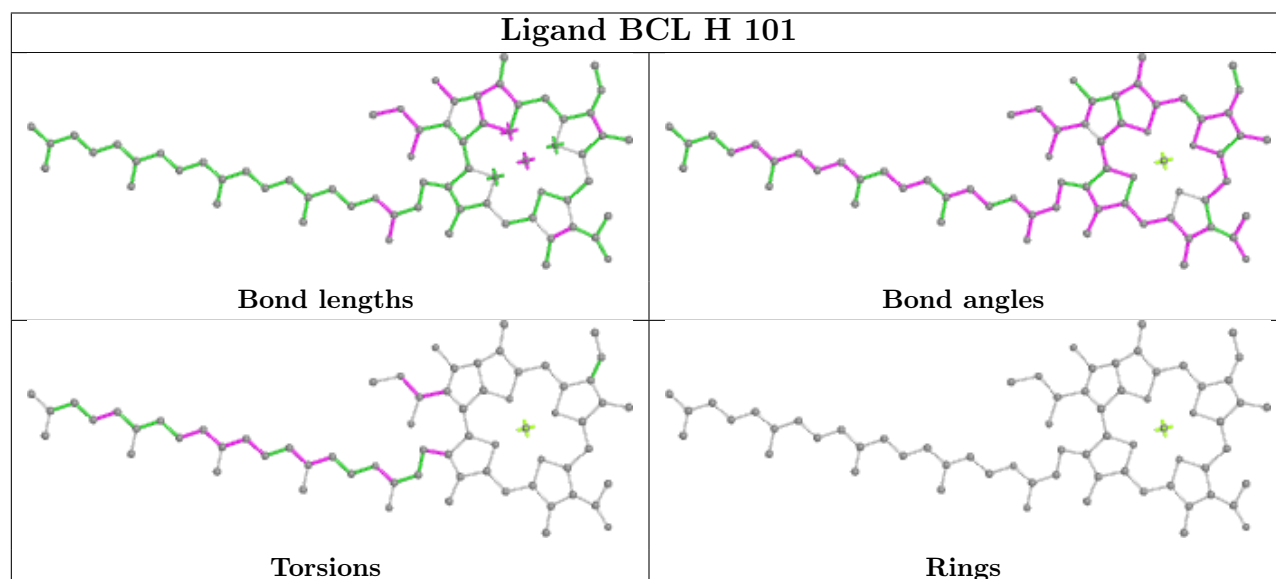
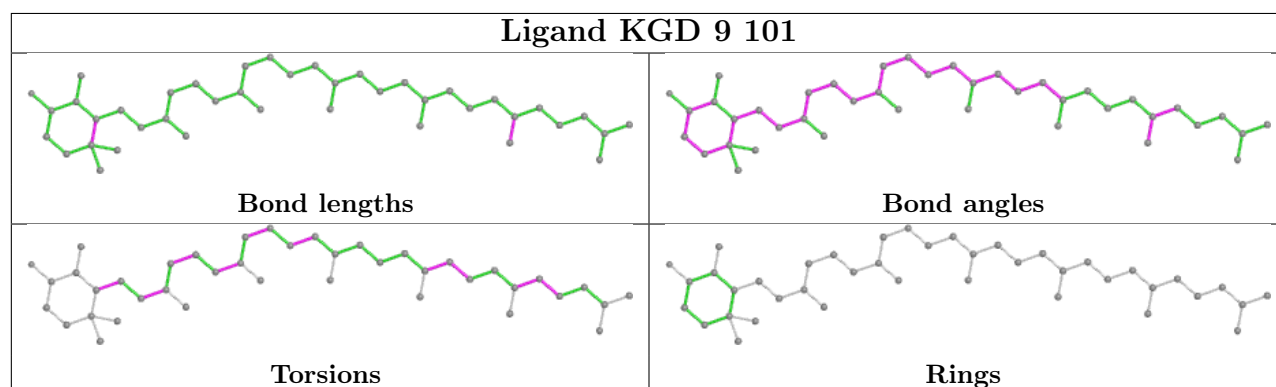
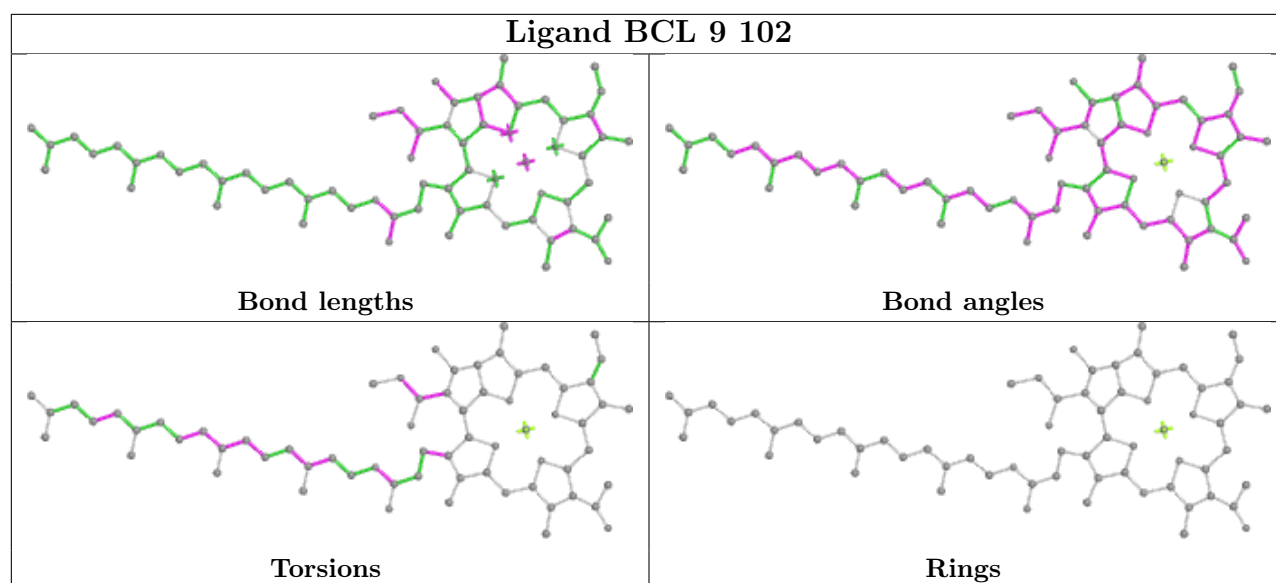
## Ligand BCL W 102



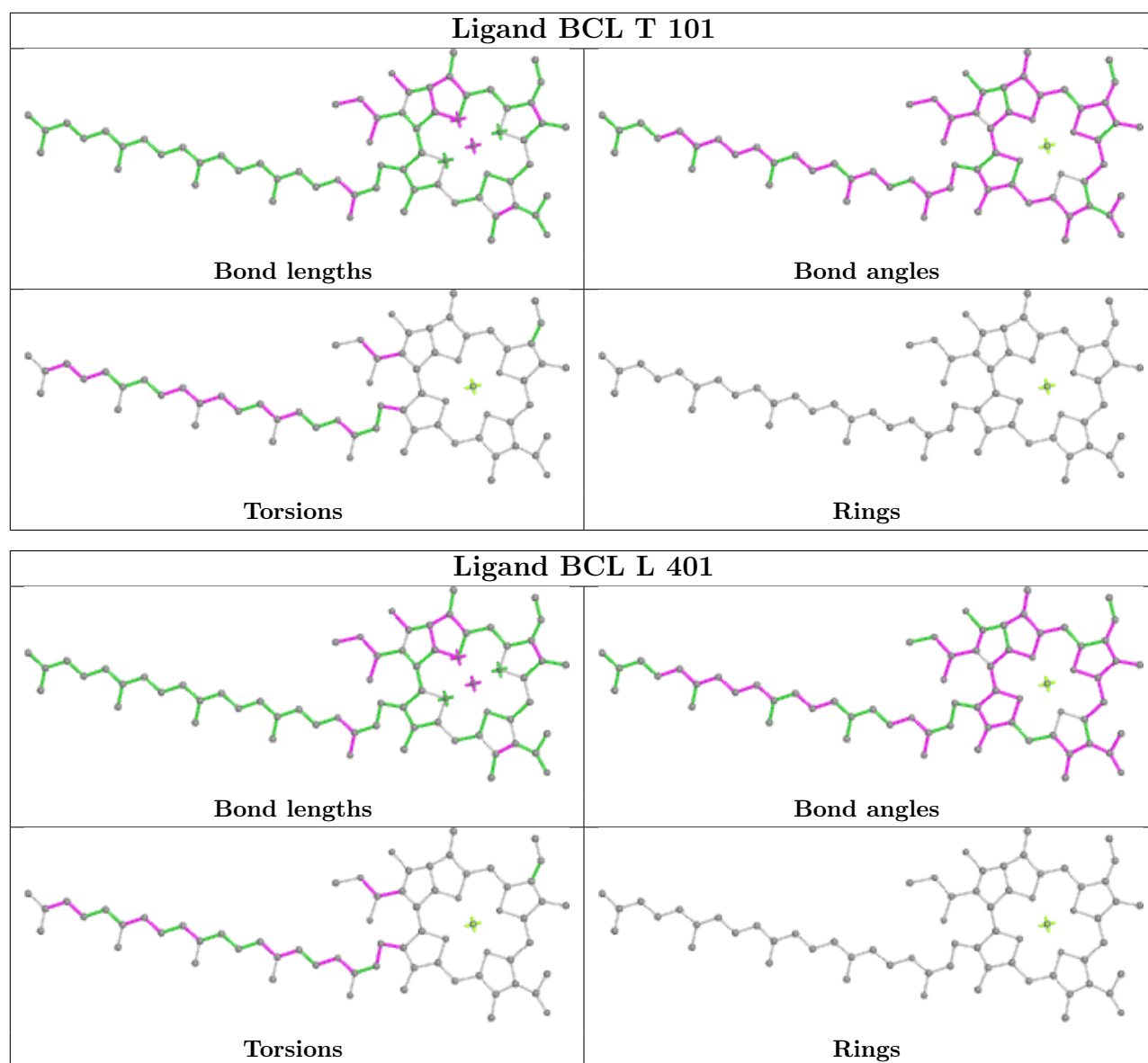












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

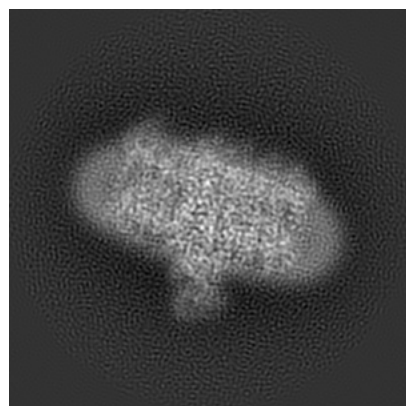
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34839. These allow visual inspection of the internal detail of the map and identification of artifacts.

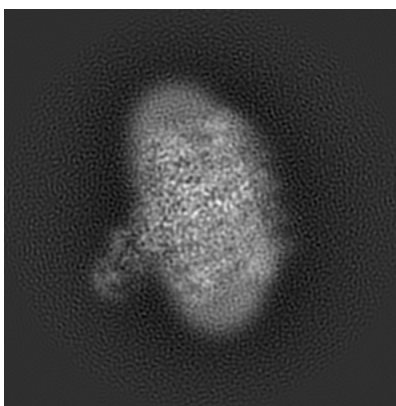
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

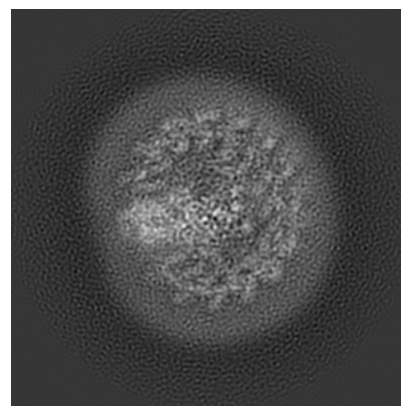
#### 6.1.1 Primary map



X

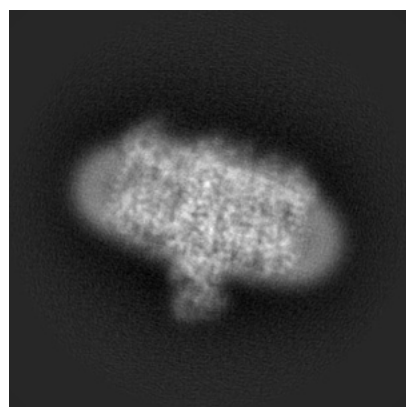


Y

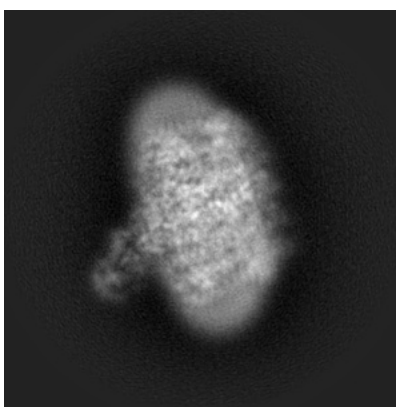


Z

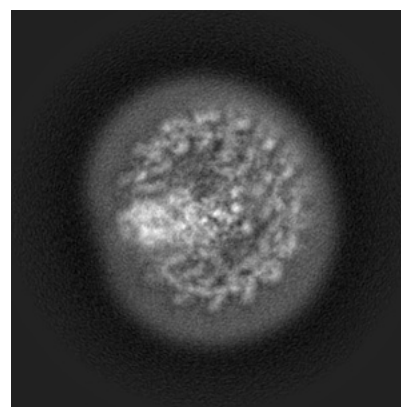
#### 6.1.2 Raw map



X



Y

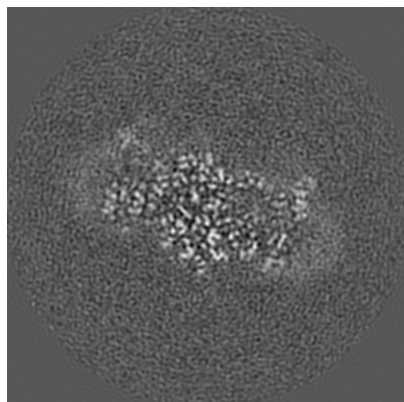


Z

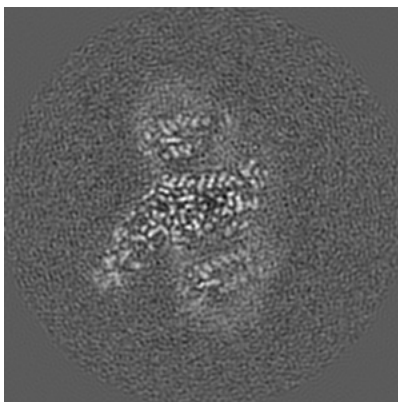
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

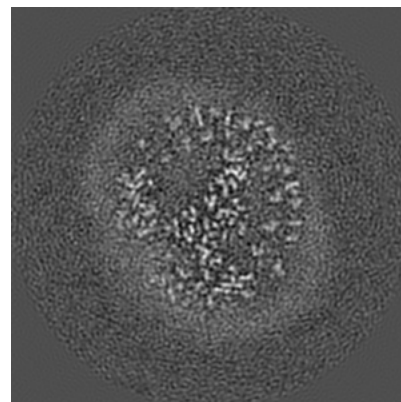
### 6.2.1 Primary map



X Index: 132

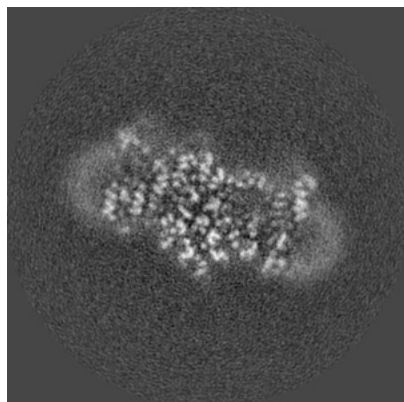


Y Index: 132

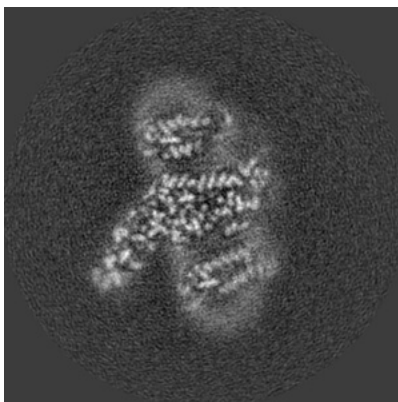


Z Index: 132

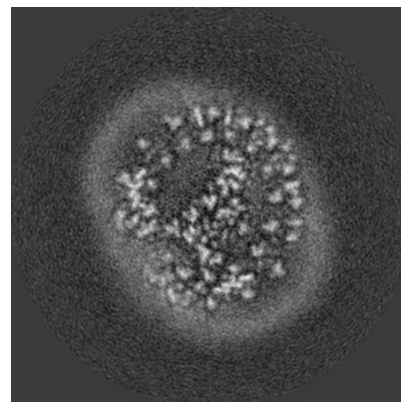
### 6.2.2 Raw map



X Index: 132



Y Index: 132

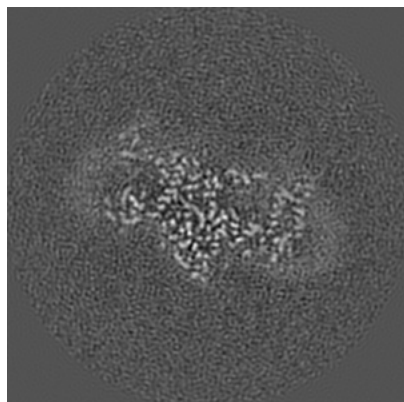


Z Index: 132

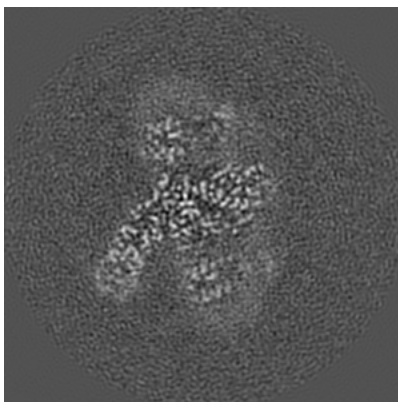
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

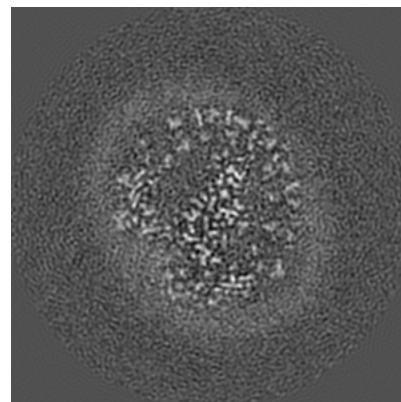
### 6.3.1 Primary map



X Index: 129

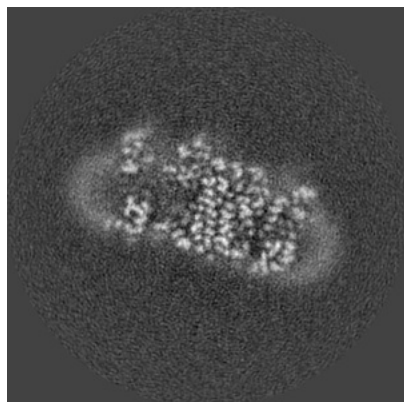


Y Index: 128

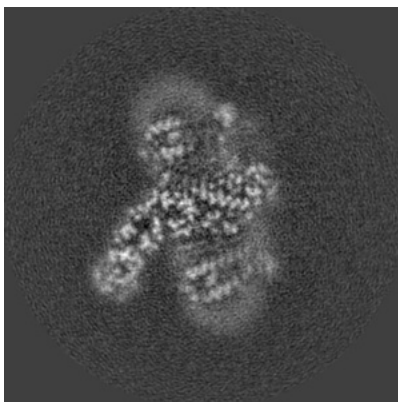


Z Index: 131

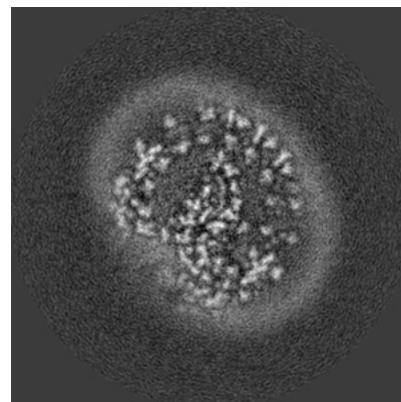
### 6.3.2 Raw map



X Index: 146



Y Index: 129



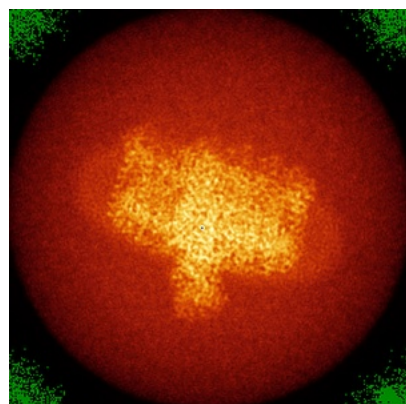
Z Index: 125

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

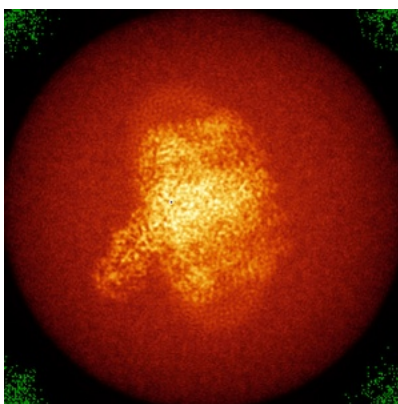


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

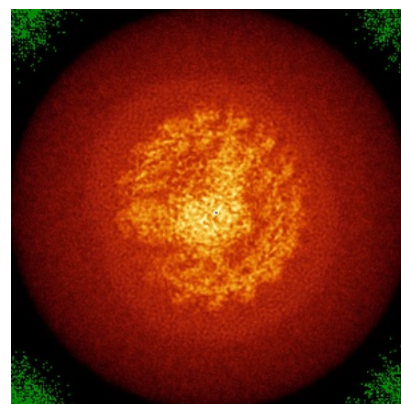
### 6.4.1 Primary map



X

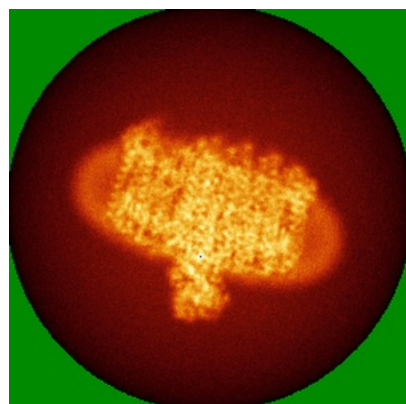


Y

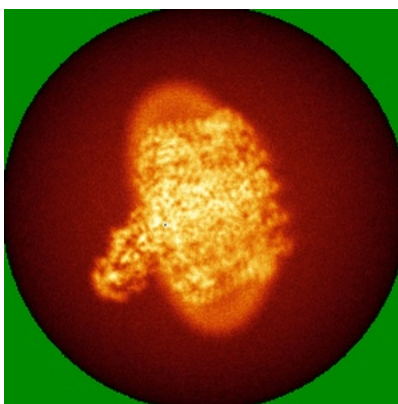


Z

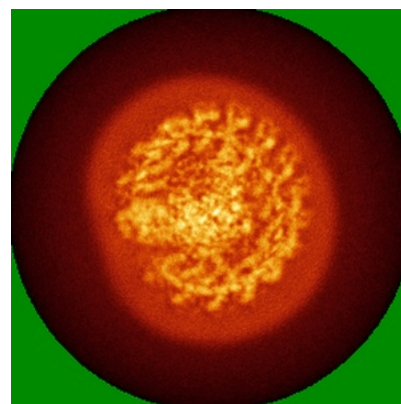
### 6.4.2 Raw map



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.

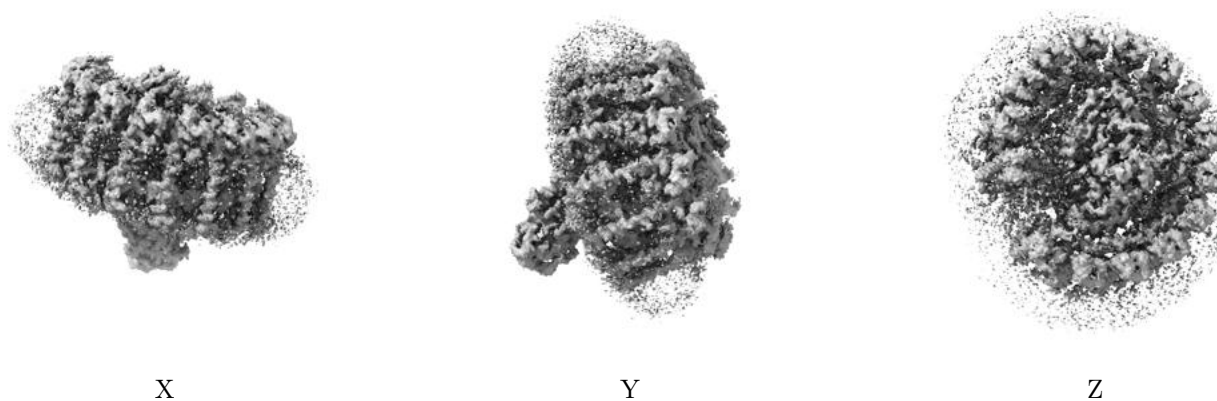
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

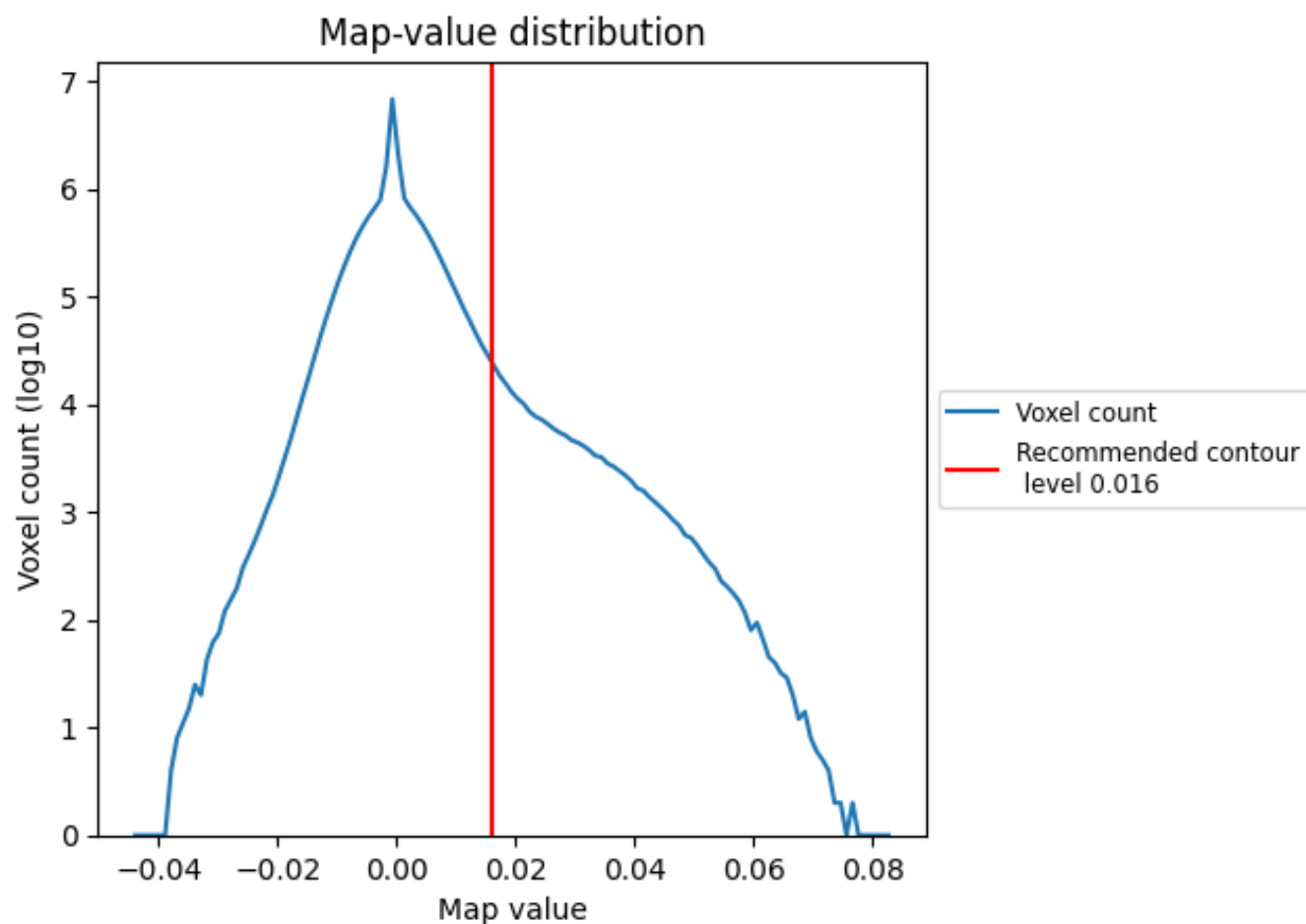
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

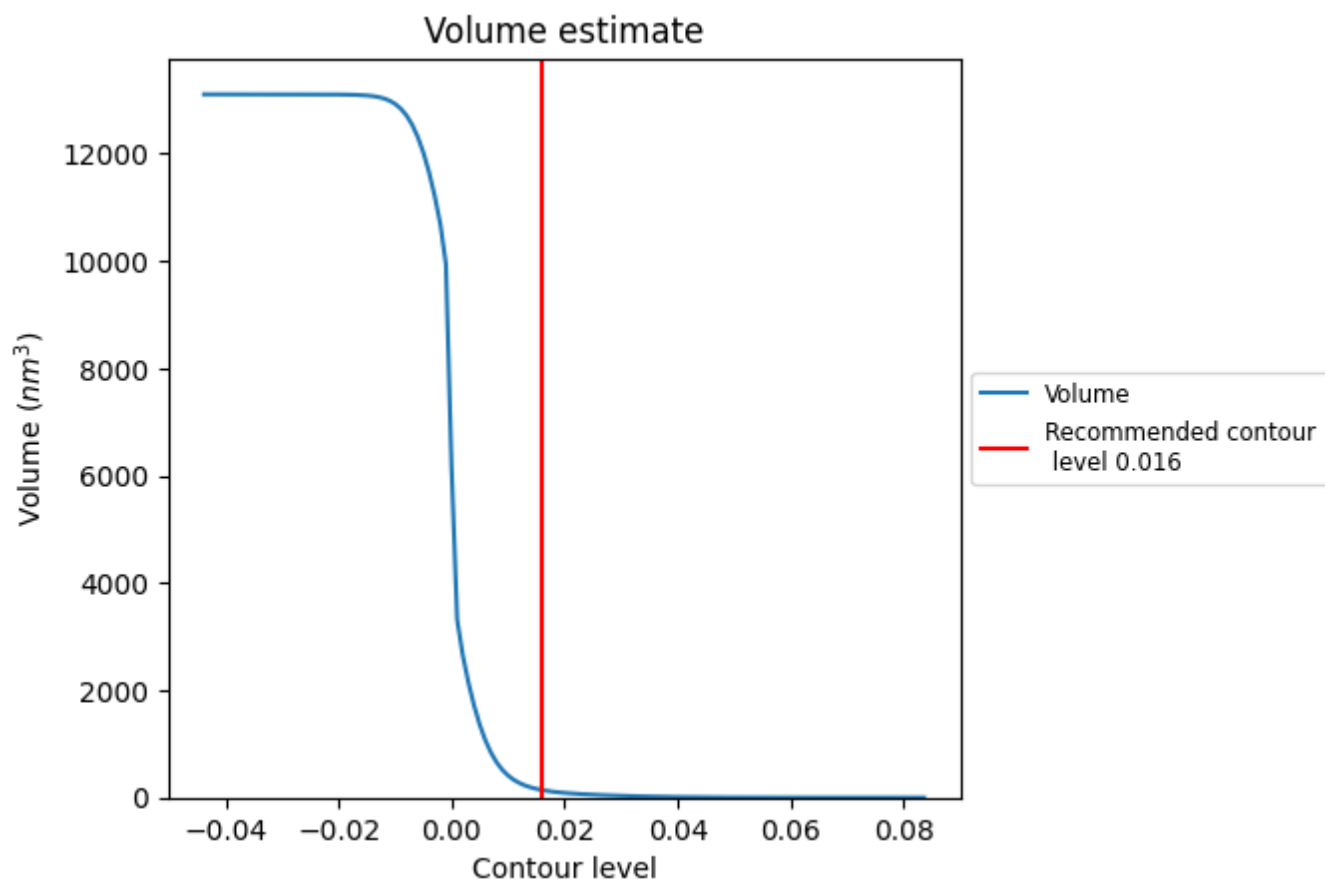
This section contains the results of statistical analysis of the map.

### 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](#)

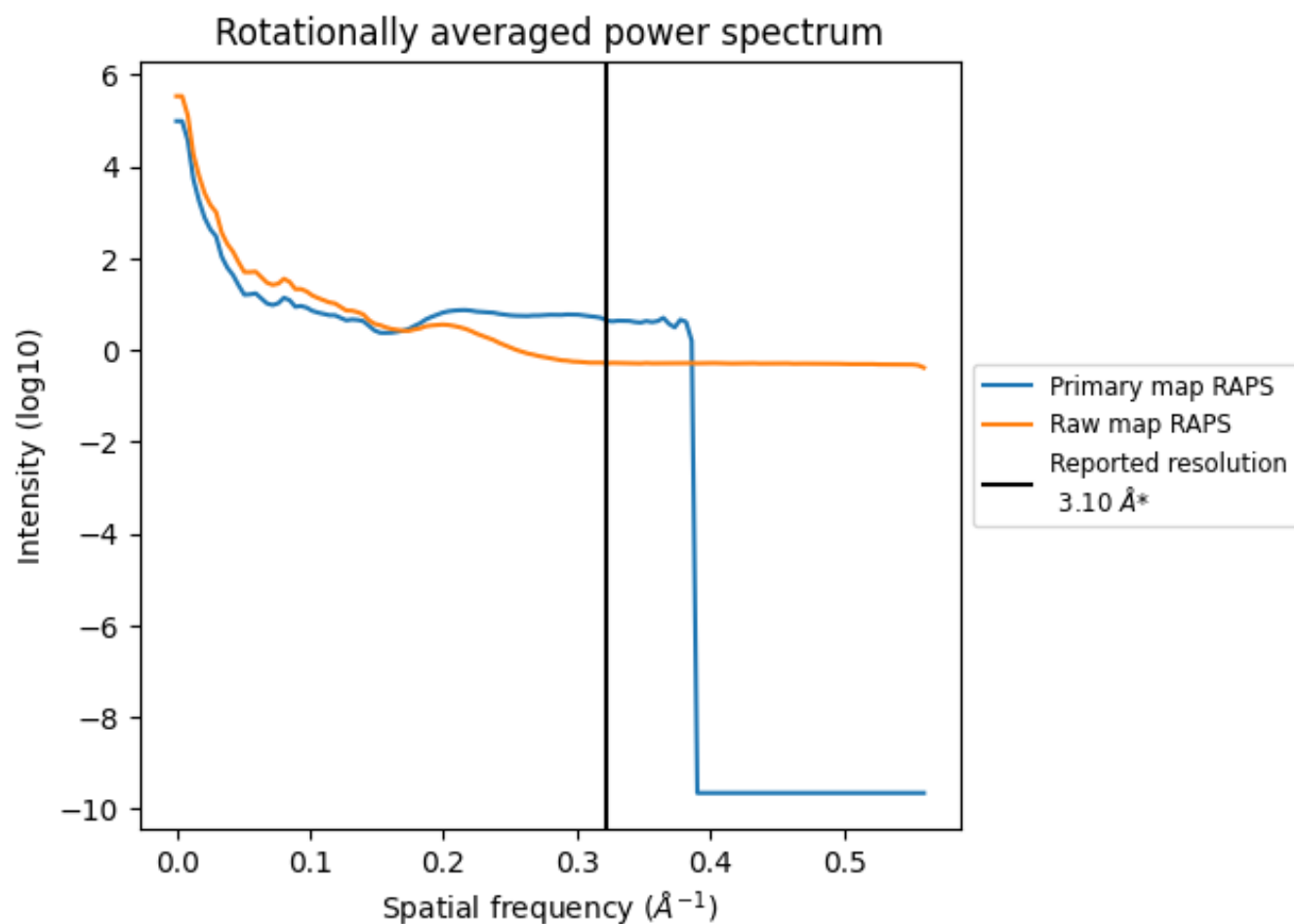


The volume at the recommended contour level is 140 nm<sup>3</sup>; this corresponds to an approximate mass of 127 kDa.

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 ⓘ

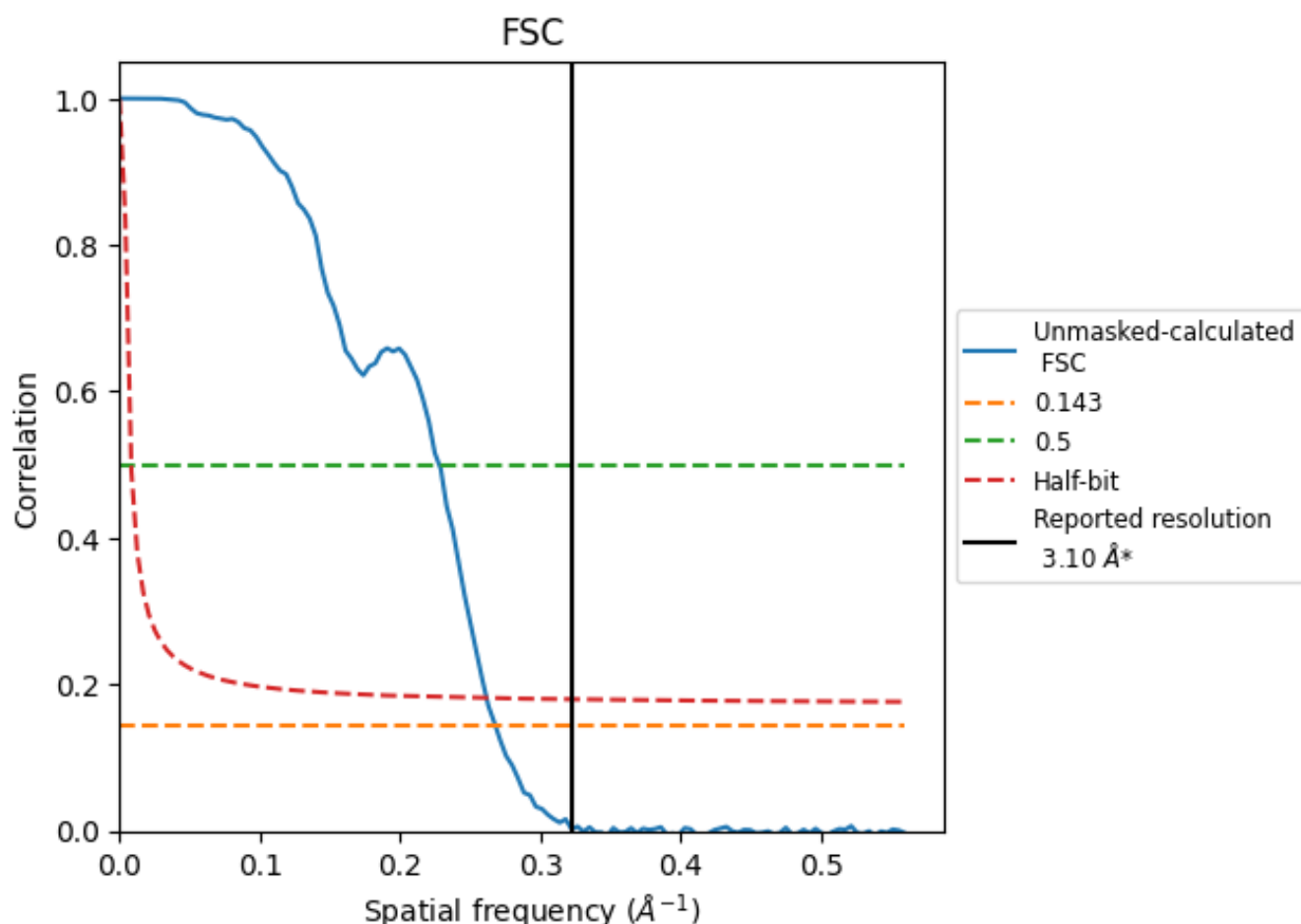


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

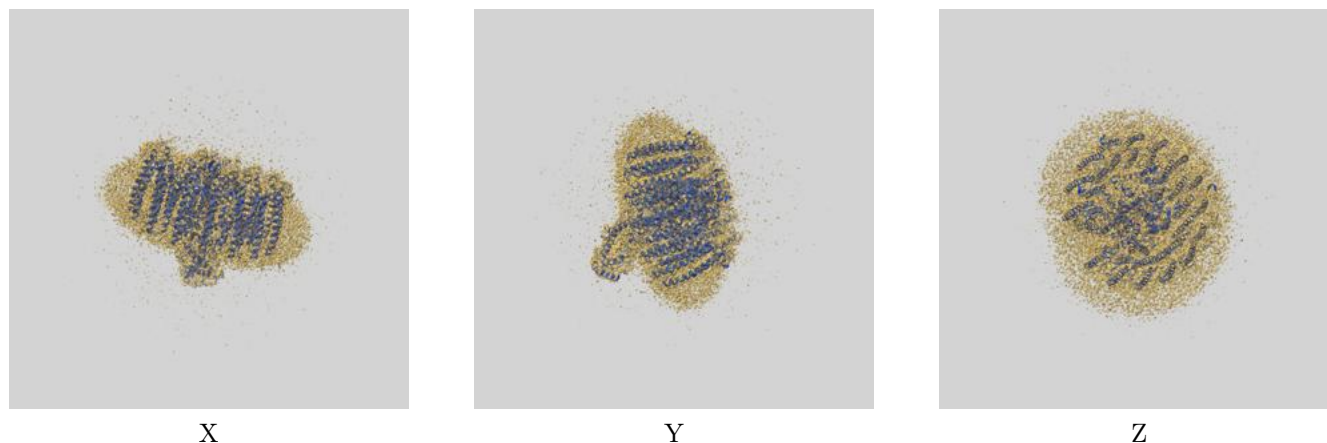
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.39	3.82

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

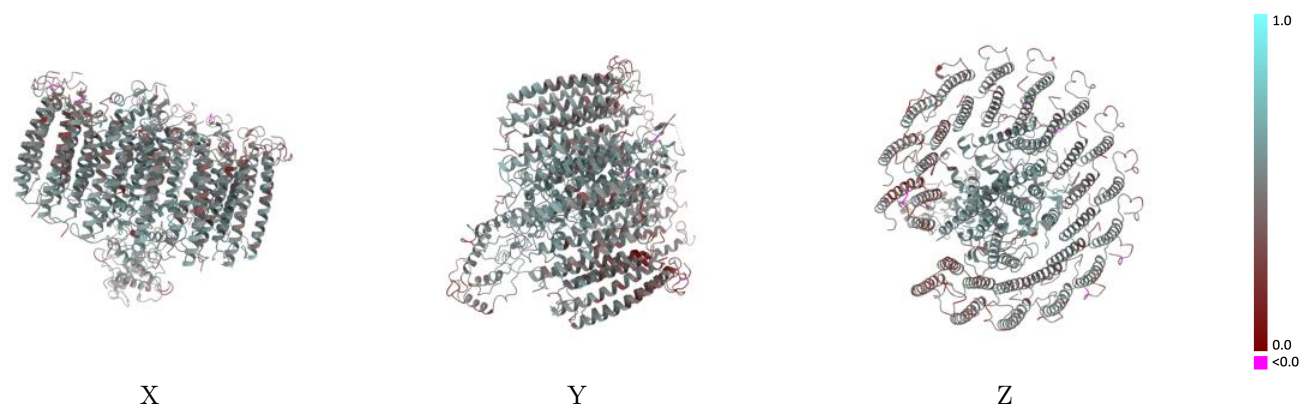
This section contains information regarding the fit between EMDB map EMD-34839 and PDB model 8HJV. Per-residue inclusion information can be found in section [3](#) on page [14](#).

### 9.1 Map-model overlay [i](#)



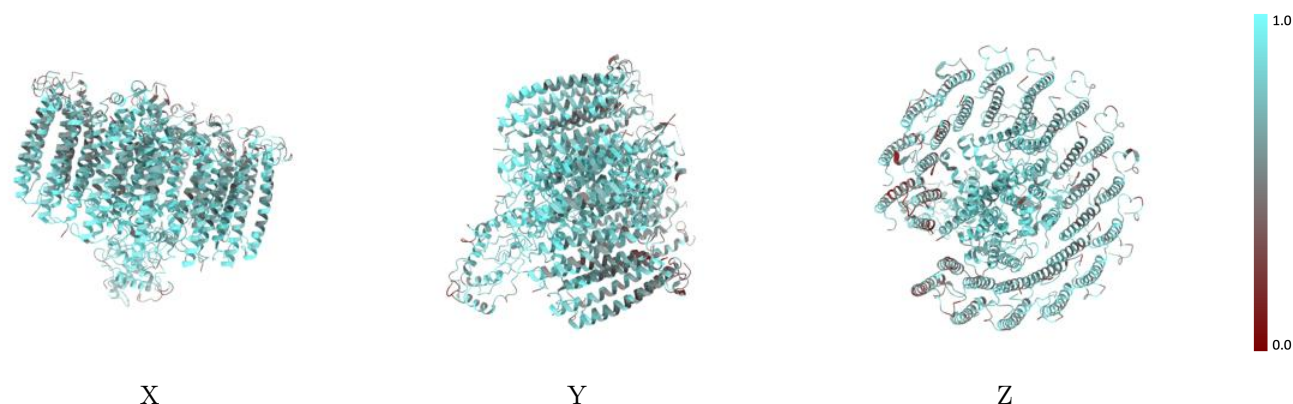
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



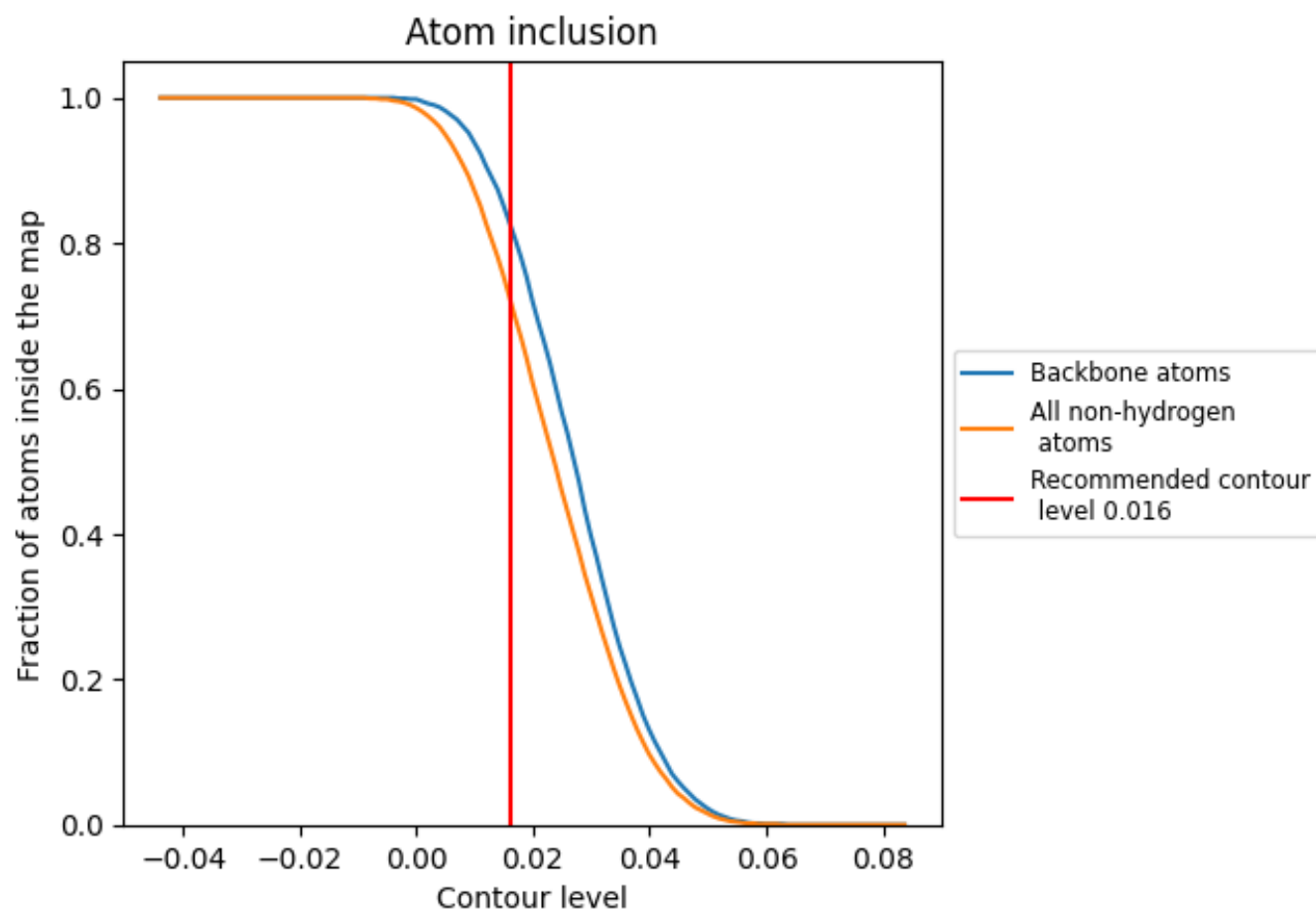
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.4780
0	 0.7440	 0.4750
1	 0.6250	 0.4370
2	 0.4760	 0.3260
3	 0.6110	 0.4170
4	 0.6180	 0.4030
5	 0.6560	 0.4360
6	 0.6630	 0.4360
7	 0.7240	 0.4890
8	 0.6730	 0.4480
9	 0.6550	 0.4520
A	 0.7630	 0.4950
B	 0.7380	 0.4830
C	 0.7700	 0.4790
D	 0.6780	 0.4480
E	 0.7210	 0.4690
F	 0.6840	 0.4710
G	 0.6900	 0.4610
H	 0.6760	 0.4500
I	 0.6810	 0.4590
J	 0.6830	 0.4900
K	 0.7400	 0.4670
L	 0.8230	 0.5480
M	 0.8440	 0.5500
N	 0.7110	 0.4840
O	 0.6980	 0.4550
P	 0.6960	 0.4610
Q	 0.7190	 0.4580
R	 0.6900	 0.4560
S	 0.7150	 0.4810
T	 0.6840	 0.4670
U	 0.6400	 0.4210
V	 0.4830	 0.3520
W	 0.4990	 0.3560
Y	 0.7930	 0.5540
Z	 0.7880	 0.5300

