



Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 08:04 PM JST

PDB ID : 5YQ7 / pdb_00005yq7
EMDB ID : EMD-6828
Title : Cryo-EM structure of the RC-LH core complex from *Roseiflexus castenholzii*
Authors : Shi, Y.; Xin, Y.Y.; Niu, T.X.; Wang, Q.Q.; Niu, W.Q.; Huang, X.J.; Ding, W.; Blankenship, R.E.; Xu, X.L.; Sun, F.
Deposited on : 2017-11-05
Resolution : 4.10 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

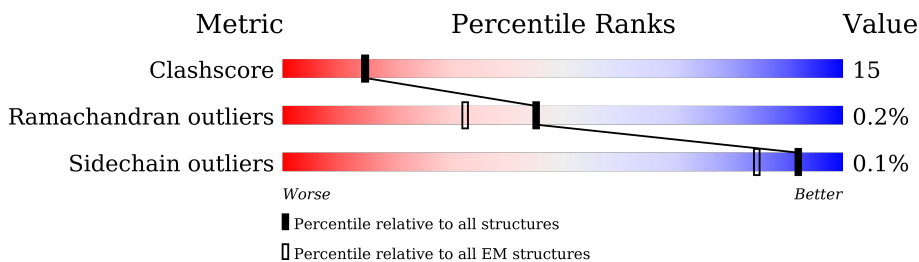
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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 ≥ 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	<div> <div>9%</div> <div>64%</div> <div>16%</div> <div>20%</div> </div>
1	2	55	<div> <div>18%</div> <div>65%</div> <div>15%</div> <div>20%</div> </div>
1	4	55	<div> <div>15%</div> <div>62%</div> <div>18%</div> <div>20%</div> </div>
1	6	55	<div> <div>15%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	8	55	<div> <div>7%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	B	55	<div> <div>5%</div> <div>71%</div> <div>9%</div> <div>20%</div> </div>
1	E	55	<div> <div>7%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	G	55	<div> <div>15%</div> <div>65%</div> <div>15%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	55	<div> <div>5%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	K	55	<div> <div>9%</div> <div>65%</div> <div>15%</div> <div>20%</div> </div>
1	O	55	<div> <div>13%</div> <div>65%</div> <div>15%</div> <div>20%</div> </div>
1	Q	55	<div> <div>13%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	S	55	<div> <div>7%</div> <div>67%</div> <div>13%</div> <div>20%</div> </div>
1	U	55	<div> <div>7%</div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	W	55	<div> <div>13%</div> <div>64%</div> <div>16%</div> <div>20%</div> </div>
2	L	310	<div> <div>13%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>
3	C	320	<div> <div>17%</div> <div>63%</div> <div>28%</div> <div>8%</div> </div>
4	1	42	<div> <div>26%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
4	3	42	<div> <div>21%</div> <div>62%</div> <div>24%</div> <div>14%</div> </div>
4	5	42	<div> <div>12%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
4	7	42	<div> <div>10%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
4	9	42	<div> <div>10%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
4	A	42	<div> <div>7%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>
4	D	42	<div> <div>10%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
4	F	42	<div> <div>10%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
4	H	42	<div> <div>60%</div> <div>26%</div> <div>14%</div> </div>
4	J	42	<div> <div>5%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
4	N	42	<div> <div>7%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
4	P	42	<div> <div>•</div> <div>67%</div> <div>19%</div> <div>14%</div> </div>
4	R	42	<div> <div>12%</div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
4	T	42	<div> <div>17%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
4	V	42	<div> <div>26%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
5	Y	25	<div> <div>8%</div> <div>96%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	X	23	<div> <div>96%</div> <div>100%</div> </div>
7	M	306	<div> <div>11%</div> <div>73%</div> <div>27%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BCL	B	102	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20009 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	E	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	B	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	0	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	8	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	6	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	4	44	Total	C	N	O	S	0	0
			319	216	54	48	1		
1	2	44	Total	C	N	O	S	0	0
			326	220	55	50	1		
1	K	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	I	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	G	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	W	44	Total	C	N	O	S	0	0
			312	208	54	49	1		
1	U	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	S	44	Total	C	N	O	S	0	0
			326	220	55	50	1		
1	Q	44	Total	C	N	O	S	0	0
			318	214	54	49	1		
1	O	44	Total	C	N	O	S	0	0
			325	220	54	50	1		

- Molecule 2 is a protein called Precursor for L subunits of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	309	Total	C	N	O	S	0	0
			2292	1526	372	389	5		

- Molecule 3 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	293	Total	C	N	O	S	0	0
			2041	1294	352	382	13		

- Molecule 4 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	V	36	Total	C	N	O	S	0	0
			263	179	40	43	1		
4	R	36	Total	C	N	O		0	0
			257	174	40	43			
4	P	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	N	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	J	36	Total	C	N	O	S	0	0
			263	179	40	43	1		
4	H	36	Total	C	N	O	S	0	0
			260	176	40	43	1		
4	F	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	D	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	A	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	9	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	7	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	5	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	3	36	Total	C	N	O	S	0	0
			260	176	40	43	1		
4	1	36	Total	C	N	O	S	0	0
			245	161	40	43	1		

- Molecule 5 is a protein called Peptide from Precursor for L and M subunits of photosynthetic

reaction center.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	25	Total	C	N	O	0	0
			125	75	25	25		

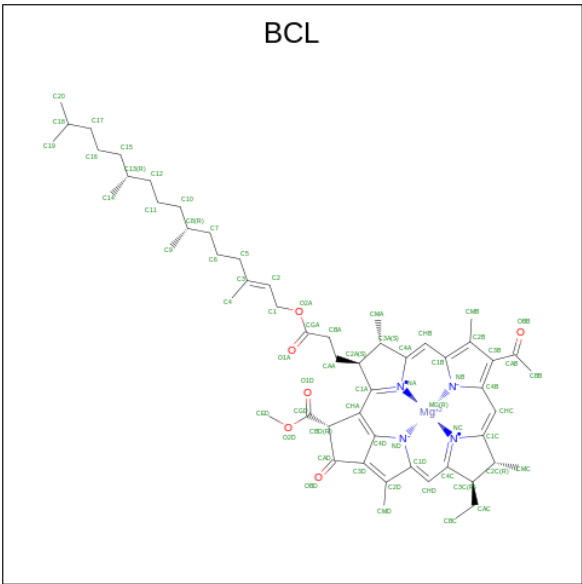
- Molecule 6 is a protein called Subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	X	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 7 is a protein called Precursor for M subunits of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	305	Total	C	N	O	S	0	0
			2373	1603	381	385	4		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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Mol	Chain	Residues	Atoms					AltConf
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	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	L	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	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	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	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	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	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	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	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	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

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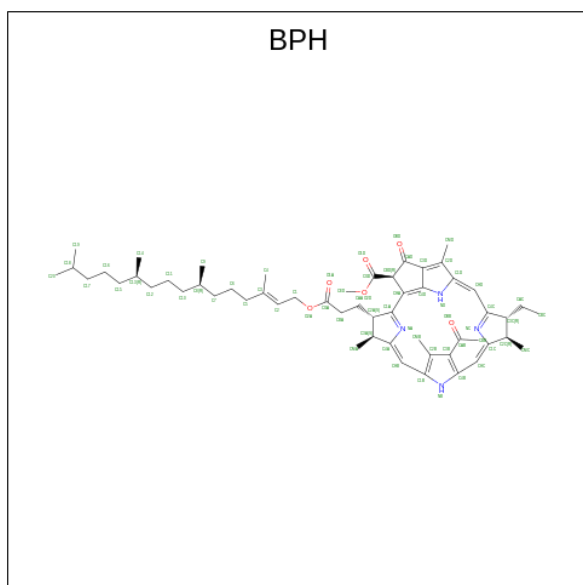
Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	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	P	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	J	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
8	F	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	A	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	7	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	3	1	Total 66	C 55	Mg 1	N 4	O 6	0

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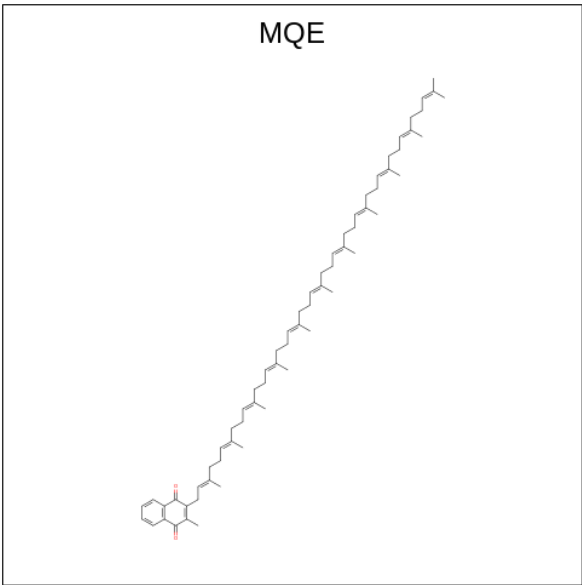
Mol	Chain	Residues	Atoms					AltConf
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



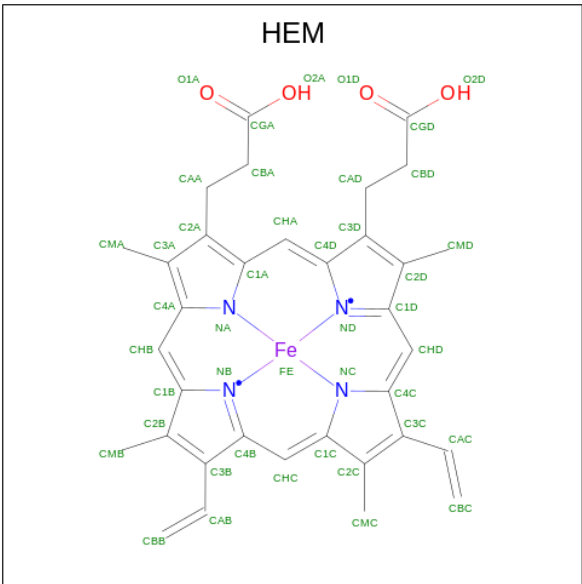
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 10 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 (CCD ID: MQE) (formula: $C_{66}H_{96}O_2$).



Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			68	66	2	
10	M	1	Total	C	O	0
			68	66	2	

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



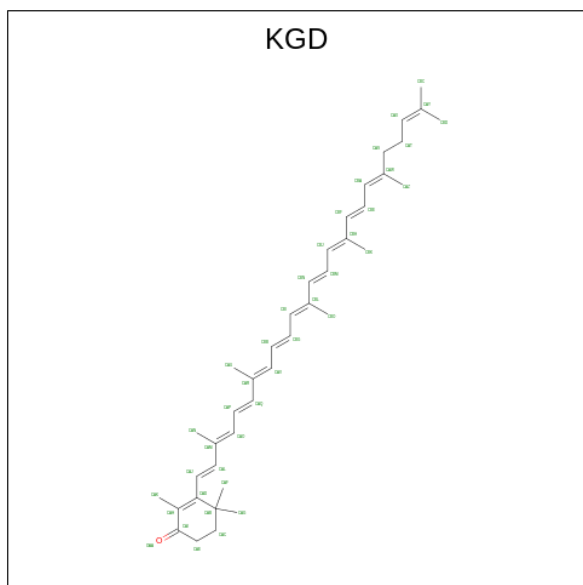
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 12 is beta,psi-caroten-4-one (CCD ID: KGD) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
12	T	1	Total	C	O	0
			41	40	1	
12	T	1	Total	C	O	0
			41	40	1	
12	R	1	Total	C	O	0
			41	40	1	
12	N	1	Total	C	O	0
			41	40	1	
12	N	1	Total	C	O	0
			41	40	1	
12	J	1	Total	C	O	0
			41	40	1	
12	H	1	Total	C	O	0
			41	40	1	
12	F	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			41	40	1	
12	9	1	Total	C	O	0
			41	40	1	
12	9	1	Total	C	O	0
			41	40	1	
12	5	1	Total	C	O	0
			41	40	1	
12	3	1	Total	C	O	0
			41	40	1	
12	3	1	Total	C	O	0
			41	40	1	

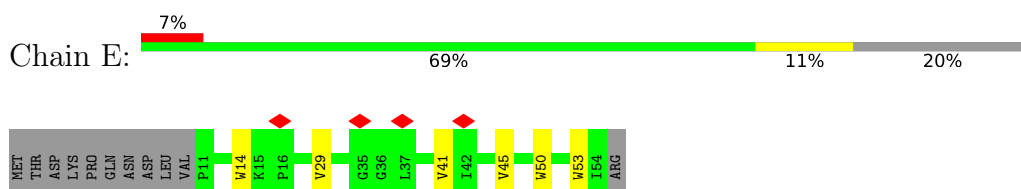
- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

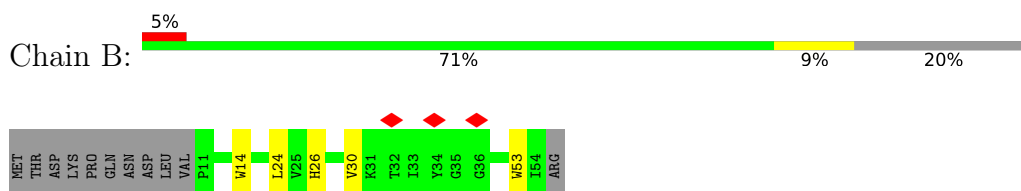
3 Residue-property plots [i](#)

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.

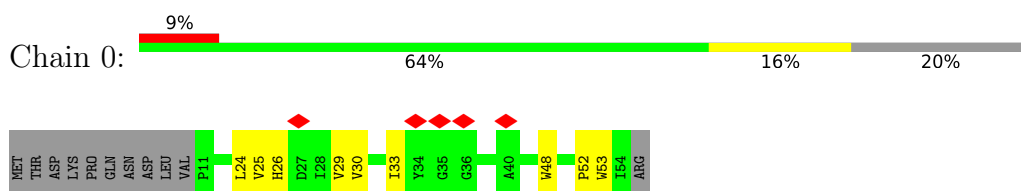
- Molecule 1: Beta subunit of light-harvesting 1



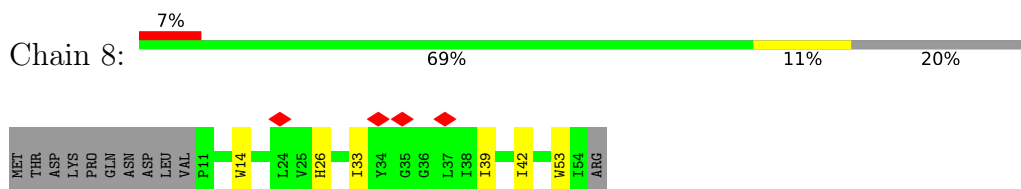
- Molecule 1: Beta subunit of light-harvesting 1



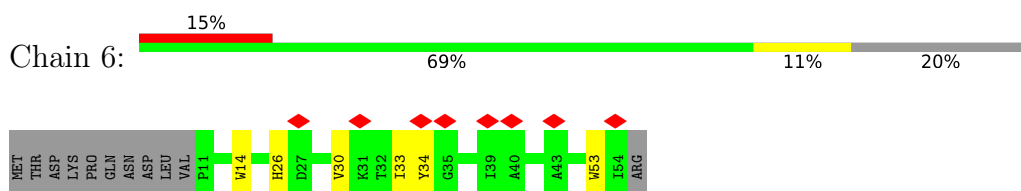
- Molecule 1: Beta subunit of light-harvesting 1



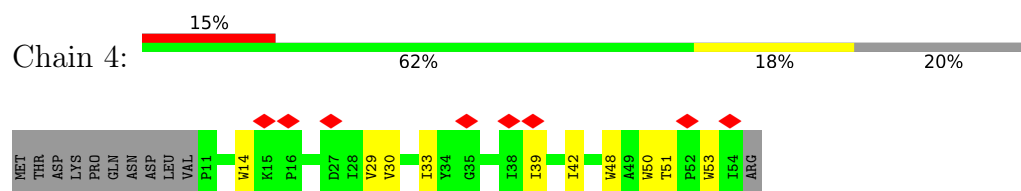
- Molecule 1: Beta subunit of light-harvesting 1



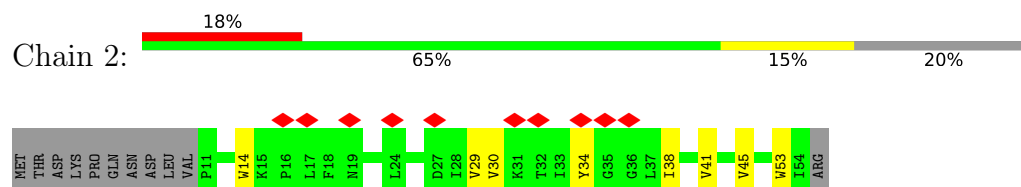
- Molecule 1: Beta subunit of light-harvesting 1



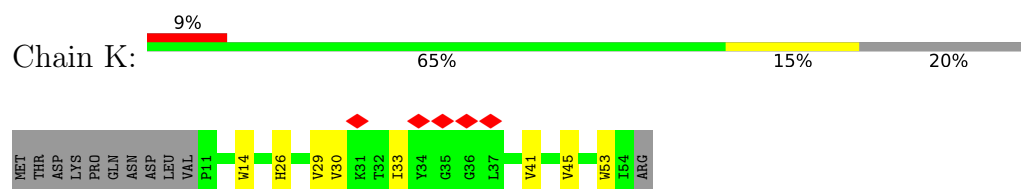
● Molecule 1: Beta subunit of light-harvesting 1



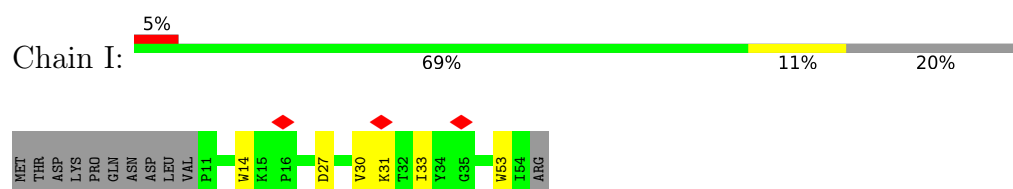
● Molecule 1: Beta subunit of light-harvesting 1



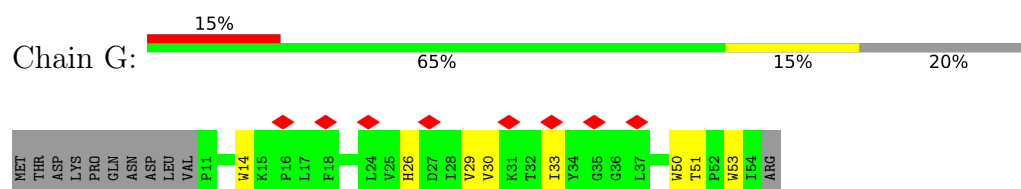
● Molecule 1: Beta subunit of light-harvesting 1



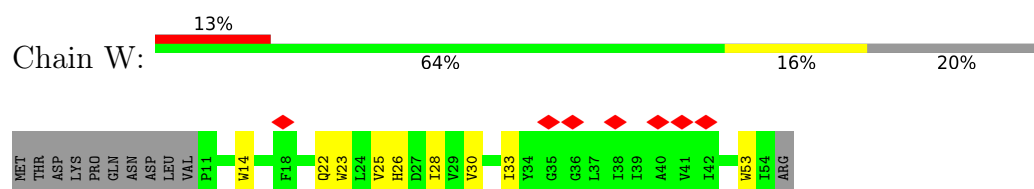
● Molecule 1: Beta subunit of light-harvesting 1



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● Molecule 1: Beta subunit of light-harvesting 1

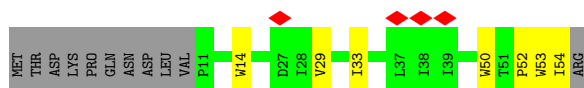


● Molecule 1: Beta subunit of light-harvesting 1





- Molecule 1: Beta subunit of light-harvesting 1



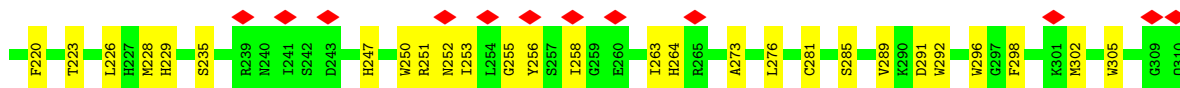
- Molecule 1: Beta subunit of light-harvesting 1



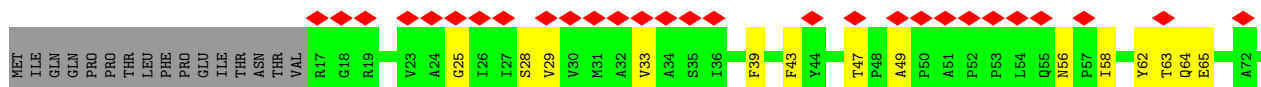
- Molecule 1: Beta subunit of light-harvesting 1

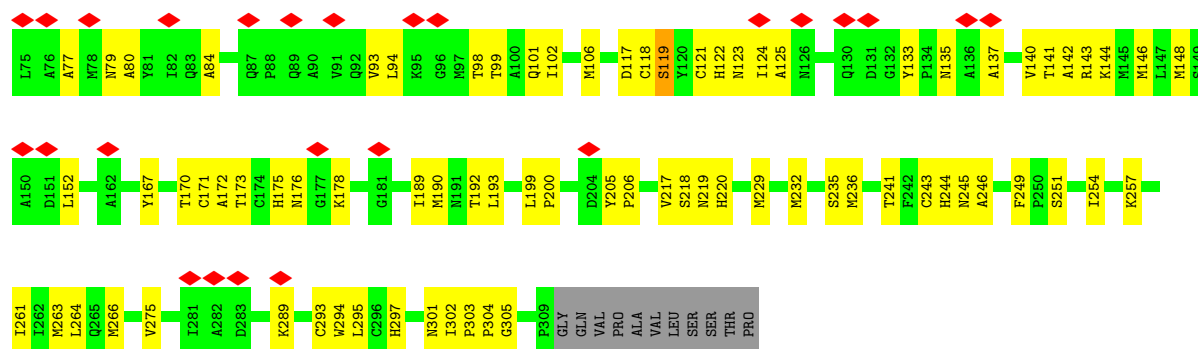


- Molecule 2: Precursor for L subunits of photosynthetic reaction center

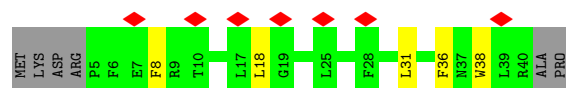
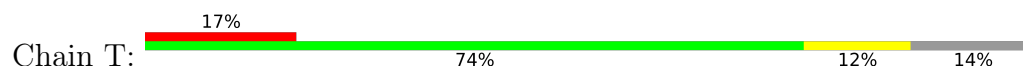


- Molecule 3: Cytochrome subunit of photosynthetic reaction center

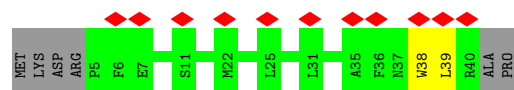
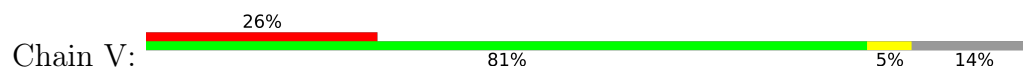




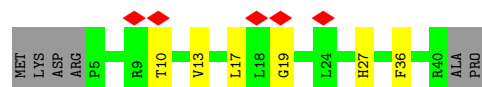
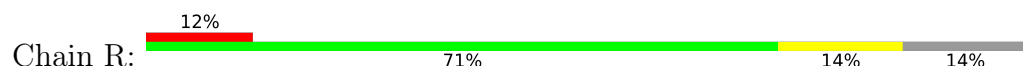
- Molecule 4: Alpha subunit of light-harvesting 1



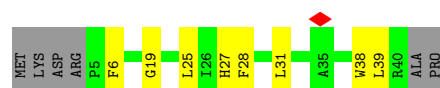
- Molecule 4: Alpha subunit of light-harvesting 1



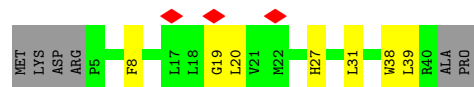
- Molecule 4: Alpha subunit of light-harvesting 1



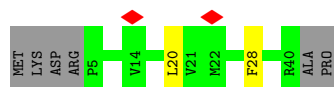
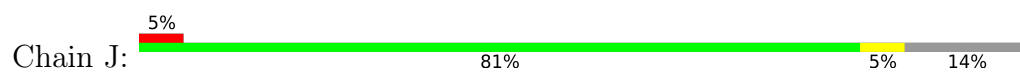
- Molecule 4: Alpha subunit of light-harvesting 1



- Molecule 4: Alpha subunit of light-harvesting 1



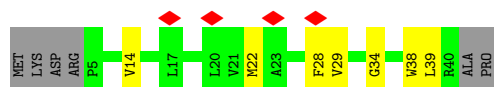
- Molecule 4: Alpha subunit of light-harvesting 1



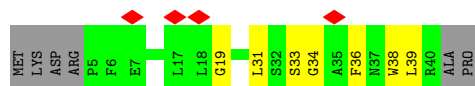
- Molecule 4: Alpha subunit of light-harvesting 1



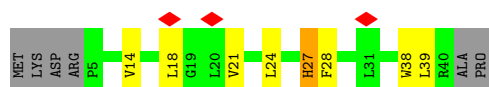
- Molecule 4: Alpha subunit of light-harvesting 1



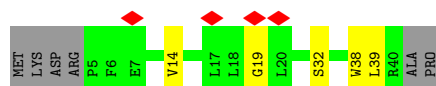
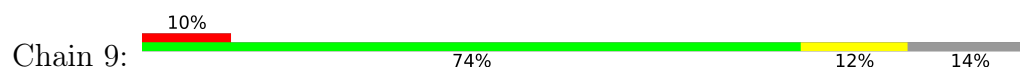
- Molecule 4: Alpha subunit of light-harvesting 1



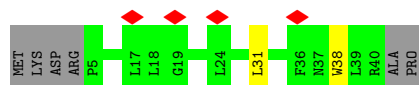
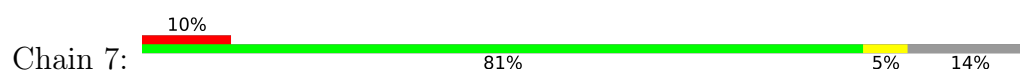
- Molecule 4: Alpha subunit of light-harvesting 1



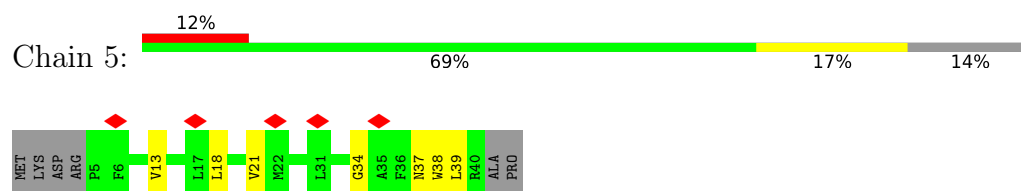
- Molecule 4: Alpha subunit of light-harvesting 1



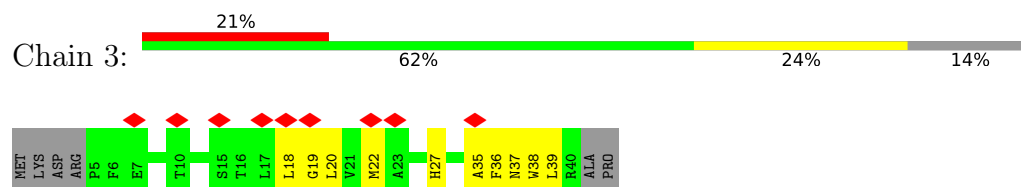
- Molecule 4: Alpha subunit of light-harvesting 1



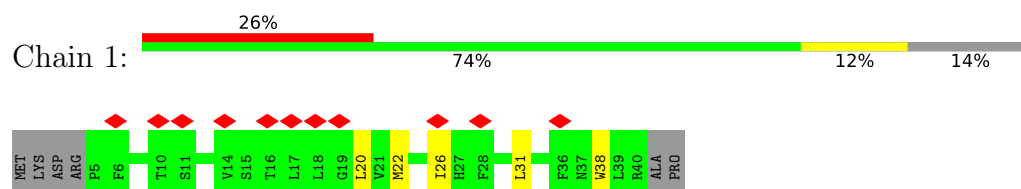
- Molecule 4: Alpha subunit of light-harvesting 1



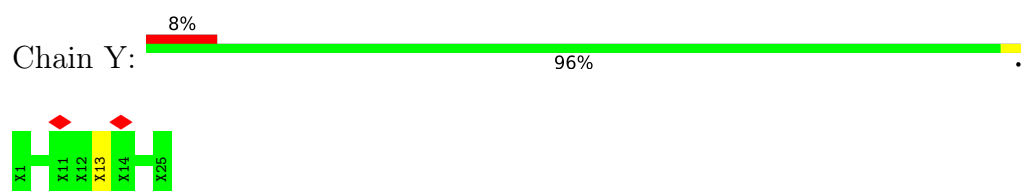
- Molecule 4: Alpha subunit of light-harvesting 1



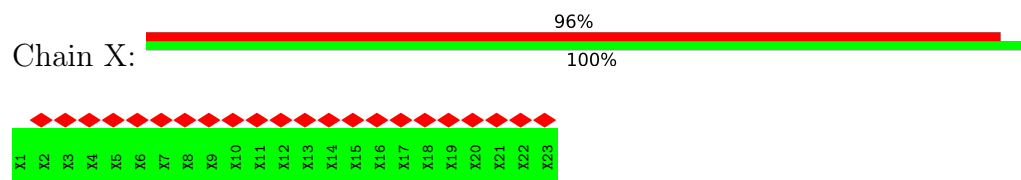
- Molecule 4: Alpha subunit of light-harvesting 1



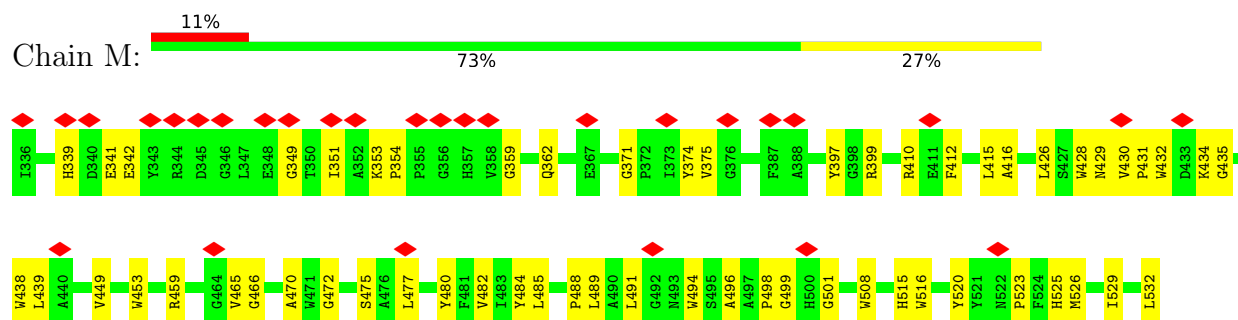
- Molecule 5: Peptide from Precursor for L and M subunits of photosynthetic reaction center



- Molecule 6: Subunit X



- Molecule 7: Precursor for M subunits of photosynthetic reaction center





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	256903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	215.04001, 215.04001, 215.04001	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/341	0.56	0/474
1	2	0.17	0/338	0.43	0/470
1	4	0.20	0/331	0.47	0/462
1	6	0.17	0/341	0.39	0/474
1	8	0.20	0/341	0.54	0/474
1	B	0.20	0/337	0.44	0/470
1	E	0.22	0/337	0.46	0/470
1	G	0.22	0/341	0.50	0/474
1	I	0.19	0/341	0.41	0/474
1	K	0.22	0/337	0.59	0/470
1	O	0.20	0/337	0.49	0/470
1	Q	0.19	0/329	0.48	0/459
1	S	0.19	0/338	0.46	0/470
1	U	0.20	0/341	0.52	0/474
1	W	0.19	0/323	0.43	0/451
2	L	0.24	0/2374	0.55	2/3262 (0.1%)
3	C	0.23	0/2093	0.67	2/2880 (0.1%)
4	1	0.20	0/248	0.45	0/341
4	3	0.22	0/265	0.61	0/363
4	5	0.24	0/272	0.53	0/372
4	7	0.24	0/272	0.48	0/372
4	9	0.21	0/272	0.55	0/372
4	A	0.24	0/272	0.55	0/372
4	D	0.23	0/272	0.59	0/372
4	F	0.18	0/272	0.55	0/372
4	H	0.26	0/265	0.80	1/363 (0.3%)
4	J	0.20	0/269	0.56	0/368
4	N	0.21	0/272	0.44	0/372
4	P	0.21	0/272	0.45	0/372
4	R	0.23	0/262	0.47	0/360
4	T	0.22	0/272	0.46	0/372
4	V	0.19	0/269	0.53	0/368

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	M	0.26	0/2478	0.52	0/3417
All	All	0.23	0/16024	0.54	5/22106 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	2
3	C	0	1
4	5	0	1
7	M	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	8	PHE	N-CA-C	8.54	120.67	111.36
3	C	295	LEU	N-CA-C	-6.07	105.42	114.64
3	C	119	SER	N-CA-C	-5.52	100.33	107.73
2	L	204	TYR	CA-C-N	5.21	131.49	121.54
2	L	204	TYR	C-N-CA	5.21	131.49	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	5	37	ASN	Peptide
3	C	62	TYR	Peptide
2	L	106	GLU	Peptide
2	L	203	TYR	Peptide
7	M	374	TYR	Peptide

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	329	0	293	11	0
1	2	326	0	284	10	0
1	4	319	0	271	16	0
1	6	329	0	293	11	0
1	8	329	0	293	12	0
1	B	325	0	282	25	0
1	E	325	0	282	9	0
1	G	329	0	293	10	0
1	I	329	0	293	17	0
1	K	325	0	282	18	0
1	O	325	0	282	8	0
1	Q	318	0	275	10	0
1	S	326	0	284	8	0
1	U	329	0	293	9	0
1	W	312	0	257	18	0
2	L	2292	0	2129	81	0
3	C	2041	0	1834	81	0
4	1	245	0	237	4	0
4	3	260	0	260	10	0
4	5	266	0	267	4	0
4	7	266	0	267	4	0
4	9	266	0	267	5	0
4	A	266	0	267	11	0
4	D	266	0	267	6	0
4	F	266	0	267	6	0
4	H	260	0	260	12	0
4	J	263	0	258	2	0
4	N	266	0	267	6	0
4	P	266	0	267	7	0
4	R	257	0	253	10	0
4	T	266	0	267	7	0
4	V	263	0	258	3	0
5	Y	125	0	27	1	0
6	X	115	0	26	0	0
7	M	2373	0	2192	60	0
8	0	132	0	148	11	0
8	1	66	0	74	4	0
8	2	132	0	148	12	0
8	3	66	0	72	4	0
8	4	132	0	147	11	0
8	5	66	0	74	3	0
8	6	132	0	148	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	7	66	0	74	7	0
8	8	132	0	148	14	0
8	9	66	0	74	2	0
8	A	66	0	74	5	0
8	B	132	0	148	30	0
8	D	66	0	74	2	0
8	E	132	0	148	8	0
8	F	66	0	74	4	0
8	G	132	0	148	12	0
8	H	66	0	74	7	0
8	I	132	0	148	19	0
8	J	66	0	74	4	0
8	K	132	0	148	19	0
8	L	132	0	148	18	0
8	M	66	0	74	5	0
8	N	66	0	74	3	0
8	O	132	0	148	11	0
8	P	66	0	74	1	0
8	Q	132	0	148	14	0
8	R	66	0	72	6	0
8	S	132	0	145	11	0
8	T	66	0	74	3	0
8	U	132	0	146	12	0
8	V	66	0	74	4	0
8	W	132	0	146	17	0
9	L	65	0	76	7	0
9	M	130	0	152	2	0
10	L	68	0	0	0	0
10	M	68	0	0	3	0
11	C	172	0	120	31	0
12	3	82	0	0	6	0
12	5	41	0	0	0	0
12	9	82	0	0	1	0
12	A	41	0	0	1	0
12	F	41	0	0	3	0
12	H	41	0	0	5	0
12	J	41	0	0	0	0
12	N	82	0	0	3	0
12	R	41	0	0	1	0
12	T	82	0	0	1	0
13	M	1	0	0	0	0
All	All	20009	0	18282	576	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 15.

All (576) 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)
1:I:33:ILE:HG13	8:I:102:BCL:CED	1.49	1.40
1:W:33:ILE:CG1	8:W:102:BCL:HED1	1.50	1.39
1:B:30:VAL:CB	8:B:102:BCL:O1D	1.78	1.32
1:B:30:VAL:CA	8:B:102:BCL:O1D	1.77	1.32
1:B:30:VAL:HA	8:B:102:BCL:O1D	1.25	1.30
1:I:33:ILE:CG1	8:I:102:BCL:CED	2.13	1.27
1:K:33:ILE:CG2	8:K:102:BCL:HED3	1.64	1.26
1:B:30:VAL:HG23	8:B:102:BCL:CED	1.67	1.24
1:I:33:ILE:HG13	8:I:102:BCL:HED1	1.20	1.17
1:I:33:ILE:HG13	8:I:102:BCL:HED3	1.26	1.15
1:W:33:ILE:HG13	8:W:102:BCL:CED	1.77	1.13
1:I:33:ILE:CG1	8:I:102:BCL:HED1	1.78	1.12
1:B:30:VAL:HG23	8:B:102:BCL:HED3	1.18	1.11
1:6:14:TRP:HE1	8:6:102:BCL:HBB1	1.10	1.07
1:I:33:ILE:CG1	8:I:102:BCL:HED3	1.77	1.07
1:B:30:VAL:CG2	8:B:102:BCL:HED3	1.84	1.07
1:K:33:ILE:HG21	8:K:102:BCL:HED3	1.34	1.07
1:B:30:VAL:HB	8:B:102:BCL:O1D	1.53	1.04
1:I:53:TRP:HZ2	8:I:101:BCL:OBB	1.39	1.04
2:L:77:ILE:HG21	10:M:702:MQE:CBF	1.88	1.03
1:E:53:TRP:HZ2	8:E:101:BCL:OBB	1.41	1.02
1:K:53:TRP:HZ2	8:K:101:BCL:OBB	1.41	1.02
1:K:33:ILE:HB	8:K:102:BCL:HED1	1.43	1.00
1:B:26:HIS:NE2	8:B:102:BCL:ND	2.10	1.00
1:O:53:TRP:HZ2	8:O:101:BCL:OBB	1.44	0.99
1:W:33:ILE:CG1	8:W:102:BCL:CED	2.34	0.99
1:6:14:TRP:NE1	8:6:102:BCL:HBB1	1.76	0.99
1:2:53:TRP:HZ2	8:2:101:BCL:OBB	1.46	0.98
1:U:14:TRP:CD1	8:U:102:BCL:OBB	2.16	0.98
4:H:10:THR:O	4:H:14:VAL:HG22	1.64	0.98
1:4:29:VAL:HG12	12:3:103:KGD:CAN	1.93	0.98
1:Q:53:TRP:HZ2	8:Q:101:BCL:OBB	1.46	0.97
1:U:53:TRP:HZ2	8:U:101:BCL:OBB	1.48	0.96
1:6:14:TRP:HE1	8:6:102:BCL:CBB	1.79	0.96
1:O:53:TRP:HZ2	8:O:101:BCL:OBB	1.49	0.96
1:4:29:VAL:CG1	12:3:103:KGD:CAN	2.44	0.95
1:K:33:ILE:HB	8:K:102:BCL:CED	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:53:TRP:HZ2	8:W:101:BCL:OBB	1.48	0.95
1:B:30:VAL:HG23	8:B:102:BCL:CGD	1.98	0.93
1:I:33:ILE:HG12	8:I:102:BCL:CED	2.02	0.90
1:4:29:VAL:HB	12:3:103:KGD:CAN	2.01	0.89
2:L:192:HIS:HE1	8:L:1001:BCL:MG	0.70	0.89
1:B:53:TRP:HZ2	8:B:101:BCL:OBB	1.54	0.89
1:O:53:TRP:CZ2	8:O:101:BCL:OBB	2.26	0.89
1:W:53:TRP:CZ2	8:W:101:BCL:OBB	2.26	0.88
2:L:77:ILE:HD12	4:R:17:LEU:CD2	2.04	0.88
1:Q:53:TRP:CZ2	8:Q:101:BCL:OBB	2.28	0.87
1:O:53:TRP:CZ2	8:O:101:BCL:OBB	2.28	0.87
1:I:53:TRP:CZ2	8:I:101:BCL:OBB	2.26	0.87
1:K:53:TRP:CZ2	8:K:101:BCL:OBB	2.27	0.86
1:E:53:TRP:CZ2	8:E:101:BCL:OBB	2.28	0.86
1:2:53:TRP:CZ2	8:2:101:BCL:OBB	2.29	0.86
1:U:53:TRP:CZ2	8:U:101:BCL:OBB	2.28	0.86
1:4:29:VAL:CB	12:3:103:KGD:CAN	2.55	0.85
1:S:53:TRP:CZ2	8:S:101:BCL:OBB	2.31	0.84
1:G:53:TRP:CZ2	8:G:101:BCL:OBB	2.31	0.83
1:G:53:TRP:HZ2	8:G:101:BCL:OBB	1.61	0.83
1:S:53:TRP:HZ2	8:S:101:BCL:OBB	1.60	0.83
1:B:53:TRP:CZ2	8:B:101:BCL:OBB	2.32	0.83
4:N:20:LEU:HD23	8:N:103:BCL:H2	1.61	0.83
1:4:53:TRP:HH2	8:4:101:BCL:H2C	1.43	0.83
2:L:192:HIS:CE1	8:L:1001:BCL:MG	1.54	0.82
2:L:77:ILE:CG2	10:M:702:MQE:CBF	2.57	0.82
1:O:14:TRP:CD1	8:O:102:BCL:OBB	2.32	0.82
1:B:30:VAL:HG23	8:B:102:BCL:O2D	1.79	0.81
1:W:14:TRP:CE2	8:W:102:BCL:OBB	2.33	0.81
1:8:53:TRP:CZ2	8:8:101:BCL:OBB	2.34	0.81
1:K:33:ILE:CB	8:K:102:BCL:HED3	2.10	0.81
1:W:33:ILE:HG13	8:W:102:BCL:HED1	0.81	0.80
2:L:77:ILE:HD12	4:R:17:LEU:HD21	1.62	0.79
1:K:33:ILE:CG2	8:K:102:BCL:CED	2.56	0.79
1:B:30:VAL:CG2	8:B:102:BCL:CGD	2.62	0.78
1:K:33:ILE:CB	8:K:102:BCL:CED	2.61	0.78
1:B:30:VAL:CG2	8:B:102:BCL:O1D	2.31	0.78
1:S:29:VAL:HG22	8:S:102:BCL:HED2	1.65	0.78
7:M:341:GLU:HG3	7:M:342:GLU:HG3	1.64	0.78
2:L:192:HIS:NE2	8:L:1001:BCL:NC	2.32	0.77
2:L:264:HIS:NE2	7:M:557:GLU:OE2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:TRP:CE2	8:K:102:BCL:OBB	2.37	0.77
1:K:33:ILE:HG22	8:K:102:BCL:HED3	1.67	0.77
1:8:14:TRP:CD2	8:8:102:BCL:OBB	2.38	0.76
3:C:93:VAL:HB	11:C:501:HEM:CGD	2.16	0.75
3:C:199:LEU:HD22	3:C:200:PRO:HD2	1.68	0.75
1:B:30:VAL:CB	8:B:102:BCL:CGD	2.64	0.75
1:G:14:TRP:HZ2	8:G:102:BCL:OBB	1.70	0.74
2:L:8:LEU:HD13	4:J:28:PHE:HB3	1.70	0.73
4:F:14:VAL:HG11	8:D:101:BCL:H162	1.70	0.73
1:8:14:TRP:CE2	8:8:102:BCL:OBB	2.42	0.72
1:B:30:VAL:HB	8:B:102:BCL:CGD	2.19	0.72
1:G:14:TRP:CZ2	8:G:102:BCL:OBB	2.43	0.72
4:A:38:TRP:HZ2	8:A:102:BCL:HHC	1.52	0.72
3:C:117:ASP:O	3:C:119:SER:N	2.23	0.72
1:W:33:ILE:CB	8:W:102:BCL:HED1	2.21	0.71
4:H:20:LEU:HD23	8:H:101:BCL:H2	1.72	0.71
3:C:98:THR:H	3:C:101:GLN:HE21	1.35	0.71
4:A:38:TRP:CZ2	8:A:102:BCL:HHC	2.25	0.71
1:I:33:ILE:CD1	12:H:102:KGD:CAU	2.69	0.71
8:I:102:BCL:H62	8:G:101:BCL:H122	1.71	0.71
3:C:303:PRO:HG2	3:C:304:PRO:HD3	1.73	0.70
1:4:50:TRP:HE1	4:3:36:PHE:HB3	1.57	0.70
3:C:93:VAL:HB	11:C:501:HEM:O1D	1.92	0.69
2:L:77:ILE:CD1	4:R:17:LEU:CD2	2.71	0.68
8:O:101:BCL:H41	8:O:101:BCL:H71	1.75	0.68
2:L:226:LEU:HD23	7:M:539:LEU:HD23	1.75	0.67
1:K:29:VAL:HG12	8:K:102:BCL:HED2	1.76	0.67
2:L:105:ILE:HG13	2:L:106:GLU:H	1.59	0.67
1:I:33:ILE:HD11	12:H:102:KGD:CAU	2.25	0.67
8:I:101:BCL:H101	8:H:101:BCL:H43	1.75	0.67
2:L:133:THR:HG22	2:L:167:TRP:HE1	1.58	0.67
3:C:245:ASN:HB2	3:C:254:ILE:HD11	1.76	0.66
3:C:122:HIS:NE2	11:C:501:HEM:C1A	2.53	0.66
2:L:256:TYR:CE2	2:L:258:ILE:HB	2.30	0.66
8:L:1001:BCL:H112	8:L:1002:BCL:H172	1.76	0.66
1:U:14:TRP:HD1	8:U:102:BCL:OBB	1.74	0.66
1:8:14:TRP:CG	8:8:102:BCL:OBB	2.48	0.65
8:L:1002:BCL:H141	9:L:1003:BPH:H6C2	1.79	0.65
2:L:133:THR:HG21	2:L:172:TRP:HE1	1.61	0.65
4:A:38:TRP:CZ2	8:A:102:BCL:OBB	2.50	0.64
3:C:244:HIS:NE2	11:C:503:HEM:C1C	2.47	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:0:102:BCL:H8	8:8:101:BCL:H141	1.78	0.64
1:4:14:TRP:CE2	8:4:102:BCL:OBB	2.51	0.64
3:C:122:HIS:NE2	11:C:501:HEM:C4A	2.53	0.64
4:7:38:TRP:HZ2	8:7:101:BCL:OBB	1.80	0.64
1:I:33:ILE:CB	8:I:102:BCL:HED3	2.27	0.64
3:C:106:MET:SD	11:C:501:HEM:C4B	2.72	0.64
1:S:33:ILE:HB	8:S:102:BCL:HED3	1.80	0.64
3:C:235:SER:HB2	3:C:294:TRP:HB3	1.80	0.64
3:C:175:HIS:HE1	11:C:502:HEM:ND	1.94	0.63
3:C:39:PHE:HB2	4:1:22:MET:HE1	1.81	0.63
7:M:545:THR:HG21	7:M:575:TRP:HE1	1.63	0.63
4:J:20:LEU:HD21	8:J:102:BCL:H52	1.80	0.63
1:B:14:TRP:CD1	8:B:102:BCL:OBB	2.52	0.63
1:B:26:HIS:NE2	8:B:102:BCL:C1D	2.62	0.63
2:L:77:ILE:CD1	4:R:17:LEU:HD21	2.29	0.62
2:L:205:ASN:O	2:L:207:PHE:N	2.32	0.62
3:C:152:LEU:HD21	3:C:266:MET:HE3	1.81	0.62
2:L:192:HIS:CE1	8:L:1001:BCL:NC	2.68	0.62
4:V:38:TRP:CZ2	8:V:101:BCL:OBB	2.53	0.61
1:8:26:HIS:NE2	8:8:102:BCL:ND	2.48	0.61
7:M:431:PRO:HB2	7:M:434:LYS:HB2	1.82	0.61
3:C:229:MET:SD	11:C:503:HEM:C4B	2.85	0.61
7:M:397:TYR:OH	7:M:412:PHE:O	2.19	0.61
4:T:38:TRP:CZ2	8:T:103:BCL:OBB	2.53	0.60
8:S:101:BCL:H62	8:R:102:BCL:H43	1.83	0.60
1:W:33:ILE:CB	8:W:102:BCL:CED	2.78	0.60
1:8:53:TRP:HZ2	8:8:101:BCL:OBB	1.83	0.60
4:H:13:VAL:HG13	8:H:101:BCL:H201	1.84	0.60
2:L:212:HIS:HB2	2:L:281:CYS:SG	2.42	0.59
1:W:14:TRP:HE1	1:W:23:TRP:HZ3	1.48	0.59
1:4:14:TRP:CZ2	8:4:102:BCL:OBB	2.55	0.59
1:2:14:TRP:CZ2	8:2:102:BCL:OBB	2.56	0.59
11:C:501:HEM:HMC1	11:C:501:HEM:HBC2	1.84	0.59
8:0:101:BCL:HMA1	8:7:101:BCL:HMA1	1.85	0.59
3:C:99:THR:HA	3:C:102:ILE:HD12	1.84	0.59
2:L:253:ILE:HG13	2:L:255:GLY:H	1.67	0.59
4:H:19:GLY:HA3	12:H:102:KGD:CBG	2.31	0.59
1:8:14:TRP:CD1	8:8:102:BCL:OBB	2.56	0.58
4:T:18:LEU:HD12	8:R:102:BCL:H172	1.86	0.58
8:R:102:BCL:H142	8:R:102:BCL:H72	1.85	0.58
4:3:38:TRP:HE3	4:3:39:LEU:HD23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:TRP:HZ3	7:M:577:TRP:NE1	2.02	0.58
7:M:426:LEU:HG	7:M:494:TRP:HB2	1.85	0.58
1:K:30:VAL:O	1:K:33:ILE:HG22	2.04	0.57
3:C:217:VAL:HG13	3:C:218:SER:H	1.68	0.57
3:C:190:MET:HA	3:C:193:LEU:HD13	1.85	0.57
1:W:33:ILE:HB	8:W:102:BCL:HED3	1.86	0.57
4:F:38:TRP:CZ2	8:F:102:BCL:OBB	2.58	0.57
3:C:106:MET:SD	11:C:501:HEM:C1B	2.78	0.57
1:W:33:ILE:HG12	8:W:102:BCL:CED	2.33	0.57
1:U:29:VAL:HG22	8:U:102:BCL:HED1	1.87	0.57
2:L:192:HIS:CE1	8:L:1001:BCL:NB	2.73	0.57
4:V:38:TRP:HZ2	8:V:101:BCL:OBB	1.87	0.57
2:L:84:VAL:HG23	9:L:1003:BPH:H9C3	1.87	0.56
3:C:219:ASN:HD22	7:M:496:ALA:HA	1.70	0.56
1:2:30:VAL:HG21	8:2:102:BCL:HMA3	1.87	0.56
11:C:501:HEM:HMB1	11:C:501:HEM:HBB2	1.87	0.56
7:M:375:VAL:HG21	7:M:459:ARG:HD3	1.88	0.56
2:L:107:PRO:HG3	2:L:186:PRO:HB3	1.88	0.56
3:C:93:VAL:HG23	3:C:94:LEU:N	2.20	0.56
4:D:31:LEU:HD22	4:D:38:TRP:CD1	2.41	0.56
8:G:101:BCL:H2	8:G:101:BCL:HED1	1.88	0.56
1:U:14:TRP:NE1	8:U:102:BCL:CAB	2.69	0.56
1:E:50:TRP:HZ3	4:D:36:PHE:HD1	1.54	0.56
3:C:232:MET:O	3:C:235:SER:OG	2.20	0.55
3:C:93:VAL:HG23	3:C:94:LEU:H	1.70	0.55
1:6:30:VAL:HG21	8:6:102:BCL:HMA1	1.89	0.55
1:8:14:TRP:CE2	8:8:102:BCL:CAB	2.89	0.55
3:C:302:ILE:HG13	11:C:504:HEM:C2D	2.42	0.55
7:M:354:PRO:HB3	7:M:371:GLY:HA2	1.88	0.55
2:L:77:ILE:CD1	4:R:17:LEU:HD22	2.36	0.55
4:T:38:TRP:CZ3	8:T:103:BCL:HMC2	2.42	0.55
1:O:30:VAL:HG23	8:O:102:BCL:HED3	1.89	0.55
11:C:504:HEM:HHC	11:C:504:HEM:HBB2	1.89	0.54
4:7:31:LEU:HD23	4:7:38:TRP:CE3	2.42	0.54
1:W:33:ILE:HB	8:W:102:BCL:CED	2.37	0.54
8:2:101:BCL:H102	8:1:101:BCL:HED1	1.89	0.54
1:E:14:TRP:HZ2	8:E:102:BCL:OBB	1.90	0.54
2:L:139:TRP:CZ3	9:L:1003:BPH:HAA2	2.43	0.54
8:S:102:BCL:HBC3	8:S:102:BCL:HHD	1.90	0.54
1:B:30:VAL:HG23	8:B:102:BCL:O1D	2.00	0.54
2:L:252:ASN:HD22	7:M:459:ARG:HH21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:VAL:HG12	12:F:101:KGD:CAN	2.38	0.53
2:L:58:ASP:N	2:L:59:PRO:HD2	2.23	0.53
8:G:101:BCL:H192	12:H:102:KGD:CBL	2.38	0.53
8:Q:102:BCL:H52	8:O:101:BCL:H172	1.91	0.53
1:O:33:ILE:HG13	8:O:102:BCL:HED3	1.91	0.53
8:B:101:BCL:HMD3	4:A:27:HIS:CE1	2.44	0.53
3:C:218:SER:HB3	3:C:220:HIS:H	1.72	0.53
3:C:244:HIS:NE2	11:C:503:HEM:C4C	2.56	0.53
8:G:102:BCL:HBC3	8:G:102:BCL:HHD	1.89	0.53
7:M:482:VAL:HG21	7:M:604:ALA:HB1	1.91	0.53
3:C:170:THR:HG23	3:C:172:ALA:H	1.74	0.53
1:8:39:ILE:HA	1:8:42:ILE:HG12	1.91	0.53
1:K:26:HIS:NE2	8:K:102:BCL:ND	2.57	0.52
3:C:302:ILE:HG22	3:C:305:GLY:H	1.73	0.52
4:3:19:GLY:HA3	12:3:103:KGD:CBG	2.39	0.52
1:4:39:ILE:HA	1:4:42:ILE:HD12	1.91	0.52
8:U:102:BCL:HBC3	8:U:102:BCL:HHD	1.91	0.52
3:C:137:ALA:O	3:C:140:VAL:HB	2.10	0.52
3:C:241:THR:C	3:C:243:CYS:H	2.17	0.52
8:I:102:BCL:CMD	4:H:11:SER:OG	2.57	0.52
3:C:263:MET:HE1	11:C:504:HEM:C1A	2.39	0.52
8:8:101:BCL:H11	8:6:101:BCL:H201	1.91	0.52
4:P:25:LEU:HD13	10:M:702:MQE:CCO	2.40	0.52
7:M:453:TRP:NE1	7:M:470:ALA:O	2.28	0.52
4:3:38:TRP:CE3	4:3:39:LEU:HD23	2.46	0.51
8:L:1001:BCL:H121	8:L:1002:BCL:H202	1.92	0.51
8:6:102:BCL:HBC3	8:6:102:BCL:HHD	1.92	0.51
1:K:14:TRP:CD2	8:K:102:BCL:OBB	2.63	0.51
3:C:244:HIS:HB3	3:C:249:PHE:CD1	2.45	0.51
8:W:101:BCL:H62	8:V:101:BCL:HED1	1.91	0.51
1:U:14:TRP:CD1	8:U:102:BCL:CAB	2.93	0.51
8:U:102:BCL:HBC2	4:T:8:PHE:CD1	2.45	0.51
7:M:472:GLY:O	7:M:475:SER:OG	2.13	0.51
8:K:102:BCL:H12	8:I:101:BCL:H203	1.92	0.51
1:6:33:ILE:HG13	8:6:102:BCL:HED3	1.92	0.51
11:C:504:HEM:HMC1	11:C:504:HEM:HBC2	1.91	0.51
1:G:50:TRP:CD1	1:G:51:THR:HG23	2.46	0.51
7:M:637:GLN:HG3	7:M:638:TYR:CE1	2.45	0.51
11:C:502:HEM:HBB2	11:C:502:HEM:HMB2	1.91	0.51
7:M:438:TRP:HH2	7:M:499:GLY:HA2	1.76	0.51
4:D:33:SER:OG	4:D:34:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:339:HIS:CE1	7:M:342:GLU:HB2	2.46	0.51
1:0:30:VAL:HA	8:0:102:BCL:HED2	1.92	0.50
8:K:101:BCL:H102	8:J:102:BCL:H43	1.93	0.50
3:C:263:MET:HE1	11:C:504:HEM:C4D	2.42	0.50
8:U:102:BCL:H41	8:S:101:BCL:H202	1.93	0.50
1:E:29:VAL:HG11	8:E:102:BCL:HED3	1.93	0.50
2:L:105:ILE:HG12	2:L:187:LEU:O	2.11	0.50
7:M:561:MET:HE3	7:M:586:TYR:HB3	1.92	0.50
8:I:102:BCL:HMD1	4:H:11:SER:OG	2.11	0.50
1:G:29:VAL:HB	8:G:102:BCL:HED2	1.94	0.50
4:A:39:LEU:H	4:A:39:LEU:HD12	1.76	0.50
2:L:10:LEU:HD23	7:M:523:PRO:HG3	1.94	0.50
8:6:102:BCL:H12	8:4:101:BCL:H201	1.94	0.50
4:P:6:PHE:HZ	8:N:103:BCL:H171	1.77	0.50
4:R:19:GLY:HA3	12:R:101:KGD:CBG	2.42	0.50
2:L:302:MET:HB2	2:L:305:TRP:HD1	1.76	0.50
1:G:26:HIS:HA	1:G:29:VAL:HG22	1.93	0.50
4:T:31:LEU:HD21	4:T:38:TRP:CD1	2.46	0.50
7:M:575:TRP:HA	7:M:578:VAL:HG22	1.93	0.50
8:E:102:BCL:HBC3	8:E:102:BCL:HHD	1.93	0.50
3:C:64:GLN:HB2	3:C:303:PRO:O	2.11	0.50
11:C:502:HEM:HMC1	11:C:502:HEM:HBC2	1.94	0.49
7:M:438:TRP:HB3	7:M:439:LEU:HD12	1.94	0.49
7:M:554:SER:HB3	7:M:567:GLY:HA3	1.94	0.49
2:L:192:HIS:NE2	8:L:1001:BCL:C1C	2.75	0.49
2:L:256:TYR:O	2:L:258:ILE:N	2.45	0.49
1:0:48:TRP:CD1	1:0:52:PRO:HA	2.47	0.49
4:F:22:MET:HG3	12:F:101:KGD:CBK	2.42	0.49
8:5:102:BCL:OBB	8:5:102:BCL:HHC	2.12	0.49
1:2:53:TRP:CH2	8:2:101:BCL:HHC	2.48	0.49
7:M:438:TRP:CH2	7:M:499:GLY:HA2	2.48	0.49
1:B:14:TRP:NE1	8:B:102:BCL:CAB	2.75	0.49
1:0:26:HIS:HA	1:0:29:VAL:HG22	1.94	0.49
1:4:30:VAL:HA	8:4:102:BCL:HED2	1.94	0.49
8:K:102:BCL:HBC3	8:K:102:BCL:HHD	1.93	0.49
3:C:244:HIS:HB3	3:C:249:PHE:HD1	1.77	0.49
3:C:263:MET:O	3:C:266:MET:HB3	2.12	0.49
4:5:38:TRP:CE3	4:5:39:LEU:HB2	2.48	0.49
3:C:189:ILE:HG22	3:C:190:MET:N	2.27	0.49
1:U:25:VAL:HA	1:U:28:ILE:HD12	1.95	0.49
4:1:20:LEU:HD21	8:1:101:BCL:H52	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:558:PHE:O	7:M:559:THR:OG1	2.21	0.49
1:E:14:TRP:CZ2	8:E:102:BCL:OBB	2.65	0.49
2:L:228:MET:HE3	2:L:250:TRP:HH2	1.77	0.49
3:C:192:THR:C	3:C:193:LEU:HD12	2.37	0.49
3:C:261:ILE:HA	3:C:264:LEU:HD12	1.95	0.49
3:C:205:TYR:CE2	3:C:264:LEU:HD13	2.48	0.49
1:O:30:VAL:HG22	1:O:34:TYR:CE2	2.48	0.49
2:L:105:ILE:HG13	2:L:106:GLU:N	2.24	0.48
8:O:101:BCL:HMD3	4:N:27:HIS:CE1	2.48	0.48
4:V:38:TRP:O	4:V:39:LEU:HG	2.13	0.48
2:L:42:PHE:O	2:L:46:PRO:HD2	2.12	0.48
2:L:229:HIS:HD1	2:L:263:ILE:HD11	1.78	0.48
1:4:48:TRP:HA	1:4:51:THR:HG22	1.96	0.48
2:L:4:VAL:HG13	2:L:5:PRO:HD2	1.96	0.48
3:C:217:VAL:HG13	3:C:218:SER:N	2.27	0.48
4:N:38:TRP:CG	4:N:39:LEU:H	2.31	0.48
1:U:50:TRP:HE1	4:T:36:PHE:HD1	1.61	0.48
8:O:102:BCL:HBC2	4:N:8:PHE:HD1	1.79	0.48
8:4:101:BCL:HAC1	8:3:102:BCL:HAC1	1.96	0.48
3:C:122:HIS:CE1	11:C:501:HEM:C4A	3.02	0.48
3:C:303:PRO:CG	3:C:304:PRO:HD3	2.41	0.48
8:W:101:BCL:H112	8:V:101:BCL:H2	1.96	0.48
1:O:26:HIS:NE2	8:O:102:BCL:ND	2.62	0.48
7:M:549:THR:HG21	7:M:571:ALA:HB2	1.95	0.48
2:L:192:HIS:CE1	8:L:1001:BCL:ND	2.82	0.48
1:2:30:VAL:HB	8:2:102:BCL:HED2	1.95	0.48
3:C:119:SER:C	3:C:121:CYS:H	2.22	0.48
3:C:176:ASN:O	3:C:178:LYS:N	2.39	0.48
1:Q:14:TRP:CD1	8:Q:102:BCL:OBB	2.66	0.48
7:M:351:ILE:HG22	7:M:353:LYS:H	1.79	0.48
8:7:101:BCL:OBB	8:7:101:BCL:HHC	2.14	0.48
7:M:637:GLN:HG3	7:M:638:TYR:CD1	2.49	0.48
4:H:10:THR:O	4:H:14:VAL:CG2	2.51	0.48
8:F:102:BCL:OBB	8:F:102:BCL:HHC	2.14	0.48
4:F:34:GLY:HA3	4:D:39:LEU:HD21	1.94	0.47
3:C:275:VAL:HG21	3:C:289:LYS:HA	1.96	0.47
1:B:26:HIS:O	1:B:30:VAL:HG12	2.14	0.47
1:6:53:TRP:CE2	8:6:101:BCL:OBB	2.67	0.47
3:C:244:HIS:CD2	11:C:503:HEM:C1C	3.02	0.47
2:L:289:VAL:HG11	2:L:292:TRP:CE2	2.50	0.47
1:8:26:HIS:NE2	8:8:102:BCL:C4D	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:11:PRO:HA	2:L:14:GLU:HG3	1.95	0.47
2:L:187:LEU:HD21	9:L:1003:BPH:H151	1.95	0.47
8:O:102:BCL:H171	8:J:102:BCL:HED1	1.96	0.47
8:O:101:BCL:HMC3	8:7:101:BCL:HBB1	1.96	0.47
2:L:14:GLU:O	2:L:17:PRO:HD2	2.14	0.47
3:C:133:TYR:O	3:C:135:ASN:N	2.43	0.47
3:C:143:ARG:O	3:C:146:MET:HB2	2.14	0.47
1:O:25:VAL:O	1:O:29:VAL:HG23	2.15	0.47
8:M:703:BCL:H102	9:M:704:BPH:HBB2	1.95	0.47
7:M:614:VAL:HG11	7:M:617:TRP:CZ2	2.50	0.47
1:S:50:TRP:HH2	4:R:36:PHE:O	1.98	0.47
4:F:28:PHE:HD2	4:F:29:VAL:HG23	1.80	0.47
1:4:29:VAL:HG12	12:3:103:KGD:CAJ	2.45	0.46
8:L:1001:BCL:H111	8:L:1001:BCL:H152	1.66	0.46
8:9:103:BCL:OBB	8:9:103:BCL:HHC	2.14	0.46
2:L:77:ILE:HD11	4:R:17:LEU:HD22	1.98	0.46
1:K:33:ILE:HG21	8:K:102:BCL:CED	2.24	0.46
3:C:63:THR:O	3:C:65:GLU:N	2.44	0.46
8:B:101:BCL:H61	8:B:101:BCL:H41	1.77	0.46
8:S:101:BCL:H92	8:R:102:BCL:H43	1.98	0.46
8:Q:102:BCL:H3A	8:Q:102:BCL:HBA2	1.62	0.46
7:M:485:LEU:C	7:M:488:PRO:HD2	2.41	0.46
7:M:499:GLY:C	7:M:501:GLY:H	2.24	0.46
7:M:525:HIS:CE1	7:M:529:ILE:HD11	2.51	0.46
1:2:53:TRP:CZ2	8:2:101:BCL:HHC	2.51	0.46
7:M:415:LEU:HD13	7:M:416:ALA:N	2.30	0.46
1:O:53:TRP:HZ3	4:7:38:TRP:HE1	1.63	0.46
4:A:24:LEU:HG	4:A:28:PHE:CE2	2.51	0.46
8:G:101:BCL:H71	8:F:102:BCL:HED1	1.98	0.46
7:M:465:VAL:HG22	7:M:466:GLY:H	1.80	0.46
7:M:477:LEU:O	7:M:480:TYR:HB3	2.16	0.46
1:4:48:TRP:HZ3	1:4:53:TRP:CD1	2.34	0.46
7:M:449:VAL:HG11	7:M:477:LEU:HD21	1.98	0.46
7:M:397:TYR:CZ	7:M:415:LEU:HB3	2.51	0.45
1:S:14:TRP:CZ2	8:S:102:BCL:HBB1	2.51	0.45
8:Q:102:BCL:HBC3	8:Q:102:BCL:HHD	1.99	0.45
2:L:57:VAL:C	2:L:59:PRO:HD2	2.41	0.45
2:L:305:TRP:CE3	7:M:410:ARG:HB2	2.52	0.45
7:M:568:THR:HA	7:M:571:ALA:HB3	1.97	0.45
1:B:26:HIS:NE2	8:B:102:BCL:C4D	2.76	0.45
8:L:1002:BCL:NB	8:M:703:BCL:HBB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:PHE:CE1	3:C:47:THR:HG21	2.51	0.45
3:C:167:TYR:HB2	11:C:504:HEM:CGD	2.47	0.45
8:S:101:BCL:HMD3	4:R:27:HIS:CE1	2.52	0.45
1:6:14:TRP:HE1	8:6:102:BCL:CAB	2.29	0.45
1:K:41:VAL:O	1:K:45:VAL:HG23	2.16	0.45
1:S:52:PRO:C	1:S:54:ILE:H	2.25	0.45
7:M:515:HIS:HD2	7:M:516:TRP:CD1	2.34	0.45
1:6:53:TRP:CZ2	8:6:101:BCL:OBB	2.70	0.45
3:C:56:ASN:O	3:C:58:ILE:N	2.49	0.45
4:H:22:MET:HG3	12:H:102:KGD:CBK	2.46	0.45
4:3:38:TRP:CE3	4:3:39:LEU:HB2	2.51	0.45
8:0:101:BCL:HBC2	8:0:101:BCL:H2C	1.65	0.45
1:W:26:HIS:O	1:W:30:VAL:HG23	2.17	0.45
4:N:38:TRP:CH2	4:N:39:LEU:HD12	2.52	0.45
8:0:101:BCL:H141	8:0:101:BCL:H161	1.81	0.45
2:L:112:GLN:NE2	2:L:117:ASP:OD2	2.40	0.45
4:H:38:TRP:CG	4:H:39:LEU:H	2.34	0.45
7:M:429:ASN:OD1	7:M:430:VAL:N	2.44	0.45
8:B:101:BCL:HBC2	8:B:101:BCL:H2C	1.69	0.45
3:C:123:ASN:O	3:C:125:ALA:N	2.50	0.45
1:W:14:TRP:CD2	8:W:102:BCL:OBB	2.70	0.45
4:5:13:VAL:HG22	8:5:102:BCL:H162	1.99	0.45
7:M:429:ASN:CG	7:M:431:PRO:HD2	2.41	0.45
1:B:14:TRP:NE1	8:B:102:BCL:OBB	2.50	0.45
2:L:162:ALA:O	2:L:165:SER:OG	2.32	0.45
3:C:297:HIS:CE1	3:C:302:ILE:HD11	2.52	0.45
1:S:14:TRP:HZ2	8:S:102:BCL:HBB1	1.82	0.45
7:M:489:LEU:C	7:M:491:LEU:H	2.25	0.45
1:8:33:ILE:HG13	8:8:102:BCL:HED3	1.99	0.44
8:D:101:BCL:H72	8:D:101:BCL:H111	1.73	0.44
7:M:416:ALA:HB1	7:M:501:GLY:HA3	1.98	0.44
7:M:430:VAL:O	7:M:432:TRP:N	2.50	0.44
2:L:139:TRP:HH2	9:L:1003:BPH:O2D	2.00	0.44
3:C:217:VAL:O	3:C:218:SER:OG	2.28	0.44
8:3:102:BCL:OBB	8:3:102:BCL:HHC	2.18	0.44
2:L:204:TYR:CE2	2:L:205:ASN:HB3	2.53	0.44
1:G:30:VAL:HG12	8:G:102:BCL:HMA2	1.99	0.44
8:U:101:BCL:H172	12:T:101:KGD:CBN	2.47	0.44
4:A:24:LEU:HG	4:A:28:PHE:HE2	1.82	0.44
7:M:431:PRO:O	7:M:435:GLY:N	2.50	0.44
7:M:558:PHE:CD2	7:M:559:THR:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:101:BCL:H61	8:E:101:BCL:H41	1.75	0.44
8:E:101:BCL:HMA1	8:A:102:BCL:HMA1	1.99	0.44
2:L:171:GLN:HE22	2:L:185:PHE:CB	2.31	0.44
3:C:148:MET:O	3:C:152:LEU:N	2.51	0.44
7:M:532:LEU:O	7:M:535:SER:OG	2.27	0.44
8:4:101:BCL:H2C	8:4:101:BCL:HBC2	1.77	0.44
3:C:106:MET:HE1	11:C:501:HEM:C4D	2.45	0.44
3:C:173:THR:HG23	3:C:304:PRO:HG2	1.98	0.44
3:C:302:ILE:HG13	11:C:504:HEM:C3D	2.53	0.44
8:R:102:BCL:H61	8:R:102:BCL:H41	1.80	0.44
2:L:105:ILE:HD11	2:L:187:LEU:HB3	2.00	0.44
2:L:273:ALA:HA	2:L:276:LEU:HD12	2.00	0.44
1:I:14:TRP:NE1	8:I:102:BCL:OBB	2.51	0.44
1:G:33:ILE:HD11	12:F:101:KGD:CAU	2.48	0.44
8:1:101:BCL:HBC2	8:1:101:BCL:H2C	1.77	0.44
8:L:1001:BCL:HED2	7:M:526:MET:SD	2.58	0.44
3:C:251:SER:O	3:C:257:LYS:NZ	2.37	0.44
4:D:31:LEU:HD22	4:D:38:TRP:HD1	1.79	0.44
2:L:136:PHE:CE1	8:L:1002:BCL:H112	2.53	0.43
1:I:27:ASP:OD1	1:I:31:LYS:HE2	2.18	0.43
4:5:34:GLY:HA2	4:3:39:LEU:CD1	2.48	0.43
4:3:20:LEU:HD12	8:3:102:BCL:H2	2.00	0.43
2:L:276:LEU:HD22	5:Y:13:UNK:CB	2.48	0.43
3:C:301:ASN:ND2	11:C:504:HEM:O1A	2.51	0.43
1:B:14:TRP:HE1	8:B:102:BCL:CAB	2.30	0.43
2:L:235:SER:OG	7:M:465:VAL:HG22	2.18	0.43
3:C:141:THR:O	3:C:144:LYS:HB3	2.19	0.43
8:U:102:BCL:H71	8:U:102:BCL:H112	1.75	0.43
4:A:14:VAL:HG21	8:9:103:BCL:H151	1.99	0.43
8:A:102:BCL:HBC2	8:A:102:BCL:H2C	1.67	0.43
3:C:297:HIS:NE2	11:C:504:HEM:C1C	2.77	0.43
4:7:38:TRP:CZ2	8:7:101:BCL:OBB	2.65	0.43
8:3:102:BCL:H62	8:3:102:BCL:H41	1.72	0.43
2:L:9:PRO:O	2:L:12:SER:OG	2.24	0.43
8:2:102:BCL:H61	8:2:102:BCL:H41	1.62	0.43
1:I:33:ILE:HG12	8:I:102:BCL:HED1	1.77	0.43
1:W:22:GLN:O	1:W:25:VAL:HG22	2.17	0.43
1:Q:47:CYS:HB3	8:Q:101:BCL:HBC1	2.01	0.43
8:R:102:BCL:HBC2	8:R:102:BCL:H2C	1.74	0.43
1:0:33:ILE:CG1	8:0:102:BCL:HED3	2.49	0.43
2:L:216:ILE:HD12	8:L:1002:BCL:HMB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:HIS:HE1	11:C:502:HEM:C4D	2.37	0.43
8:T:103:BCL:H93	8:T:103:BCL:H111	1.85	0.43
8:H:101:BCL:HBC2	8:H:101:BCL:H2C	1.87	0.43
8:B:102:BCL:H62	8:B:102:BCL:H41	1.90	0.43
2:L:140:LEU:HD12	2:L:160:PHE:HD2	1.83	0.43
2:L:203:TYR:CE2	2:L:285:SER:HB3	2.52	0.43
7:M:520:TYR:CZ	8:M:703:BCL:HMC2	2.54	0.43
1:2:29:VAL:HG12	8:2:102:BCL:HED3	2.00	0.43
8:G:101:BCL:H61	8:G:101:BCL:H41	1.63	0.43
1:O:27:ASP:O	1:O:30:VAL:HG12	2.19	0.43
4:N:19:GLY:HA2	12:N:102:KGD:CBO	2.49	0.43
8:4:102:BCL:HBC3	8:4:102:BCL:HHD	2.01	0.43
1:K:26:HIS:O	1:K:30:VAL:HG23	2.19	0.43
4:T:31:LEU:HD21	4:T:38:TRP:CG	2.54	0.43
2:L:187:LEU:HD21	9:L:1003:BPH:H171	2.00	0.42
1:I:30:VAL:HG12	8:I:102:BCL:O1D	2.19	0.42
1:O:53:TRP:CZ2	8:O:101:BCL:HHC	2.54	0.42
2:L:7:ALA:O	2:L:11:PRO:HD2	2.19	0.42
2:L:77:ILE:HG13	2:L:78:ILE:N	2.33	0.42
2:L:187:LEU:HD23	2:L:188:GLY:N	2.34	0.42
4:9:14:VAL:HG21	8:7:101:BCL:H143	2.01	0.42
7:M:359:GLY:O	7:M:362:GLN:N	2.49	0.42
8:6:102:BCL:H142	8:6:102:BCL:H112	1.90	0.42
8:2:101:BCL:H51	8:2:101:BCL:H12	1.79	0.42
8:2:102:BCL:HHC	8:2:102:BCL:HBB2	2.01	0.42
1:W:25:VAL:HA	1:W:28:ILE:HD12	2.02	0.42
4:9:32:SER:HB2	7:M:399:ARG:HE	1.85	0.42
8:B:101:BCL:H112	8:B:101:BCL:H71	1.69	0.42
2:L:8:LEU:N	2:L:9:PRO:HD2	2.34	0.42
2:L:167:TRP:CZ3	8:L:1001:BCL:HBB1	2.53	0.42
1:W:14:TRP:CZ2	8:W:102:BCL:OBB	2.71	0.42
2:L:11:PRO:O	2:L:14:GLU:HG3	2.20	0.42
8:8:101:BCL:H101	8:7:101:BCL:H62	2.02	0.42
1:Q:29:VAL:HG13	8:Q:102:BCL:HED2	2.01	0.42
4:3:18:LEU:O	4:3:22:MET:HG2	2.20	0.42
2:L:210:PRO:C	2:L:212:HIS:H	2.28	0.42
1:Q:30:VAL:HG11	8:Q:102:BCL:H2A	2.00	0.42
4:P:19:GLY:HA2	12:N:101:KGD:CBO	2.50	0.42
4:H:38:TRP:O	4:H:40:ARG:N	2.53	0.42
2:L:136:PHE:CE1	8:L:1002:BCL:H142	2.55	0.42
1:I:33:ILE:HB	8:I:102:BCL:HED3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:174:ARG:HB3	2:L:175:PRO:HD3	2.02	0.42
2:L:291:ASP:OD1	2:L:291:ASP:C	2.63	0.42
1:4:30:VAL:HA	1:4:33:ILE:HG22	2.02	0.42
3:C:47:THR:O	3:C:49:ALA:N	2.52	0.42
8:O:101:BCL:H101	8:N:103:BCL:H43	2.01	0.42
4:P:39:LEU:HD12	4:P:39:LEU:O	2.20	0.42
2:L:296:TRP:C	2:L:298:PHE:H	2.28	0.42
3:C:171:CYS:HA	11:C:502:HEM:HHC	2.02	0.42
8:1:101:BCL:H61	8:1:101:BCL:H41	1.87	0.42
7:M:428:TRP:N	7:M:428:TRP:CD1	2.88	0.42
8:W:102:BCL:H62	8:W:102:BCL:H41	1.98	0.41
4:H:10:THR:O	4:H:14:VAL:HG13	2.20	0.41
1:E:53:TRP:HZ3	4:A:38:TRP:CZ3	2.39	0.41
1:2:34:TYR:O	1:2:38:ILE:HG12	2.19	0.41
3:C:25:GLY:O	3:C:28:SER:OG	2.34	0.41
3:C:244:HIS:C	3:C:246:ALA:H	2.28	0.41
8:L:1002:BCL:C1B	8:M:703:BCL:HBB2	2.51	0.41
1:8:14:TRP:NE1	8:8:102:BCL:OBB	2.53	0.41
8:J:102:BCL:HHC	8:J:102:BCL:OBB	2.20	0.41
4:A:38:TRP:HB3	4:A:39:LEU:H	1.64	0.41
2:L:205:ASN:C	2:L:207:PHE:H	2.24	0.41
9:L:1003:BPH:OBB	7:M:533:LEU:HD13	2.20	0.41
3:C:170:THR:HG23	3:C:172:ALA:N	2.34	0.41
9:M:704:BPH:HBA2	9:M:704:BPH:H3A	1.73	0.41
1:O:25:VAL:O	1:O:29:VAL:HG13	2.20	0.41
8:6:101:BCL:H203	8:6:101:BCL:H161	1.88	0.41
3:C:293:CYS:HA	11:C:504:HEM:CBB	2.51	0.41
8:F:102:BCL:H111	8:F:102:BCL:H152	1.80	0.41
4:9:38:TRP:CE3	4:9:39:LEU:HB2	2.56	0.41
3:C:229:MET:SD	11:C:503:HEM:C1B	2.97	0.41
1:Q:26:HIS:NE2	8:Q:102:BCL:C4D	2.83	0.41
8:Q:101:BCL:HMD3	4:P:27:HIS:CE1	2.56	0.41
4:F:39:LEU:O	4:F:39:LEU:HD23	2.19	0.41
4:1:31:LEU:HB3	4:1:38:TRP:HZ3	1.86	0.41
7:M:484:TYR:O	7:M:488:PRO:HG2	2.20	0.41
2:L:72:PHE:CE2	2:L:141:LEU:HB3	2.56	0.41
8:K:101:BCL:CHC	8:H:101:BCL:HBB3	2.51	0.41
3:C:80:ALA:O	3:C:84:ALA:N	2.53	0.41
1:Q:29:VAL:HG23	12:N:101:KGD:CAN	2.51	0.41
1:Q:29:VAL:HG22	8:Q:102:BCL:HED2	2.02	0.41
3:C:142:ALA:O	3:C:146:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:20:LEU:HD23	8:H:101:BCL:C2	2.45	0.41
4:D:19:GLY:HA2	12:A:101:KGD:CBO	2.50	0.41
7:M:612:THR:HG23	7:M:613:LEU:HG	2.02	0.41
1:E:14:TRP:CE3	1:B:24:LEU:HD21	2.56	0.41
8:B:102:BCL:HBC3	8:B:102:BCL:HHD	2.03	0.41
8:B:102:BCL:HBB1	1:O:24:LEU:HD11	2.02	0.41
2:L:61:ASP:OD1	2:L:63:TRP:NE1	2.54	0.41
2:L:220:PHE:O	2:L:223:THR:HG22	2.21	0.41
2:L:247:HIS:O	2:L:251:ARG:HG2	2.20	0.41
1:6:33:ILE:CG1	8:6:102:BCL:HED3	2.50	0.41
1:4:30:VAL:O	1:4:33:ILE:HG22	2.21	0.41
1:4:33:ILE:HG21	8:4:102:BCL:O1D	2.21	0.41
1:2:41:VAL:O	1:2:45:VAL:HG23	2.21	0.41
8:Q:102:BCL:HAA1	8:Q:102:BCL:HBD	2.03	0.41
4:3:35:ALA:O	4:3:37:ASN:N	2.54	0.41
4:1:22:MET:HE3	4:1:26:ILE:HD11	2.03	0.41
7:M:515:HIS:CD2	7:M:516:TRP:CE2	3.09	0.41
8:M:703:BCL:H143	8:M:703:BCL:H161	1.75	0.41
2:L:131:ALA:O	2:L:134:ILE:HG22	2.21	0.41
8:6:101:BCL:H62	8:6:101:BCL:H41	1.82	0.41
3:C:170:THR:HG23	3:C:173:THR:H	1.84	0.41
8:H:101:BCL:H111	8:H:101:BCL:H72	1.69	0.41
1:6:26:HIS:NE2	8:6:102:BCL:ND	2.69	0.40
8:4:101:BCL:H62	8:4:101:BCL:H41	1.72	0.40
3:C:29:VAL:O	3:C:33:VAL:HG23	2.21	0.40
1:6:30:VAL:HG22	1:6:34:TYR:CE2	2.57	0.40
8:6:101:BCL:H102	8:5:102:BCL:H2	2.02	0.40
3:C:205:TYR:HB3	3:C:206:PRO:HD3	2.02	0.40
3:C:232:MET:SD	11:C:504:HEM:HAB	2.61	0.40
4:R:10:THR:HA	4:R:13:VAL:HG22	2.03	0.40
4:A:18:LEU:HA	4:A:21:VAL:HG12	2.02	0.40
4:9:39:LEU:HD23	4:9:39:LEU:O	2.22	0.40
4:5:18:LEU:HA	4:5:21:VAL:HG12	2.03	0.40
2:L:89:TYR:HD1	4:P:28:PHE:HE1	1.68	0.40
1:Q:29:VAL:HG22	8:Q:102:BCL:CED	2.51	0.40
4:P:31:LEU:HD23	4:P:38:TRP:CZ3	2.57	0.40
8:P:101:BCL:HBC2	8:P:101:BCL:H2C	1.82	0.40
4:9:19:GLY:HA2	12:9:102:KGD:CBO	2.52	0.40
7:M:498:PRO:HG3	7:M:508:TRP:CD2	2.56	0.40
1:E:41:VAL:O	1:E:45:VAL:HG23	2.21	0.40
3:C:77:ALA:C	3:C:79:ASN:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:438:TRP:HH2	7:M:498:PRO:O	2.04	0.40
2:L:89:TYR:CE1	2:L:93:VAL:HG21	2.57	0.40
2:L:118:PRO:HA	2:L:123:PHE:CE1	2.56	0.40
8:6:101:BCL:H162	8:6:101:BCL:H141	1.75	0.40
8:4:101:BCL:HMD3	4:3:27:HIS:CE1	2.57	0.40
3:C:235:SER:OG	3:C:236:MET:N	2.55	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	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	2	42/55 (76%)	36 (86%)	6 (14%)	0	100	100
1	4	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
1	6	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	8	42/55 (76%)	34 (81%)	8 (19%)	0	100	100
1	B	42/55 (76%)	39 (93%)	3 (7%)	0	100	100
1	E	42/55 (76%)	39 (93%)	3 (7%)	0	100	100
1	G	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	I	42/55 (76%)	35 (83%)	7 (17%)	0	100	100
1	K	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	O	42/55 (76%)	37 (88%)	5 (12%)	0	100	100
1	Q	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	S	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	U	42/55 (76%)	36 (86%)	6 (14%)	0	100	100
1	W	42/55 (76%)	38 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	307/310 (99%)	253 (82%)	53 (17%)	1 (0%)	37	71
3	C	291/320 (91%)	213 (73%)	76 (26%)	2 (1%)	19	56
4	1	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	3	34/42 (81%)	28 (82%)	6 (18%)	0	100	100
4	5	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
4	7	34/42 (81%)	26 (76%)	8 (24%)	0	100	100
4	9	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	A	34/42 (81%)	27 (79%)	7 (21%)	0	100	100
4	D	34/42 (81%)	31 (91%)	3 (9%)	0	100	100
4	F	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	H	34/42 (81%)	31 (91%)	3 (9%)	0	100	100
4	J	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	N	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	P	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	R	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	T	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
4	V	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
7	M	303/306 (99%)	253 (84%)	49 (16%)	1 (0%)	37	71
All	All	2041/2391 (85%)	1738 (85%)	299 (15%)	4 (0%)	45	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	206	PHE
3	C	118	CYS
3	C	124	ILE
7	M	349	GLY

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	27/49 (55%)	27 (100%)	0	100	100
1	2	26/49 (53%)	26 (100%)	0	100	100
1	4	24/49 (49%)	24 (100%)	0	100	100
1	6	27/49 (55%)	27 (100%)	0	100	100
1	8	27/49 (55%)	27 (100%)	0	100	100
1	B	26/49 (53%)	26 (100%)	0	100	100
1	E	26/49 (53%)	26 (100%)	0	100	100
1	G	27/49 (55%)	27 (100%)	0	100	100
1	I	27/49 (55%)	27 (100%)	0	100	100
1	K	26/49 (53%)	26 (100%)	0	100	100
1	O	26/49 (53%)	26 (100%)	0	100	100
1	Q	25/49 (51%)	25 (100%)	0	100	100
1	S	26/49 (53%)	26 (100%)	0	100	100
1	U	27/49 (55%)	27 (100%)	0	100	100
1	W	23/49 (47%)	23 (100%)	0	100	100
2	L	214/251 (85%)	214 (100%)	0	100	100
3	C	183/262 (70%)	183 (100%)	0	100	100
4	1	24/37 (65%)	24 (100%)	0	100	100
4	3	27/37 (73%)	27 (100%)	0	100	100
4	5	28/37 (76%)	28 (100%)	0	100	100
4	7	28/37 (76%)	28 (100%)	0	100	100
4	9	28/37 (76%)	28 (100%)	0	100	100
4	A	28/37 (76%)	27 (96%)	1 (4%)	30	53
4	D	28/37 (76%)	28 (100%)	0	100	100
4	F	28/37 (76%)	28 (100%)	0	100	100
4	H	27/37 (73%)	27 (100%)	0	100	100
4	J	27/37 (73%)	27 (100%)	0	100	100
4	N	28/37 (76%)	27 (96%)	1 (4%)	30	53
4	P	28/37 (76%)	28 (100%)	0	100	100
4	R	26/37 (70%)	26 (100%)	0	100	100
4	T	28/37 (76%)	28 (100%)	0	100	100
4	V	27/37 (73%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	M	216/244 (88%)	216 (100%)	0	100	100
All	All	1413/2047 (69%)	1411 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	31	LEU
4	A	27	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	HIS
2	L	183	HIS
2	L	252	ASN
1	4	44	HIS
1	2	44	HIS
3	C	87	GLN
3	C	101	GLN
3	C	109	GLN
3	C	168	GLN
3	C	176	ASN
3	C	219	ASN
3	C	269	HIS
3	C	298	GLN
3	C	301	ASN
1	G	44	HIS
1	Q	44	HIS
4	R	27	HIS
4	A	27	HIS
4	9	27	HIS
7	M	339	HIS
7	M	515	HIS
7	M	582	ASN
7	M	637	GLN

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 72 ligands modelled in this entry, 1 is monoatomic - leaving 71 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	T	103	4	64,74,74	1.23	6 (9%)	78,115,115	1.51	9 (11%)
9	BPH	M	705	-	51,70,70	0.99	1 (1%)	52,101,101	1.14	6 (11%)
8	BCL	S	102	1	64,74,74	1.22	5 (7%)	78,115,115	1.47	10 (12%)
8	BCL	W	101	1	64,74,74	1.26	6 (9%)	78,115,115	4.34	13 (16%)
8	BCL	V	101	4	64,74,74	1.24	6 (9%)	78,115,115	1.68	13 (16%)
10	MQE	L	1004	-	69,69,69	3.85	19 (27%)	84,87,87	2.30	22 (26%)
8	BCL	D	101	4	64,74,74	1.20	6 (9%)	78,115,115	1.64	12 (15%)
12	KGD	N	102	-	41,41,41	6.14	25 (60%)	49,53,53	4.28	23 (46%)
8	BCL	R	102	4,8	64,74,74	1.22	6 (9%)	78,115,115	1.66	14 (17%)
11	HEM	C	502	3	41,50,50	1.45	3 (7%)	45,82,82	1.28	7 (15%)
8	BCL	P	101	4	64,74,74	1.21	7 (10%)	78,115,115	1.55	10 (12%)
12	KGD	3	103	-	41,41,41	6.21	26 (63%)	49,53,53	3.38	25 (51%)
8	BCL	G	102	1	64,74,74	1.24	6 (9%)	78,115,115	1.53	10 (12%)
8	BCL	E	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	11 (14%)
8	BCL	J	102	4	64,74,74	1.26	6 (9%)	78,115,115	1.59	10 (12%)
8	BCL	6	101	1	64,74,74	1.24	7 (10%)	78,115,115	1.61	13 (16%)
8	BCL	G	101	1	64,74,74	1.28	6 (9%)	78,115,115	1.57	14 (17%)
12	KGD	R	101	-	41,41,41	5.76	25 (60%)	49,53,53	3.53	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	O	101	1	64,74,74	1.25	6 (9%)	78,115,115	1.57	12 (15%)
8	BCL	L	1001	2	64,74,74	1.25	7 (10%)	78,115,115	1.54	9 (11%)
8	BCL	F	102	4	64,74,74	1.23	6 (9%)	78,115,115	1.68	12 (15%)
8	BCL	K	101	1	64,74,74	1.24	5 (7%)	78,115,115	1.49	10 (12%)
8	BCL	U	102	1	64,74,74	1.26	7 (10%)	78,115,115	1.56	11 (14%)
8	BCL	2	102	1	64,74,74	1.24	6 (9%)	78,115,115	1.50	10 (12%)
8	BCL	8	101	1	64,74,74	1.24	6 (9%)	78,115,115	1.57	10 (12%)
12	KGD	3	101	-	41,41,41	6.01	25 (60%)	49,53,53	3.96	23 (46%)
8	BCL	W	102	1	64,74,74	1.21	6 (9%)	78,115,115	1.51	10 (12%)
8	BCL	N	103	4	64,74,74	1.22	5 (7%)	78,115,115	1.56	11 (14%)
11	HEM	C	501	3	41,50,50	1.46	4 (9%)	45,82,82	1.27	5 (11%)
8	BCL	6	102	1	64,74,74	1.23	6 (9%)	78,115,115	1.52	8 (10%)
8	BCL	2	101	1	64,74,74	1.24	6 (9%)	78,115,115	1.53	10 (12%)
8	BCL	U	101	1	64,74,74	1.24	6 (9%)	78,115,115	4.36	16 (20%)
12	KGD	J	101	-	41,41,41	5.97	25 (60%)	49,53,53	3.80	23 (46%)
8	BCL	H	101	4	64,74,74	1.24	6 (9%)	78,115,115	1.60	11 (14%)
8	BCL	E	102	-	64,74,74	1.26	5 (7%)	78,115,115	1.61	12 (15%)
12	KGD	N	101	-	41,41,41	6.10	25 (60%)	49,53,53	3.87	22 (44%)
8	BCL	4	102	1	64,74,74	1.22	5 (7%)	78,115,115	1.46	8 (10%)
12	KGD	A	101	-	41,41,41	5.87	25 (60%)	49,53,53	3.44	18 (36%)
12	KGD	9	102	-	41,41,41	6.21	26 (63%)	49,53,53	3.75	21 (42%)
8	BCL	K	102	1	64,74,74	1.24	6 (9%)	78,115,115	1.56	11 (14%)
9	BPH	L	1003	-	51,70,70	0.99	2 (3%)	52,101,101	1.24	6 (11%)
11	HEM	C	503	3	41,50,50	1.46	3 (7%)	45,82,82	1.22	4 (8%)
8	BCL	0	101	1	64,74,74	1.21	6 (9%)	78,115,115	1.49	10 (12%)
8	BCL	7	101	4	64,74,74	1.20	6 (9%)	78,115,115	1.56	10 (12%)
8	BCL	B	102	1	64,74,74	1.25	7 (10%)	78,115,115	1.66	12 (15%)
8	BCL	S	101	8,1	64,74,74	1.25	6 (9%)	78,115,115	1.54	10 (12%)
12	KGD	T	102	-	41,41,41	6.31	25 (60%)	49,53,53	4.01	21 (42%)
12	KGD	F	101	-	41,41,41	6.05	25 (60%)	49,53,53	3.75	23 (46%)
8	BCL	5	102	4	64,74,74	1.24	6 (9%)	78,115,115	1.58	10 (12%)
8	BCL	Q	101	1	64,74,74	1.24	7 (10%)	78,115,115	1.53	11 (14%)
8	BCL	9	103	4	64,74,74	1.24	5 (7%)	78,115,115	1.57	10 (12%)
12	KGD	9	101	-	41,41,41	5.86	25 (60%)	49,53,53	3.87	22 (44%)
8	BCL	I	102	1	64,74,74	1.21	6 (9%)	78,115,115	1.54	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	1	101	4	64,74,74	1.23	6 (9%)	78,115,115	1.54	9 (11%)
8	BCL	O	102	1	64,74,74	1.22	6 (9%)	78,115,115	1.49	9 (11%)
12	KGD	T	101	-	41,41,41	6.26	25 (60%)	49,53,53	3.88	23 (46%)
12	KGD	H	102	-	41,41,41	6.03	25 (60%)	49,53,53	3.16	21 (42%)
8	BCL	3	102	4,8	64,74,74	1.26	6 (9%)	78,115,115	1.65	13 (16%)
8	BCL	B	101	1	64,74,74	1.27	5 (7%)	78,115,115	1.54	10 (12%)
8	BCL	8	102	1	64,74,74	1.25	5 (7%)	78,115,115	1.53	11 (14%)
8	BCL	M	703	7	64,74,74	1.24	6 (9%)	78,115,115	1.67	11 (14%)
8	BCL	0	102	1	64,74,74	1.25	6 (9%)	78,115,115	1.61	13 (16%)
8	BCL	Q	102	1	64,74,74	1.25	6 (9%)	78,115,115	1.63	14 (17%)
10	MQE	M	702	-	69,69,69	3.74	19 (27%)	84,87,87	2.80	29 (34%)
8	BCL	I	101	1	64,74,74	1.25	6 (9%)	78,115,115	1.58	11 (14%)
12	KGD	5	101	-	41,41,41	6.52	25 (60%)	49,53,53	3.96	23 (46%)
9	BPH	M	704	-	51,70,70	0.97	1 (1%)	52,101,101	1.24	6 (11%)
8	BCL	4	101	8,1	64,74,74	1.27	7 (10%)	78,115,115	1.62	14 (17%)
8	BCL	A	102	4	64,74,74	1.23	7 (10%)	78,115,115	1.53	11 (14%)
11	HEM	C	504	3	41,50,50	1.46	5 (12%)	45,82,82	1.78	10 (22%)
8	BCL	L	1002	2	64,74,74	1.26	6 (9%)	78,115,115	1.52	9 (11%)

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	T	103	4	-	4/37/137/137	-
9	BPH	M	705	-	-	2/37/105/105	0/5/6/6
8	BCL	S	102	1	-	6/37/137/137	-
8	BCL	W	101	1	-	4/37/137/137	-
8	BCL	V	101	4	-	4/37/137/137	-
10	MQE	L	1004	-	-	12/65/85/85	0/2/2/2
8	BCL	D	101	4	-	6/37/137/137	-
12	KGD	N	102	-	-	1/36/56/56	0/1/1/1
8	BCL	R	102	4,8	-	9/37/137/137	-
11	HEM	C	502	3	-	2/12/54/54	-
8	BCL	P	101	4	-	4/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KGD	3	103	-	-	1/36/56/56	0/1/1/1
8	BCL	G	102	1	-	11/37/137/137	-
8	BCL	E	101	-	-	7/37/137/137	-
8	BCL	J	102	4	-	4/37/137/137	-
8	BCL	6	101	1	-	7/37/137/137	-
8	BCL	G	101	1	-	5/37/137/137	-
12	KGD	R	101	-	-	2/36/56/56	0/1/1/1
8	BCL	O	101	1	-	4/37/137/137	-
8	BCL	L	1001	2	-	11/37/137/137	-
8	BCL	F	102	4	-	12/37/137/137	-
8	BCL	K	101	1	-	4/37/137/137	-
8	BCL	U	102	1	-	8/37/137/137	-
8	BCL	2	102	1	-	11/37/137/137	-
8	BCL	8	101	1	-	6/37/137/137	-
12	KGD	3	101	-	-	2/36/56/56	0/1/1/1
8	BCL	W	102	1	-	11/37/137/137	-
8	BCL	N	103	4	-	10/37/137/137	-
11	HEM	C	501	3	-	1/12/54/54	-
8	BCL	6	102	1	-	8/37/137/137	-
8	BCL	2	101	1	-	8/37/137/137	-
8	BCL	U	101	1	-	5/37/137/137	-
12	KGD	J	101	-	-	0/36/56/56	0/1/1/1
8	BCL	H	101	4	-	5/37/137/137	-
8	BCL	E	102	-	-	11/37/137/137	-
12	KGD	N	101	-	-	0/36/56/56	0/1/1/1
8	BCL	4	102	1	-	13/37/137/137	-
12	KGD	A	101	-	-	2/36/56/56	0/1/1/1
12	KGD	9	102	-	-	2/36/56/56	0/1/1/1
8	BCL	K	102	1	-	7/37/137/137	-
9	BPH	L	1003	-	-	7/37/105/105	0/5/6/6
11	HEM	C	503	3	-	0/12/54/54	-
8	BCL	0	101	1	-	9/37/137/137	-
8	BCL	7	101	4	-	8/37/137/137	-
8	BCL	B	102	1	-	10/37/137/137	-
8	BCL	S	101	8,1	-	9/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KGD	T	102	-	-	1/36/56/56	0/1/1/1
12	KGD	F	101	-	-	0/36/56/56	0/1/1/1
8	BCL	5	102	4	-	7/37/137/137	-
8	BCL	Q	101	1	-	7/37/137/137	-
8	BCL	9	103	4	-	8/37/137/137	-
12	KGD	9	101	-	-	1/36/56/56	0/1/1/1
8	BCL	I	102	1	-	12/37/137/137	-
8	BCL	1	101	4	-	6/37/137/137	-
8	BCL	O	102	1	-	9/37/137/137	-
12	KGD	T	101	-	-	0/36/56/56	0/1/1/1
12	KGD	H	102	-	-	2/36/56/56	0/1/1/1
8	BCL	3	102	4,8	-	4/37/137/137	-
8	BCL	B	101	1	-	9/37/137/137	-
8	BCL	8	102	1	-	12/37/137/137	-
8	BCL	M	703	7	-	5/37/137/137	-
8	BCL	0	102	1	-	9/37/137/137	-
8	BCL	Q	102	1	-	10/37/137/137	-
10	MQE	M	702	-	-	18/65/85/85	0/2/2/2
8	BCL	I	101	1	-	0/37/137/137	-
12	KGD	5	101	-	-	2/36/56/56	0/1/1/1
9	BPH	M	704	-	-	6/37/105/105	0/5/6/6
8	BCL	4	101	8,1	-	11/37/137/137	-
8	BCL	A	102	4	-	12/37/137/137	-
11	HEM	C	504	3	-	2/12/54/54	-
8	BCL	L	1002	2	-	7/37/137/137	-

All (696) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	101	KGD	CBA-CAW	19.49	1.54	1.34
12	3	103	KGD	CBA-CAW	18.48	1.53	1.34
12	T	102	KGD	CBA-CAW	18.40	1.53	1.34
12	9	102	KGD	CBA-CAW	18.27	1.53	1.34
12	T	101	KGD	CBA-CAW	17.84	1.52	1.34
12	N	102	KGD	CBA-CAW	17.66	1.52	1.34
12	N	101	KGD	CBA-CAW	17.58	1.52	1.34
12	J	101	KGD	CBA-CAW	17.53	1.52	1.34
12	H	102	KGD	CBA-CAW	17.43	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	101	KGD	CBA-CAW	17.32	1.52	1.34
12	3	101	KGD	CBA-CAW	17.05	1.51	1.34
12	9	101	KGD	CBA-CAW	16.93	1.51	1.34
12	R	101	KGD	CBA-CAW	16.84	1.51	1.34
12	A	101	KGD	CBA-CAW	15.95	1.50	1.34
12	5	101	KGD	CAO-CAM	13.53	1.53	1.35
12	H	102	KGD	CBI-CBL	13.29	1.53	1.35
12	5	101	KGD	CBJ-CBH	13.21	1.53	1.35
12	5	101	KGD	CBI-CBL	13.19	1.53	1.35
12	5	101	KGD	CAV-CAR	13.18	1.53	1.35
12	T	101	KGD	CBJ-CBH	13.10	1.53	1.35
12	T	101	KGD	CAV-CAR	13.07	1.53	1.35
12	9	102	KGD	CAO-CAM	13.06	1.53	1.35
12	T	101	KGD	CAO-CAM	13.06	1.53	1.35
12	T	102	KGD	CAV-CAR	13.04	1.53	1.35
12	T	102	KGD	CBJ-CBH	13.03	1.53	1.35
12	N	102	KGD	CAO-CAM	12.94	1.52	1.35
12	T	102	KGD	CBI-CBL	12.93	1.52	1.35
12	3	103	KGD	CBI-CBL	12.92	1.52	1.35
12	T	101	KGD	CBI-CBL	12.86	1.52	1.35
12	T	102	KGD	CAO-CAM	12.79	1.52	1.35
12	F	101	KGD	CAV-CAR	12.77	1.52	1.35
12	N	102	KGD	CAV-CAR	12.71	1.52	1.35
12	N	101	KGD	CBI-CBL	12.71	1.52	1.35
12	3	103	KGD	CAO-CAM	12.69	1.52	1.35
12	N	101	KGD	CAO-CAM	12.61	1.52	1.35
12	9	102	KGD	CAV-CAR	12.60	1.52	1.35
12	3	101	KGD	CAV-CAR	12.56	1.52	1.35
12	F	101	KGD	CBI-CBL	12.56	1.52	1.35
12	N	102	KGD	CBI-CBL	12.56	1.52	1.35
12	9	102	KGD	CBI-CBL	12.56	1.52	1.35
12	3	101	KGD	CBI-CBL	12.54	1.52	1.35
12	N	101	KGD	CAV-CAR	12.52	1.52	1.35
12	A	101	KGD	CAV-CAR	12.50	1.52	1.35
12	F	101	KGD	CAO-CAM	12.49	1.52	1.35
12	H	102	KGD	CBJ-CBH	12.48	1.52	1.35
12	N	102	KGD	CBJ-CBH	12.40	1.52	1.35
12	3	101	KGD	CBJ-CBH	12.39	1.52	1.35
12	3	101	KGD	CAO-CAM	12.37	1.52	1.35
12	N	101	KGD	CBJ-CBH	12.37	1.52	1.35
12	3	103	KGD	CAV-CAR	12.35	1.52	1.35
12	3	103	KGD	CBJ-CBH	12.34	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	9	102	KGD	CBJ-CBH	12.32	1.52	1.35
12	A	101	KGD	CAO-CAM	12.28	1.52	1.35
12	J	101	KGD	CBJ-CBH	12.24	1.52	1.35
12	F	101	KGD	CBJ-CBH	12.21	1.52	1.35
12	9	101	KGD	CBI-CBL	12.18	1.51	1.35
12	R	101	KGD	CBI-CBL	12.18	1.51	1.35
12	J	101	KGD	CBI-CBL	12.16	1.51	1.35
12	A	101	KGD	CBI-CBL	12.13	1.51	1.35
12	J	101	KGD	CAO-CAM	12.07	1.51	1.35
12	J	101	KGD	CAV-CAR	12.06	1.51	1.35
12	9	101	KGD	CBJ-CBH	12.03	1.51	1.35
12	H	102	KGD	CAV-CAR	11.98	1.51	1.35
12	A	101	KGD	CBJ-CBH	11.89	1.51	1.35
12	R	101	KGD	CBJ-CBH	11.88	1.51	1.35
12	9	101	KGD	CAV-CAR	11.86	1.51	1.35
12	9	101	KGD	CAO-CAM	11.82	1.51	1.35
12	H	102	KGD	CAO-CAM	11.69	1.51	1.35
12	R	101	KGD	CAO-CAM	11.49	1.51	1.35
12	R	101	KGD	CAV-CAR	11.34	1.50	1.35
12	3	103	KGD	CAE-CAI	-10.32	1.37	1.50
12	9	102	KGD	CAE-CAI	-10.25	1.37	1.50
12	5	101	KGD	CAE-CAI	-10.20	1.37	1.50
12	N	102	KGD	CAE-CAI	-10.12	1.37	1.50
12	A	101	KGD	CAE-CAI	-10.07	1.37	1.50
12	F	101	KGD	CAE-CAI	-9.97	1.37	1.50
12	T	102	KGD	CAE-CAI	-9.93	1.37	1.50
12	T	101	KGD	CAE-CAI	-9.91	1.37	1.50
12	J	101	KGD	CAE-CAI	-9.88	1.37	1.50
12	R	101	KGD	CAE-CAI	-9.87	1.37	1.50
12	9	101	KGD	CAE-CAI	-9.86	1.37	1.50
12	N	101	KGD	CAE-CAI	-9.84	1.38	1.50
12	3	101	KGD	CAE-CAI	-9.81	1.38	1.50
12	H	102	KGD	CAE-CAI	-9.69	1.38	1.50
10	L	1004	MQE	CBF-CAV	8.92	1.54	1.33
10	L	1004	MQE	CBI-CAZ	8.89	1.54	1.33
10	L	1004	MQE	CBH-CAW	8.88	1.54	1.33
10	L	1004	MQE	CBG-CAT	8.85	1.54	1.33
10	L	1004	MQE	CBL-CBB	8.80	1.54	1.33
10	L	1004	MQE	CBD-CAR	8.78	1.54	1.33
10	L	1004	MQE	CBC-CAP	8.74	1.53	1.33
10	M	702	MQE	CBF-CAV	8.68	1.53	1.33
10	M	702	MQE	CBI-CAZ	8.65	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	1004	MQE	CBE-CAQ	8.63	1.53	1.33
10	M	702	MQE	CBN-CBM	8.55	1.53	1.33
10	L	1004	MQE	CCB-CCC	8.54	1.53	1.33
10	M	702	MQE	CBH-CAW	8.53	1.53	1.33
10	M	702	MQE	CCB-CCC	8.48	1.53	1.33
10	M	702	MQE	CBC-CAP	8.43	1.53	1.33
10	M	702	MQE	CBL-CBB	8.39	1.53	1.33
10	L	1004	MQE	CBN-CBM	8.38	1.53	1.33
10	M	702	MQE	CBG-CAT	8.26	1.52	1.33
10	M	702	MQE	CBE-CAQ	8.21	1.52	1.33
10	M	702	MQE	CBD-CAR	8.08	1.52	1.33
12	H	102	KGD	CAX-CAY	8.01	1.55	1.32
12	5	101	KGD	CAB-CAD	-7.96	1.42	1.53
12	T	102	KGD	CAB-CAD	-7.85	1.43	1.53
12	5	101	KGD	CBE-CBF	7.73	1.54	1.34
12	T	101	KGD	CAB-CAD	-7.67	1.43	1.53
12	5	101	KGD	CAX-CAY	7.66	1.54	1.32
12	N	101	KGD	CAB-CAD	-7.64	1.43	1.53
12	F	101	KGD	CAB-CAD	-7.59	1.43	1.53
12	N	102	KGD	CAB-CAD	-7.58	1.43	1.53
12	A	101	KGD	CAB-CAD	-7.55	1.43	1.53
12	J	101	KGD	CAX-CAY	7.53	1.54	1.32
12	A	101	KGD	CAX-CAY	7.48	1.53	1.32
12	T	102	KGD	CAP-CAQ	7.45	1.53	1.34
12	5	101	KGD	CAP-CAQ	7.41	1.53	1.34
12	3	101	KGD	CAB-CAD	-7.41	1.43	1.53
12	9	101	KGD	CAX-CAY	7.40	1.53	1.32
12	9	102	KGD	CAB-CAD	-7.38	1.43	1.53
10	M	702	MQE	CCM-CCN	7.38	1.53	1.32
12	N	102	KGD	CAX-CAY	7.37	1.53	1.32
12	3	103	KGD	CAB-CAD	-7.36	1.43	1.53
12	9	101	KGD	CAB-CAD	-7.34	1.43	1.53
12	3	103	KGD	CAX-CAY	7.33	1.53	1.32
12	R	101	KGD	CAX-CAY	7.31	1.53	1.32
10	L	1004	MQE	CCM-CCN	7.30	1.53	1.32
12	5	101	KGD	CAL-CAJ	7.29	1.55	1.33
12	3	101	KGD	CAX-CAY	7.27	1.53	1.32
12	T	101	KGD	CBM-CBN	7.23	1.53	1.34
12	T	101	KGD	CAP-CAQ	7.22	1.53	1.34
12	T	102	KGD	CBE-CBF	7.21	1.53	1.34
12	H	102	KGD	CBM-CBN	7.19	1.53	1.34
12	F	101	KGD	CAX-CAY	7.16	1.53	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	102	KGD	CAL-CAJ	7.16	1.54	1.33
12	9	102	KGD	CAP-CAQ	7.14	1.53	1.34
12	9	102	KGD	CAL-CAJ	7.14	1.54	1.33
12	T	102	KGD	CAX-CAY	7.14	1.52	1.32
12	T	101	KGD	CAX-CAY	7.14	1.52	1.32
12	3	103	KGD	CBE-CBF	7.13	1.52	1.34
10	M	702	MQE	CAY-CAX	-7.13	1.40	1.51
12	N	101	KGD	CAX-CAY	7.11	1.52	1.32
12	T	102	KGD	CBM-CBN	7.11	1.52	1.34
12	9	102	KGD	CAX-CAY	7.08	1.52	1.32
12	9	102	KGD	CBM-CBN	7.08	1.52	1.34
10	L	1004	MQE	CAY-CAX	-7.06	1.40	1.51
12	N	101	KGD	CBM-CBN	7.06	1.52	1.34
12	J	101	KGD	CAB-CAD	-7.04	1.44	1.53
12	T	101	KGD	CBE-CBF	7.03	1.52	1.34
12	N	102	KGD	CAP-CAQ	6.99	1.52	1.34
12	N	102	KGD	CBE-CBF	6.99	1.52	1.34
12	3	103	KGD	CBM-CBN	6.98	1.52	1.34
12	F	101	KGD	CAP-CAQ	6.96	1.52	1.34
12	F	101	KGD	CBM-CBN	6.94	1.52	1.34
12	H	102	KGD	CAB-CAD	-6.93	1.44	1.53
12	A	101	KGD	CAP-CAQ	6.92	1.52	1.34
12	3	101	KGD	CBM-CBN	6.92	1.52	1.34
12	N	101	KGD	CAP-CAQ	6.91	1.52	1.34
12	3	103	KGD	CAP-CAQ	6.89	1.52	1.34
12	N	101	KGD	CBE-CBF	6.89	1.52	1.34
12	N	101	KGD	CAL-CAJ	6.88	1.53	1.33
12	3	101	KGD	CAP-CAQ	6.86	1.52	1.34
12	T	101	KGD	CAL-CAJ	6.86	1.53	1.33
12	J	101	KGD	CBM-CBN	6.85	1.52	1.34
12	N	102	KGD	CBM-CBN	6.84	1.52	1.34
12	9	102	KGD	CBE-CBF	6.83	1.52	1.34
12	N	102	KGD	CAL-CAJ	6.78	1.53	1.33
12	9	101	KGD	CBM-CBN	6.77	1.52	1.34
12	R	101	KGD	CAB-CAD	-6.75	1.44	1.53
12	A	101	KGD	CBM-CBN	6.75	1.52	1.34
12	J	101	KGD	CBE-CBF	6.74	1.51	1.34
12	F	101	KGD	CBE-CBF	6.74	1.51	1.34
12	J	101	KGD	CAP-CAQ	6.73	1.51	1.34
12	3	101	KGD	CAL-CAJ	6.73	1.53	1.33
12	T	102	KGD	CBG-CBB	6.71	1.53	1.36
12	9	101	KGD	CAP-CAQ	6.70	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	101	KGD	CBE-CBF	6.70	1.51	1.34
12	H	102	KGD	CBE-CBF	6.67	1.51	1.34
12	J	101	KGD	CAL-CAJ	6.67	1.53	1.33
12	F	101	KGD	CAL-CAJ	6.64	1.53	1.33
12	R	101	KGD	CBM-CBN	6.63	1.51	1.34
12	T	101	KGD	CBG-CBB	6.62	1.53	1.36
12	H	102	KGD	CAP-CAQ	6.62	1.51	1.34
12	9	101	KGD	CBE-CBF	6.60	1.51	1.34
12	5	101	KGD	CBM-CBN	6.59	1.51	1.34
12	3	103	KGD	CAL-CAJ	6.56	1.52	1.33
12	R	101	KGD	CBE-CBF	6.49	1.51	1.34
12	A	101	KGD	CBE-CBF	6.44	1.51	1.34
12	5	101	KGD	CBG-CBB	6.43	1.52	1.36
12	9	102	KGD	CBG-CBB	6.42	1.52	1.36
12	F	101	KGD	CBG-CBB	6.42	1.52	1.36
12	H	102	KGD	CBG-CBB	6.39	1.52	1.36
12	N	101	KGD	CBG-CBB	6.39	1.52	1.36
12	R	101	KGD	CAP-CAQ	6.37	1.51	1.34
12	N	102	KGD	CBG-CBB	6.37	1.52	1.36
12	3	101	KGD	CBG-CBB	6.36	1.52	1.36
12	A	101	KGD	CAL-CAJ	6.33	1.52	1.33
12	H	102	KGD	CAL-CAJ	6.33	1.52	1.33
12	A	101	KGD	CBG-CBB	6.29	1.52	1.36
12	9	101	KGD	CAL-CAJ	6.27	1.52	1.33
12	3	103	KGD	CBG-CBB	6.25	1.52	1.36
12	9	101	KGD	CBG-CBB	6.17	1.52	1.36
12	J	101	KGD	CBG-CBB	6.09	1.51	1.36
12	R	101	KGD	CAL-CAJ	6.06	1.51	1.33
12	R	101	KGD	CBG-CBB	5.92	1.51	1.36
12	9	102	KGD	CAK-CAH	-5.73	1.38	1.50
10	M	702	MQE	CCE-CBK	-5.56	1.39	1.50
12	5	101	KGD	CAK-CAH	-5.56	1.39	1.50
10	L	1004	MQE	CCE-CBK	-5.51	1.39	1.50
12	N	102	KGD	CAK-CAH	-5.49	1.39	1.50
12	A	101	KGD	CAK-CAH	-5.41	1.39	1.50
12	N	101	KGD	CAK-CAH	-5.39	1.39	1.50
12	H	102	KGD	CAK-CAH	-5.34	1.39	1.50
12	F	101	KGD	CAK-CAH	-5.33	1.39	1.50
12	9	101	KGD	CAK-CAH	-5.32	1.39	1.50
12	J	101	KGD	CAK-CAH	-5.32	1.39	1.50
12	T	101	KGD	CAK-CAH	-5.31	1.39	1.50
12	3	103	KGD	CAK-CAH	-5.30	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	101	KGD	CAK-CAH	-5.29	1.39	1.50
12	R	101	KGD	CAK-CAH	-5.21	1.39	1.50
12	T	102	KGD	CAK-CAH	-5.19	1.39	1.50
10	M	702	MQE	CBR-CBS	-5.09	1.38	1.48
10	L	1004	MQE	CBR-CBS	-4.87	1.38	1.48
8	G	101	BCL	C1B-NB	4.85	1.39	1.35
8	G	102	BCL	C1B-NB	4.82	1.39	1.35
8	I	101	BCL	C1B-NB	4.82	1.39	1.35
8	2	101	BCL	C1B-NB	4.80	1.39	1.35
10	M	702	MQE	CBP-CBQ	-4.76	1.39	1.48
8	F	102	BCL	C1B-NB	4.75	1.39	1.35
8	6	102	BCL	C1B-NB	4.73	1.39	1.35
8	2	102	BCL	C1B-NB	4.73	1.39	1.35
9	M	705	BPH	CBD-CGD	-4.73	1.46	1.52
8	W	101	BCL	C1B-NB	4.71	1.39	1.35
8	8	101	BCL	C1B-NB	4.71	1.39	1.35
8	K	101	BCL	C1B-NB	4.71	1.39	1.35
8	9	103	BCL	MG-NA	4.70	2.17	2.06
8	B	102	BCL	C1B-NB	4.69	1.39	1.35
8	R	102	BCL	MG-NA	4.68	2.17	2.06
8	L	1002	BCL	MG-NA	4.68	2.17	2.06
8	3	102	BCL	MG-NA	4.67	2.17	2.06
8	Q	102	BCL	C1B-NB	4.66	1.39	1.35
8	E	102	BCL	C1B-NB	4.66	1.39	1.35
11	C	503	HEM	C3C-C2C	-4.66	1.33	1.40
8	B	101	BCL	C1B-NB	4.65	1.39	1.35
8	0	101	BCL	C1B-NB	4.65	1.39	1.35
8	S	101	BCL	C1B-NB	4.65	1.39	1.35
8	5	102	BCL	MG-NA	4.65	2.17	2.06
8	V	101	BCL	C1B-NB	4.65	1.39	1.35
8	0	102	BCL	C1B-NB	4.64	1.39	1.35
8	U	102	BCL	C1B-NB	4.64	1.39	1.35
8	O	102	BCL	C1B-NB	4.63	1.39	1.35
8	E	101	BCL	C1B-NB	4.62	1.39	1.35
8	8	102	BCL	MG-NA	4.62	2.17	2.06
8	U	101	BCL	C1B-NB	4.62	1.39	1.35
8	Q	102	BCL	MG-NA	4.62	2.17	2.06
9	L	1003	BPH	CBD-CGD	-4.62	1.46	1.52
8	N	103	BCL	MG-NA	4.61	2.17	2.06
8	T	103	BCL	MG-NA	4.61	2.17	2.06
8	U	102	BCL	MG-NA	4.60	2.17	2.06
8	8	102	BCL	C1B-NB	4.59	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	102	BCL	MG-NA	4.59	2.17	2.06
8	H	101	BCL	MG-NA	4.59	2.17	2.06
8	J	102	BCL	C1B-NB	4.59	1.39	1.35
8	D	101	BCL	MG-NA	4.59	2.17	2.06
8	O	101	BCL	C1B-NB	4.58	1.39	1.35
10	L	1004	MQE	CBP-CBQ	-4.58	1.39	1.48
11	C	504	HEM	C3C-C2C	-4.57	1.34	1.40
8	V	101	BCL	MG-NA	4.57	2.17	2.06
8	P	101	BCL	MG-NA	4.56	2.17	2.06
8	1	101	BCL	C1B-NB	4.56	1.39	1.35
9	M	704	BPH	CBD-CGD	-4.56	1.46	1.52
8	T	103	BCL	C1B-NB	4.55	1.39	1.35
8	1	101	BCL	MG-NA	4.55	2.17	2.06
8	4	101	BCL	C1B-NB	4.54	1.39	1.35
8	K	102	BCL	C1B-NB	4.54	1.39	1.35
8	W	102	BCL	C1B-NB	4.54	1.39	1.35
8	4	102	BCL	MG-NA	4.53	2.17	2.06
8	3	102	BCL	C1B-NB	4.52	1.39	1.35
8	J	102	BCL	MG-NA	4.52	2.17	2.06
12	H	102	KGD	CAI-CAH	-4.51	1.38	1.47
12	9	101	KGD	CAI-CAH	-4.51	1.38	1.47
12	R	101	KGD	CAI-CAH	-4.51	1.38	1.47
8	I	102	BCL	C1B-NB	4.50	1.39	1.35
8	9	103	BCL	C1B-NB	4.49	1.39	1.35
8	S	102	BCL	C1B-NB	4.49	1.39	1.35
8	I	101	BCL	MG-NA	4.49	2.16	2.06
11	C	501	HEM	C3C-C2C	-4.49	1.34	1.40
8	7	101	BCL	MG-NA	4.48	2.16	2.06
8	4	102	BCL	C1B-NB	4.48	1.39	1.35
8	S	101	BCL	MG-NA	4.48	2.16	2.06
8	5	102	BCL	C1B-NB	4.48	1.39	1.35
8	K	102	BCL	MG-NA	4.47	2.16	2.06
8	6	101	BCL	C1B-NB	4.47	1.39	1.35
8	G	101	BCL	MG-NA	4.47	2.16	2.06
8	E	102	BCL	MG-NA	4.47	2.16	2.06
8	L	1001	BCL	MG-NA	4.47	2.16	2.06
8	6	101	BCL	MG-NA	4.46	2.16	2.06
8	W	101	BCL	MG-NA	4.46	2.16	2.06
8	G	102	BCL	MG-NA	4.46	2.16	2.06
8	K	101	BCL	MG-NA	4.45	2.16	2.06
8	0	102	BCL	MG-NA	4.45	2.16	2.06
8	Q	101	BCL	MG-NA	4.45	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	102	BCL	MG-NA	4.44	2.16	2.06
8	F	102	BCL	MG-NA	4.44	2.16	2.06
8	O	102	BCL	MG-NA	4.44	2.16	2.06
8	A	102	BCL	C1B-NB	4.43	1.39	1.35
8	B	102	BCL	MG-NA	4.43	2.16	2.06
12	A	101	KGD	CAI-CAH	-4.43	1.38	1.47
8	Q	101	BCL	C1B-NB	4.42	1.39	1.35
8	M	703	BCL	C1B-NB	4.42	1.39	1.35
8	B	101	BCL	MG-NA	4.42	2.16	2.06
8	8	101	BCL	MG-NA	4.42	2.16	2.06
8	6	102	BCL	MG-NA	4.42	2.16	2.06
12	5	101	KGD	CAI-CAH	-4.40	1.38	1.47
8	O	101	BCL	MG-NA	4.40	2.16	2.06
8	D	101	BCL	C1B-NB	4.40	1.39	1.35
8	N	103	BCL	C1B-NB	4.39	1.39	1.35
8	U	101	BCL	MG-NA	4.39	2.16	2.06
8	S	102	BCL	MG-NA	4.39	2.16	2.06
8	L	1001	BCL	C1B-NB	4.38	1.39	1.35
8	H	101	BCL	C1B-NB	4.38	1.39	1.35
12	J	101	KGD	CAI-CAH	-4.38	1.38	1.47
8	L	1002	BCL	C1B-NB	4.37	1.39	1.35
8	W	102	BCL	MG-NA	4.37	2.16	2.06
8	P	101	BCL	C1B-NB	4.35	1.39	1.35
8	2	101	BCL	MG-NA	4.35	2.16	2.06
12	3	101	KGD	CAI-CAH	-4.35	1.38	1.47
8	E	101	BCL	MG-NA	4.34	2.16	2.06
10	M	702	MQE	CBK-CBS	-4.33	1.38	1.48
8	4	101	BCL	MG-NA	4.31	2.16	2.06
11	C	502	HEM	C3C-C2C	-4.30	1.34	1.40
12	N	101	KGD	CAI-CAH	-4.26	1.39	1.47
8	7	101	BCL	C1B-NB	4.26	1.39	1.35
8	0	101	BCL	MG-NA	4.25	2.16	2.06
8	R	102	BCL	C1B-NB	4.25	1.39	1.35
12	F	101	KGD	CAI-CAH	-4.24	1.39	1.47
12	T	101	KGD	CAI-CAH	-4.23	1.39	1.47
12	N	102	KGD	CAI-CAH	-4.23	1.39	1.47
8	A	102	BCL	MG-NA	4.21	2.16	2.06
12	T	102	KGD	CAI-CAH	-4.20	1.39	1.47
12	9	102	KGD	CAI-CAH	-4.18	1.39	1.47
8	M	703	BCL	MG-NA	4.14	2.16	2.06
10	L	1004	MQE	CBK-CBS	-4.11	1.39	1.48
12	3	103	KGD	CAI-CAH	-4.09	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	101	KGD	CBF-CBH	3.85	1.54	1.45
12	5	101	KGD	CBE-CBA	3.76	1.55	1.43
12	5	101	KGD	CAQ-CAR	3.59	1.53	1.45
11	C	502	HEM	C3C-CAC	3.56	1.55	1.47
11	C	501	HEM	C3C-CAC	3.55	1.55	1.47
12	5	101	KGD	CAL-CAM	3.48	1.53	1.45
11	C	503	HEM	C3C-CAC	3.46	1.54	1.47
12	T	102	KGD	CBB-CAV	3.45	1.54	1.43
12	3	103	KGD	CAD-CAH	3.45	1.40	1.35
12	3	103	KGD	CBN-CBL	3.43	1.53	1.45
11	C	504	HEM	C3C-CAC	3.43	1.54	1.47
12	5	101	KGD	CBN-CBL	3.35	1.53	1.45
12	H	102	KGD	CBN-CBL	3.35	1.53	1.45
12	5	101	KGD	CAP-CAO	3.34	1.53	1.43
12	9	102	KGD	CAL-CAM	3.33	1.53	1.45
12	T	102	KGD	CAL-CAM	3.33	1.53	1.45
12	T	102	KGD	CBN-CBL	3.32	1.53	1.45
12	T	101	KGD	CBB-CAV	3.31	1.53	1.43
12	5	101	KGD	CBB-CAV	3.30	1.53	1.43
12	T	101	KGD	CBG-CBI	3.29	1.53	1.43
12	T	102	KGD	CAD-CAH	3.29	1.40	1.35
8	G	101	BCL	MG-NC	3.28	2.14	2.06
12	T	102	KGD	CBG-CBI	3.25	1.53	1.43
12	N	101	KGD	CAD-CAH	3.21	1.40	1.35
12	9	102	KGD	CAD-CAH	3.21	1.40	1.35
12	T	101	KGD	CAD-CAH	3.21	1.40	1.35
12	J	101	KGD	CAD-CAH	3.20	1.40	1.35
12	T	101	KGD	CAQ-CAR	3.20	1.52	1.45
12	9	102	KGD	CAQ-CAR	3.19	1.52	1.45
12	3	103	KGD	CBM-CBJ	3.18	1.53	1.43
12	T	101	KGD	CAL-CAM	3.18	1.52	1.45
8	9	103	BCL	MG-NC	3.18	2.13	2.06
12	9	102	KGD	CAP-CAO	3.17	1.53	1.43
12	N	102	KGD	CAQ-CAR	3.17	1.52	1.45
12	T	102	KGD	CBF-CBH	3.16	1.52	1.45
12	N	102	KGD	CBB-CAV	3.14	1.53	1.43
12	N	101	KGD	CAQ-CAR	3.14	1.52	1.45
12	T	102	KGD	CAP-CAO	3.13	1.53	1.43
12	5	101	KGD	CBG-CBI	3.13	1.53	1.43
12	9	102	KGD	CBB-CAV	3.12	1.53	1.43
12	N	102	KGD	CAP-CAO	3.12	1.53	1.43
12	3	103	KGD	CAL-CAM	3.12	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	102	KGD	CBG-CBI	3.12	1.53	1.43
12	T	102	KGD	CAQ-CAR	3.11	1.52	1.45
8	L	1002	BCL	MG-NC	3.11	2.13	2.06
10	M	702	MQE	CAX-CBQ	-3.10	1.39	1.47
12	H	102	KGD	CBM-CBJ	3.10	1.53	1.43
12	T	102	KGD	CBM-CBJ	3.09	1.53	1.43
12	N	102	KGD	CAD-CAH	3.08	1.40	1.35
8	W	101	BCL	MG-NC	3.08	2.13	2.06
8	R	102	BCL	MG-NC	3.08	2.13	2.06
8	8	102	BCL	MG-NC	3.07	2.13	2.06
12	F	101	KGD	CBG-CBI	3.07	1.53	1.43
12	3	101	KGD	CAD-CAH	3.07	1.40	1.35
8	6	101	BCL	MG-NC	3.07	2.13	2.06
12	3	101	KGD	CBB-CAV	3.06	1.52	1.43
12	9	102	KGD	CBG-CBI	3.06	1.52	1.43
8	5	102	BCL	MG-NC	3.06	2.13	2.06
12	3	101	KGD	CBG-CBI	3.06	1.52	1.43
12	T	101	KGD	CAP-CAO	3.05	1.52	1.43
12	N	101	KGD	CBB-CAV	3.05	1.52	1.43
8	B	101	BCL	MG-NC	3.05	2.13	2.06
10	L	1004	MQE	CAX-CBQ	-3.05	1.39	1.47
12	T	101	KGD	CBN-CBL	3.05	1.52	1.45
12	R	101	KGD	CAD-CAH	3.05	1.40	1.35
8	N	103	BCL	MG-NC	3.04	2.13	2.06
12	F	101	KGD	CBB-CAV	3.04	1.52	1.43
8	B	102	BCL	MG-NC	3.04	2.13	2.06
12	5	101	KGD	CAD-CAH	3.04	1.40	1.35
12	3	103	KGD	CBF-CBH	3.04	1.52	1.45
8	4	101	BCL	C1D-C2D	-3.02	1.39	1.45
8	J	102	BCL	MG-NC	3.02	2.13	2.06
12	N	101	KGD	CAP-CAO	3.01	1.52	1.43
12	T	101	KGD	CBF-CBH	3.00	1.52	1.45
8	2	101	BCL	MG-NC	2.99	2.13	2.06
12	3	103	KGD	CBE-CBA	2.99	1.52	1.43
8	Q	101	BCL	MG-NC	2.99	2.13	2.06
8	V	101	BCL	MG-NC	2.97	2.13	2.06
12	N	102	KGD	CBN-CBL	2.97	1.52	1.45
12	F	101	KGD	CAD-CAH	2.97	1.39	1.35
8	8	101	BCL	MG-NC	2.97	2.13	2.06
8	S	102	BCL	MG-NC	2.97	2.13	2.06
12	3	101	KGD	CAL-CAM	2.97	1.52	1.45
12	9	102	KGD	CBF-CBH	2.97	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	102	BCL	MG-NC	2.97	2.13	2.06
8	P	101	BCL	MG-NC	2.96	2.13	2.06
8	3	102	BCL	MG-NC	2.96	2.13	2.06
12	T	101	KGD	CBM-CBJ	2.96	1.52	1.43
8	U	101	BCL	MG-NC	2.95	2.13	2.06
8	I	101	BCL	MG-NC	2.95	2.13	2.06
12	T	102	KGD	CBE-CBA	2.95	1.52	1.43
12	N	101	KGD	CBG-CBI	2.95	1.52	1.43
12	R	101	KGD	CBM-CBJ	2.95	1.52	1.43
8	T	103	BCL	MG-NC	2.95	2.13	2.06
8	H	101	BCL	MG-NC	2.94	2.13	2.06
12	F	101	KGD	CAP-CAO	2.93	1.52	1.43
8	2	102	BCL	MG-NC	2.93	2.13	2.06
8	I	102	BCL	MG-NC	2.93	2.13	2.06
12	N	101	KGD	CBN-CBL	2.92	1.52	1.45
8	6	102	BCL	MG-NC	2.92	2.13	2.06
12	5	101	KGD	CBM-CBJ	2.92	1.52	1.43
8	D	101	BCL	MG-NC	2.91	2.13	2.06
12	R	101	KGD	CBN-CBL	2.91	1.52	1.45
12	F	101	KGD	CAL-CAM	2.91	1.52	1.45
12	N	102	KGD	CAL-CAM	2.91	1.52	1.45
8	7	101	BCL	MG-NC	2.90	2.13	2.06
12	9	102	KGD	CBM-CBJ	2.90	1.52	1.43
8	K	101	BCL	MG-NC	2.89	2.13	2.06
8	W	102	BCL	MG-NC	2.89	2.13	2.06
8	O	101	BCL	MG-NC	2.89	2.13	2.06
8	S	101	BCL	MG-NC	2.89	2.13	2.06
8	O	102	BCL	MG-NC	2.88	2.13	2.06
11	C	502	HEM	CAB-C3B	2.88	1.55	1.47
8	K	102	BCL	MG-NC	2.88	2.13	2.06
12	9	101	KGD	CBG-CBI	2.88	1.52	1.43
12	3	103	KGD	CAP-CAO	2.88	1.52	1.43
12	A	101	KGD	CBB-CAV	2.87	1.52	1.43
12	N	101	KGD	CBM-CBJ	2.87	1.52	1.43
12	J	101	KGD	CAL-CAM	2.87	1.52	1.45
8	0	102	BCL	MG-NC	2.87	2.13	2.06
12	T	101	KGD	CBE-CBA	2.86	1.52	1.43
8	G	102	BCL	MG-NC	2.86	2.13	2.06
12	H	102	KGD	CBG-CBI	2.85	1.52	1.43
12	A	101	KGD	CAP-CAO	2.85	1.52	1.43
12	N	101	KGD	CAL-CAM	2.85	1.52	1.45
11	C	501	HEM	CAB-C3B	2.85	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	101	KGD	CAP-CAO	2.85	1.52	1.43
8	Q	102	BCL	MG-NC	2.84	2.13	2.06
12	A	101	KGD	CAD-CAH	2.84	1.39	1.35
12	A	101	KGD	CAL-CAM	2.84	1.52	1.45
8	4	102	BCL	MG-NC	2.83	2.13	2.06
12	H	102	KGD	CAD-CAH	2.83	1.39	1.35
8	E	101	BCL	MG-NC	2.83	2.13	2.06
8	0	101	BCL	MG-NC	2.83	2.13	2.06
12	3	103	KGD	CAQ-CAR	2.83	1.52	1.45
8	1	101	BCL	MG-NC	2.82	2.13	2.06
12	A	101	KGD	CBG-CBI	2.82	1.52	1.43
12	J	101	KGD	CAQ-CAR	2.82	1.52	1.45
12	3	103	KGD	CBB-CAV	2.81	1.52	1.43
12	J	101	KGD	CBM-CBJ	2.81	1.52	1.43
12	J	101	KGD	CBG-CBI	2.80	1.52	1.43
12	N	101	KGD	CBE-CBA	2.80	1.52	1.43
12	3	103	KGD	CBG-CBI	2.80	1.52	1.43
12	3	101	KGD	CAQ-CAR	2.80	1.52	1.45
8	A	102	BCL	MG-NC	2.79	2.12	2.06
12	J	101	KGD	CBN-CBL	2.78	1.51	1.45
12	9	101	KGD	CAD-CAH	2.77	1.39	1.35
12	N	102	KGD	CBF-CBH	2.77	1.51	1.45
12	9	101	KGD	CBB-CAV	2.77	1.52	1.43
12	F	101	KGD	CAQ-CAR	2.76	1.51	1.45
12	9	102	KGD	CBN-CBL	2.75	1.51	1.45
8	B	101	BCL	C1D-C2D	-2.75	1.39	1.45
12	N	102	KGD	CBE-CBA	2.74	1.51	1.43
12	J	101	KGD	CAP-CAO	2.74	1.51	1.43
8	E	102	BCL	MG-NC	2.74	2.12	2.06
12	N	102	KGD	CBM-CBJ	2.74	1.51	1.43
8	M	703	BCL	MG-NC	2.74	2.12	2.06
12	H	102	KGD	CAL-CAM	2.73	1.51	1.45
12	H	102	KGD	CAP-CAO	2.73	1.51	1.43
12	9	102	KGD	CBE-CBA	2.72	1.51	1.43
12	J	101	KGD	CBB-CAV	2.72	1.51	1.43
12	H	102	KGD	CBB-CAV	2.71	1.51	1.43
12	J	101	KGD	CBE-CBA	2.70	1.51	1.43
11	C	503	HEM	CAB-C3B	2.69	1.54	1.47
10	L	1004	MQE	CAY-CBL	2.69	1.54	1.50
8	F	102	BCL	MG-NC	2.69	2.12	2.06
12	F	101	KGD	CBF-CBH	2.69	1.51	1.45
12	F	101	KGD	CBM-CBJ	2.67	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	101	KGD	CBM-CBJ	2.67	1.51	1.43
12	9	101	KGD	CBM-CBJ	2.67	1.51	1.43
12	N	101	KGD	CBF-CBH	2.67	1.51	1.45
11	C	504	HEM	CAB-C3B	2.65	1.54	1.47
12	H	102	KGD	CBE-CBA	2.65	1.51	1.43
12	9	101	KGD	CAP-CAO	2.64	1.51	1.43
12	3	101	KGD	CBM-CBJ	2.63	1.51	1.43
12	F	101	KGD	CBE-CBA	2.61	1.51	1.43
12	3	101	KGD	CBE-CBA	2.61	1.51	1.43
12	A	101	KGD	CAQ-CAR	2.61	1.51	1.45
11	C	504	HEM	CAA-C2A	2.59	1.55	1.52
12	3	101	KGD	CBN-CBL	2.58	1.51	1.45
12	F	101	KGD	CBN-CBL	2.58	1.51	1.45
12	R	101	KGD	CBF-CBH	2.57	1.51	1.45
12	9	101	KGD	CBE-CBA	2.56	1.51	1.43
12	H	102	KGD	CAQ-CAR	2.54	1.51	1.45
12	9	101	KGD	CBF-CBH	2.53	1.51	1.45
8	U	102	BCL	CBD-CGD	-2.53	1.44	1.52
9	L	1003	BPH	C3A-C2A	-2.53	1.52	1.54
8	G	101	BCL	C1D-C2D	-2.52	1.40	1.45
8	4	101	BCL	MG-NC	2.52	2.12	2.06
8	0	102	BCL	CBD-CGD	-2.51	1.44	1.52
12	A	101	KGD	CBE-CBA	2.51	1.51	1.43
8	L	1001	BCL	MG-NC	2.51	2.12	2.06
12	R	101	KGD	CBE-CBA	2.50	1.51	1.43
8	M	703	BCL	C3D-C4D	-2.49	1.38	1.44
12	J	101	KGD	CBF-CBH	2.49	1.51	1.45
12	9	101	KGD	CBN-CBL	2.45	1.51	1.45
12	H	102	KGD	CBF-CBH	2.44	1.51	1.45
12	R	101	KGD	CAP-CAO	2.44	1.51	1.43
12	9	101	KGD	CAL-CAM	2.43	1.51	1.45
10	L	1004	MQE	CAX-CBK	2.43	1.39	1.35
12	R	101	KGD	CBG-CBI	2.42	1.50	1.43
8	5	102	BCL	C3D-C4D	-2.41	1.38	1.44
8	L	1001	BCL	C3D-C4D	-2.41	1.38	1.44
12	9	101	KGD	CAQ-CAR	2.40	1.51	1.45
12	3	101	KGD	CBF-CBH	2.39	1.51	1.45
12	R	101	KGD	CBB-CAV	2.38	1.50	1.43
8	7	101	BCL	C3D-C4D	-2.38	1.38	1.44
8	H	101	BCL	C3D-C4D	-2.37	1.38	1.44
8	U	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	E	102	BCL	C3D-C4D	-2.37	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	J	102	BCL	C3D-C4D	-2.37	1.38	1.44
8	L	1001	BCL	C1D-C2D	-2.36	1.40	1.45
8	G	101	BCL	C3D-C4D	-2.36	1.38	1.44
8	6	101	BCL	C3D-C4D	-2.36	1.38	1.44
8	L	1002	BCL	C1D-C2D	-2.35	1.40	1.45
8	D	101	BCL	C3D-C4D	-2.33	1.38	1.44
8	W	101	BCL	CHD-C1D	2.33	1.42	1.38
8	2	101	BCL	C3D-C4D	-2.33	1.38	1.44
8	L	1001	BCL	C3C-C4C	-2.33	1.48	1.51
8	A	102	BCL	C3D-C4D	-2.32	1.38	1.44
8	6	101	BCL	CHD-C1D	2.32	1.42	1.38
8	M	703	BCL	C1D-C2D	-2.32	1.40	1.45
8	N	103	BCL	CHD-C1D	2.31	1.42	1.38
8	3	102	BCL	C1D-C2D	-2.31	1.40	1.45
8	2	101	BCL	CHD-C1D	2.31	1.42	1.38
8	Q	101	BCL	C3D-C4D	-2.30	1.39	1.44
12	9	102	KGD	CAC-CAE	-2.30	1.48	1.53
8	9	103	BCL	C3D-C4D	-2.30	1.39	1.44
8	P	101	BCL	C3D-C4D	-2.30	1.39	1.44
8	4	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	S	102	BCL	C1D-C2D	-2.29	1.40	1.45
8	E	102	BCL	C1D-C2D	-2.29	1.40	1.45
10	M	702	MQE	CAX-CBK	2.28	1.39	1.35
8	B	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	4	102	BCL	C1D-C2D	-2.28	1.40	1.45
8	0	101	BCL	CHD-C1D	2.28	1.42	1.38
8	E	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	1	101	BCL	C3D-C4D	-2.27	1.39	1.44
8	U	102	BCL	C3D-C4D	-2.27	1.39	1.44
8	O	101	BCL	C3D-C4D	-2.27	1.39	1.44
8	8	101	BCL	CHD-C1D	2.26	1.42	1.38
8	K	102	BCL	C1D-C2D	-2.26	1.40	1.45
12	R	101	KGD	CAQ-CAR	2.25	1.50	1.45
8	L	1002	BCL	C3D-C4D	-2.25	1.39	1.44
8	7	101	BCL	CHD-C1D	2.24	1.42	1.38
8	O	101	BCL	C1D-C2D	-2.24	1.40	1.45
8	L	1001	BCL	C3B-CAB	-2.24	1.43	1.49
8	T	103	BCL	CHD-C1D	2.24	1.42	1.38
8	8	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	B	102	BCL	CHD-C1D	2.23	1.42	1.38
8	I	101	BCL	CHD-C1D	2.23	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	BCL	CHD-C1D	2.23	1.42	1.38
8	0	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	U	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	3	102	BCL	C3D-C4D	-2.23	1.39	1.44
8	F	102	BCL	C3D-C4D	-2.23	1.39	1.44
8	S	101	BCL	C1D-C2D	-2.23	1.40	1.45
8	R	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	1	101	BCL	CHD-C1D	2.22	1.42	1.38
8	U	102	BCL	CHD-C1D	2.21	1.42	1.38
8	K	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	N	103	BCL	C3D-C4D	-2.21	1.39	1.44
8	8	102	BCL	C1D-C2D	-2.20	1.41	1.45
12	R	101	KGD	CAL-CAM	2.20	1.50	1.45
8	R	102	BCL	CHD-C1D	2.20	1.42	1.38
8	Q	101	BCL	C1D-C2D	-2.19	1.41	1.45
8	3	102	BCL	CHD-C1D	2.19	1.42	1.38
8	W	102	BCL	C1D-C2D	-2.18	1.41	1.45
8	K	102	BCL	CBD-CGD	-2.18	1.45	1.52
8	W	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	T	103	BCL	C3D-C4D	-2.18	1.39	1.44
8	6	102	BCL	CBD-CGD	-2.18	1.45	1.52
12	A	101	KGD	CBN-CBL	2.17	1.50	1.45
8	I	102	BCL	CHD-C1D	2.17	1.42	1.38
8	E	101	BCL	CHD-C1D	2.16	1.42	1.38
8	I	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	S	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	6	102	BCL	C1D-C2D	-2.15	1.41	1.45
8	J	102	BCL	CHD-C1D	2.15	1.42	1.38
8	A	102	BCL	CHD-C1D	2.15	1.42	1.38
11	C	504	HEM	C3B-C2B	-2.15	1.32	1.37
8	0	102	BCL	C3D-C4D	-2.14	1.39	1.44
8	P	101	BCL	CHD-C1D	2.13	1.42	1.38
8	Q	102	BCL	C1D-C2D	-2.13	1.41	1.45
8	F	102	BCL	C1D-C2D	-2.12	1.41	1.45
8	Q	101	BCL	CHD-C1D	2.12	1.42	1.38
8	Q	102	BCL	C3D-C4D	-2.12	1.39	1.44
8	T	103	BCL	C4B-NB	2.12	1.37	1.35
8	B	102	BCL	O1D-CGD	2.11	1.26	1.21
10	M	702	MQE	CAY-CBL	2.11	1.53	1.50
8	9	103	BCL	CHD-C1D	2.11	1.42	1.38
8	F	102	BCL	CHD-C1D	2.11	1.42	1.38
8	6	101	BCL	C1D-C2D	-2.11	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	102	BCL	C1D-C2D	-2.11	1.41	1.45
8	A	102	BCL	C1D-C2D	-2.10	1.41	1.45
8	D	101	BCL	CHD-C1D	2.10	1.42	1.38
8	4	101	BCL	CBD-CGD	-2.09	1.45	1.52
8	4	102	BCL	C3D-C4D	-2.09	1.39	1.44
8	2	102	BCL	CHD-C1D	2.09	1.42	1.38
8	K	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	I	102	BCL	C1D-C2D	-2.08	1.41	1.45
12	3	103	KGD	CAS-CAW	2.08	1.55	1.51
8	Q	102	BCL	CBD-CGD	-2.08	1.45	1.52
8	O	102	BCL	CHD-C1D	2.08	1.42	1.38
8	I	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	G	102	BCL	C1D-C2D	-2.08	1.41	1.45
8	O	101	BCL	CHD-C1D	2.07	1.42	1.38
8	P	101	BCL	CBD-CGD	-2.07	1.45	1.52
8	Q	101	BCL	O1A-CGA	-2.07	1.16	1.22
8	W	101	BCL	C1D-C2D	-2.07	1.41	1.45
8	O	102	BCL	C3D-C4D	-2.07	1.39	1.44
8	W	102	BCL	C3D-C4D	-2.06	1.39	1.44
8	D	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	2	102	BCL	C3D-C4D	-2.06	1.39	1.44
11	C	501	HEM	CMB-C2B	2.06	1.55	1.50
8	4	101	BCL	C3C-C4C	-2.05	1.49	1.51
8	1	101	BCL	CBD-CGD	-2.05	1.46	1.52
8	2	102	BCL	CBD-CGD	-2.05	1.46	1.52
8	5	102	BCL	C1D-C2D	-2.05	1.41	1.45
8	B	102	BCL	C3D-C4D	-2.05	1.39	1.44
8	U	101	BCL	CHD-C1D	2.05	1.42	1.38
8	W	102	BCL	CHD-C1D	2.04	1.42	1.38
8	J	102	BCL	CBD-CGD	-2.04	1.46	1.52
8	G	102	BCL	C3D-C4D	-2.04	1.39	1.44
8	L	1002	BCL	CHD-C1D	2.04	1.42	1.38
8	M	703	BCL	CHD-C1D	2.03	1.42	1.38
8	V	101	BCL	CHD-C1D	2.03	1.42	1.38
8	U	102	BCL	C1D-C2D	-2.03	1.41	1.45
8	5	102	BCL	CHD-C1D	2.03	1.42	1.38
8	6	102	BCL	C3D-C4D	-2.03	1.39	1.44
8	P	101	BCL	C1D-C2D	-2.03	1.41	1.45
8	S	101	BCL	CHD-C1D	2.03	1.42	1.38
8	A	102	BCL	CBD-CGD	-2.02	1.46	1.52
12	A	101	KGD	CBF-CBH	2.02	1.50	1.45
8	S	102	BCL	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	102	BCL	C1D-ND	2.02	1.40	1.37
8	0	102	BCL	C1D-C2D	-2.02	1.41	1.45
8	H	101	BCL	C1D-C2D	-2.02	1.41	1.45
8	O	102	BCL	CBD-CGD	-2.02	1.46	1.52
8	7	101	BCL	C1D-C2D	-2.02	1.41	1.45
8	8	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	V	101	BCL	C3D-C4D	-2.01	1.39	1.44
8	0	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	2	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	I	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	6	101	BCL	CBD-CGD	-2.01	1.46	1.52
8	8	102	BCL	CBD-CGD	-2.01	1.46	1.52
8	G	102	BCL	CHD-C1D	2.01	1.42	1.38
8	G	101	BCL	CBD-CGD	-2.00	1.46	1.52
8	V	101	BCL	C1D-C2D	-2.00	1.41	1.45

All (933) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C4-C3-C5	-27.86	68.40	115.27
8	U	101	BCL	C4-C3-C5	-27.53	68.96	115.27
8	U	101	BCL	C5-C3-C2	19.65	160.88	121.12
8	W	101	BCL	C5-C3-C2	19.41	160.40	121.12
12	N	102	KGD	CBM-CBJ-CBH	-14.24	106.98	127.31
12	T	102	KGD	CBM-CBJ-CBH	-13.10	108.61	127.31
12	5	101	KGD	CBM-CBJ-CBH	-12.77	109.08	127.31
8	U	101	BCL	C4-C3-C2	-12.38	91.93	123.68
8	W	101	BCL	C4-C3-C2	-12.35	91.99	123.68
12	9	102	KGD	CBG-CBI-CBL	-12.30	109.76	127.31
12	J	101	KGD	CBG-CBI-CBL	-12.05	110.11	127.31
12	3	101	KGD	CBG-CBI-CBL	-11.98	110.21	127.31
12	3	101	KGD	CBM-CBJ-CBH	-11.51	110.88	127.31
12	N	101	KGD	CBM-CBJ-CBH	-11.47	110.95	127.31
12	5	101	KGD	CBG-CBI-CBL	-11.45	110.97	127.31
12	T	102	KGD	CBG-CBI-CBL	-11.34	111.13	127.31
12	T	101	KGD	CBM-CBJ-CBH	-11.30	111.19	127.31
12	N	101	KGD	CBG-CBI-CBL	-11.23	111.29	127.31
12	J	101	KGD	CBM-CBJ-CBH	-11.08	111.50	127.31
12	9	101	KGD	CBM-CBJ-CBH	-11.07	111.52	127.31
12	N	102	KGD	CBG-CBI-CBL	-11.05	111.54	127.31
12	9	102	KGD	CBM-CBJ-CBH	-11.04	111.56	127.31
12	F	101	KGD	CBG-CBI-CBL	-11.02	111.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	9	101	KGD	CBG-CBI-CBL	-10.96	111.66	127.31
12	T	101	KGD	CBG-CBI-CBL	-10.84	111.83	127.31
12	F	101	KGD	CBM-CBJ-CBH	-10.83	111.85	127.31
12	N	102	KGD	CAP-CAO-CAM	-10.75	111.97	127.31
12	A	101	KGD	CBG-CBI-CBL	-9.97	113.09	127.31
12	3	101	KGD	CAP-CAO-CAM	-9.63	113.57	127.31
12	5	101	KGD	CAP-CAO-CAM	-9.53	113.70	127.31
12	3	103	KGD	CBG-CBI-CBL	-9.40	113.89	127.31
12	9	101	KGD	CBB-CAV-CAR	-9.27	114.08	127.31
12	N	102	KGD	CBB-CAV-CAR	-9.21	114.17	127.31
12	N	101	KGD	CAP-CAO-CAM	-9.19	114.19	127.31
12	T	102	KGD	CAJ-CAL-CAM	-9.16	112.40	126.23
12	R	101	KGD	CBG-CBI-CBL	-9.10	114.32	127.31
12	3	103	KGD	CBM-CBJ-CBH	-9.02	114.44	127.31
12	R	101	KGD	CBM-CBJ-CBH	-8.93	114.57	127.31
12	N	102	KGD	CAJ-CAL-CAM	-8.86	112.84	126.23
12	T	101	KGD	CBB-CAV-CAR	-8.78	114.78	127.31
12	N	101	KGD	CAJ-CAL-CAM	-8.73	113.04	126.23
12	H	102	KGD	CBG-CBI-CBL	-8.71	114.88	127.31
12	T	101	KGD	CAP-CAO-CAM	-8.58	115.06	127.31
12	9	101	KGD	CAP-CAO-CAM	-8.53	115.13	127.31
12	5	101	KGD	CAJ-CAL-CAM	-8.50	113.39	126.23
12	T	102	KGD	CAP-CAO-CAM	-8.50	115.18	127.31
12	A	101	KGD	CBM-CBJ-CBH	-8.50	115.18	127.31
10	M	702	MQE	CAO-CBI-CAZ	-8.38	107.49	127.66
12	T	101	KGD	CAJ-CAL-CAM	-8.35	113.61	126.23
12	J	101	KGD	CAP-CAO-CAM	-8.35	115.40	127.31
12	F	101	KGD	CAP-CAO-CAM	-8.29	115.48	127.31
12	A	101	KGD	CBB-CAV-CAR	-8.27	115.50	127.31
12	9	102	KGD	CAP-CAO-CAM	-8.23	115.56	127.31
10	L	1004	MQE	CAY-CBL-CBB	-8.19	113.16	126.79
12	F	101	KGD	CBB-CAV-CAR	-8.02	115.87	127.31
12	3	103	KGD	CBB-CAV-CAR	-7.88	116.06	127.31
10	M	702	MQE	CAJ-CBC-CAP	-7.85	108.77	127.66
12	3	101	KGD	CBB-CAV-CAR	-7.84	116.13	127.31
12	9	101	KGD	CAJ-CAL-CAM	-7.81	114.43	126.23
12	J	101	KGD	CBB-CAV-CAR	-7.81	116.17	127.31
12	R	101	KGD	CBB-CAV-CAR	-7.77	116.22	127.31
12	F	101	KGD	CAJ-CAL-CAM	-7.76	114.51	126.23
12	3	101	KGD	CAJ-CAL-CAM	-7.71	114.58	126.23
12	N	101	KGD	CBB-CAV-CAR	-7.60	116.47	127.31
12	T	102	KGD	CBB-CAV-CAR	-7.49	116.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	101	KGD	CAJ-CAL-CAM	-7.26	115.27	126.23
12	H	102	KGD	CAJ-CAL-CAM	-7.12	115.47	126.23
12	9	102	KGD	CBB-CAV-CAR	-7.11	117.16	127.31
10	M	702	MQE	CBA-CBN-CBM	-7.08	110.61	127.66
12	5	101	KGD	CBB-CAV-CAR	-6.96	117.37	127.31
12	N	102	KGD	CBM-CBN-CBL	-6.94	106.93	126.42
12	H	102	KGD	CBG-CBB-CAV	-6.93	109.27	123.47
12	R	101	KGD	CAJ-CAL-CAM	-6.89	115.83	126.23
12	J	101	KGD	CAJ-CAL-CAM	-6.76	116.02	126.23
10	M	702	MQE	CAK-CBE-CAQ	-6.65	111.66	127.66
12	R	101	KGD	CAP-CAO-CAM	-6.62	117.86	127.31
12	R	101	KGD	CBG-CBB-CAV	-6.53	110.09	123.47
12	T	102	KGD	CBM-CBN-CBL	-6.49	108.19	126.42
10	L	1004	MQE	CBO-CCB-CCC	-6.46	112.11	127.66
12	3	101	KGD	CBM-CBN-CBL	-6.43	108.34	126.42
12	A	101	KGD	CAP-CAO-CAM	-6.40	118.18	127.31
10	M	702	MQE	CAY-CBL-CBB	-6.35	116.22	126.79
12	N	102	KGD	CBE-CBF-CBH	-6.29	108.74	126.42
12	H	102	KGD	CAP-CAO-CAM	-6.25	118.40	127.31
12	R	101	KGD	CBE-CBF-CBH	-6.23	108.90	126.42
12	J	101	KGD	CBG-CBB-CAV	-6.11	110.97	123.47
12	9	102	KGD	CBG-CBB-CAV	-6.10	110.97	123.47
12	T	101	KGD	CBM-CBN-CBL	-6.05	109.41	126.42
12	9	102	KGD	CBE-CBF-CBH	-6.04	109.44	126.42
12	T	102	KGD	CBE-CBF-CBH	-5.92	109.77	126.42
10	M	702	MQE	CAS-CBH-CAW	-5.90	113.45	127.66
12	F	101	KGD	CBM-CBN-CBL	-5.89	109.86	126.42
12	5	101	KGD	CBM-CBN-CBL	-5.89	109.87	126.42
12	9	101	KGD	CBM-CBN-CBL	-5.88	109.89	126.42
12	3	103	KGD	CAP-CAO-CAM	-5.85	118.96	127.31
12	5	101	KGD	CBG-CBB-CAV	-5.85	111.49	123.47
12	9	102	KGD	CBM-CBN-CBL	-5.84	110.02	126.42
12	H	102	KGD	CBB-CAV-CAR	-5.83	118.99	127.31
8	M	703	BCL	C1-C2-C3	-5.79	116.03	126.04
10	L	1004	MQE	CAJ-CBC-CAP	-5.77	113.77	127.66
8	Q	102	BCL	C4D-CHA-C1A	5.74	128.24	121.25
12	3	101	KGD	CBG-CBB-CAV	-5.73	111.74	123.47
12	H	102	KGD	CBM-CBJ-CBH	-5.72	119.15	127.31
12	N	101	KGD	CBG-CBB-CAV	-5.69	111.81	123.47
8	U	102	BCL	C4D-CHA-C1A	5.68	128.16	121.25
8	0	102	BCL	C4D-CHA-C1A	5.64	128.11	121.25
12	9	102	KGD	CAJ-CAL-CAM	-5.64	117.72	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	101	KGD	CBM-CBN-CBL	-5.60	110.68	126.42
12	J	101	KGD	CBM-CBN-CBL	-5.56	110.81	126.42
8	K	102	BCL	C4D-CHA-C1A	5.55	128.01	121.25
8	S	102	BCL	C4D-CHA-C1A	5.51	127.95	121.25
8	W	102	BCL	C4D-CHA-C1A	5.50	127.94	121.25
12	3	103	KGD	CBG-CBB-CAV	-5.49	112.22	123.47
8	G	102	BCL	C4D-CHA-C1A	5.47	127.90	121.25
12	5	101	KGD	CBE-CBF-CBH	-5.46	111.08	126.42
8	B	102	BCL	C4D-CHA-C1A	5.44	127.86	121.25
8	L	1002	BCL	C4D-CHA-C1A	5.42	127.84	121.25
8	H	101	BCL	C4D-CHA-C1A	5.42	127.84	121.25
10	L	1004	MQE	CAL-CBF-CAV	-5.41	114.64	127.66
8	6	102	BCL	C4D-CHA-C1A	5.40	127.83	121.25
8	N	103	BCL	C4D-CHA-C1A	5.38	127.80	121.25
8	J	102	BCL	C4D-CHA-C1A	5.37	127.79	121.25
8	7	101	BCL	C4D-CHA-C1A	5.37	127.78	121.25
8	I	102	BCL	C4D-CHA-C1A	5.36	127.78	121.25
8	L	1001	BCL	C4D-CHA-C1A	5.36	127.77	121.25
8	I	101	BCL	C4D-CHA-C1A	5.36	127.77	121.25
8	P	101	BCL	C4D-CHA-C1A	5.35	127.76	121.25
8	V	101	BCL	C11-C10-C8	5.35	133.21	115.92
12	J	101	KGD	CBE-CBF-CBH	-5.34	111.42	126.42
8	E	102	BCL	C4D-CHA-C1A	5.33	127.74	121.25
10	M	702	MQE	CAM-CBG-CAT	-5.33	114.82	127.66
8	8	102	BCL	C4D-CHA-C1A	5.33	127.73	121.25
8	1	101	BCL	C4D-CHA-C1A	5.32	127.73	121.25
8	6	101	BCL	C4D-CHA-C1A	5.31	127.71	121.25
8	M	703	BCL	C4D-CHA-C1A	5.30	127.70	121.25
8	F	102	BCL	C4D-CHA-C1A	5.29	127.68	121.25
8	O	101	BCL	C4D-CHA-C1A	5.28	127.68	121.25
8	9	103	BCL	C4D-CHA-C1A	5.27	127.66	121.25
8	W	101	BCL	C4D-CHA-C1A	5.26	127.65	121.25
8	0	101	BCL	C4D-CHA-C1A	5.25	127.63	121.25
8	O	102	BCL	C4D-CHA-C1A	5.24	127.63	121.25
8	4	101	BCL	C4D-CHA-C1A	5.24	127.62	121.25
8	D	101	BCL	C4D-CHA-C1A	5.23	127.62	121.25
12	F	101	KGD	CBG-CBB-CAV	-5.23	112.77	123.47
10	M	702	MQE	CBO-CCB-CCC	-5.22	115.08	127.66
8	D	101	BCL	CHD-C1D-ND	-5.21	119.67	124.45
8	K	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
12	9	101	KGD	CBG-CBB-CAV	-5.21	112.81	123.47
12	9	101	KGD	CBE-CBF-CBH	-5.19	111.83	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	101	BCL	C4D-CHA-C1A	5.19	127.57	121.25
12	T	102	KGD	CBG-CBB-CAV	-5.19	112.84	123.47
8	T	103	BCL	CHD-C1D-ND	-5.18	119.69	124.45
8	V	101	BCL	C4D-CHA-C1A	5.17	127.54	121.25
12	T	102	KGD	CAB-CAD-CAJ	5.17	130.39	115.78
8	8	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
12	A	101	KGD	CAB-CAD-CAJ	5.15	130.36	115.78
8	4	102	BCL	C4D-CHA-C1A	5.15	127.52	121.25
8	0	102	BCL	CHD-C1D-ND	-5.15	119.72	124.45
8	B	102	BCL	CED-O2D-CGD	5.14	127.56	115.94
8	U	101	BCL	C4D-CHA-C1A	5.14	127.50	121.25
12	H	102	KGD	CAB-CAD-CAJ	5.12	130.26	115.78
8	Q	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
8	S	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
8	R	102	BCL	C4D-CHA-C1A	5.11	127.47	121.25
8	A	102	BCL	C4D-CHA-C1A	5.10	127.46	121.25
12	A	101	KGD	CBG-CBB-CAV	-5.09	113.05	123.47
8	5	102	BCL	C4D-CHA-C1A	5.08	127.43	121.25
8	3	102	BCL	C4D-CHA-C1A	5.08	127.43	121.25
12	N	101	KGD	CBE-CBF-CBH	-5.08	112.16	126.42
8	B	101	BCL	C4D-CHA-C1A	5.07	127.42	121.25
12	3	101	KGD	CBE-CBF-CBH	-5.07	112.17	126.42
8	G	102	BCL	CHD-C1D-ND	-5.07	119.80	124.45
12	A	101	KGD	CBM-CBN-CBL	-5.06	112.20	126.42
8	L	1001	BCL	CHD-C1D-ND	-5.06	119.81	124.45
8	G	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
12	T	101	KGD	CAZ-CAW-CAS	5.05	123.76	115.27
8	U	102	BCL	CHD-C1D-ND	-5.04	119.82	124.45
12	F	101	KGD	CBE-CBF-CBH	-5.04	112.26	126.42
8	E	101	BCL	CHD-C1D-ND	-5.04	119.83	124.45
12	9	101	KGD	CAB-CAD-CAJ	5.03	130.02	115.78
8	W	102	BCL	CHD-C1D-ND	-5.03	119.83	124.45
8	O	102	BCL	CHD-C1D-ND	-5.03	119.83	124.45
8	A	102	BCL	CHD-C1D-ND	-5.03	119.83	124.45
8	1	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
8	T	103	BCL	C4D-CHA-C1A	5.02	127.36	121.25
8	E	101	BCL	C4D-CHA-C1A	5.01	127.34	121.25
8	F	102	BCL	CHD-C1D-ND	-5.01	119.85	124.45
8	9	103	BCL	CHD-C1D-ND	-5.00	119.86	124.45
8	2	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
8	I	102	BCL	CHD-C1D-ND	-5.00	119.86	124.45
8	2	102	BCL	CHD-C1D-ND	-4.99	119.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	101	KGD	CAB-CAD-CAJ	4.97	129.84	115.78
12	3	103	KGD	CAZ-CAW-CAS	4.97	123.63	115.27
8	N	103	BCL	CHD-C1D-ND	-4.96	119.89	124.45
8	I	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
8	H	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
8	3	102	BCL	CHD-C1D-ND	-4.95	119.91	124.45
8	V	101	BCL	CHD-C1D-ND	-4.95	119.91	124.45
12	R	101	KGD	CAB-CAD-CAJ	4.94	129.76	115.78
8	2	102	BCL	C4D-CHA-C1A	4.94	127.26	121.25
12	N	102	KGD	CAP-CAQ-CAR	-4.94	112.54	126.42
8	P	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
8	M	703	BCL	CHD-C1D-ND	-4.92	119.93	124.45
8	J	102	BCL	CHD-C1D-ND	-4.92	119.93	124.45
12	H	102	KGD	CAO-CAP-CAQ	-4.92	107.86	123.22
8	S	102	BCL	CHD-C1D-ND	-4.92	119.94	124.45
12	3	101	KGD	CAB-CAD-CAJ	4.91	129.68	115.78
12	T	101	KGD	CAB-CAD-CAJ	4.90	129.65	115.78
8	8	101	BCL	C1-C2-C3	-4.90	117.56	126.04
8	Q	102	BCL	CHD-C1D-ND	-4.90	119.95	124.45
8	4	102	BCL	CHD-C1D-ND	-4.90	119.95	124.45
8	7	101	BCL	CHD-C1D-ND	-4.90	119.95	124.45
8	R	102	BCL	CHD-C1D-ND	-4.89	119.96	124.45
12	N	102	KGD	CAB-CAD-CAJ	4.88	129.59	115.78
12	5	101	KGD	CAB-CAD-CAJ	4.88	129.59	115.78
8	G	101	BCL	C1-C2-C3	-4.88	117.60	126.04
8	B	102	BCL	CHD-C1D-ND	-4.87	119.98	124.45
12	J	101	KGD	CAB-CAD-CAJ	4.87	129.54	115.78
10	L	1004	MQE	CAO-CBI-CAZ	-4.86	115.96	127.66
8	W	101	BCL	CHD-C1D-ND	-4.86	119.99	124.45
8	K	102	BCL	CHD-C1D-ND	-4.85	120.00	124.45
12	R	101	KGD	CAO-CAP-CAQ	-4.85	108.09	123.22
8	8	101	BCL	CHD-C1D-ND	-4.84	120.00	124.45
10	M	702	MQE	CAL-CBF-CAV	-4.84	116.00	127.66
8	L	1002	BCL	CHD-C1D-ND	-4.83	120.01	124.45
8	8	102	BCL	CHD-C1D-ND	-4.83	120.02	124.45
8	0	101	BCL	CHD-C1D-ND	-4.82	120.02	124.45
8	E	102	BCL	CHD-C1D-ND	-4.81	120.03	124.45
8	S	101	BCL	CHD-C1D-ND	-4.81	120.03	124.45
8	6	102	BCL	CHD-C1D-ND	-4.81	120.03	124.45
10	L	1004	MQE	CBA-CBN-CBM	-4.81	116.08	127.66
12	T	101	KGD	CBE-CBF-CBH	-4.80	112.92	126.42
10	L	1004	MQE	CAI-CBD-CAR	-4.79	116.12	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CHD-C1D-ND	-4.79	120.05	124.45
8	5	102	BCL	CHD-C1D-ND	-4.78	120.06	124.45
12	3	103	KGD	CAB-CAD-CAJ	4.76	129.24	115.78
12	N	101	KGD	CAB-CAD-CAJ	4.75	129.23	115.78
10	M	702	MQE	CAI-CBD-CAR	-4.75	116.22	127.66
8	Q	101	BCL	CHD-C1D-ND	-4.73	120.11	124.45
12	N	102	KGD	CBG-CBB-CAV	-4.72	113.81	123.47
8	6	101	BCL	CHD-C1D-ND	-4.71	120.13	124.45
8	U	101	BCL	CHD-C1D-ND	-4.70	120.13	124.45
12	3	103	KGD	CBE-CBF-CBH	-4.69	113.24	126.42
12	9	102	KGD	CAB-CAD-CAJ	4.67	128.99	115.78
8	O	101	BCL	CHD-C1D-ND	-4.62	120.21	124.45
12	3	101	KGD	CAP-CAQ-CAR	-4.53	113.70	126.42
10	L	1004	MQE	CAM-CBG-CAT	-4.50	116.82	127.66
10	M	702	MQE	CAY-CAX-CBQ	4.47	123.29	118.50
12	T	101	KGD	CAP-CAQ-CAR	-4.45	113.91	126.42
8	4	101	BCL	CHD-C1D-ND	-4.44	120.37	124.45
8	G	101	BCL	CHD-C1D-ND	-4.44	120.37	124.45
8	B	101	BCL	C1-C2-C3	-4.43	118.39	126.04
12	T	101	KGD	CBG-CBB-CAV	-4.42	114.41	123.47
12	5	101	KGD	CAP-CAQ-CAR	-4.39	114.08	126.42
8	B	101	BCL	CHD-C1D-ND	-4.39	120.42	124.45
10	M	702	MQE	CBV-CAR-CAE	4.38	122.64	115.27
12	3	103	KGD	CAT-CAS-CAW	-4.38	98.58	112.98
8	5	102	BCL	C4A-NA-C1A	4.37	108.67	106.71
12	3	103	KGD	CAJ-CAL-CAM	-4.37	119.64	126.23
12	9	101	KGD	CAP-CAQ-CAR	-4.35	114.19	126.42
12	H	102	KGD	CBJ-CBM-CBN	-4.35	109.65	123.22
11	C	504	HEM	CMA-C3A-C4A	-4.29	121.87	128.46
12	F	101	KGD	CAP-CAQ-CAR	-4.25	114.47	126.42
12	R	101	KGD	CBB-CBG-CBI	-4.24	114.79	123.47
12	A	101	KGD	CAO-CAP-CAQ	-4.21	110.08	123.22
8	4	101	BCL	C4A-NA-C1A	4.21	108.60	106.71
10	L	1004	MQE	CAK-CBE-CAQ	-4.17	117.61	127.66
8	H	101	BCL	C4A-NA-C1A	4.17	108.58	106.71
8	L	1001	BCL	C4A-NA-C1A	4.17	108.58	106.71
10	M	702	MQE	CAO-CAH-CAV	-4.16	99.30	112.98
8	4	102	BCL	C4A-NA-C1A	4.13	108.56	106.71
8	6	102	BCL	C4A-NA-C1A	4.12	108.56	106.71
8	9	103	BCL	C4A-NA-C1A	4.11	108.55	106.71
12	9	102	KGD	CAT-CAX-CAY	-4.10	113.73	127.75
12	A	101	KGD	CBE-CBF-CBH	-4.09	114.93	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	103	BCL	CMB-C2B-C1B	-4.09	122.18	128.46
8	U	102	BCL	C4A-NA-C1A	4.07	108.54	106.71
12	T	102	KGD	CAT-CAX-CAY	-4.07	113.85	127.75
12	A	101	KGD	CBB-CBG-CBI	-4.07	115.14	123.47
8	D	101	BCL	C11-C10-C8	-4.05	102.81	115.92
12	H	102	KGD	CBE-CBF-CBH	-4.05	115.04	126.42
8	7	101	BCL	CMB-C2B-C1B	-4.04	122.26	128.46
8	F	102	BCL	C1-C2-C3	-4.04	119.06	126.04
8	M	703	BCL	C4A-NA-C1A	4.03	108.52	106.71
8	8	102	BCL	C4A-NA-C1A	4.03	108.52	106.71
10	L	1004	MQE	CCI-CCM-CCN	-4.02	114.00	127.75
8	V	101	BCL	C4A-NA-C1A	4.00	108.50	106.71
8	1	101	BCL	C4A-NA-C1A	3.99	108.50	106.71
8	9	103	BCL	C1D-ND-C4D	-3.99	103.50	106.33
12	H	102	KGD	CAZ-CAW-CAS	3.99	121.98	115.27
11	C	504	HEM	CBA-CAA-C2A	3.98	119.41	112.62
12	N	101	KGD	CAP-CAQ-CAR	-3.98	115.24	126.42
8	V	101	BCL	CMB-C2B-C1B	-3.96	122.38	128.46
8	R	102	BCL	C11-C10-C8	-3.96	103.13	115.92
10	L	1004	MQE	CAS-CBH-CAW	-3.95	118.16	127.66
8	3	102	BCL	C4B-C3B-CAB	-3.95	119.51	127.13
12	A	101	KGD	CAZ-CAW-CAS	3.93	121.89	115.27
8	0	102	BCL	C4A-NA-C1A	3.93	108.47	106.71
12	A	101	KGD	CBA-CBE-CBF	-3.93	110.95	123.22
8	3	102	BCL	C1D-ND-C4D	-3.93	103.55	106.33
12	H	102	KGD	CBA-CBE-CBF	-3.91	111.02	123.22
8	B	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
8	4	101	BCL	C16-C15-C13	3.89	128.50	115.92
12	3	101	KGD	CAT-CAX-CAY	-3.87	114.52	127.75
8	A	102	BCL	C4B-C3B-CAB	-3.86	119.67	127.13
8	T	103	BCL	CMB-C2B-C1B	-3.85	122.55	128.46
12	R	101	KGD	CBJ-CBM-CBN	-3.85	111.21	123.22
12	9	102	KGD	CAP-CAQ-CAR	-3.84	115.63	126.42
8	D	101	BCL	C1D-ND-C4D	-3.84	103.61	106.33
8	T	103	BCL	C1D-ND-C4D	-3.84	103.61	106.33
8	R	102	BCL	C16-C15-C13	3.82	128.28	115.92
8	4	101	BCL	C1D-ND-C4D	-3.82	103.62	106.33
8	1	101	BCL	CMB-C2B-C1B	-3.82	122.59	128.46
8	L	1001	BCL	C1D-ND-C4D	-3.82	103.62	106.33
8	K	102	BCL	C4A-NA-C1A	3.81	108.42	106.71
12	9	101	KGD	CBB-CBG-CBI	-3.81	115.67	123.47
8	F	102	BCL	C4A-NA-C1A	3.81	108.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	C4A-NA-C1A	3.80	108.42	106.71
8	0	102	BCL	C1D-ND-C4D	-3.80	103.64	106.33
8	6	102	BCL	C1D-ND-C4D	-3.80	103.64	106.33
12	T	101	KGD	CAT-CAX-CAY	-3.79	114.79	127.75
8	G	102	BCL	C1D-ND-C4D	-3.79	103.64	106.33
12	N	101	KGD	CAT-CAX-CAY	-3.79	114.81	127.75
12	3	103	KGD	CAO-CAP-CAQ	-3.78	111.41	123.22
8	A	102	BCL	C1D-ND-C4D	-3.78	103.65	106.33
8	H	101	BCL	CMB-C2B-C1B	-3.78	122.65	128.46
8	W	102	BCL	C4A-NA-C1A	3.77	108.40	106.71
8	R	102	BCL	CMB-C2B-C1B	-3.76	122.68	128.46
8	B	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
8	J	102	BCL	C4A-NA-C1A	3.75	108.39	106.71
8	E	101	BCL	C1-C2-C3	-3.75	119.56	126.04
8	I	102	BCL	C4A-NA-C1A	3.75	108.39	106.71
8	5	102	BCL	C4B-C3B-CAB	-3.75	119.89	127.13
8	J	102	BCL	C1D-ND-C4D	-3.73	103.68	106.33
8	F	102	BCL	C1D-ND-C4D	-3.72	103.69	106.33
12	T	102	KGD	CAP-CAQ-CAR	-3.72	115.98	126.42
8	I	101	BCL	C1D-ND-C4D	-3.70	103.71	106.33
12	J	101	KGD	CAO-CAP-CAQ	-3.70	111.68	123.22
8	9	103	BCL	C4B-C3B-CAB	-3.69	119.99	127.13
8	V	101	BCL	C1D-ND-C4D	-3.69	103.71	106.33
8	6	101	BCL	C4A-NA-C1A	3.69	108.36	106.71
8	F	102	BCL	CMB-C2B-C1B	-3.69	122.80	128.46
8	G	102	BCL	C4A-NA-C1A	3.69	108.36	106.71
8	O	102	BCL	CMB-C2B-C1B	-3.68	122.80	128.46
8	J	102	BCL	C4B-C3B-CAB	-3.68	120.02	127.13
8	P	101	BCL	CMB-C2B-C1B	-3.68	122.81	128.46
8	F	102	BCL	C4B-C3B-CAB	-3.68	120.03	127.13
8	W	102	BCL	C1D-ND-C4D	-3.67	103.72	106.33
8	I	102	BCL	C1D-ND-C4D	-3.67	103.73	106.33
8	3	102	BCL	C4A-NA-C1A	3.67	108.36	106.71
8	4	102	BCL	C1D-ND-C4D	-3.67	103.73	106.33
8	2	101	BCL	C1D-ND-C4D	-3.67	103.73	106.33
8	E	102	BCL	CMB-C2B-C1B	-3.66	122.83	128.46
8	1	101	BCL	C1D-ND-C4D	-3.66	103.73	106.33
12	3	103	KGD	CBB-CBG-CBI	-3.64	116.01	123.47
12	F	101	KGD	CAZ-CAW-CAS	3.64	121.39	115.27
8	S	102	BCL	C1D-ND-C4D	-3.64	103.75	106.33
12	J	101	KGD	CAP-CAQ-CAR	-3.62	116.25	126.42
8	K	102	BCL	C1D-ND-C4D	-3.62	103.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	102	BCL	C1D-ND-C4D	-3.62	103.77	106.33
8	L	1002	BCL	C1D-ND-C4D	-3.62	103.77	106.33
12	N	101	KGD	CAZ-CAW-CAS	3.61	121.35	115.27
10	M	702	MQE	CCA-CBB-CAN	3.61	121.35	115.27
8	7	101	BCL	C1D-ND-C4D	-3.61	103.77	106.33
8	L	1002	BCL	C4A-NA-C1A	3.61	108.33	106.71
8	N	103	BCL	C4A-NA-C1A	3.60	108.32	106.71
8	0	102	BCL	CMB-C2B-C1B	-3.60	122.94	128.46
8	M	703	BCL	C1D-ND-C4D	-3.59	103.78	106.33
12	5	101	KGD	CBK-CBH-CBJ	-3.59	117.89	122.92
8	8	102	BCL	C1D-ND-C4D	-3.58	103.79	106.33
10	M	702	MQE	CBA-CAU-CAZ	-3.58	101.19	112.98
8	D	101	BCL	CMB-C2B-C1B	-3.58	122.96	128.46
8	I	101	BCL	CMB-C2B-C1B	-3.57	122.98	128.46
8	6	102	BCL	CMB-C2B-C1B	-3.57	122.98	128.46
8	6	101	BCL	CMB-C2B-C1B	-3.57	122.98	128.46
8	R	102	BCL	C1D-ND-C4D	-3.57	103.80	106.33
8	I	102	BCL	CMB-C2B-C1B	-3.56	122.98	128.46
8	Q	102	BCL	C1D-ND-C4D	-3.56	103.80	106.33
8	S	102	BCL	CMB-C2B-C1B	-3.56	122.99	128.46
8	G	102	BCL	CMB-C2B-C1B	-3.56	122.99	128.46
8	P	101	BCL	C1D-ND-C4D	-3.56	103.81	106.33
12	T	102	KGD	CBK-CBH-CBJ	-3.55	117.95	122.92
12	9	101	KGD	CAZ-CAW-CAS	3.54	121.23	115.27
8	U	102	BCL	C1D-ND-C4D	-3.54	103.82	106.33
8	W	101	BCL	C4A-NA-C1A	3.54	108.30	106.71
8	N	103	BCL	C1D-ND-C4D	-3.54	103.82	106.33
8	5	102	BCL	C1D-ND-C4D	-3.54	103.82	106.33
8	O	102	BCL	C1D-ND-C4D	-3.54	103.82	106.33
8	G	101	BCL	C1D-ND-C4D	-3.52	103.83	106.33
12	9	101	KGD	CAO-CAP-CAQ	-3.51	112.26	123.22
8	9	103	BCL	CMB-C2B-C1B	-3.51	123.07	128.46
8	K	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
8	E	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
8	W	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
12	R	101	KGD	CAT-CAX-CAY	-3.50	115.79	127.75
8	S	101	BCL	C1D-ND-C4D	-3.50	103.85	106.33
12	3	101	KGD	CAZ-CAW-CAS	3.49	121.14	115.27
8	7	101	BCL	C4A-NA-C1A	3.49	108.27	106.71
8	U	101	BCL	C1D-ND-C4D	-3.48	103.86	106.33
8	Q	101	BCL	CMB-C2B-C1B	-3.48	123.12	128.46
8	E	101	BCL	CMB-C2B-C1B	-3.47	123.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33
11	C	504	HEM	C3B-C2B-C1B	3.47	109.06	106.49
8	3	102	BCL	CMB-C2B-C1B	-3.46	123.14	128.46
8	Q	102	BCL	CHA-C1A-NA	-3.46	118.48	126.40
12	N	102	KGD	CBK-CBH-CBJ	-3.46	118.08	122.92
8	0	102	BCL	C1-C2-C3	-3.45	120.07	126.04
8	J	102	BCL	CMB-C2B-C1B	-3.45	123.16	128.46
9	M	704	BPH	C16-C15-C13	3.45	127.07	115.92
8	M	703	BCL	CMB-C2B-C1B	-3.45	123.17	128.46
10	M	702	MQE	CAE-CAL-CBF	-3.44	100.56	111.88
8	B	101	BCL	C1D-ND-C4D	-3.44	103.89	106.33
8	L	1002	BCL	CMB-C2B-C1B	-3.44	123.18	128.46
10	M	702	MQE	CAC-CAI-CBD	-3.43	100.59	111.88
8	Q	101	BCL	C4A-NA-C1A	3.43	108.25	106.71
11	C	504	HEM	CAD-CBD-CGD	-3.43	106.22	113.60
12	3	103	KGD	CAP-CAQ-CAR	-3.42	116.81	126.42
12	F	101	KGD	CAT-CAX-CAY	-3.41	116.09	127.75
12	R	101	KGD	CAF-CAB-CAD	3.41	115.83	110.30
8	8	101	BCL	C4A-NA-C1A	3.41	108.24	106.71
8	U	101	BCL	C4A-NA-C1A	3.40	108.24	106.71
8	K	102	BCL	CMB-C2B-C1B	-3.40	123.24	128.46
8	2	102	BCL	C4A-NA-C1A	3.40	108.23	106.71
8	4	102	BCL	CMB-C2B-C1B	-3.39	123.26	128.46
12	T	102	KGD	CBF-CBH-CBJ	3.39	124.14	118.94
8	A	102	BCL	C4A-NA-C1A	3.39	108.23	106.71
12	F	101	KGD	CBB-CBG-CBI	-3.38	116.55	123.47
12	N	102	KGD	CBB-CBG-CBI	-3.38	116.55	123.47
8	2	102	BCL	C1D-ND-C4D	-3.38	103.94	106.33
8	Q	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
12	A	101	KGD	CAP-CAQ-CAR	-3.37	116.94	126.42
8	6	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
8	8	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
8	S	101	BCL	C4B-C3B-CAB	-3.37	120.62	127.13
8	T	103	BCL	C4A-NA-C1A	3.37	108.22	106.71
8	6	101	BCL	C4B-C3B-CAB	-3.37	120.62	127.13
8	E	102	BCL	CHA-C1A-NA	-3.35	118.72	126.40
12	R	101	KGD	CAZ-CAW-CAS	3.35	120.91	115.27
8	0	101	BCL	C4A-NA-C1A	3.35	108.21	106.71
8	O	101	BCL	CMB-C2B-C1B	-3.35	123.32	128.46
8	2	102	BCL	C6-C7-C8	3.35	126.74	115.92
8	0	101	BCL	C1D-ND-C4D	-3.35	103.96	106.33
12	J	101	KGD	CAT-CAX-CAY	-3.35	116.31	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5	102	BCL	CMB-C2B-C1B	-3.34	123.33	128.46
8	2	101	BCL	C4A-NA-C1A	3.34	108.21	106.71
12	9	101	KGD	CAT-CAX-CAY	-3.34	116.34	127.75
8	O	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
8	I	101	BCL	CHA-C1A-NA	-3.32	118.79	126.40
12	T	102	KGD	CBN-CBL-CBI	3.31	124.02	118.94
8	W	102	BCL	CMB-C2B-C1B	-3.31	123.38	128.46
8	2	101	BCL	CMB-C2B-C1B	-3.30	123.39	128.46
10	M	702	MQE	CBW-CAT-CAF	3.30	120.82	115.27
12	F	101	KGD	CAO-CAP-CAQ	-3.30	112.93	123.22
12	3	103	KGD	CBJ-CBM-CBN	-3.30	112.93	123.22
12	5	101	KGD	CBO-CBL-CBI	-3.29	118.31	122.92
10	M	702	MQE	CCI-CCM-CCN	-3.29	116.50	127.75
8	2	102	BCL	CMB-C2B-C1B	-3.29	123.41	128.46
8	Q	102	BCL	CMB-C2B-C1B	-3.28	123.42	128.46
8	6	101	BCL	C1-C2-C3	-3.27	120.39	126.04
8	K	101	BCL	CHA-C1A-NA	-3.26	118.94	126.40
10	M	702	MQE	CCL-CCC-CCD	3.25	120.75	115.27
8	L	1002	BCL	CHA-C1A-NA	-3.25	118.94	126.40
8	W	101	BCL	CMB-C2B-C1B	-3.25	123.47	128.46
8	R	102	BCL	C4A-NA-C1A	3.25	108.17	106.71
12	R	101	KGD	CAP-CAQ-CAR	-3.25	117.29	126.42
9	L	1003	BPH	OBD-CAD-CBD	-3.25	121.06	125.82
8	S	102	BCL	CHA-C1A-NA	-3.25	118.96	126.40
8	O	101	BCL	C4A-NA-C1A	3.23	108.16	106.71
12	N	102	KGD	CAT-CAX-CAY	-3.23	116.70	127.75
8	4	101	BCL	CMB-C2B-C1B	-3.23	123.50	128.46
8	U	102	BCL	CMB-C2B-C1B	-3.22	123.52	128.46
12	T	102	KGD	CBO-CBL-CBI	-3.21	118.42	122.92
8	E	102	BCL	CED-O2D-CGD	3.21	123.19	115.94
8	D	101	BCL	CHA-C1A-NA	-3.21	119.06	126.40
9	M	705	BPH	OBD-CAD-CBD	-3.20	121.12	125.82
12	A	101	KGD	CBJ-CBM-CBN	-3.20	113.22	123.22
8	U	102	BCL	CHA-C1A-NA	-3.20	119.07	126.40
8	S	102	BCL	C4A-NA-C1A	3.19	108.14	106.71
11	C	504	HEM	CHB-C1B-NB	3.19	128.33	124.38
8	5	102	BCL	C17-C16-C15	3.19	127.91	113.24
8	S	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
12	N	102	KGD	CBN-CBL-CBI	3.18	123.83	118.94
8	D	101	BCL	C1-C2-C3	-3.18	120.54	126.04
8	O	102	BCL	CHA-C1A-NA	-3.18	119.11	126.40
8	B	101	BCL	CMB-C2B-C1B	-3.18	123.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	102	BCL	C4D-C3D-CAD	-3.17	104.36	108.10
8	8	102	BCL	CHA-C1A-NA	-3.17	119.13	126.40
8	K	101	BCL	CMB-C2B-C1B	-3.16	123.61	128.46
8	E	102	BCL	C4A-NA-C1A	3.16	108.13	106.71
8	8	102	BCL	CMB-C2B-C1B	-3.16	123.61	128.46
8	K	102	BCL	CHA-C1A-NA	-3.16	119.17	126.40
8	U	101	BCL	CMB-C2B-C1B	-3.16	123.61	128.46
12	T	101	KGD	CBB-CBG-CBI	-3.16	117.01	123.47
12	N	102	KGD	CBF-CBH-CBJ	3.15	123.77	118.94
8	O	101	BCL	CHA-C1A-NA	-3.15	119.19	126.40
8	O	102	BCL	C2A-C1A-CHA	3.13	129.34	123.86
8	8	101	BCL	C4B-C3B-CAB	-3.13	121.08	127.13
8	O	102	BCL	C4A-NA-C1A	3.13	108.11	106.71
8	Q	102	BCL	CED-O2D-CGD	3.12	123.00	115.94
8	B	102	BCL	CHA-C1A-NA	-3.12	119.25	126.40
12	J	101	KGD	CBB-CBG-CBI	-3.12	117.08	123.47
8	Q	102	BCL	C4A-NA-C1A	3.12	108.11	106.71
10	L	1004	MQE	CCF-CBM-CBJ	3.12	120.52	115.27
8	O	101	BCL	C1-C2-C3	-3.11	120.66	126.04
11	C	501	HEM	CAD-CBD-CGD	-3.11	106.91	113.60
8	G	102	BCL	CHA-C1A-NA	-3.11	119.28	126.40
8	W	102	BCL	CHA-C1A-NA	-3.10	119.29	126.40
8	I	102	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	3	102	BCL	CHA-C1A-NA	-3.10	119.31	126.40
8	6	102	BCL	CHA-C1A-NA	-3.10	119.31	126.40
8	8	101	BCL	CMB-C2B-C1B	-3.09	123.71	128.46
8	J	102	BCL	C16-C15-C13	3.09	125.92	115.92
12	9	102	KGD	CBO-CBL-CBI	-3.09	118.59	122.92
12	3	101	KGD	CBN-CBL-CBI	3.09	123.69	118.94
8	L	1001	BCL	CMB-C2B-C1B	-3.09	123.71	128.46
8	B	101	BCL	C4B-C3B-CAB	-3.09	121.16	127.13
8	0	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
8	4	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
12	9	102	KGD	CBN-CBL-CBI	3.07	123.66	118.94
9	M	704	BPH	OBD-CAD-CBD	-3.07	121.32	125.82
8	S	101	BCL	C4A-NA-C1A	3.07	108.09	106.71
8	K	101	BCL	C4A-NA-C1A	3.07	108.09	106.71
8	G	101	BCL	C4A-NA-C1A	3.07	108.09	106.71
10	M	702	MQE	CBX-CAV-CAH	3.07	120.43	115.27
8	V	101	BCL	C1-C2-C3	-3.06	120.75	126.04
8	E	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
12	J	101	KGD	CAF-CAB-CAD	3.06	115.25	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	102	BCL	C1D-ND-C4D	-3.05	104.17	106.33
8	V	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
12	3	101	KGD	CBA-CBE-CBF	-3.05	113.69	123.22
12	T	101	KGD	CBN-CBL-CBI	3.05	123.62	118.94
8	S	101	BCL	CMB-C2B-C1B	-3.05	123.78	128.46
8	R	102	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	L	1001	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	H	101	BCL	C11-C10-C8	-3.04	106.10	115.92
12	J	101	KGD	CAZ-CAW-CAS	3.04	120.38	115.27
8	Q	102	BCL	C1-C2-C3	-3.03	120.80	126.04
8	W	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	H	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	P	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
12	3	103	KGD	CBM-CBN-CBL	-3.03	117.91	126.42
8	G	101	BCL	CHA-C1A-NA	-3.03	119.47	126.40
8	K	102	BCL	C16-C15-C13	3.03	125.70	115.92
8	F	102	BCL	CHA-C1A-NA	-3.03	119.47	126.40
8	0	101	BCL	CMB-C2B-C1B	-3.02	123.82	128.46
10	L	1004	MQE	CBU-CAQ-CAD	3.02	120.35	115.27
8	3	102	BCL	C16-C15-C13	3.02	125.67	115.92
8	U	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
8	2	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
12	N	101	KGD	CBB-CBG-CBI	-3.01	117.31	123.47
8	T	103	BCL	CHA-C1A-NA	-3.01	119.51	126.40
8	N	103	BCL	CHA-C1A-NA	-3.01	119.51	126.40
8	7	101	BCL	CHA-C1A-NA	-3.00	119.52	126.40
12	3	103	KGD	CAN-CAM-CAL	3.00	122.81	118.08
8	Q	101	BCL	CHA-C1A-NA	-3.00	119.52	126.40
8	7	101	BCL	CMB-C2B-C3B	3.00	130.29	124.68
8	D	101	BCL	C4A-NA-C1A	2.99	108.05	106.71
11	C	504	HEM	C4C-CHD-C1D	2.99	126.50	122.56
12	3	103	KGD	CAF-CAB-CAD	2.99	115.15	110.30
8	B	102	BCL	C4A-NA-C1A	2.99	108.05	106.71
8	2	101	BCL	CHA-C1A-NA	-2.99	119.56	126.40
12	R	101	KGD	CBM-CBN-CBL	-2.99	118.03	126.42
8	1	101	BCL	CHA-C1A-NA	-2.98	119.56	126.40
9	L	1003	BPH	C11-C10-C8	-2.98	106.27	115.92
8	I	101	BCL	C4B-C3B-CAB	-2.98	121.37	127.13
8	B	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	4	101	BCL	C15-C13-C12	-2.98	96.47	112.13
8	9	103	BCL	CHA-C1A-NA	-2.98	119.58	126.40
12	H	102	KGD	CBB-CBG-CBI	-2.97	117.39	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
8	4	101	BCL	CHA-C1A-NA	-2.97	119.60	126.40
12	9	101	KGD	CAF-CAB-CAD	2.96	115.11	110.30
8	4	102	BCL	C2A-C1A-CHA	2.96	129.04	123.86
8	D	101	BCL	C4B-C3B-CAB	-2.96	121.41	127.13
8	J	102	BCL	CHA-C1A-NA	-2.96	119.62	126.40
8	N	103	BCL	CMB-C2B-C3B	2.95	130.21	124.68
8	G	101	BCL	CMB-C2B-C1B	-2.95	123.93	128.46
8	6	101	BCL	C11-C10-C8	2.95	125.44	115.92
8	I	101	BCL	C4A-NA-C1A	2.94	108.03	106.71
12	N	102	KGD	CAZ-CAW-CAS	2.94	120.22	115.27
8	F	102	BCL	C11-C10-C8	-2.94	106.42	115.92
12	9	102	KGD	CAO-CAP-CAQ	-2.94	114.05	123.22
12	T	101	KGD	CBO-CBL-CBI	-2.94	118.81	122.92
8	A	102	BCL	CHA-C1A-NA	-2.94	119.68	126.40
12	N	101	KGD	CAO-CAP-CAQ	-2.93	114.06	123.22
8	0	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
11	C	504	HEM	CMA-C3A-C2A	2.93	130.46	124.94
8	6	101	BCL	CHA-C1A-NA	-2.92	119.70	126.40
8	I	101	BCL	C1-C2-C3	-2.92	120.99	126.04
8	K	102	BCL	C2A-C1A-CHA	2.92	128.96	123.86
8	M	703	BCL	CHA-C1A-NA	-2.92	119.72	126.40
12	3	103	KGD	CAK-CAH-CAD	-2.91	119.43	124.11
10	L	1004	MQE	CBY-CAW-CAG	2.91	120.16	115.27
8	G	102	BCL	C16-C15-C13	2.91	125.31	115.92
8	6	102	BCL	C2A-C1A-CHA	2.90	128.93	123.86
12	9	101	KGD	CBA-CBE-CBF	-2.90	114.18	123.22
8	5	102	BCL	CHA-C1A-NA	-2.89	119.77	126.40
8	I	101	BCL	C16-C15-C13	2.89	125.27	115.92
12	3	101	KGD	CAO-CAP-CAQ	-2.89	114.20	123.22
12	R	101	KGD	CBO-CBL-CBN	2.89	122.63	118.08
12	F	101	KGD	CBA-CBE-CBF	-2.88	114.23	123.22
8	E	102	BCL	CGD-CBD-CAD	-2.88	101.41	110.73
12	A	101	KGD	CAK-CAH-CAD	-2.88	119.49	124.11
8	E	101	BCL	C4B-C3B-CAB	-2.87	121.58	127.13
8	F	102	BCL	CMB-C2B-C3B	2.87	130.04	124.68
9	M	705	BPH	CMB-C2B-C3B	2.86	130.03	124.68
8	B	102	BCL	CMB-C2B-C3B	2.86	130.02	124.68
8	E	101	BCL	C4A-NA-C1A	2.85	107.99	106.71
12	N	102	KGD	CAK-CAH-CAD	-2.85	119.53	124.11
8	3	102	BCL	C6-C7-C8	2.85	125.12	115.92
12	9	101	KGD	CAK-CAH-CAD	-2.83	119.56	124.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	102	BCL	CMB-C2B-C1B	-2.82	124.12	128.46
12	H	102	KGD	CAF-CAB-CAD	2.81	114.86	110.30
8	I	102	BCL	C2A-C1A-CHA	2.81	128.78	123.86
8	L	1001	BCL	C2A-C1A-CHA	2.81	128.77	123.86
12	J	101	KGD	CBO-CBL-CBI	-2.81	118.99	122.92
8	W	102	BCL	C2A-C1A-CHA	2.80	128.76	123.86
8	V	101	BCL	CMB-C2B-C3B	2.80	129.92	124.68
8	T	103	BCL	OBG-CAB-C3B	2.80	124.96	119.99
8	B	102	BCL	O2D-CGD-CBD	-2.80	106.30	111.27
8	Q	102	BCL	C4D-C3D-CAD	-2.80	104.80	108.10
12	T	102	KGD	CAZ-CAW-CAS	2.80	119.97	115.27
12	A	101	KGD	CAF-CAB-CAD	2.80	114.83	110.30
12	F	101	KGD	CAK-CAH-CAD	-2.79	119.62	124.11
8	S	101	BCL	C6-C5-C3	2.79	120.78	113.45
12	N	102	KGD	CAN-CAM-CAO	-2.79	119.01	122.92
12	N	102	KGD	CBO-CBL-CBI	-2.79	119.02	122.92
12	T	101	KGD	CAK-CAH-CAD	-2.79	119.63	124.11
12	J	101	KGD	CBA-CBE-CBF	-2.79	114.52	123.22
8	3	102	BCL	C1-C2-C3	-2.79	121.22	126.04
8	0	102	BCL	C2A-C1A-CHA	2.78	128.73	123.86
12	N	101	KGD	CBA-CBE-CBF	-2.78	114.56	123.22
8	K	101	BCL	C4B-C3B-CAB	-2.78	121.77	127.13
12	5	101	KGD	CBF-CBH-CBJ	2.77	123.20	118.94
8	R	102	BCL	CMB-C2B-C3B	2.77	129.87	124.68
8	1	101	BCL	CMB-C2B-C3B	2.76	129.85	124.68
8	I	101	BCL	CMB-C2B-C3B	2.76	129.84	124.68
8	4	101	BCL	C17-C16-C15	2.75	125.89	113.24
12	H	102	KGD	CAK-CAH-CAD	-2.75	119.68	124.11
8	U	102	BCL	C2A-C1A-CHA	2.75	128.66	123.86
10	M	702	MQE	CAJ-CAD-CAQ	-2.75	103.94	112.98
12	T	101	KGD	CAO-CAP-CAQ	-2.74	114.66	123.22
8	R	102	BCL	C2A-C1A-CHA	2.74	128.65	123.86
8	8	102	BCL	C2A-C1A-CHA	2.74	128.65	123.86
8	W	101	BCL	C4B-C3B-CAB	-2.74	121.84	127.13
8	E	101	BCL	CMB-C2B-C3B	2.74	129.80	124.68
10	L	1004	MQE	CBV-CAR-CAE	2.73	119.86	115.27
12	T	101	KGD	CBA-CBE-CBF	-2.73	114.71	123.22
8	R	102	BCL	C4B-C3B-CAB	-2.72	121.86	127.13
8	U	101	BCL	C2A-C1A-CHA	2.72	128.61	123.86
8	I	102	BCL	C4B-C3B-CAB	-2.72	121.88	127.13
8	9	103	BCL	CMB-C2B-C3B	2.72	129.76	124.68
12	3	101	KGD	CAF-CAB-CAD	2.71	114.70	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	101	KGD	CAK-CAH-CAD	-2.71	119.75	124.11
11	C	503	HEM	CBA-CAA-C2A	-2.71	108.00	112.62
12	3	103	KGD	CBA-CBE-CBF	-2.71	114.76	123.22
12	N	101	KGD	CBK-CBH-CBJ	-2.71	119.13	122.92
8	E	102	BCL	CMB-C2B-C3B	2.70	129.74	124.68
8	P	101	BCL	C4B-C3B-CAB	-2.70	121.91	127.13
8	V	101	BCL	C2A-C1A-CHA	2.70	128.58	123.86
8	H	101	BCL	CMB-C2B-C3B	2.70	129.73	124.68
8	0	102	BCL	CMB-C2B-C3B	2.70	129.72	124.68
8	0	101	BCL	C1-C2-C3	-2.69	121.38	126.04
8	2	102	BCL	C2A-C1A-CHA	2.69	128.57	123.86
8	D	101	BCL	CMB-C2B-C3B	2.68	129.70	124.68
12	5	101	KGD	CAK-CAH-CAD	-2.68	119.81	124.11
8	P	101	BCL	C2A-C1A-CHA	2.68	128.54	123.86
8	4	101	BCL	C1-C2-C3	-2.68	121.42	126.04
8	P	101	BCL	CMB-C2B-C3B	2.67	129.68	124.68
12	3	101	KGD	CAK-CAH-CAD	-2.67	119.81	124.11
8	U	102	BCL	CAC-C3C-C4C	2.67	118.51	112.58
8	8	102	BCL	C16-C15-C13	2.67	124.54	115.92
9	L	1003	BPH	CMB-C2B-C3B	2.67	129.67	124.68
12	3	101	KGD	CBO-CBL-CBI	-2.67	119.19	122.92
12	9	102	KGD	CAK-CAH-CAD	-2.66	119.83	124.11
8	F	102	BCL	C2A-C1A-CHA	2.66	128.52	123.86
8	B	102	BCL	C2A-C1A-CHA	2.66	128.52	123.86
12	R	101	KGD	CAK-CAH-CAD	-2.66	119.83	124.11
12	3	101	KGD	CBB-CBG-CBI	-2.66	118.03	123.47
8	7	101	BCL	C4B-C3B-CAB	-2.66	122.00	127.13
12	N	101	KGD	CAF-CAB-CAD	2.66	114.61	110.30
8	G	102	BCL	CMB-C2B-C3B	2.65	129.64	124.68
8	G	102	BCL	C2A-C1A-CHA	2.65	128.49	123.86
8	7	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
8	I	102	BCL	CMB-C2B-C3B	2.65	129.63	124.68
8	O	101	BCL	C6-C5-C3	2.64	120.39	113.45
8	O	102	BCL	CMB-C2B-C3B	2.64	129.62	124.68
8	Q	101	BCL	CMB-C2B-C3B	2.64	129.62	124.68
12	T	102	KGD	CBB-CBG-CBI	-2.64	118.07	123.47
8	Q	101	BCL	C4B-C3B-CAB	-2.64	122.04	127.13
12	F	101	KGD	CBN-CBL-CBI	2.63	122.98	118.94
12	T	102	KGD	CAO-CAP-CAQ	-2.63	115.00	123.22
8	T	103	BCL	C2A-C1A-CHA	2.63	128.46	123.86
8	6	101	BCL	CMB-C2B-C3B	2.63	129.59	124.68
12	J	101	KGD	CAK-CAH-CAD	-2.62	119.89	124.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	102	KGD	CAU-CAR-CAQ	2.62	122.20	118.08
8	O	101	BCL	C4B-C3B-CAB	-2.62	122.07	127.13
8	T	103	BCL	CMB-C2B-C3B	2.61	129.57	124.68
8	J	102	BCL	CMB-C2B-C3B	2.61	129.56	124.68
8	2	101	BCL	CMB-C2B-C3B	2.60	129.54	124.68
8	2	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
8	I	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
8	6	102	BCL	CMB-C2B-C3B	2.59	129.53	124.68
12	R	101	KGD	CAT-CAS-CAW	-2.59	104.44	112.98
12	9	102	KGD	CBK-CBH-CBJ	-2.59	119.29	122.92
8	6	101	BCL	C16-C15-C13	-2.59	107.54	115.92
12	3	101	KGD	CAT-CAS-CAW	-2.59	104.46	112.98
8	G	101	BCL	C6-C7-C8	-2.59	107.55	115.92
8	3	102	BCL	CMB-C2B-C3B	2.59	129.52	124.68
8	L	1002	BCL	C2A-C1A-CHA	2.59	128.38	123.86
12	5	101	KGD	CBB-CBG-CBI	-2.59	118.17	123.47
12	F	101	KGD	CBO-CBL-CBI	-2.59	119.30	122.92
8	1	101	BCL	C4B-C3B-CAB	-2.58	122.15	127.13
8	S	102	BCL	CMB-C2B-C3B	2.58	129.50	124.68
10	L	1004	MQE	CBW-CAT-CAF	2.57	119.60	115.27
12	H	102	KGD	CAP-CAQ-CAR	-2.57	119.19	126.42
8	O	101	BCL	CMB-C2B-C3B	2.57	129.49	124.68
12	R	101	KGD	CAU-CAR-CAQ	2.57	122.12	118.08
8	5	102	BCL	CMB-C2B-C3B	2.57	129.48	124.68
8	E	101	BCL	C2A-C1A-CHA	2.56	128.34	123.86
8	3	102	BCL	C2A-C1A-CHA	2.56	128.33	123.86
12	N	101	KGD	CBO-CBL-CBI	-2.55	119.35	122.92
12	T	102	KGD	CAF-CAB-CAD	2.55	114.44	110.30
8	H	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86
12	9	102	KGD	CAZ-CAW-CAS	2.55	119.56	115.27
8	W	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86
12	N	102	KGD	CAF-CAB-CAD	2.55	114.43	110.30
12	F	101	KGD	CAF-CAB-CAD	2.54	114.42	110.30
8	S	102	BCL	C2A-C1A-CHA	2.54	128.30	123.86
8	H	101	BCL	C4B-C3B-CAB	-2.54	122.22	127.13
8	9	103	BCL	C2A-C1A-CHA	2.54	128.30	123.86
8	I	102	BCL	C1-C2-C3	-2.54	121.65	126.04
12	5	101	KGD	CAT-CAX-CAY	-2.54	119.08	127.75
8	B	101	BCL	C2A-C1A-CHA	2.53	128.29	123.86
8	N	103	BCL	C4B-C3B-CAB	-2.53	122.24	127.13
9	L	1003	BPH	CMD-C2D-C3D	2.53	129.41	124.68
8	U	101	BCL	C17-C16-C15	2.53	124.85	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	0	101	BCL	C4B-C3B-CAB	-2.52	122.26	127.13
12	9	102	KGD	CBD-CAY-CBC	2.52	120.16	114.60
10	M	702	MQE	CCP-CCN-CCO	2.51	120.15	114.60
12	3	103	KGD	CBO-CBL-CBN	2.51	122.03	118.08
12	3	103	KGD	CAL-CAM-CAO	-2.51	115.09	118.94
8	L	1002	BCL	CMB-C2B-C3B	2.51	129.37	124.68
12	T	101	KGD	CBD-CAY-CBC	2.51	120.14	114.60
9	M	704	BPH	CMB-C2B-C3B	2.51	129.37	124.68
12	A	101	KGD	CBD-CAY-CBC	2.51	120.14	114.60
12	3	103	KGD	CAT-CAX-CAY	-2.51	119.19	127.75
8	A	102	BCL	C2A-C1A-CHA	2.50	128.23	123.86
8	N	103	BCL	C2A-C1A-CHA	2.49	128.22	123.86
8	K	102	BCL	C17-C16-C15	2.49	124.69	113.24
12	N	101	KGD	CBN-CBL-CBI	2.49	122.76	118.94
10	L	1004	MQE	CCL-CCC-CCD	2.49	119.45	115.27
8	W	102	BCL	C6-C7-C8	2.48	123.94	115.92
10	M	702	MQE	CCF-CBM-CBJ	2.48	119.44	115.27
10	L	1004	MQE	CBX-CAV-CAH	2.48	119.44	115.27
12	T	102	KGD	CBD-CAY-CBC	2.47	120.06	114.60
8	U	101	BCL	C11-C10-C8	-2.47	107.93	115.92
11	C	501	HEM	CBA-CAA-C2A	-2.47	108.40	112.62
8	M	703	BCL	CMB-C2B-C3B	2.47	129.30	124.68
8	D	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
8	Q	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
8	1	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
8	L	1002	BCL	C6-C5-C3	2.47	119.92	113.45
8	0	101	BCL	C2A-C1A-CHA	2.47	128.17	123.86
12	H	102	KGD	CBO-CBL-CBN	2.47	121.96	118.08
12	N	101	KGD	CBD-CAY-CBC	2.47	120.05	114.60
8	K	102	BCL	CMB-C2B-C3B	2.46	129.28	124.68
11	C	503	HEM	C4C-CHD-C1D	2.46	125.81	122.56
12	5	101	KGD	CAN-CAM-CAO	-2.46	119.48	122.92
8	4	102	BCL	CMB-C2B-C3B	2.46	129.28	124.68
8	8	101	BCL	CMB-C2B-C3B	2.46	129.28	124.68
8	B	101	BCL	CMB-C2B-C3B	2.45	129.27	124.68
8	3	102	BCL	C11-C10-C8	-2.45	108.01	115.92
9	M	705	BPH	CMD-C2D-C3D	2.44	129.25	124.68
8	U	101	BCL	C4B-C3B-CAB	-2.44	122.41	127.13
12	3	103	KGD	CBK-CBH-CBJ	-2.44	119.51	122.92
12	T	101	KGD	CAF-CAB-CAD	2.43	114.24	110.30
8	S	101	BCL	CMB-C2B-C3B	2.43	129.22	124.68
8	Q	102	BCL	CMB-C2B-C3B	2.42	129.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	101	BCL	CMB-C2B-C3B	2.42	129.21	124.68
8	Q	102	BCL	C1-O2A-CGA	2.42	122.79	116.44
12	9	102	KGD	CAF-CAB-CAD	2.42	114.22	110.30
12	T	101	KGD	CBK-CBH-CBJ	-2.42	119.54	122.92
10	M	702	MQE	CCE-CBK-CAX	-2.42	120.46	124.40
11	C	504	HEM	C4D-ND-C1D	2.42	107.57	105.07
8	W	102	BCL	CMB-C2B-C3B	2.42	129.20	124.68
8	U	102	BCL	CMB-C2B-C3B	2.42	129.20	124.68
8	L	1001	BCL	CAA-CBA-CGA	2.41	120.31	113.25
10	L	1004	MQE	CCP-CCN-CCO	2.41	119.94	114.60
8	6	101	BCL	C2A-C1A-CHA	2.41	128.08	123.86
8	Q	102	BCL	C2A-C1A-CHA	2.41	128.07	123.86
8	F	102	BCL	C16-C15-C13	2.41	123.70	115.92
8	S	101	BCL	C2A-C1A-CHA	2.40	128.06	123.86
12	9	102	KGD	CAN-CAM-CAO	-2.40	119.56	122.92
8	M	703	BCL	C2A-C1A-CHA	2.40	128.06	123.86
8	U	101	BCL	C6-C7-C8	-2.40	108.16	115.92
8	W	101	BCL	CMB-C2B-C3B	2.40	129.17	124.68
12	R	101	KGD	CBD-CAY-CBC	2.39	119.89	114.60
12	5	101	KGD	CBN-CBL-CBI	2.39	122.61	118.94
10	M	702	MQE	CBY-CAW-CAG	2.39	119.29	115.27
10	L	1004	MQE	CCE-CBK-CAX	-2.39	120.50	124.40
9	M	705	BPH	C17-C16-C15	2.39	124.21	113.24
10	L	1004	MQE	CBZ-CAZ-CAU	2.38	119.28	115.27
8	Q	102	BCL	O2A-C1-C2	-2.38	102.38	108.64
8	U	101	BCL	CMB-C2B-C3B	2.38	129.13	124.68
8	B	102	BCL	C16-C15-C13	2.37	123.58	115.92
8	E	102	BCL	C2A-C1A-CHA	2.37	128.00	123.86
8	0	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
12	5	101	KGD	CAS-CAT-CAX	-2.37	104.10	111.88
9	L	1003	BPH	O2D-CGD-CBD	2.37	113.99	111.00
8	K	101	BCL	C2A-C1A-CHA	2.37	128.00	123.86
9	M	704	BPH	CAA-CBA-CGA	2.36	120.16	113.25
8	4	101	BCL	CMB-C2B-C3B	2.35	129.08	124.68
8	O	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
8	8	102	BCL	CMB-C2B-C3B	2.35	129.08	124.68
8	4	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
8	4	101	BCL	C4B-C3B-CAB	-2.35	122.59	127.13
8	E	101	BCL	CBA-CAA-C2A	-2.35	106.93	113.86
12	5	101	KGD	CAF-CAB-CAD	2.34	114.10	110.30
8	E	102	BCL	C16-C15-C13	2.34	123.48	115.92
8	0	102	BCL	C1C-NC-C4C	2.34	107.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	705	BPH	C1-C2-C3	-2.33	122.01	126.04
8	2	101	BCL	C4B-C3B-CAB	-2.33	122.62	127.13
12	F	101	KGD	CBD-CAY-CBC	2.33	119.75	114.60
12	J	101	KGD	CBK-CBH-CBJ	-2.32	119.67	122.92
12	3	103	KGD	CBD-CAY-CBC	2.32	119.72	114.60
12	9	102	KGD	CBB-CBG-CBI	-2.32	118.73	123.47
8	4	101	BCL	C2D-C1D-ND	2.32	111.81	110.10
8	O	101	BCL	C11-C10-C8	-2.31	108.45	115.92
8	V	101	BCL	C4B-C3B-CAB	-2.31	122.66	127.13
8	G	101	BCL	CMB-C2B-C3B	2.31	129.00	124.68
8	8	101	BCL	C2A-C1A-CHA	2.31	127.90	123.86
11	C	504	HEM	CMC-C2C-C3C	2.31	129.00	124.68
8	0	102	BCL	C16-C15-C13	2.30	123.36	115.92
8	J	102	BCL	C2A-C1A-CHA	2.30	127.88	123.86
8	U	102	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
12	N	102	KGD	CAU-CAR-CAV	-2.30	119.71	122.92
11	C	503	HEM	CBD-CAD-C3D	-2.29	106.26	112.63
8	A	102	BCL	CMB-C2B-C3B	2.29	128.96	124.68
8	V	101	BCL	OB B-CAB-CBB	-2.29	115.02	120.17
12	T	102	KGD	CAK-CAH-CAD	-2.28	120.44	124.11
12	3	101	KGD	CAN-CAM-CAO	-2.28	119.73	122.92
8	U	101	BCL	C1-C2-C3	-2.28	122.11	126.04
8	M	703	BCL	C4B-C3B-CAB	-2.27	122.74	127.13
8	W	101	BCL	C16-C15-C13	2.26	123.24	115.92
11	C	501	HEM	CMC-C2C-C3C	2.26	128.91	124.68
8	Q	101	BCL	C1-C2-C3	-2.26	122.13	126.04
9	M	704	BPH	CMD-C2D-C3D	2.26	128.91	124.68
8	M	703	BCL	C11-C10-C8	-2.26	108.62	115.92
8	9	103	BCL	C17-C16-C15	2.26	123.60	113.24
8	N	103	BCL	C1-C2-C3	-2.25	122.15	126.04
8	2	102	BCL	CMB-C2B-C3B	2.24	128.88	124.68
8	7	101	BCL	OB B-CAB-CBB	-2.24	115.13	120.17
12	N	102	KGD	CBD-CAY-CBC	2.24	119.54	114.60
12	3	101	KGD	CBD-CAY-CBC	2.23	119.53	114.60
8	A	102	BCL	C17-C16-C15	2.22	123.44	113.24
12	9	101	KGD	CBD-CAY-CBC	2.22	119.51	114.60
8	5	102	BCL	C2A-C1A-CHA	2.22	127.74	123.86
8	0	102	BCL	C11-C10-C8	-2.22	108.75	115.92
11	C	502	HEM	CHB-C1B-NB	2.22	127.12	124.38
9	L	1003	BPH	C15-C13-C12	-2.21	100.50	112.13
11	C	502	HEM	C1B-NB-C4B	2.20	107.34	105.07
12	J	101	KGD	CBD-CAY-CBC	2.19	119.44	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	9	101	KGD	CBO-CBL-CBI	-2.19	119.86	122.92
12	9	101	KGD	CBJ-CBM-CBN	-2.18	116.40	123.22
12	H	102	KGD	CAQ-CAR-CAV	-2.18	115.59	118.94
10	M	702	MQE	CBL-CAY-CAX	2.16	117.87	112.05
8	K	101	BCL	C1C-NC-C4C	2.16	107.67	106.71
8	2	102	BCL	C11-C10-C8	2.15	122.88	115.92
9	M	705	BPH	O2D-CGD-CBD	2.15	113.72	111.00
11	C	502	HEM	C3B-C2B-C1B	2.15	108.08	106.49
8	V	101	BCL	OB B-CAB-C3B	2.15	123.80	119.99
10	M	702	MQE	CBU-CAQ-CAD	2.14	118.88	115.27
12	H	102	KGD	CBM-CBN-CBL	-2.14	120.39	126.42
8	G	102	BCL	C4B-C3B-CAB	-2.14	122.99	127.13
12	5	101	KGD	CAZ-CAW-CAS	2.14	118.88	115.27
8	G	101	BCL	C4B-C3B-CAB	-2.14	123.00	127.13
12	F	101	KGD	CBK-CBH-CBJ	-2.13	119.94	122.92
12	9	101	KGD	CBK-CBH-CBJ	-2.13	119.94	122.92
8	H	101	BCL	OB B-CAB-CBB	-2.13	115.37	120.17
11	C	502	HEM	CMC-C2C-C3C	2.13	128.66	124.68
8	A	102	BCL	C16-C15-C13	2.12	122.78	115.92
8	G	101	BCL	C11-C10-C8	2.12	122.78	115.92
12	H	102	KGD	CAN-CAM-CAL	2.12	121.42	118.08
12	T	101	KGD	CAU-CAR-CAV	-2.12	119.96	122.92
8	L	1001	BCL	CMB-C2B-C3B	2.11	128.63	124.68
12	J	101	KGD	CBJ-CBM-CBN	-2.11	116.62	123.22
11	C	502	HEM	CAA-CBA-CGA	-2.11	107.85	113.76
12	5	101	KGD	CBD-CAY-CBC	2.11	119.25	114.60
11	C	502	HEM	CMB-C2B-C1B	-2.11	121.83	125.04
11	C	504	HEM	C1B-NB-C4B	2.10	107.24	105.07
10	M	702	MQE	CBZ-CAZ-CBI	-2.10	118.29	123.68
8	R	102	BCL	C17-C16-C15	2.10	122.88	113.24
8	2	101	BCL	C1-C2-C3	-2.10	122.42	126.04
11	C	502	HEM	C4C-CHD-C1D	2.09	125.31	122.56
8	D	101	BCL	C11-C12-C13	-2.09	109.17	115.92
11	C	501	HEM	C4D-ND-C1D	2.08	107.22	105.07
8	G	101	BCL	C2A-C1A-CHA	2.08	127.49	123.86
8	S	102	BCL	C2D-C1D-ND	2.07	111.63	110.10
10	L	1004	MQE	CCA-CBB-CAN	2.07	118.76	115.27
12	3	101	KGD	CBK-CBH-CBJ	-2.07	120.02	122.92
12	N	101	KGD	CAN-CAM-CAO	-2.06	120.03	122.92
12	F	101	KGD	CAE-CAC-CAB	-2.05	109.88	113.18
12	F	101	KGD	CBJ-CBM-CBN	-2.05	116.81	123.22
8	8	102	BCL	C4B-C3B-CAB	-2.05	123.16	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	102	KGD	CAO-CAP-CAQ	-2.05	116.82	123.22
8	P	101	BCL	C1-C2-C3	-2.05	122.50	126.04
12	T	101	KGD	CAN-CAM-CAO	-2.05	120.06	122.92
8	W	102	BCL	C1-C2-C3	-2.05	122.50	126.04
12	3	103	KGD	CBO-CBL-CBI	-2.04	120.06	122.92
11	C	501	HEM	C4C-CHD-C1D	2.04	125.25	122.56
8	G	101	BCL	C1C-NC-C4C	2.04	107.62	106.71
8	B	102	BCL	C1-C2-C3	-2.03	122.52	126.04
8	S	102	BCL	C1C-NC-C4C	2.03	107.62	106.71
12	5	101	KGD	CAO-CAP-CAQ	-2.03	116.88	123.22
8	0	102	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
8	8	102	BCL	C4D-C3D-CAD	-2.02	105.71	108.10
12	9	101	KGD	CBN-CBL-CBI	2.02	122.05	118.94
8	G	101	BCL	C15-C13-C12	-2.02	101.49	112.13
9	M	704	BPH	C15-C13-C12	-2.02	101.49	112.13
8	K	102	BCL	C1-C2-C3	2.02	129.53	126.04
8	O	102	BCL	O2A-C1-C2	-2.02	103.34	108.64
8	Q	102	BCL	C1C-NC-C4C	2.02	107.61	106.71
12	J	101	KGD	CAU-CAR-CAQ	2.01	121.25	118.08
8	Q	101	BCL	C11-C10-C8	-2.01	109.42	115.92
8	N	103	BCL	OBG-CAB-CBB	-2.01	115.64	120.17
11	C	503	HEM	CHD-C1D-ND	2.01	126.62	124.43
8	R	102	BCL	CED-O2D-CGD	2.01	120.48	115.94
8	6	101	BCL	C16-C17-C18	-2.01	106.53	115.98
12	R	101	KGD	CAN-CAM-CAL	2.00	121.24	118.08
8	U	102	BCL	C11-C10-C8	-2.00	109.44	115.92
12	J	101	KGD	CBN-CBL-CBI	2.00	122.01	118.94
8	R	102	BCL	OBG-CAB-CBB	-2.00	115.67	120.17

There are no chirality outliers.

All (435) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	101	BCL	CHA-CBD-CGD-O1D
8	E	101	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	C2-C3-C5-C6
8	E	101	BCL	C4-C3-C5-C6
8	E	102	BCL	CAD-CBD-CGD-O1D
8	E	102	BCL	CAD-CBD-CGD-O2D
8	B	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C4C-C3C-CAC-CBC
8	B	101	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	B	101	BCL	CHA-CBD-CGD-O2D
8	B	101	BCL	C2-C3-C5-C6
8	B	101	BCL	C4-C3-C5-C6
8	B	102	BCL	CHA-CBD-CGD-O1D
8	B	102	BCL	CHA-CBD-CGD-O2D
8	0	101	BCL	C2C-C3C-CAC-CBC
8	0	101	BCL	C4C-C3C-CAC-CBC
8	0	101	BCL	CHA-CBD-CGD-O1D
8	0	101	BCL	CHA-CBD-CGD-O2D
8	0	102	BCL	C2C-C3C-CAC-CBC
8	0	102	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	CHA-CBD-CGD-O1D
8	0	102	BCL	CHA-CBD-CGD-O2D
8	0	102	BCL	CAD-CBD-CGD-O1D
8	0	102	BCL	C2-C3-C5-C6
8	0	102	BCL	C4-C3-C5-C6
8	L	1001	BCL	C1A-C2A-CAA-CBA
8	L	1001	BCL	C4C-C3C-CAC-CBC
8	L	1001	BCL	CHA-CBD-CGD-O1D
8	L	1001	BCL	CHA-CBD-CGD-O2D
8	8	101	BCL	CHA-CBD-CGD-O1D
8	8	101	BCL	CHA-CBD-CGD-O2D
8	8	102	BCL	C2A-CAA-CBA-CGA
8	8	102	BCL	C2C-C3C-CAC-CBC
8	8	102	BCL	C4C-C3C-CAC-CBC
8	8	102	BCL	CAD-CBD-CGD-O1D
8	8	102	BCL	CAD-CBD-CGD-O2D
8	8	102	BCL	C2-C3-C5-C6
8	8	102	BCL	C4-C3-C5-C6
8	6	101	BCL	CHA-CBD-CGD-O1D
8	6	101	BCL	CHA-CBD-CGD-O2D
8	6	101	BCL	C2-C3-C5-C6
8	6	101	BCL	C4-C3-C5-C6
8	6	102	BCL	C4C-C3C-CAC-CBC
8	6	102	BCL	CHA-CBD-CGD-O1D
8	6	102	BCL	CHA-CBD-CGD-O2D
8	6	102	BCL	CAD-CBD-CGD-O1D
8	6	102	BCL	CAD-CBD-CGD-O2D
8	4	101	BCL	C4C-C3C-CAC-CBC
8	4	101	BCL	CHA-CBD-CGD-O1D
8	4	101	BCL	CHA-CBD-CGD-O2D
8	4	102	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	4	102	BCL	C4C-C3C-CAC-CBC
8	4	102	BCL	CHA-CBD-CGD-O1D
8	4	102	BCL	CHA-CBD-CGD-O2D
8	2	101	BCL	CHA-CBD-CGD-O1D
8	2	101	BCL	CHA-CBD-CGD-O2D
8	2	102	BCL	C2C-C3C-CAC-CBC
8	2	102	BCL	C4C-C3C-CAC-CBC
8	2	102	BCL	C2-C3-C5-C6
8	2	102	BCL	C4-C3-C5-C6
8	K	102	BCL	O2A-C1-C2-C3
8	I	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C4C-C3C-CAC-CBC
8	G	101	BCL	C2-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
8	G	102	BCL	CAD-CBD-CGD-O1D
8	G	102	BCL	CAD-CBD-CGD-O2D
8	W	101	BCL	C2-C3-C5-C6
8	W	102	BCL	C2-C3-C5-C6
8	W	102	BCL	C4-C3-C5-C6
8	U	102	BCL	CHA-CBD-CGD-O1D
8	U	102	BCL	CHA-CBD-CGD-O2D
8	U	102	BCL	CAD-CBD-CGD-O1D
8	T	103	BCL	C2-C3-C5-C6
8	T	103	BCL	C4-C3-C5-C6
8	S	101	BCL	CHA-CBD-CGD-O1D
8	S	101	BCL	CHA-CBD-CGD-O2D
8	Q	101	BCL	CHA-CBD-CGD-O1D
8	Q	101	BCL	CHA-CBD-CGD-O2D
8	Q	102	BCL	C1A-C2A-CAA-CBA
8	Q	102	BCL	C2C-C3C-CAC-CBC
8	Q	102	BCL	C4C-C3C-CAC-CBC
8	O	101	BCL	CHA-CBD-CGD-O1D
8	O	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C4C-C3C-CAC-CBC
8	O	102	BCL	CHA-CBD-CGD-O1D
8	O	102	BCL	CHA-CBD-CGD-O2D
8	R	102	BCL	C2C-C3C-CAC-CBC
8	R	102	BCL	C2-C3-C5-C6
8	R	102	BCL	C4-C3-C5-C6
8	P	101	BCL	CHA-CBD-CGD-O1D
8	P	101	BCL	CHA-CBD-CGD-O2D
8	N	103	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	N	103	BCL	C4C-C3C-CAC-CBC
8	N	103	BCL	CHA-CBD-CGD-O1D
8	N	103	BCL	CHA-CBD-CGD-O2D
8	N	103	BCL	C2-C3-C5-C6
8	N	103	BCL	C4-C3-C5-C6
8	J	102	BCL	C2-C3-C5-C6
8	J	102	BCL	C4-C3-C5-C6
8	F	102	BCL	C2C-C3C-CAC-CBC
8	F	102	BCL	C4C-C3C-CAC-CBC
8	F	102	BCL	CHA-CBD-CGD-O1D
8	F	102	BCL	CHA-CBD-CGD-O2D
8	A	102	BCL	C2C-C3C-CAC-CBC
8	A	102	BCL	C4C-C3C-CAC-CBC
8	9	103	BCL	CHA-CBD-CGD-O1D
8	9	103	BCL	CHA-CBD-CGD-O2D
8	7	101	BCL	C2C-C3C-CAC-CBC
8	7	101	BCL	C4C-C3C-CAC-CBC
8	7	101	BCL	CHA-CBD-CGD-O1D
8	7	101	BCL	CHA-CBD-CGD-O2D
8	1	101	BCL	C2C-C3C-CAC-CBC
8	1	101	BCL	C4C-C3C-CAC-CBC
8	1	101	BCL	CHA-CBD-CGD-O1D
8	1	101	BCL	CHA-CBD-CGD-O2D
8	1	101	BCL	C2-C3-C5-C6
8	1	101	BCL	C4-C3-C5-C6
9	M	704	BPH	C3A-C2A-CAA-CBA
10	L	1004	MQE	CAO-CAH-CAV-CBF
10	L	1004	MQE	CAO-CAH-CAV-CBX
10	L	1004	MQE	CCB-CCC-CCD-CCI
10	L	1004	MQE	CCL-CCC-CCD-CCI
10	M	702	MQE	CAJ-CAD-CAQ-CBE
10	M	702	MQE	CAJ-CAD-CAQ-CBU
10	M	702	MQE	CAL-CAE-CAR-CBD
10	M	702	MQE	CAL-CAE-CAR-CBV
10	M	702	MQE	CAS-CAN-CBB-CBL
10	M	702	MQE	CAS-CAN-CBB-CCA
11	C	504	HEM	C1A-C2A-CAA-CBA
11	C	504	HEM	C3A-C2A-CAA-CBA
12	H	102	KGD	CAS-CAT-CAX-CAY
8	4	101	BCL	C4-C3-C5-C6
8	H	101	BCL	C4-C3-C5-C6
8	5	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	L	1004	MQE	CAK-CAF-CAT-CBW
10	L	1004	MQE	CAM-CAG-CAW-CBY
10	M	702	MQE	CCL-CCC-CCD-CCI
8	H	101	BCL	C2-C3-C5-C6
10	L	1004	MQE	CAM-CAG-CAW-CBH
8	4	102	BCL	C2A-CAA-CBA-CGA
8	K	102	BCL	C2A-CAA-CBA-CGA
8	L	1002	BCL	C4-C3-C5-C6
8	8	101	BCL	C4-C3-C5-C6
8	Q	101	BCL	C4-C3-C5-C6
8	L	1002	BCL	C2-C3-C5-C6
8	8	101	BCL	C2-C3-C5-C6
8	Q	101	BCL	C2-C3-C5-C6
8	O	102	BCL	C2A-CAA-CBA-CGA
8	K	102	BCL	C10-C11-C12-C13
8	3	102	BCL	C4-C3-C5-C6
8	M	703	BCL	C4-C3-C5-C6
8	4	101	BCL	C2-C3-C5-C6
10	L	1004	MQE	CAK-CAF-CAT-CBG
8	S	101	BCL	C6-C7-C8-C9
8	O	102	BCL	C6-C7-C8-C9
8	5	102	BCL	C14-C13-C15-C16
8	B	101	BCL	C15-C16-C17-C18
8	L	1002	BCL	C5-C6-C7-C8
8	B	102	BCL	C10-C11-C12-C13
10	M	702	MQE	CBO-CBJ-CBM-CCF
8	I	102	BCL	C12-C13-C15-C16
8	F	102	BCL	C6-C7-C8-C10
8	4	101	BCL	C2A-CAA-CBA-CGA
8	O	101	BCL	C13-C15-C16-C17
10	M	702	MQE	CCB-CCC-CCD-CCI
8	A	102	BCL	C4-C3-C5-C6
8	9	103	BCL	C4-C3-C5-C6
10	M	702	MQE	CAM-CAG-CAW-CBY
8	5	102	BCL	C2-C3-C5-C6
8	2	102	BCL	C2A-CAA-CBA-CGA
8	L	1001	BCL	C3A-C2A-CAA-CBA
8	9	103	BCL	C2-C3-C5-C6
10	M	702	MQE	CAM-CAG-CAW-CBH
10	M	702	MQE	CBO-CBJ-CBM-CBN
10	M	702	MQE	CBA-CAU-CAZ-CBZ
8	A	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	3	102	BCL	C2-C3-C5-C6
8	U	102	BCL	C2A-CAA-CBA-CGA
8	8	102	BCL	C13-C15-C16-C17
8	K	102	BCL	C4-C3-C5-C6
8	W	101	BCL	C4-C3-C5-C6
8	M	703	BCL	C2-C3-C5-C6
10	M	702	MQE	CBA-CAU-CAZ-CBI
8	E	102	BCL	C13-C15-C16-C17
8	O	102	BCL	C4-C3-C5-C6
8	E	102	BCL	C2C-C3C-CAC-CBC
8	B	102	BCL	C2C-C3C-CAC-CBC
8	L	1001	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C2C-C3C-CAC-CBC
8	4	101	BCL	C2C-C3C-CAC-CBC
8	K	102	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C2A-CAA-CBA-CGA
10	M	702	MQE	CBK-CAX-CAY-CBL
8	0	102	BCL	C10-C11-C12-C13
8	2	101	BCL	C13-C15-C16-C17
8	G	102	BCL	C10-C11-C12-C13
10	M	702	MQE	CBQ-CAX-CAY-CBL
8	S	101	BCL	C5-C6-C7-C8
8	S	102	BCL	C5-C6-C7-C8
8	G	102	BCL	C5-C6-C7-C8
8	L	1001	BCL	C4-C3-C5-C6
8	L	1001	BCL	C2-C3-C5-C6
8	L	1001	BCL	C11-C10-C8-C7
8	2	102	BCL	C11-C10-C8-C7
8	I	102	BCL	C11-C12-C13-C15
8	O	102	BCL	C2-C3-C5-C6
9	L	1003	BPH	C6-C7-C8-C10
8	S	101	BCL	C11-C10-C8-C9
8	Q	102	BCL	C6-C7-C8-C9
8	K	101	BCL	C16-C17-C18-C19
8	4	102	BCL	C4-C3-C5-C6
12	5	101	KGD	CAT-CAS-CAW-CAZ
12	5	101	KGD	CAT-CAS-CAW-CBA
8	K	101	BCL	C16-C17-C18-C20
8	S	102	BCL	O2A-C1-C2-C3
8	G	102	BCL	C13-C15-C16-C17
9	M	705	BPH	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	8	102	BCL	C2-C1-O2A-CGA
8	A	102	BCL	C2-C1-O2A-CGA
8	3	102	BCL	C2-C1-O2A-CGA
8	K	101	BCL	C11-C10-C8-C9
8	W	102	BCL	C10-C11-C12-C13
8	E	102	BCL	C4C-C3C-CAC-CBC
8	B	102	BCL	C4C-C3C-CAC-CBC
8	K	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C4C-C3C-CAC-CBC
8	S	102	BCL	C4C-C3C-CAC-CBC
8	R	102	BCL	C4C-C3C-CAC-CBC
8	I	102	BCL	C5-C6-C7-C8
8	S	101	BCL	C11-C10-C8-C7
8	D	101	BCL	C12-C13-C15-C16
8	A	102	BCL	C8-C10-C11-C12
8	6	101	BCL	C8-C10-C11-C12
9	L	1003	BPH	C8-C10-C11-C12
11	C	501	HEM	C2A-CAA-CBA-CGA
8	U	102	BCL	CAD-CBD-CGD-O2D
10	L	1004	MQE	CBO-CBJ-CBM-CCF
8	L	1001	BCL	C10-C11-C12-C13
8	O	101	BCL	CHA-CBD-CGD-O2D
8	F	102	BCL	C6-C7-C8-C9
8	4	101	BCL	C1A-C2A-CAA-CBA
8	K	102	BCL	C2-C3-C5-C6
10	M	702	MQE	CAX-CAY-CBL-CBB
8	4	102	BCL	CAD-CBD-CGD-O1D
8	I	102	BCL	CAD-CBD-CGD-O1D
8	Q	102	BCL	CAD-CBD-CGD-O1D
8	Q	102	BCL	C13-C15-C16-C17
8	8	102	BCL	C6-C7-C8-C10
8	S	101	BCL	C6-C7-C8-C10
8	S	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C6-C7-C8-C10
8	5	102	BCL	C12-C13-C15-C16
11	C	502	HEM	C2A-CAA-CBA-CGA
8	E	102	BCL	O2A-C1-C2-C3
9	L	1003	BPH	O2A-C1-C2-C3
8	D	101	BCL	C4-C3-C5-C6
8	0	101	BCL	C15-C16-C17-C18
8	L	1001	BCL	C11-C10-C8-C9
8	2	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	I	102	BCL	C11-C12-C13-C14
8	I	102	BCL	C14-C13-C15-C16
8	D	101	BCL	C14-C13-C15-C16
8	A	102	BCL	C14-C13-C15-C16
9	L	1003	BPH	C6-C7-C8-C9
8	E	102	BCL	C10-C11-C12-C13
10	L	1004	MQE	CBO-CBJ-CBM-CBN
8	3	102	BCL	C13-C15-C16-C17
8	I	102	BCL	C2-C1-O2A-CGA
9	M	704	BPH	CHA-CBD-CGD-O1D
9	M	704	BPH	CHA-CBD-CGD-O2D
8	2	101	BCL	C11-C12-C13-C15
8	J	102	BCL	C11-C10-C8-C7
8	8	102	BCL	C6-C7-C8-C9
8	J	102	BCL	C11-C10-C8-C9
12	3	101	KGD	CAT-CAS-CAW-CAZ
8	4	102	BCL	C2-C3-C5-C6
8	W	102	BCL	C8-C10-C11-C12
8	U	102	BCL	C2-C1-O2A-CGA
8	N	103	BCL	C2-C1-O2A-CGA
8	F	102	BCL	C2-C1-O2A-CGA
8	E	101	BCL	C15-C16-C17-C18
8	4	101	BCL	C3A-C2A-CAA-CBA
8	Q	102	BCL	C3A-C2A-CAA-CBA
8	H	101	BCL	C16-C17-C18-C19
8	I	102	BCL	CAA-CBA-CGA-O2A
8	8	102	BCL	C14-C13-C15-C16
8	4	101	BCL	C6-C7-C8-C9
8	P	101	BCL	C11-C12-C13-C14
8	N	103	BCL	C6-C7-C8-C9
8	N	103	BCL	C11-C10-C8-C9
8	5	102	BCL	C6-C7-C8-C9
8	H	101	BCL	C16-C17-C18-C20
8	4	102	BCL	O2A-C1-C2-C3
8	G	102	BCL	O2A-C1-C2-C3
8	U	102	BCL	O2A-C1-C2-C3
8	L	1002	BCL	C6-C7-C8-C10
8	4	101	BCL	C6-C7-C8-C10
8	W	102	BCL	C11-C10-C8-C7
8	N	103	BCL	C6-C7-C8-C10
8	2	102	BCL	C5-C6-C7-C8
8	L	1002	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	E	102	BCL	C5-C6-C7-C8
8	U	101	BCL	C4-C3-C5-C6
12	A	101	KGD	CAT-CAS-CAW-CAZ
8	D	101	BCL	C2-C3-C5-C6
11	C	502	HEM	C3D-CAD-CBD-CGD
8	4	102	BCL	C5-C6-C7-C8
8	B	102	BCL	C4-C3-C5-C6
8	0	101	BCL	C2-C1-O2A-CGA
8	2	102	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C2-C1-O2A-CGA
8	5	102	BCL	C2-C1-O2A-CGA
12	3	101	KGD	CAT-CAS-CAW-CBA
8	E	101	BCL	CAA-CBA-CGA-O2A
8	G	102	BCL	C4-C3-C5-C6
10	M	702	MQE	CAK-CAF-CAT-CBW
12	R	101	KGD	CAT-CAS-CAW-CAZ
12	9	102	KGD	CAT-CAS-CAW-CAZ
8	U	102	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	CAA-CBA-CGA-O2A
8	R	102	BCL	C10-C11-C12-C13
8	P	101	BCL	C4-C3-C5-C6
12	R	101	KGD	CAT-CAS-CAW-CBA
8	U	101	BCL	CAA-CBA-CGA-O2A
8	E	102	BCL	C4-C3-C5-C6
8	S	101	BCL	C4-C3-C5-C6
10	L	1004	MQE	CAJ-CAD-CAQ-CBU
12	9	101	KGD	CAT-CAS-CAW-CAZ
8	8	101	BCL	CAA-CBA-CGA-O2A
8	E	102	BCL	C6-C7-C8-C9
8	2	102	BCL	C11-C10-C8-C9
8	R	102	BCL	C11-C12-C13-C14
8	H	101	BCL	C11-C12-C13-C14
8	9	103	BCL	C11-C12-C13-C14
9	M	704	BPH	C6-C7-C8-C9
8	Q	101	BCL	C3-C5-C6-C7
8	0	102	BCL	CAD-CBD-CGD-O2D
8	W	102	BCL	CAD-CBD-CGD-O2D
8	S	102	BCL	CAD-CBD-CGD-O2D
8	5	102	BCL	CAD-CBD-CGD-O2D
8	M	703	BCL	CAD-CBD-CGD-O2D
8	E	101	BCL	C2A-CAA-CBA-CGA
8	4	102	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	T	102	KGD	CAT-CAS-CAW-CAZ
12	N	102	KGD	CAT-CAS-CAW-CAZ
12	A	101	KGD	CAT-CAS-CAW-CBA
8	B	102	BCL	CAA-CBA-CGA-O2A
8	T	103	BCL	CAA-CBA-CGA-O2A
8	7	101	BCL	CAA-CBA-CGA-O2A
8	2	101	BCL	C8-C10-C11-C12
8	B	101	BCL	CAA-CBA-CGA-O2A
8	0	101	BCL	CAA-CBA-CGA-O2A
8	D	101	BCL	CAA-CBA-CGA-O2A
8	9	103	BCL	CAA-CBA-CGA-O2A
8	6	102	BCL	O2A-C1-C2-C3
9	M	704	BPH	O2A-C1-C2-C3
8	R	102	BCL	CAA-CBA-CGA-O2A
9	M	705	BPH	C16-C17-C18-C19
8	G	102	BCL	CHA-CBD-CGD-O1D
8	G	102	BCL	CHA-CBD-CGD-O2D
8	U	101	BCL	CHA-CBD-CGD-O1D
8	U	101	BCL	CHA-CBD-CGD-O2D
8	A	102	BCL	CHA-CBD-CGD-O1D
8	A	102	BCL	CHA-CBD-CGD-O2D
12	3	103	KGD	CAT-CAS-CAW-CAZ
12	9	102	KGD	CAT-CAS-CAW-CBA
8	Q	102	BCL	CAA-CBA-CGA-O2A
8	V	101	BCL	CAA-CBA-CGA-O2A
8	F	102	BCL	C13-C15-C16-C17
8	K	101	BCL	CAA-CBA-CGA-O2A
8	W	102	BCL	CAA-CBA-CGA-O2A
8	E	102	BCL	C6-C7-C8-C10
8	7	101	BCL	C6-C7-C8-C10
9	M	704	BPH	C6-C7-C8-C10
8	M	703	BCL	CAA-CBA-CGA-O2A
9	L	1003	BPH	CAA-CBA-CGA-O2A
8	B	102	BCL	C14-C13-C15-C16
8	6	101	BCL	C6-C7-C8-C9
8	W	102	BCL	C14-C13-C15-C16
8	V	101	BCL	C6-C7-C8-C9
8	F	102	BCL	C14-C13-C15-C16
8	Q	102	BCL	C5-C6-C7-C8
8	Q	101	BCL	CAA-CBA-CGA-O2A
8	S	102	BCL	C4-C3-C5-C6
8	T	103	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	7	101	BCL	CAA-CBA-CGA-O1A
8	4	102	BCL	C1A-C2A-CAA-CBA
8	O	101	BCL	C1A-C2A-CAA-CBA
8	B	102	BCL	CAA-CBA-CGA-O1A
8	9	103	BCL	CAA-CBA-CGA-O1A
8	I	102	BCL	C15-C16-C17-C18
8	B	101	BCL	CAA-CBA-CGA-O1A
8	8	101	BCL	CAA-CBA-CGA-O1A
8	U	101	BCL	CAA-CBA-CGA-O1A
8	R	102	BCL	CAA-CBA-CGA-O1A
8	G	101	BCL	C16-C17-C18-C19
8	0	101	BCL	CAA-CBA-CGA-O1A
9	L	1003	BPH	C4-C3-C5-C6
8	4	102	BCL	CAA-CBA-CGA-O1A
8	D	101	BCL	CAA-CBA-CGA-O1A
8	M	703	BCL	CAA-CBA-CGA-O1A
8	F	102	BCL	CAA-CBA-CGA-O2A
9	L	1003	BPH	CAA-CBA-CGA-O1A
8	2	102	BCL	CAA-CBA-CGA-O2A
8	S	101	BCL	CAA-CBA-CGA-O2A
8	Q	102	BCL	CAA-CBA-CGA-O1A
12	H	102	KGD	CAT-CAS-CAW-CAZ
8	F	102	BCL	C10-C11-C12-C13
8	2	102	BCL	CAD-CBD-CGD-O1D
8	A	102	BCL	CAD-CBD-CGD-O1D
8	2	101	BCL	C11-C10-C8-C9
8	W	101	BCL	C11-C10-C8-C9
8	R	102	BCL	C11-C10-C8-C9
8	7	101	BCL	C6-C7-C8-C9
8	G	101	BCL	CAA-CBA-CGA-O2A
8	I	102	BCL	C10-C11-C12-C13
8	W	102	BCL	CAA-CBA-CGA-O1A
8	B	102	BCL	C2-C3-C5-C6
8	0	101	BCL	C11-C10-C8-C7
8	6	101	BCL	C6-C7-C8-C10
8	W	102	BCL	C6-C7-C8-C10
8	W	102	BCL	C12-C13-C15-C16
8	V	101	BCL	C6-C7-C8-C10
8	F	102	BCL	C12-C13-C15-C16
8	A	102	BCL	C12-C13-C15-C16
10	L	1004	MQE	CAJ-CAD-CAQ-CBE
8	L	1002	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
8	Q	101	BCL	CAA-CBA-CGA-O1A
8	V	101	BCL	CAA-CBA-CGA-O1A
8	A	102	BCL	C10-C11-C12-C13
8	W	101	BCL	CAA-CBA-CGA-O2A
8	9	103	BCL	C8-C10-C11-C12
8	L	1002	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

64 monomers are involved in 335 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	103	BCL	3	0
8	S	102	BCL	5	0
8	W	101	BCL	4	0
8	V	101	BCL	4	0
8	D	101	BCL	2	0
12	N	102	KGD	1	0
8	R	102	BCL	6	0
11	C	502	HEM	5	0
8	P	101	BCL	1	0
12	3	103	KGD	6	0
8	G	102	BCL	5	0
8	E	101	BCL	4	0
8	J	102	BCL	4	0
8	6	101	BCL	7	0
8	G	101	BCL	7	0
12	R	101	KGD	1	0
8	O	101	BCL	6	0
8	L	1001	BCL	12	0
8	F	102	BCL	4	0
8	K	101	BCL	4	0
8	U	102	BCL	9	0
8	2	102	BCL	6	0
8	8	101	BCL	5	0
8	W	102	BCL	13	0
8	N	103	BCL	3	0
11	C	501	HEM	10	0
8	6	102	BCL	11	0
8	2	101	BCL	6	0
8	U	101	BCL	3	0
8	H	101	BCL	7	0
8	E	102	BCL	4	0

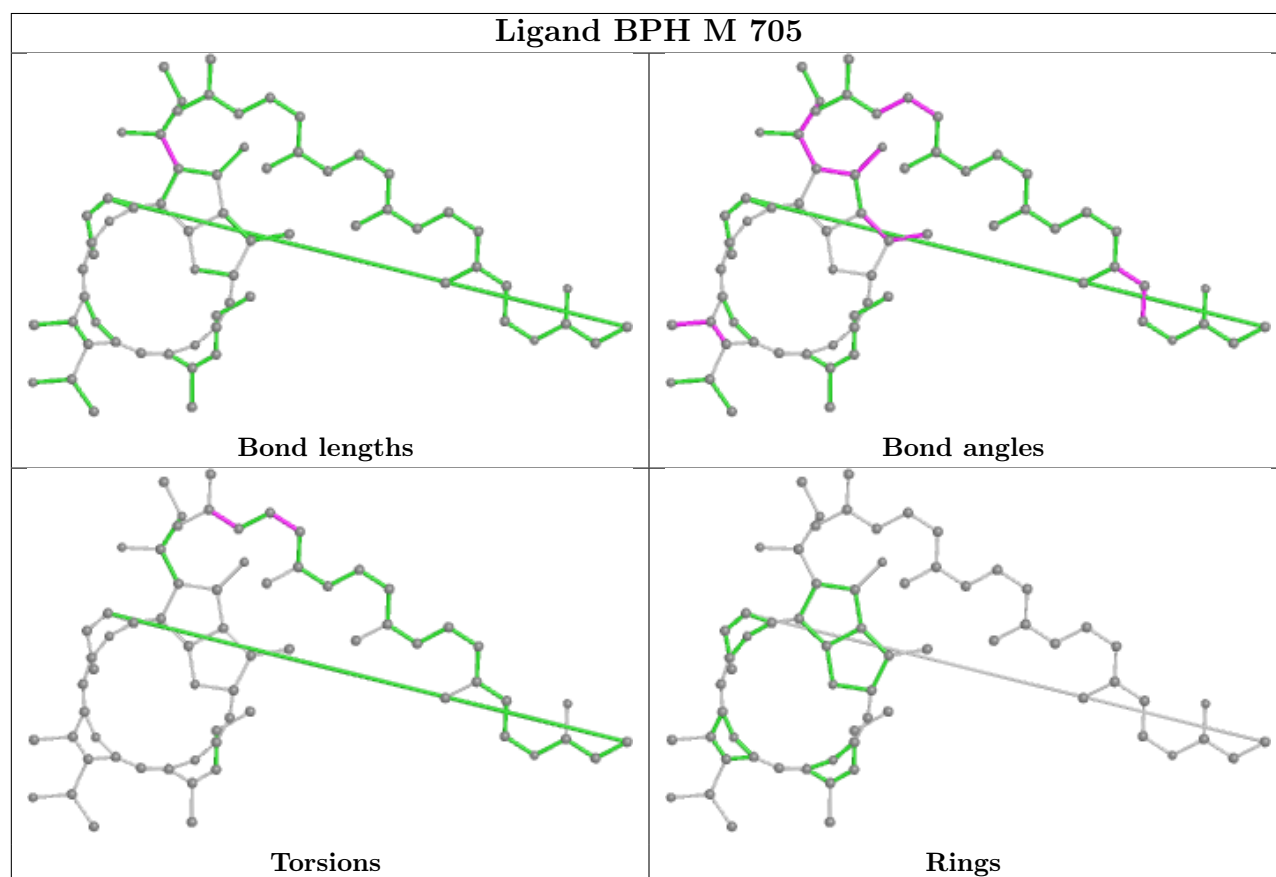
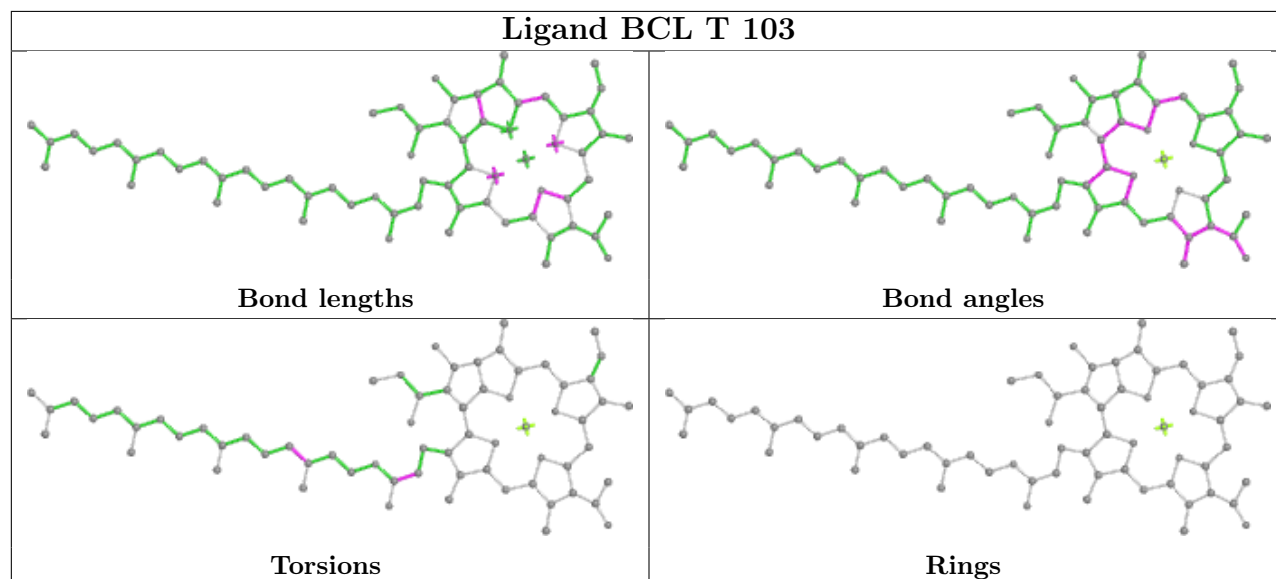
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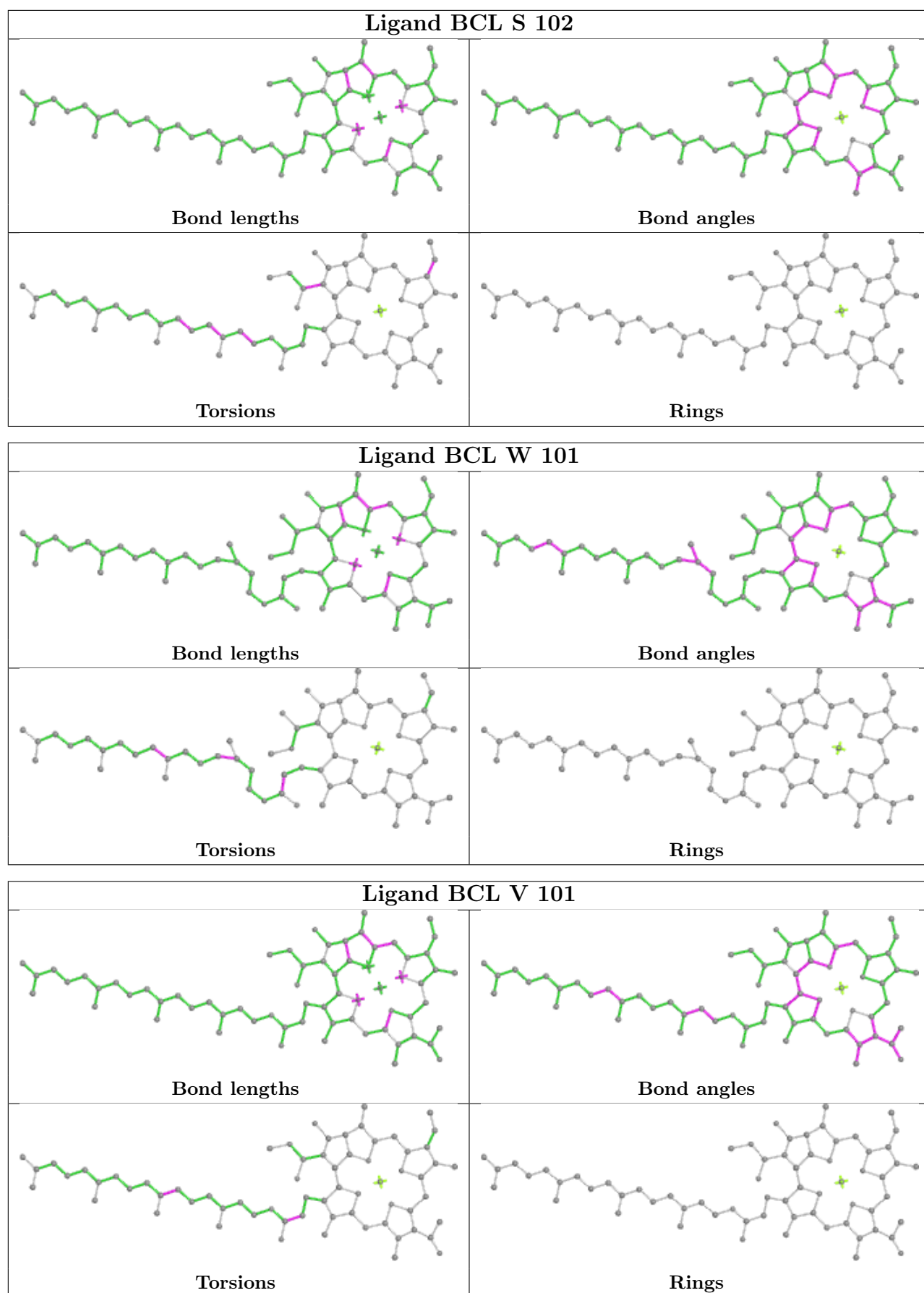
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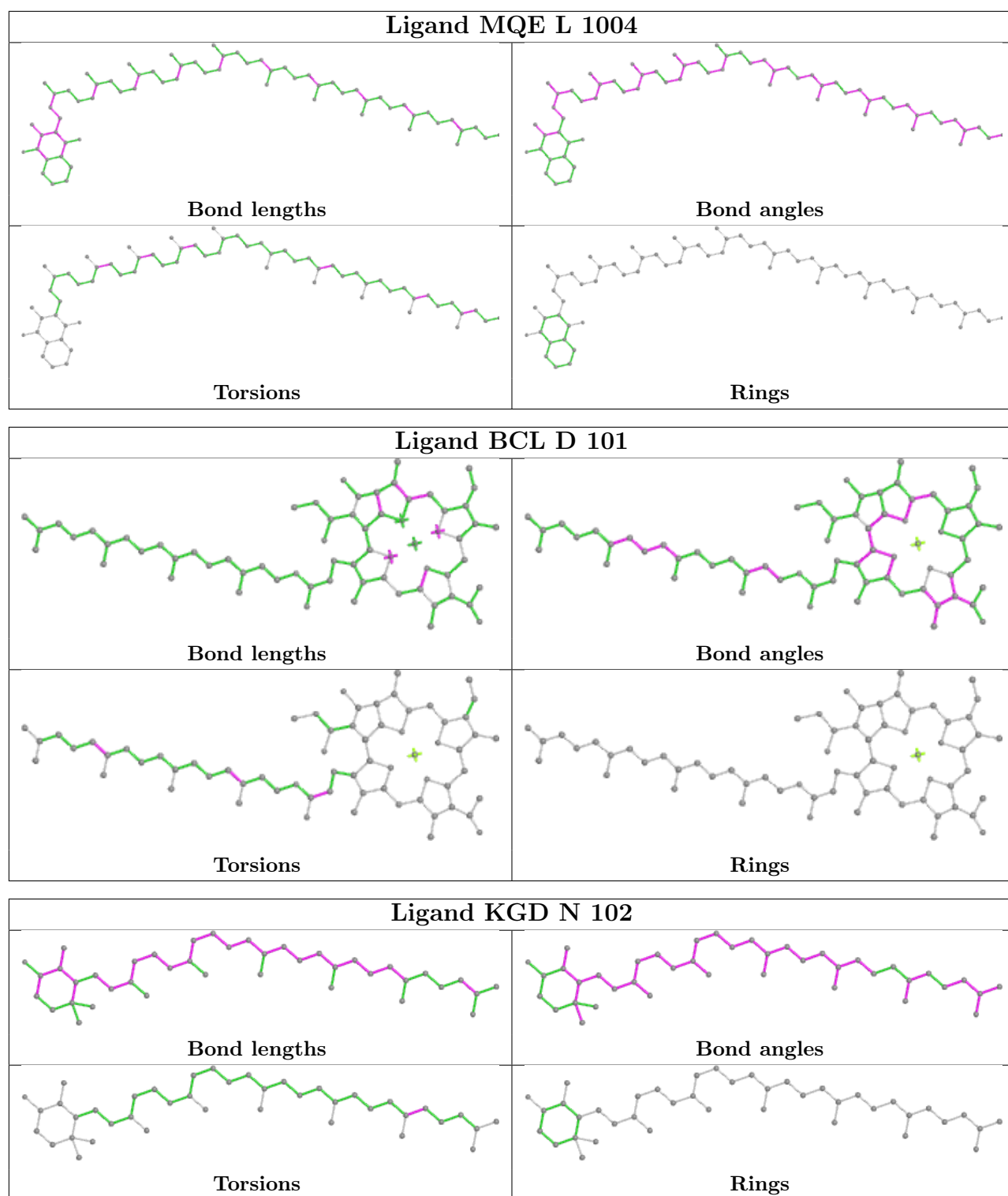
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	101	KGD	2	0
8	4	102	BCL	5	0
12	A	101	KGD	1	0
12	9	102	KGD	1	0
8	K	102	BCL	15	0
9	L	1003	BPH	7	0
11	C	503	HEM	5	0
8	0	101	BCL	7	0
8	7	101	BCL	7	0
8	B	102	BCL	24	0
8	S	101	BCL	6	0
12	F	101	KGD	3	0
8	5	102	BCL	3	0
8	Q	101	BCL	4	0
8	9	103	BCL	2	0
8	I	102	BCL	15	0
8	1	101	BCL	4	0
8	O	102	BCL	5	0
12	T	101	KGD	1	0
12	H	102	KGD	5	0
8	3	102	BCL	4	0
8	B	101	BCL	6	0
8	8	102	BCL	9	0
8	M	703	BCL	5	0
8	0	102	BCL	4	0
8	Q	102	BCL	10	0
10	M	702	MQE	3	0
8	I	101	BCL	4	0
9	M	704	BPH	2	0
8	4	101	BCL	6	0
8	A	102	BCL	5	0
11	C	504	HEM	11	0
8	L	1002	BCL	8	0

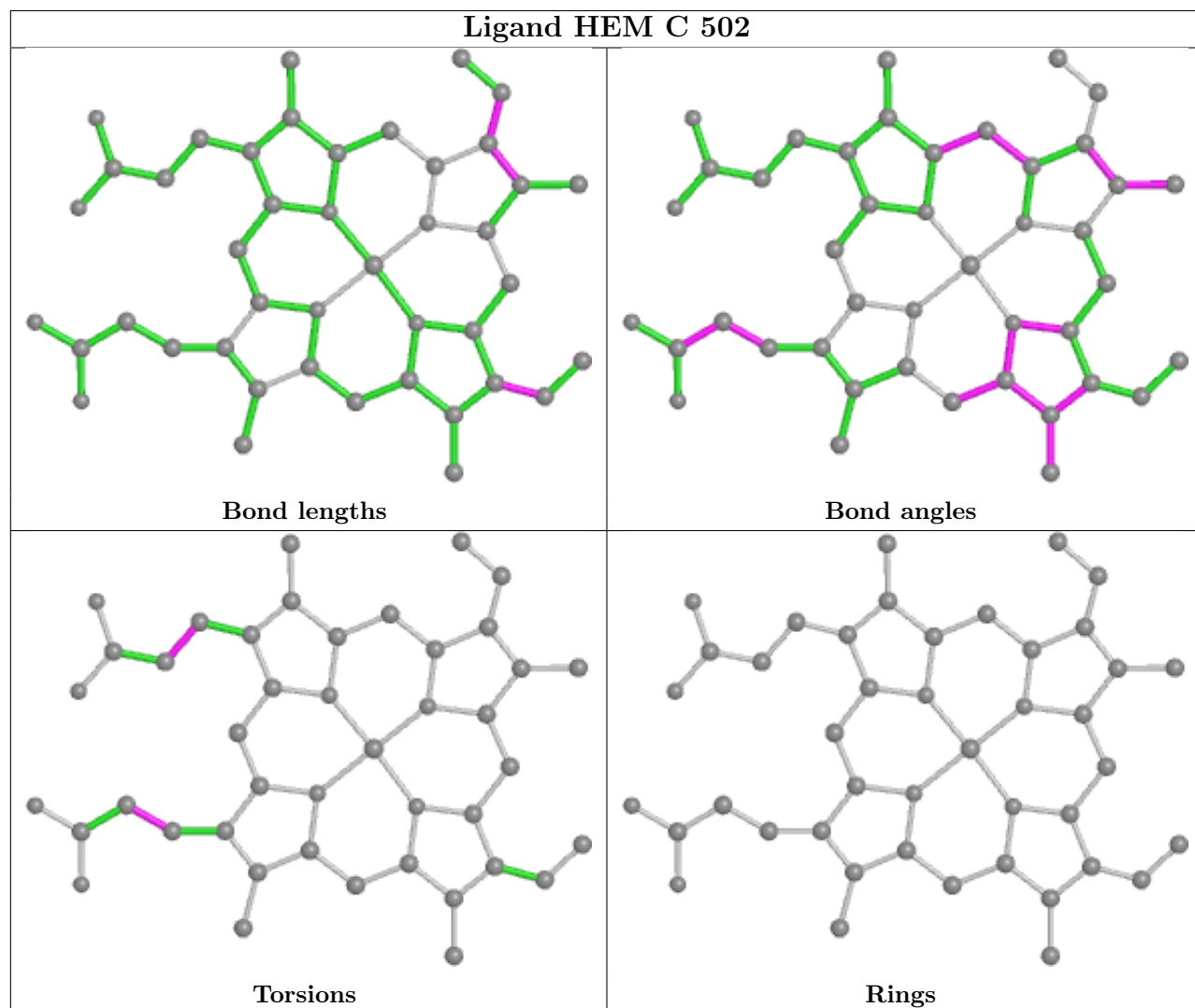
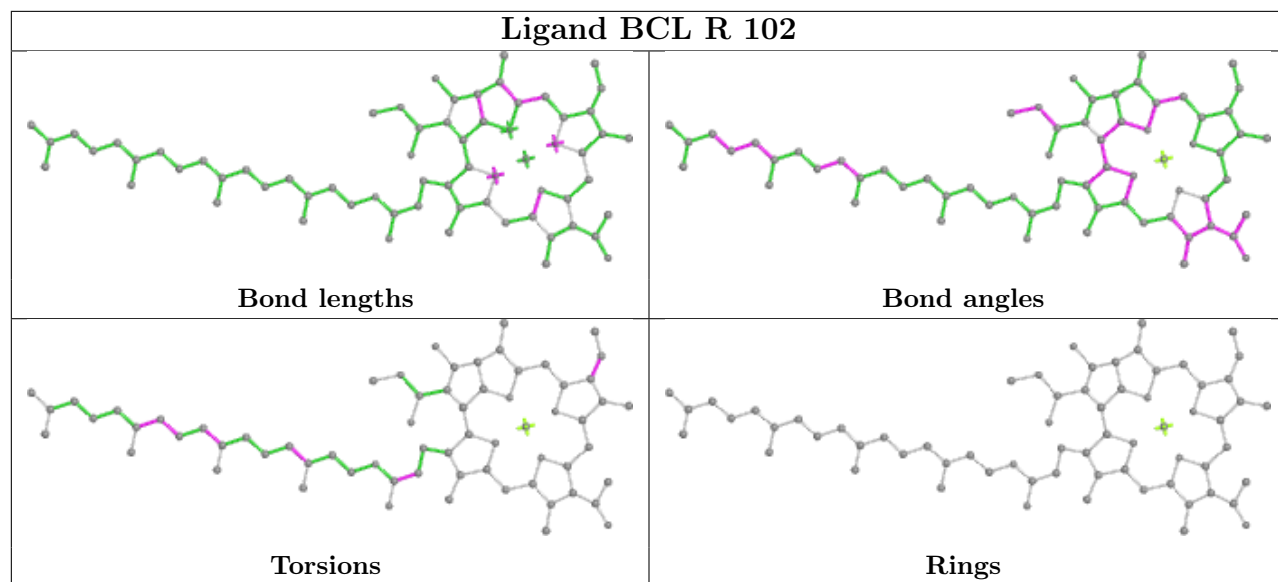
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

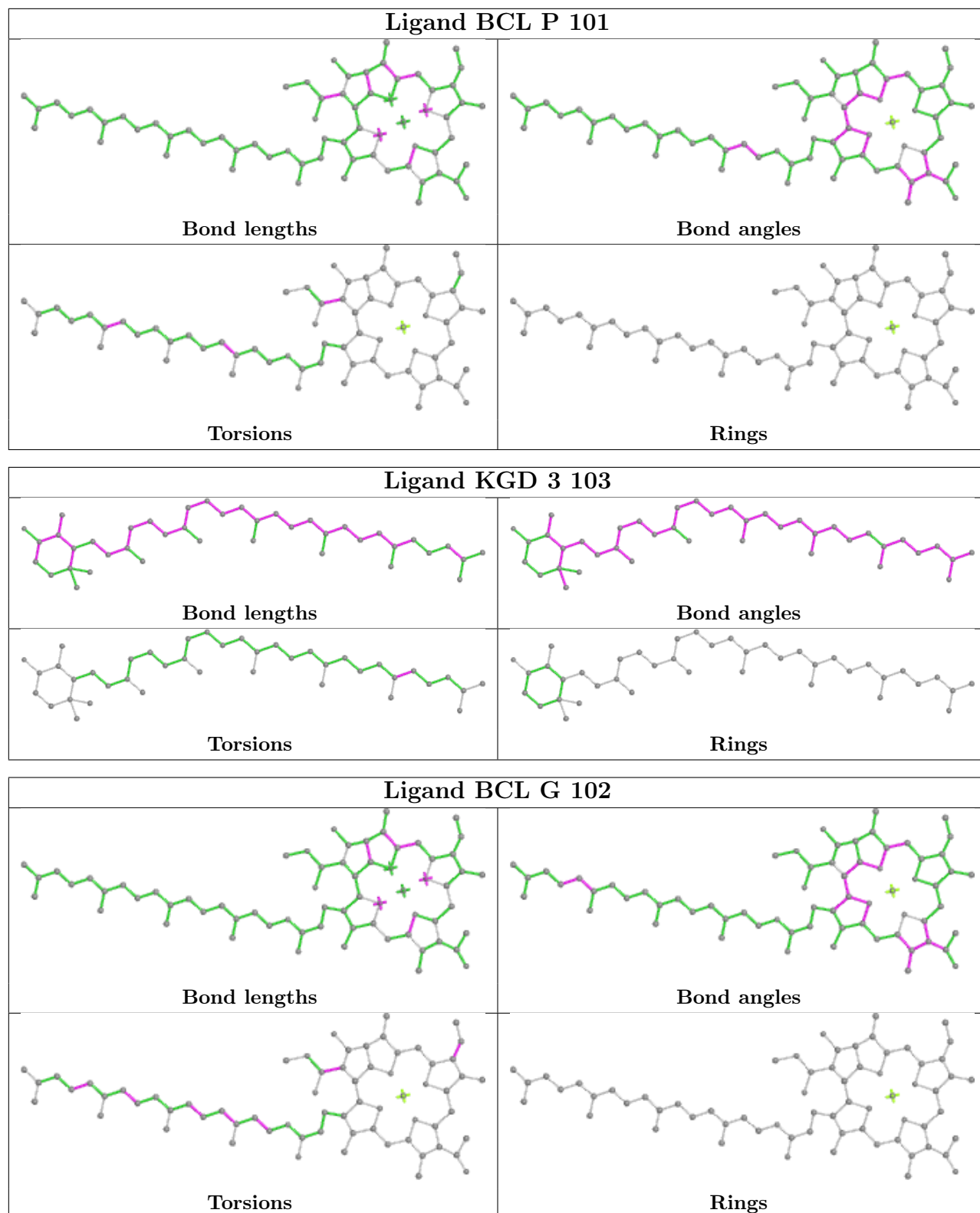
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

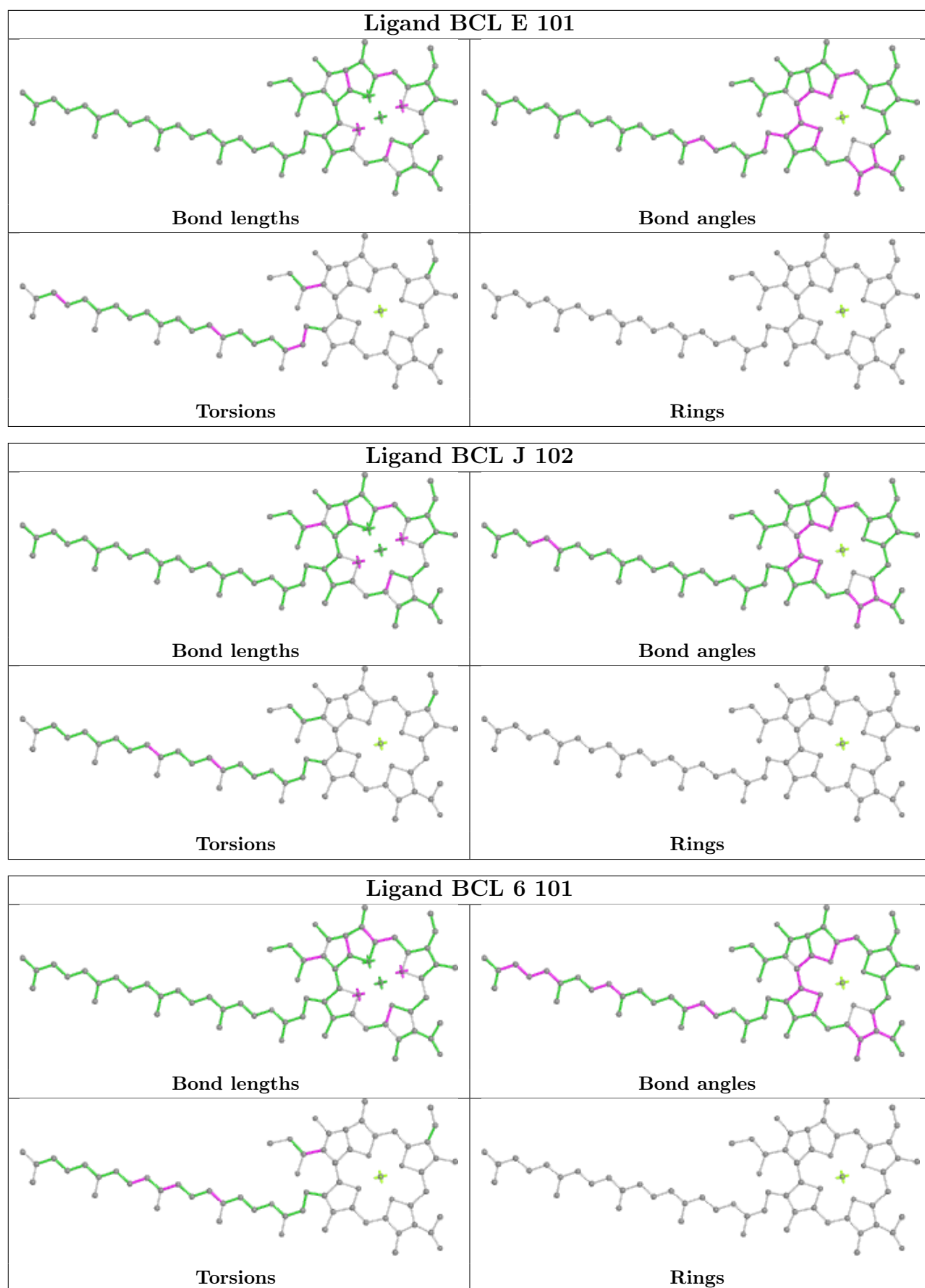


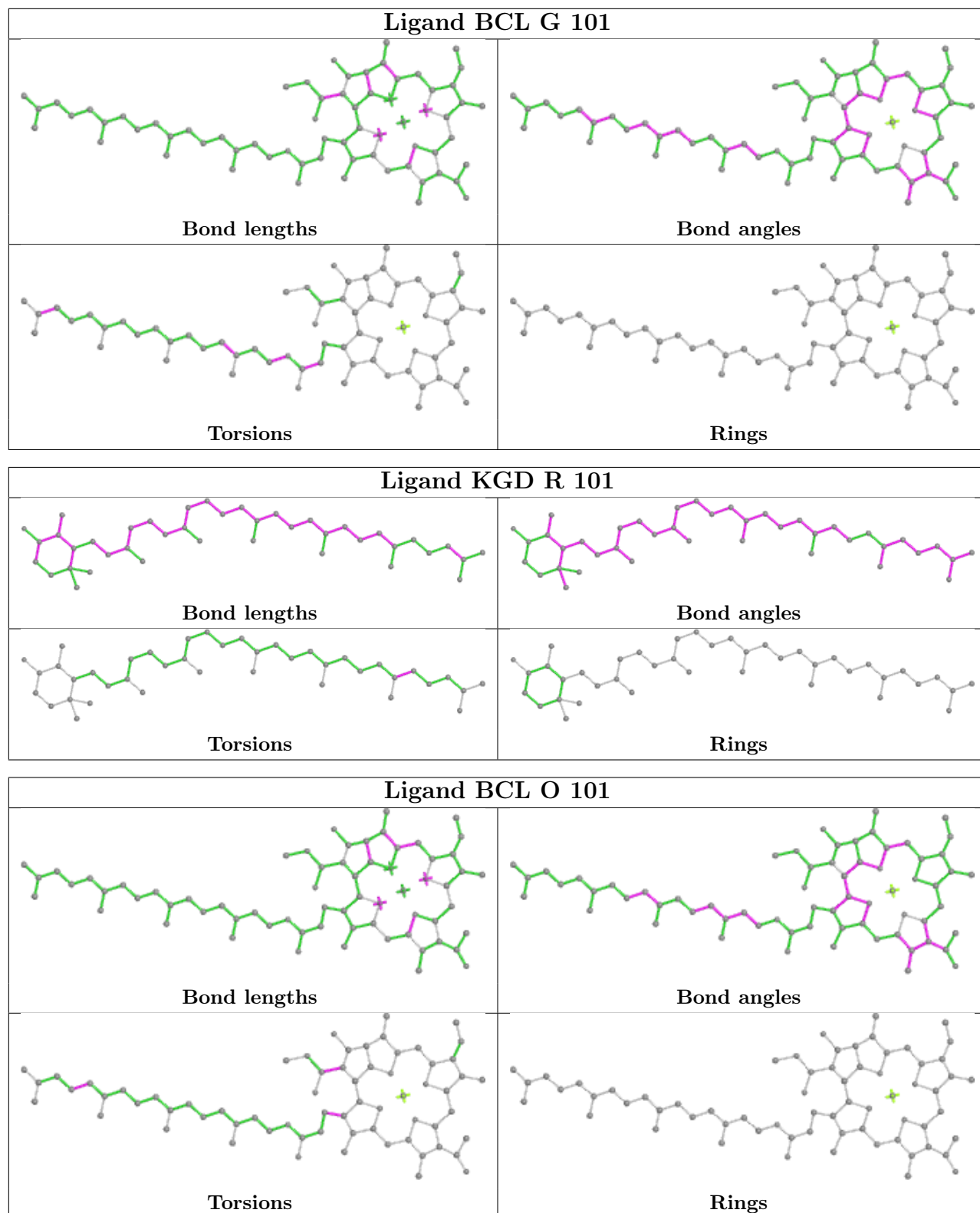


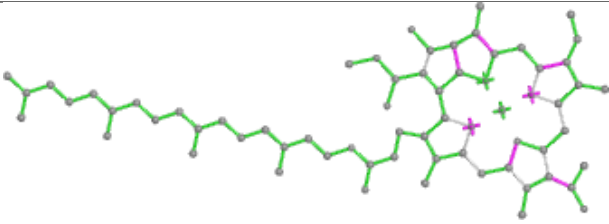
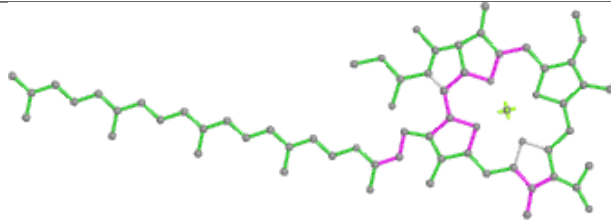
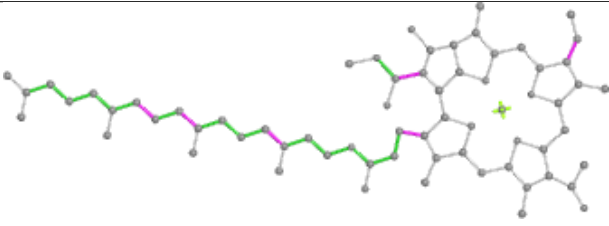
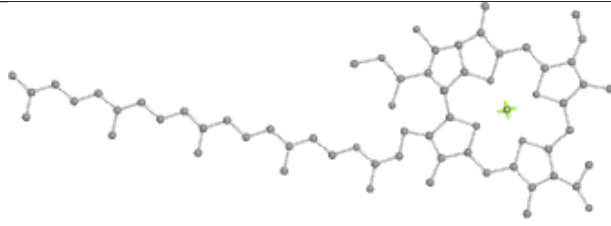
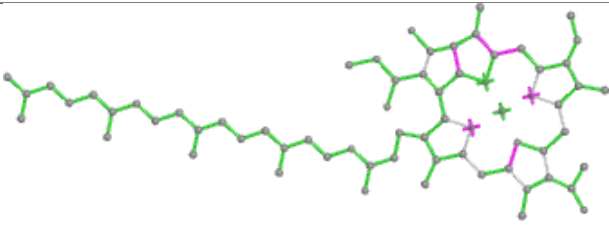
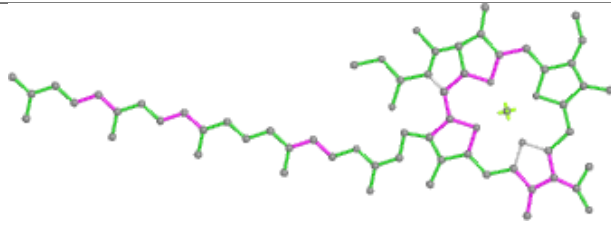
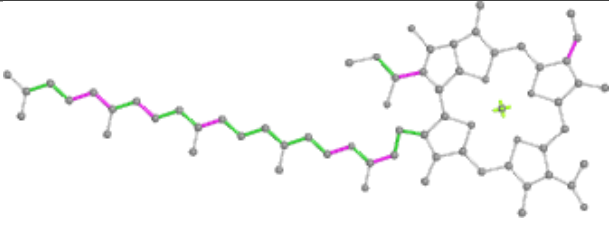
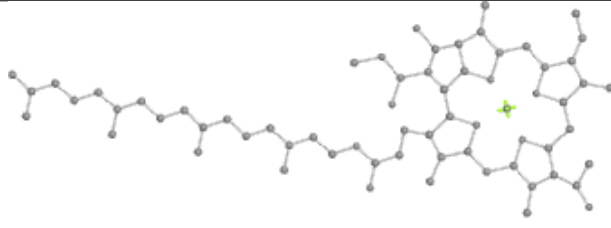
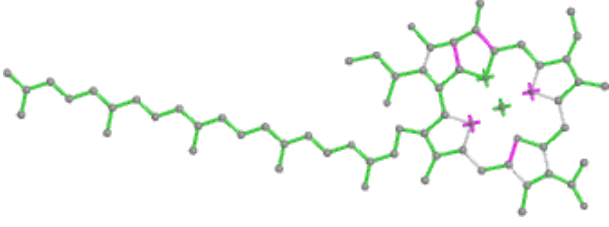
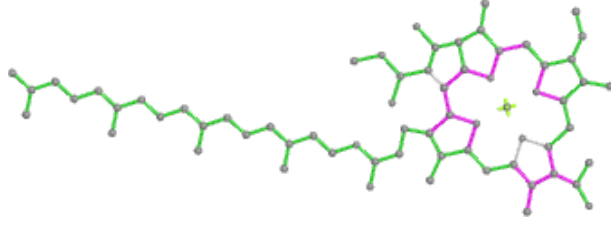
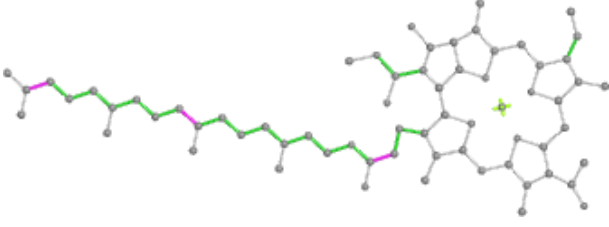
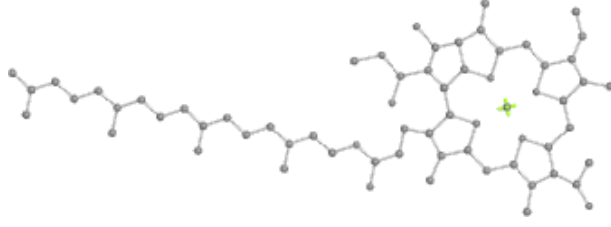


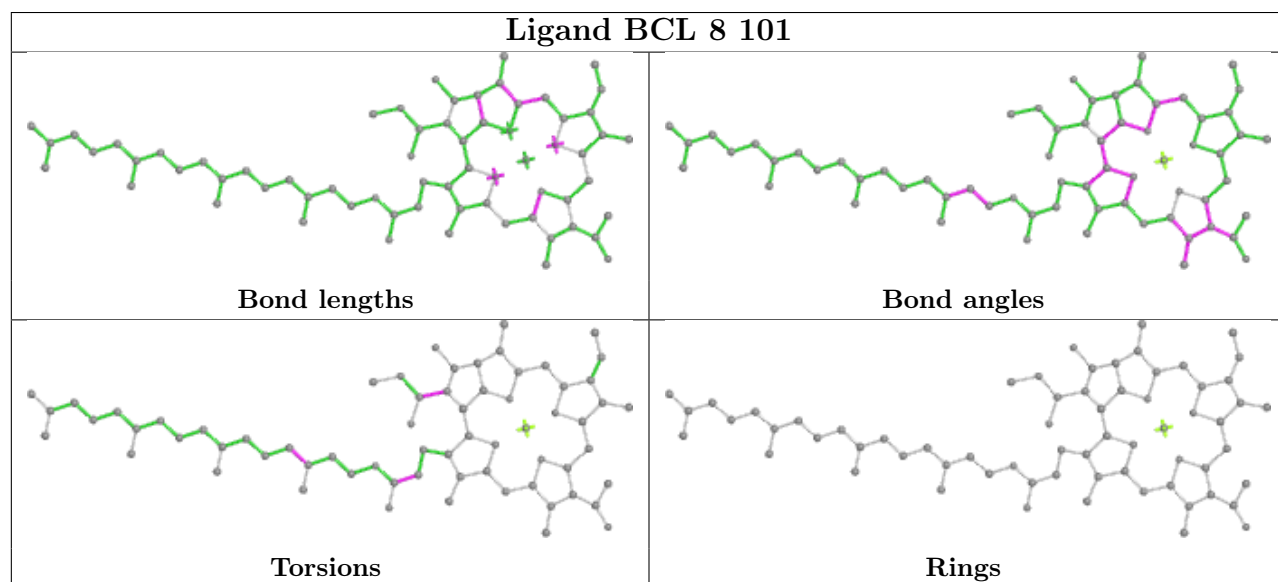
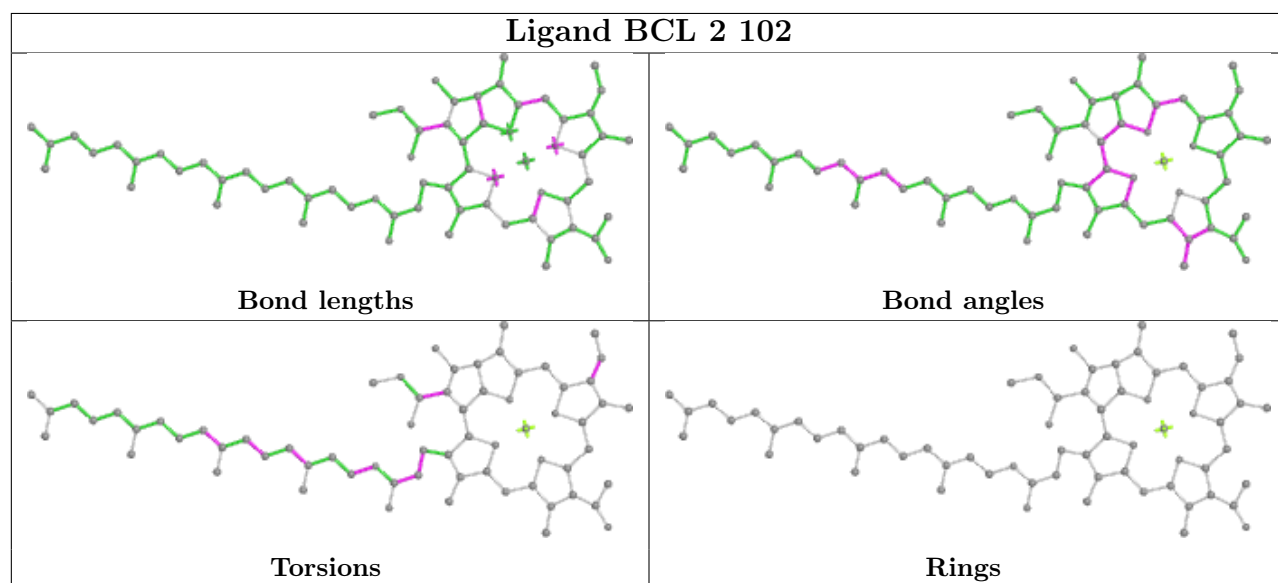
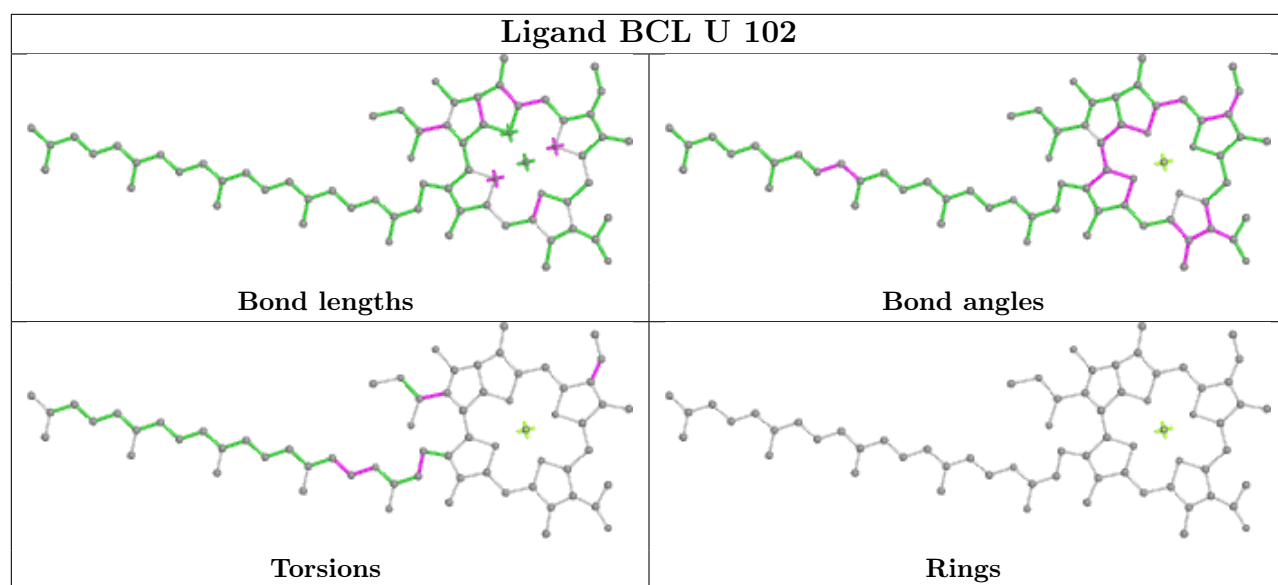


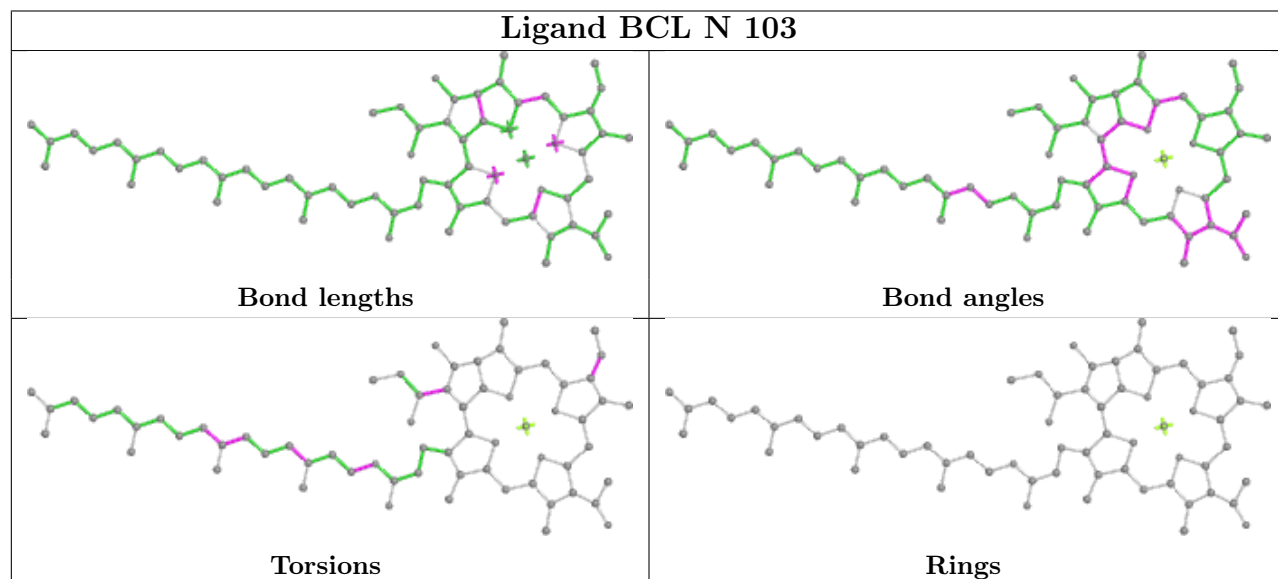
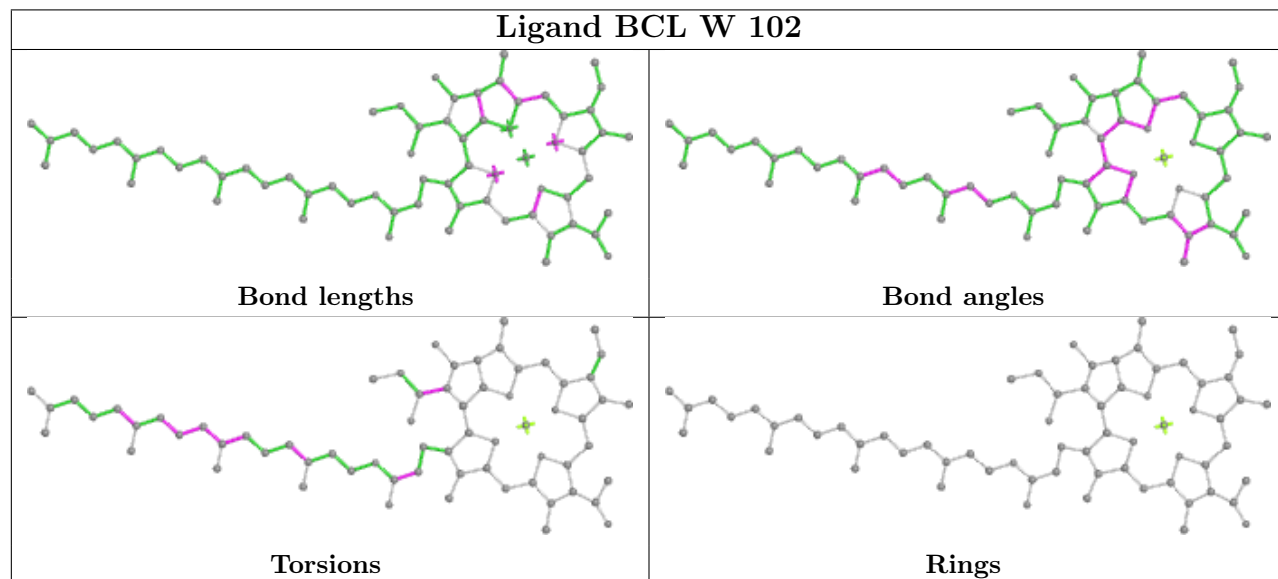
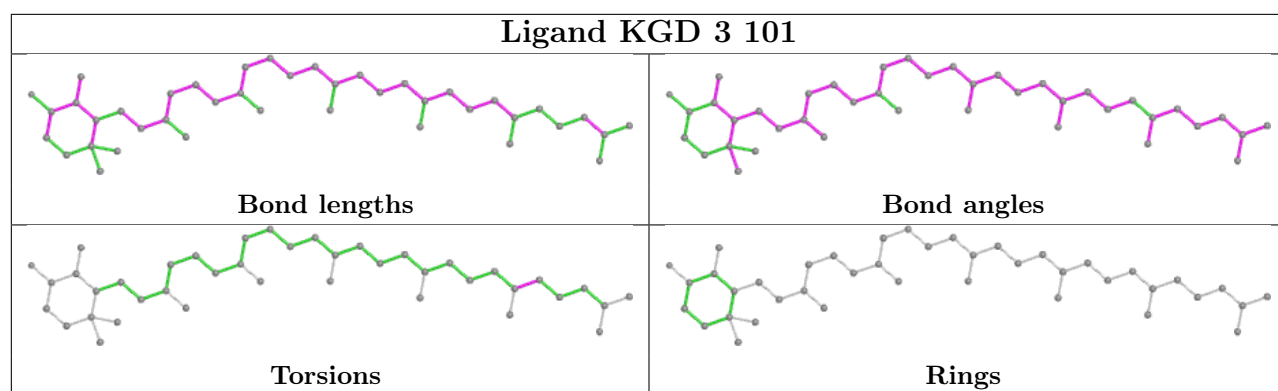


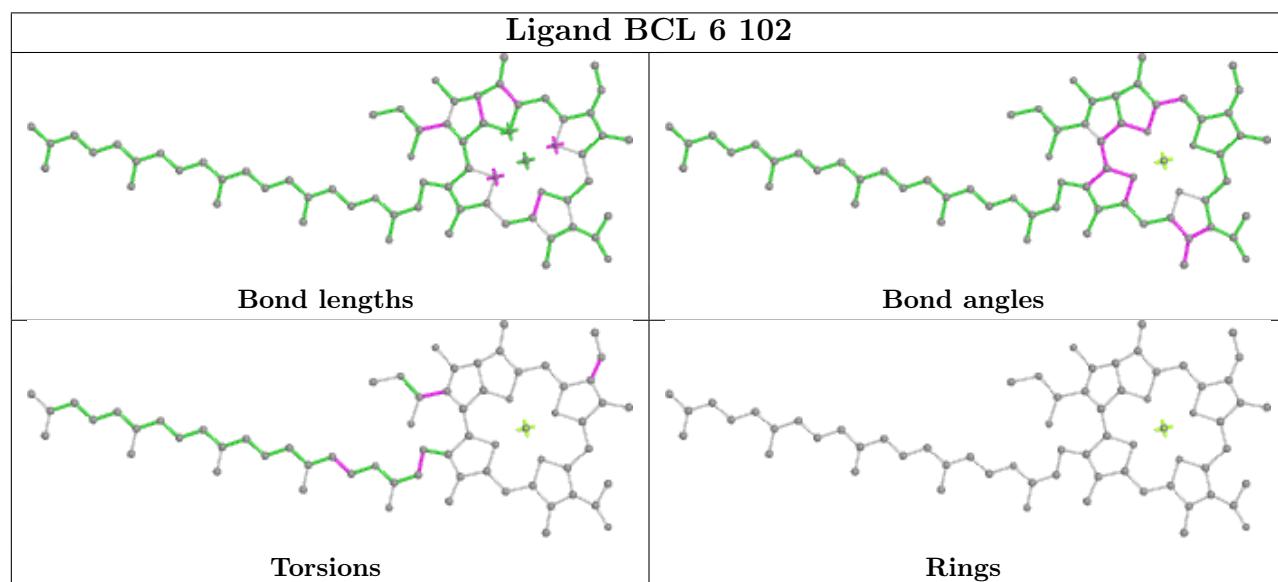
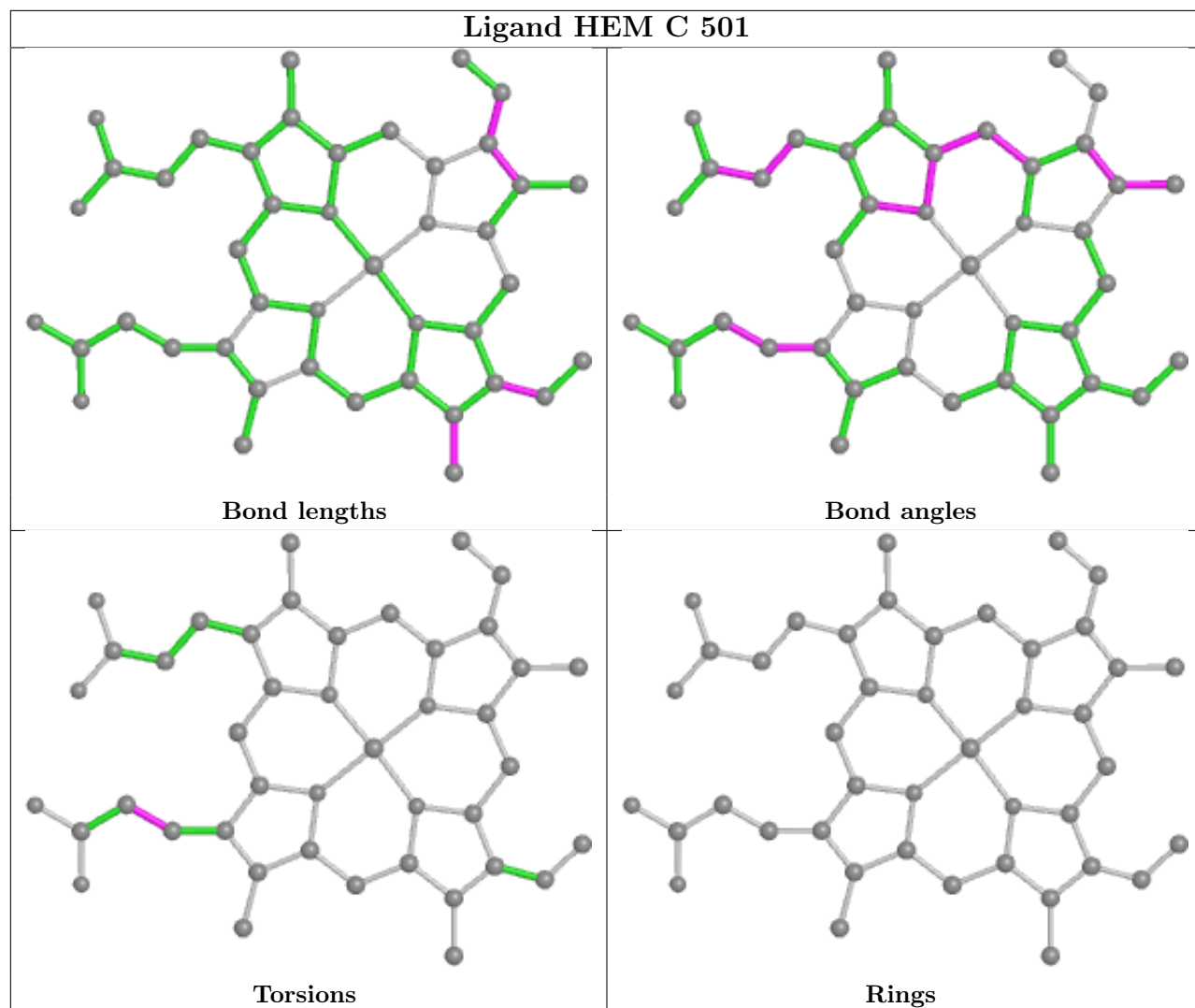


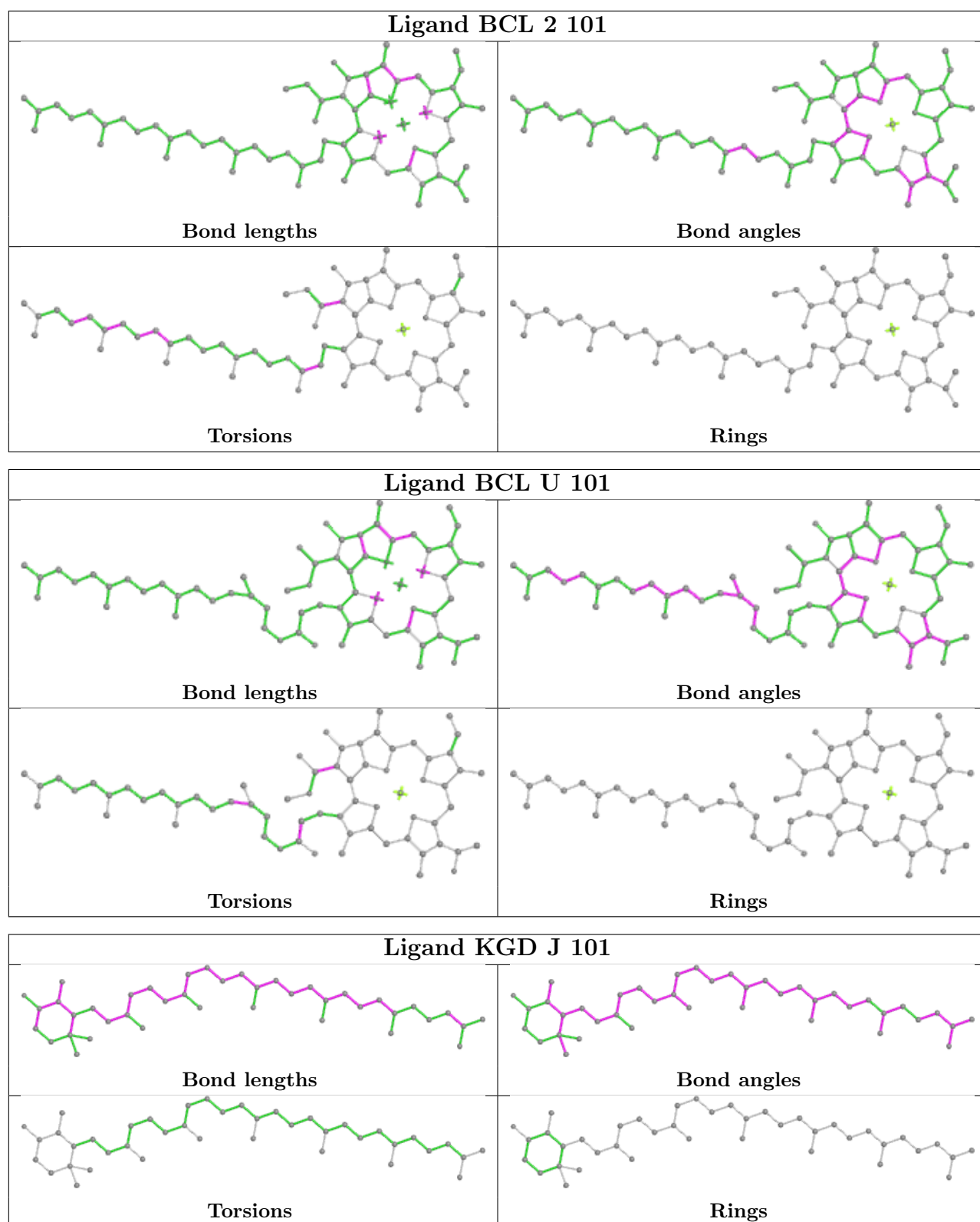


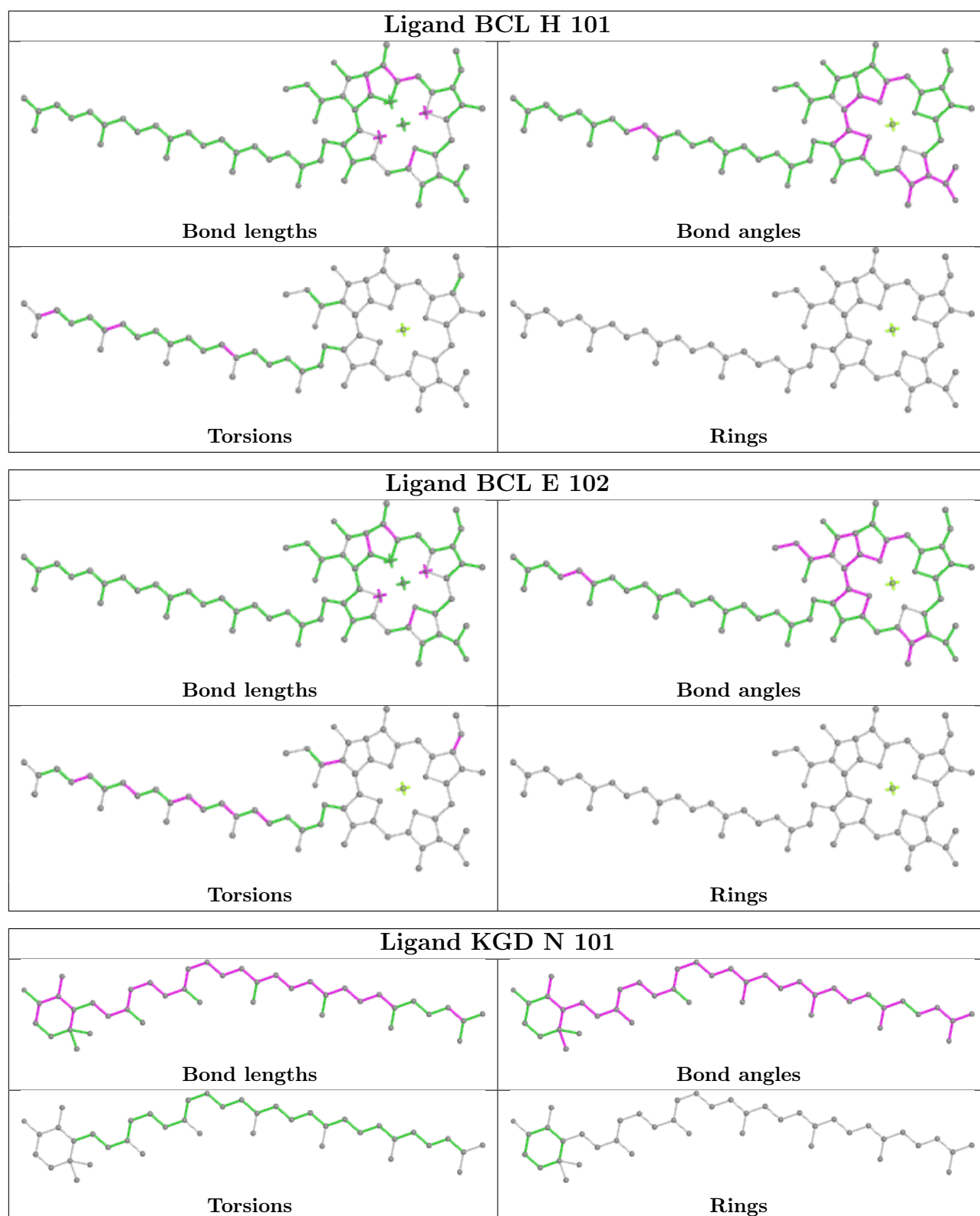
Ligand BCL L 1001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL F 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL K 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

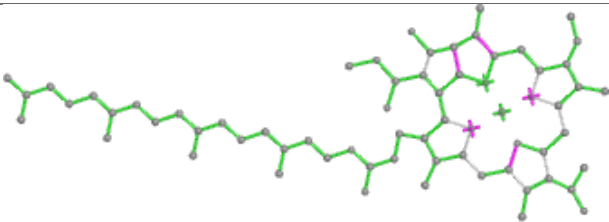
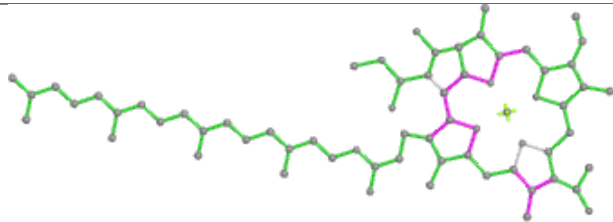
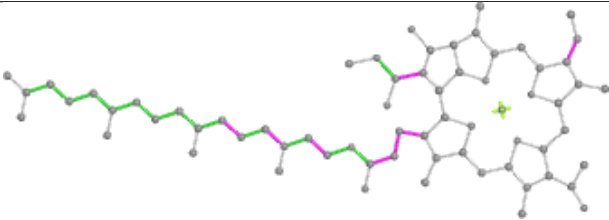
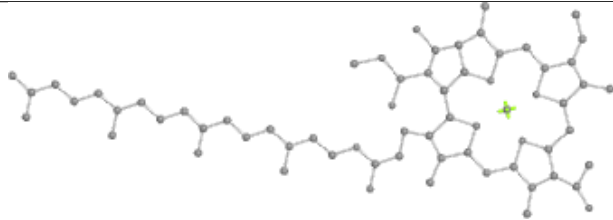


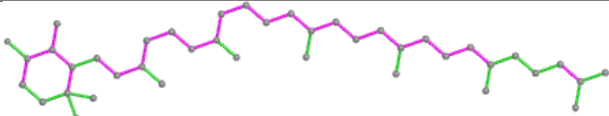
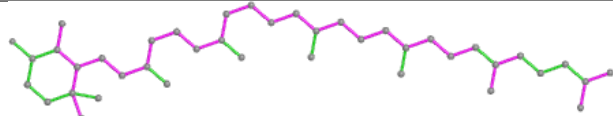
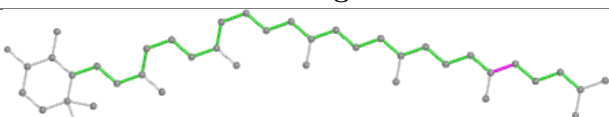
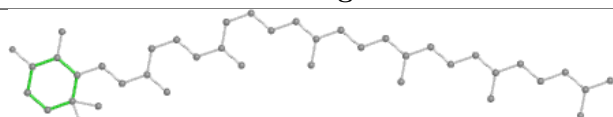


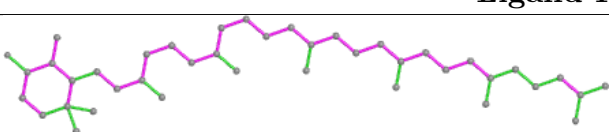
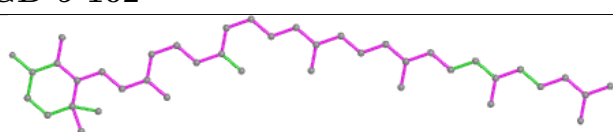
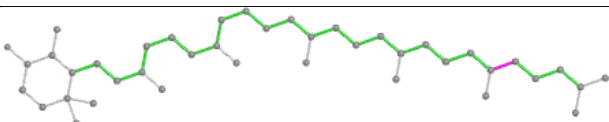
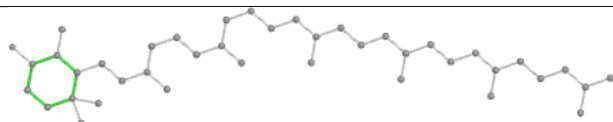


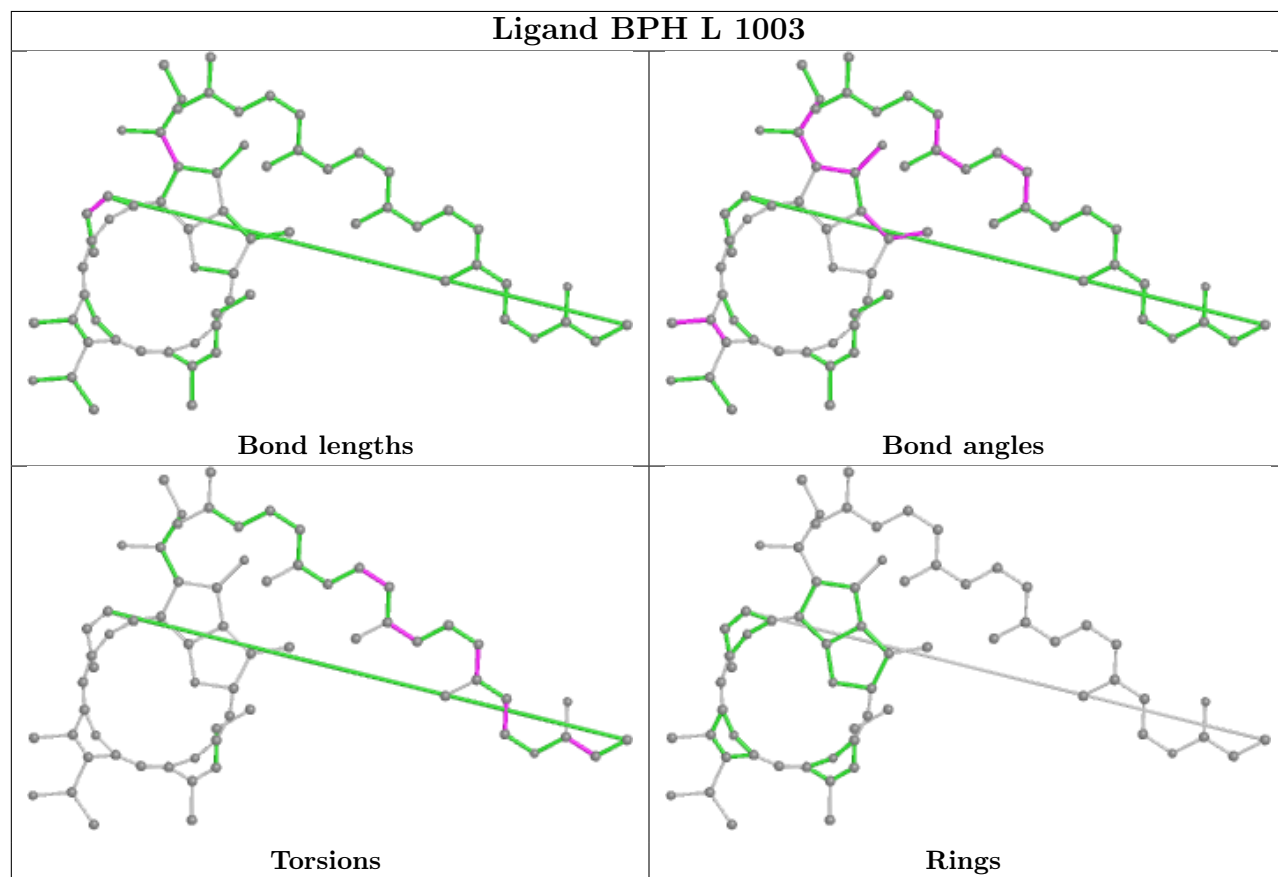
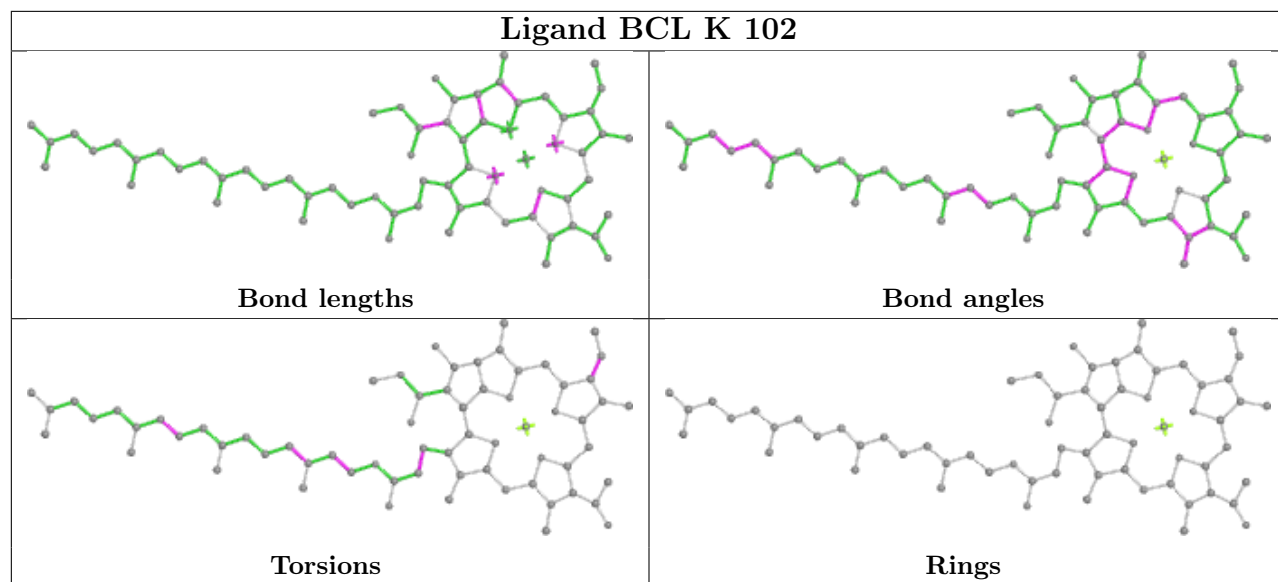


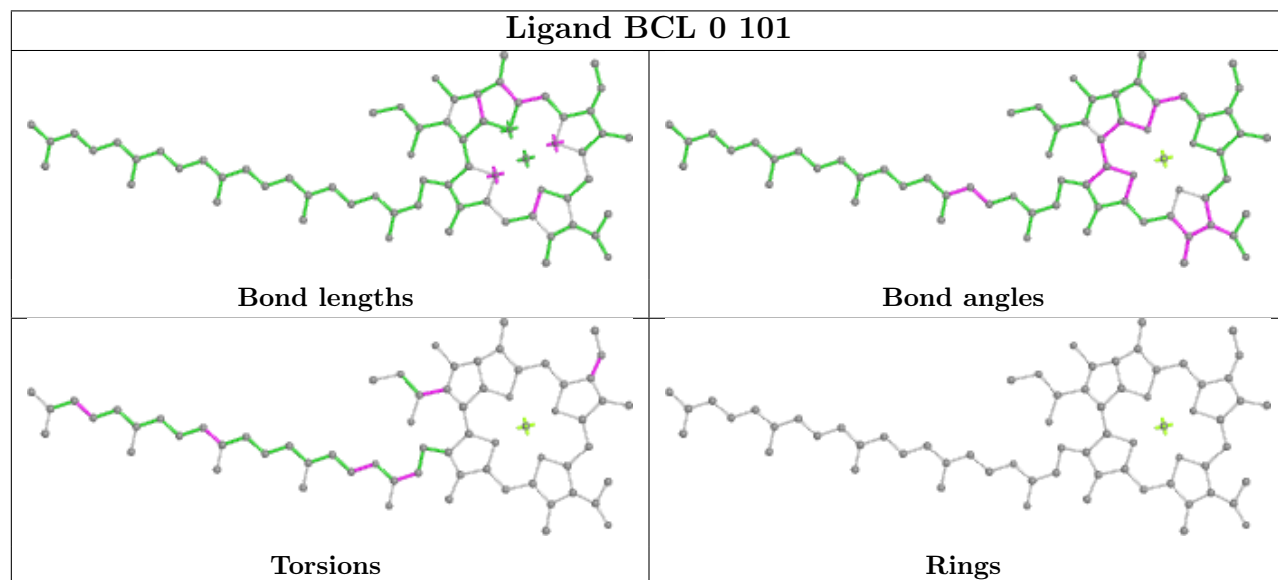
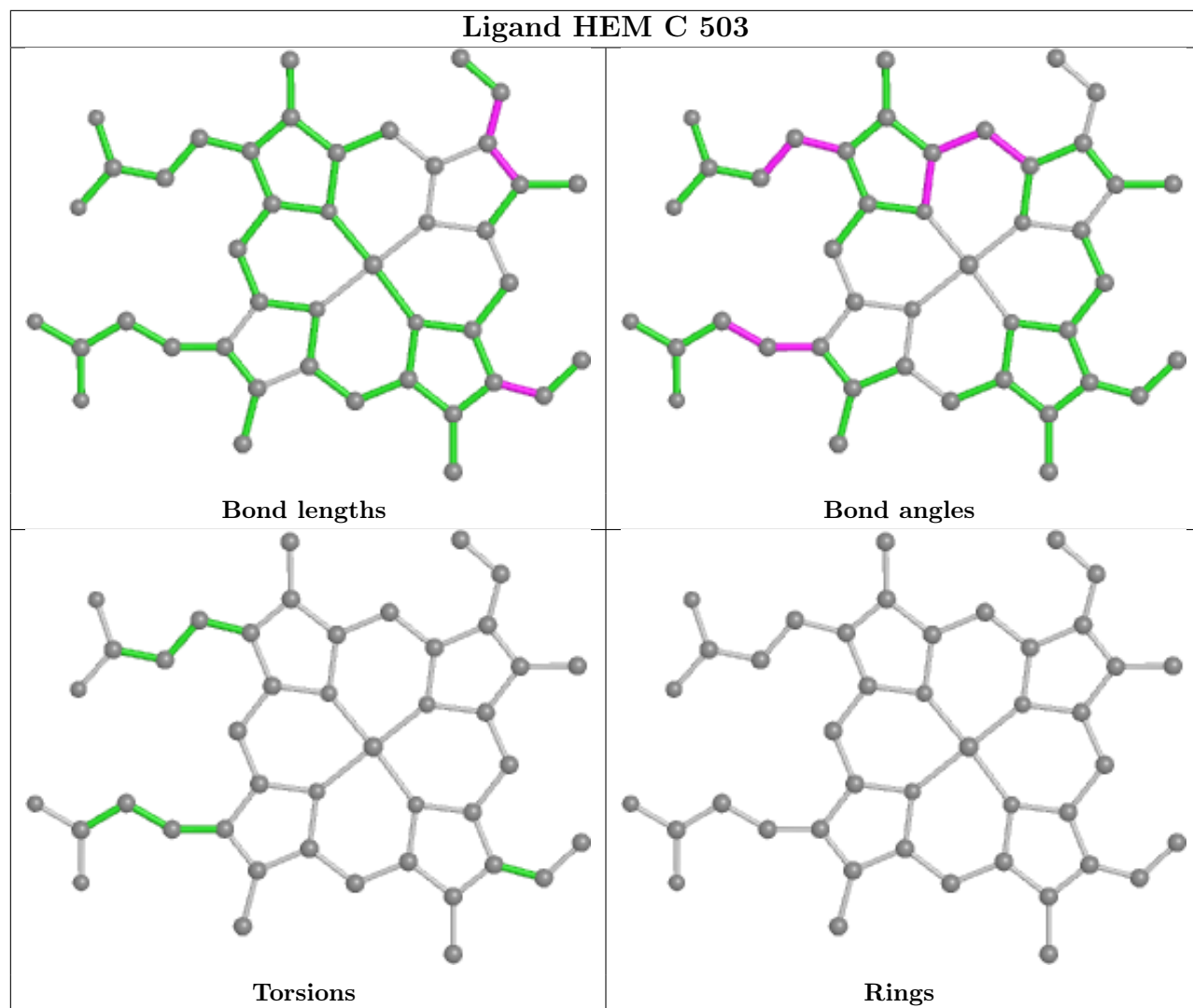


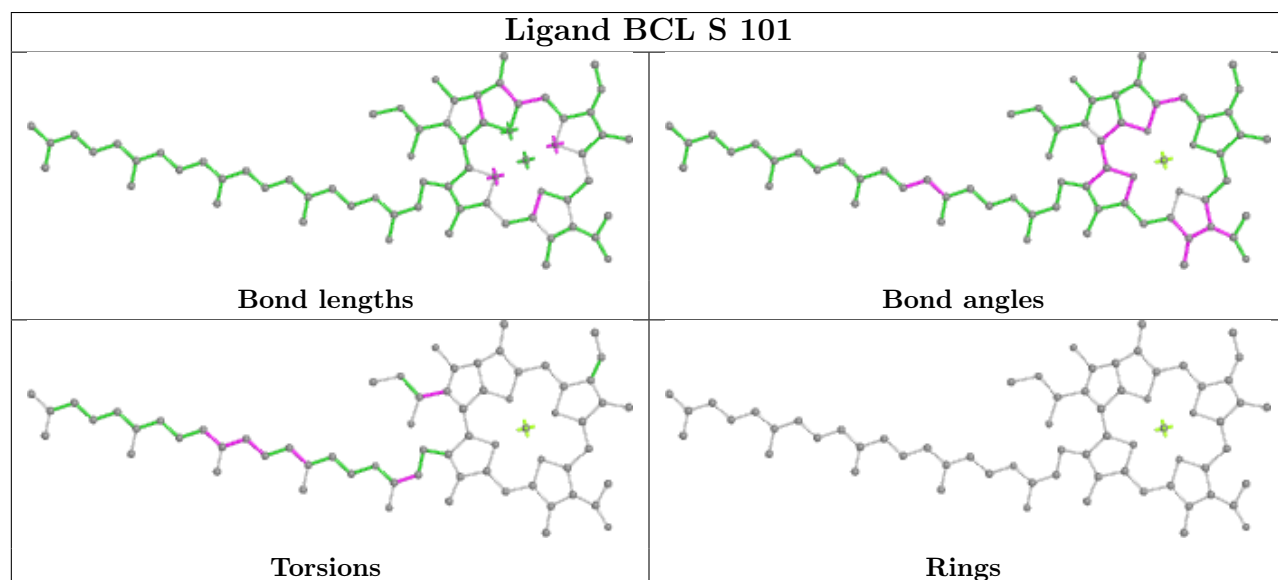
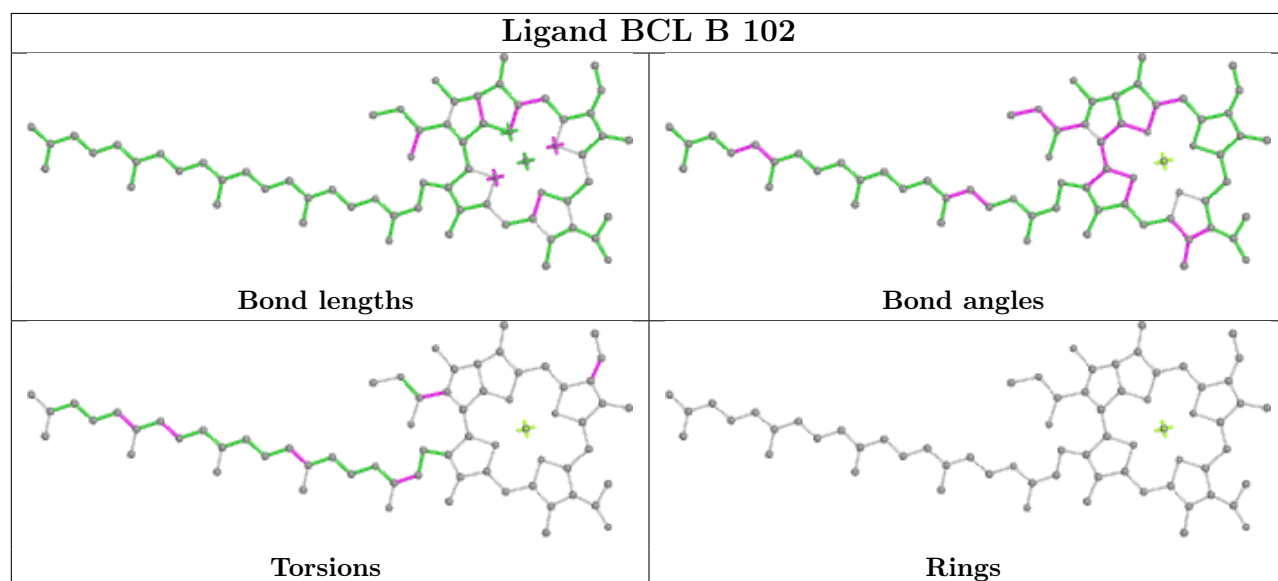
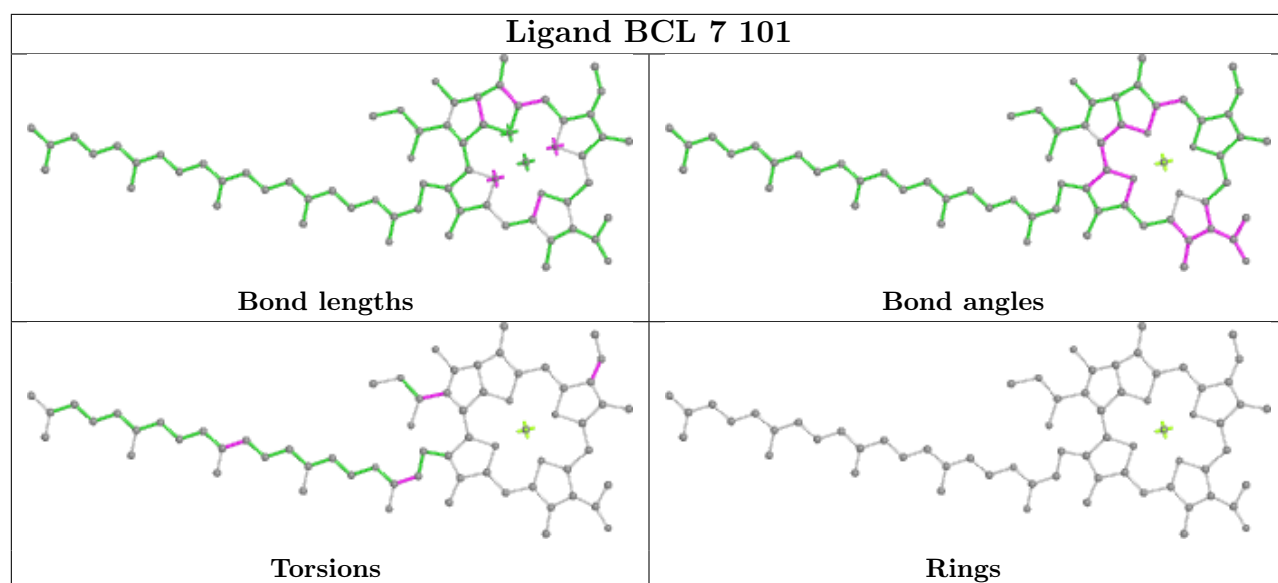
Ligand BCL 4 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

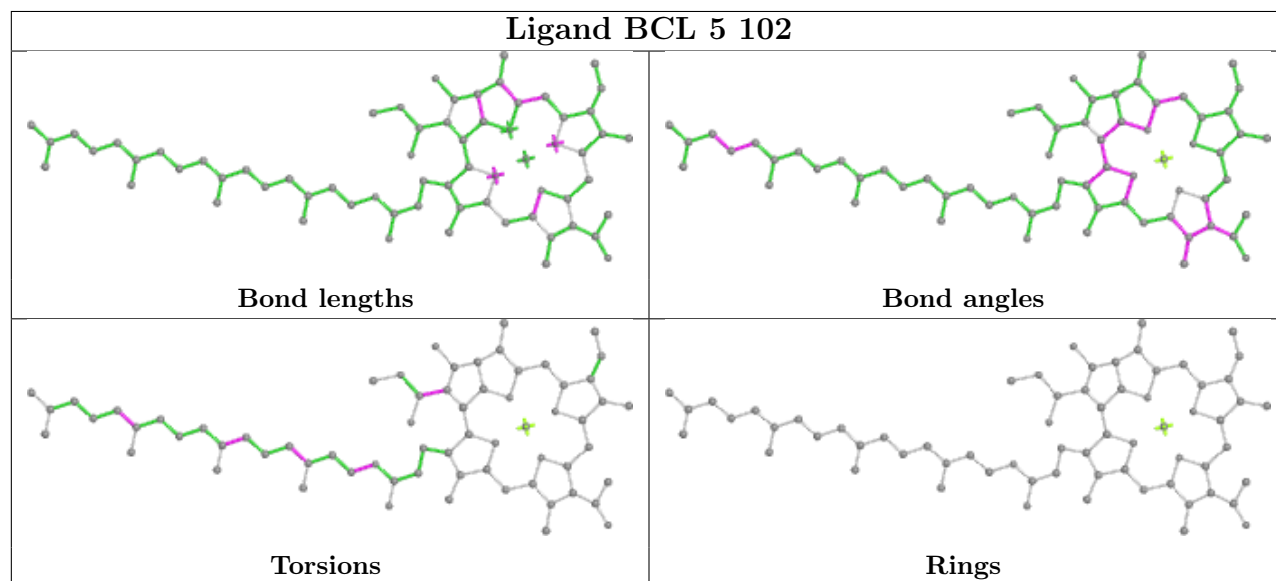
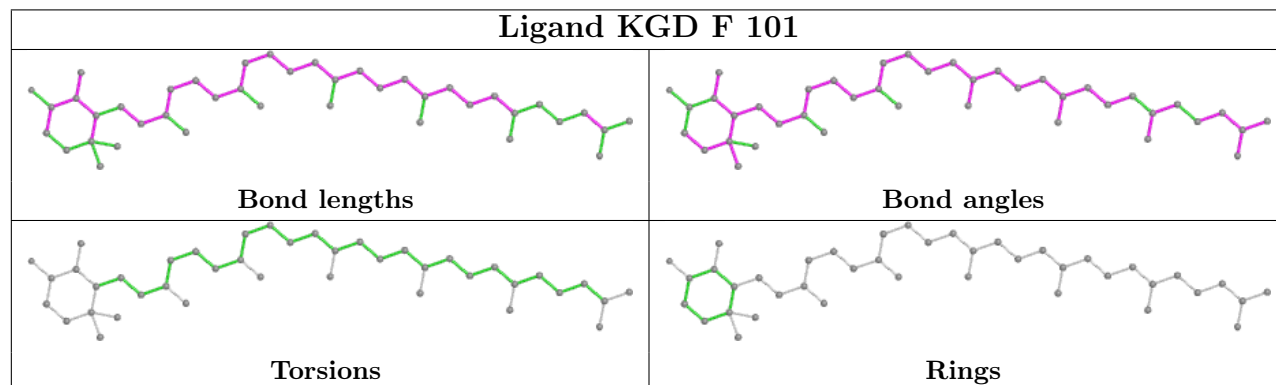
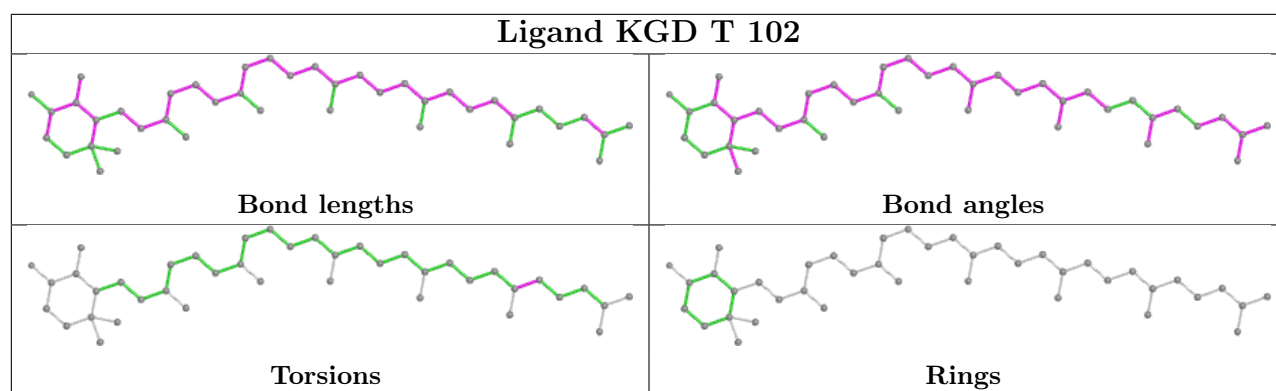
Ligand KGD A 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

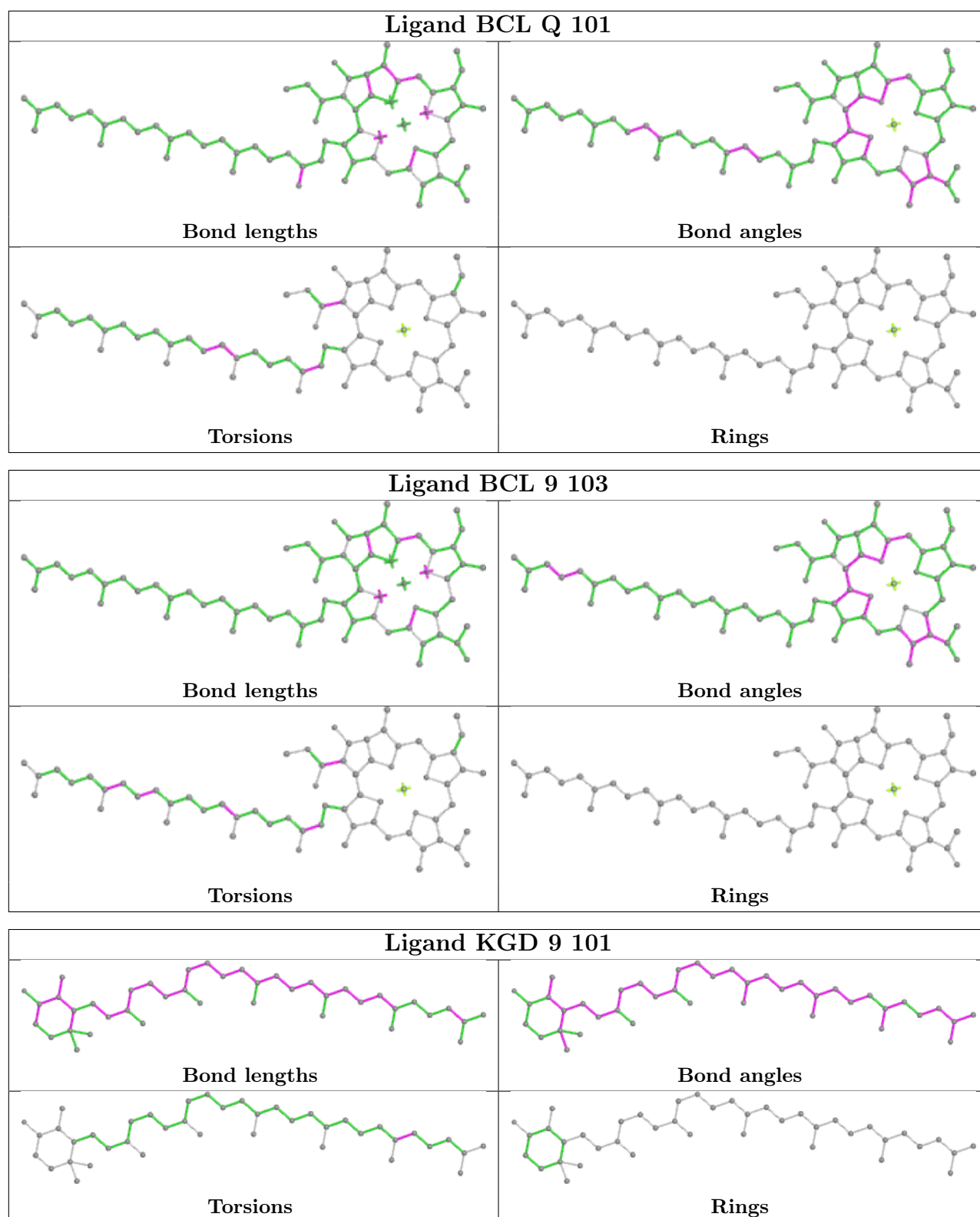
Ligand KGD 9 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

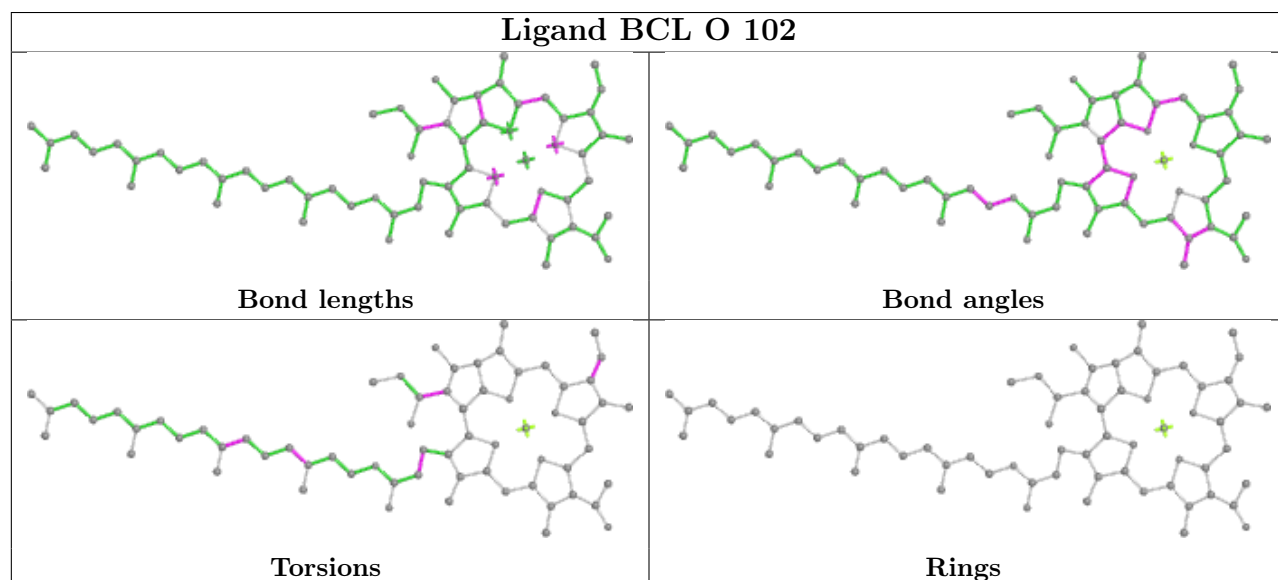
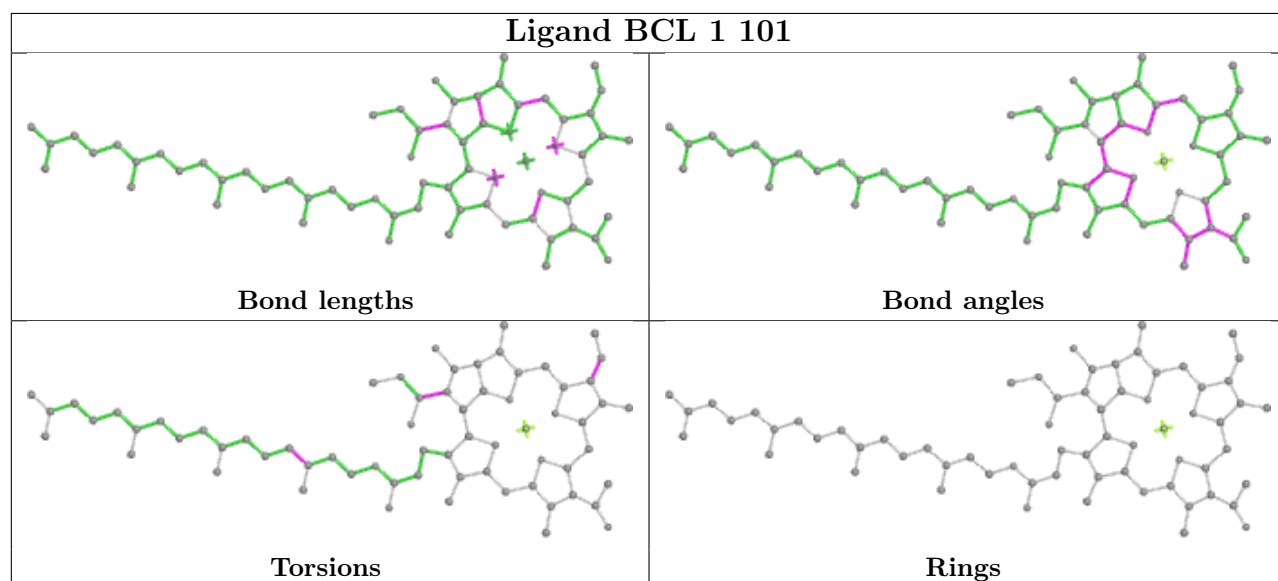
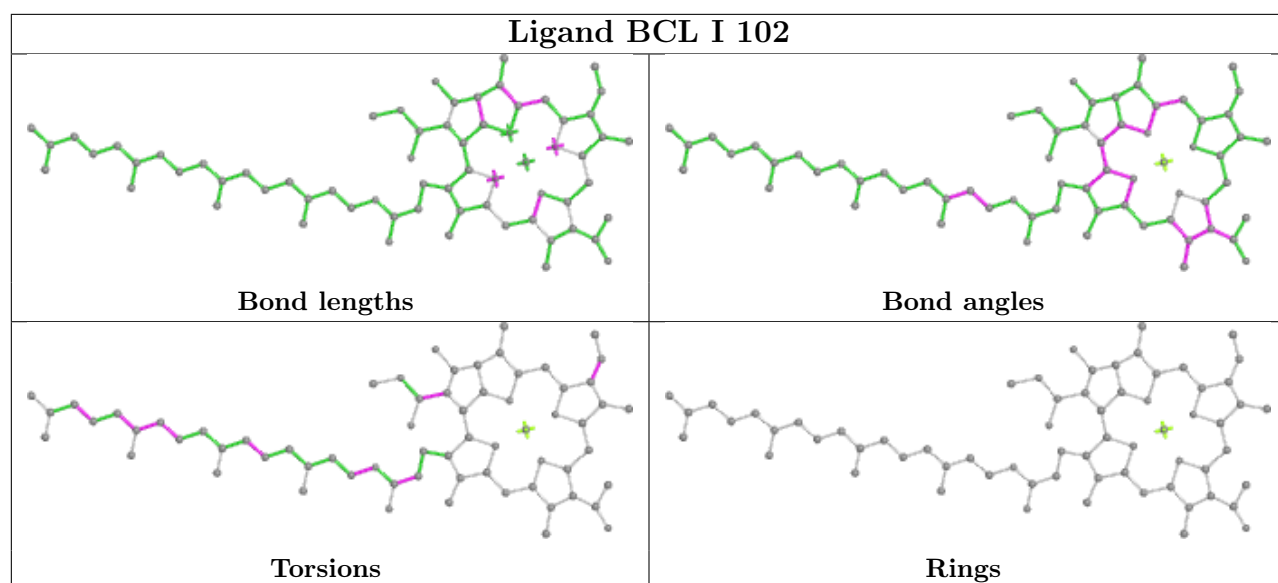


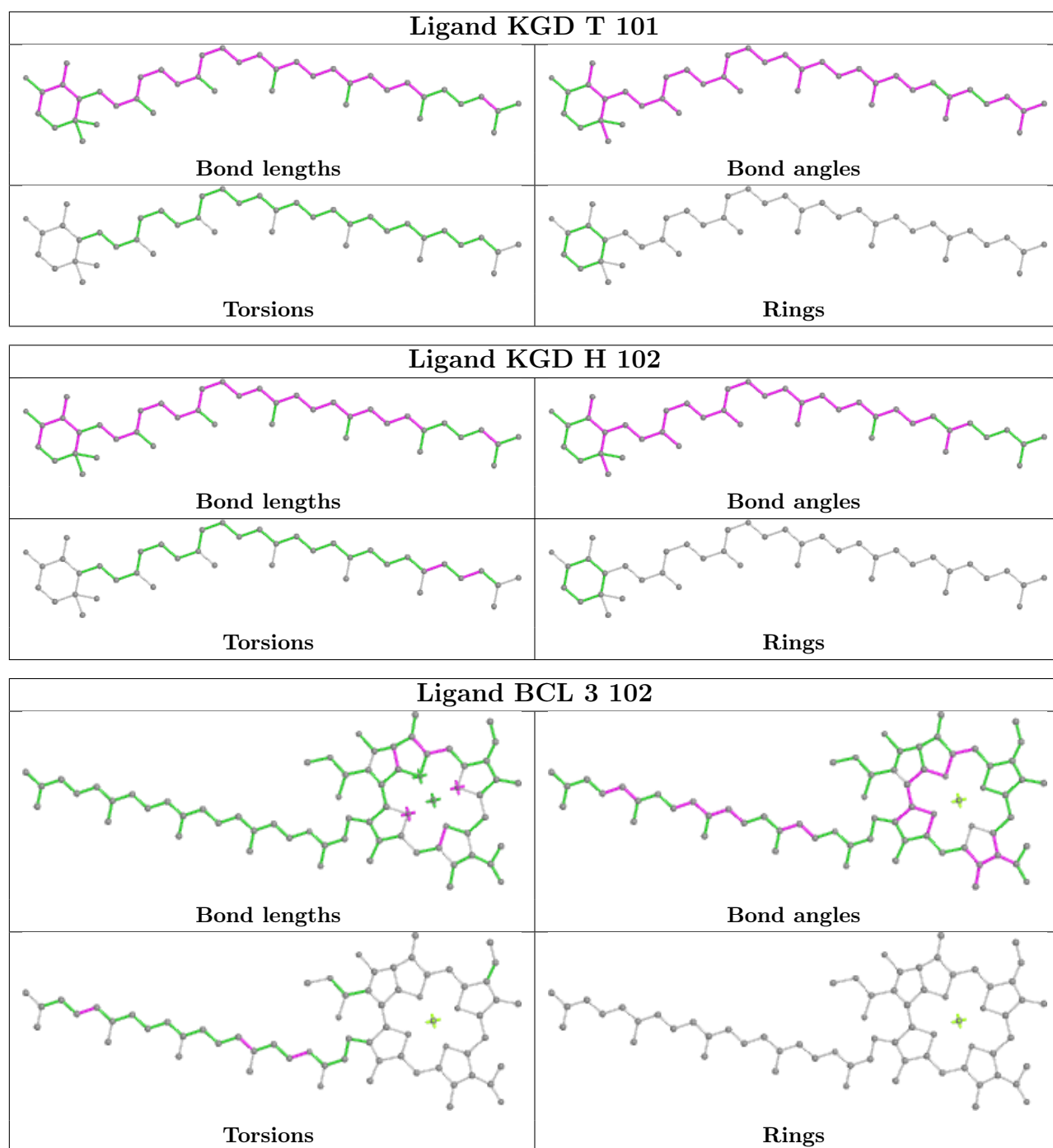


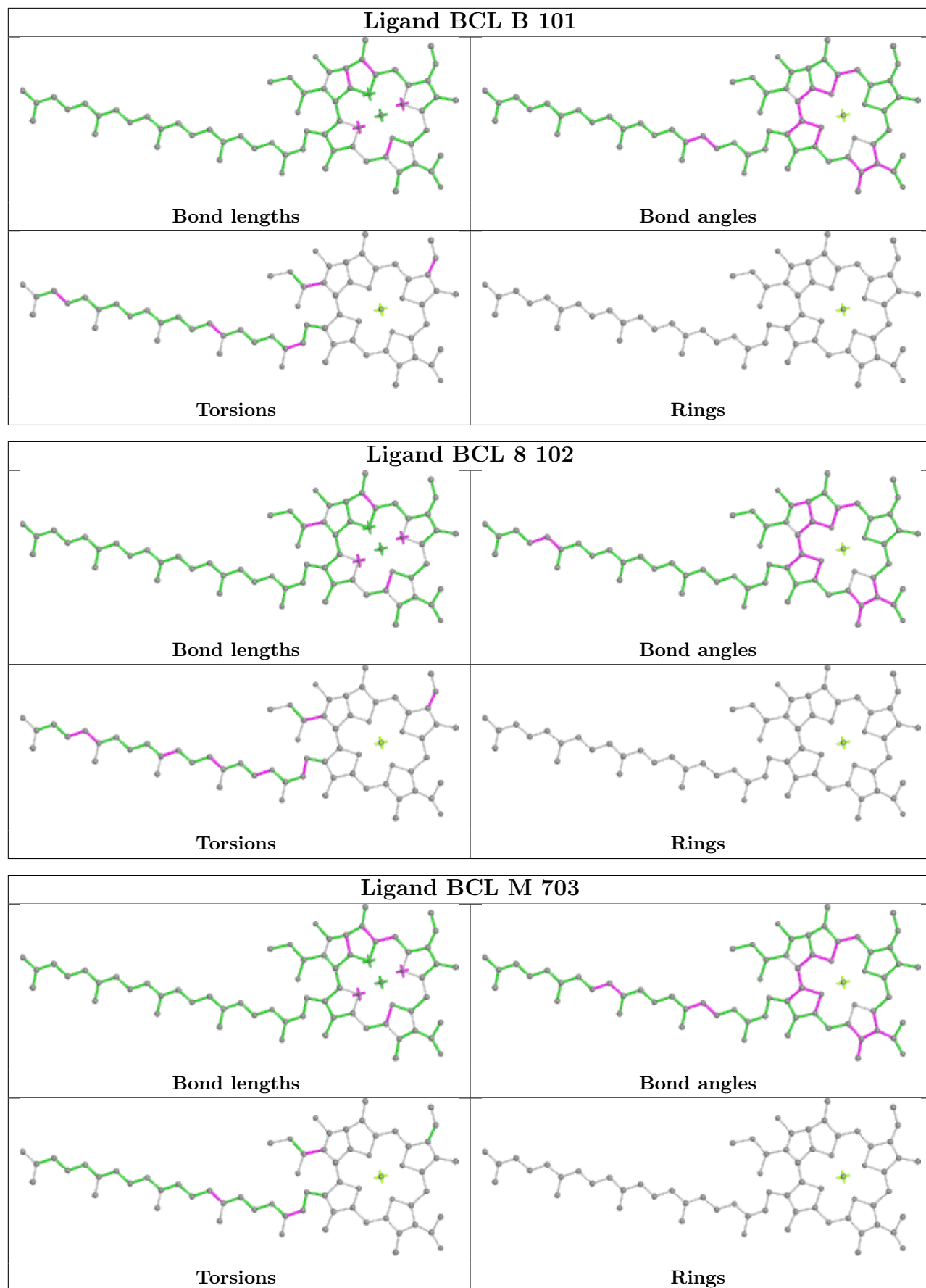


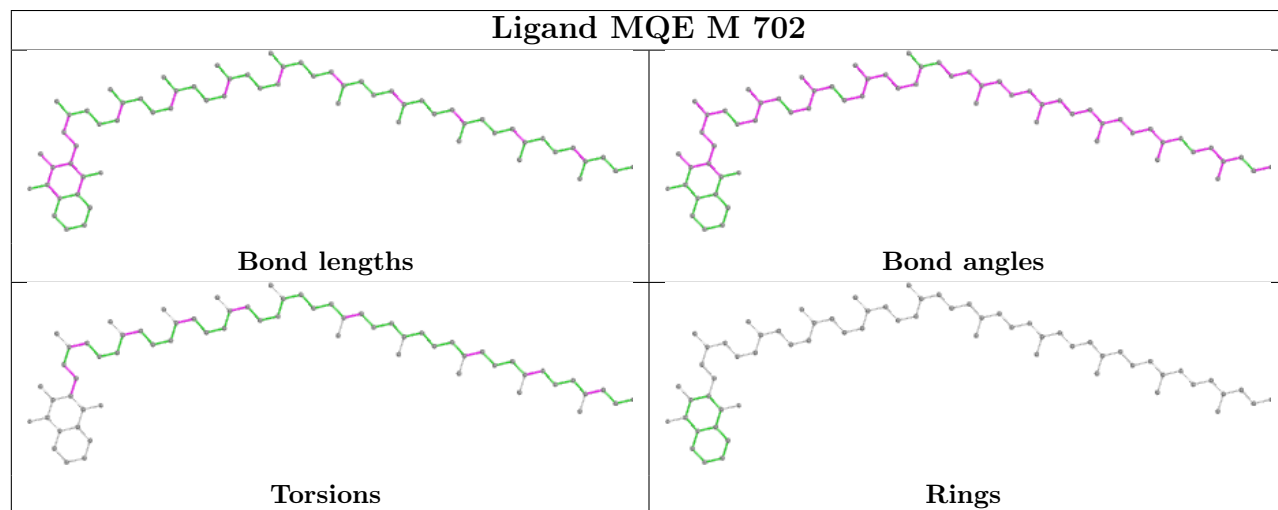
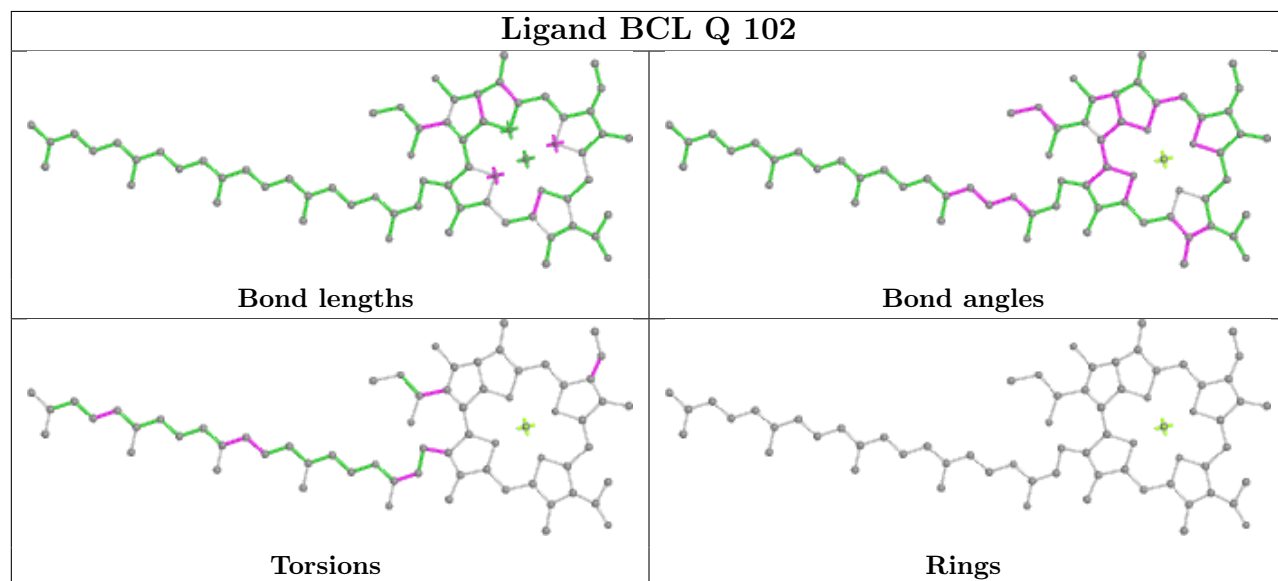
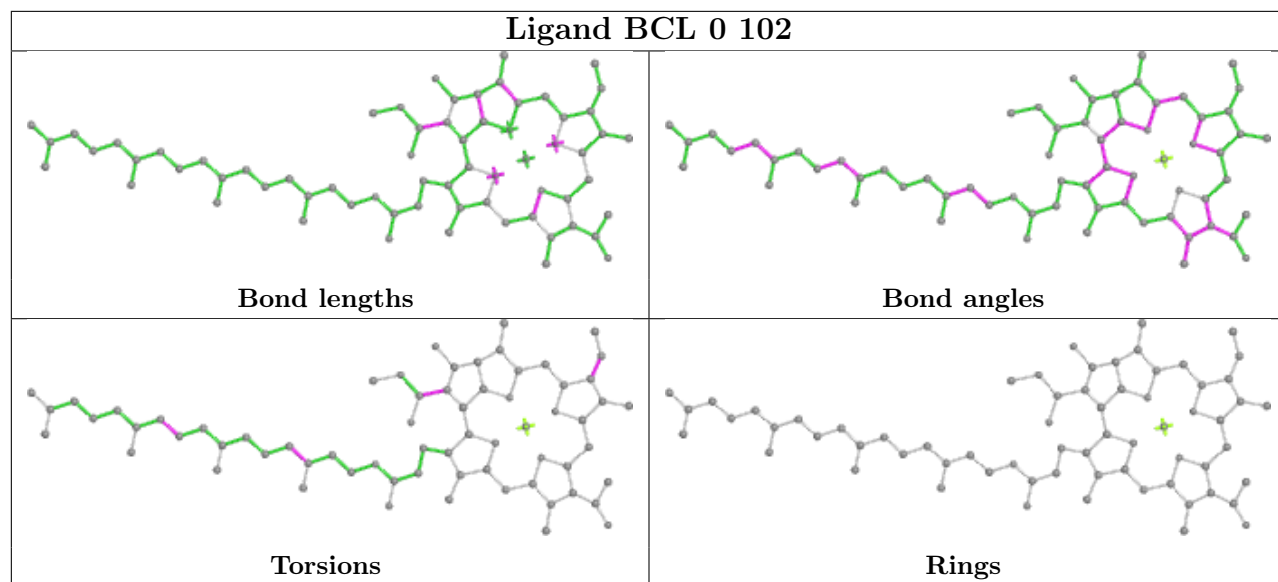


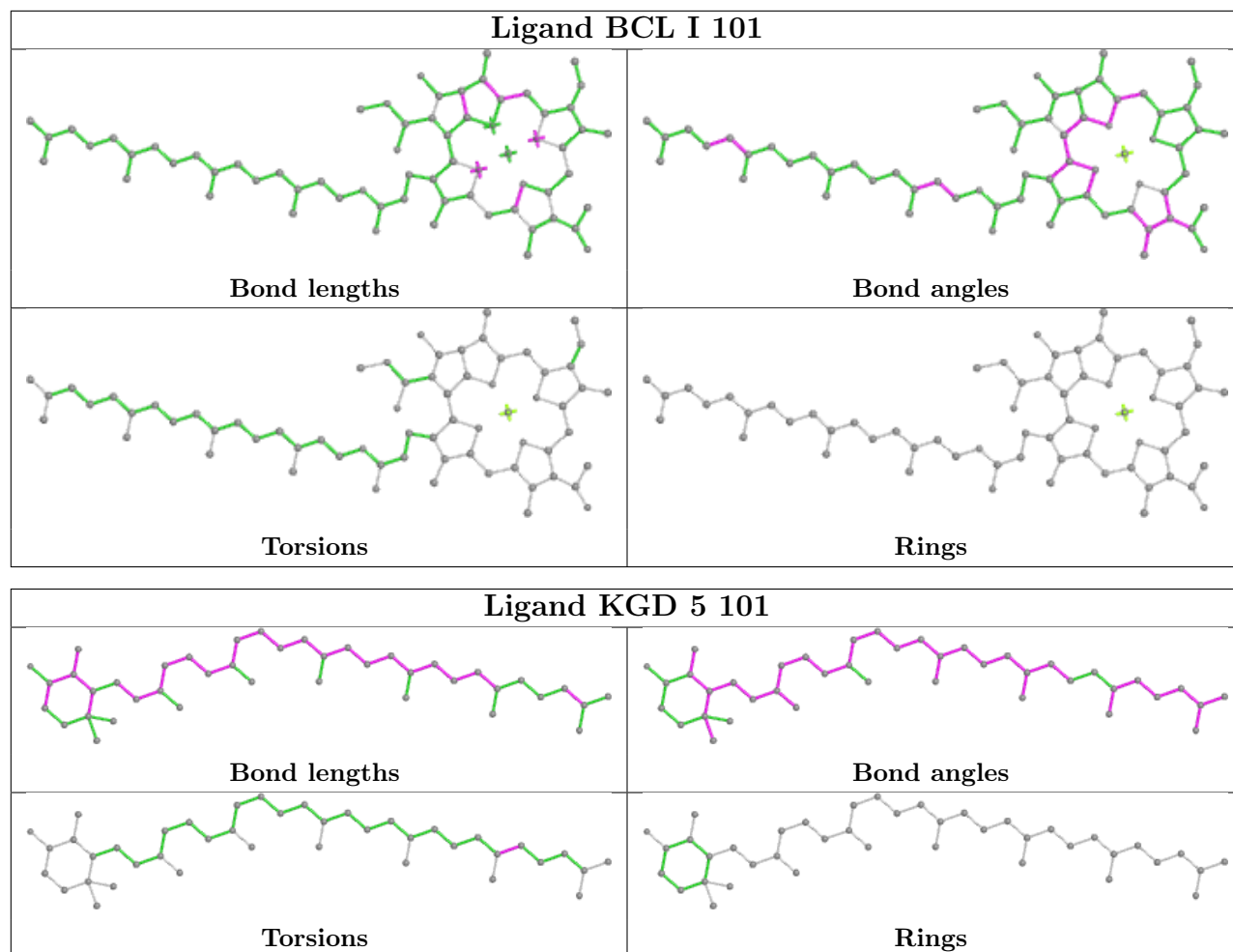


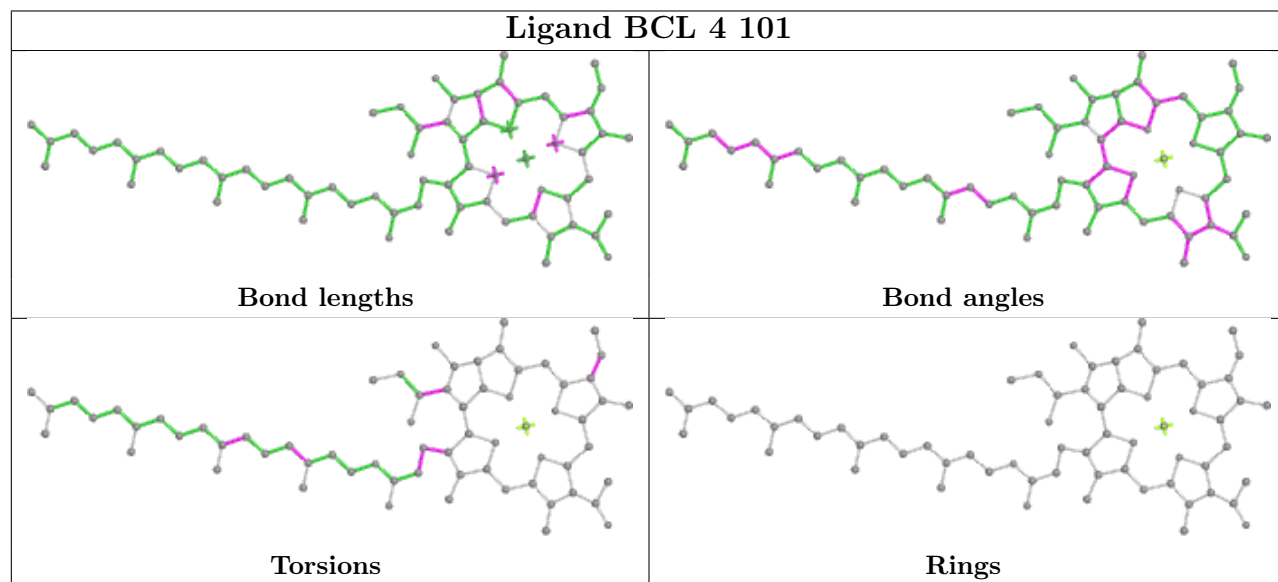
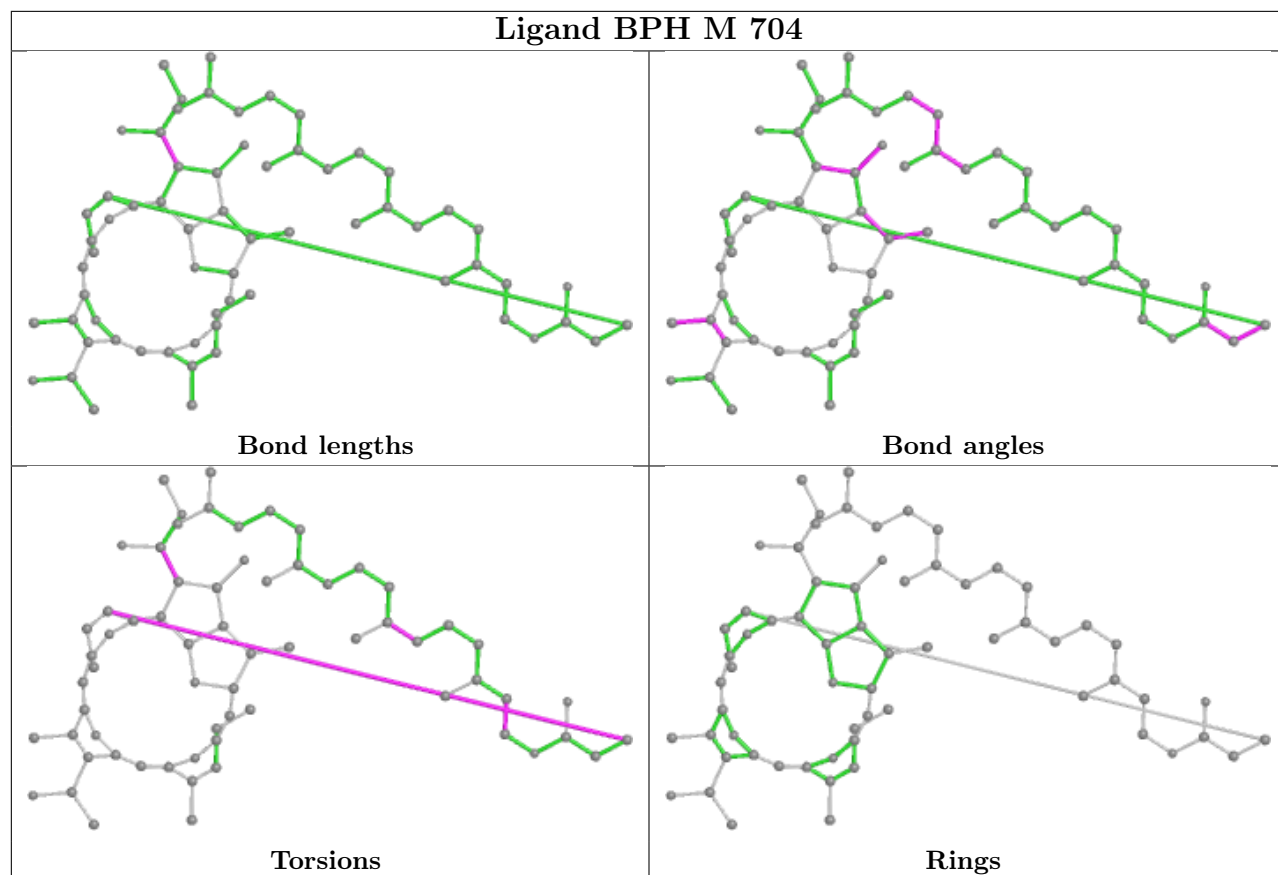


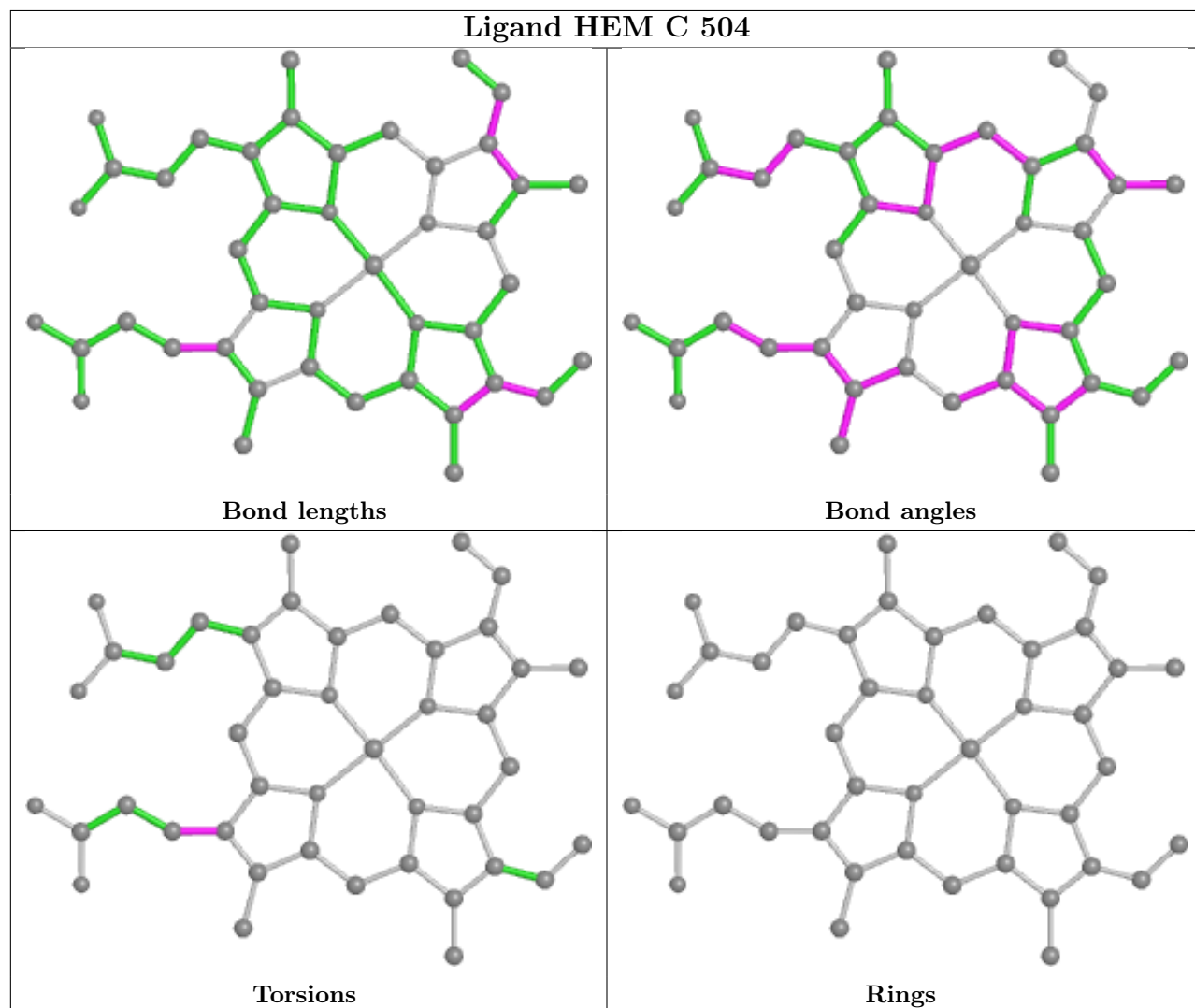
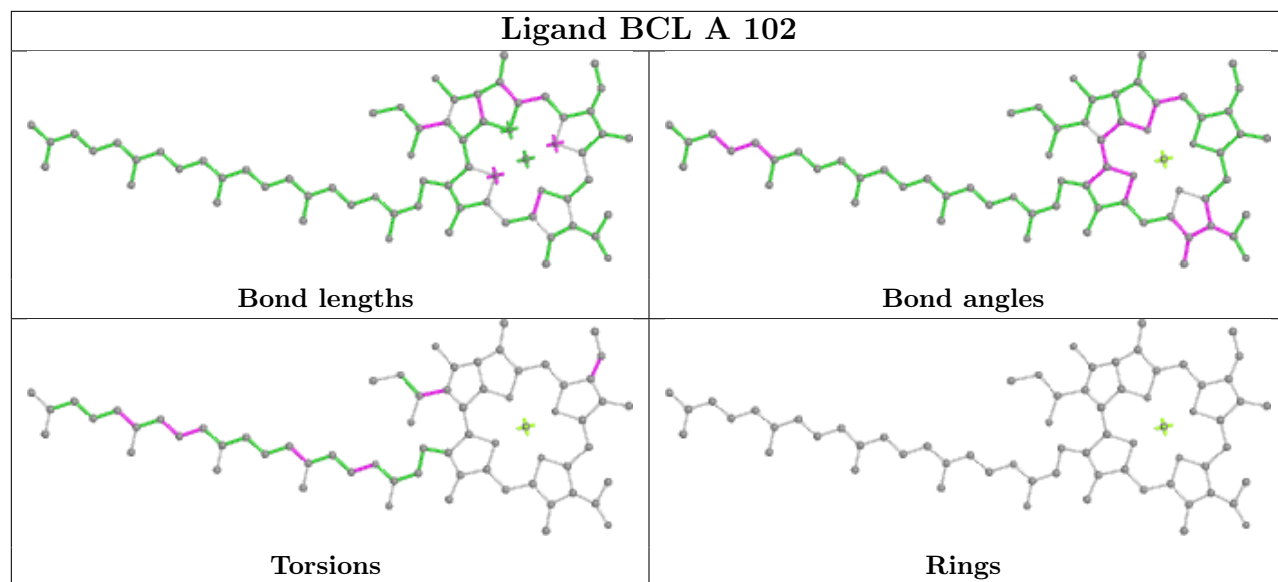


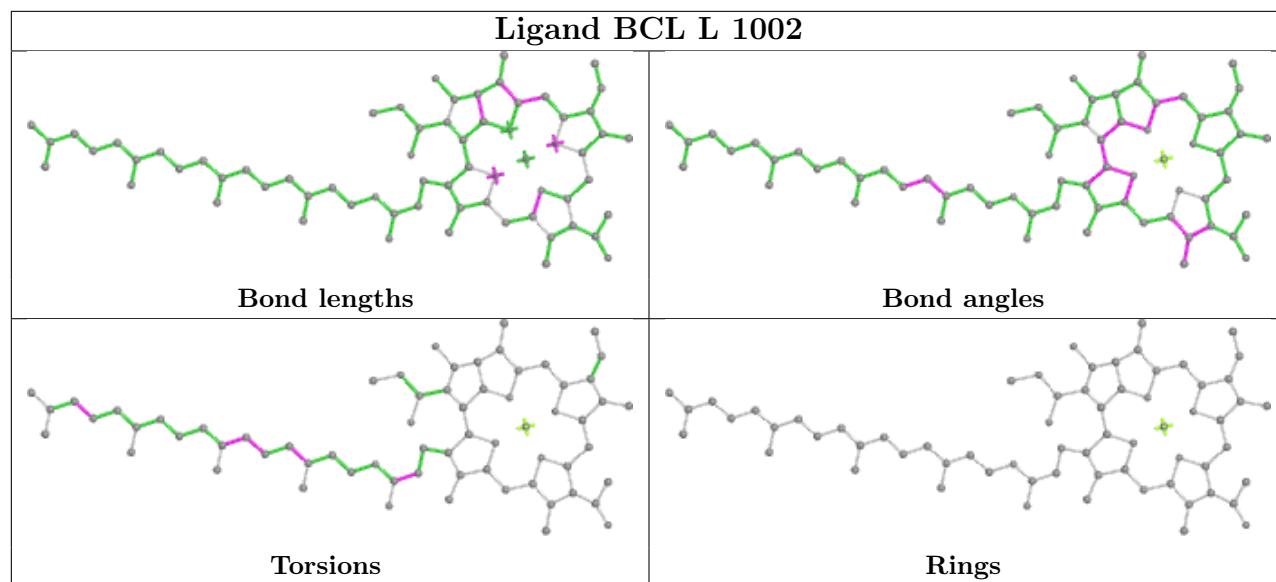












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

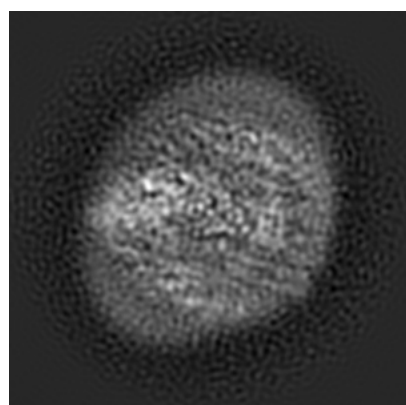
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6828. These allow visual inspection of the internal detail of the map and identification of artifacts.

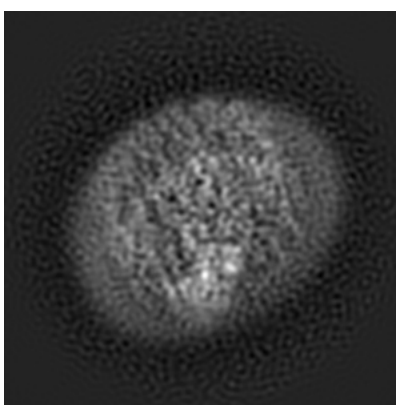
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

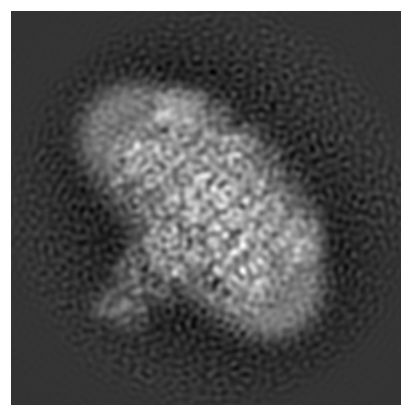
6.1.1 Primary map



X



Y

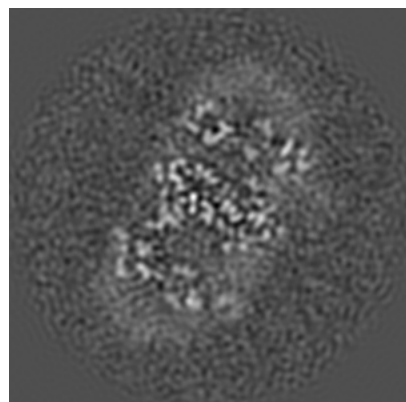


Z

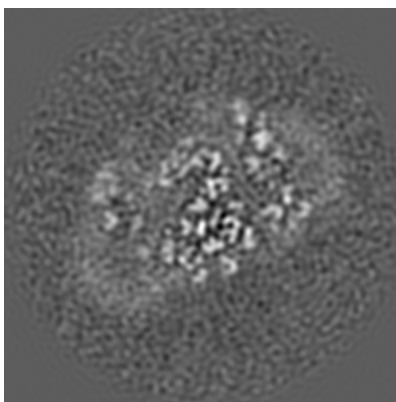
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

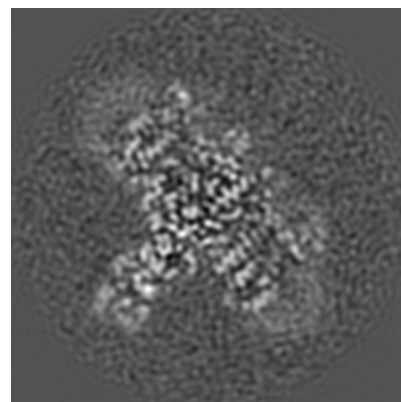
6.2.1 Primary map



X Index: 96



Y Index: 96

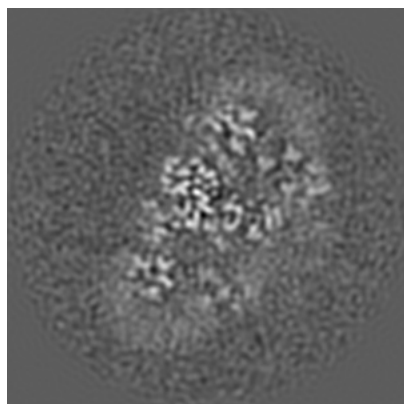


Z Index: 96

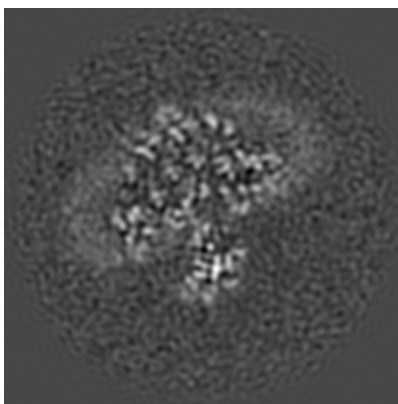
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

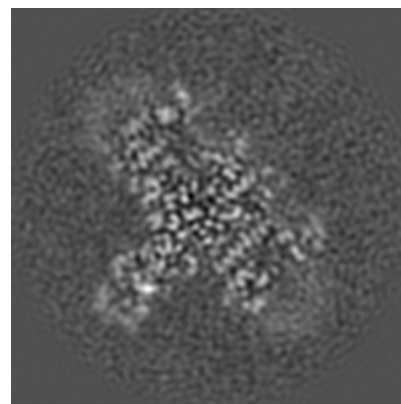
6.3.1 Primary map



X Index: 88



Y Index: 71

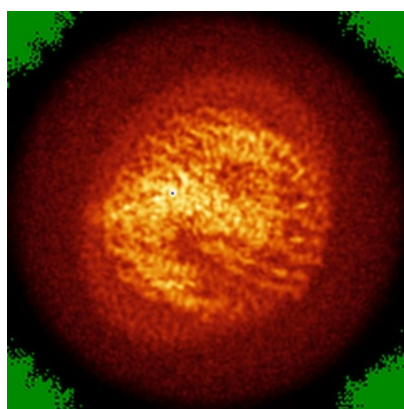


Z Index: 97

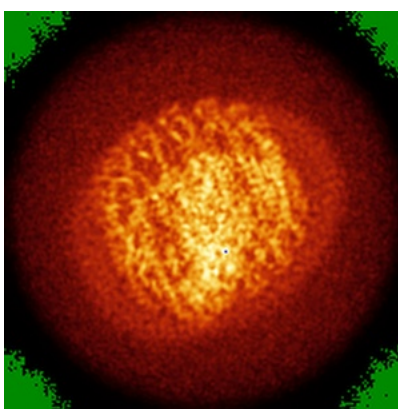
The images above show the largest variance slices of the map in three orthogonal directions.

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

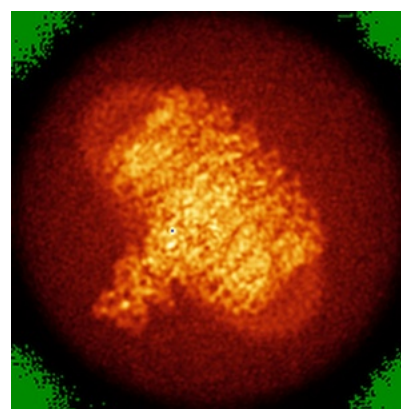
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

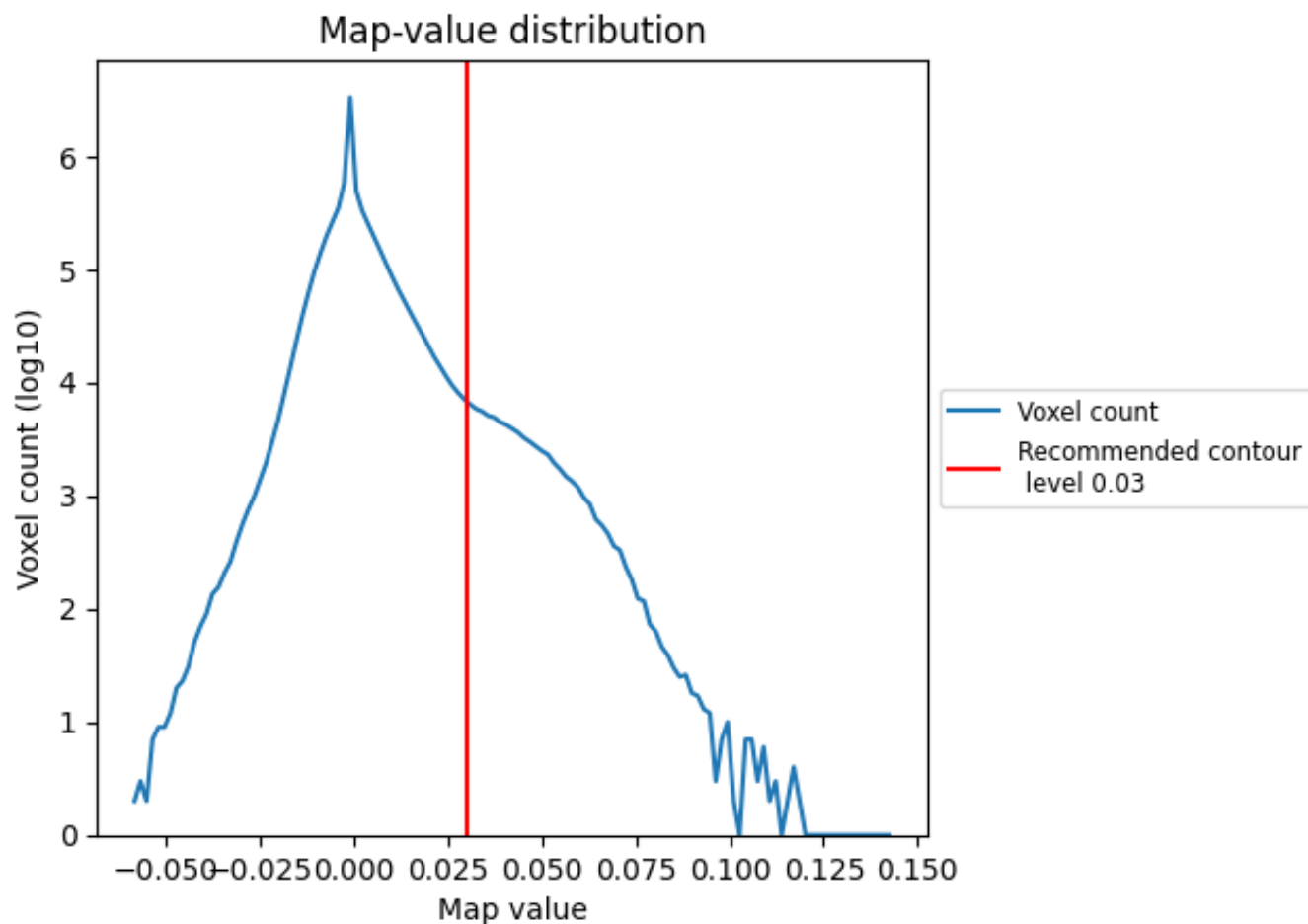
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

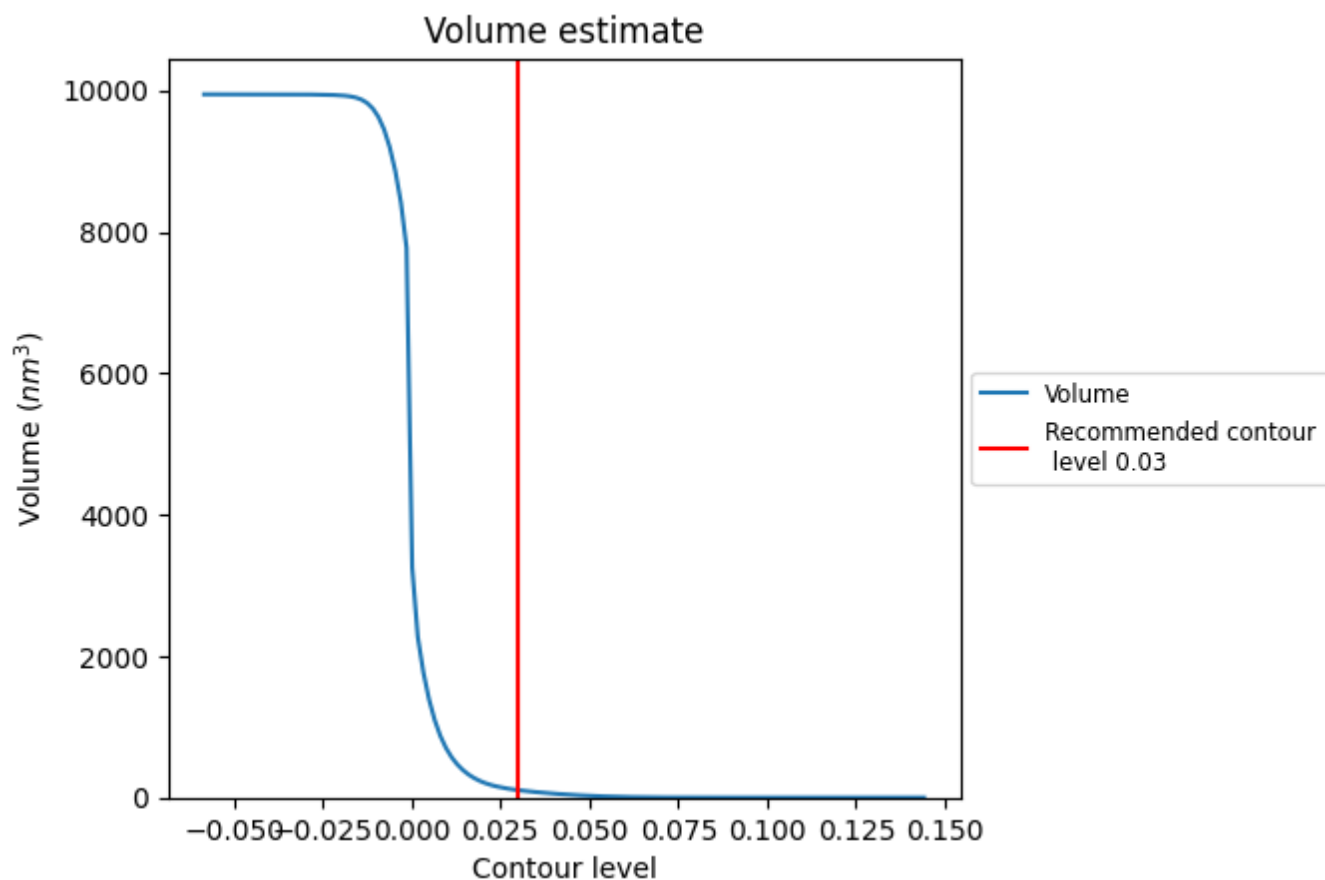
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

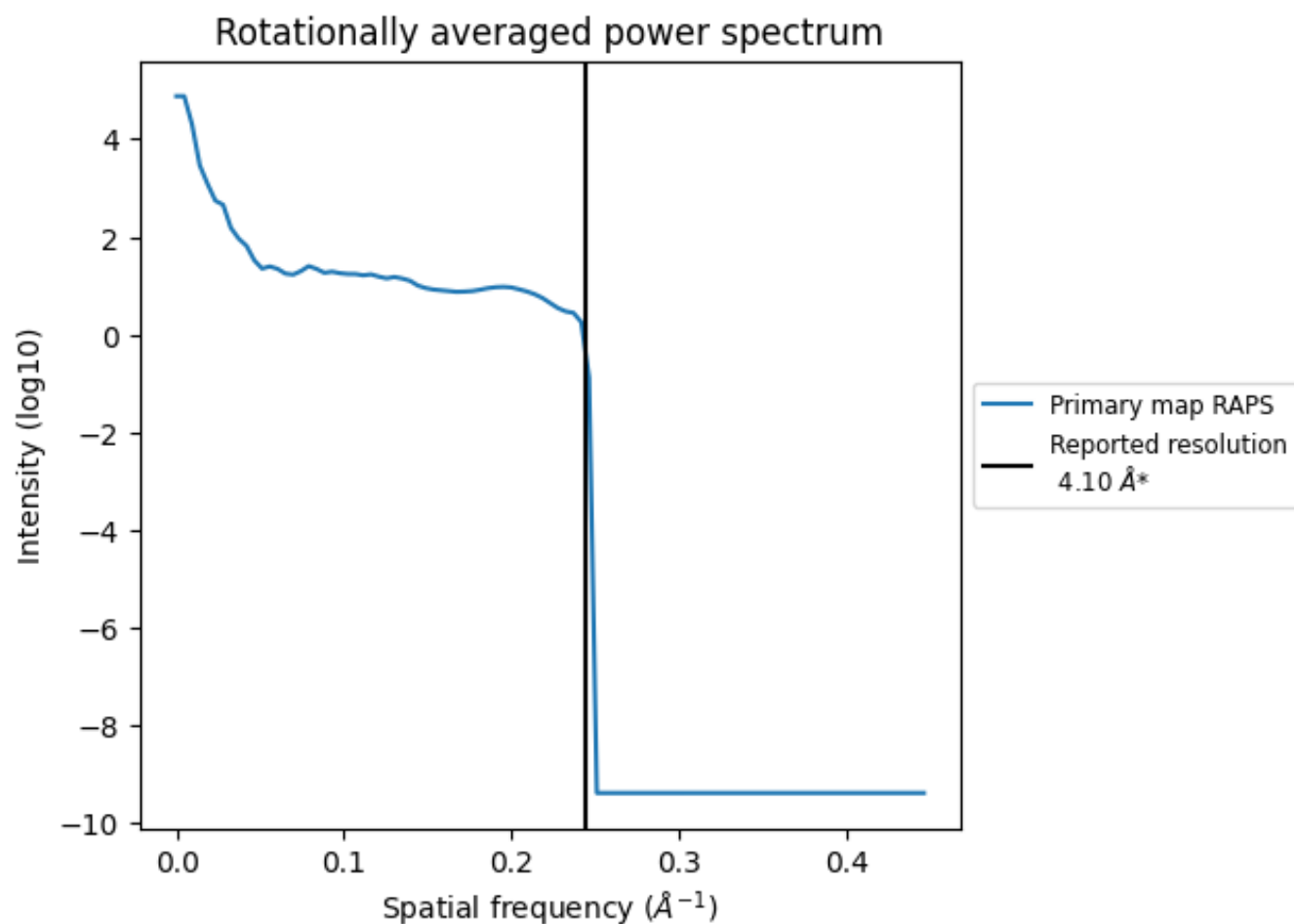
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 0.244 Å⁻¹

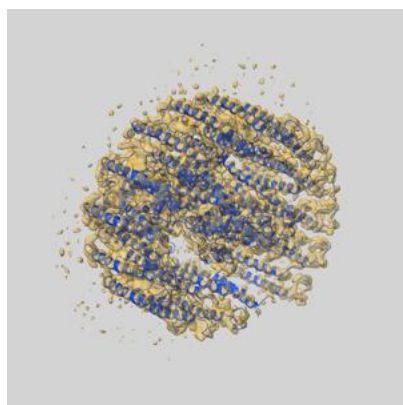
8 Fourier-Shell correlation ⓘ

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

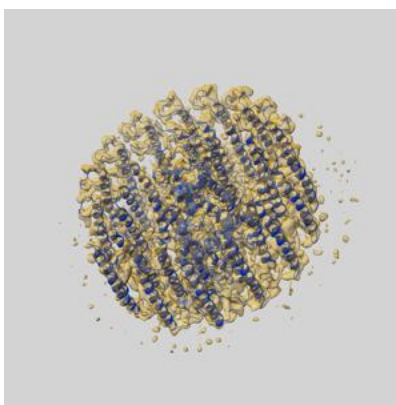
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6828 and PDB model 5YQ7. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

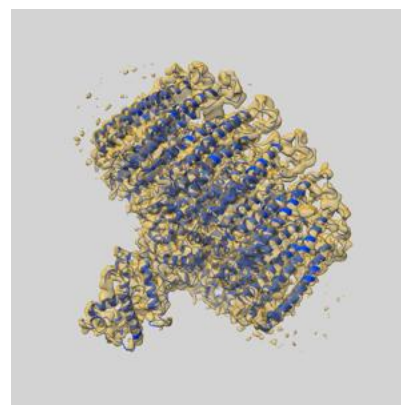
9.1 Map-model overlay [i](#)



X



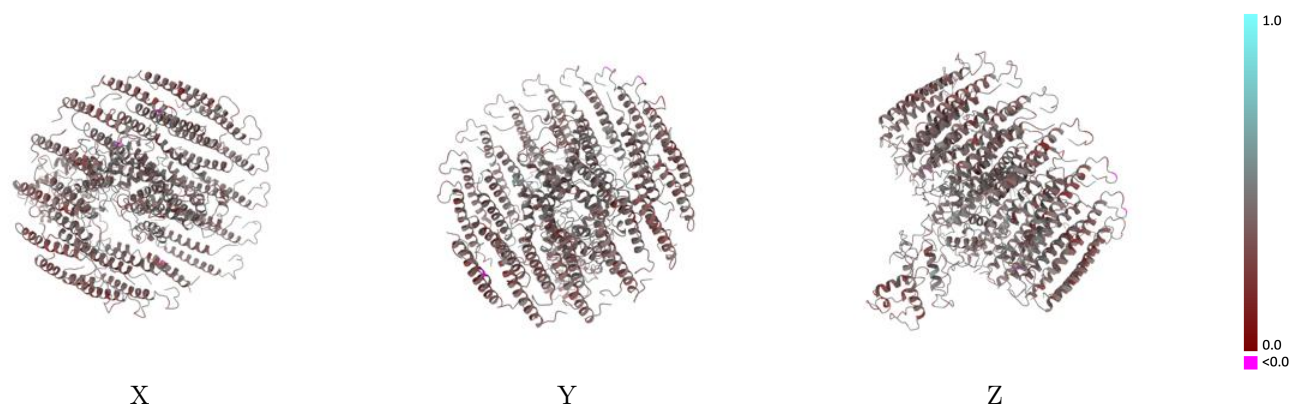
Y



Z

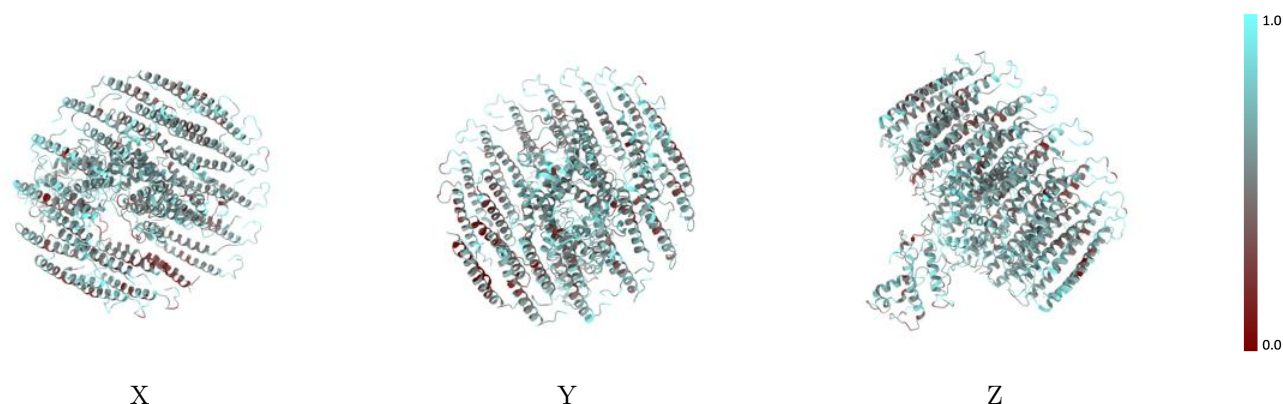
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



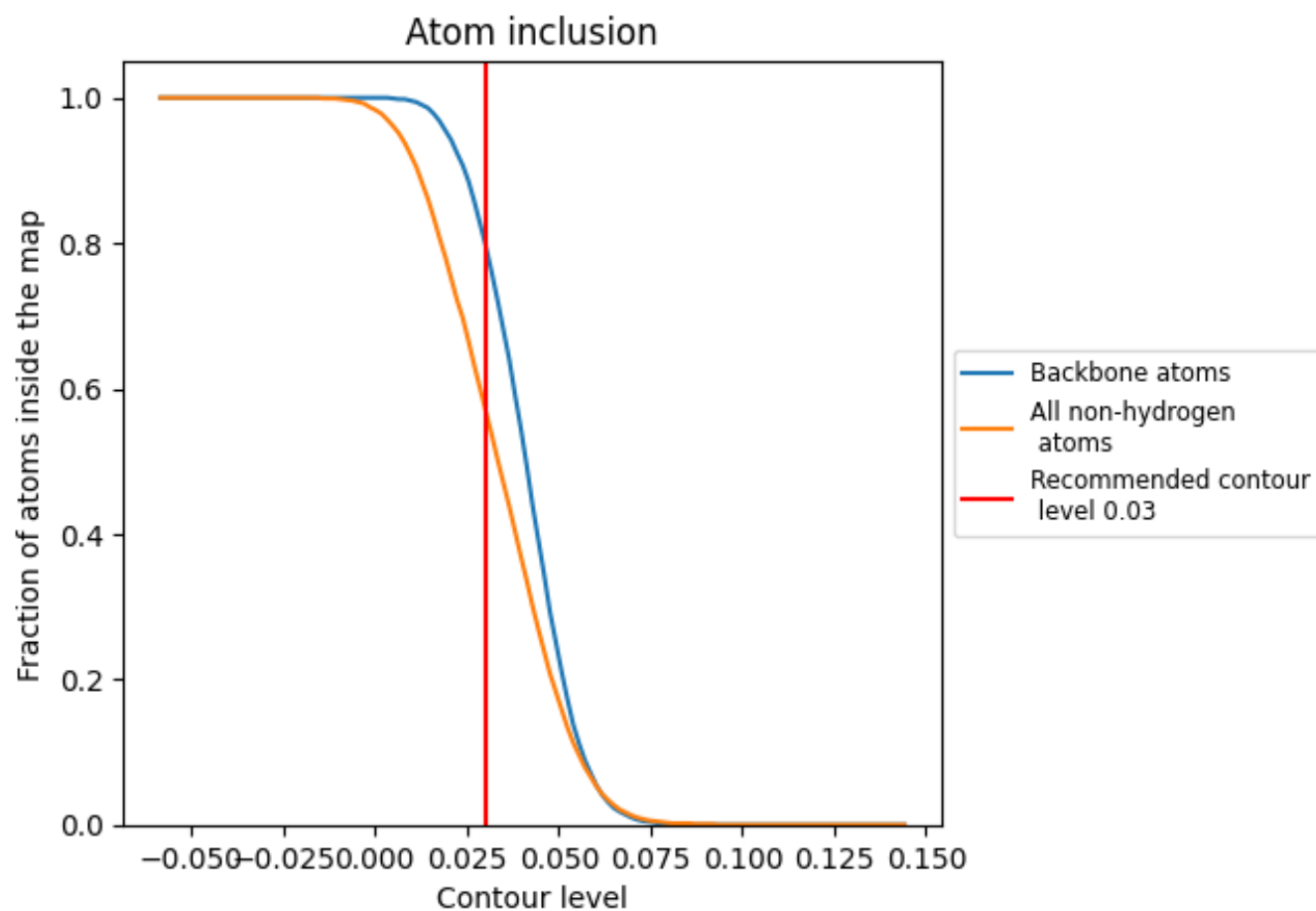
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5730	 0.4020
0	 0.6020	 0.3920
1	 0.5000	 0.4110
2	 0.5200	 0.3830
3	 0.4660	 0.3850
4	 0.5610	 0.3770
5	 0.5080	 0.3910
6	 0.5770	 0.3830
7	 0.5750	 0.4120
8	 0.5910	 0.3740
9	 0.5060	 0.4030
A	 0.5460	 0.4000
B	 0.6300	 0.3980
C	 0.6340	 0.3950
D	 0.5870	 0.4120
E	 0.6120	 0.3990
F	 0.5160	 0.4020
G	 0.5790	 0.3880
H	 0.5470	 0.4010
I	 0.5860	 0.3860
J	 0.5320	 0.3990
K	 0.5940	 0.4020
L	 0.5970	 0.4220
M	 0.6170	 0.4280
N	 0.4690	 0.3990
O	 0.5910	 0.3910
P	 0.5960	 0.4190
Q	 0.5810	 0.3960
R	 0.5180	 0.3920
S	 0.5990	 0.4020
T	 0.4440	 0.3910
U	 0.5590	 0.3950
V	 0.4480	 0.3660
W	 0.5290	 0.3790
X	 0.0430	 0.2960
Y	 0.7280	 0.4360

