



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:51 PM UTC

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:

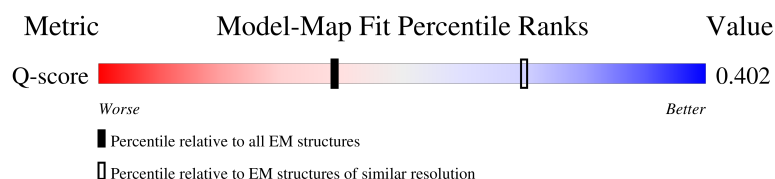
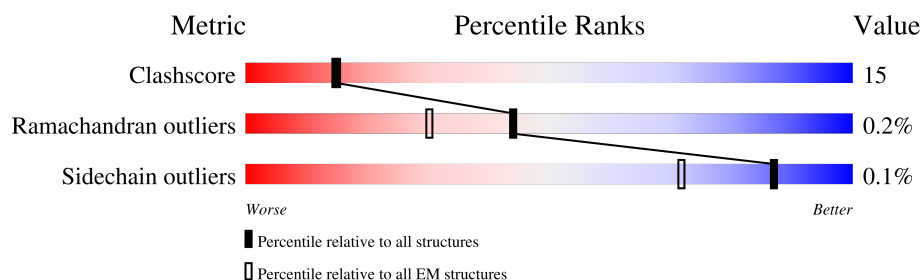
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	9% 64% 16% 20%
1	2	55	18% 65% 15% 20%
1	4	55	15% 62% 18% 20%
1	6	55	15% 69% 11% 20%

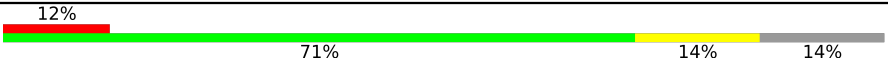
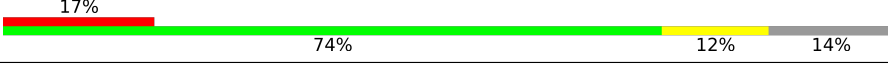
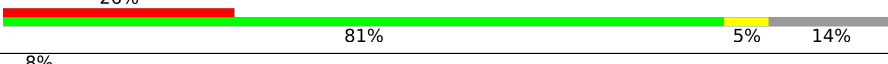
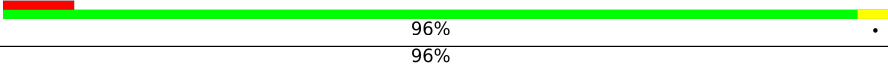
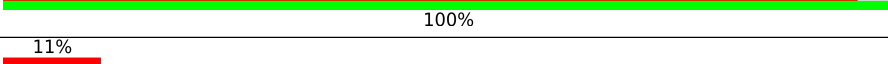
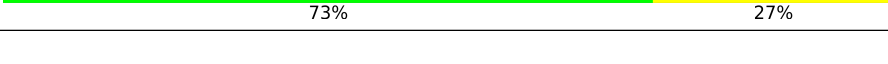
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Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	L	310	
3	C	320	
4	1	42	
4	3	42	
4	5	42	
4	7	42	
4	9	42	
4	A	42	
4	D	42	
4	F	42	
4	H	42	
4	J	42	
4	N	42	
4	P	42	

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Mol	Chain	Length	Quality of chain
4	R	42	
4	T	42	
4	V	42	
5	Y	25	
6	X	23	
7	M	306	

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		

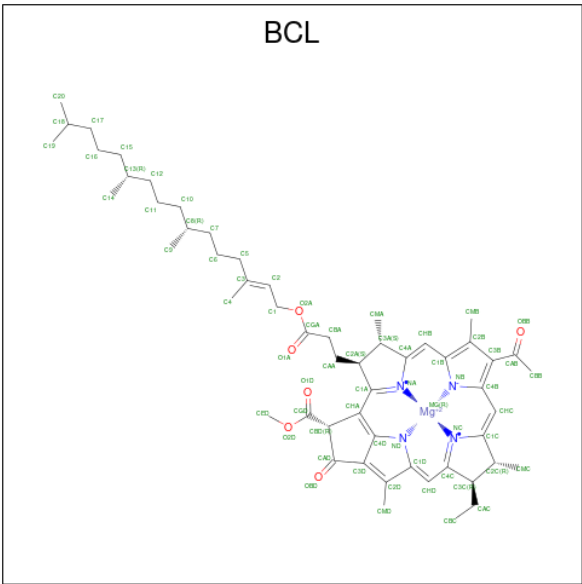
- Molecule 6 is a protein called Subunit X.

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).



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

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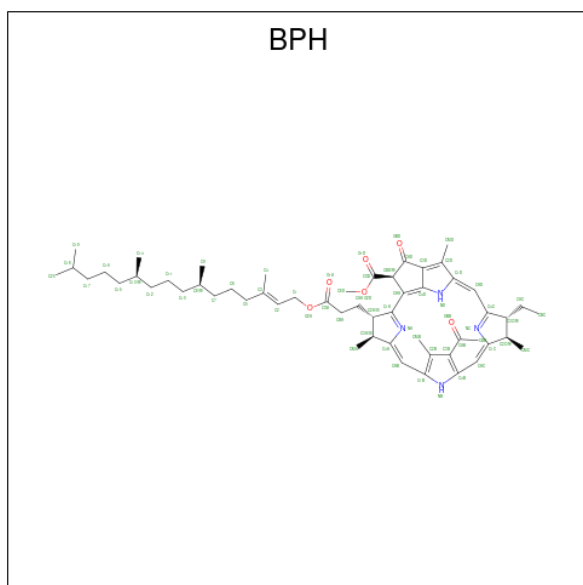
Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55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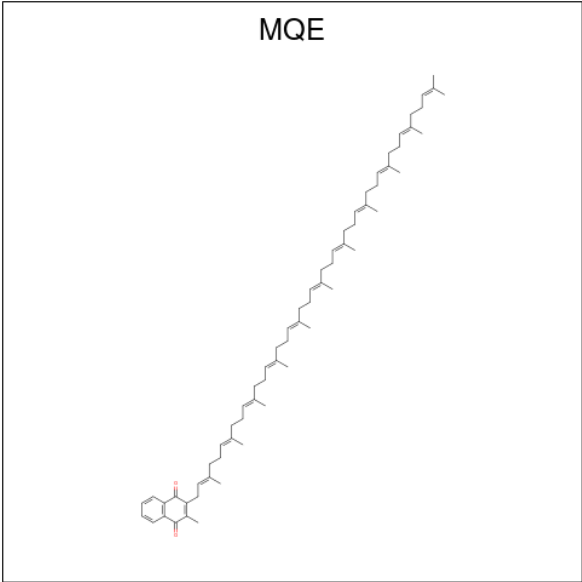
Mol	Chain	Residues	Atoms					AltConf
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



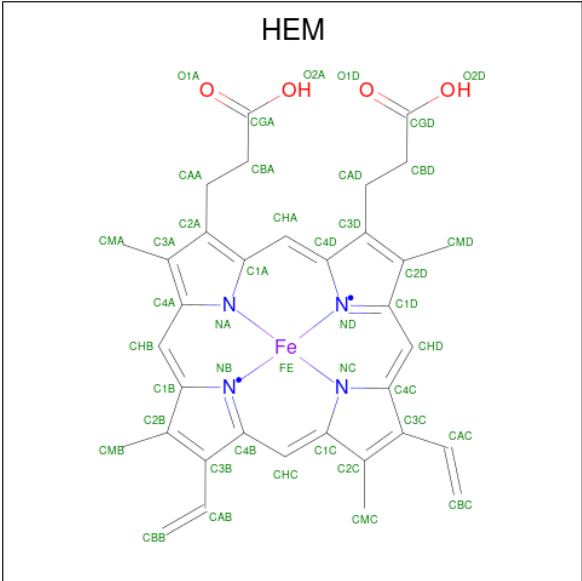
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	

- 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: $C_{34}H_{32}FeN_4O_4$).



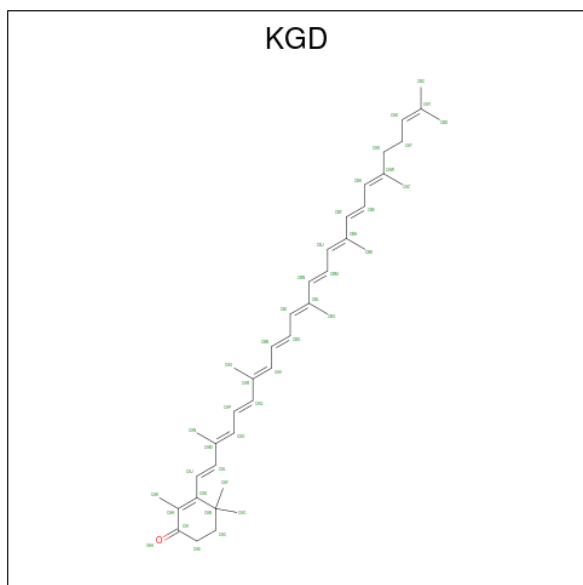
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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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	

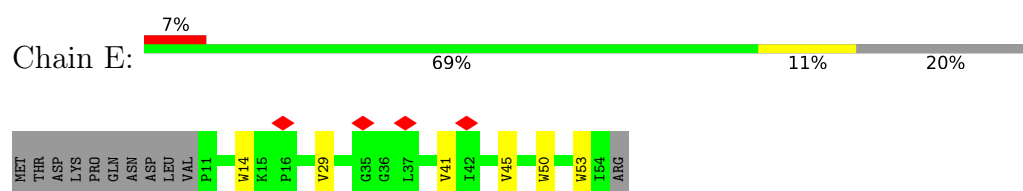
- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

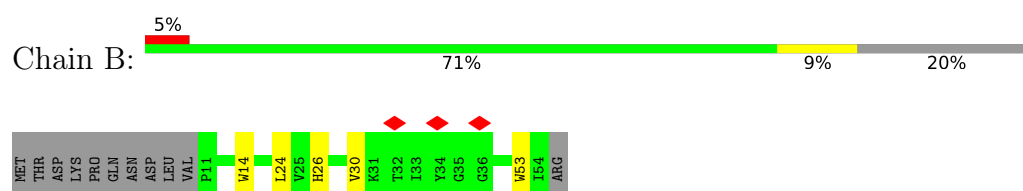
3 Residue-property plots [i](#)

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.

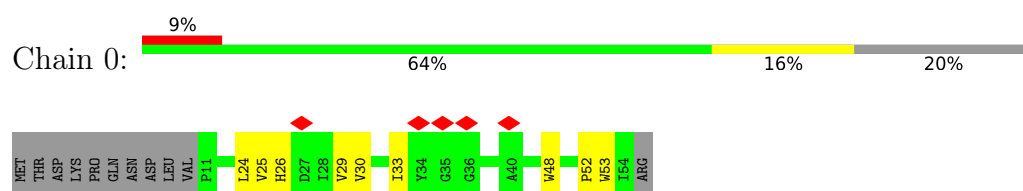
- Molecule 1: Beta subunit of light-harvesting 1



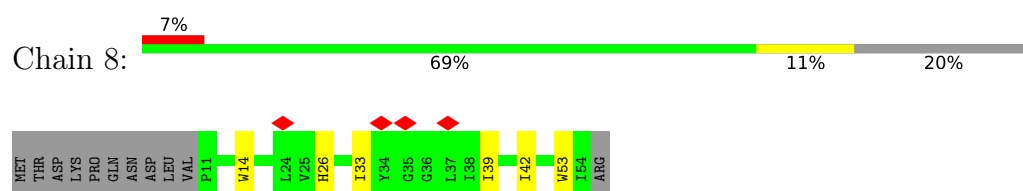
- Molecule 1: Beta subunit of light-harvesting 1



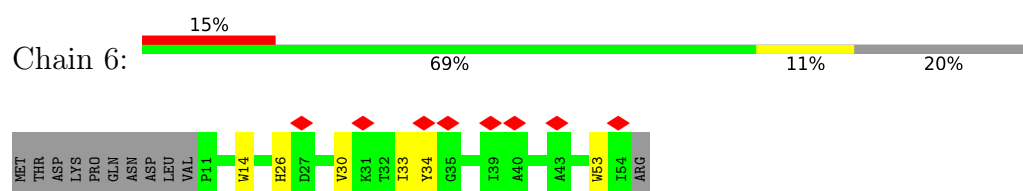
- Molecule 1: Beta subunit of light-harvesting 1



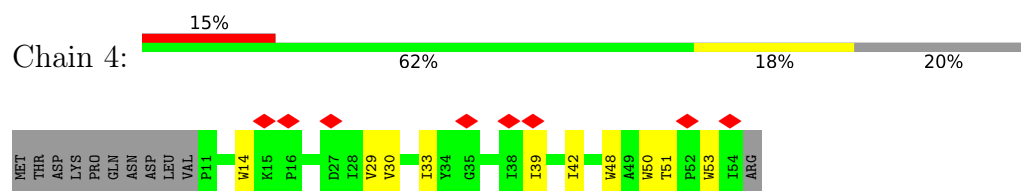
- Molecule 1: Beta subunit of light-harvesting 1



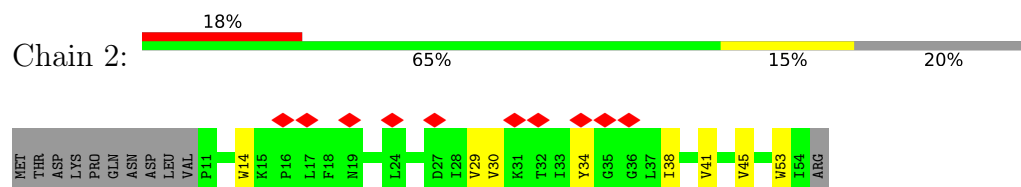
- Molecule 1: Beta subunit of light-harvesting 1



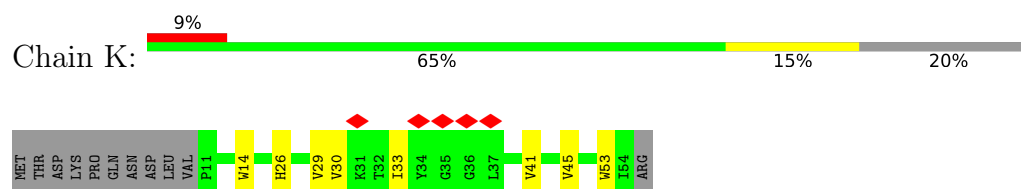
● Molecule 1: Beta subunit of light-harvesting 1



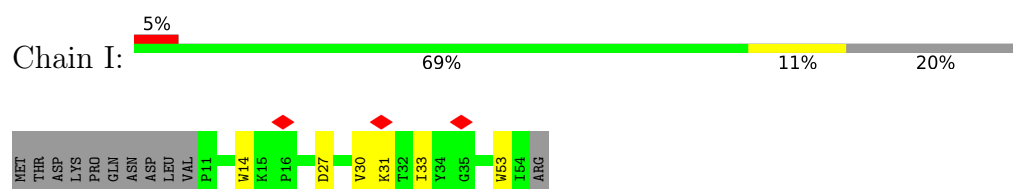
● Molecule 1: Beta subunit of light-harvesting 1



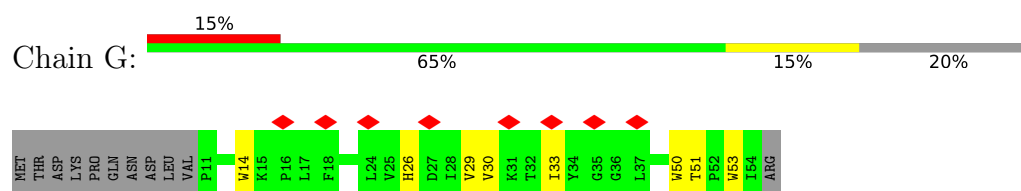
● Molecule 1: Beta subunit of light-harvesting 1



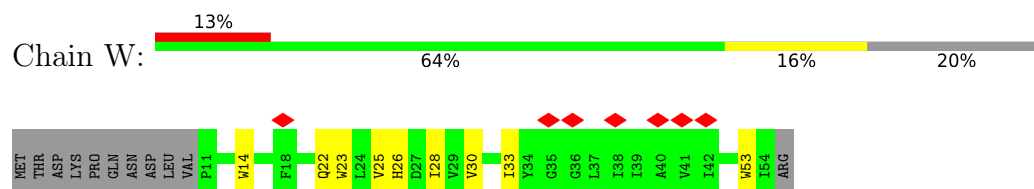
● Molecule 1: Beta subunit of light-harvesting 1



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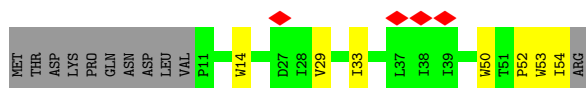


● Molecule 1: Beta subunit of light-harvesting 1





- Molecule 1: Beta subunit of light-harvesting 1



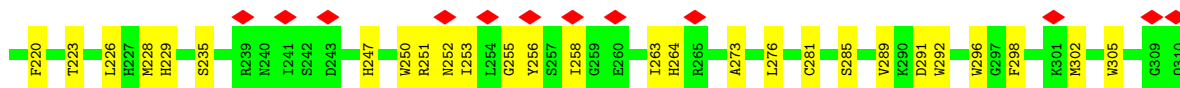
- Molecule 1: Beta subunit of light-harvesting 1



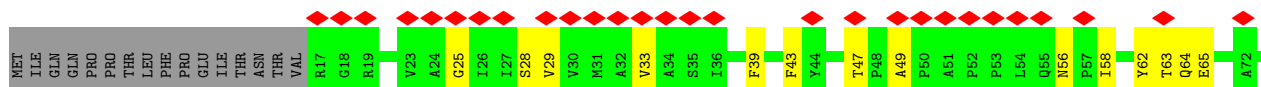
- Molecule 1: Beta subunit of light-harvesting 1

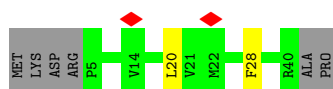
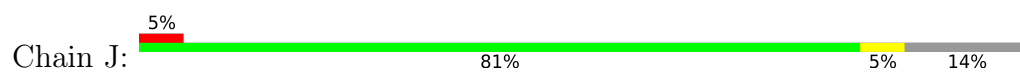


- Molecule 2: Precursor for L subunits of photosynthetic reaction center



- Molecule 3: Cytochrome subunit of photosynthetic reaction center

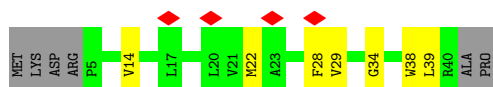




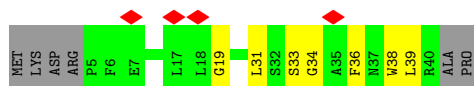
- Molecule 4: Alpha subunit of light-harvesting 1



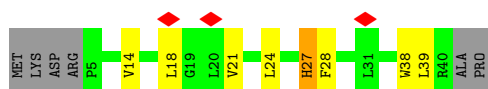
- Molecule 4: Alpha subunit of light-harvesting 1



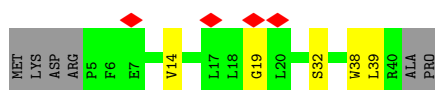
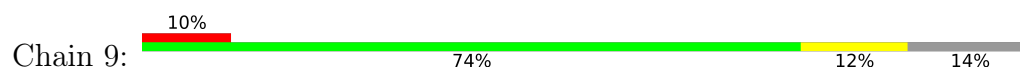
- Molecule 4: Alpha subunit of light-harvesting 1



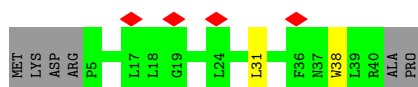
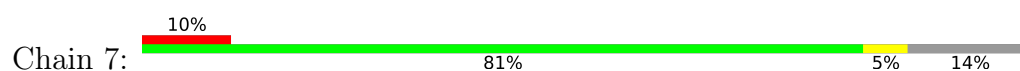
- Molecule 4: Alpha subunit of light-harvesting 1



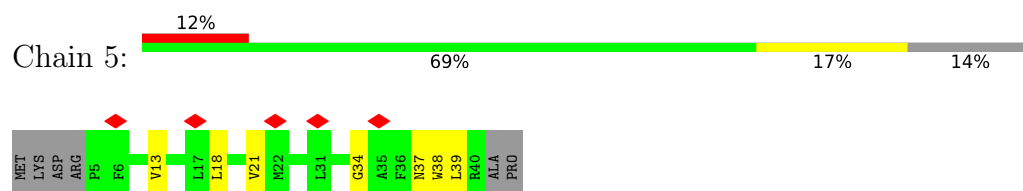
- Molecule 4: Alpha subunit of light-harvesting 1



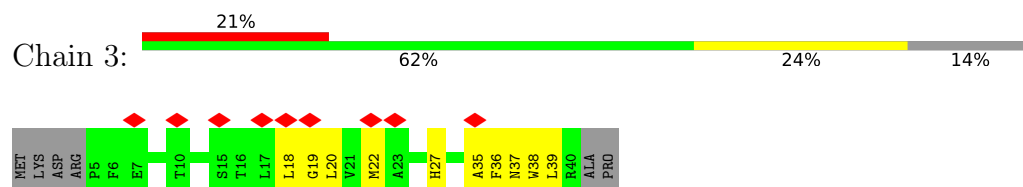
- Molecule 4: Alpha subunit of light-harvesting 1



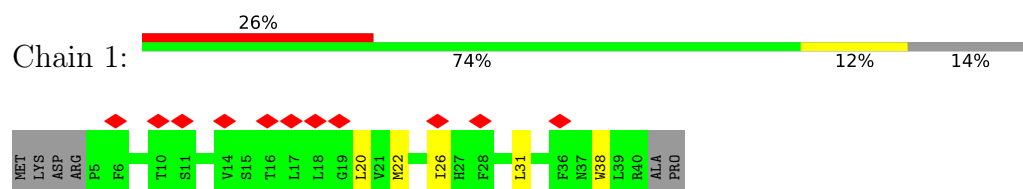
- Molecule 4: Alpha subunit of light-harvesting 1



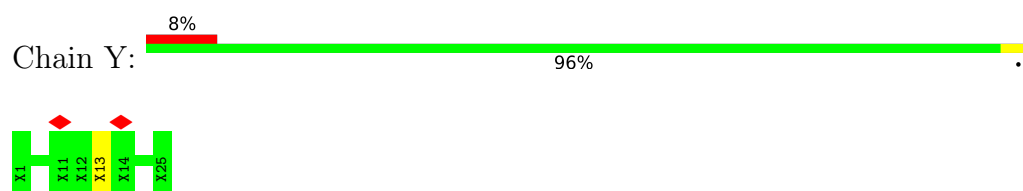
- Molecule 4: Alpha subunit of light-harvesting 1



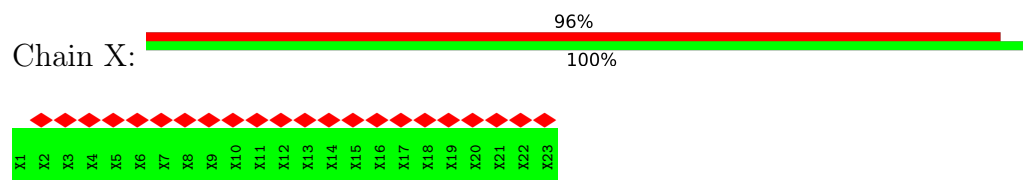
- Molecule 4: Alpha subunit of light-harvesting 1



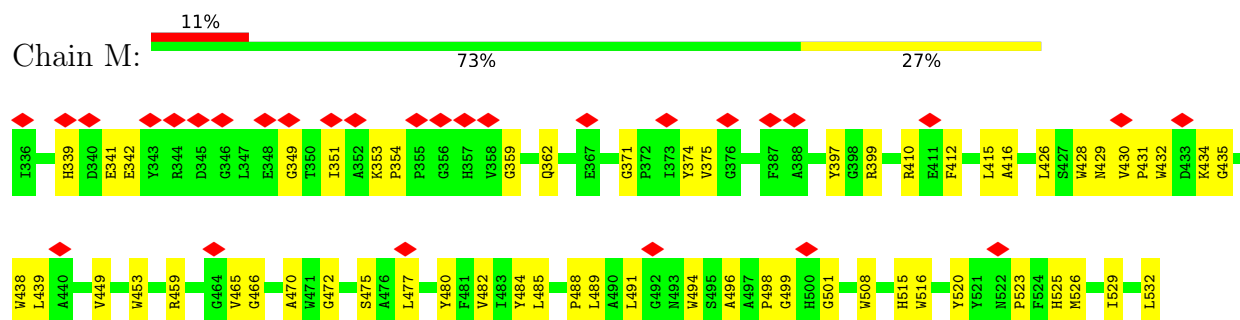
- Molecule 5: Peptide from Precursor for L and M subunits of photosynthetic reaction center



- 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 (Å)	215.04001, 215.04001, 215.04001	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: HEM, BCL, MQE, KGD, BPH, FE

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%)	36	70
3	C	291/320 (91%)	213 (73%)	76 (26%)	2 (1%)	18	55
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%)	36	70
All	All	2041/2391 (85%)	1738 (85%)	299 (15%)	4 (0%)	44	76

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%)	31	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%)	31	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%)	87	89

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	E	101	-	69,74,74	1.07	4 (5%)	79,115,115	1.46	10 (12%)
8	BCL	B	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.51	10 (12%)
8	BCL	O	101	1	69,74,74	1.07	5 (7%)	79,115,115	1.35	8 (10%)
8	BCL	Q	102	1	69,74,74	1.10	6 (8%)	79,115,115	1.50	11 (13%)
8	BCL	R	102	4,8	69,74,74	1.09	5 (7%)	79,115,115	1.50	11 (13%)
8	BCL	W	102	1	69,74,74	1.07	5 (7%)	79,115,115	1.36	8 (10%)
8	BCL	T	103	4	69,74,74	1.10	5 (7%)	79,115,115	1.34	7 (8%)
8	BCL	W	101	1	69,74,74	1.10	5 (7%)	79,115,115	4.09	11 (13%)
8	BCL	F	102	4	69,74,74	1.07	6 (8%)	79,115,115	1.54	10 (12%)
10	MQE	L	1004	-	69,69,69	3.94	19 (27%)	85,87,87	2.34	23 (27%)
8	BCL	Q	101	1	69,74,74	1.10	7 (10%)	79,115,115	1.38	9 (11%)
8	BCL	O	101	1	69,74,74	1.11	5 (7%)	79,115,115	1.45	10 (12%)
8	BCL	7	101	4	69,74,74	1.08	6 (8%)	79,115,115	1.39	9 (11%)
8	BCL	5	102	4	69,74,74	1.10	5 (7%)	79,115,115	1.43	8 (10%)
8	BCL	I	102	1	69,74,74	1.07	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	G	101	1	69,74,74	1.13	5 (7%)	79,115,115	1.47	11 (13%)
8	BCL	K	102	1	69,74,74	1.10	5 (7%)	79,115,115	1.41	9 (11%)
8	BCL	4	102	1	69,74,74	1.09	4 (5%)	79,115,115	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	C	504	3	50,50,50	1.30	5 (10%)	67,82,82	1.30	8 (11%)
8	BCL	P	101	4	69,74,74	1.08	6 (8%)	79,115,115	1.40	8 (10%)
8	BCL	M	703	7	69,74,74	1.10	6 (8%)	79,115,115	1.57	9 (11%)
8	BCL	V	101	4	69,74,74	1.09	6 (8%)	79,115,115	1.54	10 (12%)
12	KGD	5	101	-	41,41,41	4.74	25 (60%)	50,53,53	4.29	24 (48%)
8	BCL	L	1001	2	69,74,74	1.10	6 (8%)	79,115,115	1.40	7 (8%)
8	BCL	U	101	1	69,74,74	1.09	5 (7%)	79,115,115	4.11	14 (17%)
8	BCL	L	1002	2	69,74,74	1.12	5 (7%)	79,115,115	1.38	7 (8%)
9	BPH	M	704	-	59,70,70	1.17	3 (5%)	59,101,101	1.99	11 (18%)
12	KGD	H	102	-	41,41,41	4.40	25 (60%)	50,53,53	3.38	23 (46%)
8	BCL	S	102	1	69,74,74	1.08	5 (7%)	79,115,115	1.30	7 (8%)
8	BCL	8	102	1	69,74,74	1.10	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	K	101	1	69,74,74	1.08	4 (5%)	79,115,115	1.35	8 (10%)
8	BCL	N	103	4	69,74,74	1.09	6 (8%)	79,115,115	1.40	9 (11%)
8	BCL	S	101	1,8	69,74,74	1.08	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	9	103	4	69,74,74	1.09	5 (7%)	79,115,115	1.41	8 (10%)
8	BCL	0	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.47	10 (12%)
8	BCL	A	102	4	69,74,74	1.08	7 (10%)	79,115,115	1.38	9 (11%)
8	BCL	D	101	4	69,74,74	1.07	6 (8%)	79,115,115	1.49	10 (12%)
12	KGD	F	101	-	41,41,41	4.43	26 (63%)	50,53,53	4.01	23 (46%)
9	BPH	M	705	-	59,70,70	1.17	3 (5%)	59,101,101	1.85	10 (16%)
8	BCL	E	102	-	69,74,74	1.11	5 (7%)	79,115,115	1.47	10 (12%)
8	BCL	6	102	1	69,74,74	1.08	6 (8%)	79,115,115	1.38	7 (8%)
8	BCL	O	102	1	69,74,74	1.09	6 (8%)	79,115,115	1.32	6 (7%)
8	BCL	J	102	4	69,74,74	1.11	5 (7%)	79,115,115	1.44	8 (10%)
11	HEM	C	501	3	50,50,50	1.28	6 (12%)	67,82,82	0.98	1 (1%)
8	BCL	2	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.36	9 (11%)
8	BCL	B	101	1	69,74,74	1.12	4 (5%)	79,115,115	1.41	8 (10%)
11	HEM	C	502	3	50,50,50	1.29	6 (12%)	67,82,82	1.06	5 (7%)
11	HEM	C	503	3	50,50,50	1.28	5 (10%)	67,82,82	0.98	2 (2%)
12	KGD	N	102	-	41,41,41	4.50	25 (60%)	50,53,53	4.61	23 (46%)
12	KGD	T	101	-	41,41,41	4.58	25 (60%)	50,53,53	4.11	22 (44%)
12	KGD	9	102	-	41,41,41	4.54	26 (63%)	50,53,53	4.11	23 (46%)
8	BCL	6	101	1	69,74,74	1.10	6 (8%)	79,115,115	1.47	11 (13%)
9	BPH	L	1003	-	59,70,70	1.16	3 (5%)	59,101,101	1.92	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	KGD	N	101	-	41,41,41	4.47	26 (63%)	50,53,53	4.11	23 (46%)
12	KGD	9	101	-	41,41,41	4.30	25 (60%)	50,53,53	4.15	20 (40%)
12	KGD	J	101	-	41,41,41	4.36	25 (60%)	50,53,53	4.08	23 (46%)
8	BCL	G	102	1	69,74,74	1.08	5 (7%)	79,115,115	1.38	7 (8%)
8	BCL	U	102	1	69,74,74	1.10	6 (8%)	79,115,115	1.41	7 (8%)
12	KGD	T	102	-	41,41,41	4.61	25 (60%)	50,53,53	4.30	23 (46%)
8	BCL	2	101	1	69,74,74	1.09	6 (8%)	79,115,115	1.39	7 (8%)
8	BCL	4	101	1,8	69,74,74	1.12	6 (8%)	79,115,115	1.48	11 (13%)
12	KGD	R	101	-	41,41,41	4.21	25 (60%)	50,53,53	4.04	24 (48%)
12	KGD	A	101	-	41,41,41	4.35	25 (60%)	50,53,53	3.69	20 (40%)
8	BCL	3	102	4,8	69,74,74	1.10	6 (8%)	79,115,115	1.51	11 (13%)
8	BCL	H	101	4	69,74,74	1.11	7 (10%)	79,115,115	1.45	8 (10%)
8	BCL	1	101	4	69,74,74	1.09	5 (7%)	79,115,115	1.37	7 (8%)
8	BCL	8	101	1	69,74,74	1.07	5 (7%)	79,115,115	1.45	8 (10%)
10	MQE	M	702	-	69,69,69	3.81	19 (27%)	85,87,87	2.85	30 (35%)
12	KGD	3	101	-	41,41,41	4.40	25 (60%)	50,53,53	4.20	23 (46%)
8	BCL	I	101	1	69,74,74	1.09	6 (8%)	79,115,115	1.44	9 (11%)
12	KGD	3	103	-	41,41,41	4.53	26 (63%)	50,53,53	3.61	25 (50%)

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	E	101	-	-	5/41/137/137	-
8	BCL	B	102	1	-	7/41/137/137	-
8	BCL	0	101	1	-	7/41/137/137	-
8	BCL	Q	102	1	-	12/41/137/137	-
8	BCL	R	102	4,8	-	8/41/137/137	-
8	BCL	W	102	1	-	10/41/137/137	-
8	BCL	T	103	4	-	4/41/137/137	-
8	BCL	W	101	1	-	3/41/137/137	-
8	BCL	F	102	4	-	11/41/137/137	-
10	MQE	L	1004	-	-	12/65/85/85	0/2/2/2
8	BCL	Q	101	1	-	5/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	O	101	1	-	2/41/137/137	-
8	BCL	7	101	4	-	4/41/137/137	-
8	BCL	5	102	4	-	6/41/137/137	-
8	BCL	I	102	1	-	12/41/137/137	-
8	BCL	G	101	1	-	5/41/137/137	-
8	BCL	K	102	1	-	8/41/137/137	-
8	BCL	4	102	1	-	12/41/137/137	-
11	HEM	C	504	3	-	2/14/54/54	-
8	BCL	P	101	4	-	2/41/137/137	-
8	BCL	M	703	7	-	4/41/137/137	-
8	BCL	V	101	4	-	3/41/137/137	-
12	KGD	5	101	-	-	2/36/56/56	0/1/1/1
8	BCL	L	1001	2	-	13/41/137/137	-
8	BCL	U	101	1	-	3/41/137/137	-
8	BCL	L	1002	2	-	5/41/137/137	-
9	BPH	M	704	-	-	5/37/105/105	0/5/6/6
12	KGD	H	102	-	-	2/36/56/56	0/1/1/1
8	BCL	S	102	1	-	5/41/137/137	-
8	BCL	8	102	1	-	12/41/137/137	-
8	BCL	K	101	1	-	4/41/137/137	-
8	BCL	N	103	4	-	6/41/137/137	-
8	BCL	S	101	1,8	-	7/41/137/137	-
8	BCL	9	103	4	-	6/41/137/137	-
8	BCL	0	102	1	-	7/41/137/137	-
8	BCL	A	102	4	-	8/41/137/137	-
8	BCL	D	101	4	-	6/41/137/137	-
12	KGD	F	101	-	-	0/36/56/56	0/1/1/1
9	BPH	M	705	-	-	2/37/105/105	0/5/6/6
8	BCL	E	102	-	-	11/41/137/137	-
8	BCL	6	102	1	-	5/41/137/137	-
8	BCL	O	102	1	-	7/41/137/137	-
8	BCL	J	102	4	-	2/41/137/137	-
11	HEM	C	501	3	-	2/14/54/54	-
8	BCL	2	102	1	-	14/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	B	101	1	-	7/41/137/137	-
11	HEM	C	502	3	-	2/14/54/54	-
11	HEM	C	503	3	-	0/14/54/54	-
12	KGD	N	102	-	-	1/36/56/56	0/1/1/1
12	KGD	T	101	-	-	0/36/56/56	0/1/1/1
12	KGD	9	102	-	-	2/36/56/56	0/1/1/1
8	BCL	6	101	1	-	5/41/137/137	-
9	BPH	L	1003	-	-	7/37/105/105	0/5/6/6
12	KGD	N	101	-	-	0/36/56/56	0/1/1/1
12	KGD	9	101	-	-	1/36/56/56	0/1/1/1
12	KGD	J	101	-	-	0/36/56/56	0/1/1/1
8	BCL	G	102	1	-	10/41/137/137	-
8	BCL	U	102	1	-	8/41/137/137	-
12	KGD	T	102	-	-	1/36/56/56	0/1/1/1
8	BCL	2	101	1	-	3/41/137/137	-
8	BCL	4	101	1,8	-	9/41/137/137	-
12	KGD	R	101	-	-	2/36/56/56	0/1/1/1
12	KGD	A	101	-	-	2/36/56/56	0/1/1/1
8	BCL	3	102	4,8	-	4/41/137/137	-
8	BCL	H	101	4	-	5/41/137/137	-
8	BCL	1	101	4	-	4/41/137/137	-
8	BCL	8	101	1	-	4/41/137/137	-
10	MQE	M	702	-	-	17/65/85/85	0/2/2/2
12	KGD	3	101	-	-	2/36/56/56	0/1/1/1
8	BCL	I	101	1	-	0/41/137/137	-
12	KGD	3	103	-	-	1/36/56/56	0/1/1/1

All (685) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	103	KGD	CAE-CAI	-10.12	1.37	1.50
12	9	102	KGD	CAE-CAI	-10.05	1.37	1.50
12	5	101	KGD	CAE-CAI	-10.00	1.37	1.50
12	N	102	KGD	CAE-CAI	-9.92	1.37	1.50
12	A	101	KGD	CAE-CAI	-9.87	1.37	1.50
12	F	101	KGD	CAE-CAI	-9.78	1.37	1.50
12	T	102	KGD	CAE-CAI	-9.73	1.37	1.50
12	T	101	KGD	CAE-CAI	-9.72	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	101	KGD	CAE-CAI	-9.68	1.37	1.50
12	R	101	KGD	CAE-CAI	-9.68	1.37	1.50
12	9	101	KGD	CAE-CAI	-9.66	1.37	1.50
12	N	101	KGD	CAE-CAI	-9.65	1.38	1.50
12	3	101	KGD	CAE-CAI	-9.61	1.38	1.50
12	H	102	KGD	CAE-CAI	-9.50	1.38	1.50
10	L	1004	MQE	CBF-CAV	9.26	1.54	1.33
10	L	1004	MQE	CBI-CAZ	9.22	1.54	1.33
10	L	1004	MQE	CBH-CAW	9.22	1.54	1.33
10	L	1004	MQE	CBG-CAT	9.19	1.54	1.33
10	L	1004	MQE	CBL-CBB	9.13	1.54	1.33
10	L	1004	MQE	CBD-CAR	9.11	1.54	1.33
10	L	1004	MQE	CBC-CAP	9.07	1.53	1.33
10	M	702	MQE	CBF-CAV	9.01	1.53	1.33
10	M	702	MQE	CBI-CAZ	8.98	1.53	1.33
10	L	1004	MQE	CBE-CAQ	8.96	1.53	1.33
10	M	702	MQE	CBN-CBM	8.87	1.53	1.33
10	L	1004	MQE	CCB-CCC	8.87	1.53	1.33
10	M	702	MQE	CBH-CAW	8.85	1.53	1.33
10	M	702	MQE	CCB-CCC	8.80	1.53	1.33
10	M	702	MQE	CBC-CAP	8.75	1.53	1.33
10	M	702	MQE	CBL-CBB	8.71	1.53	1.33
10	L	1004	MQE	CBN-CBM	8.69	1.53	1.33
10	M	702	MQE	CBG-CAT	8.58	1.52	1.33
12	5	101	KGD	CAB-CAD	-8.55	1.42	1.53
10	M	702	MQE	CBE-CAQ	8.52	1.52	1.33
12	T	102	KGD	CAB-CAD	-8.44	1.43	1.53
10	M	702	MQE	CBD-CAR	8.38	1.52	1.33
12	T	101	KGD	CAB-CAD	-8.24	1.43	1.53
12	N	101	KGD	CAB-CAD	-8.21	1.43	1.53
12	F	101	KGD	CAB-CAD	-8.16	1.43	1.53
12	N	102	KGD	CAB-CAD	-8.14	1.43	1.53
12	A	101	KGD	CAB-CAD	-8.12	1.43	1.53
12	3	101	KGD	CAB-CAD	-7.96	1.43	1.53
12	9	102	KGD	CAB-CAD	-7.93	1.43	1.53
12	3	103	KGD	CAB-CAD	-7.91	1.43	1.53
12	9	101	KGD	CAB-CAD	-7.88	1.43	1.53
12	5	101	KGD	CAO-CAM	7.75	1.53	1.35
12	H	102	KGD	CAX-CAY	7.68	1.55	1.32
12	H	102	KGD	CBI-CBL	7.61	1.53	1.35
12	5	101	KGD	CBE-CBF	7.59	1.54	1.34
12	5	101	KGD	CBJ-CBH	7.56	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	101	KGD	CAB-CAD	-7.56	1.44	1.53
12	5	101	KGD	CBI-CBL	7.56	1.53	1.35
12	5	101	KGD	CAV-CAR	7.55	1.53	1.35
12	T	101	KGD	CBJ-CBH	7.50	1.53	1.35
12	T	101	KGD	CAV-CAR	7.49	1.53	1.35
12	9	102	KGD	CAO-CAM	7.48	1.53	1.35
12	T	101	KGD	CAO-CAM	7.48	1.53	1.35
12	T	102	KGD	CAV-CAR	7.47	1.53	1.35
12	T	102	KGD	CBJ-CBH	7.46	1.53	1.35
12	H	102	KGD	CAB-CAD	-7.45	1.44	1.53
12	N	102	KGD	CAO-CAM	7.41	1.52	1.35
12	T	102	KGD	CBI-CBL	7.41	1.52	1.35
12	5	101	KGD	CAL-CAJ	7.40	1.55	1.33
12	3	103	KGD	CBI-CBL	7.40	1.52	1.35
12	T	101	KGD	CBI-CBL	7.36	1.52	1.35
12	5	101	KGD	CAX-CAY	7.34	1.54	1.32
12	T	102	KGD	CAO-CAM	7.32	1.52	1.35
12	T	102	KGD	CAP-CAQ	7.32	1.53	1.34
12	F	101	KGD	CAV-CAR	7.31	1.52	1.35
12	5	101	KGD	CAP-CAQ	7.28	1.53	1.34
12	N	102	KGD	CAV-CAR	7.28	1.52	1.35
12	N	101	KGD	CBI-CBL	7.28	1.52	1.35
12	3	103	KGD	CAO-CAM	7.27	1.52	1.35
12	T	102	KGD	CAL-CAJ	7.26	1.54	1.33
12	R	101	KGD	CAB-CAD	-7.26	1.44	1.53
12	9	102	KGD	CAL-CAJ	7.24	1.54	1.33
12	N	101	KGD	CAO-CAM	7.22	1.52	1.35
12	9	102	KGD	CAV-CAR	7.22	1.52	1.35
12	J	101	KGD	CAX-CAY	7.22	1.54	1.32
12	3	101	KGD	CAV-CAR	7.19	1.52	1.35
12	F	101	KGD	CBI-CBL	7.19	1.52	1.35
12	N	102	KGD	CBI-CBL	7.19	1.52	1.35
12	9	102	KGD	CBI-CBL	7.19	1.52	1.35
12	3	101	KGD	CBI-CBL	7.18	1.52	1.35
12	N	101	KGD	CAV-CAR	7.17	1.52	1.35
12	A	101	KGD	CAX-CAY	7.17	1.53	1.32
12	A	101	KGD	CAV-CAR	7.16	1.52	1.35
12	F	101	KGD	CAO-CAM	7.15	1.52	1.35
12	H	102	KGD	CBJ-CBH	7.15	1.52	1.35
12	N	102	KGD	CBJ-CBH	7.10	1.52	1.35
12	3	101	KGD	CBJ-CBH	7.10	1.52	1.35
12	T	101	KGD	CBM-CBN	7.10	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	101	KGD	CAP-CAQ	7.09	1.53	1.34
12	9	101	KGD	CAX-CAY	7.09	1.53	1.32
12	3	101	KGD	CAO-CAM	7.08	1.52	1.35
12	N	101	KGD	CBJ-CBH	7.08	1.52	1.35
12	T	102	KGD	CBE-CBF	7.08	1.53	1.34
12	3	103	KGD	CAV-CAR	7.07	1.52	1.35
10	M	702	MQE	CCM-CCN	7.07	1.53	1.32
12	3	103	KGD	CBJ-CBH	7.07	1.52	1.35
12	N	102	KGD	CAX-CAY	7.06	1.53	1.32
12	H	102	KGD	CBM-CBN	7.06	1.53	1.34
12	9	102	KGD	CBJ-CBH	7.06	1.52	1.35
12	A	101	KGD	CAO-CAM	7.03	1.52	1.35
12	3	103	KGD	CAX-CAY	7.02	1.53	1.32
12	9	102	KGD	CAP-CAQ	7.01	1.53	1.34
12	J	101	KGD	CBJ-CBH	7.01	1.52	1.35
12	R	101	KGD	CAX-CAY	7.01	1.53	1.32
12	3	103	KGD	CBE-CBF	7.00	1.52	1.34
10	L	1004	MQE	CCM-CCN	7.00	1.53	1.32
12	F	101	KGD	CBJ-CBH	6.99	1.52	1.35
12	T	102	KGD	CBM-CBN	6.98	1.52	1.34
12	N	101	KGD	CAL-CAJ	6.98	1.53	1.33
12	9	101	KGD	CBI-CBL	6.98	1.51	1.35
12	R	101	KGD	CBI-CBL	6.97	1.51	1.35
12	J	101	KGD	CBI-CBL	6.97	1.51	1.35
12	3	101	KGD	CAX-CAY	6.96	1.53	1.32
12	T	101	KGD	CAL-CAJ	6.96	1.53	1.33
12	9	102	KGD	CBM-CBN	6.95	1.52	1.34
12	A	101	KGD	CBI-CBL	6.94	1.51	1.35
12	N	101	KGD	CBM-CBN	6.93	1.52	1.34
12	J	101	KGD	CAO-CAM	6.91	1.51	1.35
12	J	101	KGD	CAV-CAR	6.91	1.51	1.35
12	T	101	KGD	CBE-CBF	6.90	1.52	1.34
12	9	101	KGD	CBJ-CBH	6.89	1.51	1.35
12	N	102	KGD	CAL-CAJ	6.88	1.53	1.33
12	N	102	KGD	CAP-CAQ	6.86	1.52	1.34
12	H	102	KGD	CAV-CAR	6.86	1.51	1.35
12	F	101	KGD	CAX-CAY	6.86	1.53	1.32
12	N	102	KGD	CBE-CBF	6.86	1.52	1.34
12	3	103	KGD	CBM-CBN	6.85	1.52	1.34
12	T	102	KGD	CAX-CAY	6.84	1.52	1.32
12	T	101	KGD	CAX-CAY	6.84	1.52	1.32
12	F	101	KGD	CAP-CAQ	6.84	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	101	KGD	CAL-CAJ	6.82	1.53	1.33
12	N	101	KGD	CAX-CAY	6.82	1.52	1.32
12	A	101	KGD	CBJ-CBH	6.81	1.51	1.35
12	F	101	KGD	CBM-CBN	6.81	1.52	1.34
12	R	101	KGD	CBJ-CBH	6.80	1.51	1.35
12	A	101	KGD	CAP-CAQ	6.80	1.52	1.34
12	3	101	KGD	CBM-CBN	6.79	1.52	1.34
12	9	101	KGD	CAV-CAR	6.79	1.51	1.35
12	9	102	KGD	CAX-CAY	6.78	1.52	1.32
12	N	101	KGD	CAP-CAQ	6.78	1.52	1.34
12	3	103	KGD	CAP-CAQ	6.77	1.52	1.34
12	J	101	KGD	CAL-CAJ	6.77	1.53	1.33
12	9	101	KGD	CAO-CAM	6.77	1.51	1.35
12	N	101	KGD	CBE-CBF	6.76	1.52	1.34
12	3	101	KGD	CAP-CAQ	6.74	1.52	1.34
12	F	101	KGD	CAL-CAJ	6.74	1.53	1.33
12	J	101	KGD	CBM-CBN	6.73	1.52	1.34
12	N	102	KGD	CBM-CBN	6.72	1.52	1.34
12	9	102	KGD	CBE-CBF	6.70	1.52	1.34
12	H	102	KGD	CAO-CAM	6.70	1.51	1.35
12	3	103	KGD	CAL-CAJ	6.65	1.52	1.33
12	9	101	KGD	CBM-CBN	6.65	1.52	1.34
12	A	101	KGD	CBM-CBN	6.62	1.52	1.34
12	J	101	KGD	CBE-CBF	6.62	1.51	1.34
12	F	101	KGD	CBE-CBF	6.61	1.51	1.34
12	J	101	KGD	CAP-CAQ	6.61	1.51	1.34
12	R	101	KGD	CAO-CAM	6.58	1.51	1.35
12	9	101	KGD	CAP-CAQ	6.58	1.51	1.34
12	3	101	KGD	CBE-CBF	6.58	1.51	1.34
12	H	102	KGD	CBE-CBF	6.55	1.51	1.34
12	R	101	KGD	CBM-CBN	6.50	1.51	1.34
12	H	102	KGD	CAP-CAQ	6.50	1.51	1.34
12	R	101	KGD	CAV-CAR	6.50	1.50	1.35
12	9	101	KGD	CBE-CBF	6.48	1.51	1.34
12	5	101	KGD	CBM-CBN	6.47	1.51	1.34
12	A	101	KGD	CAL-CAJ	6.42	1.52	1.33
12	H	102	KGD	CAL-CAJ	6.42	1.52	1.33
10	M	702	MQE	CAY-CAX	-6.40	1.40	1.51
12	R	101	KGD	CBE-CBF	6.36	1.51	1.34
12	9	101	KGD	CAL-CAJ	6.36	1.52	1.33
10	L	1004	MQE	CAY-CAX	-6.34	1.40	1.51
12	A	101	KGD	CBE-CBF	6.32	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	102	KGD	CBG-CBB	6.30	1.53	1.36
12	R	101	KGD	CAP-CAQ	6.25	1.51	1.34
12	T	101	KGD	CBG-CBB	6.22	1.53	1.36
12	R	101	KGD	CAL-CAJ	6.14	1.51	1.33
12	5	101	KGD	CBG-CBB	6.04	1.52	1.36
12	9	102	KGD	CBG-CBB	6.03	1.52	1.36
12	F	101	KGD	CBG-CBB	6.03	1.52	1.36
12	H	102	KGD	CBG-CBB	6.00	1.52	1.36
12	N	101	KGD	CBG-CBB	5.99	1.52	1.36
12	N	102	KGD	CBG-CBB	5.98	1.52	1.36
12	3	101	KGD	CBG-CBB	5.97	1.52	1.36
12	5	101	KGD	CBA-CAW	5.95	1.54	1.35
12	9	102	KGD	CAK-CAH	-5.90	1.38	1.50
12	A	101	KGD	CBG-CBB	5.90	1.52	1.36
12	3	103	KGD	CBG-CBB	5.86	1.52	1.36
12	9	101	KGD	CBG-CBB	5.79	1.52	1.36
10	M	702	MQE	CCE-CBK	-5.74	1.39	1.50
12	5	101	KGD	CAK-CAH	-5.73	1.39	1.50
12	J	101	KGD	CBG-CBB	5.71	1.51	1.36
10	L	1004	MQE	CCE-CBK	-5.68	1.39	1.50
12	N	102	KGD	CAK-CAH	-5.66	1.39	1.50
12	3	103	KGD	CBA-CAW	5.63	1.53	1.35
12	T	102	KGD	CBA-CAW	5.60	1.53	1.35
12	A	101	KGD	CAK-CAH	-5.58	1.39	1.50
12	N	101	KGD	CAK-CAH	-5.56	1.39	1.50
12	9	102	KGD	CBA-CAW	5.56	1.53	1.35
12	R	101	KGD	CBG-CBB	5.55	1.51	1.36
12	H	102	KGD	CAK-CAH	-5.51	1.39	1.50
12	F	101	KGD	CAK-CAH	-5.50	1.39	1.50
12	9	101	KGD	CAK-CAH	-5.49	1.39	1.50
12	J	101	KGD	CAK-CAH	-5.48	1.39	1.50
12	T	101	KGD	CAK-CAH	-5.48	1.39	1.50
12	3	103	KGD	CAK-CAH	-5.46	1.39	1.50
12	3	101	KGD	CAK-CAH	-5.45	1.39	1.50
12	T	101	KGD	CBA-CAW	5.42	1.52	1.35
12	R	101	KGD	CAK-CAH	-5.38	1.39	1.50
12	N	102	KGD	CBA-CAW	5.36	1.52	1.35
12	T	102	KGD	CAK-CAH	-5.35	1.39	1.50
12	N	101	KGD	CBA-CAW	5.34	1.52	1.35
12	J	101	KGD	CBA-CAW	5.32	1.52	1.35
12	H	102	KGD	CBA-CAW	5.29	1.52	1.35
12	F	101	KGD	CBA-CAW	5.25	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	101	KGD	CBA-CAW	5.17	1.51	1.35
12	9	101	KGD	CBA-CAW	5.13	1.51	1.35
12	R	101	KGD	CBA-CAW	5.10	1.51	1.35
9	M	705	BPH	CBD-CGD	-5.10	1.46	1.52
9	L	1003	BPH	CBD-CGD	-4.98	1.46	1.52
10	M	702	MQE	CBR-CBS	-4.97	1.38	1.48
9	M	704	BPH	CBD-CGD	-4.91	1.46	1.52
12	A	101	KGD	CBA-CAW	4.82	1.50	1.35
10	L	1004	MQE	CBR-CBS	-4.76	1.38	1.48
8	9	103	BCL	MG-NA	4.70	2.17	2.06
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
10	M	702	MQE	CBP-CBQ	-4.65	1.39	1.48
8	5	102	BCL	MG-NA	4.65	2.17	2.06
8	8	102	BCL	MG-NA	4.62	2.17	2.06
8	Q	102	BCL	MG-NA	4.62	2.17	2.06
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	2	102	BCL	MG-NA	4.59	2.17	2.06
8	H	101	BCL	MG-NA	4.59	2.17	2.06
8	D	101	BCL	MG-NA	4.59	2.17	2.06
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	MG-NA	4.55	2.17	2.06
8	4	102	BCL	MG-NA	4.53	2.17	2.06
8	J	102	BCL	MG-NA	4.52	2.17	2.06
8	I	101	BCL	MG-NA	4.49	2.16	2.06
8	7	101	BCL	MG-NA	4.48	2.16	2.06
8	S	101	BCL	MG-NA	4.48	2.16	2.06
8	K	102	BCL	MG-NA	4.47	2.16	2.06
10	L	1004	MQE	CBP-CBQ	-4.47	1.39	1.48
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	B	102	BCL	MG-NA	4.43	2.16	2.06
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
8	O	101	BCL	MG-NA	4.40	2.16	2.06
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	W	102	BCL	MG-NA	4.37	2.16	2.06
8	2	101	BCL	MG-NA	4.35	2.16	2.06
8	E	101	BCL	MG-NA	4.34	2.16	2.06
12	H	102	KGD	CAI-CAH	-4.33	1.38	1.47
12	9	101	KGD	CAI-CAH	-4.32	1.38	1.47
12	R	101	KGD	CAI-CAH	-4.32	1.38	1.47
8	4	101	BCL	MG-NA	4.31	2.16	2.06
8	0	101	BCL	MG-NA	4.25	2.16	2.06
12	A	101	KGD	CAI-CAH	-4.24	1.38	1.47
12	5	101	KGD	CAI-CAH	-4.22	1.38	1.47
8	A	102	BCL	MG-NA	4.21	2.16	2.06
12	J	101	KGD	CAI-CAH	-4.19	1.38	1.47
12	3	101	KGD	CAI-CAH	-4.16	1.38	1.47
8	M	703	BCL	MG-NA	4.14	2.16	2.06
12	N	101	KGD	CAI-CAH	-4.08	1.39	1.47
12	F	101	KGD	CAI-CAH	-4.06	1.39	1.47
12	T	101	KGD	CAI-CAH	-4.05	1.39	1.47
12	N	102	KGD	CAI-CAH	-4.05	1.39	1.47
12	T	102	KGD	CAI-CAH	-4.03	1.39	1.47
12	9	102	KGD	CAI-CAH	-4.00	1.39	1.47
12	3	103	KGD	CAI-CAH	-3.92	1.39	1.47
10	M	702	MQE	CBK-CBS	-3.89	1.38	1.47
12	5	101	KGD	CBF-CBH	3.86	1.54	1.46
12	5	101	KGD	CBE-CBA	3.85	1.55	1.43
10	L	1004	MQE	CBK-CBS	-3.68	1.39	1.47
12	5	101	KGD	CAQ-CAR	3.60	1.53	1.46
9	M	704	BPH	C3D-CAD	-3.56	1.41	1.47
12	T	102	KGD	CBB-CAV	3.54	1.54	1.43
12	5	101	KGD	CAL-CAM	3.49	1.53	1.46
12	3	103	KGD	CAD-CAH	3.45	1.40	1.35
12	3	103	KGD	CBN-CBL	3.44	1.53	1.46
12	5	101	KGD	CAP-CAO	3.43	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	101	KGD	CBB-CAV	3.39	1.53	1.43
12	5	101	KGD	CBB-CAV	3.38	1.53	1.43
12	T	101	KGD	CBG-CBI	3.37	1.53	1.43
12	5	101	KGD	CBN-CBL	3.36	1.53	1.46
9	M	705	BPH	C3D-CAD	-3.36	1.41	1.47
12	H	102	KGD	CBN-CBL	3.35	1.53	1.46
12	9	102	KGD	CAL-CAM	3.33	1.53	1.46
12	T	102	KGD	CAL-CAM	3.33	1.53	1.46
12	T	102	KGD	CBG-CBI	3.33	1.53	1.43
12	T	102	KGD	CBN-CBL	3.32	1.53	1.46
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	3	103	KGD	CBM-CBJ	3.27	1.53	1.43
12	9	102	KGD	CAP-CAO	3.26	1.53	1.43
12	N	102	KGD	CBB-CAV	3.23	1.53	1.43
12	T	102	KGD	CAP-CAO	3.22	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	5	101	KGD	CBG-CBI	3.21	1.53	1.43
12	T	101	KGD	CAD-CAH	3.21	1.40	1.35
12	9	102	KGD	CBB-CAV	3.20	1.53	1.43
12	N	102	KGD	CAP-CAO	3.20	1.53	1.43
12	T	101	KGD	CAQ-CAR	3.20	1.52	1.46
12	J	101	KGD	CAD-CAH	3.20	1.40	1.35
12	N	102	KGD	CBG-CBI	3.20	1.53	1.43
12	9	102	KGD	CAQ-CAR	3.19	1.52	1.46
12	T	101	KGD	CAL-CAM	3.19	1.52	1.46
12	H	102	KGD	CBM-CBJ	3.18	1.53	1.43
8	9	103	BCL	MG-NC	3.18	2.13	2.06
9	L	1003	BPH	C3D-CAD	-3.18	1.41	1.47
12	T	102	KGD	CBM-CBJ	3.18	1.53	1.43
12	N	102	KGD	CAQ-CAR	3.18	1.52	1.46
12	T	102	KGD	CBF-CBH	3.17	1.52	1.46
12	F	101	KGD	CBG-CBI	3.16	1.53	1.43
12	N	101	KGD	CAQ-CAR	3.14	1.52	1.46
12	3	101	KGD	CBB-CAV	3.14	1.52	1.43
12	9	102	KGD	CBG-CBI	3.14	1.52	1.43
12	3	101	KGD	CBG-CBI	3.14	1.52	1.43
12	T	101	KGD	CAP-CAO	3.14	1.52	1.43
12	N	101	KGD	CBB-CAV	3.14	1.52	1.43
12	3	103	KGD	CAL-CAM	3.13	1.52	1.46
12	F	101	KGD	CBB-CAV	3.12	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	102	KGD	CAQ-CAR	3.11	1.52	1.46
11	C	504	HEM	FE-NC	3.11	2.05	1.95
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	N	101	KGD	CAP-CAO	3.09	1.52	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	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	103	KGD	CBE-CBA	3.07	1.52	1.43
8	5	102	BCL	MG-NC	3.06	2.13	2.06
12	T	101	KGD	CBN-CBL	3.05	1.52	1.46
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	R	101	KGD	CAD-CAH	3.05	1.40	1.35
8	N	103	BCL	MG-NC	3.04	2.13	2.06
12	3	103	KGD	CBF-CBH	3.04	1.52	1.46
12	T	101	KGD	CBM-CBJ	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	T	102	KGD	CBE-CBA	3.03	1.52	1.43
12	N	101	KGD	CBG-CBI	3.03	1.52	1.43
12	R	101	KGD	CBM-CBJ	3.03	1.52	1.43
8	J	102	BCL	MG-NC	3.02	2.13	2.06
8	4	101	BCL	C1D-C2D	-3.02	1.39	1.45
12	F	101	KGD	CAP-CAO	3.02	1.52	1.43
12	T	101	KGD	CBF-CBH	3.01	1.52	1.46
12	5	101	KGD	CBM-CBJ	3.00	1.52	1.43
8	2	101	BCL	MG-NC	2.99	2.13	2.06
8	Q	101	BCL	MG-NC	2.99	2.13	2.06
12	9	102	KGD	CBM-CBJ	2.98	1.52	1.43
12	N	102	KGD	CBN-CBL	2.98	1.52	1.46
12	3	101	KGD	CAL-CAM	2.98	1.52	1.46
8	V	101	BCL	MG-NC	2.97	2.13	2.06
12	9	102	KGD	CBF-CBH	2.97	1.52	1.46
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
8	U	102	BCL	MG-NC	2.97	2.13	2.06
8	P	101	BCL	MG-NC	2.96	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	102	BCL	MG-NC	2.96	2.13	2.06
12	9	101	KGD	CBG-CBI	2.96	1.52	1.43
12	3	103	KGD	CAP-CAO	2.96	1.52	1.43
12	A	101	KGD	CBB-CAV	2.96	1.52	1.43
12	N	101	KGD	CBM-CBJ	2.96	1.52	1.43
11	C	502	HEM	CAB-C3B	2.95	1.55	1.47
8	U	101	BCL	MG-NC	2.95	2.13	2.06
8	I	101	BCL	MG-NC	2.95	2.13	2.06
11	C	504	HEM	FE-NB	2.95	2.04	1.94
8	T	103	BCL	MG-NC	2.95	2.13	2.06
12	T	101	KGD	CBE-CBA	2.94	1.52	1.43
12	H	102	KGD	CBG-CBI	2.94	1.52	1.43
8	H	101	BCL	MG-NC	2.94	2.13	2.06
12	A	101	KGD	CAP-CAO	2.93	1.52	1.43
8	2	102	BCL	MG-NC	2.93	2.13	2.06
12	N	101	KGD	CBN-CBL	2.93	1.52	1.46
12	3	101	KGD	CAP-CAO	2.93	1.52	1.43
8	I	102	BCL	MG-NC	2.93	2.13	2.06
11	C	501	HEM	CAB-C3B	2.93	1.55	1.47
8	6	102	BCL	MG-NC	2.92	2.13	2.06
12	R	101	KGD	CBN-CBL	2.92	1.52	1.46
12	F	101	KGD	CAL-CAM	2.92	1.52	1.46
8	D	101	BCL	MG-NC	2.91	2.13	2.06
12	N	102	KGD	CAL-CAM	2.91	1.52	1.46
12	A	101	KGD	CBG-CBI	2.91	1.52	1.43
8	7	101	BCL	MG-NC	2.90	2.13	2.06
12	3	103	KGD	CBB-CAV	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
11	C	502	HEM	CAC-C3C	2.89	1.55	1.47
8	O	101	BCL	MG-NC	2.89	2.13	2.06
12	J	101	KGD	CBM-CBJ	2.89	1.52	1.43
8	S	101	BCL	MG-NC	2.89	2.13	2.06
12	J	101	KGD	CBG-CBI	2.88	1.52	1.43
12	N	101	KGD	CBE-CBA	2.88	1.52	1.43
11	C	501	HEM	CAC-C3C	2.88	1.55	1.47
12	3	103	KGD	CBG-CBI	2.88	1.52	1.43
8	O	102	BCL	MG-NC	2.88	2.13	2.06
12	J	101	KGD	CAL-CAM	2.88	1.52	1.46
8	K	102	BCL	MG-NC	2.88	2.13	2.06
8	0	102	BCL	MG-NC	2.87	2.13	2.06
12	N	101	KGD	CAL-CAM	2.86	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	102	BCL	MG-NC	2.86	2.13	2.06
12	9	101	KGD	CBB-CAV	2.85	1.52	1.43
12	A	101	KGD	CAL-CAM	2.85	1.52	1.46
8	Q	102	BCL	MG-NC	2.84	2.13	2.06
12	A	101	KGD	CAD-CAH	2.84	1.39	1.35
8	4	102	BCL	MG-NC	2.83	2.13	2.06
12	3	103	KGD	CAQ-CAR	2.83	1.52	1.46
12	H	102	KGD	CAD-CAH	2.83	1.39	1.35
8	E	101	BCL	MG-NC	2.83	2.13	2.06
11	C	502	HEM	FE-NB	2.83	2.03	1.94
8	0	101	BCL	MG-NC	2.83	2.13	2.06
12	N	102	KGD	CBE-CBA	2.83	1.51	1.43
8	1	101	BCL	MG-NC	2.82	2.13	2.06
12	J	101	KGD	CAQ-CAR	2.82	1.52	1.46
12	J	101	KGD	CAP-CAO	2.82	1.51	1.43
12	N	102	KGD	CBM-CBJ	2.82	1.51	1.43
11	C	503	HEM	CAC-C3C	2.81	1.54	1.47
12	H	102	KGD	CAP-CAO	2.81	1.51	1.43
12	9	102	KGD	CBE-CBA	2.80	1.51	1.43
12	3	101	KGD	CAQ-CAR	2.80	1.52	1.46
12	J	101	KGD	CBB-CAV	2.80	1.51	1.43
12	H	102	KGD	CBB-CAV	2.79	1.51	1.43
11	C	504	HEM	CAC-C3C	2.79	1.54	1.47
8	A	102	BCL	MG-NC	2.79	2.12	2.06
12	J	101	KGD	CBN-CBL	2.79	1.51	1.46
12	J	101	KGD	CBE-CBA	2.78	1.51	1.43
12	N	102	KGD	CBF-CBH	2.78	1.51	1.46
12	9	101	KGD	CAD-CAH	2.77	1.39	1.35
11	C	503	HEM	CAB-C3B	2.77	1.54	1.47
12	F	101	KGD	CAQ-CAR	2.77	1.51	1.46
12	F	101	KGD	CBM-CBJ	2.76	1.51	1.43
12	9	102	KGD	CBN-CBL	2.76	1.51	1.46
12	A	101	KGD	CBM-CBJ	2.75	1.51	1.43
12	9	101	KGD	CBM-CBJ	2.75	1.51	1.43
8	B	101	BCL	C1D-C2D	-2.74	1.39	1.45
8	E	102	BCL	MG-NC	2.74	2.12	2.06
8	M	703	BCL	MG-NC	2.74	2.12	2.06
12	H	102	KGD	CAL-CAM	2.73	1.51	1.46
12	H	102	KGD	CBE-CBA	2.73	1.51	1.43
12	9	101	KGD	CAP-CAO	2.72	1.51	1.43
11	C	504	HEM	CAB-C3B	2.72	1.54	1.47
12	3	101	KGD	CBM-CBJ	2.71	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	101	KGD	CBE-CBA	2.70	1.51	1.43
11	C	503	HEM	FE-NB	2.70	2.03	1.94
12	3	101	KGD	CBE-CBA	2.69	1.51	1.43
12	F	101	KGD	CBF-CBH	2.69	1.51	1.46
8	F	102	BCL	MG-NC	2.69	2.12	2.06
9	L	1003	BPH	C3A-C2A	-2.68	1.52	1.54
12	N	101	KGD	CBF-CBH	2.67	1.51	1.46
12	9	101	KGD	CBE-CBA	2.64	1.51	1.43
8	U	102	BCL	CBD-CGD	-2.63	1.44	1.52
12	A	101	KGD	CAQ-CAR	2.62	1.51	1.46
8	0	102	BCL	CBD-CGD	-2.61	1.44	1.52
11	C	502	HEM	FE-NC	2.60	2.03	1.95
12	A	101	KGD	CBE-CBA	2.59	1.51	1.43
12	3	101	KGD	CBN-CBL	2.59	1.51	1.46
12	F	101	KGD	CBN-CBL	2.59	1.51	1.46
12	R	101	KGD	CBE-CBA	2.59	1.51	1.43
12	R	101	KGD	CBF-CBH	2.58	1.51	1.46
12	H	102	KGD	CAQ-CAR	2.55	1.51	1.46
12	9	101	KGD	CBF-CBH	2.54	1.51	1.46
10	L	1004	MQE	CAY-CBL	2.53	1.54	1.50
11	C	503	HEM	C2A-C3A	-2.53	1.32	1.38
12	R	101	KGD	CAP-CAO	2.52	1.51	1.43
8	G	101	BCL	C1D-C2D	-2.52	1.40	1.45
8	4	101	BCL	MG-NC	2.52	2.12	2.06
11	C	503	HEM	FE-NC	2.51	2.03	1.95
8	L	1001	BCL	MG-NC	2.51	2.12	2.06
8	M	703	BCL	C3D-C4D	-2.50	1.38	1.44
12	R	101	KGD	CBG-CBI	2.50	1.50	1.43
12	J	101	KGD	CBF-CBH	2.49	1.51	1.46
10	L	1004	MQE	CAX-CBK	2.48	1.39	1.35
12	R	101	KGD	CBB-CAV	2.46	1.50	1.43
11	C	501	HEM	FE-NA	2.46	2.03	1.95
12	9	101	KGD	CBN-CBL	2.45	1.51	1.46
12	H	102	KGD	CBF-CBH	2.45	1.51	1.46
12	9	101	KGD	CAL-CAM	2.44	1.51	1.46
8	2	102	BCL	C3B-C4B	2.43	1.45	1.41
8	5	102	BCL	C3D-C4D	-2.43	1.38	1.44
8	L	1001	BCL	C3D-C4D	-2.42	1.38	1.44
12	9	101	KGD	CAQ-CAR	2.40	1.51	1.46
8	7	101	BCL	C3D-C4D	-2.39	1.38	1.44
12	3	101	KGD	CBF-CBH	2.39	1.51	1.46
8	H	101	BCL	C3D-C4D	-2.39	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	102	BCL	C3D-C4D	-2.39	1.38	1.44
8	J	102	BCL	C3D-C4D	-2.38	1.38	1.44
8	G	101	BCL	C3D-C4D	-2.38	1.38	1.44
8	U	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	6	101	BCL	C3D-C4D	-2.37	1.38	1.44
8	K	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	T	103	BCL	C3B-C4B	2.37	1.45	1.41
8	L	1001	BCL	C1D-C2D	-2.36	1.40	1.45
12	9	102	KGD	CAC-CAE	-2.36	1.48	1.53
8	L	1002	BCL	C1D-C2D	-2.35	1.40	1.45
8	D	101	BCL	C3D-C4D	-2.34	1.38	1.44
8	2	101	BCL	C3D-C4D	-2.34	1.38	1.44
8	A	102	BCL	C3D-C4D	-2.33	1.38	1.44
10	M	702	MQE	CAX-CBK	2.33	1.39	1.35
8	L	1001	BCL	C3C-C4C	-2.33	1.48	1.51
8	Q	101	BCL	C3D-C4D	-2.32	1.39	1.44
8	M	703	BCL	C1D-C2D	-2.32	1.40	1.45
8	9	103	BCL	C3D-C4D	-2.32	1.39	1.44
8	W	101	BCL	CHD-C1D	2.32	1.42	1.38
8	P	101	BCL	C3D-C4D	-2.31	1.39	1.44
8	4	101	BCL	C3D-C4D	-2.31	1.39	1.44
8	3	102	BCL	C1D-C2D	-2.31	1.40	1.45
8	6	101	BCL	CHD-C1D	2.30	1.42	1.38
8	B	101	BCL	C3D-C4D	-2.30	1.39	1.44
8	N	103	BCL	CHD-C1D	2.30	1.42	1.38
8	S	102	BCL	C1D-C2D	-2.29	1.40	1.45
8	2	101	BCL	CHD-C1D	2.29	1.42	1.38
8	E	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	1	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	U	102	BCL	C3D-C4D	-2.29	1.39	1.44
8	E	102	BCL	C1D-C2D	-2.28	1.40	1.45
8	O	102	BCL	C3B-C4B	2.28	1.45	1.41
8	4	102	BCL	C1D-C2D	-2.28	1.40	1.45
8	O	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	K	102	BCL	CBD-CGD	-2.27	1.45	1.52
8	L	1002	BCL	C3D-C4D	-2.26	1.39	1.44
8	0	101	BCL	CHD-C1D	2.26	1.42	1.38
8	6	102	BCL	CBD-CGD	-2.26	1.45	1.52
12	R	101	KGD	CAQ-CAR	2.26	1.50	1.46
8	K	102	BCL	C1D-C2D	-2.26	1.40	1.45
8	8	101	BCL	CHD-C1D	2.25	1.42	1.38
8	8	101	BCL	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	102	BCL	C3B-C4B	2.25	1.45	1.41
8	0	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	U	101	BCL	C3D-C4D	-2.24	1.39	1.44
8	3	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	F	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	O	101	BCL	C1D-C2D	-2.24	1.40	1.45
8	R	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	7	101	BCL	CHD-C1D	2.23	1.42	1.38
8	A	102	BCL	OBG-CAB	2.23	1.28	1.23
8	K	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	S	101	BCL	C1D-C2D	-2.23	1.40	1.45
8	N	103	BCL	C3D-C4D	-2.23	1.39	1.44
8	T	103	BCL	CHD-C1D	2.22	1.42	1.38
8	N	103	BCL	C3B-C4B	2.22	1.45	1.41
8	B	102	BCL	CHD-C1D	2.22	1.42	1.38
8	I	101	BCL	CHD-C1D	2.22	1.42	1.38
8	H	101	BCL	CHD-C1D	2.22	1.42	1.38
8	1	101	BCL	CHD-C1D	2.21	1.42	1.38
12	R	101	KGD	CAL-CAM	2.20	1.50	1.46
8	U	102	BCL	CHD-C1D	2.20	1.42	1.38
8	8	102	BCL	C1D-C2D	-2.20	1.41	1.45
8	W	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	Q	101	BCL	C1D-C2D	-2.19	1.41	1.45
8	T	103	BCL	C3D-C4D	-2.19	1.39	1.44
8	0	102	BCL	C3B-C4B	2.19	1.45	1.41
11	C	501	HEM	FE-NB	2.19	2.01	1.94
8	R	102	BCL	CHD-C1D	2.18	1.42	1.38
8	W	102	BCL	C1D-C2D	-2.18	1.41	1.45
12	A	101	KGD	CBN-CBL	2.18	1.50	1.46
8	V	101	BCL	C3B-C4B	2.18	1.45	1.41
8	3	102	BCL	CHD-C1D	2.18	1.42	1.38
8	4	101	BCL	CBD-CGD	-2.17	1.45	1.52
8	I	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	S	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	Q	102	BCL	CBD-CGD	-2.16	1.45	1.52
9	M	705	BPH	C3B-C4B	2.16	1.45	1.41
8	I	102	BCL	CHD-C1D	2.16	1.42	1.38
8	0	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	P	101	BCL	CBD-CGD	-2.15	1.45	1.52
8	6	102	BCL	C1D-C2D	-2.15	1.41	1.45
8	E	101	BCL	CHD-C1D	2.15	1.42	1.38
11	C	502	HEM	C2A-C3A	-2.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	102	BCL	CHD-C1D	2.14	1.42	1.38
11	C	501	HEM	CMB-C2B	2.14	1.55	1.50
8	A	102	BCL	CHD-C1D	2.14	1.42	1.38
8	1	101	BCL	CBD-CGD	-2.13	1.46	1.52
8	Q	102	BCL	C3D-C4D	-2.13	1.39	1.44
8	2	102	BCL	CBD-CGD	-2.13	1.46	1.52
8	Q	102	BCL	C1D-C2D	-2.13	1.41	1.45
8	J	102	BCL	CBD-CGD	-2.12	1.46	1.52
8	F	102	BCL	C1D-C2D	-2.12	1.41	1.45
8	P	101	BCL	CHD-C1D	2.12	1.42	1.38
8	Q	101	BCL	CHD-C1D	2.11	1.42	1.38
8	A	102	BCL	CBD-CGD	-2.11	1.46	1.52
8	6	101	BCL	C1D-C2D	-2.10	1.41	1.45
8	R	102	BCL	C1D-C2D	-2.10	1.41	1.45
8	9	103	BCL	CHD-C1D	2.10	1.42	1.38
8	F	102	BCL	CHD-C1D	2.10	1.42	1.38
8	4	102	BCL	C3D-C4D	-2.10	1.39	1.44
8	A	102	BCL	C1D-C2D	-2.10	1.41	1.45
8	O	102	BCL	CBD-CGD	-2.10	1.46	1.52
12	3	103	KGD	CAS-CAW	2.10	1.55	1.51
8	B	102	BCL	C3B-C4B	2.10	1.45	1.41
8	K	102	BCL	C3D-C4D	-2.10	1.39	1.44
8	B	102	BCL	O1D-CGD	2.09	1.26	1.21
8	6	101	BCL	CBD-CGD	-2.09	1.46	1.52
8	I	102	BCL	C3D-C4D	-2.09	1.39	1.44
8	8	102	BCL	CBD-CGD	-2.09	1.46	1.52
8	D	101	BCL	CHD-C1D	2.09	1.42	1.38
8	2	101	BCL	C3B-C4B	2.08	1.45	1.41
8	G	101	BCL	CBD-CGD	-2.08	1.46	1.52
11	C	504	HEM	C3B-C2B	-2.08	1.32	1.37
8	I	102	BCL	C1D-C2D	-2.08	1.41	1.45
8	O	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	W	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	G	102	BCL	C1D-C2D	-2.08	1.41	1.45
8	2	102	BCL	CHD-C1D	2.07	1.42	1.38
9	M	704	BPH	C2C-C3C	-2.07	1.52	1.54
8	I	101	BCL	CBD-CGD	-2.07	1.46	1.52
8	2	102	BCL	C3D-C4D	-2.07	1.39	1.44
8	H	101	BCL	CBD-CGD	-2.07	1.46	1.52
8	7	101	BCL	C3B-C4B	2.07	1.45	1.41
8	E	102	BCL	CBD-CGD	-2.07	1.46	1.52
8	3	102	BCL	OBB-CAB	2.07	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	101	BCL	C1D-C2D	-2.07	1.41	1.45
8	O	102	BCL	CHD-C1D	2.07	1.42	1.38
8	D	101	BCL	CBD-CGD	-2.06	1.46	1.52
8	O	101	BCL	CHD-C1D	2.06	1.42	1.38
8	D	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	L	1001	BCL	CBD-CGD	-2.06	1.46	1.52
8	G	102	BCL	CBD-CGD	-2.06	1.46	1.52
11	C	502	HEM	CMB-C2B	2.06	1.55	1.50
8	B	102	BCL	C3D-C4D	-2.06	1.39	1.44
8	F	102	BCL	CBD-CGD	-2.06	1.46	1.52
8	H	101	BCL	C3B-C4B	2.05	1.45	1.41
8	4	101	BCL	C3C-C4C	-2.05	1.49	1.51
8	Q	102	BCL	C3B-C4B	2.05	1.45	1.41
8	M	703	BCL	CBD-CGD	-2.05	1.46	1.52
8	G	102	BCL	C3D-C4D	-2.05	1.39	1.44
8	Q	101	BCL	CBD-CGD	-2.05	1.46	1.52
8	Q	101	BCL	O1A-CGA	-2.05	1.16	1.22
8	5	102	BCL	C1D-C2D	-2.05	1.41	1.45
8	6	102	BCL	C3D-C4D	-2.04	1.39	1.44
8	9	103	BCL	CBD-CGD	-2.04	1.46	1.52
8	U	101	BCL	CHD-C1D	2.04	1.42	1.38
8	S	102	BCL	CBD-CGD	-2.04	1.46	1.52
8	S	102	BCL	C3D-C4D	-2.03	1.39	1.44
8	W	102	BCL	CHD-C1D	2.03	1.42	1.38
8	U	102	BCL	C1D-C2D	-2.03	1.41	1.45
12	N	101	KGD	CAC-CAE	-2.03	1.49	1.53
8	P	101	BCL	C1D-C2D	-2.03	1.41	1.45
8	L	1002	BCL	CHD-C1D	2.03	1.42	1.38
8	V	101	BCL	C3D-C4D	-2.03	1.39	1.44
12	A	101	KGD	CBF-CBH	2.03	1.50	1.46
8	M	703	BCL	CHD-C1D	2.02	1.42	1.38
8	V	101	BCL	CHD-C1D	2.02	1.42	1.38
8	5	102	BCL	CHD-C1D	2.02	1.42	1.38
8	0	102	BCL	C1D-C2D	-2.02	1.41	1.45
8	H	101	BCL	C1D-C2D	-2.02	1.41	1.45
11	C	501	HEM	CMC-C2C	2.02	1.54	1.50
8	S	101	BCL	CHD-C1D	2.02	1.42	1.38
8	7	101	BCL	C1D-C2D	-2.02	1.41	1.45
12	F	101	KGD	CAC-CAE	-2.01	1.49	1.53
8	8	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	0	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	2	101	BCL	C1D-C2D	-2.01	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	101	BCL	C1D-C2D	-2.01	1.41	1.45
10	M	702	MQE	CAY-CBL	2.00	1.53	1.50
8	8	102	BCL	C3D-C4D	-2.00	1.39	1.44
8	N	103	BCL	CBD-CGD	-2.00	1.46	1.52
8	V	101	BCL	C1D-C2D	-2.00	1.41	1.45

All (841) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C4-C3-C5	-26.98	68.40	115.23
8	U	101	BCL	C4-C3-C5	-26.66	68.96	115.23
8	U	101	BCL	C5-C3-C2	17.69	160.88	121.17
8	W	101	BCL	C5-C3-C2	17.47	160.40	121.17
12	N	102	KGD	CBM-CBJ-CBH	-14.47	106.98	127.28
12	R	101	KGD	CBE-CBA-CAW	-13.67	108.47	127.69
12	T	102	KGD	CBM-CBJ-CBH	-13.31	108.61	127.28
12	5	101	KGD	CBM-CBJ-CBH	-12.98	109.08	127.28
12	9	102	KGD	CBG-CBI-CBL	-12.49	109.76	127.28
8	U	101	BCL	C4-C3-C2	-12.34	91.93	123.63
8	W	101	BCL	C4-C3-C2	-12.32	91.99	123.63
12	J	101	KGD	CBG-CBI-CBL	-12.24	110.11	127.28
12	N	102	KGD	CBE-CBA-CAW	-12.20	110.53	127.69
12	3	101	KGD	CBG-CBI-CBL	-12.17	110.21	127.28
12	5	101	KGD	CBE-CBA-CAW	-12.05	110.75	127.69
12	9	102	KGD	CBE-CBA-CAW	-11.92	110.93	127.69
12	3	101	KGD	CBM-CBJ-CBH	-11.69	110.88	127.28
12	N	101	KGD	CBM-CBJ-CBH	-11.64	110.95	127.28
12	5	101	KGD	CBG-CBI-CBL	-11.63	110.97	127.28
12	T	102	KGD	CBG-CBI-CBL	-11.51	111.13	127.28
12	T	101	KGD	CBM-CBJ-CBH	-11.48	111.19	127.28
12	N	101	KGD	CBG-CBI-CBL	-11.40	111.29	127.28
12	J	101	KGD	CBM-CBJ-CBH	-11.25	111.50	127.28
12	9	101	KGD	CBM-CBJ-CBH	-11.24	111.52	127.28
12	N	102	KGD	CBG-CBI-CBL	-11.22	111.54	127.28
12	9	102	KGD	CBM-CBJ-CBH	-11.21	111.56	127.28
12	F	101	KGD	CBG-CBI-CBL	-11.19	111.59	127.28
12	9	101	KGD	CBG-CBI-CBL	-11.13	111.66	127.28
12	T	102	KGD	CBE-CBA-CAW	-11.03	112.18	127.69
12	T	101	KGD	CBG-CBI-CBL	-11.01	111.83	127.28
12	F	101	KGD	CBM-CBJ-CBH	-11.00	111.85	127.28
12	N	102	KGD	CAP-CAO-CAM	-10.92	111.97	127.28
12	9	101	KGD	CBE-CBA-CAW	-10.50	112.92	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	704	BPH	C4D-CHA-CBD	-10.27	103.53	108.45
12	J	101	KGD	CBE-CBA-CAW	-10.26	113.26	127.69
12	A	101	KGD	CBG-CBI-CBL	-10.12	113.09	127.28
12	F	101	KGD	CBE-CBA-CAW	-9.89	113.78	127.69
12	3	101	KGD	CBE-CBA-CAW	-9.85	113.84	127.69
12	3	101	KGD	CAP-CAO-CAM	-9.77	113.57	127.28
12	N	101	KGD	CBE-CBA-CAW	-9.75	113.97	127.69
12	T	101	KGD	CBE-CBA-CAW	-9.73	114.01	127.69
12	5	101	KGD	CAP-CAO-CAM	-9.68	113.70	127.28
12	3	103	KGD	CBG-CBI-CBL	-9.55	113.89	127.28
12	9	101	KGD	CBB-CAV-CAR	-9.41	114.08	127.28
12	T	102	KGD	CAJ-CAL-CAM	-9.35	112.40	126.23
12	N	102	KGD	CBB-CAV-CAR	-9.35	114.17	127.28
12	N	101	KGD	CAP-CAO-CAM	-9.33	114.19	127.28
9	L	1003	BPH	C4D-CHA-CBD	-9.32	103.99	108.45
12	R	101	KGD	CBG-CBI-CBL	-9.24	114.32	127.28
12	3	103	KGD	CBM-CBJ-CBH	-9.15	114.44	127.28
12	A	101	KGD	CBE-CBA-CAW	-9.12	114.87	127.69
9	M	705	BPH	C4D-CHA-CBD	-9.11	104.09	108.45
12	R	101	KGD	CBM-CBJ-CBH	-9.06	114.57	127.28
12	N	102	KGD	CAJ-CAL-CAM	-9.05	112.84	126.23
12	N	101	KGD	CAJ-CAL-CAM	-8.92	113.04	126.23
12	T	101	KGD	CBB-CAV-CAR	-8.91	114.78	127.28
12	H	102	KGD	CBG-CBI-CBL	-8.84	114.88	127.28
10	M	702	MQE	CAO-CBI-CAZ	-8.80	107.49	127.62
12	3	103	KGD	CBE-CBA-CAW	-8.79	115.33	127.69
12	T	101	KGD	CAP-CAO-CAM	-8.71	115.06	127.28
12	5	101	KGD	CAJ-CAL-CAM	-8.68	113.39	126.23
12	9	101	KGD	CAP-CAO-CAM	-8.66	115.13	127.28
12	T	102	KGD	CAP-CAO-CAM	-8.63	115.18	127.28
12	A	101	KGD	CBM-CBJ-CBH	-8.62	115.18	127.28
12	T	101	KGD	CAJ-CAL-CAM	-8.53	113.61	126.23
12	J	101	KGD	CAP-CAO-CAM	-8.47	115.40	127.28
12	F	101	KGD	CAP-CAO-CAM	-8.41	115.48	127.28
12	A	101	KGD	CBB-CAV-CAR	-8.40	115.50	127.28
12	9	102	KGD	CAP-CAO-CAM	-8.35	115.56	127.28
10	M	702	MQE	CAJ-CBC-CAP	-8.24	108.77	127.62
12	F	101	KGD	CBB-CAV-CAR	-8.13	115.87	127.28
12	3	103	KGD	CBB-CAV-CAR	-8.00	116.06	127.28
12	9	101	KGD	CAJ-CAL-CAM	-7.98	114.43	126.23
12	H	102	KGD	CBE-CBA-CAW	-7.96	116.49	127.69
12	3	101	KGD	CBB-CAV-CAR	-7.95	116.13	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	1004	MQE	CAY-CBL-CBB	-7.94	113.16	126.83
12	F	101	KGD	CAJ-CAL-CAM	-7.93	114.51	126.23
12	J	101	KGD	CBB-CAV-CAR	-7.92	116.17	127.28
12	R	101	KGD	CBB-CAV-CAR	-7.88	116.22	127.28
12	3	101	KGD	CAJ-CAL-CAM	-7.88	114.58	126.23
12	N	101	KGD	CBB-CAV-CAR	-7.71	116.47	127.28
12	T	102	KGD	CBB-CAV-CAR	-7.60	116.62	127.28
10	M	702	MQE	CBA-CBN-CBM	-7.43	110.61	127.62
12	A	101	KGD	CAJ-CAL-CAM	-7.42	115.27	126.23
12	H	102	KGD	CAJ-CAL-CAM	-7.27	115.47	126.23
12	9	102	KGD	CBB-CAV-CAR	-7.22	117.16	127.28
12	N	102	KGD	CBM-CBN-CBL	-7.09	106.93	126.36
12	5	101	KGD	CBB-CAV-CAR	-7.06	117.37	127.28
12	R	101	KGD	CAJ-CAL-CAM	-7.04	115.83	126.23
10	M	702	MQE	CAK-CBE-CAQ	-6.98	111.66	127.62
12	H	102	KGD	CBG-CBB-CAV	-6.96	109.27	123.52
12	J	101	KGD	CAJ-CAL-CAM	-6.90	116.02	126.23
10	L	1004	MQE	CBO-CCB-CCC	-6.78	112.11	127.62
12	R	101	KGD	CAP-CAO-CAM	-6.72	117.86	127.28
12	T	102	KGD	CBM-CBN-CBL	-6.63	108.19	126.36
12	3	101	KGD	CBM-CBN-CBL	-6.57	108.34	126.36
12	R	101	KGD	CBG-CBB-CAV	-6.56	110.09	123.52
12	A	101	KGD	CAP-CAO-CAM	-6.49	118.18	127.28
12	N	102	KGD	CBE-CBF-CBH	-6.43	108.74	126.36
12	R	101	KGD	CBE-CBF-CBH	-6.37	108.90	126.36
12	H	102	KGD	CAP-CAO-CAM	-6.33	118.40	127.28
8	M	703	BCL	C1-C2-C3	-6.21	116.03	126.20
10	M	702	MQE	CAS-CBH-CAW	-6.19	113.45	127.62
12	T	101	KGD	CBM-CBN-CBL	-6.18	109.41	126.36
12	9	102	KGD	CBE-CBF-CBH	-6.17	109.44	126.36
10	M	702	MQE	CAY-CBL-CBB	-6.16	116.22	126.83
12	J	101	KGD	CBG-CBB-CAV	-6.13	110.97	123.52
12	9	102	KGD	CBG-CBB-CAV	-6.13	110.97	123.52
10	L	1004	MQE	CAJ-CBC-CAP	-6.05	113.77	127.62
12	T	102	KGD	CBE-CBF-CBH	-6.05	109.77	126.36
12	F	101	KGD	CBM-CBN-CBL	-6.02	109.86	126.36
12	5	101	KGD	CBM-CBN-CBL	-6.02	109.87	126.36
12	9	101	KGD	CBM-CBN-CBL	-6.01	109.89	126.36
12	9	102	KGD	CBM-CBN-CBL	-5.96	110.02	126.36
12	3	103	KGD	CAP-CAO-CAM	-5.93	118.96	127.28
12	H	102	KGD	CBB-CAV-CAR	-5.91	118.99	127.28
12	5	101	KGD	CBG-CBB-CAV	-5.88	111.49	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	102	BCL	C4D-CHA-C1A	5.86	128.24	121.24
8	U	102	BCL	C4D-CHA-C1A	5.80	128.16	121.24
12	H	102	KGD	CBM-CBJ-CBH	-5.80	119.15	127.28
8	0	102	BCL	C4D-CHA-C1A	5.76	128.11	121.24
12	3	101	KGD	CBG-CBB-CAV	-5.76	111.74	123.52
12	9	102	KGD	CAJ-CAL-CAM	-5.76	117.72	126.23
12	N	101	KGD	CBG-CBB-CAV	-5.72	111.81	123.52
12	N	101	KGD	CBM-CBN-CBL	-5.72	110.68	126.36
12	J	101	KGD	CBM-CBN-CBL	-5.67	110.81	126.36
8	K	102	BCL	C4D-CHA-C1A	5.67	128.01	121.24
10	L	1004	MQE	CAL-CBF-CAV	-5.67	114.64	127.62
8	S	102	BCL	C4D-CHA-C1A	5.62	127.95	121.24
8	W	102	BCL	C4D-CHA-C1A	5.61	127.94	121.24
10	M	702	MQE	CAM-CBG-CAT	-5.60	114.82	127.62
8	G	102	BCL	C4D-CHA-C1A	5.58	127.90	121.24
12	5	101	KGD	CBE-CBF-CBH	-5.57	111.08	126.36
8	B	102	BCL	C4D-CHA-C1A	5.55	127.86	121.24
8	L	1002	BCL	C4D-CHA-C1A	5.53	127.84	121.24
8	H	101	BCL	C4D-CHA-C1A	5.53	127.84	121.24
12	3	103	KGD	CBG-CBB-CAV	-5.52	112.22	123.52
8	6	102	BCL	C4D-CHA-C1A	5.52	127.83	121.24
8	N	103	BCL	C4D-CHA-C1A	5.50	127.80	121.24
8	J	102	BCL	C4D-CHA-C1A	5.49	127.79	121.24
8	7	101	BCL	C4D-CHA-C1A	5.48	127.78	121.24
10	M	702	MQE	CBO-CCB-CCC	-5.48	115.08	127.62
8	I	102	BCL	C4D-CHA-C1A	5.48	127.78	121.24
8	L	1001	BCL	C4D-CHA-C1A	5.47	127.77	121.24
8	I	101	BCL	C4D-CHA-C1A	5.47	127.77	121.24
8	P	101	BCL	C4D-CHA-C1A	5.47	127.76	121.24
12	J	101	KGD	CBE-CBF-CBH	-5.45	111.42	126.36
8	E	102	BCL	C4D-CHA-C1A	5.45	127.74	121.24
8	8	102	BCL	C4D-CHA-C1A	5.44	127.73	121.24
8	1	101	BCL	C4D-CHA-C1A	5.44	127.73	121.24
12	T	102	KGD	CAB-CAD-CAJ	5.44	130.39	115.65
12	A	101	KGD	CAB-CAD-CAJ	5.42	130.36	115.65
8	6	101	BCL	C4D-CHA-C1A	5.42	127.71	121.24
8	M	703	BCL	C4D-CHA-C1A	5.41	127.70	121.24
8	F	102	BCL	C4D-CHA-C1A	5.40	127.68	121.24
8	O	101	BCL	C4D-CHA-C1A	5.40	127.68	121.24
12	H	102	KGD	CAB-CAD-CAJ	5.39	130.26	115.65
8	9	103	BCL	C4D-CHA-C1A	5.38	127.66	121.24
8	W	101	BCL	C4D-CHA-C1A	5.37	127.65	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	0	101	BCL	C4D-CHA-C1A	5.36	127.63	121.24
8	O	102	BCL	C4D-CHA-C1A	5.35	127.63	121.24
8	4	101	BCL	C4D-CHA-C1A	5.35	127.62	121.24
8	D	101	BCL	C4D-CHA-C1A	5.34	127.62	121.24
8	K	101	BCL	C4D-CHA-C1A	5.32	127.59	121.24
8	2	101	BCL	C4D-CHA-C1A	5.30	127.57	121.24
12	9	101	KGD	CBE-CBF-CBH	-5.30	111.83	126.36
12	9	101	KGD	CAB-CAD-CAJ	5.30	130.02	115.65
12	H	102	KGD	CAO-CAP-CAQ	-5.29	107.86	123.20
8	V	101	BCL	C4D-CHA-C1A	5.28	127.54	121.24
8	8	101	BCL	C1-C2-C3	-5.27	117.56	126.20
8	8	101	BCL	C4D-CHA-C1A	5.27	127.53	121.24
8	4	102	BCL	C4D-CHA-C1A	5.26	127.52	121.24
12	F	101	KGD	CBG-CBB-CAV	-5.26	112.77	123.52
8	U	101	BCL	C4D-CHA-C1A	5.25	127.50	121.24
8	G	101	BCL	C1-C2-C3	-5.25	117.60	126.20
12	9	101	KGD	CBG-CBB-CAV	-5.23	112.81	123.52
12	F	101	KGD	CAB-CAD-CAJ	5.23	129.84	115.65
8	Q	101	BCL	C4D-CHA-C1A	5.22	127.47	121.24
12	T	102	KGD	CBG-CBB-CAV	-5.22	112.84	123.52
8	S	101	BCL	C4D-CHA-C1A	5.22	127.47	121.24
8	R	102	BCL	C4D-CHA-C1A	5.22	127.47	121.24
12	R	101	KGD	CAO-CAP-CAQ	-5.21	108.09	123.20
8	A	102	BCL	C4D-CHA-C1A	5.21	127.46	121.24
12	R	101	KGD	CAB-CAD-CAJ	5.20	129.76	115.65
8	V	101	BCL	C11-C10-C8	5.19	133.21	115.97
8	5	102	BCL	C4D-CHA-C1A	5.19	127.43	121.24
8	3	102	BCL	C4D-CHA-C1A	5.19	127.43	121.24
12	N	101	KGD	CBE-CBF-CBH	-5.18	112.16	126.36
8	B	101	BCL	C4D-CHA-C1A	5.18	127.42	121.24
12	3	101	KGD	CBE-CBF-CBH	-5.18	112.17	126.36
12	3	101	KGD	CAB-CAD-CAJ	5.17	129.68	115.65
12	A	101	KGD	CBM-CBN-CBL	-5.16	112.20	126.36
12	T	101	KGD	CAB-CAD-CAJ	5.16	129.65	115.65
8	G	101	BCL	C4D-CHA-C1A	5.16	127.39	121.24
12	F	101	KGD	CBE-CBF-CBH	-5.14	112.26	126.36
12	N	102	KGD	CAB-CAD-CAJ	5.14	129.59	115.65
12	5	101	KGD	CAB-CAD-CAJ	5.14	129.59	115.65
8	B	102	BCL	CED-O2D-CGD	5.13	127.56	115.92
8	T	103	BCL	C4D-CHA-C1A	5.13	127.36	121.24
12	J	101	KGD	CAB-CAD-CAJ	5.12	129.54	115.65
12	A	101	KGD	CBG-CBB-CAV	-5.12	113.05	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	101	BCL	C4D-CHA-C1A	5.12	127.34	121.24
10	L	1004	MQE	CAO-CBI-CAZ	-5.09	115.96	127.62
10	M	702	MQE	CAL-CBF-CAV	-5.08	116.00	127.62
8	2	102	BCL	C4D-CHA-C1A	5.05	127.26	121.24
10	L	1004	MQE	CBA-CBN-CBM	-5.04	116.08	127.62
12	N	102	KGD	CAP-CAQ-CAR	-5.04	112.54	126.36
10	L	1004	MQE	CAI-CBD-CAR	-5.03	116.12	127.62
12	3	103	KGD	CAB-CAD-CAJ	5.01	129.24	115.65
12	N	101	KGD	CAB-CAD-CAJ	5.01	129.23	115.65
10	M	702	MQE	CAI-CBD-CAR	-4.98	116.22	127.62
12	9	102	KGD	CAB-CAD-CAJ	4.92	128.99	115.65
12	T	101	KGD	CAZ-CAW-CAS	4.91	123.76	115.23
12	T	101	KGD	CBE-CBF-CBH	-4.90	112.92	126.36
12	3	103	KGD	CAZ-CAW-CAS	4.84	123.63	115.23
12	3	103	KGD	CBE-CBF-CBH	-4.78	113.24	126.36
8	B	101	BCL	C1-C2-C3	-4.77	118.39	126.20
12	N	102	KGD	CBG-CBB-CAV	-4.74	113.81	123.52
10	L	1004	MQE	CAM-CBG-CAT	-4.72	116.82	127.62
12	H	102	KGD	CBJ-CBM-CBN	-4.68	109.65	123.20
12	3	101	KGD	CAP-CAQ-CAR	-4.62	113.70	126.36
12	T	101	KGD	CAP-CAQ-CAR	-4.54	113.91	126.36
12	A	101	KGD	CAO-CAP-CAQ	-4.53	110.08	123.20
12	5	101	KGD	CAP-CAQ-CAR	-4.48	114.08	126.36
10	M	702	MQE	CAY-CAX-CBQ	4.47	123.29	118.58
12	3	103	KGD	CAJ-CAL-CAM	-4.46	119.64	126.23
12	T	101	KGD	CBG-CBB-CAV	-4.45	114.41	123.52
12	9	101	KGD	CAP-CAQ-CAR	-4.44	114.19	126.36
12	3	103	KGD	CAT-CAS-CAW	-4.41	98.58	113.19
10	L	1004	MQE	CAK-CBE-CAQ	-4.37	117.61	127.62
8	5	102	BCL	C4A-NA-C1A	4.37	108.67	106.68
8	F	102	BCL	C1-C2-C3	-4.35	119.06	126.20
9	M	704	BPH	C4D-ND-C1D	-4.34	103.67	108.87
12	F	101	KGD	CAP-CAQ-CAR	-4.34	114.47	126.36
10	M	702	MQE	CAY-CAX-CBK	-4.33	117.47	124.89
9	M	705	BPH	C4D-ND-C1D	-4.29	103.73	108.87
10	M	702	MQE	CBV-CAR-CAE	4.27	122.64	115.23
12	R	101	KGD	CBB-CBG-CBI	-4.27	114.79	123.52
12	A	101	KGD	CBA-CBE-CBF	-4.23	110.95	123.20
8	4	101	BCL	C4A-NA-C1A	4.20	108.60	106.68
12	H	102	KGD	CBA-CBE-CBF	-4.20	111.02	123.20
10	M	702	MQE	CAO-CAH-CAV	-4.19	99.30	113.19
12	9	102	KGD	CAT-CAX-CAY	-4.17	113.73	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	101	KGD	CBE-CBF-CBH	-4.17	114.93	126.36
8	H	101	BCL	C4A-NA-C1A	4.17	108.58	106.68
8	L	1001	BCL	C4A-NA-C1A	4.16	108.58	106.68
12	T	102	KGD	CAT-CAX-CAY	-4.14	113.85	127.64
12	R	101	KGD	CBJ-CBM-CBN	-4.14	111.21	123.20
10	L	1004	MQE	CAS-CBH-CAW	-4.14	118.16	127.62
12	H	102	KGD	CBE-CBF-CBH	-4.13	115.04	126.36
8	4	102	BCL	C4A-NA-C1A	4.13	108.56	106.68
8	6	102	BCL	C4A-NA-C1A	4.12	108.56	106.68
9	L	1003	BPH	C4D-ND-C1D	-4.12	103.94	108.87
8	9	103	BCL	C4A-NA-C1A	4.11	108.55	106.68
12	A	101	KGD	CBB-CBG-CBI	-4.09	115.14	123.52
10	L	1004	MQE	CCI-CCM-CCN	-4.09	114.00	127.64
8	U	102	BCL	C4A-NA-C1A	4.07	108.54	106.68
12	3	103	KGD	CAO-CAP-CAQ	-4.07	111.41	123.20
12	N	101	KGD	CAP-CAQ-CAR	-4.06	115.24	126.36
8	E	101	BCL	C1-C2-C3	-4.05	119.56	126.20
8	M	703	BCL	C4A-NA-C1A	4.03	108.52	106.68
8	8	102	BCL	C4A-NA-C1A	4.03	108.52	106.68
8	9	103	BCL	C1D-ND-C4D	-4.01	103.50	106.31
8	V	101	BCL	C4A-NA-C1A	4.00	108.50	106.68
8	1	101	BCL	C4A-NA-C1A	3.99	108.50	106.68
12	J	101	KGD	CAO-CAP-CAQ	-3.98	111.68	123.20
8	D	101	BCL	C11-C10-C8	-3.96	102.81	115.97
8	3	102	BCL	C1D-ND-C4D	-3.94	103.55	106.31
12	3	101	KGD	CAT-CAX-CAY	-3.93	114.52	127.64
8	0	102	BCL	C4A-NA-C1A	3.93	108.47	106.68
12	9	102	KGD	CAP-CAQ-CAR	-3.92	115.63	126.36
12	H	102	KGD	CAZ-CAW-CAS	3.89	121.98	115.23
8	R	102	BCL	C11-C10-C8	-3.86	103.13	115.97
12	T	101	KGD	CAT-CAX-CAY	-3.85	114.79	127.64
8	D	101	BCL	C1D-ND-C4D	-3.85	103.61	106.31
8	T	103	BCL	C1D-ND-C4D	-3.85	103.61	106.31
12	N	101	KGD	CAT-CAX-CAY	-3.85	114.81	127.64
12	A	101	KGD	CAZ-CAW-CAS	3.84	121.89	115.23
12	9	101	KGD	CBB-CBG-CBI	-3.84	115.67	123.52
8	4	101	BCL	C1D-ND-C4D	-3.84	103.62	106.31
8	L	1001	BCL	C1D-ND-C4D	-3.83	103.62	106.31
8	K	102	BCL	C4A-NA-C1A	3.82	108.42	106.68
8	0	102	BCL	C1D-ND-C4D	-3.82	103.64	106.31
8	F	102	BCL	C4A-NA-C1A	3.81	108.42	106.68
8	6	102	BCL	C1D-ND-C4D	-3.81	103.64	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	C4A-NA-C1A	3.81	108.42	106.68
8	G	102	BCL	C1D-ND-C4D	-3.80	103.64	106.31
8	A	102	BCL	C1D-ND-C4D	-3.80	103.65	106.31
12	T	102	KGD	CAP-CAQ-CAR	-3.79	115.98	126.36
12	9	101	KGD	CAO-CAP-CAQ	-3.77	112.26	123.20
8	W	102	BCL	C4A-NA-C1A	3.77	108.40	106.68
8	4	101	BCL	C16-C15-C13	3.77	128.50	115.97
8	B	101	BCL	C4A-NA-C1A	3.75	108.39	106.68
8	J	102	BCL	C4A-NA-C1A	3.75	108.39	106.68
8	I	102	BCL	C4A-NA-C1A	3.75	108.39	106.68
8	J	102	BCL	C1D-ND-C4D	-3.75	103.68	106.31
8	0	102	BCL	C1-C2-C3	-3.74	120.07	126.20
8	F	102	BCL	C1D-ND-C4D	-3.74	103.69	106.31
8	I	101	BCL	C1D-ND-C4D	-3.71	103.71	106.31
8	V	101	BCL	C1D-ND-C4D	-3.71	103.71	106.31
8	R	102	BCL	C16-C15-C13	3.71	128.28	115.97
8	6	101	BCL	C4A-NA-C1A	3.70	108.36	106.68
8	G	102	BCL	C4A-NA-C1A	3.69	108.36	106.68
12	J	101	KGD	CAP-CAQ-CAR	-3.69	116.25	126.36
8	W	102	BCL	C1D-ND-C4D	-3.69	103.72	106.31
8	I	102	BCL	C1D-ND-C4D	-3.69	103.73	106.31
8	4	102	BCL	C1D-ND-C4D	-3.68	103.73	106.31
8	2	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
8	3	102	BCL	C4A-NA-C1A	3.68	108.36	106.68
8	1	101	BCL	C1D-ND-C4D	-3.67	103.73	106.31
12	3	103	KGD	CBB-CBG-CBI	-3.67	116.01	123.52
8	D	101	BCL	CHD-C1D-ND	-3.65	119.67	124.80
8	S	102	BCL	C1D-ND-C4D	-3.65	103.75	106.31
8	3	102	BCL	CAB-C3B-C2B	3.64	135.31	127.74
8	K	102	BCL	C1D-ND-C4D	-3.63	103.76	106.31
8	E	102	BCL	C1D-ND-C4D	-3.63	103.77	106.31
8	L	1002	BCL	C1D-ND-C4D	-3.63	103.77	106.31
8	T	103	BCL	CHD-C1D-ND	-3.63	119.69	124.80
8	7	101	BCL	C1D-ND-C4D	-3.62	103.77	106.31
10	M	702	MQE	CBA-CAU-CAZ	-3.62	101.19	113.19
8	L	1002	BCL	C4A-NA-C1A	3.61	108.33	106.68
8	0	102	BCL	CHD-C1D-ND	-3.61	119.72	124.80
8	N	103	BCL	C4A-NA-C1A	3.60	108.32	106.68
8	M	703	BCL	C1D-ND-C4D	-3.60	103.78	106.31
9	L	1003	BPH	C3D-C4D-ND	3.60	112.33	107.71
9	M	705	BPH	C3D-C4D-ND	3.60	112.32	107.71
8	8	102	BCL	C1D-ND-C4D	-3.60	103.79	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	BCL	C1D-ND-C4D	-3.58	103.80	106.31
8	Q	102	BCL	C1D-ND-C4D	-3.57	103.80	106.31
8	P	101	BCL	C1D-ND-C4D	-3.57	103.81	106.31
12	R	101	KGD	CAF-CAB-CAD	3.56	115.83	110.24
8	G	102	BCL	CHD-C1D-ND	-3.56	119.80	124.80
12	R	101	KGD	CAT-CAX-CAY	-3.55	115.79	127.64
8	U	102	BCL	C1D-ND-C4D	-3.55	103.82	106.31
12	F	101	KGD	CAZ-CAW-CAS	3.55	121.39	115.23
8	N	103	BCL	C1D-ND-C4D	-3.55	103.82	106.31
8	5	102	BCL	C1D-ND-C4D	-3.55	103.82	106.31
8	O	102	BCL	C1D-ND-C4D	-3.55	103.82	106.31
8	L	1001	BCL	CHD-C1D-ND	-3.55	119.81	124.80
8	W	101	BCL	C4A-NA-C1A	3.55	108.30	106.68
12	F	101	KGD	CAO-CAP-CAQ	-3.54	112.93	123.20
12	3	103	KGD	CBJ-CBM-CBN	-3.54	112.93	123.20
8	U	102	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	6	101	BCL	C1-C2-C3	-3.54	120.39	126.20
8	E	101	BCL	CHD-C1D-ND	-3.54	119.83	124.80
8	W	102	BCL	CHD-C1D-ND	-3.53	119.83	124.80
8	O	102	BCL	CHD-C1D-ND	-3.53	119.83	124.80
8	G	101	BCL	C1D-ND-C4D	-3.53	103.83	106.31
8	A	102	BCL	CHD-C1D-ND	-3.53	119.83	124.80
8	1	101	BCL	CHD-C1D-ND	-3.53	119.84	124.80
12	N	101	KGD	CAZ-CAW-CAS	3.53	121.35	115.23
10	M	702	MQE	CCA-CBB-CAN	3.52	121.35	115.23
11	C	504	HEM	C3B-C2B-C1B	3.52	109.06	106.41
8	5	102	BCL	CAB-C3B-C2B	3.52	135.06	127.74
8	K	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	E	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	F	102	BCL	CHD-C1D-ND	-3.52	119.85	124.80
8	W	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	9	103	BCL	CHD-C1D-ND	-3.51	119.86	124.80
8	2	101	BCL	CHD-C1D-ND	-3.51	119.86	124.80
8	I	102	BCL	CHD-C1D-ND	-3.51	119.86	124.80
8	S	101	BCL	C1D-ND-C4D	-3.51	103.85	106.31
9	M	704	BPH	C3D-C4D-ND	3.51	112.20	107.71
8	2	102	BCL	CHD-C1D-ND	-3.50	119.87	124.80
8	U	101	BCL	C1D-ND-C4D	-3.49	103.86	106.31
8	Q	102	BCL	CHA-C1A-NA	-3.49	118.48	126.39
8	7	101	BCL	C4A-NA-C1A	3.49	108.27	106.68
8	N	103	BCL	CHD-C1D-ND	-3.49	119.89	124.80
8	F	102	BCL	CAB-C3B-C2B	3.48	134.98	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	101	BCL	C1D-ND-C4D	-3.48	103.87	106.31
12	3	103	KGD	CAP-CAQ-CAR	-3.48	116.81	126.36
8	I	101	BCL	CHD-C1D-ND	-3.48	119.90	124.80
8	H	101	BCL	CHD-C1D-ND	-3.48	119.90	124.80
8	3	102	BCL	CHD-C1D-ND	-3.48	119.91	124.80
8	V	101	BCL	CHD-C1D-ND	-3.48	119.91	124.80
8	A	102	BCL	CAB-C3B-C2B	3.47	134.96	127.74
8	P	101	BCL	CHD-C1D-ND	-3.47	119.92	124.80
12	F	101	KGD	CAT-CAX-CAY	-3.46	116.09	127.64
8	M	703	BCL	CHD-C1D-ND	-3.46	119.93	124.80
8	J	102	BCL	CHD-C1D-ND	-3.46	119.93	124.80
12	9	101	KGD	CAZ-CAW-CAS	3.46	121.23	115.23
8	S	102	BCL	CHD-C1D-ND	-3.46	119.94	124.80
8	E	102	BCL	C4D-C3D-CAD	-3.45	104.36	108.11
8	D	101	BCL	C1-C2-C3	-3.45	120.54	126.20
8	B	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
8	Q	102	BCL	CHD-C1D-ND	-3.45	119.95	124.80
8	4	102	BCL	CHD-C1D-ND	-3.44	119.95	124.80
8	7	101	BCL	CHD-C1D-ND	-3.44	119.95	124.80
12	A	101	KGD	CBJ-CBM-CBN	-3.44	113.22	123.20
8	R	102	BCL	CHD-C1D-ND	-3.44	119.96	124.80
8	Q	101	BCL	C4A-NA-C1A	3.44	108.25	106.68
12	A	101	KGD	CAP-CAQ-CAR	-3.44	116.94	126.36
8	B	102	BCL	CHD-C1D-ND	-3.43	119.98	124.80
8	W	101	BCL	CHD-C1D-ND	-3.42	119.99	124.80
8	8	101	BCL	C4A-NA-C1A	3.41	108.24	106.68
8	K	102	BCL	CHD-C1D-ND	-3.41	120.00	124.80
8	U	101	BCL	C4A-NA-C1A	3.41	108.24	106.68
8	8	101	BCL	CHD-C1D-ND	-3.41	120.00	124.80
8	2	102	BCL	C4A-NA-C1A	3.41	108.23	106.68
12	3	101	KGD	CAZ-CAW-CAS	3.41	121.14	115.23
12	F	101	KGD	CBB-CBG-CBI	-3.41	116.55	123.52
12	N	102	KGD	CBB-CBG-CBI	-3.40	116.55	123.52
8	L	1002	BCL	CHD-C1D-ND	-3.40	120.01	124.80
8	8	102	BCL	CHD-C1D-ND	-3.40	120.02	124.80
12	J	101	KGD	CAT-CAX-CAY	-3.40	116.31	127.64
8	0	101	BCL	CHD-C1D-ND	-3.40	120.02	124.80
8	A	102	BCL	C4A-NA-C1A	3.40	108.23	106.68
8	E	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	S	101	BCL	CHD-C1D-ND	-3.39	120.03	124.80
12	9	101	KGD	CAT-CAX-CAY	-3.39	116.34	127.64
8	6	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	102	BCL	CHA-C1A-NA	-3.39	118.72	126.39
8	2	102	BCL	C1D-ND-C4D	-3.39	103.94	106.31
8	Q	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
8	6	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
8	O	101	BCL	C1-C2-C3	-3.38	120.66	126.20
8	8	101	BCL	C1D-ND-C4D	-3.38	103.94	106.31
8	T	103	BCL	C4A-NA-C1A	3.38	108.22	106.68
8	9	103	BCL	CAB-C3B-C2B	3.38	134.76	127.74
8	K	101	BCL	CHD-C1D-ND	-3.37	120.05	124.80
8	5	102	BCL	CHD-C1D-ND	-3.37	120.06	124.80
8	J	102	BCL	CAB-C3B-C2B	3.36	134.73	127.74
8	0	101	BCL	C4A-NA-C1A	3.36	108.21	106.68
8	0	101	BCL	C1D-ND-C4D	-3.36	103.96	106.31
8	I	101	BCL	CHA-C1A-NA	-3.36	118.79	126.39
8	2	101	BCL	C4A-NA-C1A	3.35	108.21	106.68
10	M	702	MQE	CCI-CCM-CCN	-3.34	116.50	127.64
9	M	704	BPH	C16-C15-C13	3.34	127.07	115.97
8	O	101	BCL	C1D-ND-C4D	-3.34	103.97	106.31
8	Q	101	BCL	CHD-C1D-ND	-3.34	120.11	124.80
8	V	101	BCL	C1-C2-C3	-3.33	120.75	126.20
8	6	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
8	U	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
12	R	101	KGD	CAP-CAQ-CAR	-3.31	117.29	126.36
8	Q	102	BCL	C1-C2-C3	-3.30	120.80	126.20
8	K	101	BCL	CHA-C1A-NA	-3.29	118.94	126.39
8	L	1002	BCL	CHA-C1A-NA	-3.29	118.94	126.39
12	3	101	KGD	CBA-CBE-CBF	-3.28	113.69	123.20
8	S	102	BCL	CHA-C1A-NA	-3.28	118.96	126.39
12	N	102	KGD	CAT-CAX-CAY	-3.28	116.70	127.64
12	R	101	KGD	CAZ-CAW-CAS	3.27	120.91	115.23
8	O	101	BCL	CHD-C1D-ND	-3.27	120.21	124.80
8	5	102	BCL	C17-C16-C15	3.27	127.91	113.28
8	R	102	BCL	C4A-NA-C1A	3.26	108.17	106.68
12	T	102	KGD	CBF-CBH-CBJ	3.26	124.14	119.01
9	L	1003	BPH	OBD-CAD-CBD	-3.25	121.06	125.82
8	O	101	BCL	C4A-NA-C1A	3.24	108.16	106.68
8	2	102	BCL	C6-C7-C8	3.24	126.74	115.97
8	D	101	BCL	CHA-C1A-NA	-3.24	119.06	126.39
8	U	102	BCL	CHA-C1A-NA	-3.23	119.07	126.39
8	S	101	BCL	CHA-C1A-NA	-3.23	119.09	126.39
10	M	702	MQE	CBW-CAT-CAF	3.22	120.82	115.23
8	O	102	BCL	CHA-C1A-NA	-3.21	119.11	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	102	BCL	C4A-NA-C1A	3.21	108.14	106.68
8	E	102	BCL	CED-O2D-CGD	3.21	123.19	115.92
8	8	102	BCL	CHA-C1A-NA	-3.21	119.13	126.39
9	M	705	BPH	OBD-CAD-CBD	-3.20	121.12	125.82
11	C	504	HEM	CHB-C1B-NB	3.20	128.33	124.37
12	J	101	KGD	CAF-CAB-CAD	3.20	115.25	110.24
8	K	102	BCL	CHA-C1A-NA	-3.19	119.17	126.39
12	T	102	KGD	CBN-CBL-CBI	3.19	124.02	119.01
12	T	101	KGD	CBB-CBG-CBI	-3.18	117.01	123.52
8	I	101	BCL	C1-C2-C3	-3.18	120.99	126.20
10	M	702	MQE	CCL-CCC-CCD	3.18	120.75	115.23
8	O	101	BCL	CHA-C1A-NA	-3.18	119.19	126.39
8	E	102	BCL	C4A-NA-C1A	3.17	108.13	106.68
12	9	102	KGD	CAO-CAP-CAQ	-3.16	114.05	123.20
12	N	101	KGD	CAO-CAP-CAQ	-3.15	114.06	123.20
8	B	102	BCL	CHA-C1A-NA	-3.15	119.25	126.39
8	O	102	BCL	C2A-C1A-CHA	3.15	129.34	123.87
8	4	101	BCL	CHD-C1D-ND	-3.15	120.37	124.80
8	G	101	BCL	CHD-C1D-ND	-3.15	120.37	124.80
12	J	101	KGD	CBB-CBG-CBI	-3.14	117.08	123.52
8	O	102	BCL	C4A-NA-C1A	3.14	108.11	106.68
8	G	102	BCL	CHA-C1A-NA	-3.14	119.28	126.39
8	W	102	BCL	CHA-C1A-NA	-3.14	119.29	126.39
8	I	102	BCL	CHA-C1A-NA	-3.13	119.30	126.39
8	Q	102	BCL	C4A-NA-C1A	3.13	108.11	106.68
8	3	102	BCL	CHA-C1A-NA	-3.13	119.31	126.39
12	3	103	KGD	CAF-CAB-CAD	3.13	115.15	110.24
8	6	102	BCL	CHA-C1A-NA	-3.13	119.31	126.39
8	Q	102	BCL	CED-O2D-CGD	3.12	123.00	115.92
8	0	102	BCL	CHA-C1A-NA	-3.12	119.33	126.39
8	4	102	BCL	CHA-C1A-NA	-3.12	119.33	126.39
12	9	101	KGD	CBA-CBE-CBF	-3.11	114.18	123.20
8	B	101	BCL	CHD-C1D-ND	-3.11	120.42	124.80
12	3	101	KGD	CAO-CAP-CAQ	-3.10	114.20	123.20
12	9	101	KGD	CAF-CAB-CAD	3.10	115.11	110.24
12	F	101	KGD	CBA-CBE-CBF	-3.10	114.23	123.20
8	E	101	BCL	CHA-C1A-NA	-3.09	119.39	126.39
12	3	103	KGD	CAN-CAM-CAL	3.09	122.81	118.09
8	S	101	BCL	C4A-NA-C1A	3.09	108.09	106.68
12	3	103	KGD	CBM-CBN-CBL	-3.08	117.91	126.36
8	V	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	K	101	BCL	C4A-NA-C1A	3.08	108.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	BCL	C4A-NA-C1A	3.08	108.09	106.68
8	4	101	BCL	C15-C13-C12	-3.08	96.47	112.07
8	R	102	BCL	CHA-C1A-NA	-3.08	119.43	126.39
8	L	1001	BCL	CHA-C1A-NA	-3.08	119.43	126.39
9	M	704	BPH	OBD-CAD-CBD	-3.07	121.32	125.82
8	W	101	BCL	CHA-C1A-NA	-3.06	119.45	126.39
8	H	101	BCL	CHA-C1A-NA	-3.06	119.45	126.39
12	N	102	KGD	CBN-CBL-CBI	3.06	123.83	119.01
8	P	101	BCL	CHA-C1A-NA	-3.06	119.45	126.39
8	B	102	BCL	C1D-ND-C4D	-3.06	104.17	106.31
8	G	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	F	102	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	6	101	BCL	CAB-C3B-C2B	3.05	134.09	127.74
8	U	101	BCL	CHA-C1A-NA	-3.05	119.49	126.39
10	L	1004	MQE	CCF-CBM-CBJ	3.05	120.52	115.23
8	Q	102	BCL	C4D-C3D-CAD	-3.04	104.80	108.11
8	2	102	BCL	CHA-C1A-NA	-3.04	119.50	126.39
8	T	103	BCL	CHA-C1A-NA	-3.04	119.51	126.39
12	R	101	KGD	CBM-CBN-CBL	-3.04	118.03	126.36
12	5	101	KGD	CBK-CBH-CBJ	-3.04	117.89	122.82
8	N	103	BCL	CHA-C1A-NA	-3.04	119.51	126.39
12	N	101	KGD	CBB-CBG-CBI	-3.04	117.31	123.52
8	7	101	BCL	CHA-C1A-NA	-3.03	119.52	126.39
8	3	102	BCL	C1-C2-C3	-3.03	121.22	126.20
8	Q	101	BCL	CHA-C1A-NA	-3.03	119.52	126.39
12	N	102	KGD	CBF-CBH-CBJ	3.03	123.77	119.01
8	2	101	BCL	CHA-C1A-NA	-3.02	119.56	126.39
8	1	101	BCL	CHA-C1A-NA	-3.02	119.56	126.39
8	D	101	BCL	C4A-NA-C1A	3.01	108.05	106.68
8	B	101	BCL	CHA-C1A-NA	-3.01	119.58	126.39
8	9	103	BCL	CHA-C1A-NA	-3.01	119.58	126.39
8	B	102	BCL	C4A-NA-C1A	3.01	108.05	106.68
8	S	101	BCL	C6-C5-C3	3.00	120.78	113.47
12	T	102	KGD	CBK-CBH-CBJ	-3.00	117.95	122.82
8	8	101	BCL	CHA-C1A-NA	-3.00	119.60	126.39
8	4	101	BCL	CHA-C1A-NA	-3.00	119.60	126.39
10	M	702	MQE	CBX-CAV-CAH	3.00	120.43	115.23
12	J	101	KGD	CBA-CBE-CBF	-3.00	114.52	123.20
8	J	102	BCL	C16-C15-C13	3.00	125.92	115.97
12	H	102	KGD	CBB-CBG-CBI	-2.99	117.39	123.52
8	J	102	BCL	CHA-C1A-NA	-2.99	119.62	126.39
12	N	101	KGD	CBA-CBE-CBF	-2.98	114.56	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	102	BCL	C2A-C1A-CHA	2.98	129.04	123.87
12	3	101	KGD	CBN-CBL-CBI	2.97	123.69	119.01
12	R	101	KGD	CBO-CBL-CBN	2.97	122.63	118.09
8	H	101	BCL	C11-C10-C8	-2.97	106.10	115.97
12	J	101	KGD	CAZ-CAW-CAS	2.97	120.38	115.23
8	A	102	BCL	CHA-C1A-NA	-2.97	119.68	126.39
8	I	101	BCL	C4A-NA-C1A	2.96	108.03	106.68
8	0	101	BCL	CHA-C1A-NA	-2.96	119.69	126.39
12	9	102	KGD	CBN-CBL-CBI	2.95	123.66	119.01
8	6	101	BCL	CHA-C1A-NA	-2.95	119.70	126.39
10	L	1004	MQE	CBU-CAQ-CAD	2.95	120.35	115.23
12	T	101	KGD	CAO-CAP-CAQ	-2.95	114.66	123.20
12	H	102	KGD	CAF-CAB-CAD	2.95	114.86	110.24
8	M	703	BCL	CHA-C1A-NA	-2.95	119.72	126.39
8	0	101	BCL	C1-C2-C3	-2.94	121.38	126.20
12	T	101	KGD	CBN-CBL-CBI	2.93	123.62	119.01
8	K	102	BCL	C2A-C1A-CHA	2.93	128.96	123.87
12	T	101	KGD	CBA-CBE-CBF	-2.93	114.71	123.20
8	K	102	BCL	C16-C15-C13	2.93	125.70	115.97
12	A	101	KGD	CAF-CAB-CAD	2.93	114.83	110.24
8	5	102	BCL	CHA-C1A-NA	-2.92	119.77	126.39
12	N	102	KGD	CBK-CBH-CBJ	-2.92	118.08	122.82
8	3	102	BCL	C16-C15-C13	2.92	125.67	115.97
8	4	101	BCL	C1-C2-C3	-2.92	121.42	126.20
8	6	102	BCL	C2A-C1A-CHA	2.92	128.93	123.87
9	L	1003	BPH	C11-C10-C8	-2.92	106.27	115.97
8	E	102	BCL	CGD-CBD-CAD	-2.91	101.41	110.85
12	3	103	KGD	CBA-CBE-CBF	-2.91	114.76	123.20
12	3	103	KGD	CAK-CAH-CAD	-2.91	119.43	124.11
12	A	101	KGD	CAK-CAH-CAD	-2.88	119.49	124.11
8	S	101	BCL	CAB-C3B-C2B	2.87	133.71	127.74
12	N	102	KGD	CAZ-CAW-CAS	2.87	120.22	115.23
8	F	102	BCL	C11-C10-C8	-2.87	106.42	115.97
8	E	101	BCL	C4A-NA-C1A	2.87	107.99	106.68
8	6	101	BCL	C11-C10-C8	2.85	125.44	115.97
12	N	102	KGD	CAK-CAH-CAD	-2.85	119.53	124.11
12	3	101	KGD	CAF-CAB-CAD	2.84	114.70	110.24
10	L	1004	MQE	CBY-CAW-CAG	2.84	120.16	115.23
8	O	101	BCL	C6-C5-C3	2.84	120.39	113.47
8	I	102	BCL	C2A-C1A-CHA	2.83	128.78	123.87
12	9	101	KGD	CAK-CAH-CAD	-2.83	119.56	124.11
12	T	102	KGD	CAO-CAP-CAQ	-2.83	115.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1001	BCL	C2A-C1A-CHA	2.83	128.77	123.87
8	B	102	BCL	O2D-CGD-CBD	-2.82	106.30	111.23
8	W	102	BCL	C2A-C1A-CHA	2.82	128.76	123.87
8	4	101	BCL	C17-C16-C15	2.82	125.89	113.28
8	G	102	BCL	C16-C15-C13	2.81	125.31	115.97
11	C	504	HEM	CAD-CBD-CGD	-2.81	106.22	113.67
8	0	102	BCL	C2A-C1A-CHA	2.80	128.73	123.87
8	I	101	BCL	C16-C15-C13	2.80	125.27	115.97
12	F	101	KGD	CAK-CAH-CAD	-2.79	119.62	124.11
10	M	702	MQE	CAJ-CAD-CAQ	-2.79	103.94	113.19
12	T	101	KGD	CAK-CAH-CAD	-2.79	119.63	124.11
12	N	101	KGD	CAF-CAB-CAD	2.78	114.61	110.24
12	5	101	KGD	CBO-CBL-CBI	-2.78	118.31	122.82
8	I	102	BCL	C1-C2-C3	-2.77	121.65	126.20
9	L	1003	BPH	O2D-CGD-CBD	2.77	113.99	110.95
8	U	102	BCL	C2A-C1A-CHA	2.76	128.66	123.87
8	R	102	BCL	C2A-C1A-CHA	2.76	128.65	123.87
8	8	102	BCL	C2A-C1A-CHA	2.76	128.65	123.87
8	3	102	BCL	C6-C7-C8	2.76	125.12	115.97
12	H	102	KGD	CAK-CAH-CAD	-2.75	119.68	124.11
12	T	102	KGD	CAZ-CAW-CAS	2.73	119.97	115.23
8	U	101	BCL	C2A-C1A-CHA	2.73	128.61	123.87
8	V	101	BCL	C2A-C1A-CHA	2.72	128.58	123.87
12	T	102	KGD	CBO-CBL-CBI	-2.71	118.42	122.82
12	N	101	KGD	CAK-CAH-CAD	-2.71	119.75	124.11
8	2	102	BCL	C2A-C1A-CHA	2.71	128.57	123.87
12	H	102	KGD	CAU-CAR-CAQ	2.69	122.20	118.09
8	P	101	BCL	C2A-C1A-CHA	2.69	128.54	123.87
12	3	101	KGD	CBB-CBG-CBI	-2.68	118.03	123.52
8	D	101	BCL	CAB-C3B-C2B	2.68	133.32	127.74
9	M	705	BPH	C2D-C1D-ND	2.68	111.37	109.43
8	F	102	BCL	C2A-C1A-CHA	2.68	128.52	123.87
8	B	102	BCL	C2A-C1A-CHA	2.68	128.52	123.87
12	5	101	KGD	CAK-CAH-CAD	-2.68	119.81	124.11
12	T	102	KGD	CAF-CAB-CAD	2.68	114.44	110.24
9	M	705	BPH	CMB-C2B-C3B	2.67	130.03	124.68
12	3	101	KGD	CAK-CAH-CAD	-2.67	119.81	124.11
12	N	102	KGD	CAF-CAB-CAD	2.67	114.43	110.24
8	U	102	BCL	CAC-C3C-C4C	2.67	118.51	112.58
10	L	1004	MQE	CBV-CAR-CAE	2.67	119.86	115.23
12	F	101	KGD	CAF-CAB-CAD	2.67	114.42	110.24
12	T	102	KGD	CBB-CBG-CBI	-2.67	118.07	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	9	102	KGD	CAK-CAH-CAD	-2.66	119.83	124.11
8	G	102	BCL	C2A-C1A-CHA	2.66	128.49	123.87
12	5	101	KGD	CBF-CBH-CBJ	2.66	123.20	119.01
8	7	101	BCL	C2A-C1A-CHA	2.66	128.49	123.87
12	R	101	KGD	CAK-CAH-CAD	-2.66	119.83	124.11
8	L	1002	BCL	C6-C5-C3	2.65	119.92	113.47
8	T	103	BCL	C2A-C1A-CHA	2.64	128.46	123.87
12	R	101	KGD	CAU-CAR-CAQ	2.64	122.12	118.09
12	R	101	KGD	CAT-CAS-CAW	-2.64	104.44	113.19
10	L	1004	MQE	CAY-CAX-CBK	-2.63	120.38	124.89
12	3	101	KGD	CAT-CAS-CAW	-2.63	104.46	113.19
8	B	101	BCL	CAB-C3B-C2B	2.63	133.20	127.74
12	J	101	KGD	CAK-CAH-CAD	-2.62	119.89	124.11
8	I	101	BCL	CAB-C3B-C2B	2.62	133.19	127.74
12	H	102	KGD	CAP-CAQ-CAR	-2.61	119.19	126.36
8	2	101	BCL	C2A-C1A-CHA	2.61	128.40	123.87
12	5	101	KGD	CBB-CBG-CBI	-2.61	118.17	123.52
8	I	101	BCL	C2A-C1A-CHA	2.61	128.40	123.87
12	9	102	KGD	CBO-CBL-CBI	-2.61	118.59	122.82
8	7	101	BCL	CAB-C3B-C2B	2.61	133.16	127.74
8	L	1002	BCL	C2A-C1A-CHA	2.60	128.38	123.87
9	L	1003	BPH	C2D-C1D-ND	2.60	111.31	109.43
9	M	704	BPH	C2D-C1D-ND	2.59	111.30	109.43
8	U	101	BCL	C17-C16-C15	2.58	124.85	113.28
12	3	103	KGD	CBO-CBL-CBN	2.58	122.03	118.09
8	8	102	BCL	C16-C15-C13	2.58	124.54	115.97
8	8	101	BCL	CAB-C3B-C2B	2.58	133.10	127.74
8	E	101	BCL	C2A-C1A-CHA	2.58	128.34	123.87
8	3	102	BCL	C2A-C1A-CHA	2.57	128.33	123.87
12	5	101	KGD	CAT-CAX-CAY	-2.57	119.08	127.64
8	H	101	BCL	C2A-C1A-CHA	2.57	128.32	123.87
8	W	101	BCL	C2A-C1A-CHA	2.56	128.32	123.87
8	T	103	BCL	OBG-CAB-C3B	2.56	124.96	120.43
9	M	705	BPH	C1-C2-C3	-2.56	122.01	126.20
8	S	102	BCL	C2A-C1A-CHA	2.56	128.30	123.87
8	9	103	BCL	C2A-C1A-CHA	2.55	128.30	123.87
12	T	101	KGD	CAF-CAB-CAD	2.55	114.24	110.24
8	R	102	BCL	CAB-C3B-C2B	2.55	133.04	127.74
11	C	501	HEM	CAD-CBD-CGD	-2.55	106.91	113.67
8	B	101	BCL	C2A-C1A-CHA	2.55	128.29	123.87
8	K	102	BCL	C17-C16-C15	2.55	124.69	113.28
8	Q	102	BCL	C1-O2A-CGA	2.54	122.79	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	9	102	KGD	CAF-CAB-CAD	2.54	114.22	110.24
12	3	103	KGD	CAT-CAX-CAY	-2.54	119.19	127.64
12	H	102	KGD	CBO-CBL-CBN	2.54	121.96	118.09
8	6	101	BCL	C16-C15-C13	-2.53	107.54	115.97
8	G	101	BCL	C6-C7-C8	-2.53	107.55	115.97
12	F	101	KGD	CBN-CBL-CBI	2.53	122.98	119.01
9	M	705	BPH	O2D-CGD-CBD	2.52	113.72	110.95
10	L	1004	MQE	CBW-CAT-CAF	2.52	119.60	115.23
8	A	102	BCL	C2A-C1A-CHA	2.52	128.23	123.87
8	E	101	BCL	CAB-C3B-C2B	2.51	132.96	127.74
8	N	103	BCL	C2A-C1A-CHA	2.51	128.22	123.87
8	L	1001	BCL	CAA-CBA-CGA	2.50	120.31	113.21
8	U	101	BCL	C1-C2-C3	-2.50	122.11	126.20
12	9	102	KGD	CAZ-CAW-CAS	2.50	119.56	115.23
9	L	1003	BPH	CMB-C2B-C3B	2.49	129.67	124.68
12	3	103	KGD	CAL-CAM-CAO	-2.49	115.09	119.01
11	C	504	HEM	CBA-CAA-C2A	2.49	119.41	112.53
8	N	103	BCL	CAB-C3B-C2B	2.49	132.91	127.74
8	H	101	BCL	CAB-C3B-C2B	2.49	132.91	127.74
8	D	101	BCL	C2A-C1A-CHA	2.48	128.18	123.87
8	Q	101	BCL	C2A-C1A-CHA	2.48	128.17	123.87
8	1	101	BCL	C2A-C1A-CHA	2.48	128.17	123.87
8	0	101	BCL	C2A-C1A-CHA	2.48	128.17	123.87
8	Q	101	BCL	C1-C2-C3	-2.48	122.13	126.20
12	T	101	KGD	CBO-CBL-CBI	-2.47	118.81	122.82
8	N	103	BCL	C1-C2-C3	-2.47	122.15	126.20
8	P	101	BCL	CAB-C3B-C2B	2.46	132.86	127.74
12	5	101	KGD	CAF-CAB-CAD	2.46	114.10	110.24
9	M	704	BPH	CAA-CBA-CGA	2.45	120.16	113.21
9	M	705	BPH	C17-C16-C15	2.44	124.21	113.28
10	L	1004	MQE	CCL-CCC-CCD	2.43	119.45	115.23
10	M	702	MQE	CCE-CBK-CAX	-2.43	120.46	124.45
8	6	101	BCL	C2A-C1A-CHA	2.43	128.08	123.87
10	M	702	MQE	CCF-CBM-CBJ	2.43	119.44	115.23
10	L	1004	MQE	CBX-CAV-CAH	2.43	119.44	115.23
8	Q	102	BCL	C2A-C1A-CHA	2.42	128.07	123.87
12	9	102	KGD	CBD-CAY-CBC	2.42	120.16	114.59
8	S	101	BCL	C2A-C1A-CHA	2.42	128.06	123.87
8	U	101	BCL	C11-C10-C8	-2.42	107.93	115.97
10	M	702	MQE	CCP-CCN-CCO	2.42	120.15	114.59
8	M	703	BCL	C2A-C1A-CHA	2.42	128.06	123.87
12	T	101	KGD	CBD-CAY-CBC	2.41	120.14	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	101	KGD	CBD-CAY-CBC	2.41	120.14	114.59
8	W	102	BCL	C6-C7-C8	2.40	123.94	115.97
10	L	1004	MQE	CCE-CBK-CAX	-2.40	120.50	124.45
8	I	102	BCL	CAB-C3B-C2B	2.40	132.72	127.74
8	3	102	BCL	C11-C10-C8	-2.39	108.01	115.97
12	N	101	KGD	CBN-CBL-CBI	2.39	122.76	119.01
8	1	101	BCL	CAB-C3B-C2B	2.39	132.70	127.74
8	E	102	BCL	C2A-C1A-CHA	2.38	128.00	123.87
12	T	102	KGD	CBD-CAY-CBC	2.38	120.06	114.59
8	K	101	BCL	C2A-C1A-CHA	2.38	128.00	123.87
12	N	101	KGD	CBD-CAY-CBC	2.37	120.05	114.59
8	O	101	BCL	C2A-C1A-CHA	2.37	127.97	123.87
9	L	1003	BPH	CMD-C2D-C3D	2.37	129.41	124.68
8	4	101	BCL	C2A-C1A-CHA	2.36	127.97	123.87
12	J	101	KGD	CBO-CBL-CBI	-2.36	118.99	122.82
8	0	102	BCL	C1C-NC-C4C	2.36	107.76	106.68
8	V	101	BCL	CAB-C3B-C2B	2.36	132.64	127.74
10	M	702	MQE	CBL-CAY-CAX	2.35	117.87	112.08
12	N	102	KGD	CAN-CAM-CAO	-2.35	119.01	122.82
8	U	101	BCL	C6-C7-C8	-2.35	108.16	115.97
12	9	101	KGD	CBJ-CBM-CBN	-2.35	116.40	123.20
12	N	102	KGD	CBO-CBL-CBI	-2.35	119.02	122.82
9	M	704	BPH	CMB-C2B-C3B	2.34	129.37	124.68
12	9	102	KGD	CBB-CBG-CBI	-2.34	118.73	123.52
8	Q	101	BCL	CAB-C3B-C2B	2.34	132.61	127.74
10	M	702	MQE	CBY-CAW-CAG	2.34	119.29	115.23
10	L	1004	MQE	CBZ-CAZ-CAU	2.33	119.28	115.23
11	C	504	HEM	CMA-C3A-C4A	-2.33	121.87	125.42
8	F	102	BCL	C16-C15-C13	2.33	123.70	115.97
10	L	1004	MQE	CCP-CCN-CCO	2.32	119.94	114.59
8	8	101	BCL	C2A-C1A-CHA	2.32	127.90	123.87
10	M	702	MQE	CAE-CAL-CBF	-2.32	100.56	112.02
8	W	101	BCL	CAB-C3B-C2B	2.32	132.55	127.74
8	J	102	BCL	C2A-C1A-CHA	2.31	127.88	123.87
10	M	702	MQE	CAC-CAI-CBD	-2.31	100.59	112.02
8	2	101	BCL	C1-C2-C3	-2.31	122.42	126.20
8	E	101	BCL	CBA-CAA-C2A	-2.31	106.93	113.79
12	R	101	KGD	CBD-CAY-CBC	2.30	119.89	114.59
8	9	103	BCL	C17-C16-C15	2.30	123.60	113.28
11	C	504	HEM	CAA-C2A-C3A	2.30	132.23	127.07
8	K	101	BCL	CAB-C3B-C2B	2.30	132.52	127.74
8	B	102	BCL	C16-C15-C13	2.29	123.58	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	101	KGD	CBN-CBL-CBI	2.29	122.61	119.01
9	M	705	BPH	CMD-C2D-C3D	2.29	129.25	124.68
9	L	1003	BPH	C15-C13-C12	-2.28	100.50	112.07
12	T	102	KGD	CAK-CAH-CAD	-2.28	120.44	124.11
11	C	504	HEM	CMA-C3A-C2A	2.28	130.46	125.62
12	N	101	KGD	CBK-CBH-CBJ	-2.28	119.13	122.82
12	F	101	KGD	CAE-CAC-CAB	-2.27	109.88	113.21
12	J	101	KGD	CBJ-CBM-CBN	-2.27	116.62	123.20
11	C	503	HEM	CBD-CAD-C3D	-2.27	106.26	112.53
8	A	102	BCL	C17-C16-C15	2.27	123.44	113.28
8	O	101	BCL	C11-C10-C8	-2.26	108.45	115.97
8	E	102	BCL	C16-C15-C13	2.26	123.48	115.97
8	O	101	BCL	CAB-C3B-C2B	2.26	132.44	127.74
8	P	101	BCL	C1-C2-C3	-2.26	122.50	126.20
8	W	102	BCL	C1-C2-C3	-2.25	122.50	126.20
8	B	102	BCL	C1-C2-C3	-2.24	122.52	126.20
12	F	101	KGD	CBD-CAY-CBC	2.24	119.75	114.59
12	3	101	KGD	CBO-CBL-CBI	-2.24	119.19	122.82
8	5	102	BCL	C2A-C1A-CHA	2.23	127.74	123.87
12	3	103	KGD	CBD-CAY-CBC	2.23	119.72	114.59
11	C	502	HEM	CHB-C1B-NB	2.22	127.12	124.37
8	0	102	BCL	C16-C15-C13	2.22	123.36	115.97
11	C	502	HEM	CHD-C4C-NC	2.22	126.87	124.45
11	C	502	HEM	C3B-C2B-C1B	2.22	108.08	106.41
9	M	704	BPH	O2D-CGD-CBD	2.22	113.38	110.95
8	M	703	BCL	C11-C10-C8	-2.21	108.62	115.97
12	F	101	KGD	CBJ-CBM-CBN	-2.21	116.81	123.20
8	8	102	BCL	C4D-C3D-CAD	-2.21	105.71	108.11
12	N	102	KGD	CAO-CAP-CAQ	-2.20	116.82	123.20
8	M	703	BCL	C1-O2A-CGA	-2.20	111.33	116.65
11	C	502	HEM	CAA-CBA-CGA	-2.19	107.85	113.67
8	W	101	BCL	C16-C15-C13	2.19	123.24	115.97
8	K	101	BCL	C1C-NC-C4C	2.18	107.67	106.68
12	5	101	KGD	CAO-CAP-CAQ	-2.18	116.88	123.20
12	H	102	KGD	CAN-CAM-CAL	2.18	121.42	118.09
12	H	102	KGD	CBM-CBN-CBL	-2.18	120.39	126.36
12	9	102	KGD	CBK-CBH-CBJ	-2.18	119.29	122.82
12	R	101	KGD	CAE-CAC-CAB	-2.18	110.03	113.21
8	0	102	BCL	C11-C10-C8	-2.17	108.75	115.97
12	H	102	KGD	CAQ-CAR-CAV	-2.17	115.59	119.01
12	F	101	KGD	CBO-CBL-CBI	-2.17	119.30	122.82
12	J	101	KGD	CAE-CAC-CAB	-2.16	110.05	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	102	KGD	CBD-CAY-CBC	2.15	119.54	114.59
12	3	101	KGD	CBD-CAY-CBC	2.15	119.53	114.59
8	R	102	BCL	C17-C16-C15	2.14	122.88	113.28
12	N	101	KGD	CBO-CBL-CBI	-2.14	119.35	122.82
12	A	101	KGD	CAE-CAC-CAB	-2.14	110.08	113.21
12	9	101	KGD	CBD-CAY-CBC	2.14	119.51	114.59
8	2	102	BCL	C1-C2-C3	-2.14	122.70	126.20
8	N	103	BCL	CMB-C2B-C1B	-2.13	122.18	125.42
8	V	101	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
12	N	101	KGD	CAE-CAC-CAB	-2.12	110.11	113.21
9	M	704	BPH	CMD-C2D-C3D	2.11	128.91	124.68
8	6	101	BCL	C16-C17-C18	-2.11	106.53	115.94
8	4	101	BCL	CAB-C3B-C2B	2.11	132.12	127.74
12	J	101	KGD	CBD-CAY-CBC	2.11	119.44	114.59
10	M	702	MQE	CBU-CAQ-CAD	2.10	118.88	115.23
12	5	101	KGD	CAZ-CAW-CAS	2.10	118.88	115.23
8	G	101	BCL	C15-C13-C12	-2.09	101.49	112.07
9	M	704	BPH	C15-C13-C12	-2.09	101.49	112.07
8	G	101	BCL	C2A-C1A-CHA	2.09	127.49	123.87
12	5	101	KGD	CAE-CAC-CAB	-2.08	110.16	113.21
8	2	102	BCL	C11-C10-C8	2.08	122.88	115.97
8	7	101	BCL	CMB-C2B-C1B	-2.08	122.26	125.42
10	M	702	MQE	CBZ-CAZ-CBI	-2.08	118.29	123.63
12	3	101	KGD	CAE-CAC-CAB	-2.07	110.18	113.21
8	7	101	BCL	OBB-CAB-CBB	-2.07	115.13	119.77
12	J	101	KGD	CAU-CAR-CAQ	2.07	121.25	118.09
8	Q	101	BCL	C6-C5-C3	2.07	118.50	113.47
8	G	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
8	S	102	BCL	C1C-NC-C4C	2.06	107.62	106.68
12	R	101	KGD	CAN-CAM-CAL	2.06	121.24	118.09
12	5	101	KGD	CAN-CAM-CAO	-2.06	119.48	122.82
8	A	102	BCL	C16-C15-C13	2.05	122.78	115.97
8	G	101	BCL	C11-C10-C8	2.05	122.78	115.97
11	C	502	HEM	CMB-C2B-C1B	-2.05	121.83	125.03
8	Q	102	BCL	C1C-NC-C4C	2.05	107.61	106.68
8	D	101	BCL	C11-C12-C13	-2.04	109.17	115.97
12	T	102	KGD	CAE-CAC-CAB	-2.04	110.22	113.21
12	9	102	KGD	CAE-CAC-CAB	-2.04	110.22	113.21
12	3	103	KGD	CBK-CBH-CBJ	-2.04	119.51	122.82
11	C	504	HEM	CAA-C2A-C1A	-2.04	120.95	124.94
11	C	503	HEM	CHD-C1D-ND	2.04	126.62	124.42
12	H	102	KGD	CAE-CAC-CAB	-2.04	110.23	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	102	BCL	C1-C2-C3	2.04	129.53	126.20
10	L	1004	MQE	CCA-CBB-CAN	2.03	118.76	115.23
8	6	102	BCL	C4D-C3D-CAD	-2.03	105.90	108.11
12	5	101	KGD	CBD-CAY-CBC	2.03	119.25	114.59
12	T	101	KGD	CBK-CBH-CBJ	-2.02	119.54	122.82
8	U	101	BCL	CAB-C3B-C2B	2.02	131.93	127.74
12	9	102	KGD	CAN-CAM-CAO	-2.01	119.56	122.82
8	E	101	BCL	C1C-NC-C4C	2.01	107.60	106.68
8	R	102	BCL	CED-O2D-CGD	2.01	120.48	115.92
8	0	101	BCL	CAB-C3B-C2B	2.00	131.90	127.74

There are no chirality outliers.

All (375) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	0	101	BCL	C2C-C3C-CAC-CBC
8	0	101	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	C2C-C3C-CAC-CBC
8	0	102	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	CAD-CBD-CGD-O1D
8	0	102	BCL	CAD-CBD-CGD-O2D
8	L	1001	BCL	C1A-C2A-CAA-CBA
8	L	1001	BCL	C4C-C3C-CAC-CBC
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	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	CAD-CBD-CGD-O1D
8	6	102	BCL	CAD-CBD-CGD-O2D
8	4	101	BCL	C4C-C3C-CAC-CBC
8	4	102	BCL	C2C-C3C-CAC-CBC
8	4	102	BCL	C4C-C3C-CAC-CBC
8	2	102	BCL	C2B-C3B-CAB-OB
8	2	102	BCL	C2B-C3B-CAB-CB
8	2	102	BCL	C4B-C3B-CAB-OB

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Mol	Chain	Res	Type	Atoms
8	2	102	BCL	C4B-C3B-CAB-CBB
8	2	102	BCL	C2C-C3C-CAC-CBC
8	2	102	BCL	C4C-C3C-CAC-CBC
8	I	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	CAD-CBD-CGD-O1D
8	G	102	BCL	CAD-CBD-CGD-O2D
8	W	102	BCL	C2-C3-C5-C6
8	W	102	BCL	C4-C3-C5-C6
8	U	102	BCL	CAD-CBD-CGD-O1D
8	U	102	BCL	CAD-CBD-CGD-O2D
8	T	103	BCL	C2-C3-C5-C6
8	T	103	BCL	C4-C3-C5-C6
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	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C4C-C3C-CAC-CBC
8	R	102	BCL	C2C-C3C-CAC-CBC
8	N	103	BCL	C2C-C3C-CAC-CBC
8	N	103	BCL	C4C-C3C-CAC-CBC
8	F	102	BCL	C2C-C3C-CAC-CBC
8	F	102	BCL	C4C-C3C-CAC-CBC
8	A	102	BCL	C2C-C3C-CAC-CBC
8	A	102	BCL	C4C-C3C-CAC-CBC
8	7	101	BCL	C2C-C3C-CAC-CBC
8	7	101	BCL	C4C-C3C-CAC-CBC
8	1	101	BCL	C2C-C3C-CAC-CBC
8	1	101	BCL	C4C-C3C-CAC-CBC
9	M	704	BPH	C3A-C2A-CAA-CBA
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	CAS-CAN-CBB-CCA
11	C	504	HEM	C3A-C2A-CAA-CBA
12	H	102	KGD	CAS-CAT-CAX-CAY
8	E	101	BCL	C4-C3-C5-C6
8	B	101	BCL	C4-C3-C5-C6
8	0	102	BCL	C4-C3-C5-C6
8	8	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	4	101	BCL	C4-C3-C5-C6
8	2	102	BCL	C4-C3-C5-C6
8	G	101	BCL	C4-C3-C5-C6
8	R	102	BCL	C4-C3-C5-C6
8	N	103	BCL	C4-C3-C5-C6
8	J	102	BCL	C4-C3-C5-C6
8	H	101	BCL	C4-C3-C5-C6
8	1	101	BCL	C4-C3-C5-C6
10	L	1004	MQE	CAM-CAG-CAW-CBY
10	M	702	MQE	CAL-CAE-CAR-CBV
8	E	101	BCL	C2-C3-C5-C6
8	B	101	BCL	C2-C3-C5-C6
8	0	102	BCL	C2-C3-C5-C6
8	8	102	BCL	C2-C3-C5-C6
8	2	102	BCL	C2-C3-C5-C6
8	G	101	BCL	C2-C3-C5-C6
8	W	101	BCL	C2-C3-C5-C6
8	R	102	BCL	C2-C3-C5-C6
8	N	103	BCL	C2-C3-C5-C6
8	J	102	BCL	C2-C3-C5-C6
8	H	101	BCL	C2-C3-C5-C6
8	1	101	BCL	C2-C3-C5-C6
10	L	1004	MQE	CAM-CAG-CAW-CBH
10	L	1004	MQE	CAO-CAH-CAV-CBF
10	M	702	MQE	CAL-CAE-CAR-CBD
10	M	702	MQE	CAS-CAN-CBB-CBL
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	5	102	BCL	C4-C3-C5-C6
10	L	1004	MQE	CAK-CAF-CAT-CBW
10	M	702	MQE	CCL-CCC-CCD-CCI
8	L	1002	BCL	C2-C3-C5-C6
8	8	101	BCL	C2-C3-C5-C6
8	Q	101	BCL	C2-C3-C5-C6
11	C	504	HEM	C1A-C2A-CAA-CBA
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	8	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
8	K	102	BCL	C10-C11-C12-C13
8	I	102	BCL	C12-C13-C15-C16
8	F	102	BCL	C6-C7-C8-C10
8	3	102	BCL	C4-C3-C5-C6
8	M	703	BCL	C4-C3-C5-C6
8	B	101	BCL	C15-C16-C17-C18
8	4	101	BCL	C2A-CAA-CBA-CGA
8	4	102	BCL	C2A-CAA-CBA-CGA
8	K	102	BCL	C2A-CAA-CBA-CGA
8	L	1002	BCL	C5-C6-C7-C8
10	M	702	MQE	CBO-CBJ-CBM-CCF
10	M	702	MQE	CCB-CCC-CCD-CCI
8	B	102	BCL	C10-C11-C12-C13
8	O	102	BCL	C2A-CAA-CBA-CGA
8	5	102	BCL	C2-C3-C5-C6
8	O	101	BCL	C13-C15-C16-C17
8	L	1001	BCL	C4B-C3B-CAB-OB
8	2	102	BCL	C2A-CAA-CBA-CGA
10	M	702	MQE	CBO-CBJ-CBM-CBN
8	L	1001	BCL	C3A-C2A-CAA-CBA
8	3	102	BCL	C2-C3-C5-C6
10	M	702	MQE	CBA-CAU-CAZ-CBZ
8	M	703	BCL	C2-C3-C5-C6
10	M	702	MQE	CBA-CAU-CAZ-CBI
8	K	102	BCL	C4-C3-C5-C6
8	9	103	BCL	C4-C3-C5-C6
10	M	702	MQE	CAM-CAG-CAW-CBY
8	8	102	BCL	C13-C15-C16-C17
10	M	702	MQE	CAM-CAG-CAW-CBH
8	U	102	BCL	C2A-CAA-CBA-CGA
8	2	102	BCL	C11-C10-C8-C7
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	9	103	BCL	C2-C3-C5-C6
8	E	102	BCL	C13-C15-C16-C17
8	L	1001	BCL	C4B-C3B-CAB-CBB
8	U	102	BCL	C4B-C3B-CAB-OB
8	6	102	BCL	C2A-CAA-CBA-CGA
8	S	101	BCL	C11-C10-C8-C9
8	0	102	BCL	C10-C11-C12-C13
8	2	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	G	102	BCL	C10-C11-C12-C13
8	K	102	BCL	O2A-C1-C2-C3
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	4	102	BCL	C4-C3-C5-C6
8	K	101	BCL	C16-C17-C18-C19
8	K	101	BCL	C16-C17-C18-C20
8	O	102	BCL	C4-C3-C5-C6
8	Q	102	BCL	C6-C7-C8-C9
8	L	1001	BCL	C11-C10-C8-C7
8	I	102	BCL	C11-C12-C13-C15
8	S	101	BCL	C11-C10-C8-C7
9	L	1003	BPH	C6-C7-C8-C10
8	L	1001	BCL	C4-C3-C5-C6
12	5	101	KGD	CAT-CAS-CAW-CAZ
8	A	102	BCL	C4-C3-C5-C6
12	5	101	KGD	CAT-CAS-CAW-CBA
9	M	705	BPH	C13-C15-C16-C17
8	W	101	BCL	C4-C3-C5-C6
8	L	1001	BCL	C2-C3-C5-C6
8	O	102	BCL	C2-C3-C5-C6
8	G	102	BCL	C13-C15-C16-C17
8	4	102	BCL	C4B-C3B-CAB-OB
8	F	102	BCL	C6-C7-C8-C9
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	A	102	BCL	C2-C3-C5-C6
8	A	102	BCL	C8-C10-C11-C12
8	6	101	BCL	C8-C10-C11-C12
8	W	102	BCL	C10-C11-C12-C13
8	D	101	BCL	C12-C13-C15-C16
10	M	702	MQE	CBK-CAX-CAY-CBL
8	L	1001	BCL	C10-C11-C12-C13
10	L	1004	MQE	CBO-CBJ-CBM-CCF
8	S	102	BCL	O2A-C1-C2-C3
8	K	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	M	702	MQE	CBQ-CAX-CAY-CBL
9	L	1003	BPH	C8-C10-C11-C12
8	K	101	BCL	C11-C10-C8-C9
8	I	102	BCL	C11-C12-C13-C14
8	D	101	BCL	C14-C13-C15-C16
9	L	1003	BPH	C6-C7-C8-C9
8	4	101	BCL	C1A-C2A-CAA-CBA
8	D	101	BCL	C4-C3-C5-C6
8	8	102	BCL	C6-C7-C8-C10
8	S	101	BCL	C6-C7-C8-C10
8	O	102	BCL	C6-C7-C8-C10
8	5	102	BCL	C12-C13-C15-C16
8	E	102	BCL	C2C-C3C-CAC-CBC
8	B	102	BCL	C2C-C3C-CAC-CBC
8	K	102	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C2C-C3C-CAC-CBC
8	U	102	BCL	C4B-C3B-CAB-CBB
8	L	1001	BCL	C11-C10-C8-C9
8	0	101	BCL	C15-C16-C17-C18
8	Q	102	BCL	C13-C15-C16-C17
10	L	1004	MQE	CBO-CBJ-CBM-CBN
8	4	102	BCL	CAD-CBD-CGD-O2D
8	Q	102	BCL	CAD-CBD-CGD-O2D
8	E	102	BCL	C10-C11-C12-C13
8	3	102	BCL	C13-C15-C16-C17
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	E	102	BCL	O2A-C1-C2-C3
8	L	1001	BCL	C2B-C3B-CAB-OB
8	8	102	BCL	C6-C7-C8-C9
8	A	102	BCL	C14-C13-C15-C16
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	4	102	BCL	C4B-C3B-CAB-CBB
8	K	102	BCL	C4B-C3B-CAB-OB
8	W	102	BCL	C4B-C3B-CAB-OB
11	C	501	HEM	C2A-CAA-CBA-CGA
8	H	101	BCL	C16-C17-C18-C19
8	E	101	BCL	C15-C16-C17-C18
8	U	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	101	KGD	CAT-CAS-CAW-CAZ
8	D	101	BCL	C2-C3-C5-C6
12	3	101	KGD	CAT-CAS-CAW-CBA
8	L	1002	BCL	C6-C7-C8-C10
8	W	102	BCL	C11-C10-C8-C7
8	H	101	BCL	C16-C17-C18-C20
8	4	101	BCL	C3A-C2A-CAA-CBA
8	Q	102	BCL	C3A-C2A-CAA-CBA
8	8	102	BCL	C2-C1-O2A-CGA
8	2	102	BCL	C5-C6-C7-C8
12	R	101	KGD	CAT-CAS-CAW-CAZ
12	9	102	KGD	CAT-CAS-CAW-CAZ
11	C	502	HEM	C2A-CAA-CBA-CGA
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	C11-C10-C8-C9
8	5	102	BCL	C6-C7-C8-C9
8	L	1002	BCL	C15-C16-C17-C18
9	L	1003	BPH	O2A-C1-C2-C3
8	E	102	BCL	C5-C6-C7-C8
8	B	102	BCL	C4-C3-C5-C6
8	I	102	BCL	CAA-CBA-CGA-O2A
12	R	101	KGD	CAT-CAS-CAW-CBA
8	4	102	BCL	C5-C6-C7-C8
8	G	102	BCL	C4-C3-C5-C6
10	M	702	MQE	CAK-CAF-CAT-CBW
11	C	502	HEM	C3D-CAD-CBD-CGD
8	4	101	BCL	C6-C7-C8-C10
8	S	102	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C4-C3-C5-C6
12	A	101	KGD	CAT-CAS-CAW-CBA
8	E	102	BCL	C4-C3-C5-C6
12	9	101	KGD	CAT-CAS-CAW-CAZ
12	9	102	KGD	CAT-CAS-CAW-CBA
8	Q	101	BCL	C3-C5-C6-C7
8	R	102	BCL	C10-C11-C12-C13
8	U	102	BCL	C4C-C3C-CAC-CBC
8	S	101	BCL	C4-C3-C5-C6
10	L	1004	MQE	CAJ-CAD-CAQ-CBU
12	T	102	KGD	CAT-CAS-CAW-CAZ
12	N	102	KGD	CAT-CAS-CAW-CAZ

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Mol	Chain	Res	Type	Atoms
8	E	101	BCL	CAA-CBA-CGA-O2A
9	M	704	BPH	CHA-CBD-CGD-O1D
9	M	704	BPH	CHA-CBD-CGD-O2D
8	2	101	BCL	CAA-CBA-CGA-O2A
12	3	103	KGD	CAT-CAS-CAW-CAZ
8	N	103	BCL	C2-C1-O2A-CGA
8	3	102	BCL	C2-C1-O2A-CGA
9	M	705	BPH	C16-C17-C18-C19
8	L	1001	BCL	C2B-C3B-CAB-CBB
8	U	102	BCL	O2A-C1-C2-C3
8	2	101	BCL	C8-C10-C11-C12
8	S	102	BCL	C4-C3-C5-C6
8	W	102	BCL	C4B-C3B-CAB-CBB
8	F	102	BCL	C13-C15-C16-C17
8	U	101	BCL	CAA-CBA-CGA-O2A
9	L	1003	BPH	C4-C3-C5-C6
8	E	102	BCL	C6-C7-C8-C10
8	0	101	BCL	C11-C10-C8-C7
9	M	704	BPH	C6-C7-C8-C10
8	8	101	BCL	CAA-CBA-CGA-O2A
8	K	101	BCL	CAA-CBA-CGA-O2A
8	I	102	BCL	C2-C1-O2A-CGA
8	U	102	BCL	C2-C1-O2A-CGA
8	A	102	BCL	C2-C1-O2A-CGA
8	4	102	BCL	CAA-CBA-CGA-O2A
8	Q	102	BCL	C5-C6-C7-C8
12	H	102	KGD	CAT-CAS-CAW-CAZ
8	T	103	BCL	CAA-CBA-CGA-O2A
8	B	102	BCL	CAA-CBA-CGA-O2A
8	7	101	BCL	CAA-CBA-CGA-O2A
8	B	101	BCL	CAA-CBA-CGA-O2A
8	D	101	BCL	CAA-CBA-CGA-O2A
8	I	102	BCL	C15-C16-C17-C18
8	9	103	BCL	CAA-CBA-CGA-O2A
8	B	102	BCL	C2-C3-C5-C6
10	L	1004	MQE	CAJ-CAD-CAQ-CBE
8	0	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

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Mol	Chain	Res	Type	Atoms
9	M	704	BPH	C6-C7-C8-C9
8	R	102	BCL	CAA-CBA-CGA-O2A
8	W	102	BCL	CAA-CBA-CGA-O2A
8	M	703	BCL	CAA-CBA-CGA-O2A
8	Q	102	BCL	CAA-CBA-CGA-O2A
8	V	101	BCL	CAA-CBA-CGA-O2A
8	E	101	BCL	C2A-CAA-CBA-CGA
9	L	1003	BPH	CAA-CBA-CGA-O2A
8	0	101	BCL	C2-C1-O2A-CGA
8	G	101	BCL	C2-C1-O2A-CGA
8	F	102	BCL	C2-C1-O2A-CGA
8	5	102	BCL	C2-C1-O2A-CGA
8	6	101	BCL	C6-C7-C8-C10
8	W	102	BCL	C6-C7-C8-C10
8	V	101	BCL	C6-C7-C8-C10
8	F	102	BCL	C12-C13-C15-C16
8	G	101	BCL	C16-C17-C18-C19
8	G	102	BCL	O2A-C1-C2-C3
8	2	102	BCL	CAA-CBA-CGA-O2A
8	Q	102	BCL	C4-C3-C5-C6
8	Q	101	BCL	CAA-CBA-CGA-O2A
8	F	102	BCL	C10-C11-C12-C13
8	T	103	BCL	CAA-CBA-CGA-O1A
8	9	103	BCL	CAA-CBA-CGA-O1A
8	I	102	BCL	C10-C11-C12-C13
8	6	101	BCL	C6-C7-C8-C9
8	V	101	BCL	C6-C7-C8-C9
8	F	102	BCL	C14-C13-C15-C16
8	F	102	BCL	CAA-CBA-CGA-O2A
8	B	101	BCL	CAA-CBA-CGA-O1A
8	R	102	BCL	CAA-CBA-CGA-O1A
8	7	101	BCL	CAA-CBA-CGA-O1A
8	A	102	BCL	C10-C11-C12-C13
8	O	101	BCL	C4-C3-C5-C6
8	B	102	BCL	CAA-CBA-CGA-O1A
8	0	101	BCL	CAA-CBA-CGA-O1A
8	D	101	BCL	CAA-CBA-CGA-O1A
8	4	102	BCL	CAA-CBA-CGA-O1A
8	S	101	BCL	CAA-CBA-CGA-O2A
8	8	101	BCL	CAA-CBA-CGA-O1A
8	U	101	BCL	CAA-CBA-CGA-O1A
8	M	703	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	9	103	BCL	C8-C10-C11-C12
9	L	1003	BPH	CAA-CBA-CGA-O1A
11	C	501	HEM	C2B-C3B-CAB-CBB
8	I	102	BCL	CAD-CBD-CGD-O2D
8	G	101	BCL	CAA-CBA-CGA-O2A
8	W	101	BCL	CAA-CBA-CGA-O2A
8	Q	102	BCL	CAA-CBA-CGA-O1A
8	2	102	BCL	C2-C1-O2A-CGA
8	G	102	BCL	C15-C16-C17-C18
8	W	102	BCL	CAA-CBA-CGA-O1A
8	Q	101	BCL	CAA-CBA-CGA-O1A
8	F	102	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	E	101	BCL	4	0
8	B	102	BCL	24	0
8	0	101	BCL	7	0
8	Q	102	BCL	10	0
8	R	102	BCL	6	0
8	W	102	BCL	13	0
8	T	103	BCL	3	0
8	W	101	BCL	4	0
8	F	102	BCL	4	0
8	Q	101	BCL	4	0
8	O	101	BCL	6	0
8	7	101	BCL	7	0
8	5	102	BCL	3	0
8	I	102	BCL	15	0
8	G	101	BCL	7	0
8	K	102	BCL	15	0
8	4	102	BCL	5	0
11	C	504	HEM	11	0
8	P	101	BCL	1	0
8	M	703	BCL	5	0
8	V	101	BCL	4	0
8	L	1001	BCL	12	0
8	U	101	BCL	3	0
8	L	1002	BCL	8	0
9	M	704	BPH	2	0

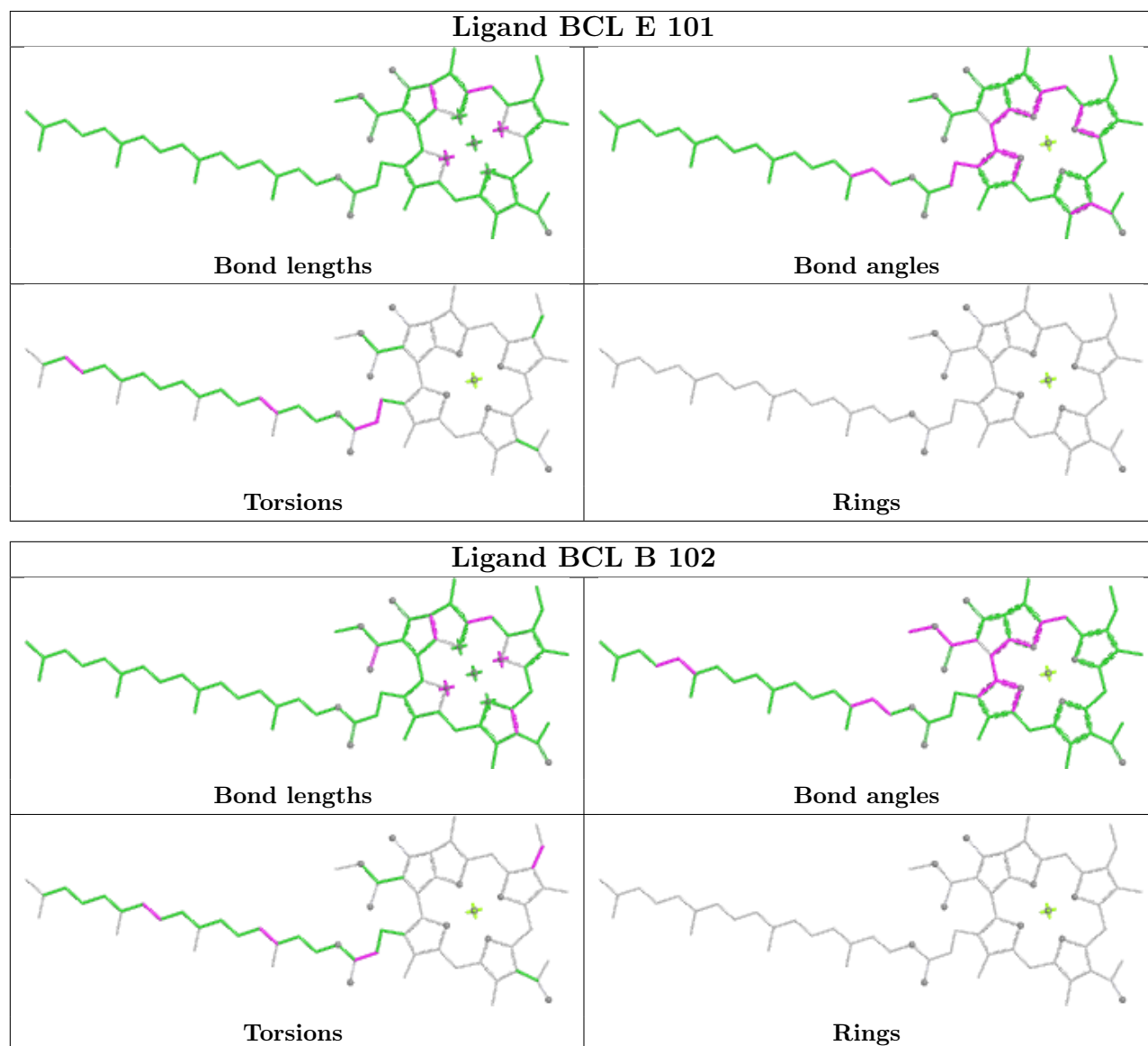
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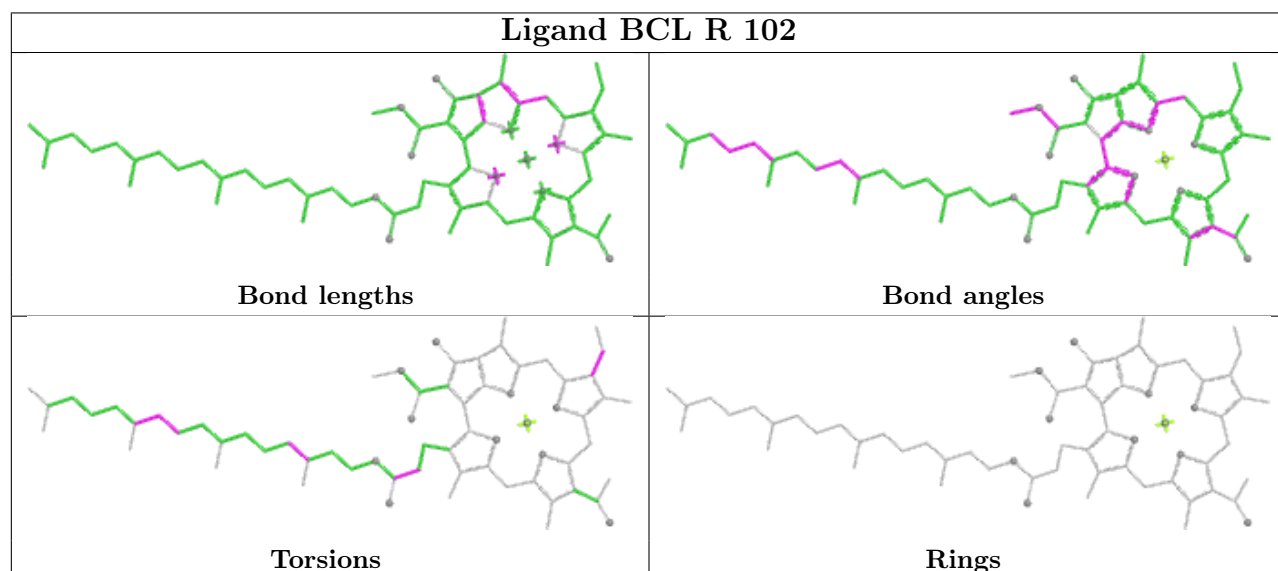
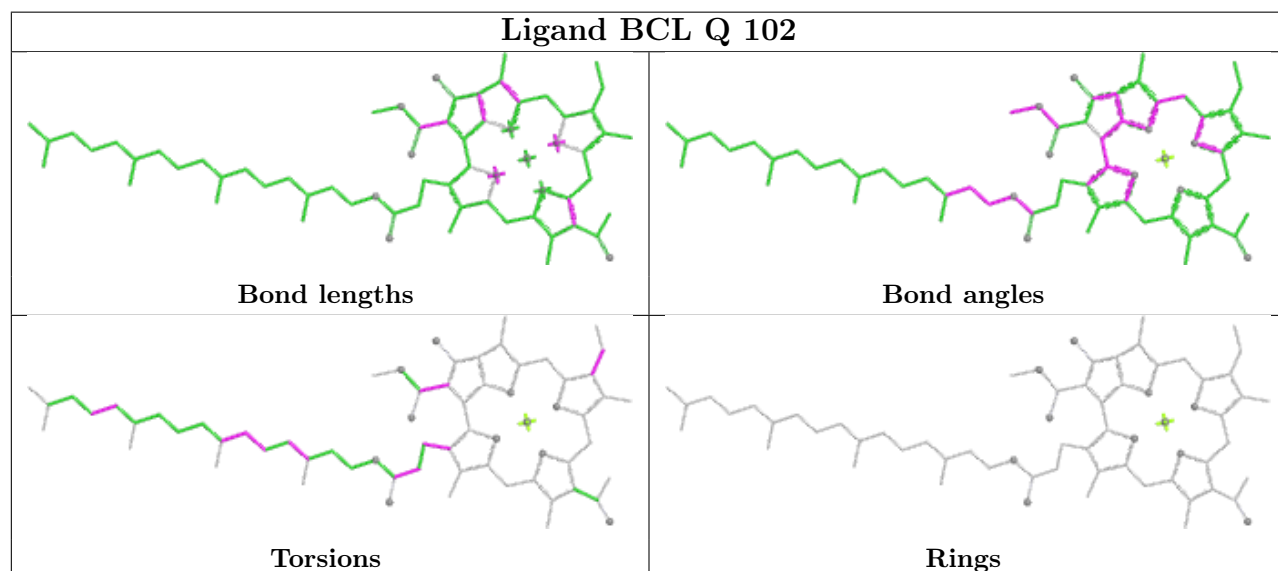
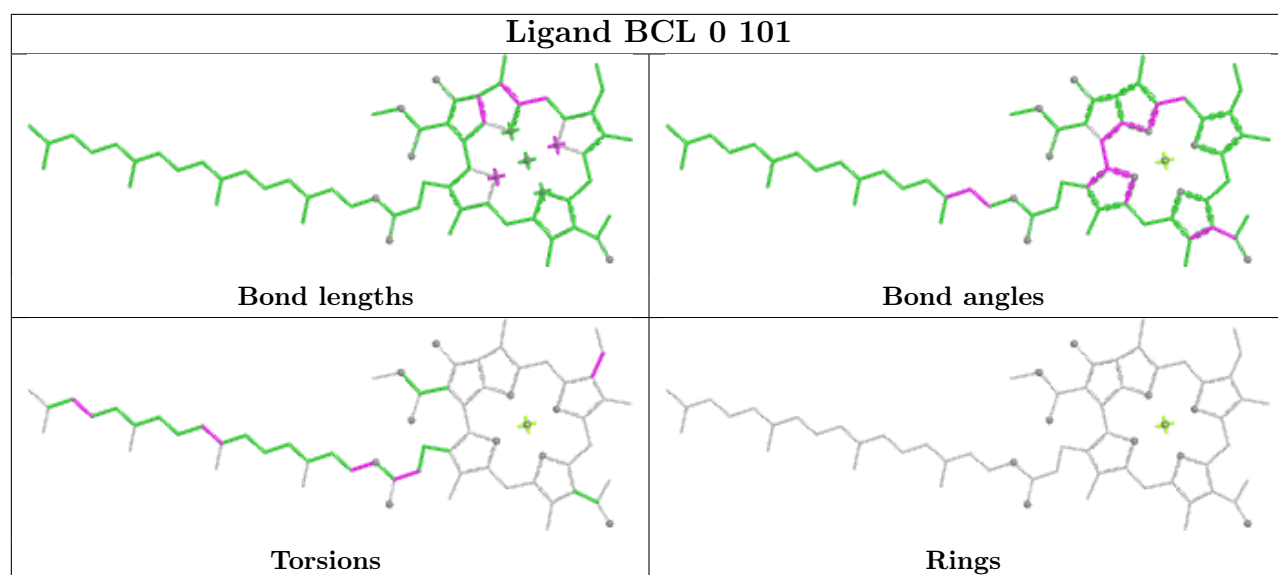
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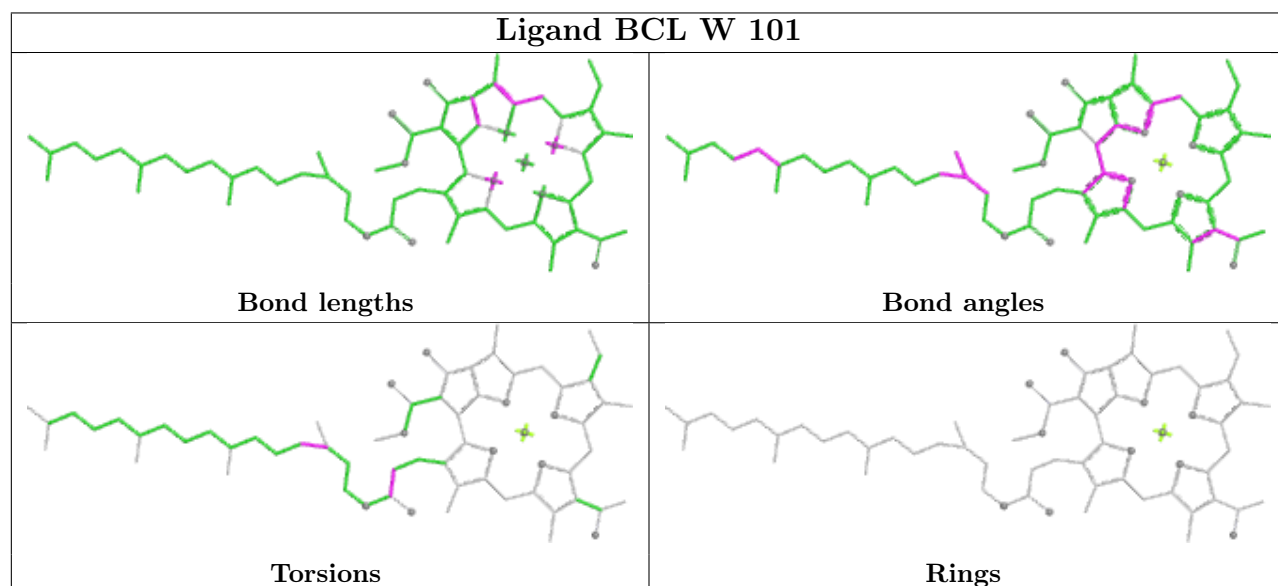
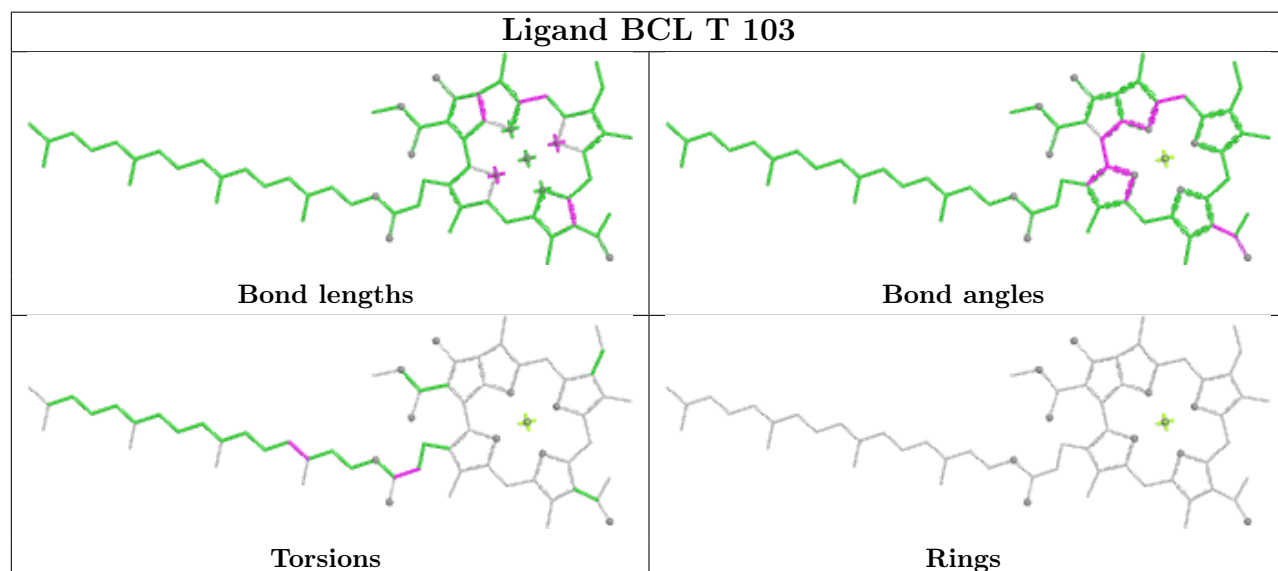
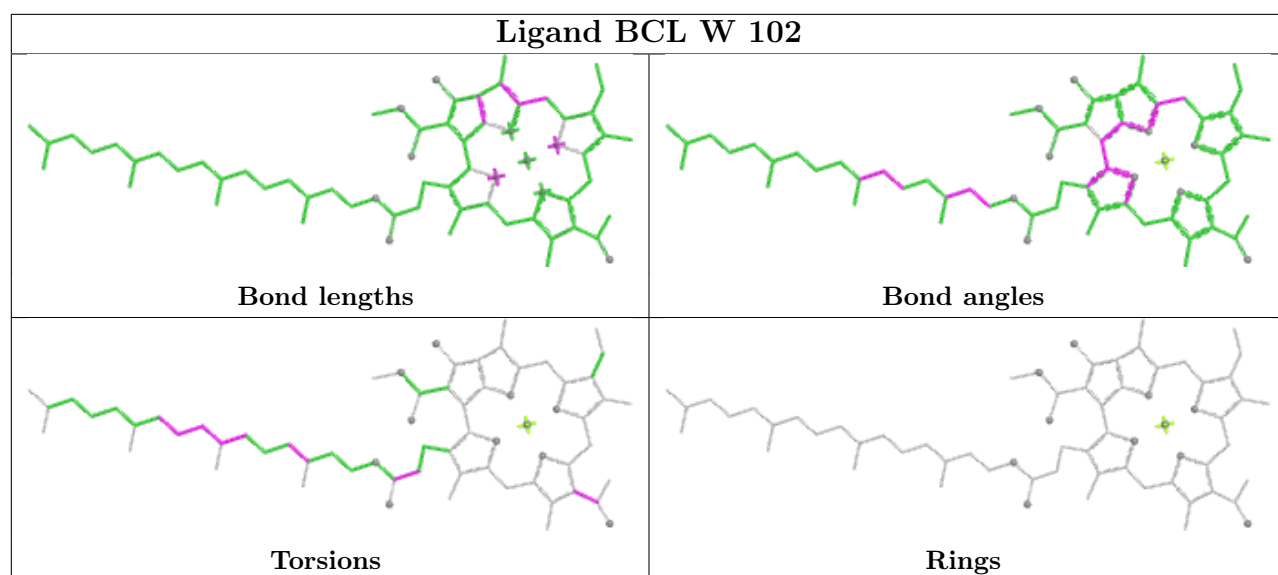
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	102	KGD	5	0
8	S	102	BCL	5	0
8	8	102	BCL	9	0
8	K	101	BCL	4	0
8	N	103	BCL	3	0
8	S	101	BCL	6	0
8	9	103	BCL	2	0
8	0	102	BCL	4	0
8	A	102	BCL	5	0
8	D	101	BCL	2	0
12	F	101	KGD	3	0
8	E	102	BCL	4	0
8	6	102	BCL	11	0
8	O	102	BCL	5	0
8	J	102	BCL	4	0
11	C	501	HEM	10	0
8	2	102	BCL	6	0
8	B	101	BCL	6	0
11	C	502	HEM	5	0
11	C	503	HEM	5	0
12	N	102	KGD	1	0
12	T	101	KGD	1	0
12	9	102	KGD	1	0
8	6	101	BCL	7	0
9	L	1003	BPH	7	0
12	N	101	KGD	2	0
8	G	102	BCL	5	0
8	U	102	BCL	9	0
8	2	101	BCL	6	0
8	4	101	BCL	6	0
12	R	101	KGD	1	0
12	A	101	KGD	1	0
8	3	102	BCL	4	0
8	H	101	BCL	7	0
8	1	101	BCL	4	0
8	8	101	BCL	5	0
10	M	702	MQE	3	0
8	I	101	BCL	4	0
12	3	103	KGD	6	0

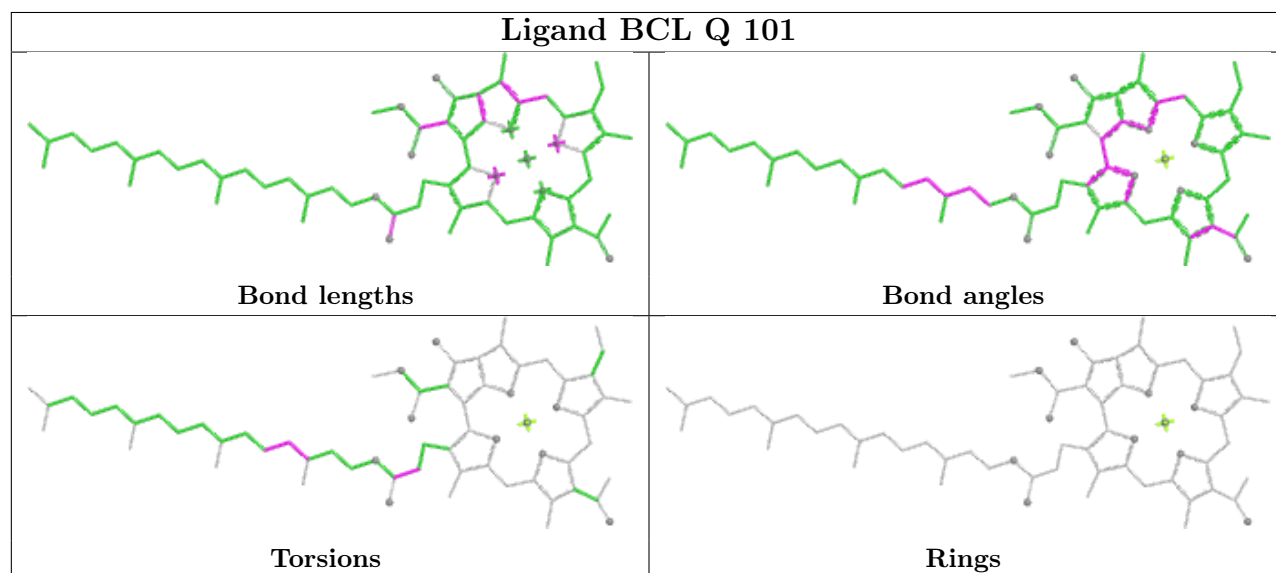
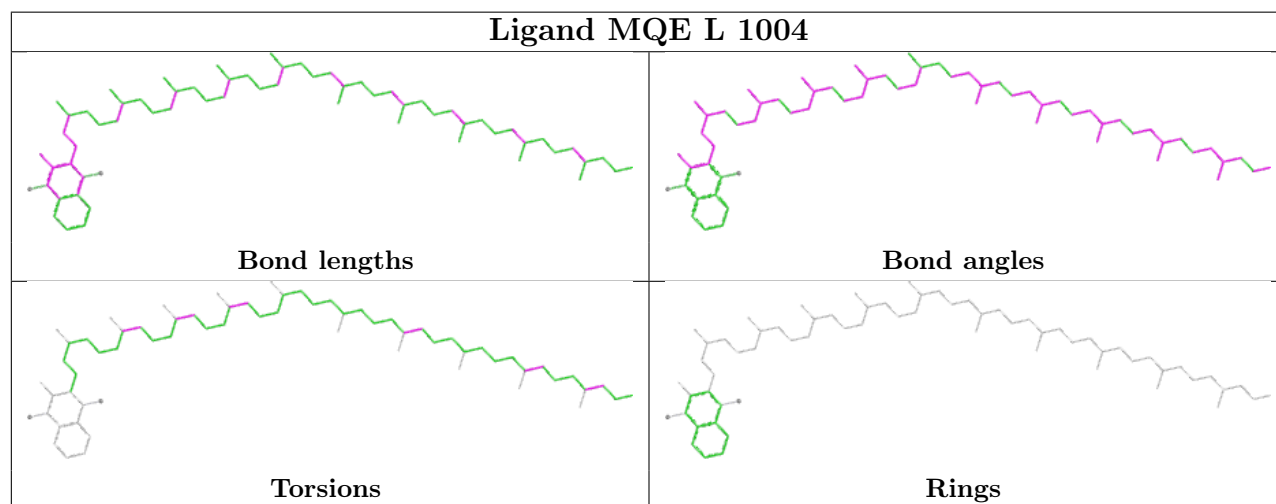
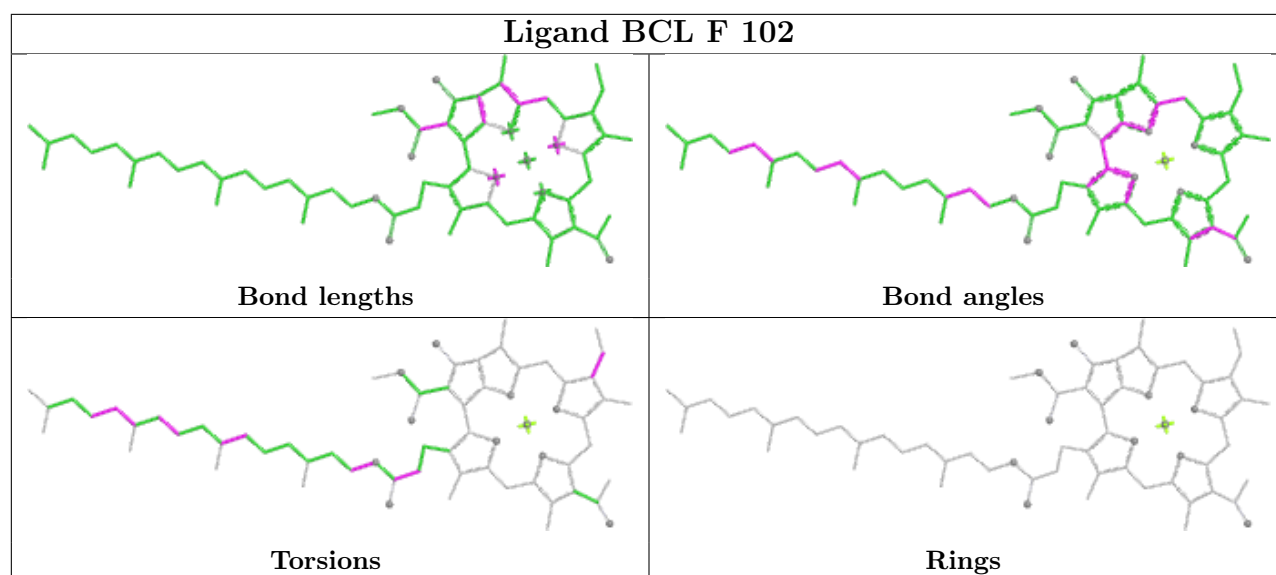
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

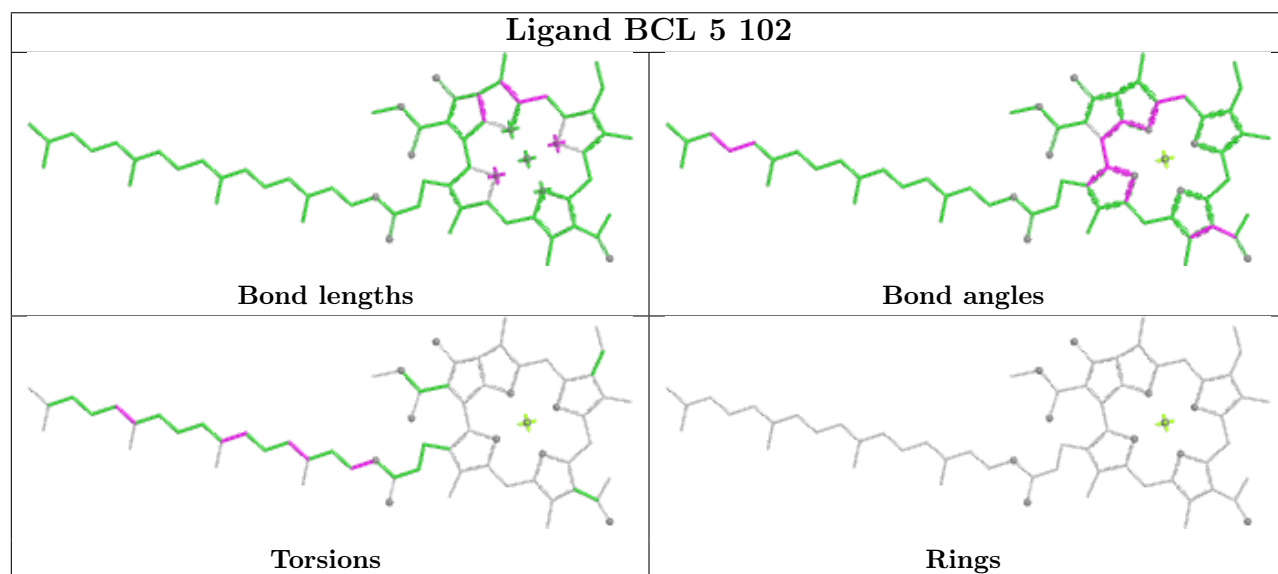
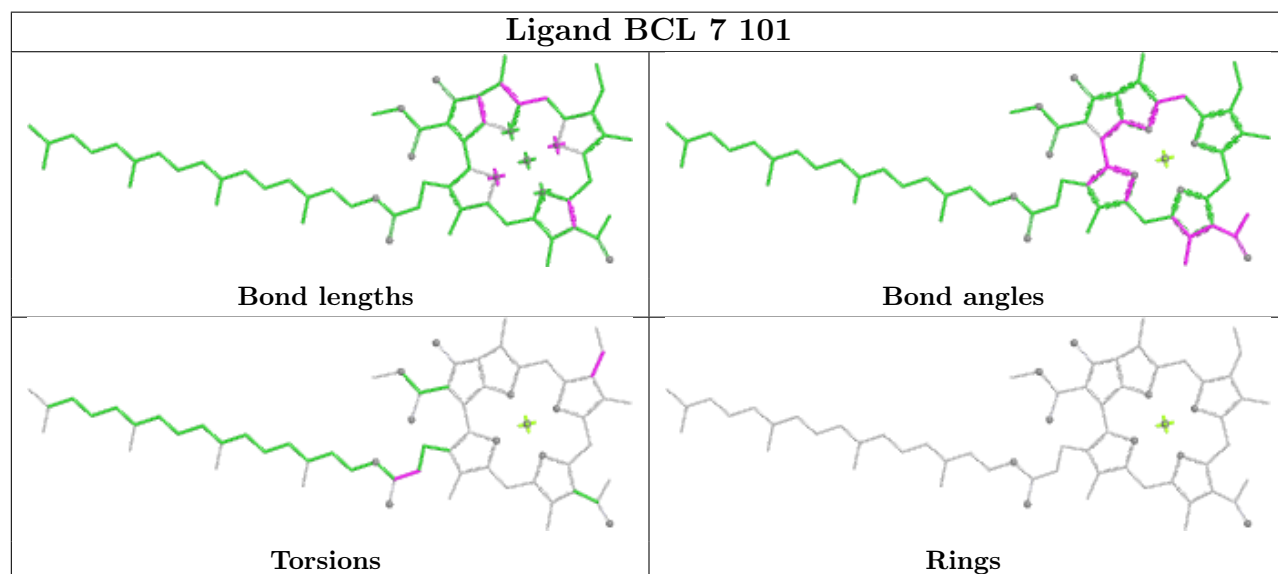
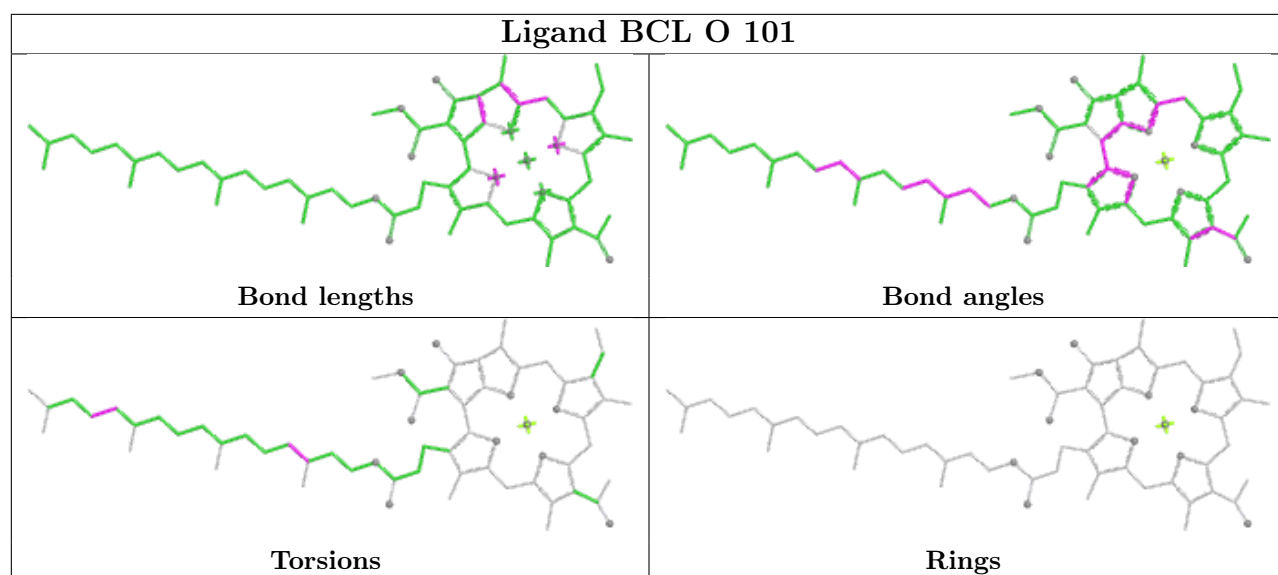
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

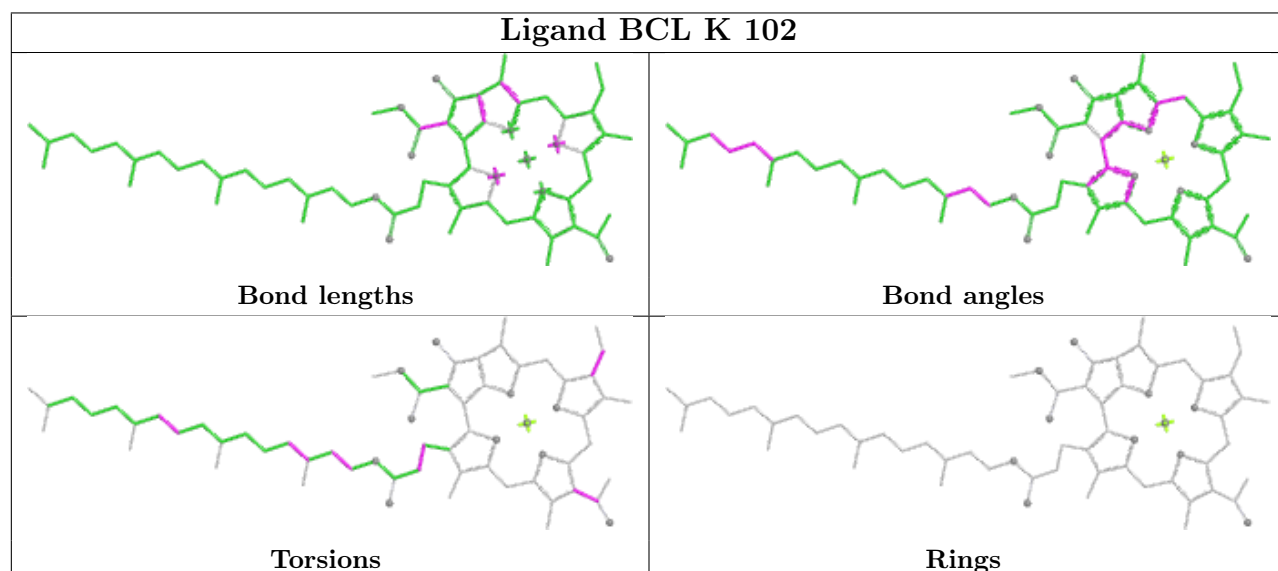
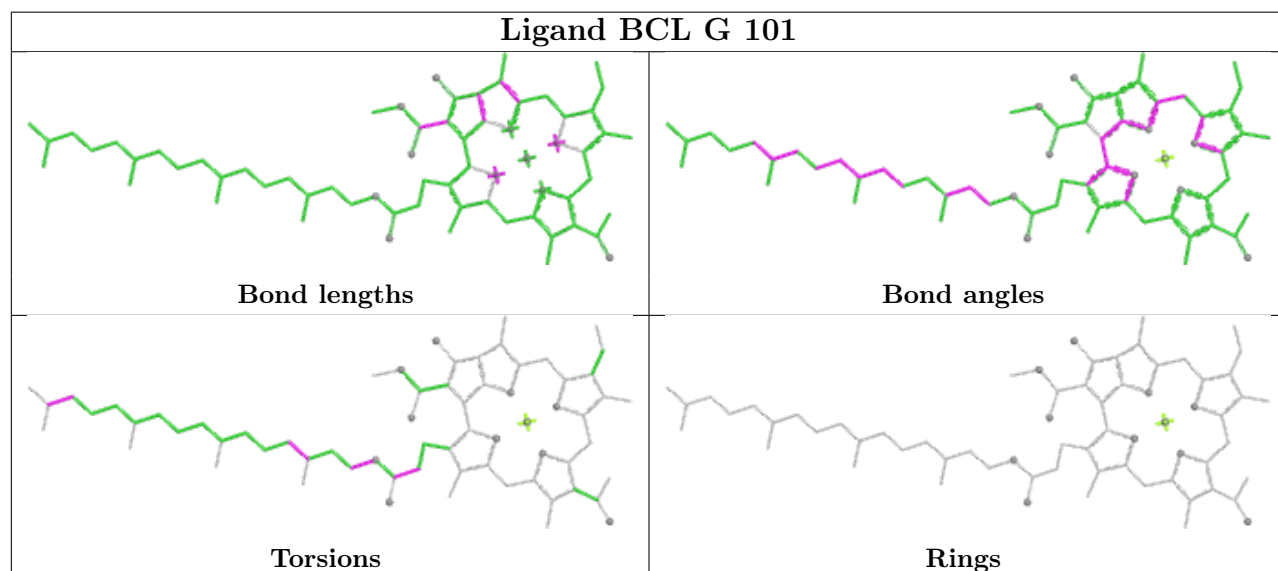
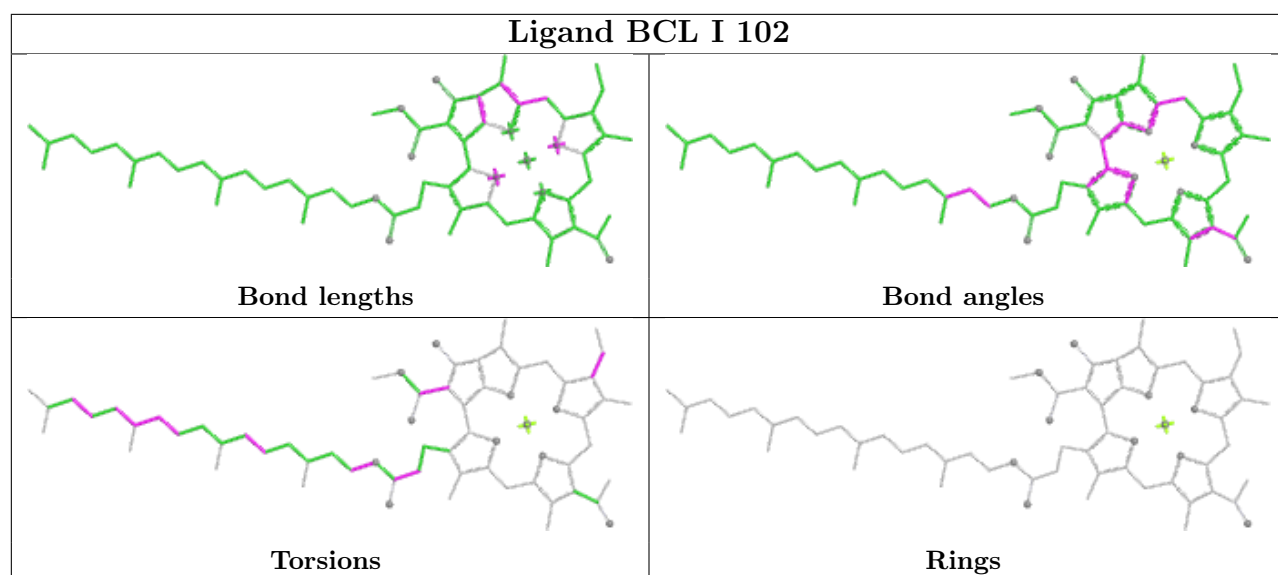


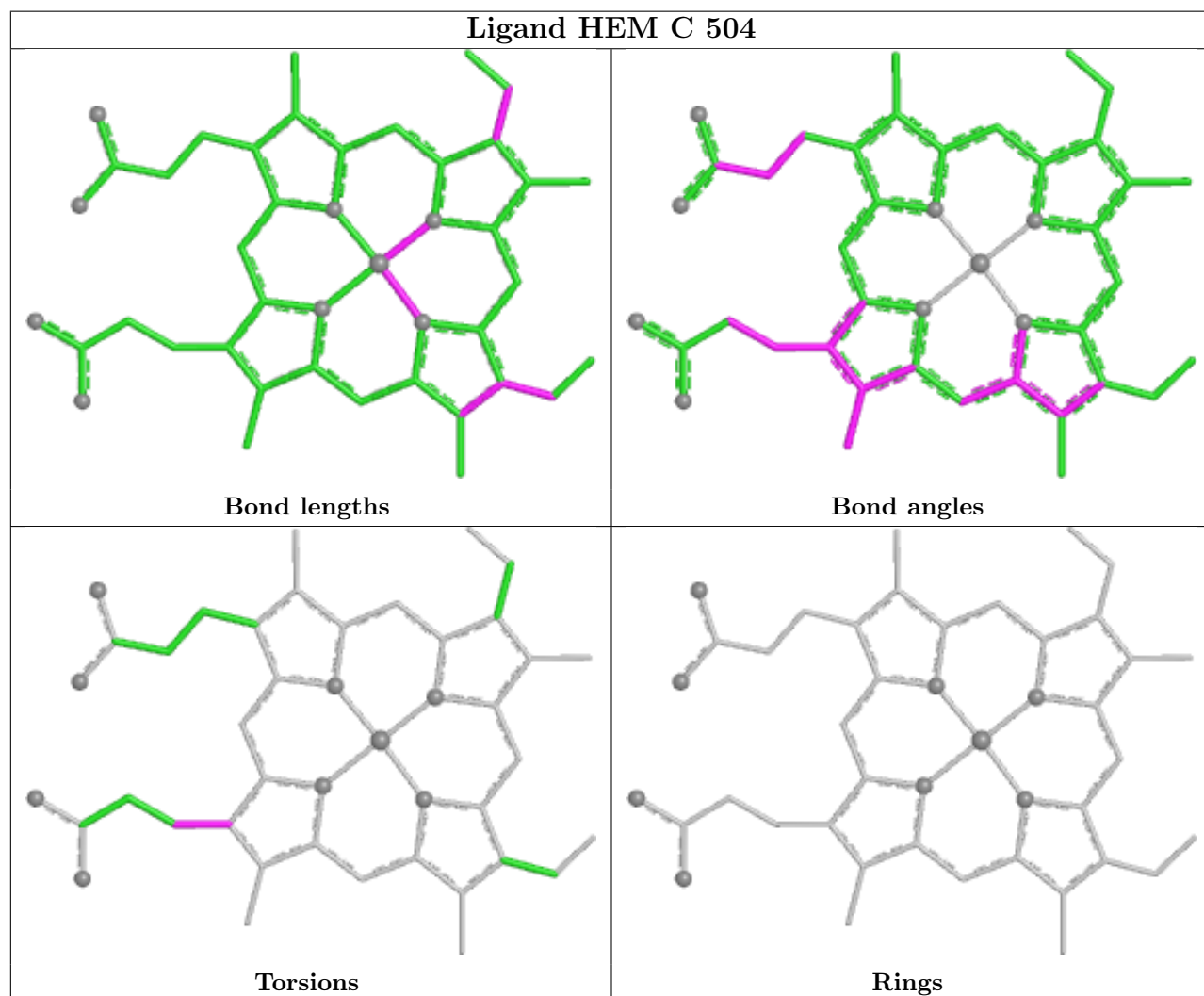
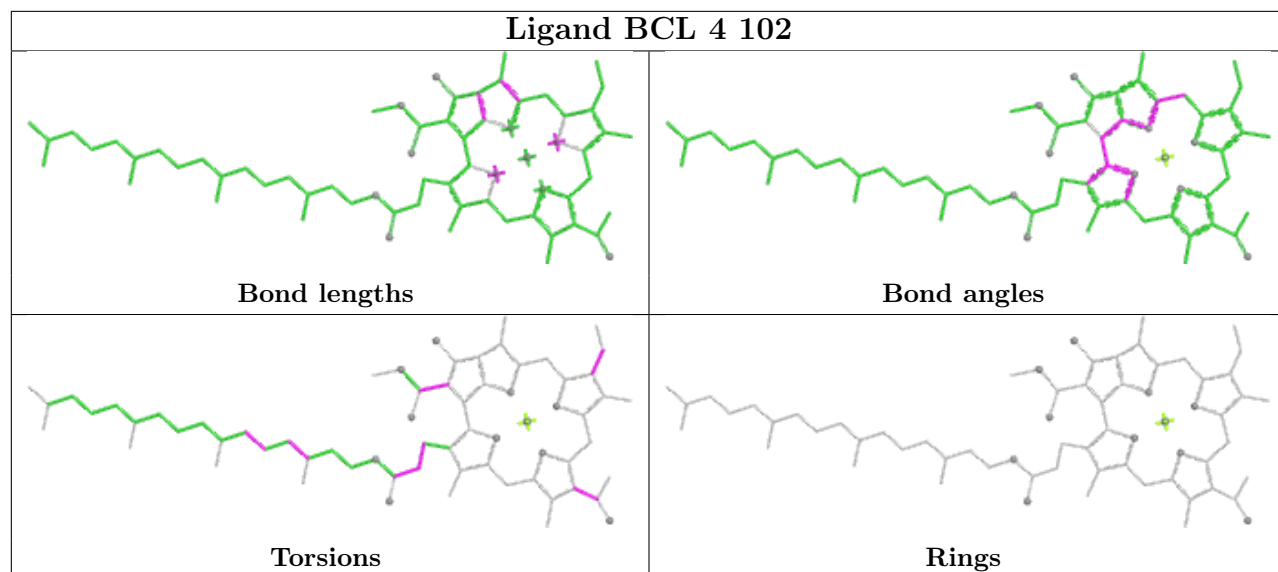


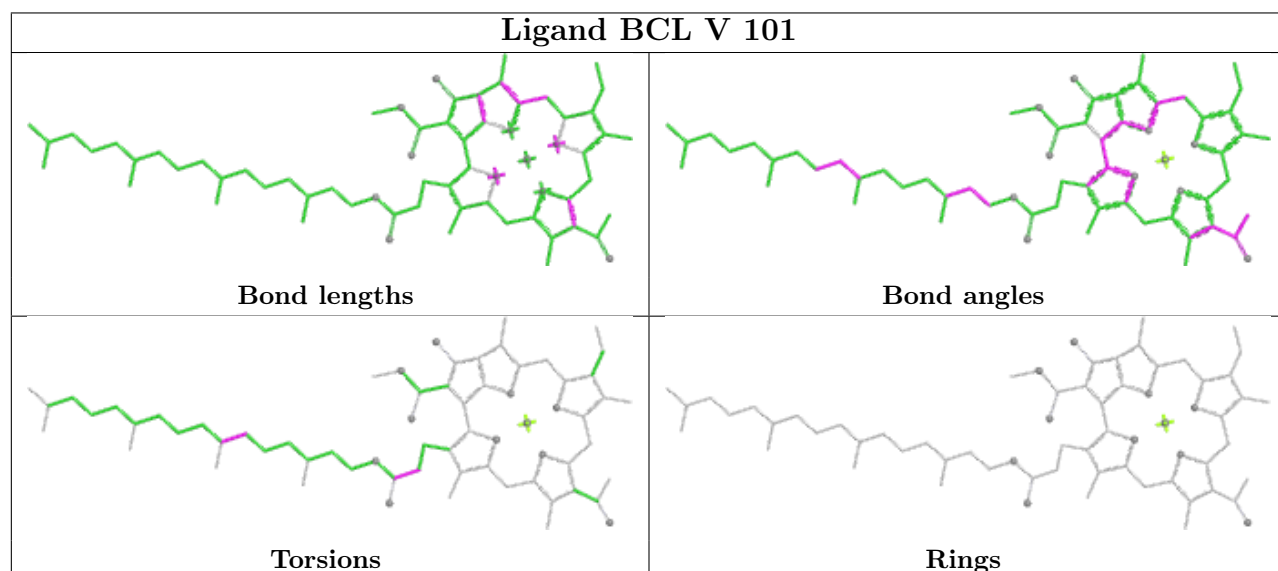
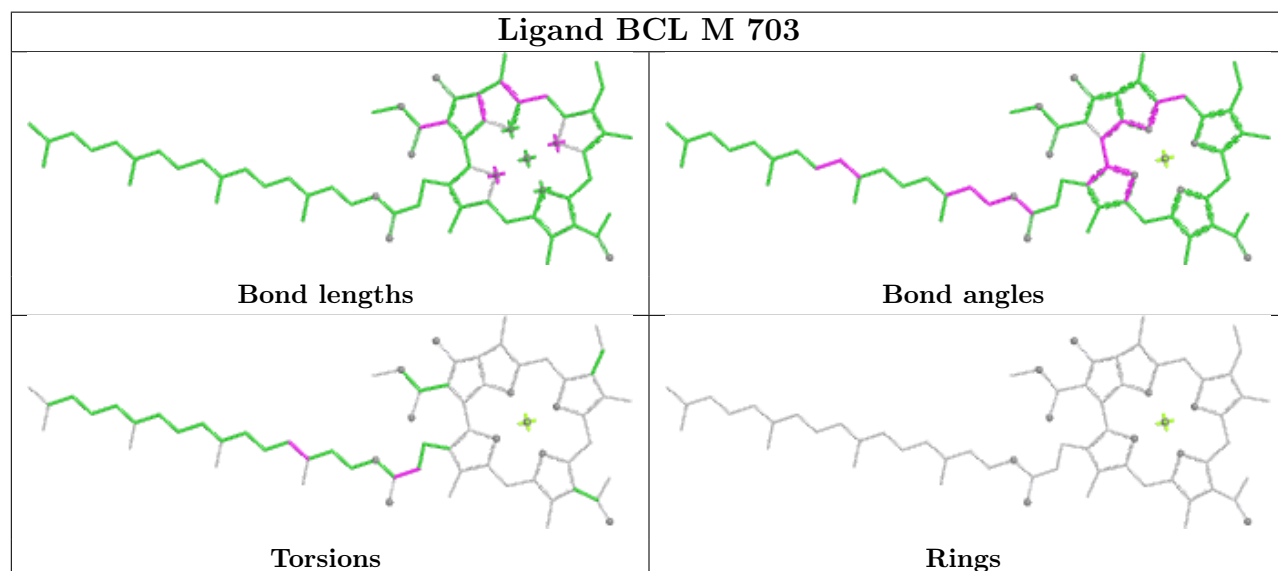
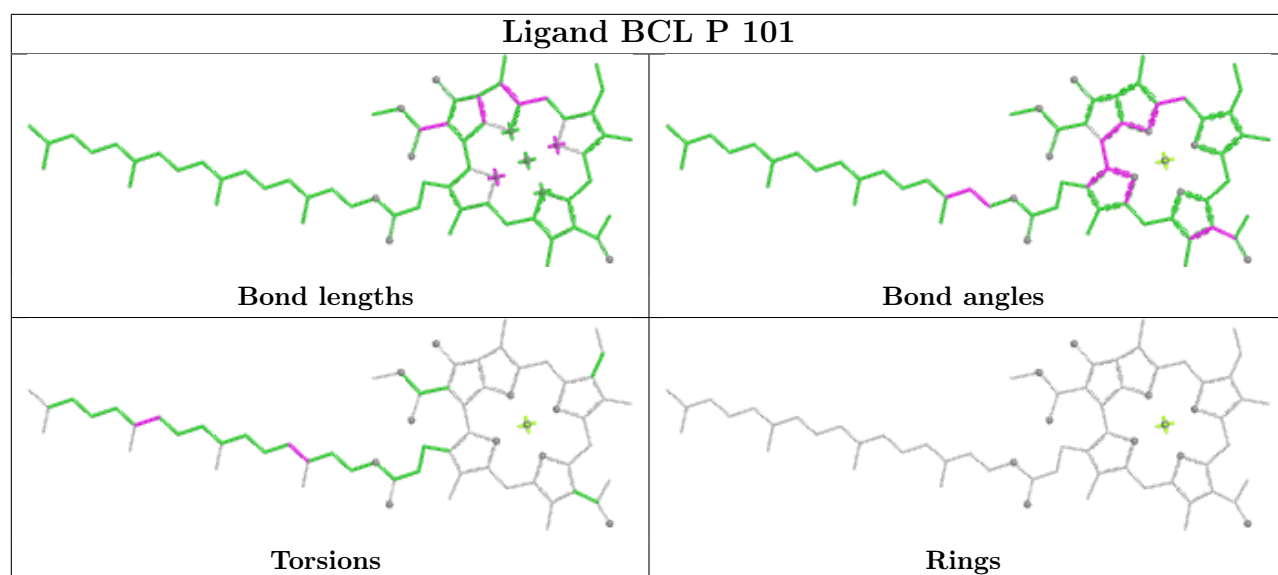


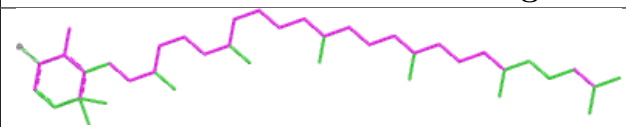
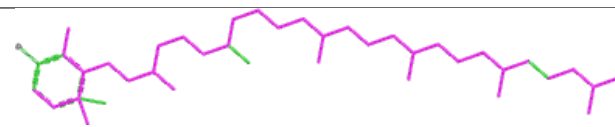
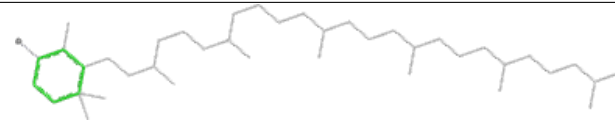


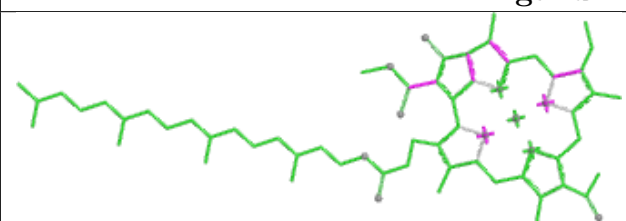
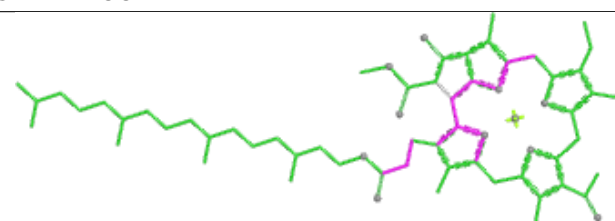
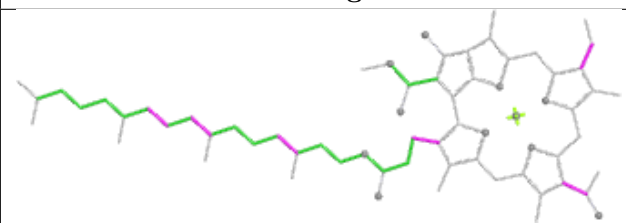
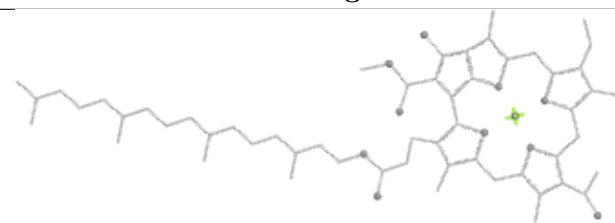


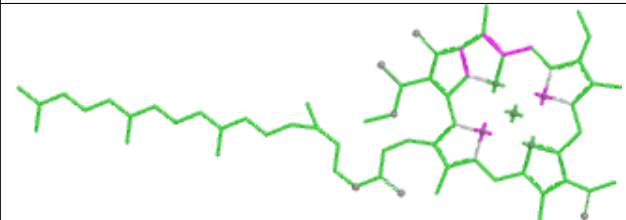
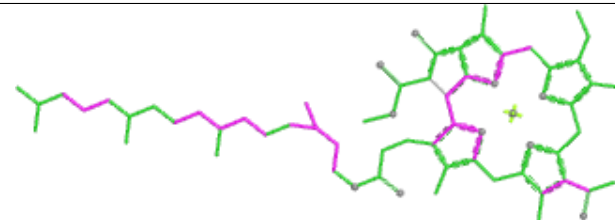
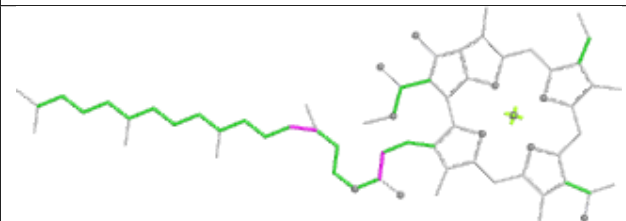
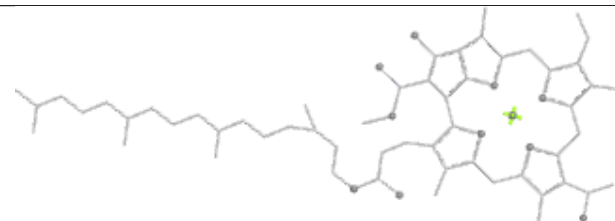


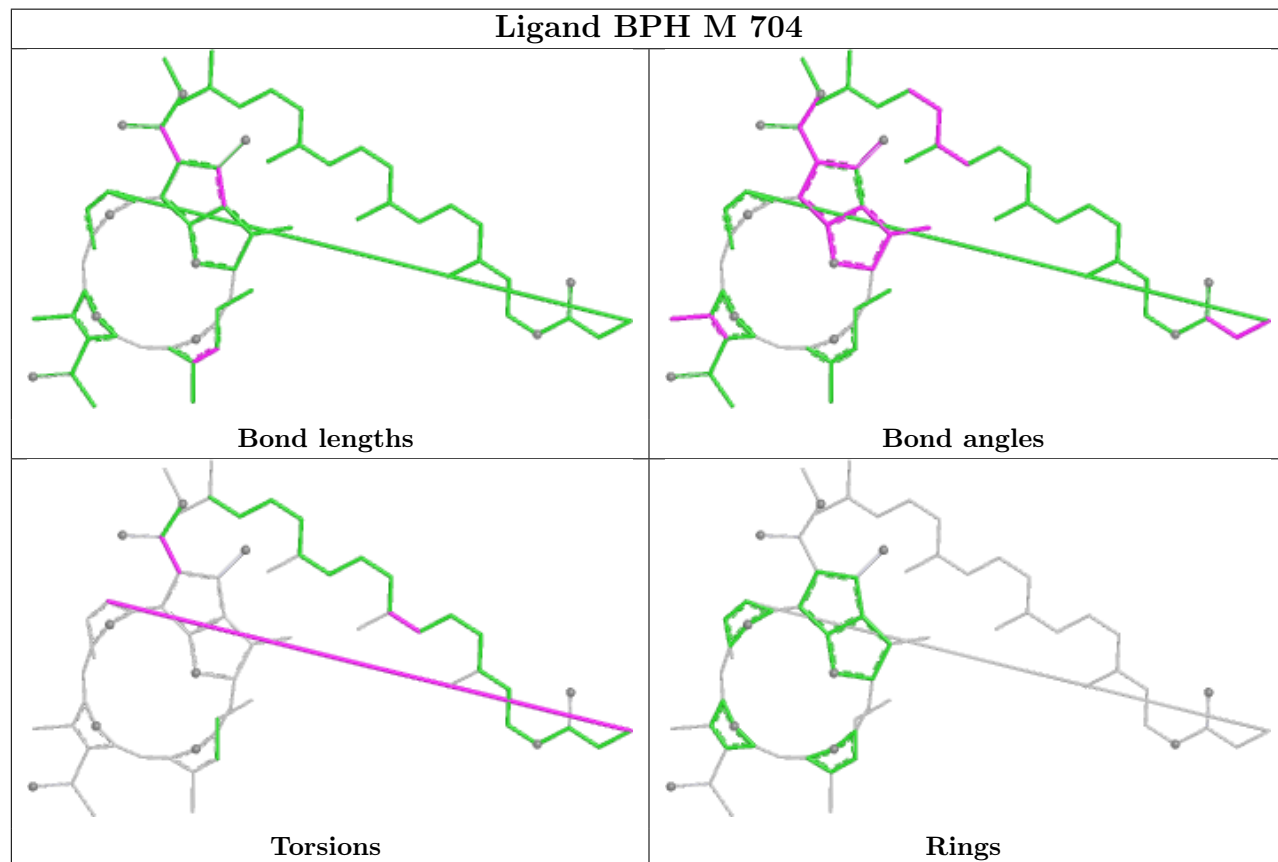
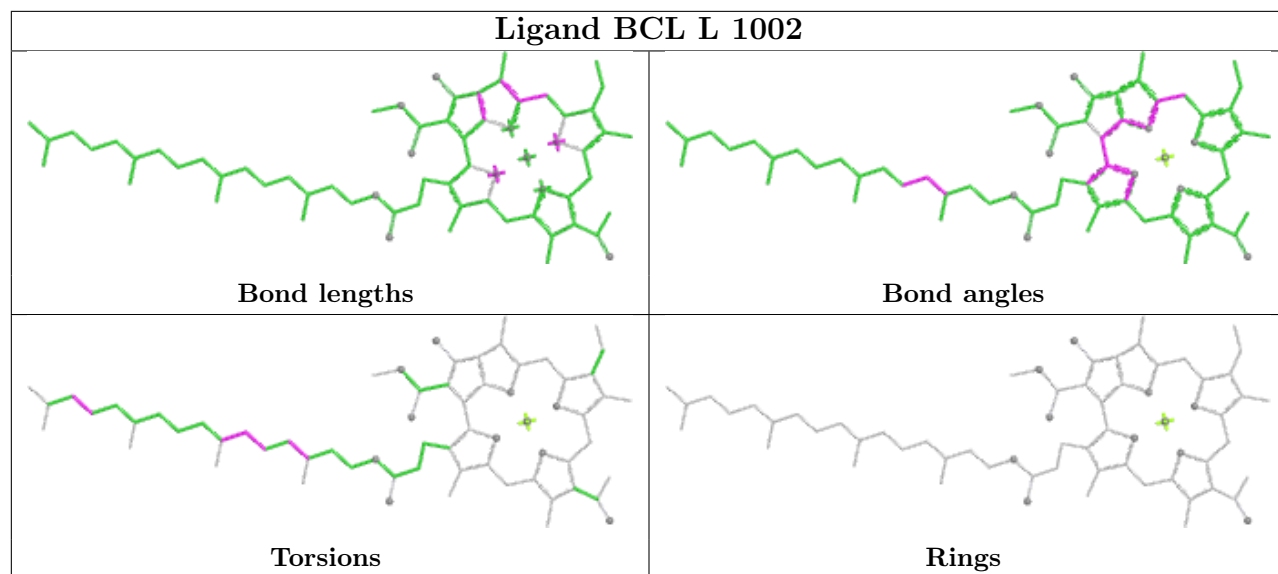


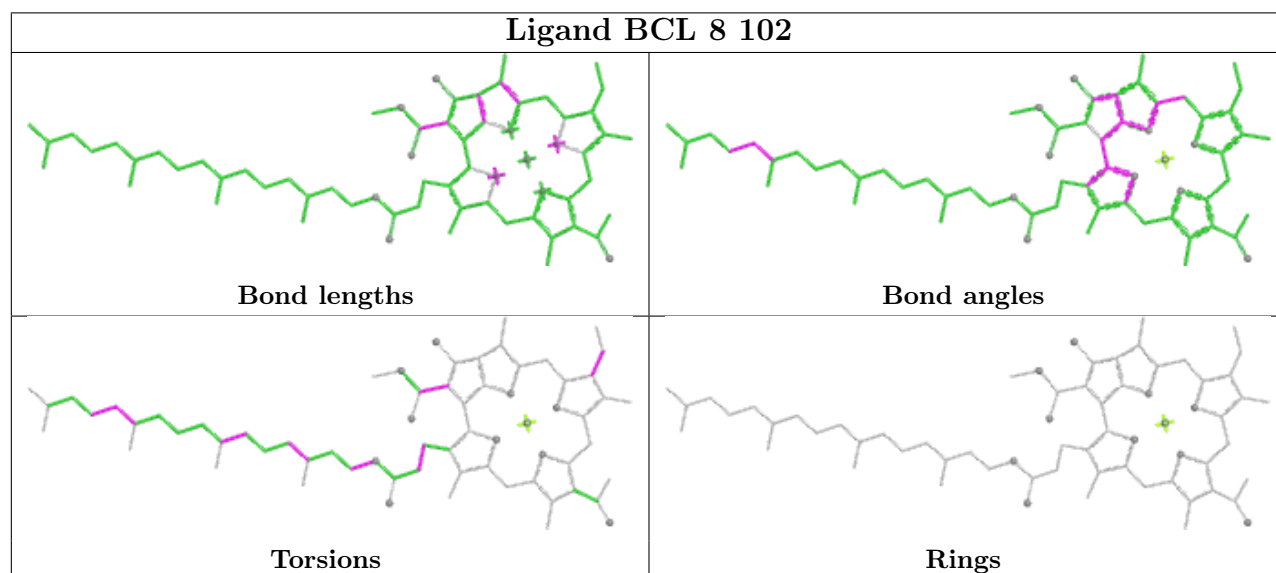
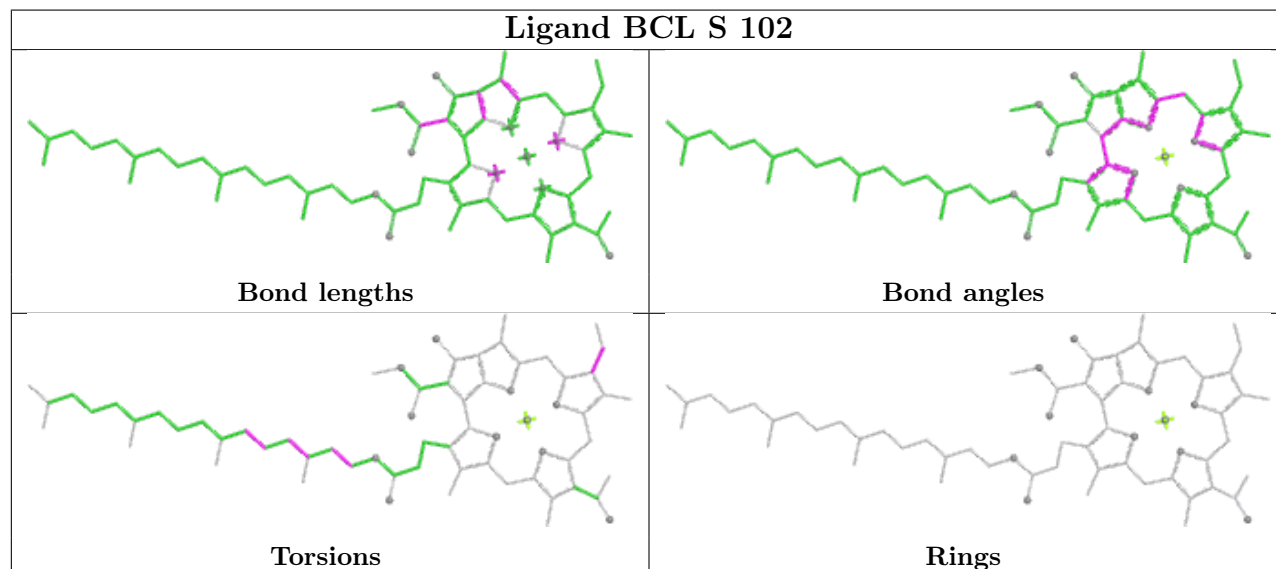
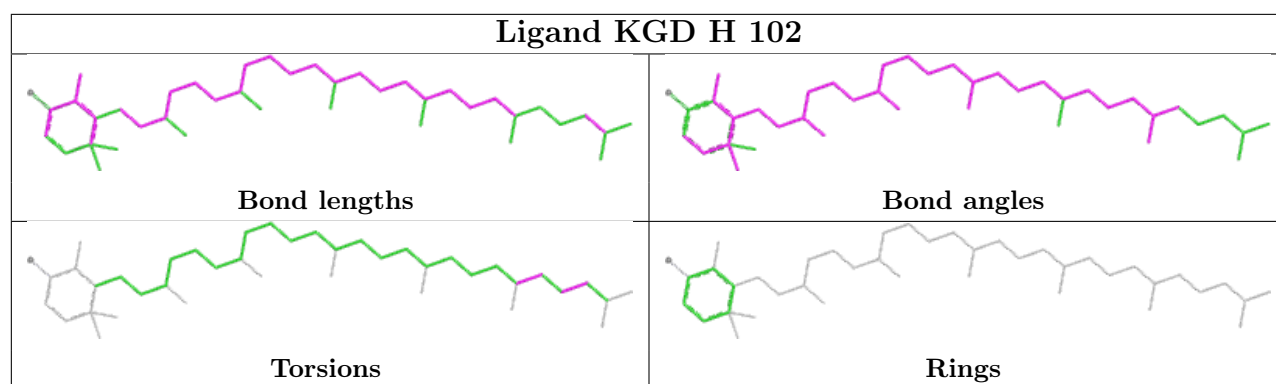


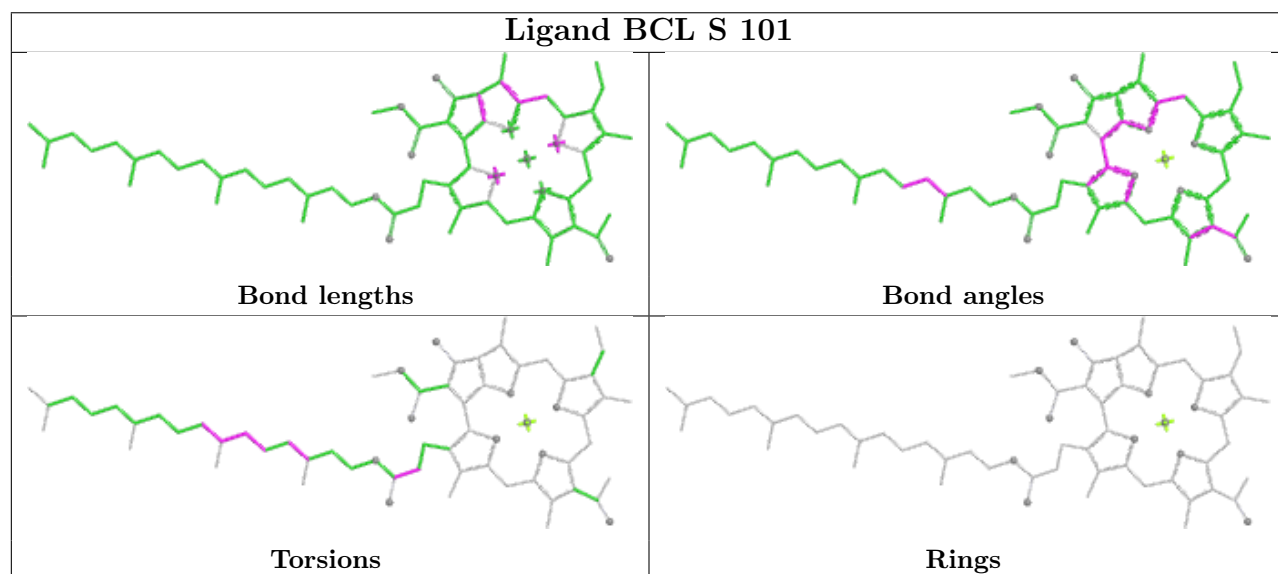
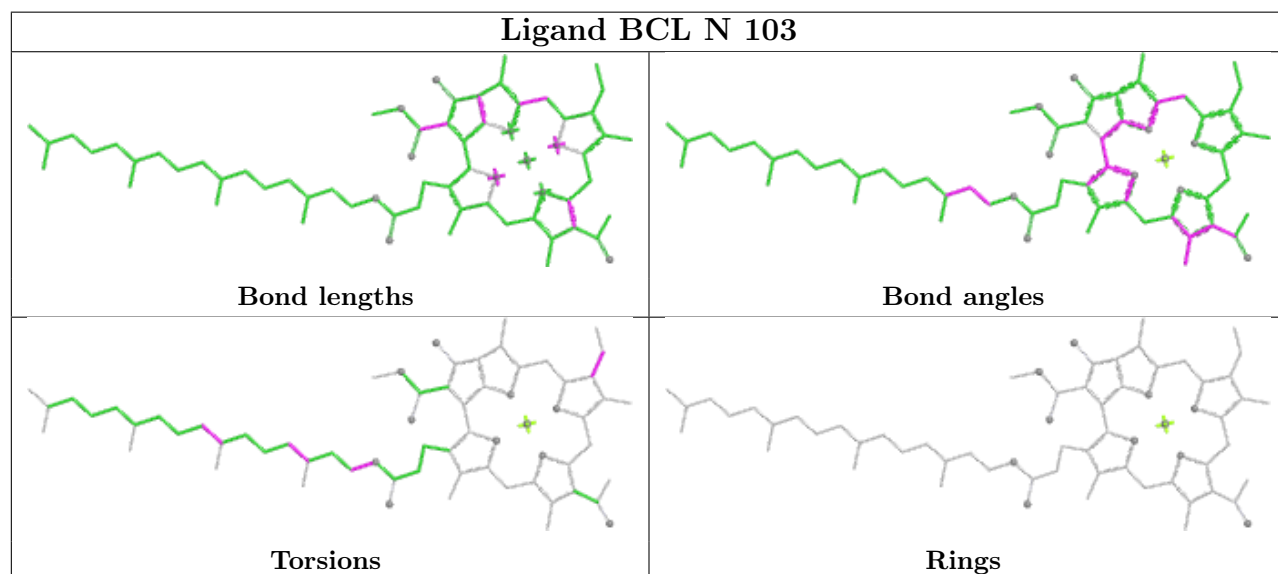
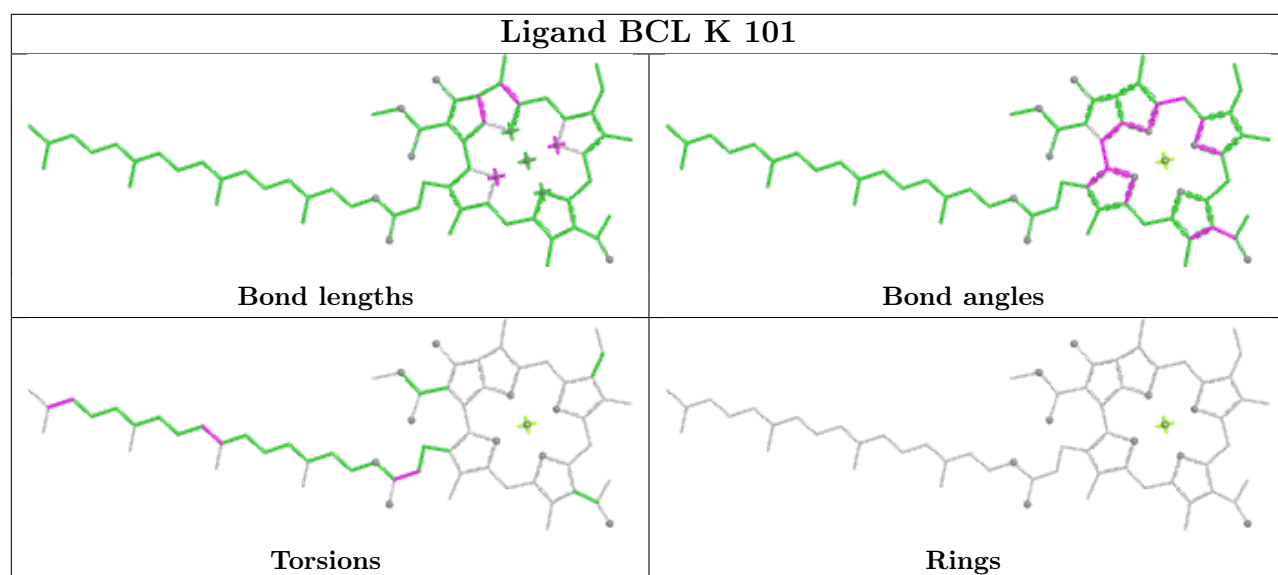
Ligand KGD 5 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

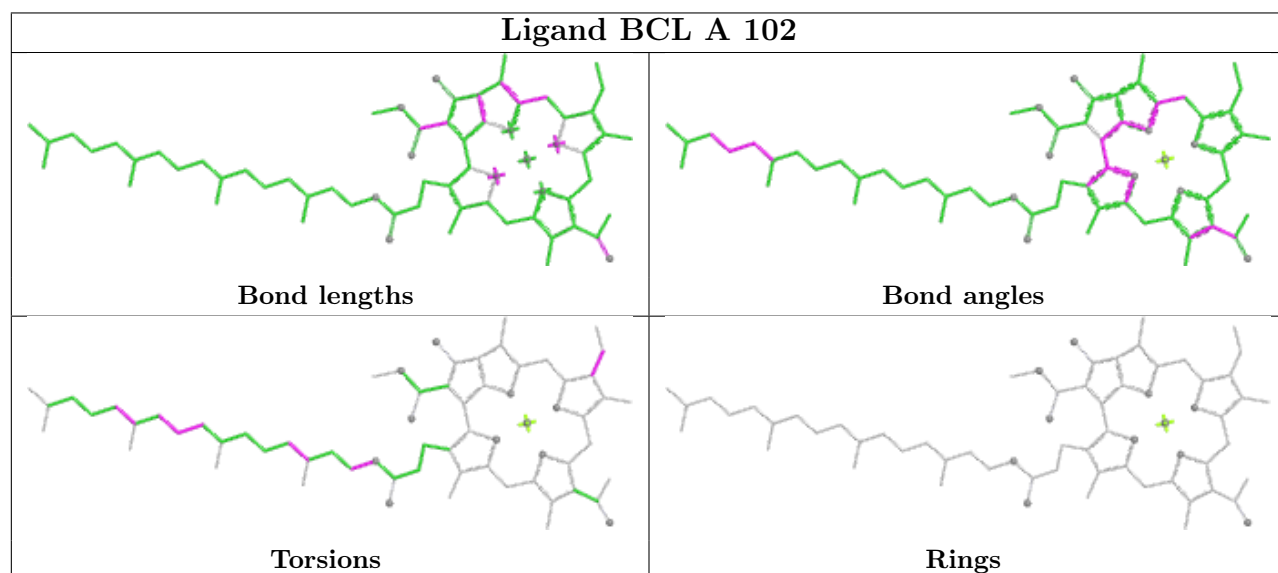
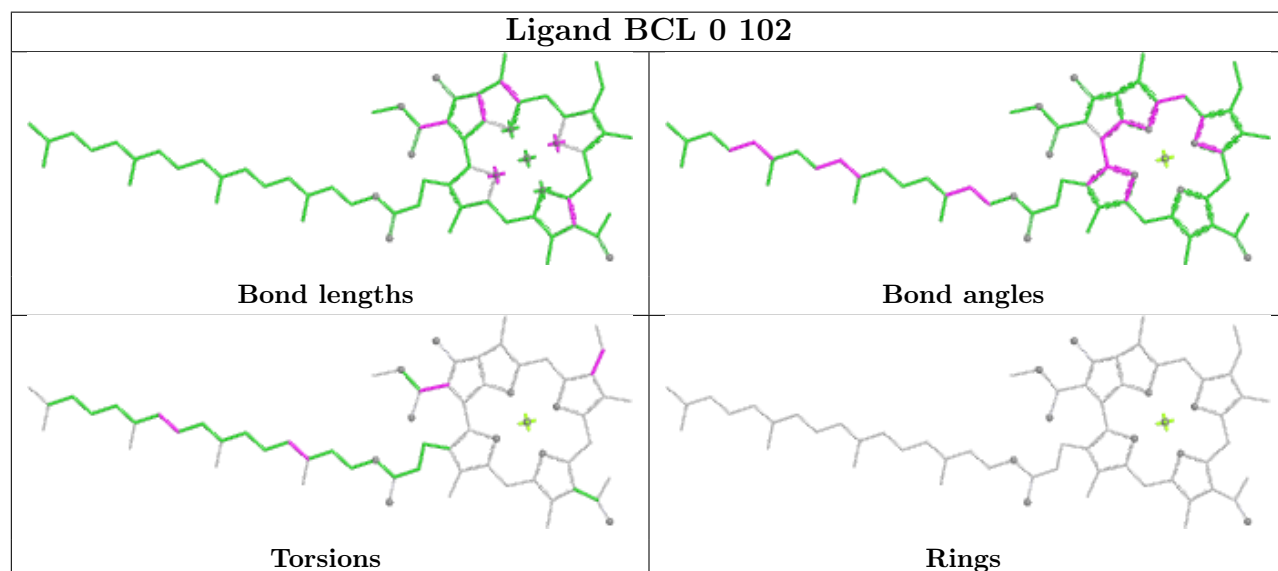
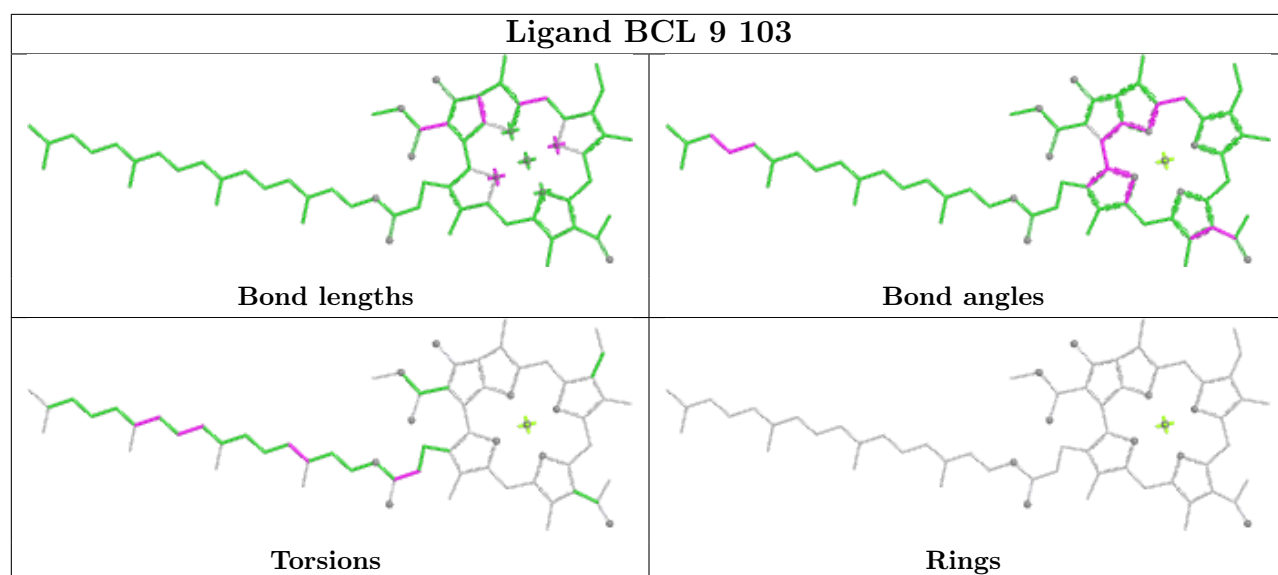
Ligand BCL L 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

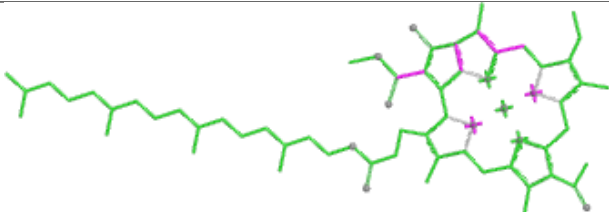
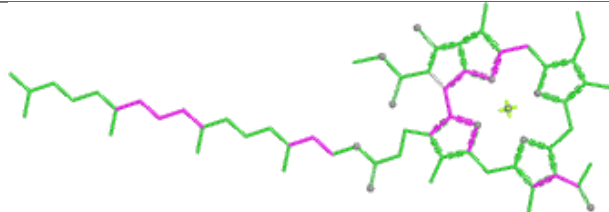
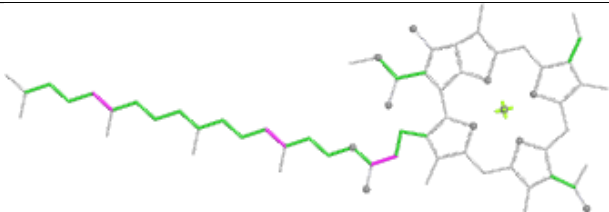
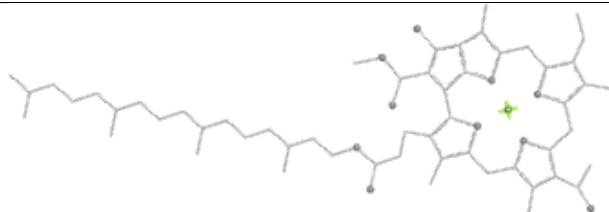
Ligand BCL U 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

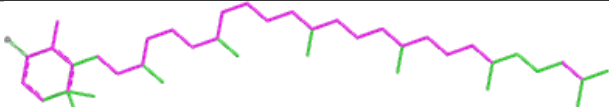
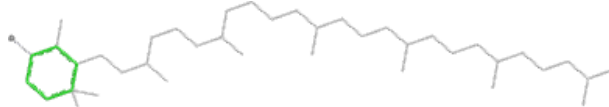


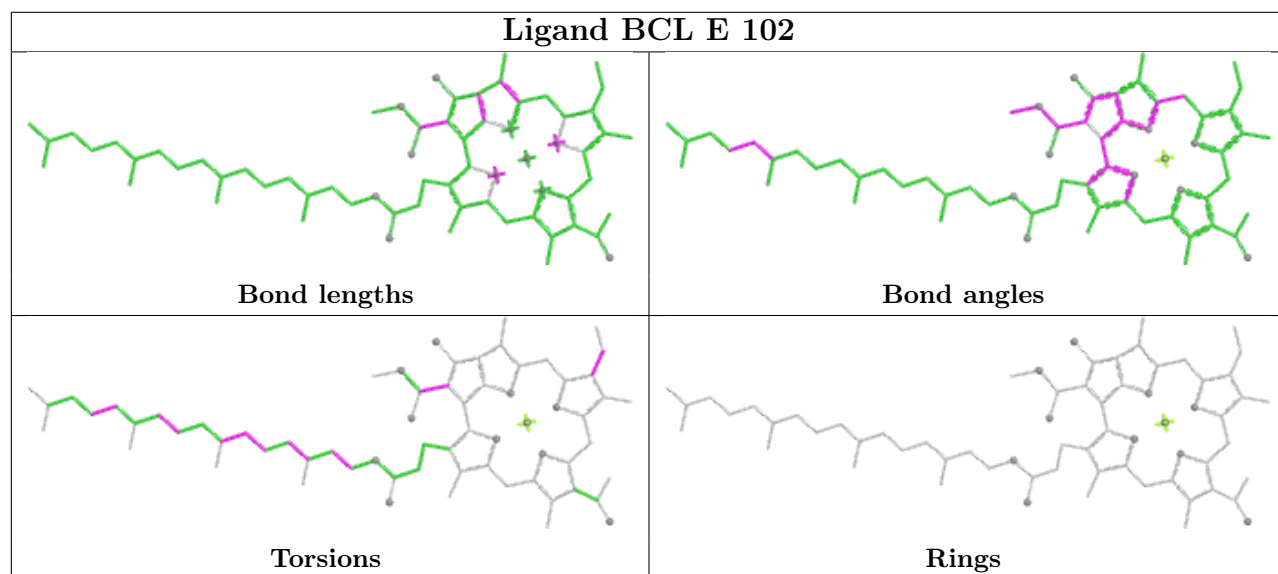
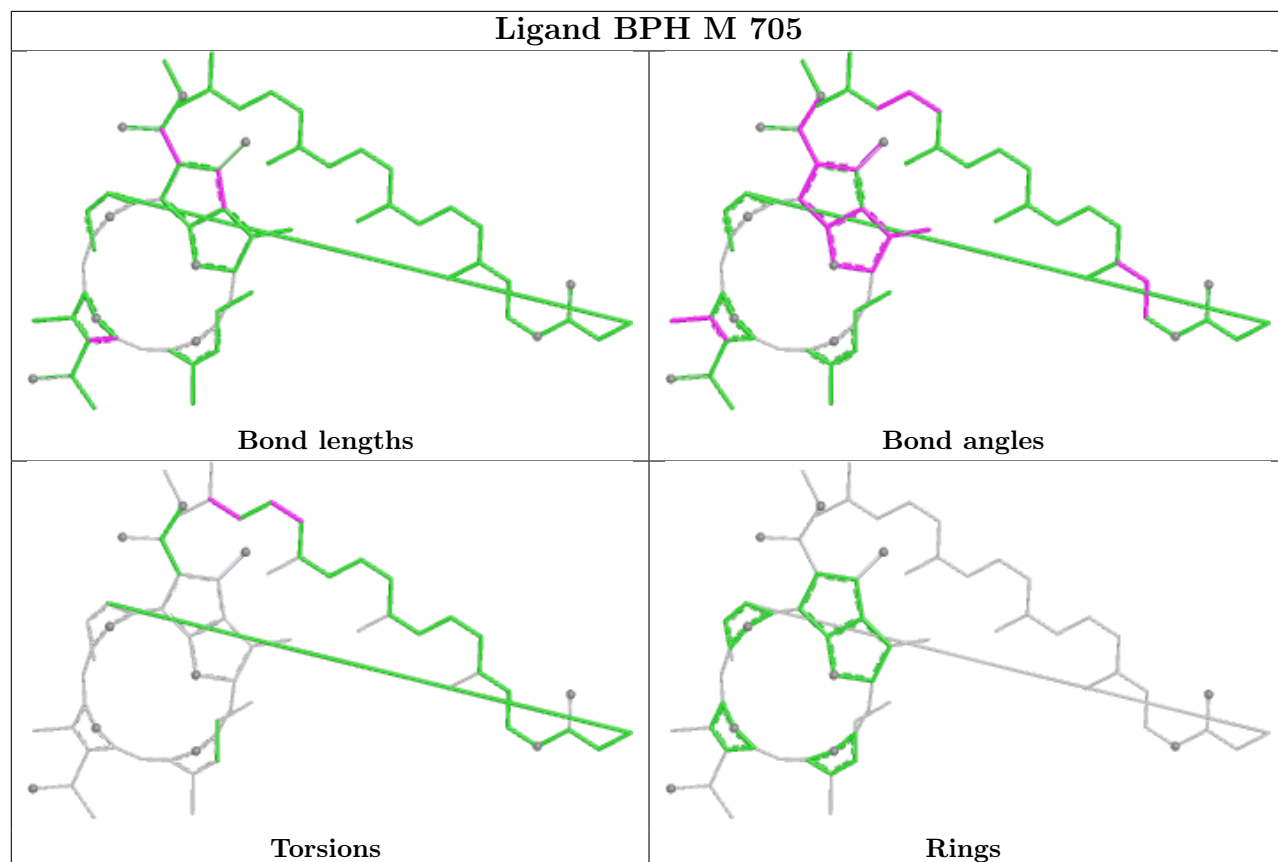


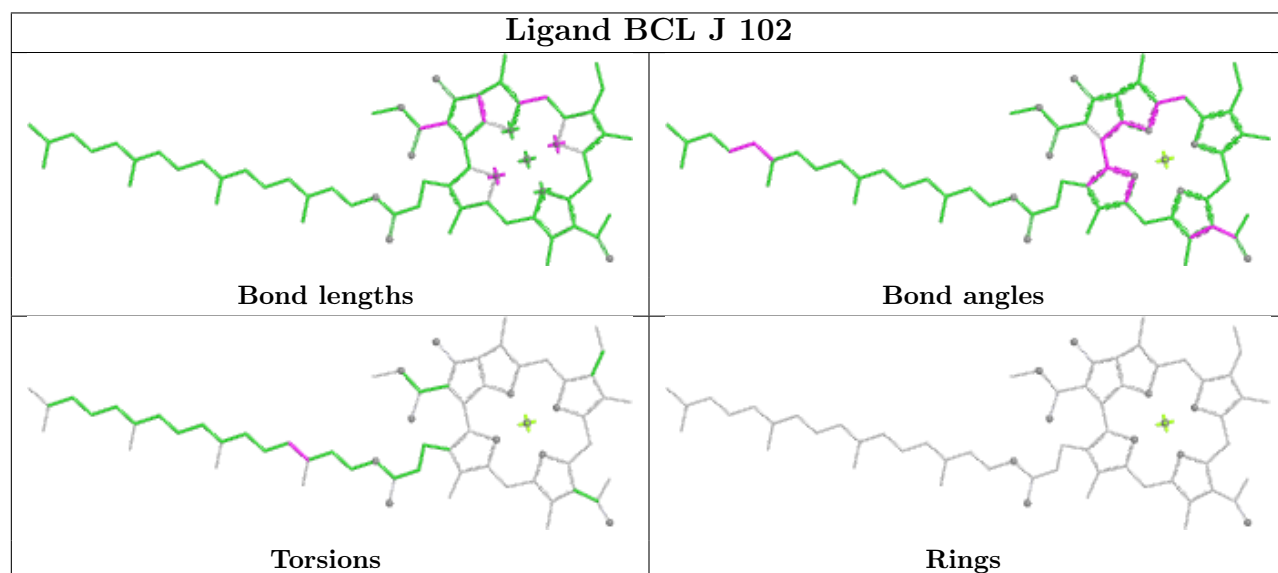
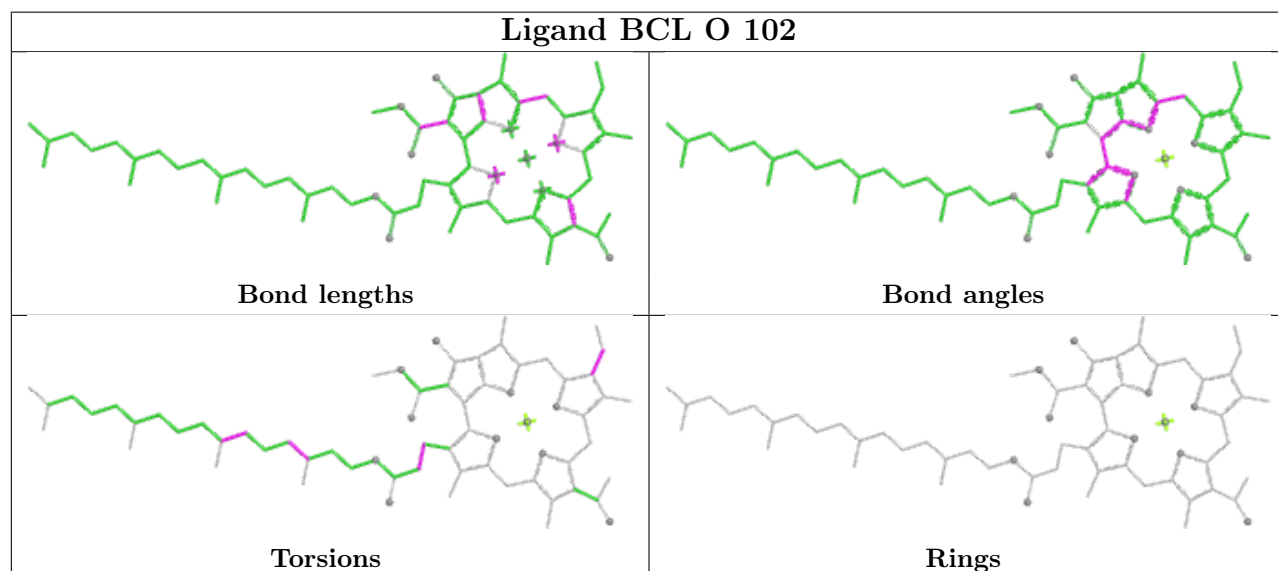
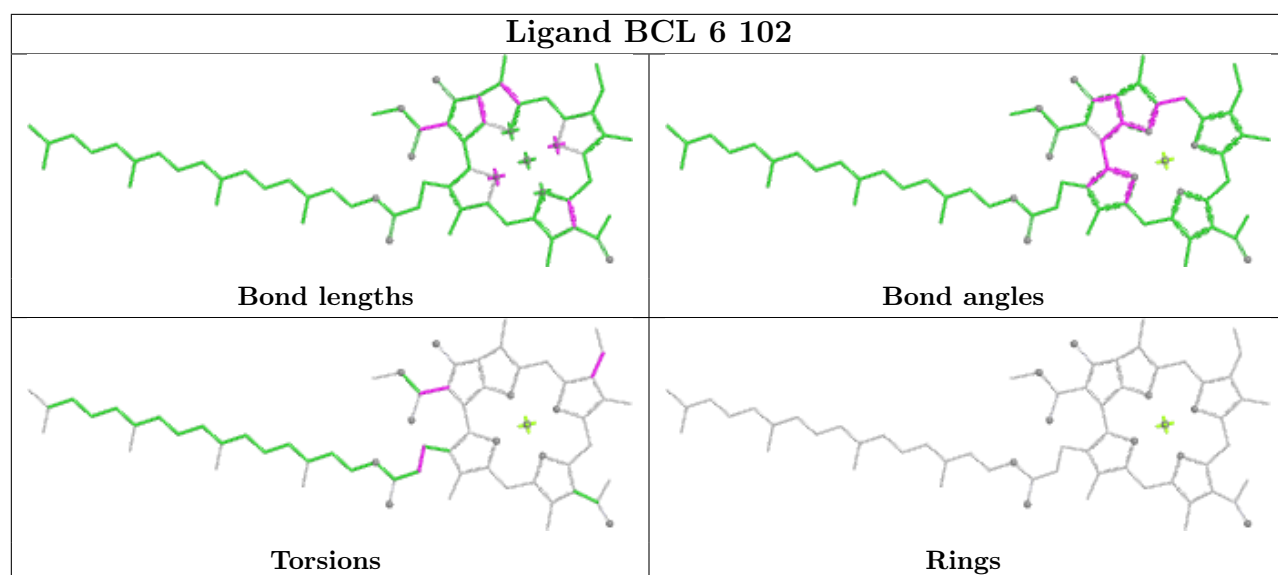


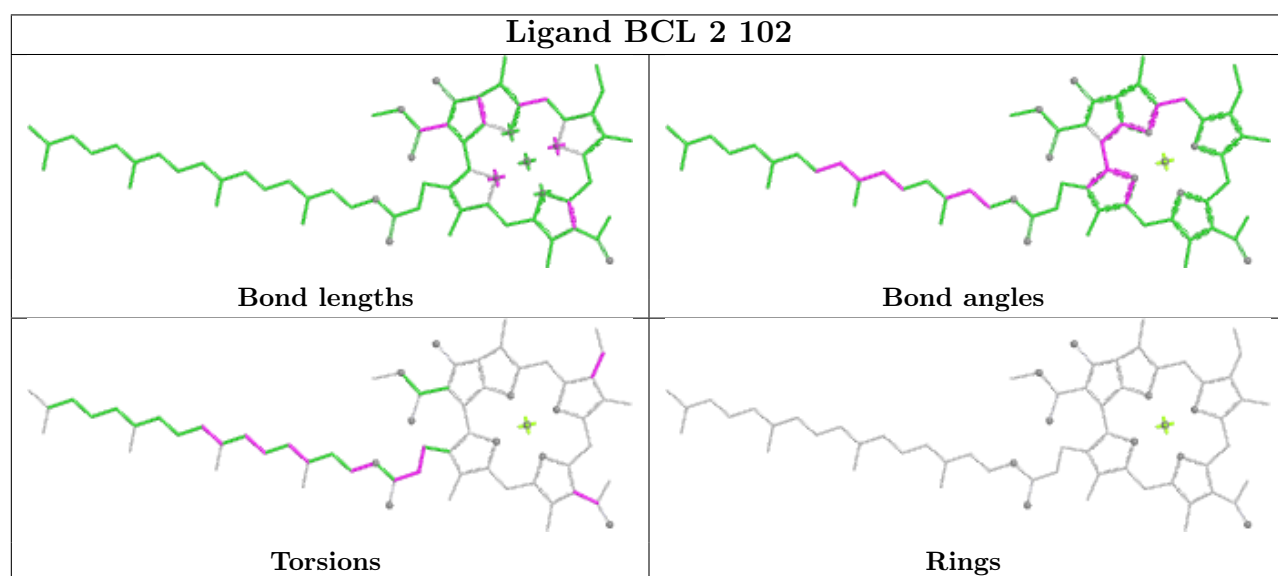
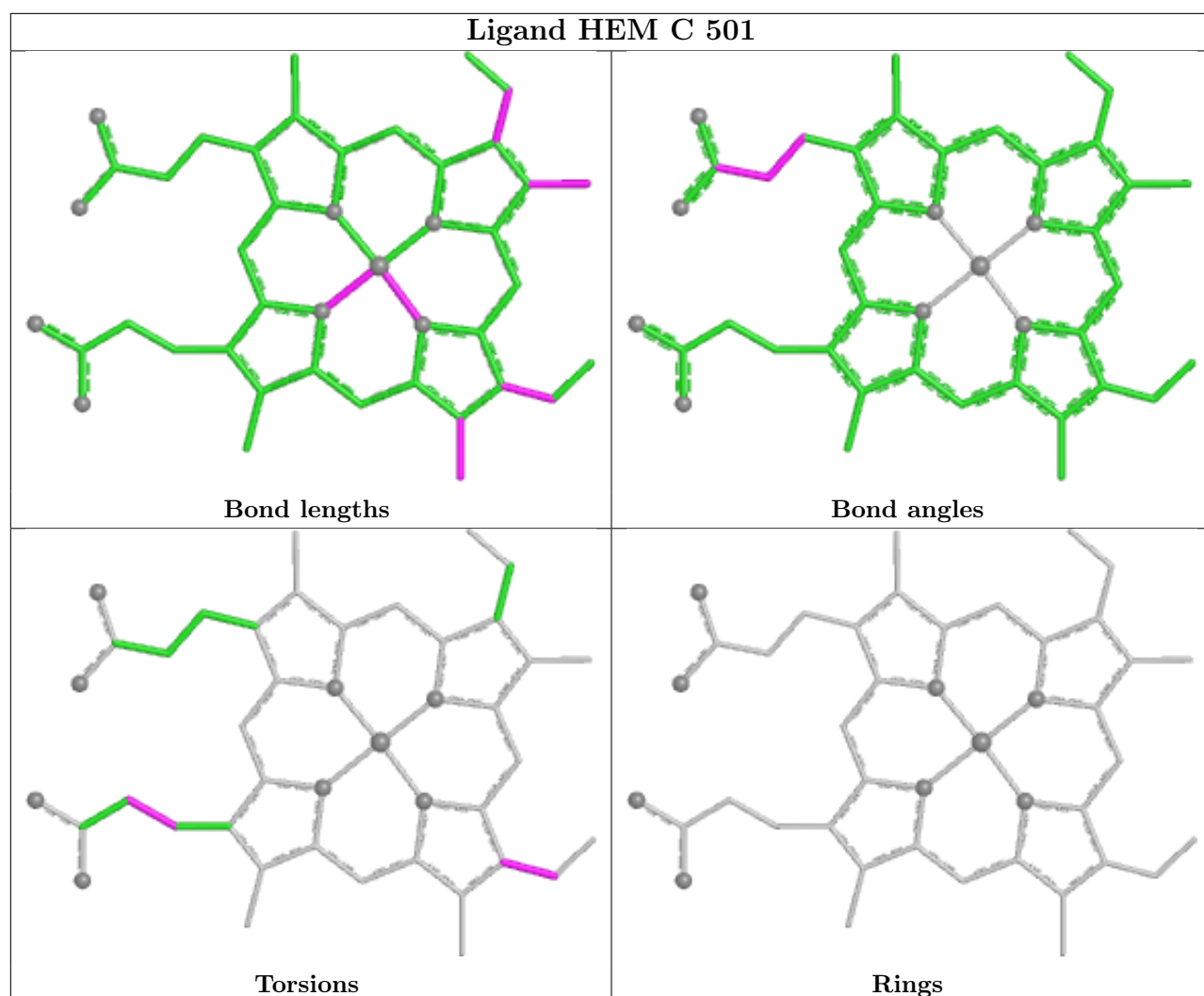


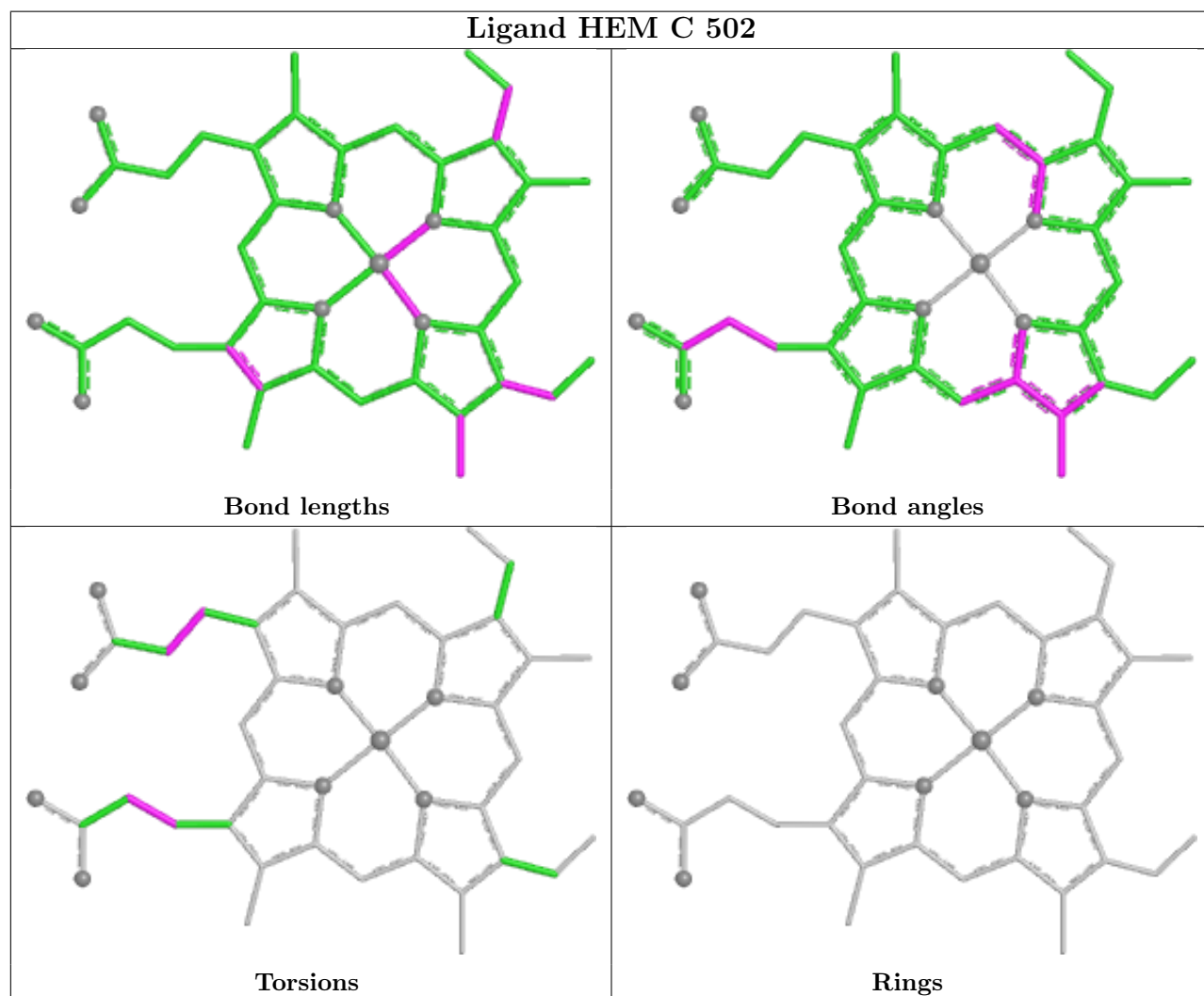
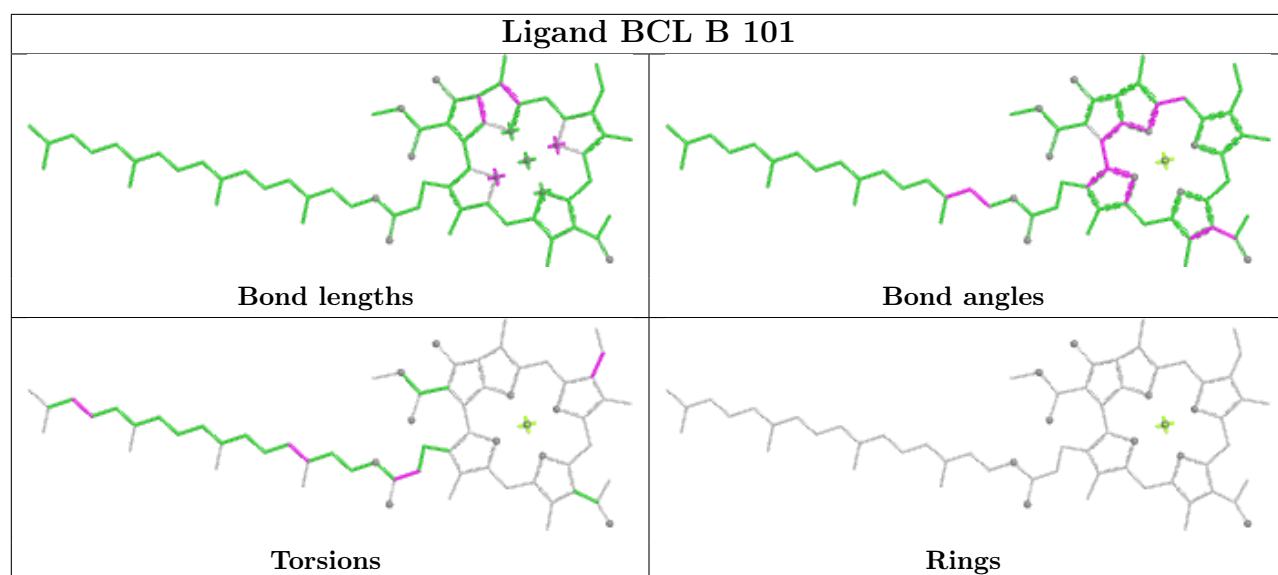
Ligand BCL D 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

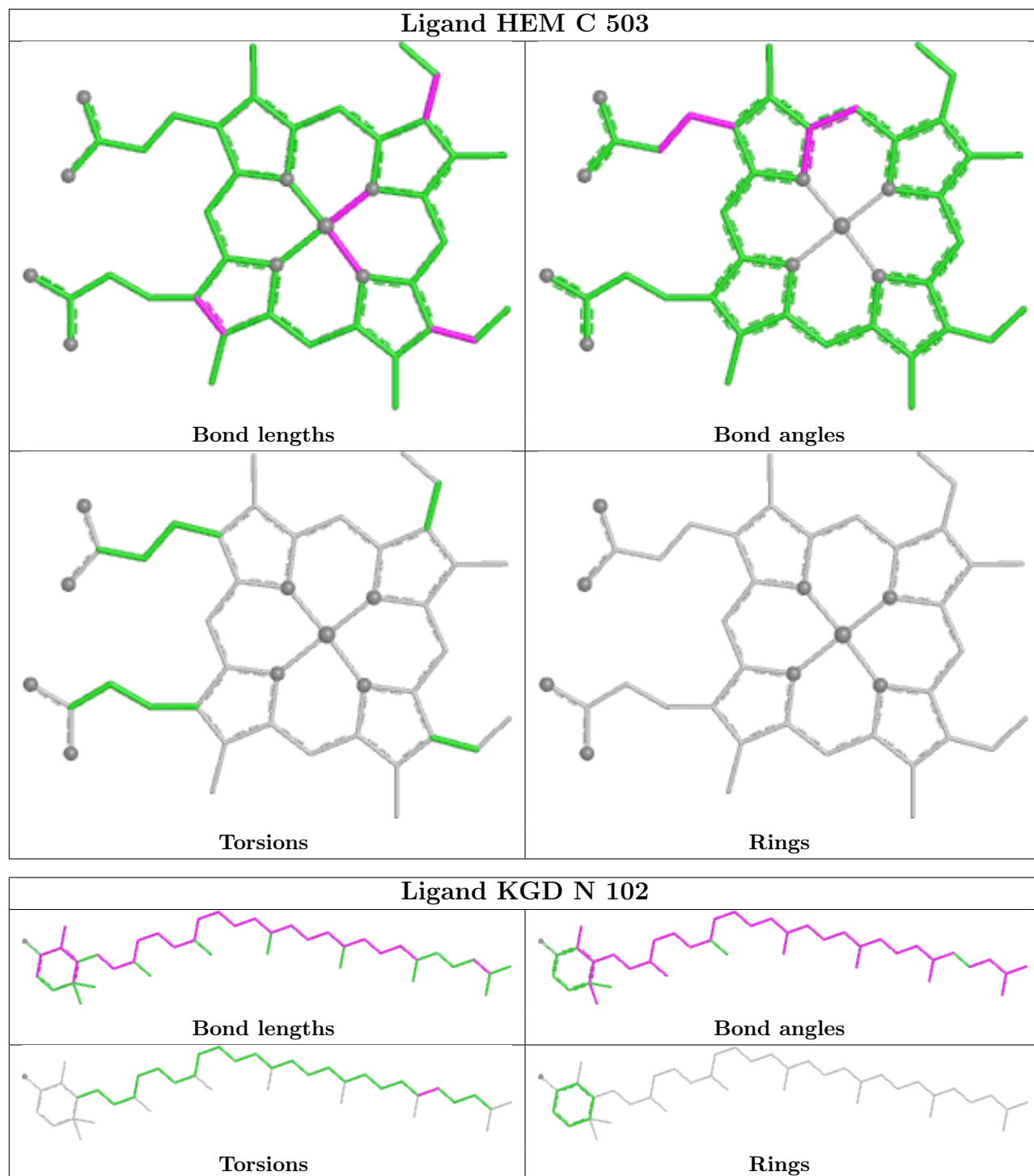
Ligand KGD F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

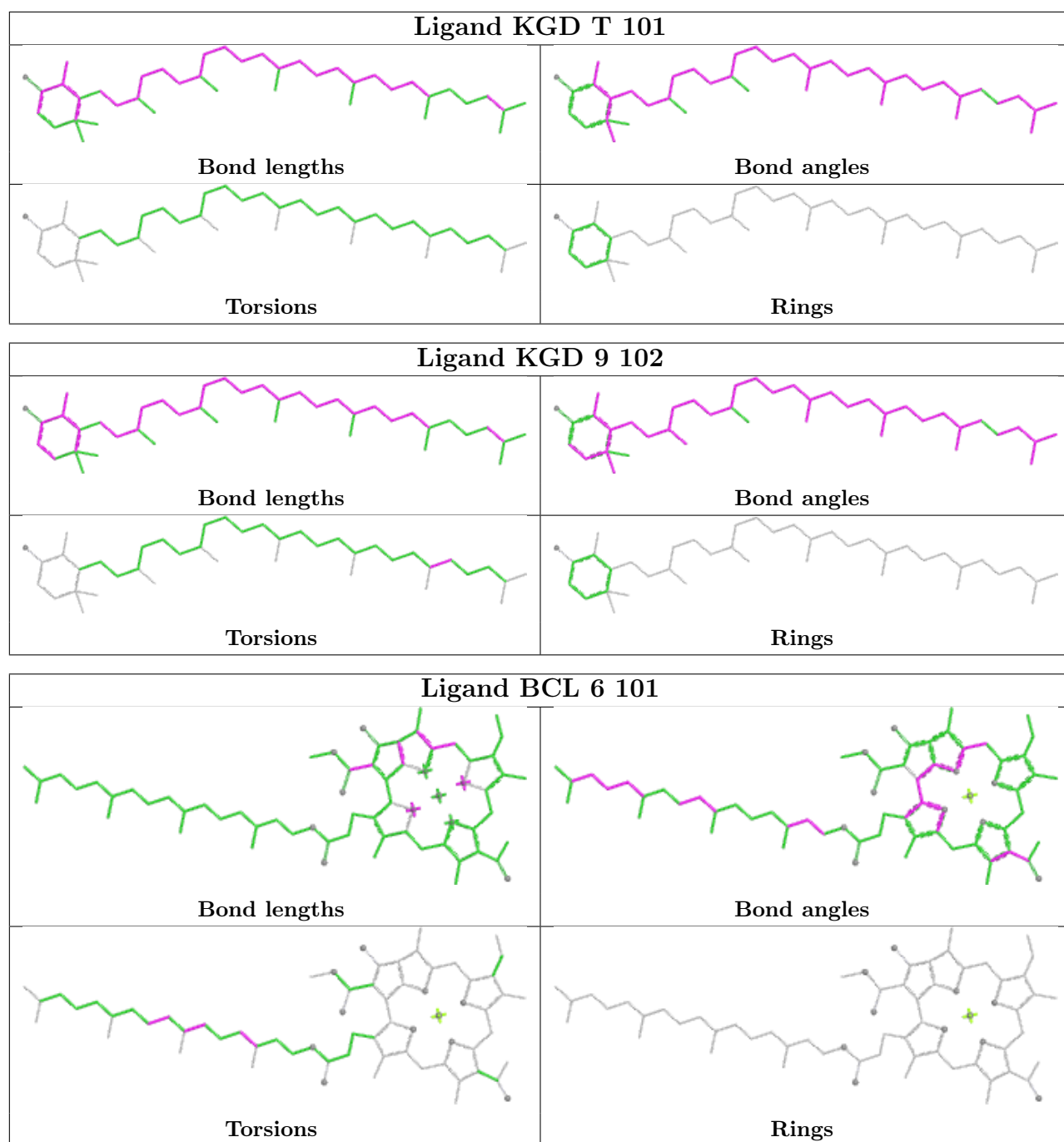


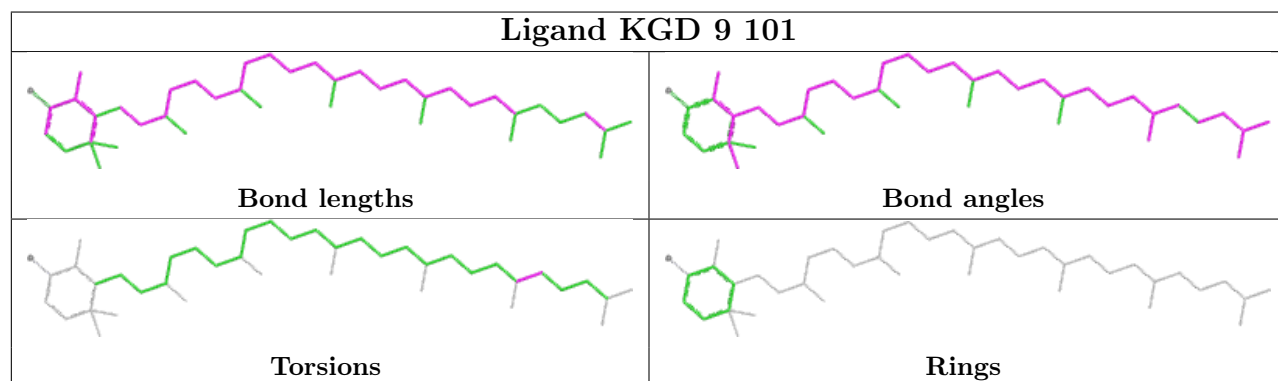
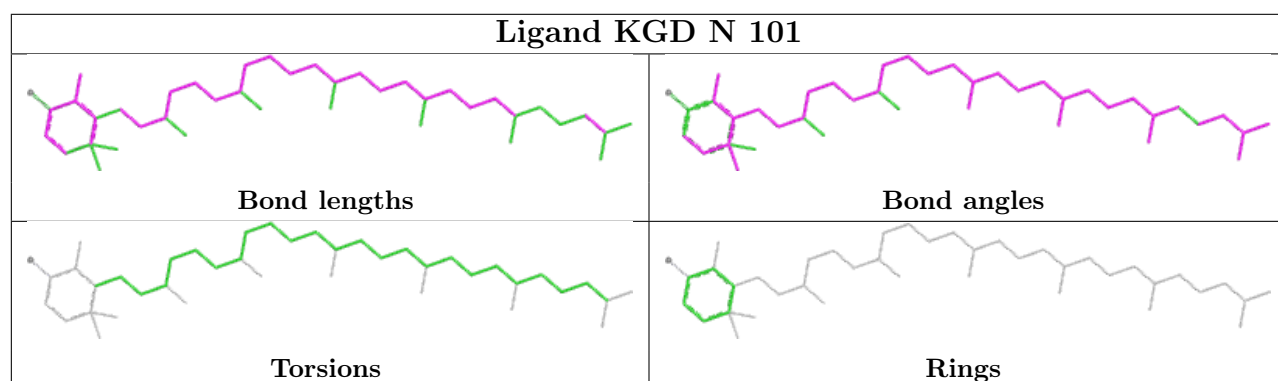
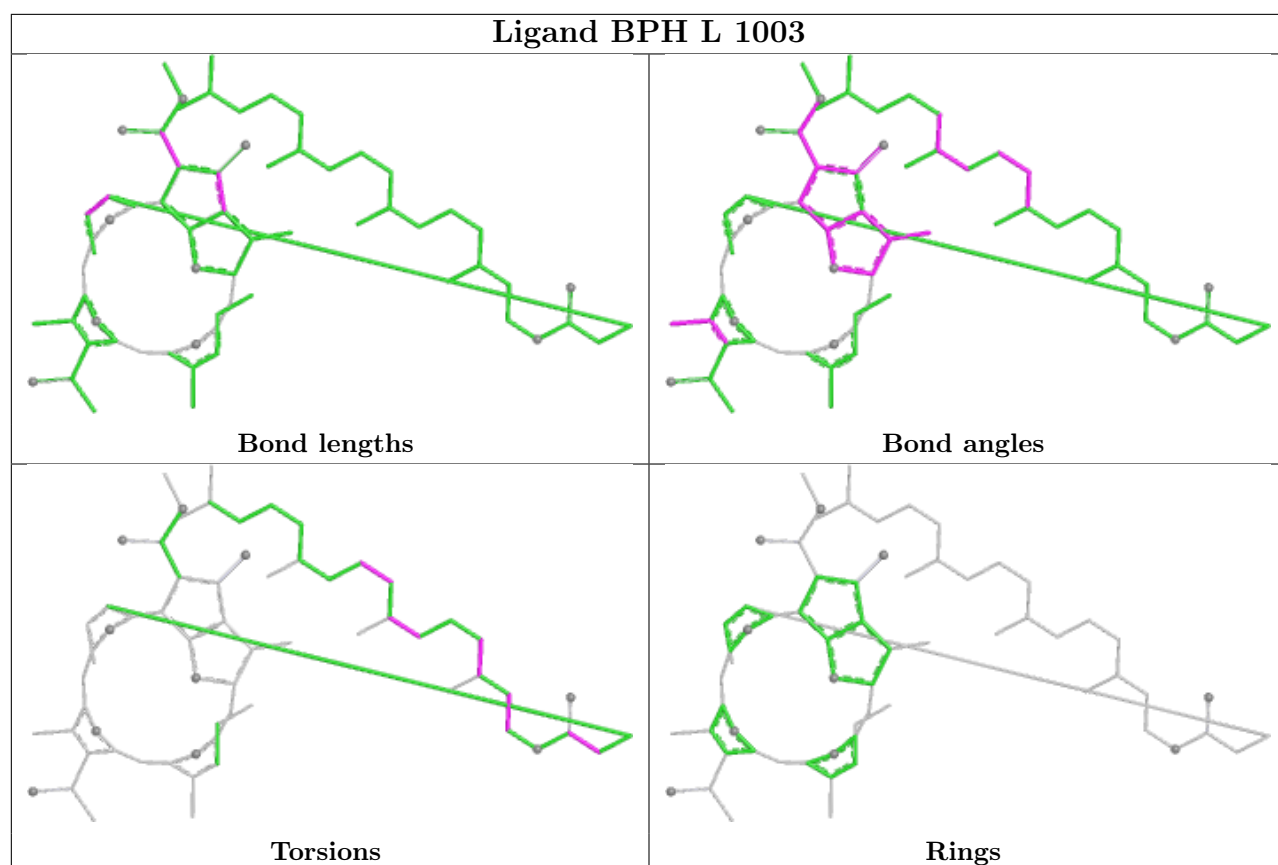


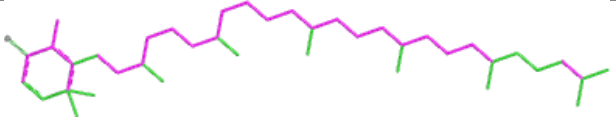
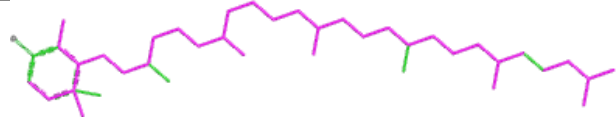
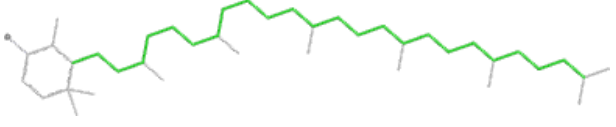
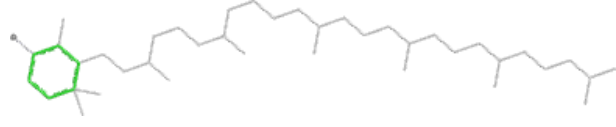


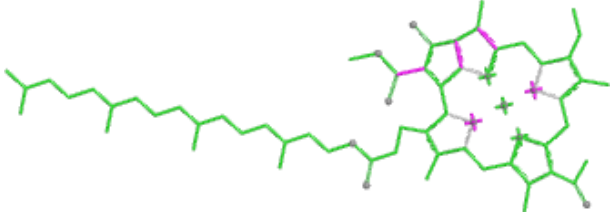
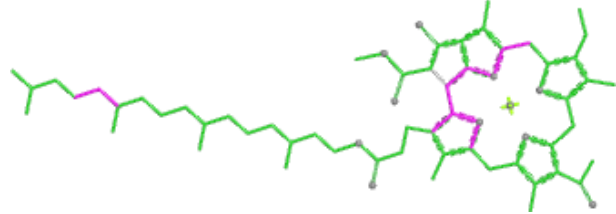
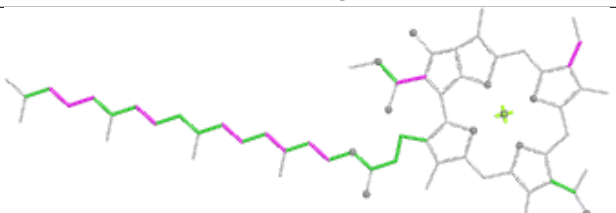
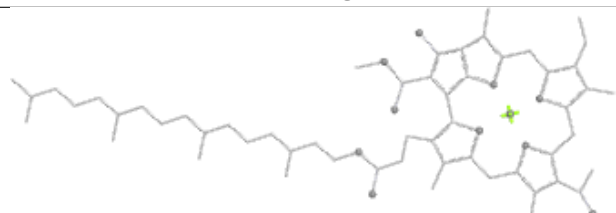


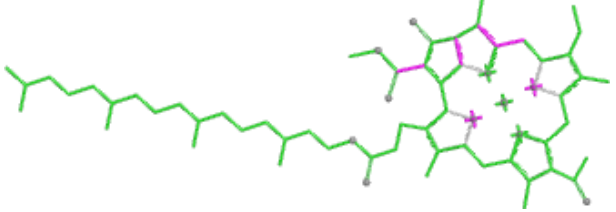
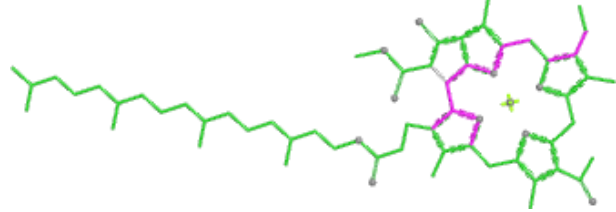
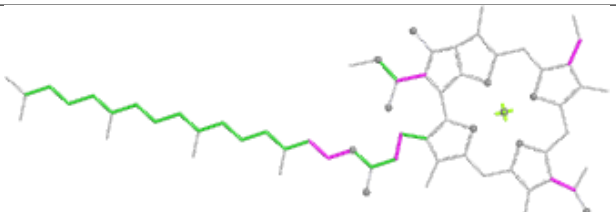
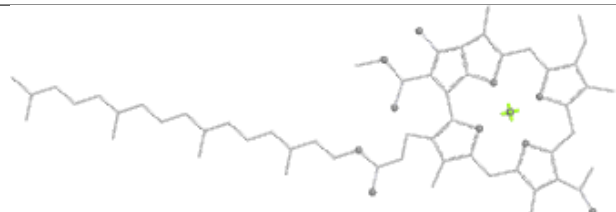


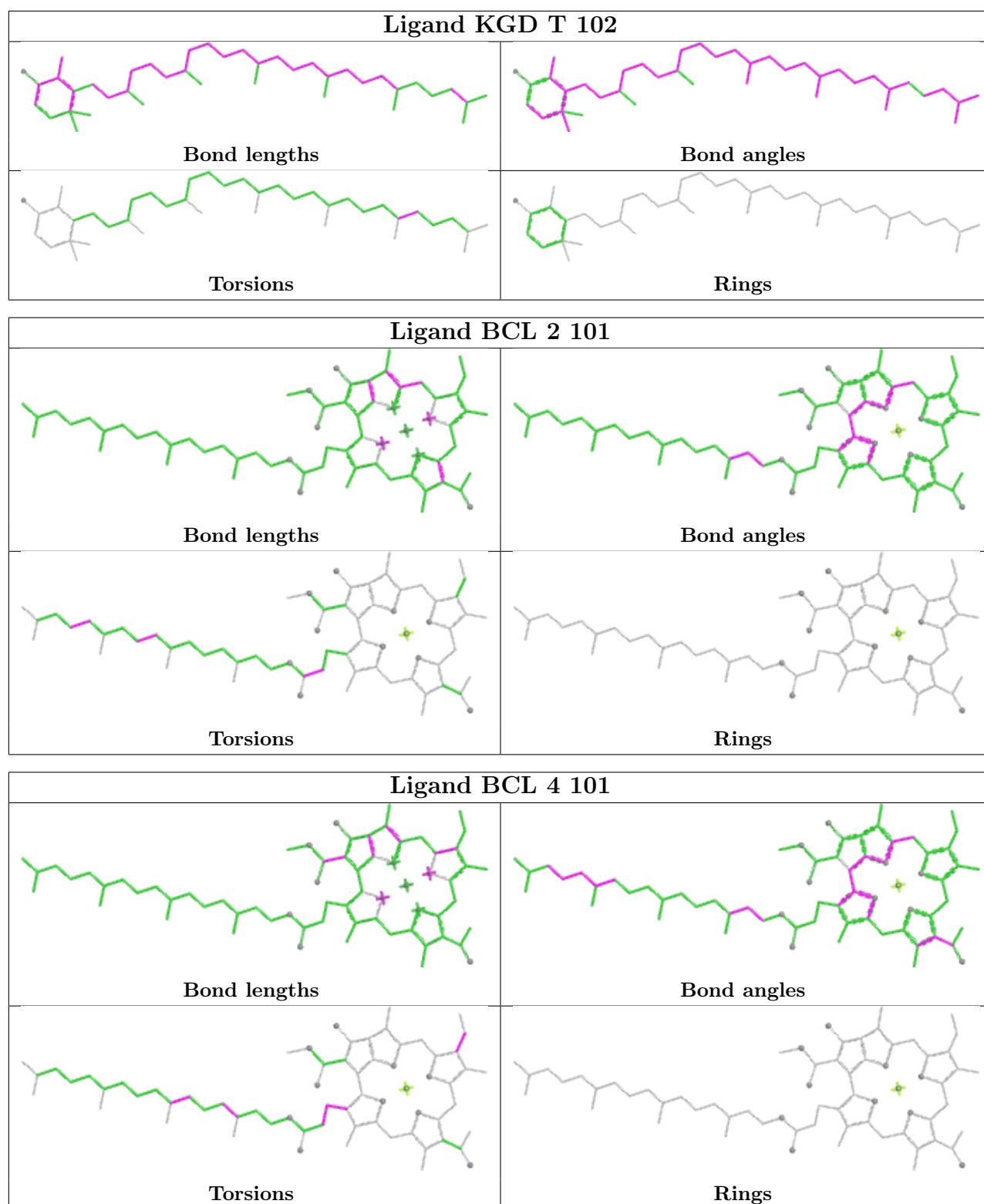


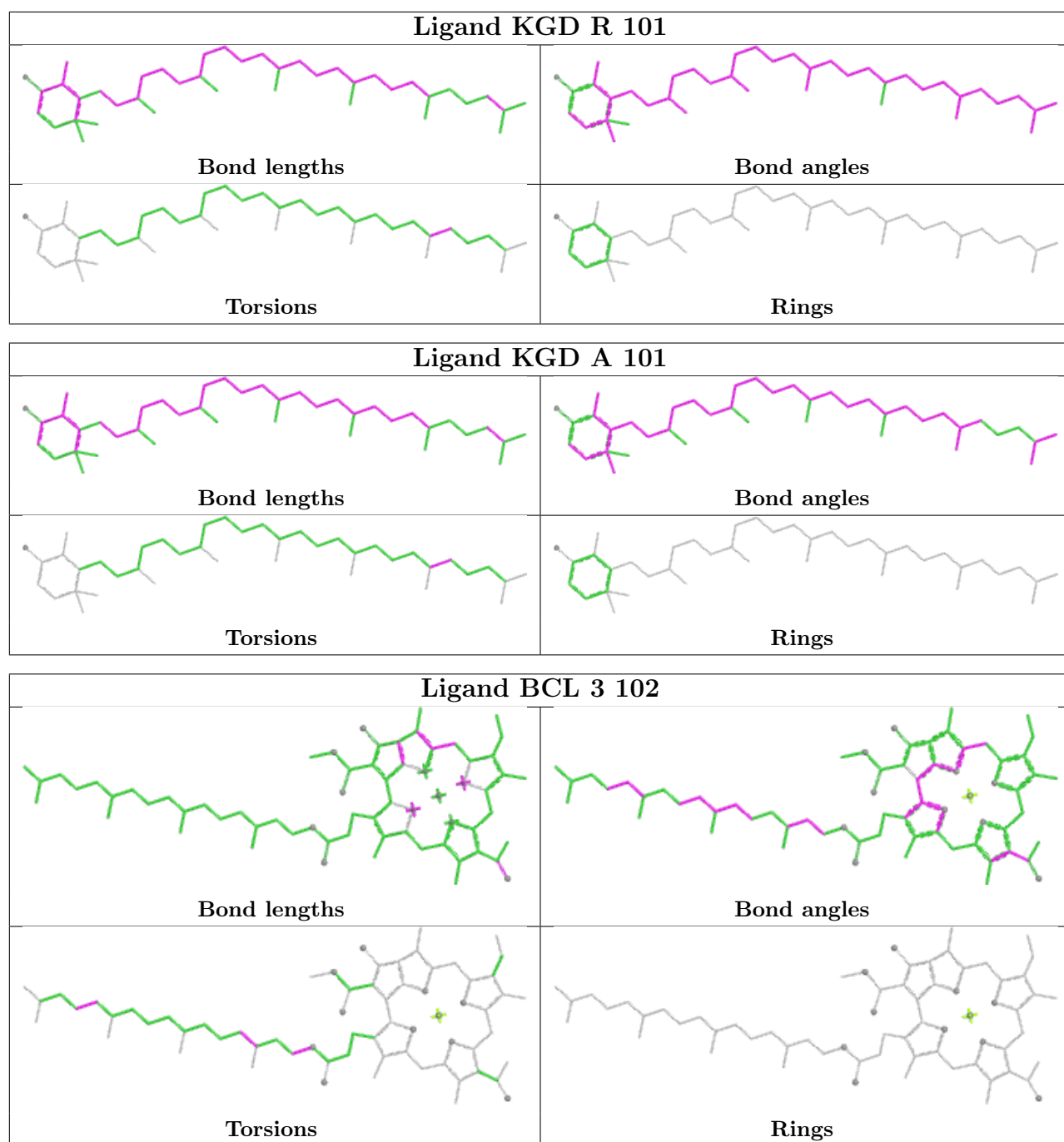


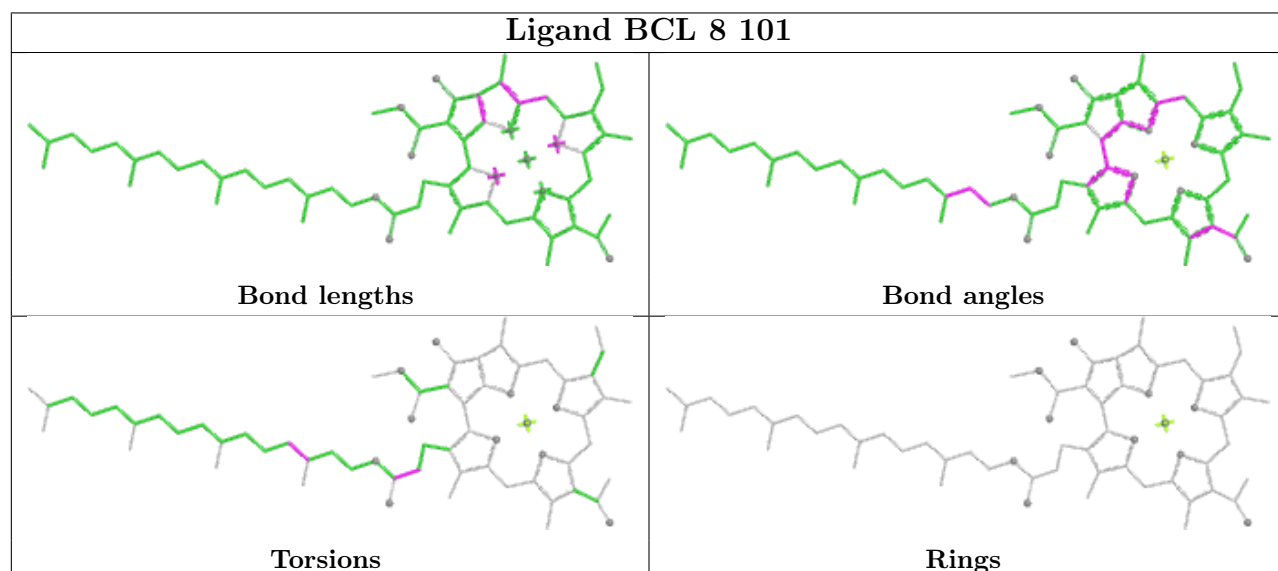
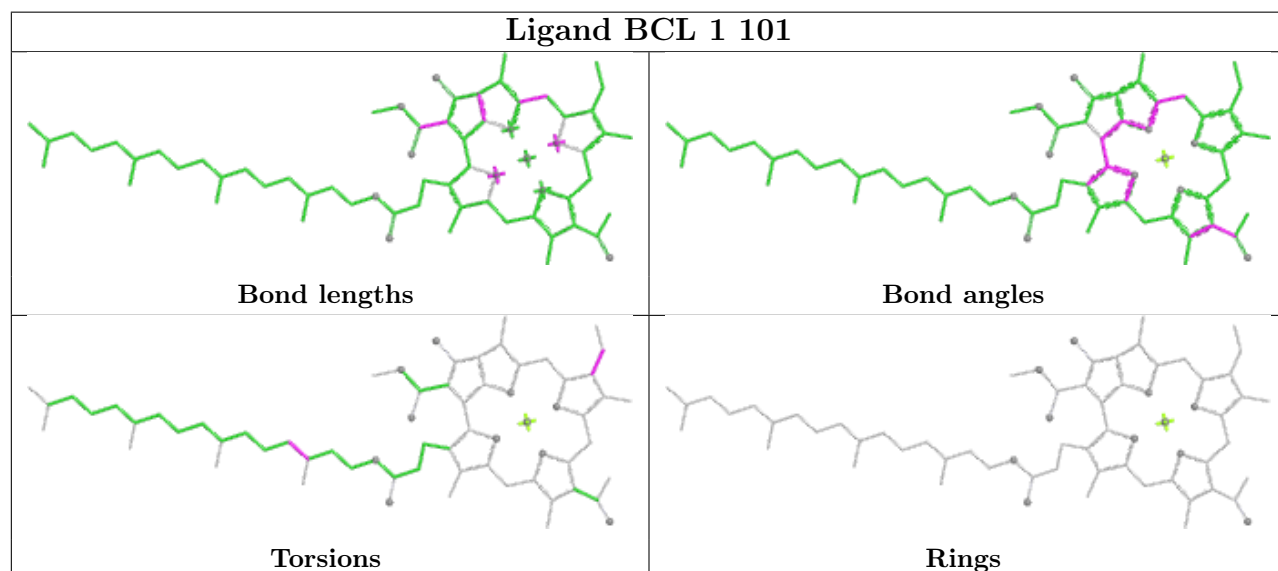
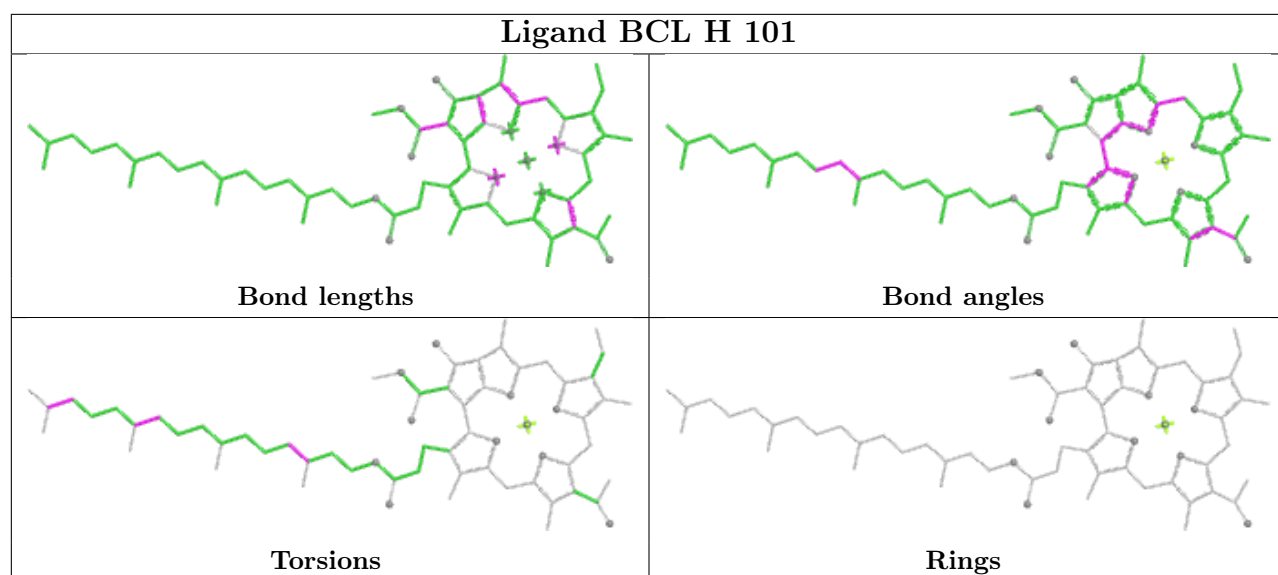
Ligand KGD J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

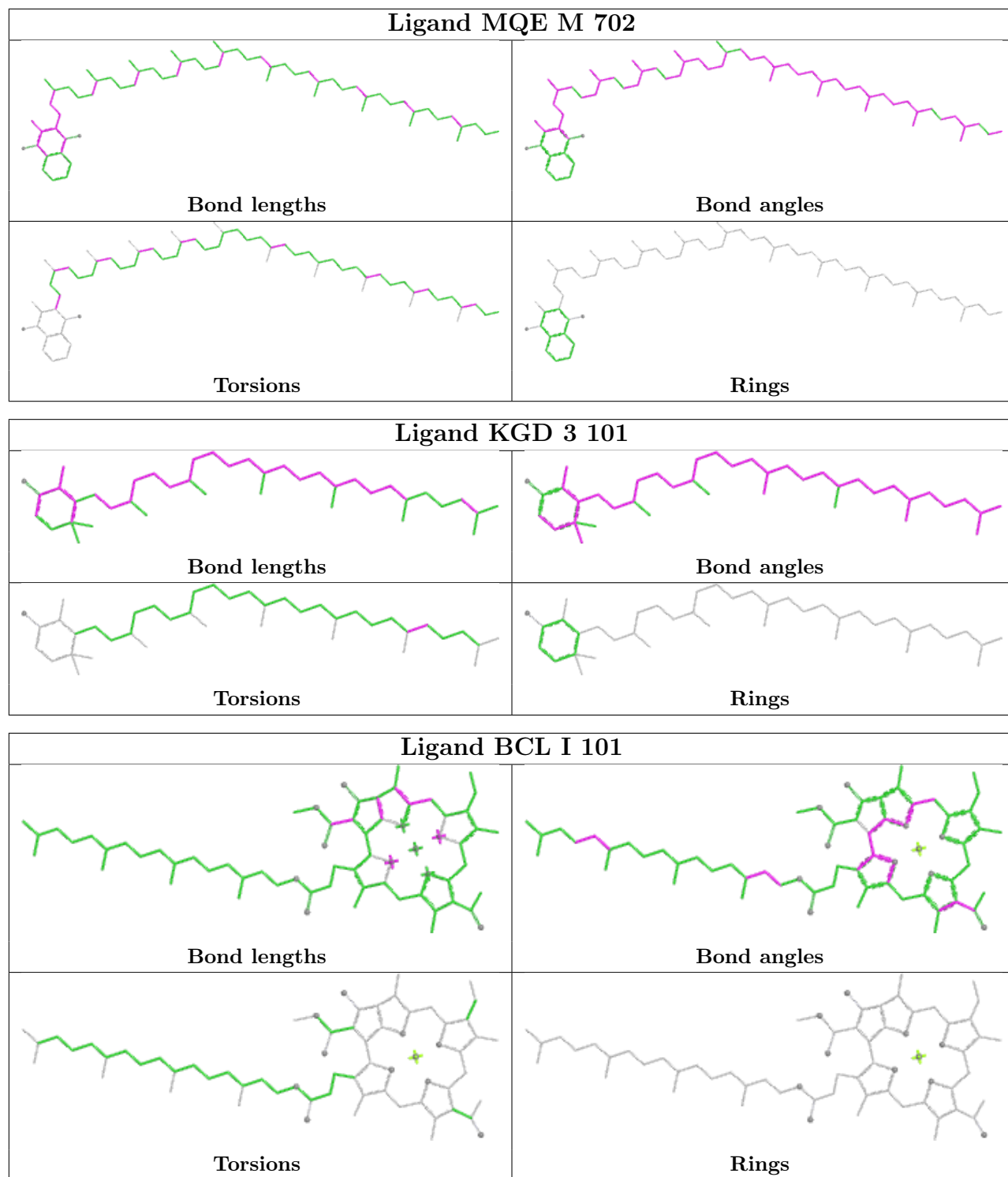
Ligand BCL G 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

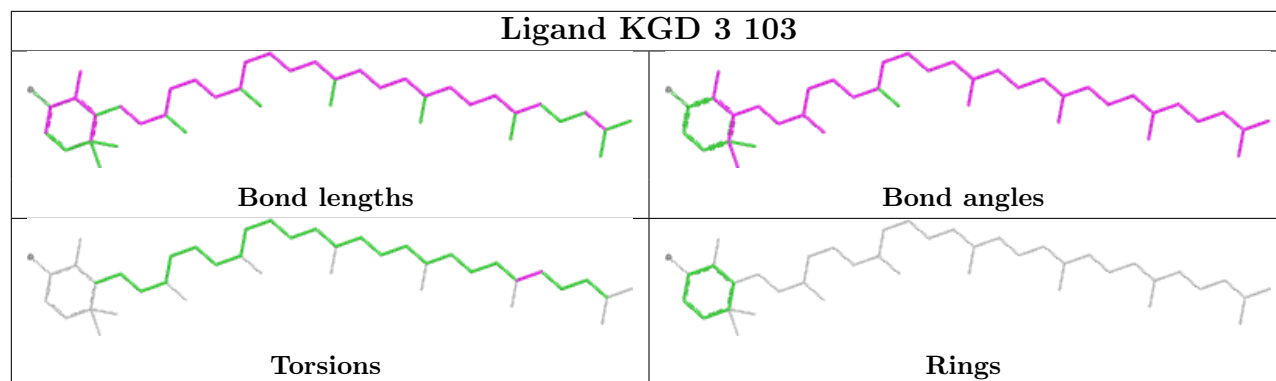
Ligand BCL U 102	
	
Bond lengths	Bond angles
	
Torsions	Rings











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.

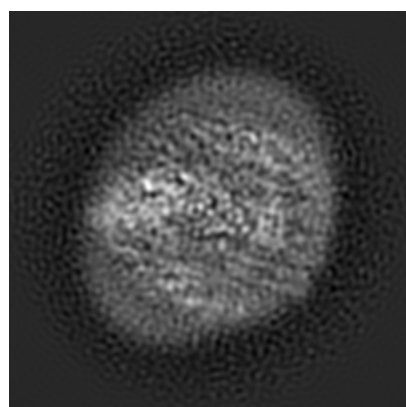
6 Map visualisation [i](#)

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.

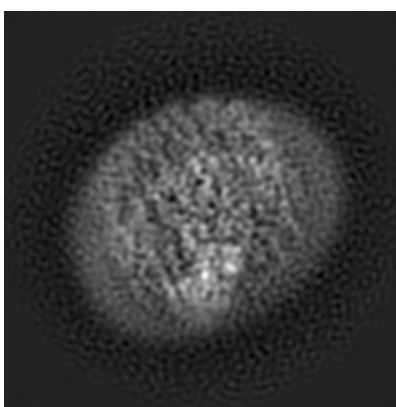
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

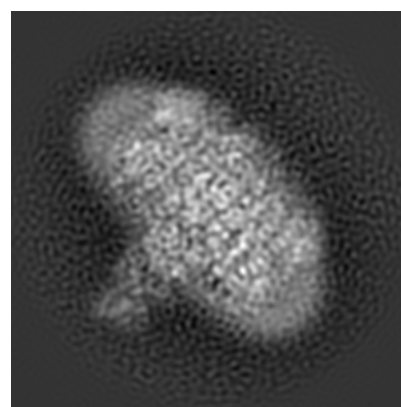
6.1.1 Primary map



X



Y

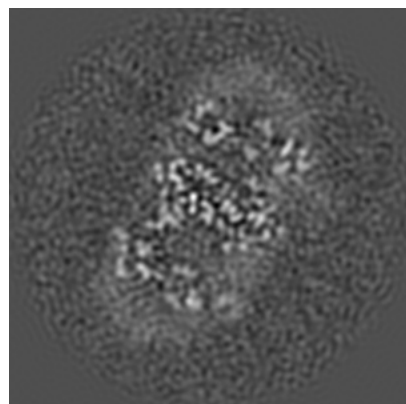


Z

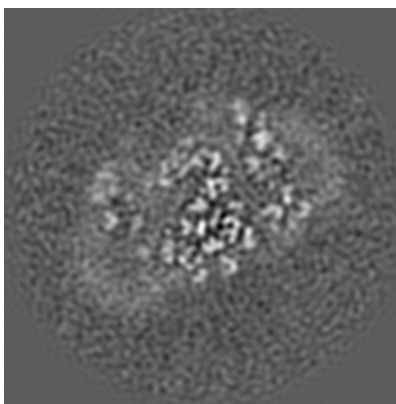
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

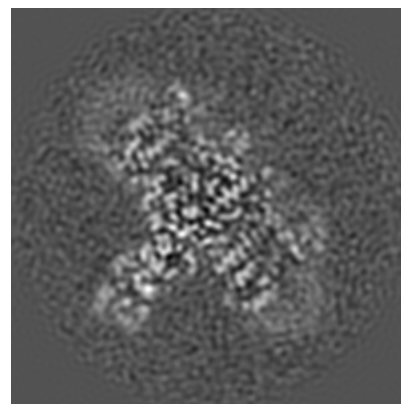
6.2.1 Primary map



X Index: 96



Y Index: 96

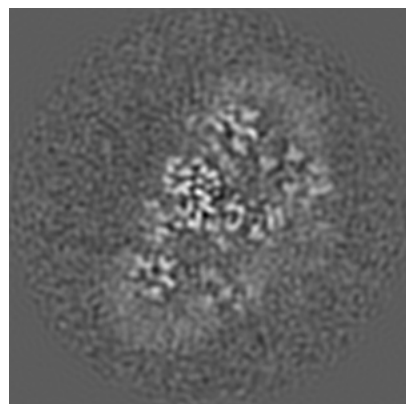


Z Index: 96

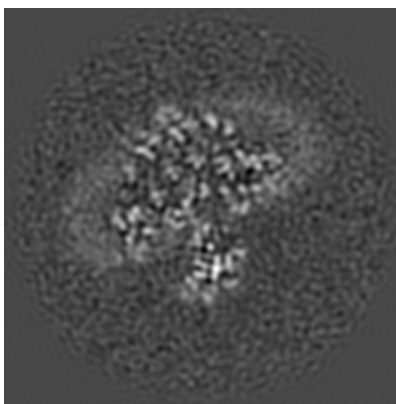
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

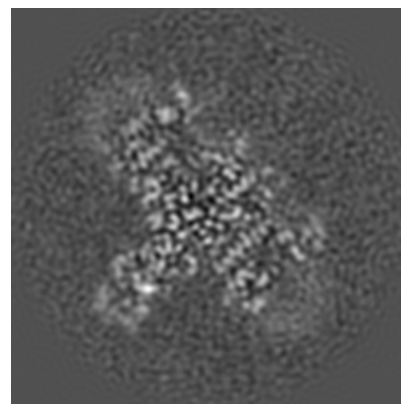
6.3.1 Primary map



X Index: 88



Y Index: 71

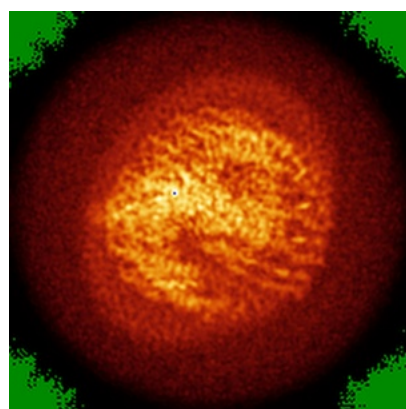


Z Index: 97

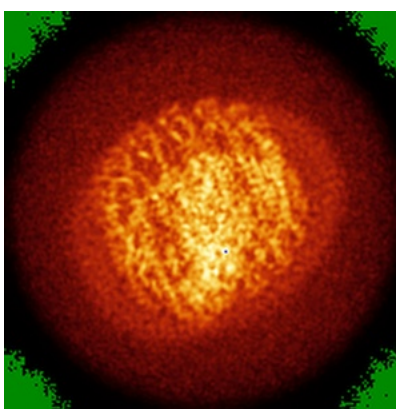
The images above show the largest variance slices of the map in three orthogonal directions.

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

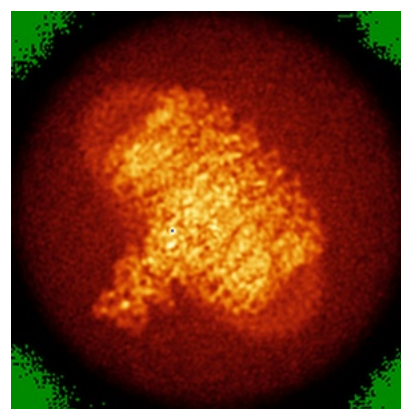
6.4.1 Primary map



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.

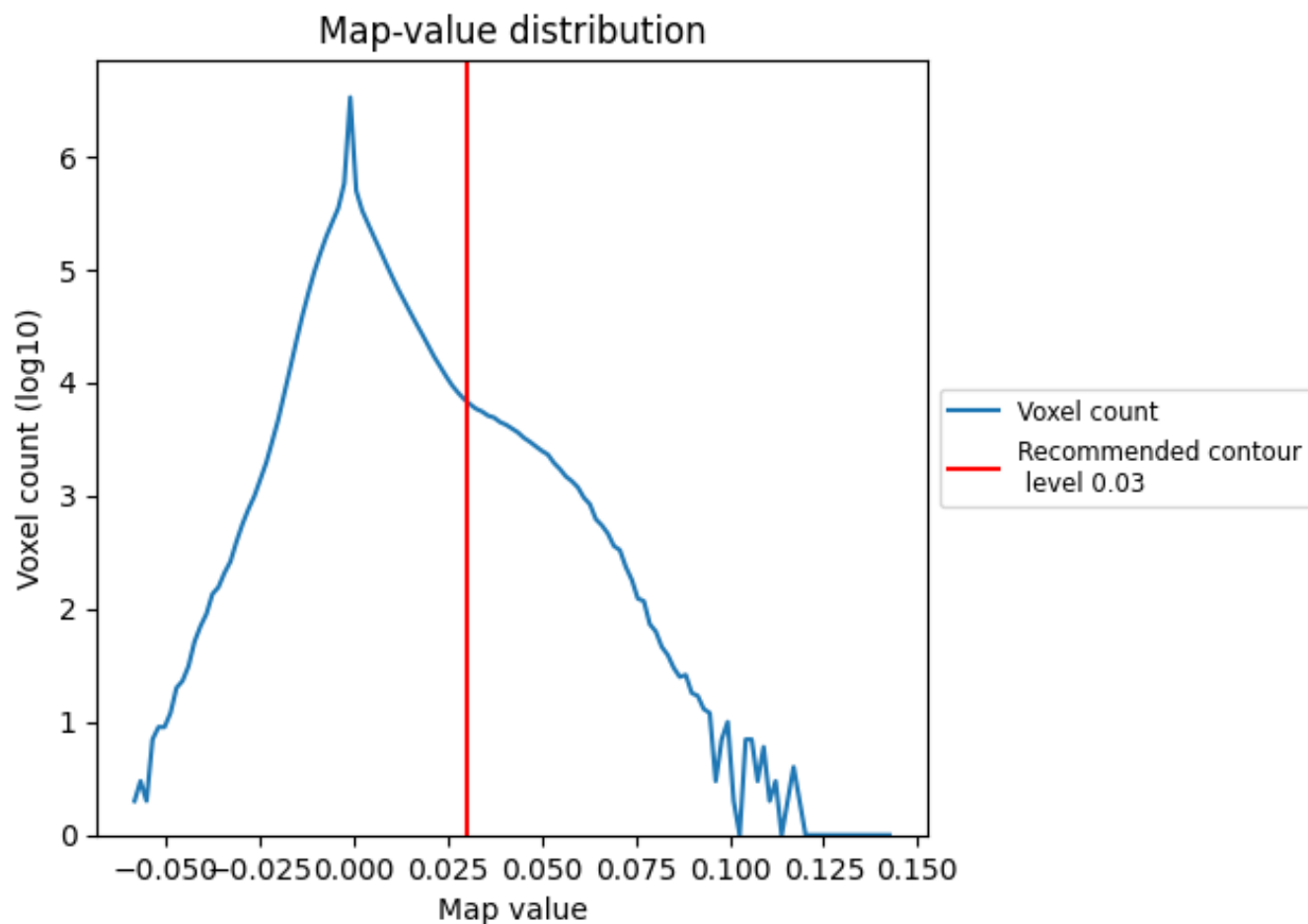
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

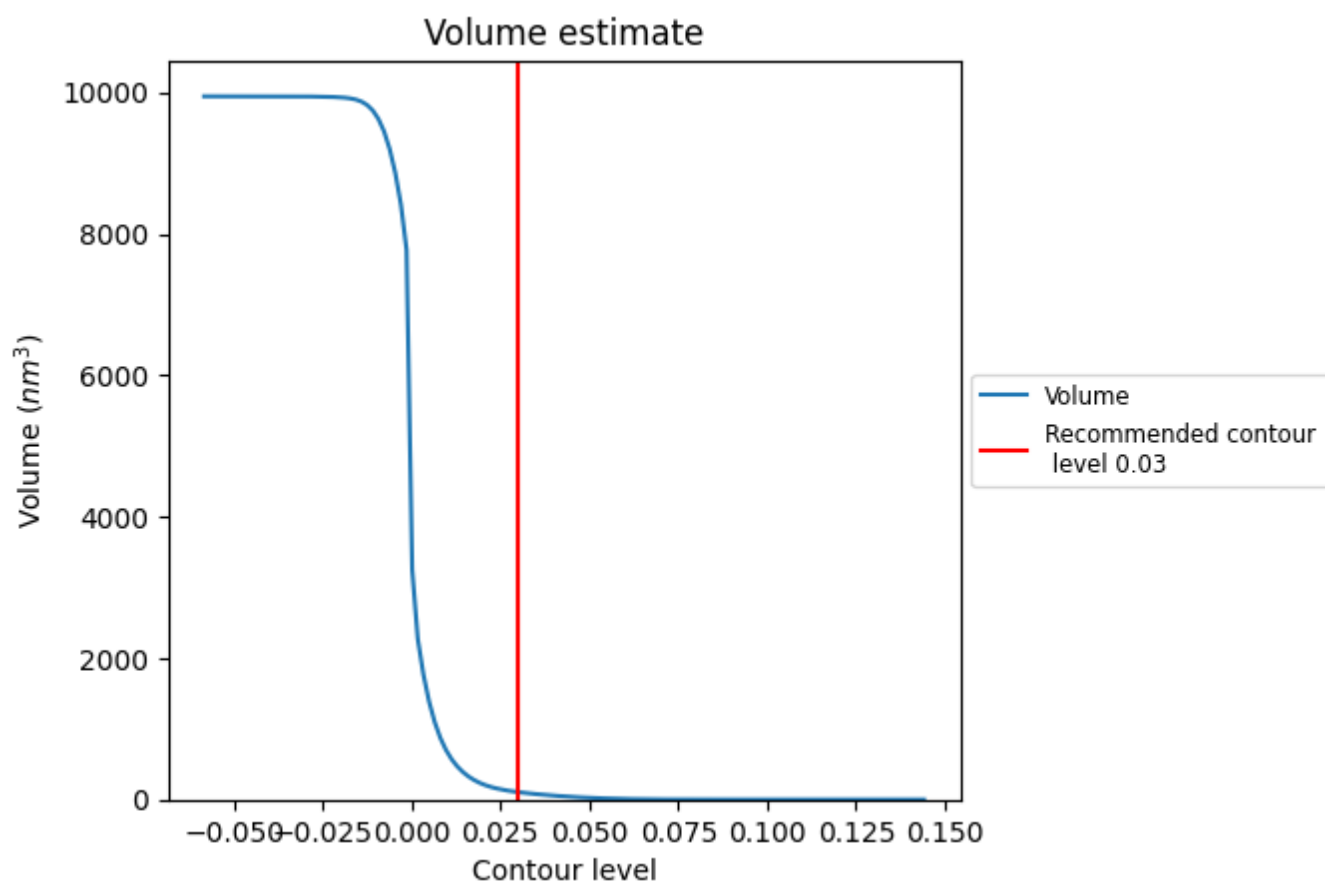
This section contains the results of statistical analysis of the map.

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.

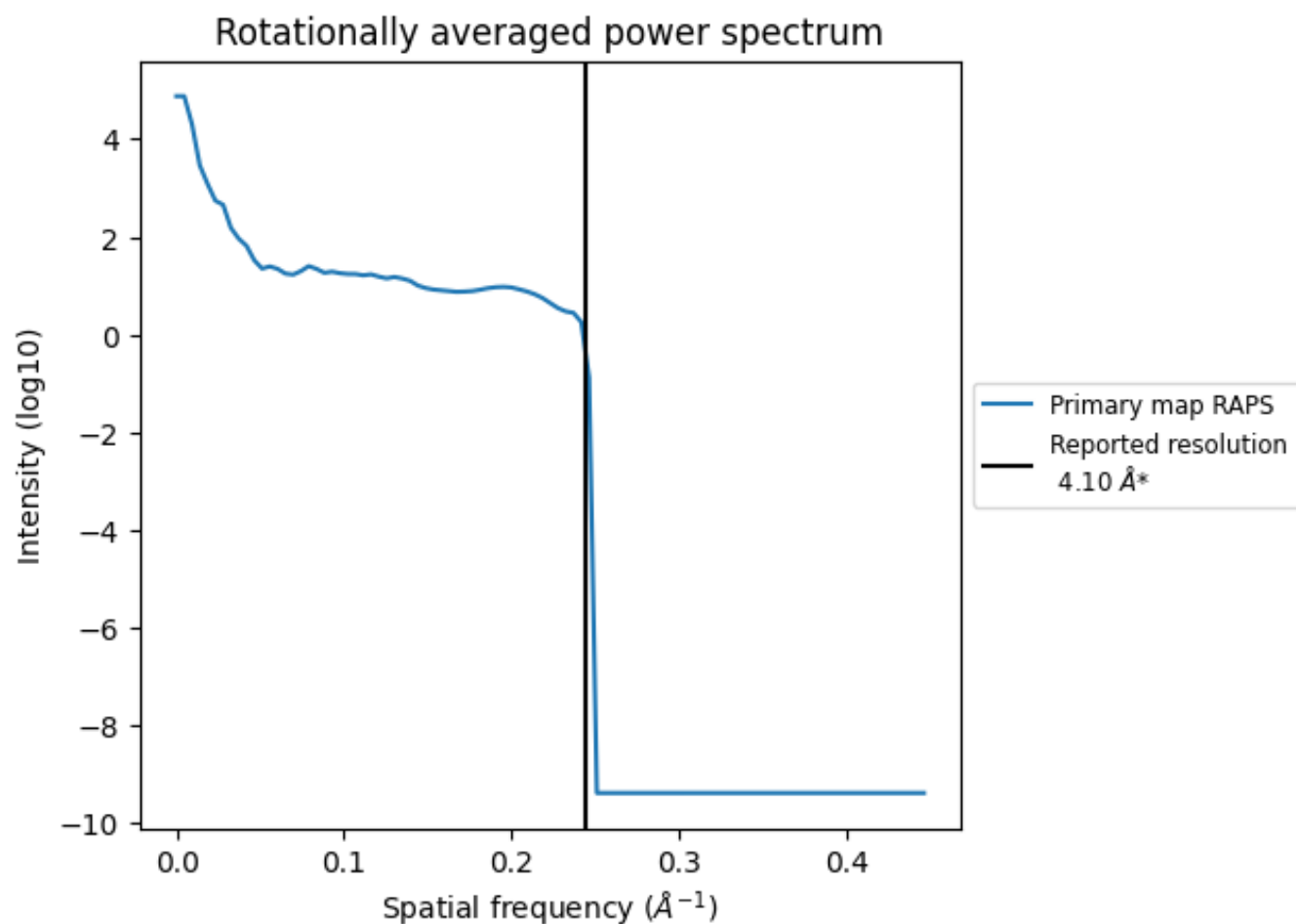
7.2 Volume estimate [i](#)



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

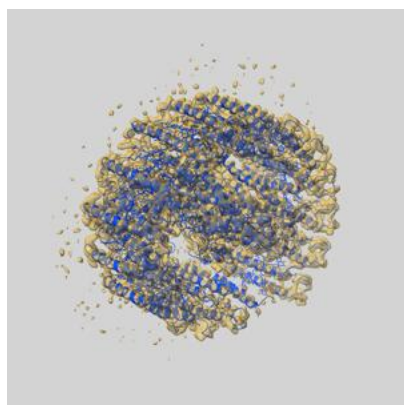
8 Fourier-Shell correlation

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

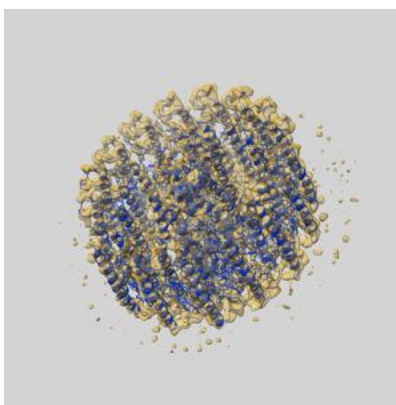
9 Map-model fit [i](#)

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](#).

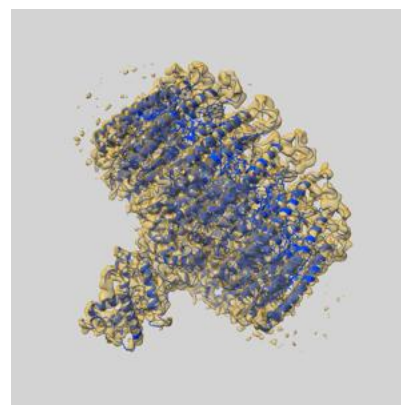
9.1 Map-model overlay [i](#)



X



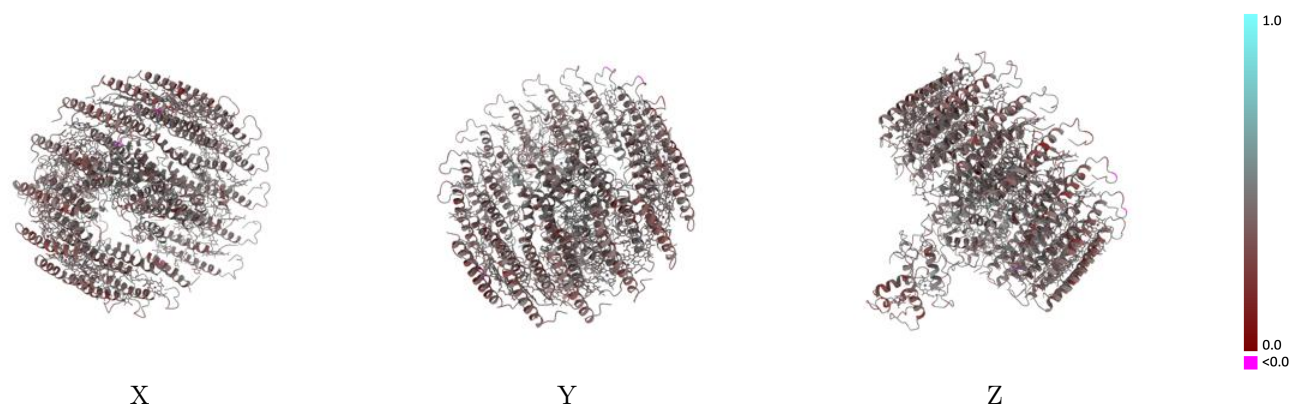
Y



Z

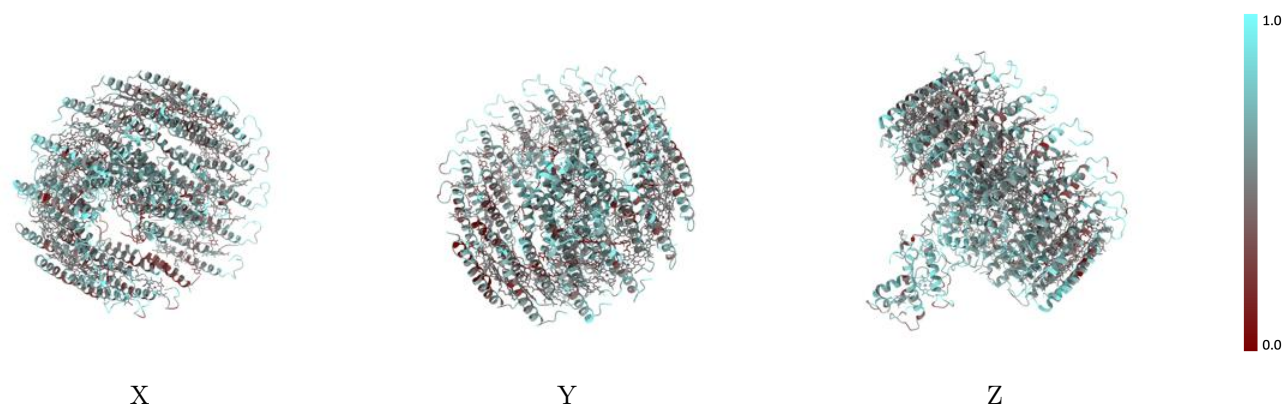
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



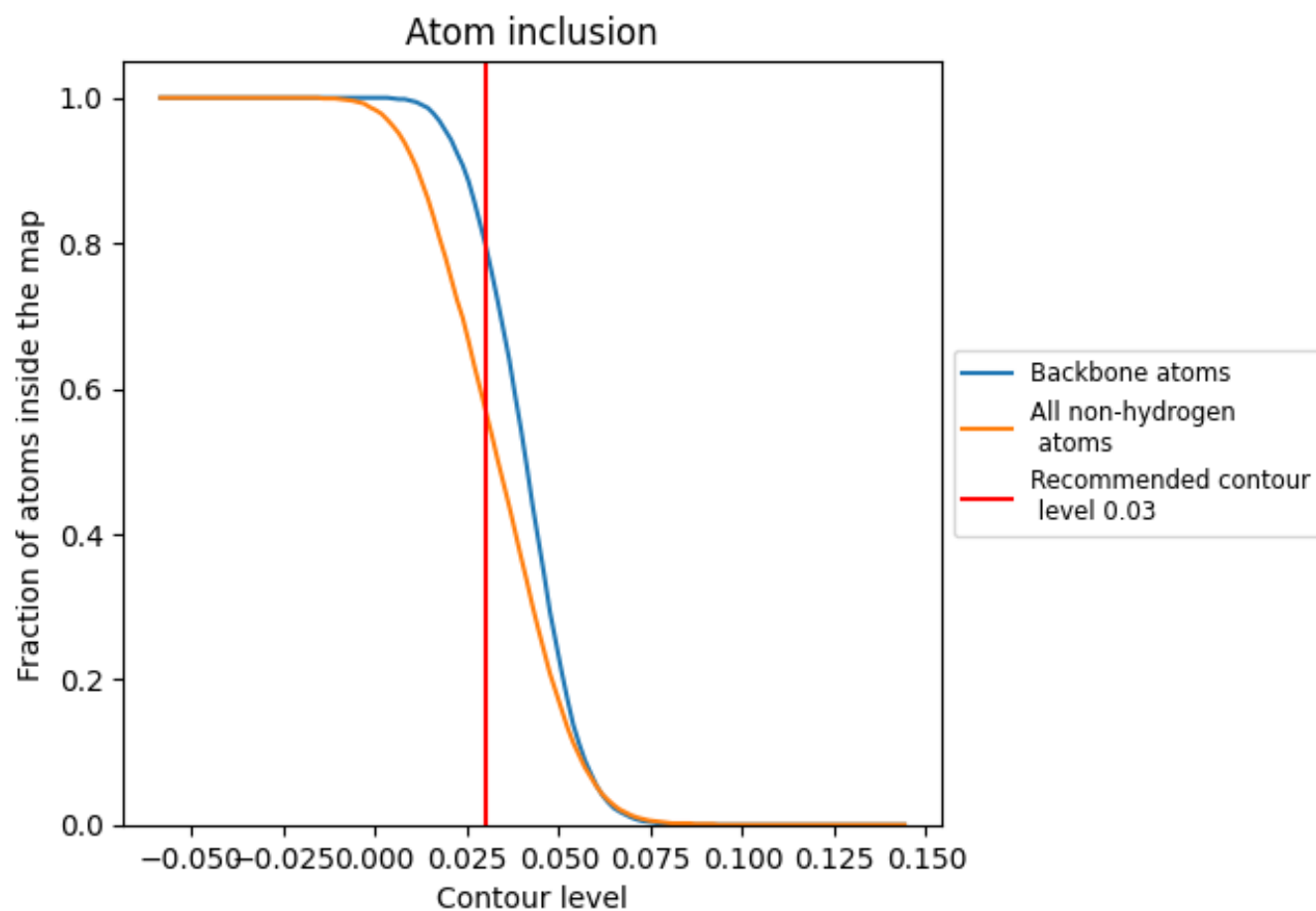
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

