



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:18 AM JST

PDB ID : 8J5P
EMDB ID : EMD-35989
Title : Cryo-EM structure of native RC-LH complex from *Roseiflexus castenholzii* at 2,000lux
Authors : Xu, X.; Xin, J.
Deposited on : 2023-04-24
Resolution : 3.10 Å(reported)

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

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

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

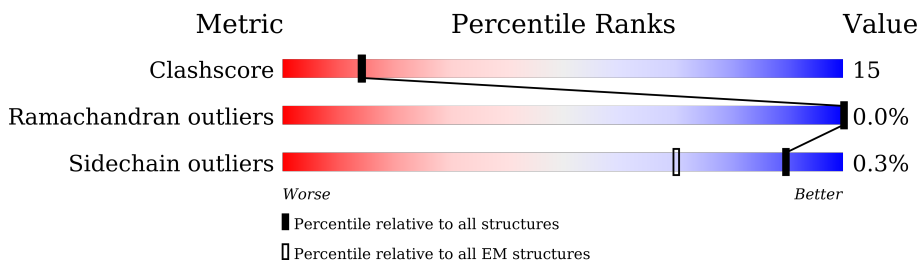
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	60% 29% 11%
1	2	55	58% 31% 11%
1	4	55	64% 24% 11%
1	6	55	58% 31% 11%
1	8	55	76% 13% 11%
1	B	55	58% 31% 11%
1	E	55	56% 33% 11%
1	G	55	65% 24% 11%




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Mol	Chain	Length	Quality of chain
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	1	42	
2	3	42	
2	5	42	
2	7	42	
2	9	42	
2	A	42	
2	D	42	
2	F	42	
2	H	42	
2	J	42	
2	N	42	
2	P	42	
2	R	42	
2	T	42	
2	V	42	
3	C	320	
4	L	315	
5	M	307	

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Mol	Chain	Length	Quality of chain
6	X	32	 38% 44% 19%
7	Y	39	 5% 54% 28% 18%
8	Z	63	 5% 52% 22% 25%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23737 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	3	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	5	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	7	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	J	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	N	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	P	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	R	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 3 is a protein called MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	315	Total	C	N	O	S	0	0
			2404	1532	407	443	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	300	Total	C	N	O	S	0	0
			2375	1589	384	394	8		

- Molecule 5 is a protein called Reaction center protein M chain.

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

- Molecule 6 is a protein called Subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	26	Total	C	N	O	S	0	0
			206	145	26	31	4		

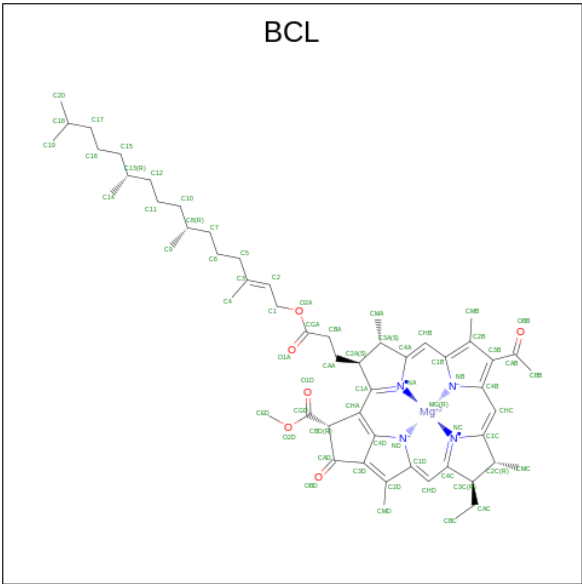
- Molecule 7 is a protein called Subunit Y.

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

- Molecule 8 is a protein called Subunit Z.

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

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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

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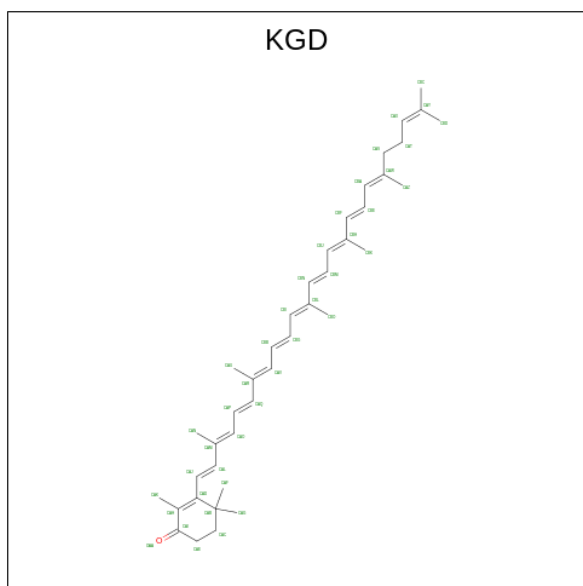
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55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

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Mol	Chain	Residues	Atoms					AltConf
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is beta,psi-caroten-4-one (three-letter code: KGD) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
10	0	1	Total	C	O	0
			41	40	1	
10	2	1	Total	C	O	0
			41	40	1	
10	3	1	Total	C	O	0
			41	40	1	
10	4	1	Total	C	O	0
			41	40	1	
10	5	1	Total	C	O	0
			41	40	1	
10	5	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
10	6	1	Total 41	C 40	O 1	0
10	8	1	Total 41	C 40	O 1	0
10	9	1	Total 41	C 40	O 1	0
10	A	1	Total 41	C 40	O 1	0
10	B	1	Total 41	C 40	O 1	0
10	C	1	Total 41	C 40	O 1	0
10	C	1	Total 41	C 40	O 1	0
10	E	1	Total 41	C 40	O 1	0
10	E	1	Total 41	C 40	O 1	0
10	G	1	Total 41	C 40	O 1	0
10	H	1	Total 41	C 40	O 1	0
10	I	1	Total 41	C 40	O 1	0
10	I	1	Total 41	C 40	O 1	0
10	J	1	Total 41	C 40	O 1	0
10	K	1	Total 41	C 40	O 1	0
10	O	1	Total 41	C 40	O 1	0
10	P	1	Total 41	C 40	O 1	0
10	P	1	Total 41	C 40	O 1	0
10	Q	1	Total 41	C 40	O 1	0
10	R	1	Total 41	C 40	O 1	0
10	S	1	Total 41	C 40	O 1	0

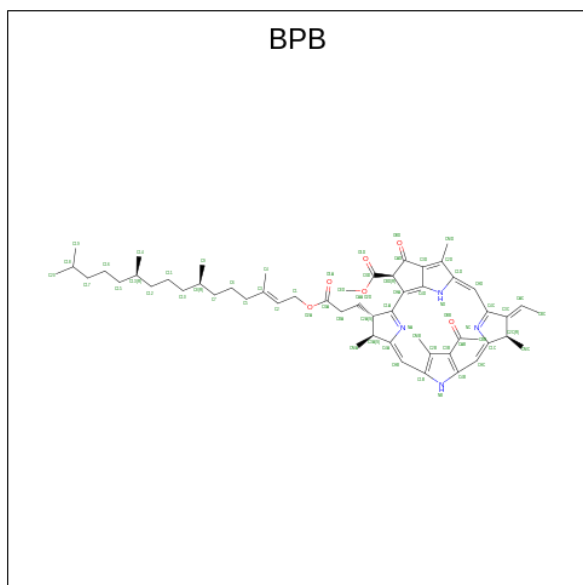
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Mol	Chain	Residues	Atoms			AltConf
10	T	1	Total 41	C 40	O 1	0
10	U	1	Total 41	C 40	O 1	0
10	W	1	Total 41	C 40	O 1	0

- # HEM

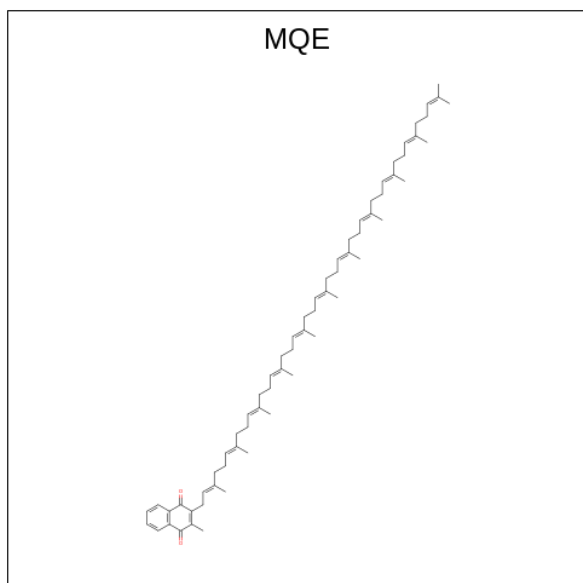
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

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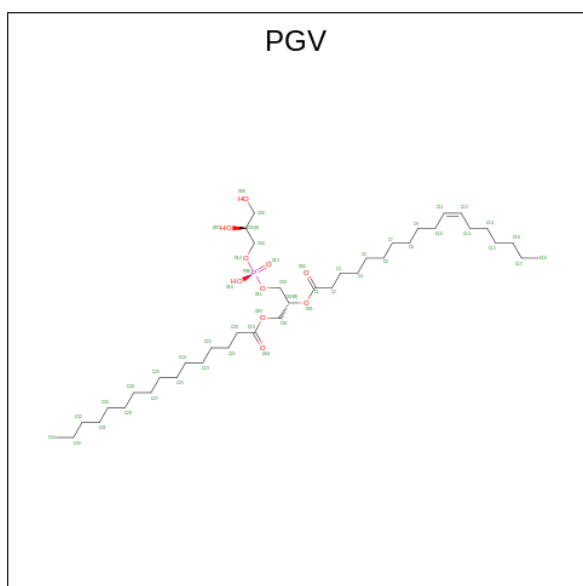
Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			65	55	4	6	
12	L	1	Total	C	N	O	0
			65	55	4	6	
12	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 13 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (three-letter code: MQE) (formula: C₆₆H₉₆O₂).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			68	66	2	
13	M	1	Total	C	O	0
			68	66	2	
13	M	1	Total	C	O	0
			24	22	2	

- Molecule 14 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			32	21	10	1	
14	L	1	Total	C	O	P	0
			45	34	10	1	
14	P	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
15	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.

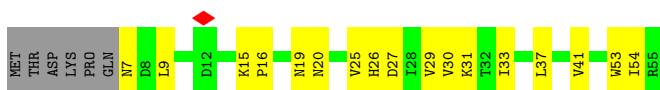
- Molecule 1: Beta subunit of light-harvesting 1

Chain 0: 



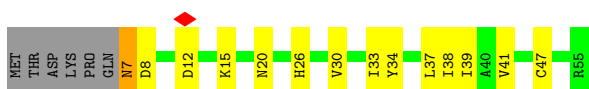
- Molecule 1: Beta subunit of light-harvesting 1

Chain 2: 



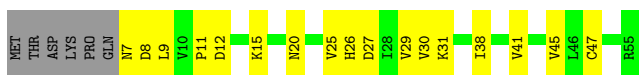
- Molecule 1: Beta subunit of light-harvesting 1

Chain 4: 




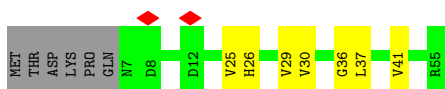
- Molecule 1: Beta subunit of light-harvesting 1

Chain 6: 



- Molecule 1: Beta subunit of light-harvesting 1

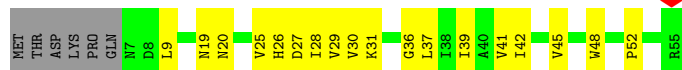
Chain 8: 



- Molecule 1: Beta subunit of light-harvesting 1



- Molecule 1: Beta subunit of light-harvesting 1



- Molecule 1: Beta subunit of light-harvesting 1



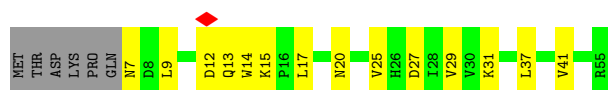
- Molecule 1: Beta subunit of light-harvesting 1



- 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

Chain S:  65% 24% 11%



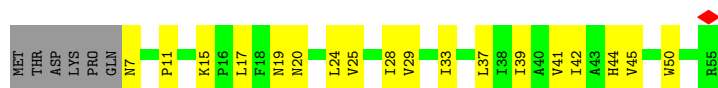
- Molecule 1: Beta subunit of light-harvesting 1

Chain U:  64% 25% 11%



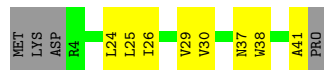
- Molecule 1: Beta subunit of light-harvesting 1

Chain W:  56% 33% 11%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 1:  71% 19% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 3:  69% 21% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 5:  62% 29% 10%



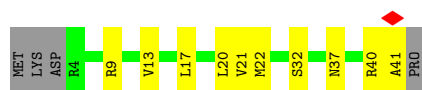
- Molecule 2: Alpha subunit of light-harvesting 1

Chain 7:  67% 24% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:  67% 24% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain A:  69% 21% 10%



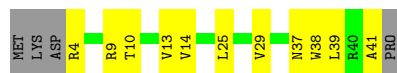
- Molecule 2: Alpha subunit of light-harvesting 1

Chain D:  57% 33% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain F:  64% 26% 10%



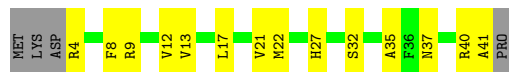
- Molecule 2: Alpha subunit of light-harvesting 1

Chain H:  50% 40% 10%



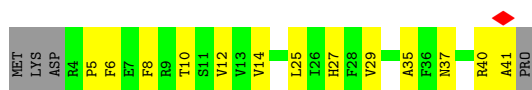
- Molecule 2: Alpha subunit of light-harvesting 1

Chain J:  57% 33% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

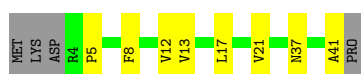
Chain N:  60% 31% 10%



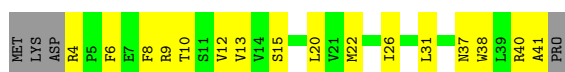
- Molecule 2: Alpha subunit of light-harvesting 1



- Molecule 2: Alpha subunit of light-harvesting 1



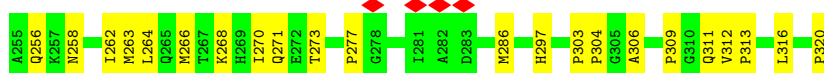
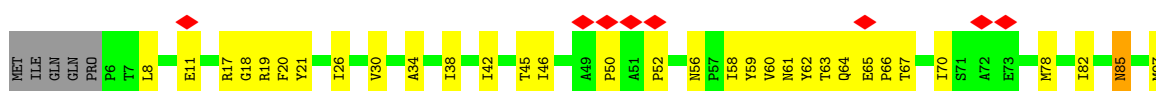
- Molecule 2: Alpha subunit of light-harvesting 1



- Molecule 2: Alpha subunit of light-harvesting 1

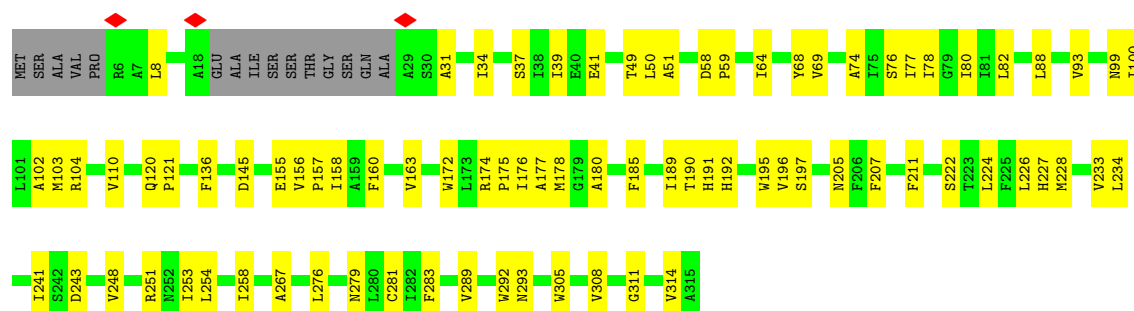


- Molecule 3: MULTHEME_CYTC DOMAIN-CONTAINING PROTEIN

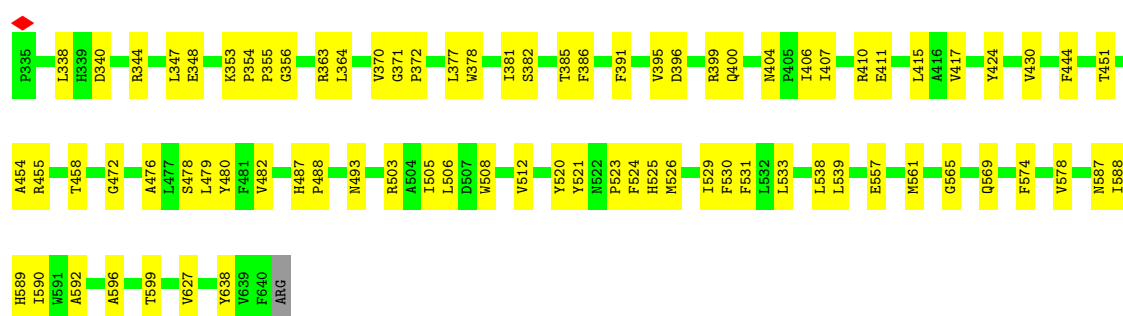


- Molecule 4: Reaction center protein L chain

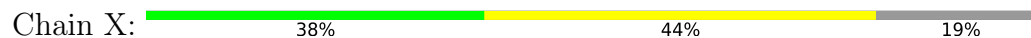




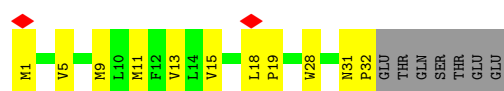
• Molecule 5: Reaction center protein M chain



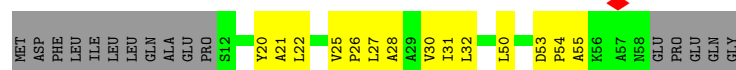
• Molecule 6: Subunit X



• Molecule 7: Subunit Y



• Molecule 8: Subunit Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272617	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	235.752, 235.752, 235.752	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.893, 0.893, 0.893	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.25	0/423	0.39	0/585
1	2	0.24	0/423	0.41	0/585
1	4	0.25	0/423	0.39	0/585
1	6	0.26	0/423	0.41	0/585
1	8	0.24	0/423	0.38	0/585
1	B	0.28	0/423	0.44	0/585
1	E	0.30	0/423	0.46	0/585
1	G	0.24	0/423	0.39	0/585
1	I	0.24	0/423	0.40	0/585
1	K	0.25	0/423	0.42	0/585
1	O	0.25	0/423	0.41	0/585
1	Q	0.25	0/423	0.45	0/585
1	S	0.26	0/423	0.42	0/585
1	U	0.26	0/423	0.44	0/585
1	W	0.24	0/423	0.44	0/585
2	1	0.35	0/307	0.55	0/417
2	3	0.26	0/307	0.49	0/417
2	5	0.26	0/307	0.51	0/417
2	7	0.28	0/307	0.54	0/417
2	9	0.25	0/307	0.51	0/417
2	A	0.27	0/307	0.48	0/417
2	D	0.25	0/307	0.47	0/417
2	F	0.25	0/307	0.49	0/417
2	H	0.29	0/307	0.52	0/417
2	J	0.25	0/307	0.49	0/417
2	N	0.24	0/307	0.48	0/417
2	P	0.27	0/307	0.51	0/417
2	R	0.25	0/307	0.50	0/417
2	T	0.26	0/307	0.54	0/417
2	V	0.28	0/307	0.51	0/417
3	C	0.27	0/2469	0.46	0/3371
4	L	0.29	0/2459	0.48	0/3356

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.26	0/2597	0.46	0/3566
6	X	0.27	0/211	0.36	0/285
7	Y	0.30	0/268	0.46	0/370
8	Z	0.25	0/374	0.45	0/513
All	All	0.27	0/19328	0.46	0/26491

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	407	0	407	9	0
1	2	407	0	407	14	0
1	4	407	0	407	11	0
1	6	407	0	407	12	0
1	8	407	0	407	5	0
1	B	407	0	407	11	0
1	E	407	0	407	11	0
1	G	407	0	407	10	0
1	I	407	0	407	12	0
1	K	407	0	407	16	0
1	O	407	0	407	12	0
1	Q	407	0	407	9	0
1	S	407	0	407	11	0
1	U	407	0	407	12	0
1	W	407	0	407	16	0
2	1	300	0	316	5	0
2	3	300	0	316	6	0
2	5	300	0	316	8	0
2	7	300	0	316	8	0
2	9	300	0	316	9	0
2	A	300	0	316	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	300	0	316	12	0
2	F	300	0	316	7	0
2	H	300	0	316	14	0
2	J	300	0	316	14	0
2	N	300	0	316	12	0
2	P	300	0	316	11	0
2	R	300	0	316	5	0
2	T	300	0	316	17	0
2	V	300	0	316	15	0
3	C	2404	0	2360	87	0
4	L	2375	0	2337	81	0
5	M	2488	0	2373	67	0
6	X	206	0	224	17	0
7	Y	259	0	272	14	0
8	Z	362	0	366	13	0
9	0	132	0	148	8	0
9	1	66	0	74	4	0
9	2	132	0	148	6	0
9	3	66	0	74	5	0
9	4	132	0	148	14	0
9	5	66	0	74	5	0
9	6	132	0	148	12	0
9	7	66	0	74	6	0
9	8	132	0	148	8	0
9	9	66	0	74	3	0
9	A	66	0	74	6	0
9	B	132	0	148	9	0
9	D	132	0	148	12	0
9	E	66	0	74	3	0
9	F	66	0	74	4	0
9	G	132	0	148	11	0
9	H	66	0	74	2	0
9	I	132	0	148	14	0
9	J	66	0	74	3	0
9	K	132	0	148	15	0
9	L	132	0	148	14	0
9	M	66	0	74	8	0
9	N	66	0	74	3	0
9	O	132	0	148	11	0
9	P	66	0	74	3	0
9	Q	132	0	148	9	0
9	R	66	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	S	132	0	148	8	0
9	T	66	0	74	3	0
9	U	132	0	148	9	0
9	V	66	0	74	7	0
9	W	66	0	74	4	0
9	X	66	0	74	12	0
10	0	41	0	0	0	0
10	2	41	0	0	1	0
10	3	41	0	0	3	0
10	4	41	0	0	1	0
10	5	82	0	0	1	0
10	6	41	0	0	0	0
10	8	41	0	0	0	0
10	9	41	0	0	2	0
10	A	41	0	0	0	0
10	B	41	0	0	0	0
10	C	82	0	0	6	0
10	E	82	0	0	9	0
10	G	41	0	0	3	0
10	H	41	0	0	0	0
10	I	82	0	0	6	0
10	J	41	0	0	1	0
10	K	41	0	0	1	0
10	O	41	0	0	2	0
10	P	82	0	0	5	0
10	Q	41	0	0	2	0
10	R	41	0	0	1	0
10	S	41	0	0	1	0
10	T	41	0	0	1	0
10	U	41	0	0	1	0
10	W	41	0	0	0	0
11	C	172	0	120	15	0
12	L	130	0	148	15	0
12	M	65	0	74	5	0
13	L	68	0	0	2	0
13	M	92	0	0	2	0
14	L	77	0	95	2	0
14	P	35	0	40	0	0
15	M	1	0	0	0	0
All	All	23737	0	22806	715	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 (715) 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)
3:C:286:MET:HE3	11:C:403:HEM:HMD2	1.34	1.08
3:C:145:MET:HE3	3:C:145:MET:HA	1.36	1.06
1:Q:39:ILE:HD11	9:S:102:BCL:H122	1.43	0.98
3:C:175:HIS:HA	3:C:182:LEU:HD11	1.45	0.96
1:U:7:ASN:HA	1:U:20:ASN:HB2	1.50	0.90
4:L:248:VAL:HG21	5:M:338:LEU:HD12	1.53	0.90
1:W:7:ASN:HA	1:W:20:ASN:HB2	1.57	0.86
3:C:185:TYR:HA	3:C:189:ILE:HD11	1.55	0.86
3:C:286:MET:HE3	11:C:403:HEM:CMD	2.06	0.85
4:L:8:LEU:HB3	8:Z:50:LEU:HD11	1.59	0.84
5:M:538:LEU:HD11	5:M:588:ILE:HD11	1.60	0.84
2:F:4:ARG:HG3	1:G:17:LEU:HD23	1.59	0.83
2:F:37:ASN:HA	2:F:41:ALA:HA	1.60	0.83
3:C:286:MET:CE	11:C:403:HEM:HMD2	2.09	0.83
2:N:37:ASN:HA	2:N:41:ALA:HA	1.61	0.82
3:C:106:MET:HA	3:C:110:VAL:HG22	1.62	0.81
2:D:37:ASN:HA	2:D:41:ALA:HA	1.62	0.81
5:M:378:TRP:HB3	5:M:455:ARG:HB2	1.62	0.80
4:L:211:PHE:HB2	4:L:281:CYS:HB3	1.63	0.79
3:C:145:MET:HA	3:C:145:MET:CE	2.10	0.79
2:P:37:ASN:HA	2:P:41:ALA:HA	1.62	0.79
2:H:37:ASN:HA	2:H:41:ALA:HA	1.67	0.77
10:I:104:KGD:CAG	9:K:102:BCL:H51	2.14	0.76
2:A:40:ARG:HB2	2:D:35:ALA:HB2	1.67	0.76
2:J:40:ARG:HB2	2:N:35:ALA:HB2	1.68	0.75
1:S:7:ASN:HA	1:S:20:ASN:HB2	1.66	0.75
3:C:20:PHE:HE1	10:C:406:KGD:CBA	1.99	0.75
3:C:241:THR:HG21	5:M:638:TYR:HB3	1.69	0.75
12:L:1005:BPB:H44	9:M:703:BCL:H203	1.69	0.74
10:I:104:KGD:CAG	9:K:102:BCL:H62	2.17	0.74
10:9:101:KGD:CAE	9:B:102:BCL:HBB3	2.18	0.74
2:3:37:ASN:HA	2:3:41:ALA:HA	1.69	0.73
3:C:124:ILE:HA	3:C:127:PHE:HE1	1.53	0.73
10:J:102:KGD:CAE	9:O:102:BCL:HBB3	2.19	0.73
3:C:138:LYS:HE3	11:C:403:HEM:O1A	1.88	0.73
9:6:101:BCL:H192	9:6:101:BCL:H152	1.71	0.72
2:J:37:ASN:HA	2:J:41:ALA:HA	1.70	0.72
6:X:17:THR:HA	9:X:101:BCL:H172	1.72	0.72
7:Y:5:VAL:O	7:Y:9:MET:HG2	1.90	0.71
2:A:37:ASN:HA	2:A:41:ALA:HA	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:37:ASN:HA	2:7:41:ALA:HA	1.71	0.71
4:L:305:TRP:HB3	5:M:410:ARG:HD3	1.72	0.70
2:V:37:ASN:HA	2:V:41:ALA:HA	1.72	0.70
4:L:31:ALA:HB1	8:Z:50:LEU:HD23	1.73	0.70
1:S:31:LYS:HB2	9:U:102:BCL:H42	1.73	0.69
10:I:104:KGD:CAG	9:K:102:BCL:C5	2.69	0.69
5:M:385:THR:CG2	5:M:444:PHE:O	2.40	0.69
3:C:202:GLU:HG3	3:C:203:LEU:HD23	1.75	0.68
1:S:27:ASP:O	1:S:31:LYS:HG3	1.92	0.68
9:B:101:BCL:H192	9:B:101:BCL:H152	1.76	0.68
4:L:93:VAL:HG21	2:P:31:LEU:HD23	1.75	0.68
5:M:587:ASN:HA	5:M:590:ILE:HD12	1.75	0.68
1:O:25:VAL:O	1:O:29:VAL:HG23	1.94	0.68
5:M:340:ASP:O	5:M:344:ARG:HG3	1.94	0.67
2:9:20:LEU:HD21	2:A:18:LEU:HD11	1.76	0.67
5:M:353:LYS:HA	5:M:372:PRO:HB3	1.77	0.67
9:O:101:BCL:H152	9:O:101:BCL:H192	1.76	0.67
1:2:7:ASN:HA	1:2:20:ASN:HB2	1.76	0.67
12:L:1003:BPB:HMB	12:L:1003:BPB:HBBA	1.77	0.67
9:D:102:BCL:H192	9:D:102:BCL:H152	1.76	0.67
2:H:40:ARG:HG2	2:J:35:ALA:HB2	1.75	0.67
3:C:20:PHE:CE1	10:C:406:KGD:CBA	2.78	0.67
5:M:454:ALA:O	5:M:458:THR:HG23	1.95	0.67
9:8:101:BCL:H192	9:8:101:BCL:H152	1.77	0.66
10:I:104:KGD:CAG	9:K:102:BCL:C6	2.73	0.66
1:O:31:LYS:HB2	9:Q:102:BCL:H42	1.77	0.66
1:K:31:LYS:HB2	9:O:102:BCL:H42	1.77	0.66
9:G:101:BCL:H192	9:G:101:BCL:H152	1.78	0.66
9:S:101:BCL:H192	9:S:101:BCL:H152	1.77	0.66
1:K:22:GLN:HG2	2:N:5:PRO:HG3	1.76	0.66
3:C:18:GLY:HA2	3:C:21:TYR:HD2	1.61	0.66
2:D:25:LEU:O	2:D:29:VAL:HG23	1.96	0.65
8:Z:27:LEU:O	8:Z:31:ILE:HG13	1.96	0.65
5:M:424:TYR:HE1	5:M:430:VAL:HG12	1.60	0.65
9:J:101:BCL:HBB2	10:P:101:KGD:CBC	2.27	0.65
4:L:76:SER:O	4:L:80:ILE:HG13	1.96	0.65
4:L:211:PHE:HB2	4:L:281:CYS:CB	2.26	0.65
3:C:263:MET:HG3	11:C:405:HEM:C4A	2.32	0.65
10:C:406:KGD:CAK	7:Y:11:MET:HE2	2.27	0.65
4:L:189:ILE:HD11	9:L:1001:BCL:H141	1.78	0.65
4:L:254:LEU:HD23	12:L:1005:BPB:H15	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:103:KGD:CAF	9:G:102:BCL:H62	2.28	0.64
9:2:101:BCL:H192	9:2:101:BCL:H152	1.79	0.64
1:E:19:ASN:OD1	1:E:20:ASN:N	2.30	0.64
4:L:37:SER:O	4:L:41:GLU:HG2	1.98	0.64
9:U:101:BCL:H192	9:U:101:BCL:H152	1.80	0.64
1:O:34:TYR:O	1:O:38:ILE:HG13	1.98	0.64
9:B:101:BCL:H151	10:E:102:KGD:CBJ	2.28	0.64
9:H:102:BCL:HMB1	9:H:102:BCL:HBB3	1.79	0.64
9:R:101:BCL:H13	10:R:102:KGD:CAF	2.28	0.64
9:G:101:BCL:H162	10:I:103:KGD:CBN	2.28	0.63
1:W:50:TRP:NE1	6:X:1:MET:HB2	2.13	0.63
9:1:101:BCL:HMB1	9:1:101:BCL:HBB3	1.81	0.63
1:B:39:ILE:HD11	9:E:101:BCL:H122	1.80	0.63
5:M:411:GLU:O	5:M:415:LEU:HG	1.98	0.63
2:R:13:VAL:HG22	9:R:101:BCL:H193	1.81	0.63
1:4:7:ASN:N	1:4:7:ASN:HD22	1.97	0.63
1:8:37:LEU:O	1:8:41:VAL:HG23	1.99	0.63
9:4:101:BCL:H192	9:4:101:BCL:H152	1.81	0.62
1:I:19:ASN:OD1	1:I:20:ASN:N	2.32	0.62
9:O:101:BCL:H192	9:O:101:BCL:H152	1.81	0.62
12:L:1005:BPB:HBBB	12:L:1005:BPB:HHC	1.80	0.62
1:E:39:ILE:HD11	9:G:102:BCL:H122	1.81	0.62
5:M:480:TYR:HB2	9:M:703:BCL:H62	1.81	0.62
4:L:99:ASN:ND2	14:L:1006:PGV:O02	2.33	0.62
1:I:25:VAL:O	1:I:29:VAL:HG23	1.99	0.61
9:T:101:BCL:HBB3	9:T:101:BCL:HMB1	1.82	0.61
2:7:38:TRP:CZ2	9:7:101:BCL:HHC	2.34	0.61
2:T:9:ARG:HD3	2:V:5:PRO:O	2.00	0.61
2:1:26:ILE:O	2:1:30:VAL:HG23	2.00	0.61
3:C:56:ASN:ND2	3:C:62:TYR:O	2.31	0.61
6:X:13:LEU:HD12	9:X:101:BCL:H151	1.82	0.61
10:E:103:KGD:CAU	9:G:102:BCL:H162	2.30	0.61
1:4:34:TYR:O	1:4:38:ILE:HG12	2.00	0.61
3:C:67:THR:HG23	3:C:70:ILE:HD12	1.81	0.61
11:C:402:HEM:HBB2	11:C:402:HEM:HMB2	1.82	0.61
4:L:59:PRO:HB3	2:T:10:THR:HG23	1.82	0.61
9:R:101:BCL:HMB1	9:R:101:BCL:HBB3	1.83	0.61
4:L:110:VAL:HG13	4:L:180:ALA:HB1	1.83	0.61
5:M:385:THR:HG22	5:M:444:PHE:O	2.00	0.61
2:R:37:ASN:HA	2:R:41:ALA:HA	1.83	0.61
9:S:101:BCL:HMB1	9:S:101:BCL:HBB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ILE:O	3:C:46:ILE:HG12	2.00	0.60
4:L:100:ILE:HA	4:L:103:MET:CE	2.31	0.60
9:8:101:BCL:HMB1	9:8:101:BCL:HBB2	1.83	0.60
2:3:8:PHE:HD1	9:4:102:BCL:HBB2	1.65	0.60
2:T:37:ASN:HA	2:T:41:ALA:HA	1.83	0.60
9:D:102:BCL:HMB1	9:D:102:BCL:HBB2	1.83	0.60
2:V:38:TRP:HE1	6:X:6:MET:HG3	1.65	0.60
9:4:101:BCL:HMB1	9:4:101:BCL:HBB2	1.84	0.60
2:J:8:PHE:O	2:J:12:VAL:HG23	2.01	0.60
3:C:145:MET:HE1	3:C:148:MET:CE	2.31	0.60
9:2:101:BCL:HMB1	9:2:101:BCL:HBB2	1.83	0.59
9:B:101:BCL:HMB1	9:B:101:BCL:HBB2	1.83	0.59
1:Q:7:ASN:HA	1:Q:20:ASN:HB2	1.83	0.59
2:V:27:HIS:O	2:V:31:LEU:HD23	2.02	0.59
10:2:103:KGD:CAG	9:4:102:BCL:H62	2.31	0.59
1:6:12:ASP:HA	1:6:15:LYS:HE2	1.82	0.59
3:C:201:LEU:HA	3:C:205:TYR:OH	2.03	0.59
4:L:241:ILE:HG22	4:L:243:ASP:H	1.66	0.59
3:C:145:MET:CE	3:C:148:MET:CE	2.80	0.59
4:L:51:ALA:HB3	4:L:58:ASP:OD1	2.02	0.59
3:C:204:ASP:OD1	3:C:206:PRO:HD2	2.02	0.59
10:K:103:KGD:CAU	9:O:102:BCL:H162	2.33	0.59
9:5:101:BCL:HMB1	9:5:101:BCL:HBB3	1.83	0.59
9:6:101:BCL:HMB1	9:6:101:BCL:HBB2	1.83	0.59
9:A:101:BCL:HMB1	9:A:101:BCL:HBB3	1.83	0.59
1:Q:11:PRO:O	1:Q:15:LYS:HG3	2.03	0.59
9:O:101:BCL:HMB1	9:O:101:BCL:HBB2	1.84	0.59
9:9:102:BCL:HMB1	9:9:102:BCL:HBB3	1.84	0.59
2:J:32:SER:HB3	8:Z:20:TYR:HE2	1.66	0.59
4:L:267:ALA:HB1	5:M:539:LEU:HG	1.84	0.59
9:L:1001:BCL:HMB1	9:L:1001:BCL:HBB2	1.85	0.59
10:C:406:KGD:CAK	7:Y:11:MET:CE	2.81	0.58
2:5:37:ASN:HA	2:5:41:ALA:HA	1.85	0.58
9:P:102:BCL:HMB1	9:P:102:BCL:HBB3	1.84	0.58
9:U:101:BCL:HBB2	9:U:101:BCL:HMB1	1.85	0.58
8:Z:25:VAL:HB	8:Z:26:PRO:HD3	1.84	0.58
2:J:32:SER:HB3	8:Z:20:TYR:CE2	2.37	0.58
5:M:353:LYS:HB2	5:M:354:PRO:HD3	1.86	0.58
6:X:17:THR:HB	9:X:101:BCL:H162	1.85	0.58
9:O:101:BCL:HBB2	9:O:101:BCL:HMB1	1.85	0.58
2:1:24:LEU:HD12	10:3:102:KGD:CAZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:248:VAL:CG2	5:M:338:LEU:HD12	2.32	0.58
1:Q:27:ASP:OD1	1:Q:31:LYS:HE2	2.03	0.58
9:Q:101:BCL:H192	9:Q:101:BCL:H152	1.84	0.58
3:C:141:THR:O	3:C:145:MET:HG2	2.04	0.58
3:C:254:ILE:HG22	3:C:256:GLN:OE1	2.04	0.58
9:I:101:BCL:HMB1	9:I:101:BCL:HBB2	1.86	0.58
2:9:37:ASN:HA	2:9:41:ALA:HA	1.86	0.58
3:C:124:ILE:HA	3:C:127:PHE:CE1	2.36	0.58
2:T:20:LEU:HD21	2:V:18:LEU:HD11	1.85	0.58
9:3:101:BCL:HMB1	9:3:101:BCL:HBB3	1.86	0.57
2:P:18:LEU:O	2:P:22:MET:HG2	2.04	0.57
9:7:101:BCL:HBB3	9:7:101:BCL:HMB1	1.84	0.57
9:B:102:BCL:HHC	9:B:102:BCL:HBB2	1.85	0.57
3:C:18:GLY:HA2	3:C:21:TYR:CD2	2.39	0.57
9:K:102:BCL:HHC	9:K:102:BCL:HBB2	1.86	0.57
2:J:17:LEU:O	2:J:21:VAL:HG23	2.04	0.57
4:L:104:ARG:HG3	4:L:191:HIS:CD2	2.40	0.57
4:L:189:ILE:O	4:L:190:THR:OG1	2.21	0.57
2:N:40:ARG:HB2	2:P:35:ALA:HB2	1.87	0.57
9:G:101:BCL:HMB1	9:G:101:BCL:HBB2	1.87	0.57
4:L:254:LEU:CD2	12:L:1005:BPB:H15	2.34	0.57
9:L:1001:BCL:HBC1	9:L:1002:BCL:HAA1	1.85	0.57
9:K:101:BCL:H192	9:K:101:BCL:H152	1.86	0.57
4:L:100:ILE:HA	4:L:103:MET:HE2	1.86	0.57
1:B:26:HIS:O	1:B:30:VAL:HG23	2.04	0.57
3:C:85:ASN:O	3:C:85:ASN:ND2	2.38	0.57
9:J:101:BCL:HBB3	9:J:101:BCL:HMB1	1.87	0.57
5:M:525:HIS:CE1	5:M:529:ILE:HD11	2.40	0.57
1:E:25:VAL:O	1:E:29:VAL:HG23	2.04	0.56
2:N:27:HIS:CE1	9:O:101:BCL:HMD1	2.40	0.56
2:V:13:VAL:HG22	9:V:101:BCL:H193	1.87	0.56
3:C:38:ILE:HB	10:C:401:KGD:CAZ	2.34	0.56
9:G:102:BCL:HHC	9:G:102:BCL:HBB2	1.87	0.56
5:M:565:GLY:O	5:M:569:GLN:HG3	2.06	0.56
2:T:22:MET:O	2:T:26:ILE:HG13	2.05	0.56
14:L:1007:PGV:C12	12:M:704:BPB:HED	2.36	0.56
2:5:9:ARG:HD3	2:7:5:PRO:O	2.05	0.56
3:C:145:MET:HE1	3:C:148:MET:HE1	1.88	0.56
10:G:103:KGD:CAF	9:I:102:BCL:H51	2.35	0.56
4:L:50:LEU:HB2	4:L:145:ASP:OD1	2.06	0.56
5:M:347:LEU:HD23	5:M:348:GLU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:101:BCL:HMB1	9:F:101:BCL:HBB3	1.87	0.56
1:I:9:LEU:HB2	1:I:20:ASN:OD1	2.05	0.56
1:K:11:PRO:O	1:K:15:LYS:HG3	2.06	0.56
1:4:7:ASN:N	1:4:7:ASN:ND2	2.52	0.56
1:U:7:ASN:HA	1:U:20:ASN:CB	2.30	0.56
2:9:40:ARG:HB2	2:A:35:ALA:HB2	1.88	0.55
1:G:31:LYS:HB2	9:I:102:BCL:H42	1.87	0.55
4:L:49:THR:HG21	4:L:68:TYR:OH	2.07	0.55
5:M:531:PHE:HB3	5:M:599:THR:OG1	2.06	0.55
8:Z:26:PRO:O	8:Z:30:VAL:HG23	2.06	0.55
2:A:13:VAL:HG22	9:A:101:BCL:H193	1.88	0.55
4:L:233:VAL:HG11	5:M:589:HIS:CE1	2.41	0.55
2:J:40:ARG:HB2	2:N:35:ALA:CB	2.35	0.55
9:O:101:BCL:H202	10:O:103:KGD:CAK	2.37	0.55
2:5:10:THR:O	2:5:14:VAL:HG23	2.05	0.55
1:E:28:ILE:HG21	10:E:102:KGD:CAF	2.36	0.55
1:G:25:VAL:O	1:G:29:VAL:HG23	2.06	0.55
1:0:9:LEU:HD12	1:0:20:ASN:OD1	2.06	0.55
9:Q:102:BCL:HBB2	9:Q:102:BCL:HHC	1.89	0.55
1:K:7:ASN:HA	1:K:20:ASN:HB2	1.89	0.55
1:6:9:LEU:HD12	1:6:20:ASN:OD1	2.07	0.55
4:L:155:GLU:HA	4:L:158:ILE:HD12	1.88	0.55
9:O:102:BCL:HHC	9:O:102:BCL:HBB2	1.88	0.55
9:S:102:BCL:HHC	9:S:102:BCL:HBB2	1.89	0.55
3:C:97:MET:HB3	3:C:102:ILE:HG13	1.89	0.55
4:L:205:ASN:HB2	4:L:293:ASN:HD21	1.72	0.54
2:H:4:ARG:NH1	2:H:7:GLU:OE1	2.40	0.54
5:M:524:PHE:CE2	8:Z:22:LEU:HD11	2.42	0.54
1:S:34:TYR:OH	9:S:102:BCL:OBD	2.23	0.54
9:Q:101:BCL:HMB1	9:Q:101:BCL:HBB2	1.88	0.54
1:S:41:VAL:O	1:S:45:VAL:HG23	2.07	0.54
1:S:35:GLY:O	1:S:38:ILE:HG22	2.08	0.54
9:0:102:BCL:HHC	9:0:102:BCL:HBB2	1.88	0.54
1:0:26:HIS:O	1:0:30:VAL:HG23	2.07	0.54
3:C:56:ASN:HD21	3:C:63:THR:HA	1.73	0.54
1:6:11:PRO:O	1:6:15:LYS:HG3	2.08	0.54
10:S:103:KGD:CAG	9:U:102:BCL:H51	2.37	0.54
1:W:50:TRP:CD1	6:X:1:MET:HB2	2.42	0.54
3:C:166:GLY:HA3	3:C:309:PRO:HB3	1.89	0.54
1:U:26:HIS:O	1:U:30:VAL:HG23	2.08	0.54
2:J:27:HIS:CE1	9:K:101:BCL:HMD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:224:LEU:O	4:L:228:MET:HG3	2.07	0.54
4:L:192:HIS:O	4:L:196:VAL:HG23	2.08	0.54
6:X:13:LEU:CD1	9:X:101:BCL:H151	2.37	0.54
5:M:385:THR:HG21	5:M:444:PHE:O	2.07	0.53
2:5:8:PHE:O	2:5:12:VAL:HG23	2.08	0.53
1:6:38:ILE:O	1:6:41:VAL:HG12	2.08	0.53
1:K:26:HIS:O	1:K:30:VAL:HG23	2.08	0.53
4:L:34:ILE:HD11	4:L:39:ILE:HD11	1.91	0.53
4:L:59:PRO:CA	2:T:10:THR:HG23	2.39	0.53
4:L:93:VAL:HG22	2:P:32:SER:HB3	1.89	0.53
9:U:102:BCL:HHC	9:U:102:BCL:HBB2	1.90	0.53
9:Q:101:BCL:H142	10:Q:103:KGD:CAQ	2.38	0.53
2:H:31:LEU:HD13	2:H:38:TRP:CZ3	2.44	0.53
4:L:59:PRO:HA	2:T:10:THR:HG23	1.90	0.53
9:L:1001:BCL:H43	5:M:530:PHE:CE1	2.44	0.53
10:9:101:KGD:CAC	9:B:102:BCL:HBB3	2.39	0.53
4:L:31:ALA:HB1	8:Z:50:LEU:CD2	2.38	0.53
9:2:101:BCL:HMC3	3:C:42:ILE:HG23	1.91	0.53
2:H:31:LEU:HD13	2:H:38:TRP:HZ3	1.73	0.53
5:M:391:PHE:O	5:M:395:VAL:HG23	2.08	0.53
2:1:37:ASN:HA	2:1:41:ALA:HA	1.91	0.53
1:2:9:LEU:HB2	1:2:20:ASN:OD1	2.09	0.53
1:4:7:ASN:HA	1:4:20:ASN:HB2	1.90	0.53
1:8:26:HIS:O	1:8:30:VAL:HG23	2.09	0.53
1:S:47:CYS:SG	9:S:101:BCL:HBC1	2.49	0.53
1:B:11:PRO:O	1:B:15:LYS:HG3	2.08	0.52
5:M:404:ASN:HD22	5:M:407:ILE:HG13	1.74	0.52
10:4:103:KGD:CAF	9:6:102:BCL:H51	2.39	0.52
9:B:101:BCL:H162	10:E:102:KGD:CBN	2.40	0.52
2:T:31:LEU:HD13	2:T:38:TRP:CE3	2.44	0.52
1:U:7:ASN:O	1:U:10:VAL:HG22	2.10	0.52
2:V:31:LEU:HD11	2:V:38:TRP:CZ3	2.45	0.52
3:C:150:ALA:HB2	3:C:316:LEU:HD22	1.91	0.52
2:D:31:LEU:HD13	2:D:38:TRP:CE3	2.45	0.52
4:L:110:VAL:HG13	4:L:180:ALA:CB	2.39	0.52
3:C:203:LEU:O	3:C:268:LYS:HE2	2.09	0.52
2:D:27:HIS:CE1	9:D:102:BCL:HMD1	2.45	0.52
1:G:7:ASN:HA	1:G:20:ASN:HB2	1.90	0.52
4:L:226:LEU:HG	5:M:592:ALA:HB1	1.92	0.52
5:M:557:GLU:O	5:M:561:MET:HG3	2.09	0.52
2:7:31:LEU:HD13	2:7:38:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:TRP:O	3:C:198:ARG:HD2	2.08	0.52
9:L:1001:BCL:O1A	5:M:533:LEU:HD12	2.10	0.52
9:T:101:BCL:HMC3	9:X:101:BCL:HBB1	1.90	0.52
2:H:40:ARG:HG2	2:J:35:ALA:CB	2.40	0.52
4:L:39:ILE:HD13	8:Z:54:PRO:HG3	1.92	0.52
4:L:227:HIS:HD2	12:L:1005:BPB:HMDB	1.75	0.52
2:J:22:MET:HB3	9:K:101:BCL:HED1	1.91	0.52
4:L:227:HIS:NE2	5:M:472:GLY:HA3	2.25	0.52
1:E:26:HIS:O	1:E:30:VAL:HG23	2.10	0.52
9:N:101:BCL:HMB1	9:N:101:BCL:HBB3	1.90	0.52
2:T:8:PHE:O	2:T:12:VAL:HG23	2.10	0.52
2:V:26:ILE:O	2:V:30:VAL:HG23	2.09	0.52
1:E:9:LEU:HB2	1:E:20:ASN:OD1	2.09	0.51
4:L:174:ARG:HB3	4:L:175:PRO:HD3	1.91	0.51
5:M:478:SER:O	5:M:482:VAL:HG23	2.09	0.51
2:T:40:ARG:O	2:T:40:ARG:HG3	2.10	0.51
1:W:11:PRO:O	1:W:15:LYS:HG2	2.11	0.51
1:4:26:HIS:O	1:4:30:VAL:HG23	2.10	0.51
5:M:404:ASN:ND2	5:M:407:ILE:HG13	2.25	0.51
1:S:37:LEU:O	1:S:41:VAL:HG23	2.10	0.51
4:L:80:ILE:HG23	12:L:1003:BPB:H5	1.91	0.51
4:L:74:ALA:O	4:L:78:ILE:HG13	2.10	0.51
1:O:7:ASN:HA	1:O:20:ASN:HD22	1.75	0.51
2:A:38:TRP:CZ2	9:A:101:BCL:HHC	2.46	0.51
5:M:476:ALA:HB1	9:M:703:BCL:C9	2.41	0.51
1:S:31:LYS:HD3	9:U:102:BCL:H12	1.93	0.51
4:L:136:PHE:CZ	9:L:1002:BCL:H102	2.45	0.51
4:L:207:PHE:CD2	5:M:506:LEU:HB3	2.46	0.51
7:Y:11:MET:O	7:Y:15:VAL:HG23	2.10	0.51
2:7:9:ARG:HA	2:7:12:VAL:HG12	1.92	0.50
5:M:487:HIS:HB3	5:M:488:PRO:HD3	1.92	0.50
9:5:101:BCL:HMB3	9:8:101:BCL:CHB	2.40	0.50
9:6:102:BCL:HBB2	9:6:102:BCL:HHC	1.93	0.50
9:F:101:BCL:HMC3	9:I:101:BCL:HBB1	1.92	0.50
1:K:42:ILE:O	1:K:46:LEU:HD23	2.10	0.50
6:X:16:ALA:HB3	9:X:101:BCL:H141	1.92	0.50
2:T:4:ARG:HD3	2:T:6:PHE:O	2.11	0.50
2:T:12:VAL:HG11	10:T:102:KGD:CAK	2.42	0.50
2:V:38:TRP:CZ2	9:V:101:BCL:HHC	2.47	0.50
2:9:22:MET:HE3	2:9:22:MET:HA	1.92	0.50
2:5:38:TRP:CZ2	9:5:101:BCL:HHC	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:9:LEU:HD12	1:U:20:ASN:OD1	2.12	0.50
1:W:37:LEU:O	1:W:41:VAL:HG23	2.11	0.50
3:C:263:MET:HG3	11:C:405:HEM:C1B	2.47	0.50
4:L:174:ARG:O	4:L:178:MET:HG3	2.10	0.50
1:W:25:VAL:O	1:W:29:VAL:HG23	2.12	0.50
3:C:273:THR:O	3:C:277:PRO:HG3	2.11	0.50
7:Y:1:MET:O	7:Y:5:VAL:HG22	2.12	0.50
9:1:101:BCL:HBB2	10:3:102:KGD:CBD	2.41	0.50
4:L:276:LEU:HA	4:L:279:ASN:ND2	2.26	0.50
12:L:1003:BPB:H4B	12:L:1003:BPB:O1A	2.12	0.50
3:C:175:HIS:CA	3:C:182:LEU:HD11	2.31	0.50
2:D:31:LEU:HD13	2:D:38:TRP:CZ3	2.46	0.50
1:E:27:ASP:OD1	1:E:31:LYS:HE2	2.12	0.50
3:C:56:ASN:ND2	3:C:63:THR:HA	2.26	0.49
1:I:7:ASN:HA	1:I:20:ASN:HB2	1.94	0.49
2:P:27:HIS:CE1	9:Q:101:BCL:HMD1	2.47	0.49
1:6:26:HIS:O	1:6:30:VAL:HG23	2.11	0.49
1:Q:31:LYS:HE3	9:S:102:BCL:H12	1.93	0.49
1:2:26:HIS:O	1:2:30:VAL:HG23	2.12	0.49
1:4:47:CYS:SG	9:4:101:BCL:HBC1	2.52	0.49
9:A:101:BCL:HBB2	10:E:102:KGD:CBD	2.42	0.49
3:C:312:VAL:HB	3:C:313:PRO:HD2	1.94	0.49
5:M:396:ASP:O	5:M:400:GLN:HG3	2.12	0.49
9:D:101:BCL:HMC3	9:G:101:BCL:HBB1	1.93	0.49
1:K:27:ASP:OD1	1:K:31:LYS:NZ	2.43	0.49
4:L:283:PHE:CZ	7:Y:9:MET:HB2	2.47	0.49
9:4:102:BCL:HBB2	9:4:102:BCL:HHC	1.95	0.49
3:C:145:MET:HB3	11:C:403:HEM:C4B	2.48	0.49
1:K:25:VAL:O	1:K:29:VAL:HG23	2.13	0.49
4:L:251:ARG:HD3	5:M:371:GLY:HA3	1.94	0.49
1:U:19:ASN:OD1	1:U:20:ASN:N	2.42	0.49
1:W:41:VAL:O	1:W:45:VAL:HG23	2.13	0.49
1:G:27:ASP:OD1	1:G:31:LYS:HE3	2.12	0.49
1:I:26:HIS:O	1:I:30:VAL:HG23	2.12	0.49
5:M:574:PHE:O	5:M:578:VAL:HG23	2.12	0.49
2:N:8:PHE:O	2:N:12:VAL:HG23	2.13	0.49
9:D:101:BCL:HMB1	9:D:101:BCL:HBB3	1.93	0.49
1:6:27:ASP:O	1:6:31:LYS:HG3	2.13	0.49
3:C:205:TYR:CD2	3:C:264:LEU:HB3	2.48	0.49
3:C:313:PRO:HG2	3:C:316:LEU:HG	1.95	0.49
1:2:25:VAL:O	1:2:29:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:LEU:O	1:K:41:VAL:HG23	2.12	0.48
1:O:7:ASN:OD1	1:O:15:LYS:HG2	2.13	0.48
2:7:9:ARG:O	2:7:13:VAL:HG23	2.13	0.48
9:K:101:BCL:HBB2	9:K:101:BCL:HMB1	1.95	0.48
6:X:8:PHE:O	6:X:12:VAL:HG23	2.13	0.48
4:L:59:PRO:CB	2:T:10:THR:HG23	2.43	0.48
6:X:16:ALA:CB	9:X:101:BCL:H141	2.43	0.48
4:L:74:ALA:O	4:L:77:ILE:HG22	2.14	0.48
12:M:704:BPB:HMB	12:M:704:BPB:HBBA	1.95	0.48
9:1:101:BCL:HMB3	9:4:101:BCL:CHB	2.44	0.48
3:C:8:LEU:HD23	2:V:9:ARG:HG3	1.94	0.48
1:G:12:ASP:OD1	1:G:12:ASP:N	2.44	0.48
2:H:8:PHE:HA	9:I:102:BCL:CBB	2.44	0.48
1:I:34:TYR:O	1:I:38:ILE:HG12	2.12	0.48
9:M:703:BCL:CBB	9:M:703:BCL:HMB1	2.44	0.48
9:2:102:BCL:HHC	9:2:102:BCL:HBB2	1.95	0.48
9:L:1002:BCL:HMB1	9:L:1002:BCL:HBB2	1.95	0.48
1:W:39:ILE:O	1:W:42:ILE:HG22	2.14	0.48
1:8:37:LEU:HD12	9:8:101:BCL:H12	1.95	0.48
2:A:17:LEU:O	2:A:21:VAL:HG23	2.14	0.48
2:H:8:PHE:HA	9:I:102:BCL:HBB1	1.96	0.48
4:L:289:VAL:HG21	4:L:292:TRP:CZ2	2.48	0.48
9:N:101:BCL:H111	9:N:101:BCL:H152	1.61	0.47
4:L:120:GLN:HB3	4:L:121:PRO:HD2	1.97	0.47
4:L:207:PHE:CE1	9:L:1002:BCL:HMC2	2.48	0.47
3:C:64:GLN:OE1	3:C:64:GLN:N	2.40	0.47
5:M:424:TYR:CE1	5:M:430:VAL:HG12	2.47	0.47
2:J:9:ARG:O	2:J:13:VAL:HG23	2.15	0.47
9:O:101:BCL:H142	10:O:103:KGD:CAQ	2.44	0.47
1:2:37:LEU:HD22	9:2:101:BCL:H12	1.96	0.47
2:H:22:MET:O	2:H:26:ILE:HD12	2.15	0.47
1:I:37:LEU:O	1:I:41:VAL:HG23	2.15	0.47
2:J:9:ARG:HG3	2:N:6:PHE:CE1	2.50	0.47
4:L:205:ASN:HB2	4:L:293:ASN:ND2	2.29	0.47
4:L:222:SER:O	5:M:539:LEU:HD22	2.15	0.47
9:P:102:BCL:H152	9:P:102:BCL:H111	1.66	0.47
1:Q:37:LEU:O	1:Q:41:VAL:HG23	2.12	0.47
9:X:101:BCL:CBB	9:X:101:BCL:HMB1	2.44	0.47
1:2:37:LEU:O	1:2:41:VAL:HG23	2.14	0.47
10:G:103:KGD:CAF	9:I:102:BCL:H62	2.45	0.47
1:K:9:LEU:HD13	1:K:20:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:102:BCL:H13	10:P:103:KGD:CAG	2.44	0.47
10:U:103:KGD:CAF	9:W:101:BCL:H51	2.45	0.47
6:X:11:ILE:O	6:X:15:VAL:HG12	2.14	0.47
1:2:27:ASP:OD1	1:2:31:LYS:HE2	2.15	0.47
2:5:25:LEU:O	2:5:29:VAL:HG23	2.15	0.47
1:6:25:VAL:O	1:6:29:VAL:HG23	2.14	0.47
1:U:25:VAL:O	1:U:29:VAL:HG23	2.14	0.47
1:K:38:ILE:O	1:K:42:ILE:HG12	2.15	0.47
9:K:101:BCL:HMB1	9:K:101:BCL:CBB	2.45	0.47
5:M:503:ARG:O	5:M:503:ARG:HG2	2.15	0.47
2:7:25:LEU:O	2:7:29:VAL:HG23	2.15	0.46
3:C:50:PRO:O	3:C:52:PRO:HD3	2.15	0.46
9:G:101:BCL:H61	9:G:101:BCL:H41	1.80	0.46
4:L:185:PHE:HB3	4:L:195:TRP:CE3	2.50	0.46
2:P:12:VAL:O	2:P:16:THR:HG23	2.15	0.46
1:W:19:ASN:OD1	1:W:20:ASN:N	2.46	0.46
4:L:253:ILE:HG22	4:L:254:LEU:HG	1.98	0.46
9:T:101:BCL:H111	9:T:101:BCL:H152	1.56	0.46
9:3:101:BCL:H111	9:3:101:BCL:H152	1.59	0.46
1:E:42:ILE:O	1:E:45:VAL:HG12	2.15	0.46
2:F:38:TRP:NE1	2:F:39:LEU:HG	2.31	0.46
3:C:202:GLU:HG3	3:C:203:LEU:CD2	2.43	0.46
1:U:7:ASN:CA	1:U:20:ASN:HB2	2.36	0.46
3:C:145:MET:HE2	3:C:148:MET:HE2	1.97	0.46
4:L:172:TRP:O	4:L:176:ILE:HG13	2.15	0.46
9:L:1002:BCL:HAA2	9:L:1002:BCL:HBD	1.97	0.46
1:O:27:ASP:O	1:O:31:LYS:HG3	2.15	0.46
3:C:263:MET:HG3	11:C:405:HEM:CHB	2.45	0.46
9:I:101:BCL:H192	9:I:101:BCL:H152	1.98	0.46
4:L:160:PHE:HA	4:L:163:VAL:HG12	1.98	0.46
2:T:9:ARG:O	2:T:13:VAL:HG23	2.16	0.46
1:6:31:LYS:HB2	9:8:102:BCL:H42	1.97	0.46
9:8:102:BCL:CBB	9:8:102:BCL:HHC	2.45	0.46
3:C:42:ILE:HA	3:C:45:THR:HG22	1.98	0.46
3:C:98:THR:HB	3:C:101:GLN:OE1	2.16	0.46
5:M:353:LYS:O	5:M:355:PRO:HD3	2.16	0.46
1:O:9:LEU:H	1:O:20:ASN:HD21	1.64	0.46
8:Z:28:ALA:O	8:Z:32:LEU:HD23	2.16	0.46
2:5:24:LEU:HD23	10:5:103:KGD:CAZ	2.46	0.46
2:D:38:TRP:CZ2	9:D:101:BCL:HHC	2.51	0.46
9:E:101:BCL:CBB	9:E:101:BCL:HHC	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1005:BPB:HBBA	12:M:704:BPB:H1A	1.98	0.46
9:G:101:BCL:H151	10:I:103:KGD:CBJ	2.46	0.46
9:H:102:BCL:H111	9:H:102:BCL:H152	1.79	0.46
1:U:8:ASP:OD1	1:U:9:LEU:HG	2.16	0.46
1:W:24:LEU:O	1:W:28:ILE:HG12	2.16	0.46
1:6:41:VAL:O	1:6:45:VAL:HG23	2.16	0.46
1:G:9:LEU:HB2	1:G:20:ASN:OD1	2.16	0.46
4:L:254:LEU:HD21	12:L:1005:BPB:HEDB	1.98	0.46
9:V:101:BCL:H101	9:X:101:BCL:H191	1.96	0.46
3:C:186:PRO:HD2	3:C:189:ILE:HG12	1.98	0.45
4:L:258:ILE:HG22	13:L:1004:MQE:CBQ	2.45	0.45
6:X:7:ALA:O	6:X:11:ILE:HG13	2.16	0.45
2:9:40:ARG:HB2	2:A:35:ALA:CB	2.45	0.45
3:C:145:MET:CE	3:C:148:MET:HE2	2.46	0.45
4:L:99:ASN:OD1	4:L:102:ALA:HB3	2.16	0.45
5:M:363:ARG:HH21	7:Y:32:PRO:HD2	1.80	0.45
1:O:25:VAL:O	1:O:29:VAL:HG23	2.16	0.45
9:0:101:BCL:H71	9:0:101:BCL:H112	1.75	0.45
3:C:185:TYR:OH	3:C:199:LEU:HB2	2.16	0.45
11:C:404:HEM:HBD1	11:C:404:HEM:HHA	1.98	0.45
2:D:22:MET:HB3	9:D:102:BCL:HED1	1.97	0.45
1:G:11:PRO:O	1:G:15:LYS:HG3	2.16	0.45
1:Q:8:ASP:OD1	1:Q:9:LEU:HD12	2.15	0.45
2:F:38:TRP:CD1	2:F:39:LEU:HG	2.51	0.45
1:I:7:ASN:O	1:I:15:LYS:HE3	2.16	0.45
1:8:25:VAL:O	1:8:29:VAL:HG23	2.16	0.45
3:C:111:SER:O	3:C:115:LYS:N	2.45	0.45
9:I:101:BCL:H61	9:I:101:BCL:H41	1.81	0.45
5:M:520:TYR:CZ	9:M:703:BCL:HMC2	2.52	0.45
9:R:101:BCL:H111	9:R:101:BCL:H152	1.71	0.45
4:L:189:ILE:HD11	9:L:1001:BCL:C14	2.46	0.45
12:L:1005:BPB:HBCA	12:L:1005:BPB:H43	1.76	0.45
2:P:9:ARG:HD3	2:R:5:PRO:O	2.16	0.45
4:L:100:ILE:HG22	4:L:103:MET:HE3	1.99	0.45
9:W:101:BCL:H62	9:W:101:BCL:H41	1.85	0.45
2:9:9:ARG:O	2:9:13:VAL:HG23	2.17	0.45
1:B:12:ASP:HA	1:B:15:LYS:HE2	1.99	0.45
9:K:101:BCL:H151	10:P:101:KGD:CBJ	2.47	0.45
9:2:101:BCL:H61	9:2:101:BCL:H41	1.85	0.45
2:9:20:LEU:HD21	2:A:18:LEU:CD1	2.44	0.45
4:L:88:LEU:HD13	13:M:701:MQE:CCN	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ASP:OD2	1:O:31:LYS:HE3	2.17	0.45
1:Q:12:ASP:OD1	1:Q:13:GLN:N	2.49	0.45
9:F:101:BCL:H152	9:F:101:BCL:H111	1.67	0.45
1:K:41:VAL:O	1:K:45:VAL:HG23	2.17	0.45
1:O:14:TRP:HE3	1:O:17:LEU:HD12	1.82	0.45
2:1:38:TRP:CZ2	9:1:101:BCL:HHC	2.51	0.44
10:3:102:KGD:CAE	9:6:102:BCL:HBB3	2.47	0.44
3:C:8:LEU:CD1	1:W:25:VAL:HG21	2.47	0.44
3:C:26:ILE:O	3:C:30:VAL:HG23	2.16	0.44
2:V:4:ARG:NH1	1:W:17:LEU:O	2.50	0.44
3:C:45:THR:HG23	3:C:46:ILE:HG23	1.98	0.44
1:G:27:ASP:O	1:G:30:VAL:HG12	2.17	0.44
9:M:703:BCL:H61	9:M:703:BCL:H41	1.75	0.44
9:L:1001:BCL:HED2	5:M:526:MET:SD	2.56	0.44
9:L:1002:BCL:HMB1	9:L:1002:BCL:CBB	2.47	0.44
1:U:37:LEU:O	1:U:41:VAL:HG23	2.17	0.44
6:X:14:ILE:O	6:X:18:LEU:HG	2.18	0.44
1:I:47:CYS:SG	9:I:101:BCL:HBC1	2.57	0.44
5:M:523:PRO:HA	5:M:526:MET:CE	2.48	0.44
9:A:101:BCL:CHB	10:E:102:KGD:CAS	2.95	0.44
7:Y:18:LEU:HB3	7:Y:19:PRO:HD3	2.00	0.44
1:B:27:ASP:O	1:B:31:LYS:HG3	2.17	0.44
9:D:102:BCL:C4	1:E:36:GLY:HA3	2.47	0.44
1:2:31:LYS:HD2	9:4:102:BCL:H12	1.98	0.44
2:3:25:LEU:O	2:3:29:VAL:HG23	2.18	0.44
1:4:33:ILE:O	1:4:37:LEU:HG	2.16	0.44
1:K:22:GLN:CG	2:N:5:PRO:HG3	2.46	0.44
9:O:101:BCL:H61	9:O:101:BCL:H41	1.81	0.44
2:V:31:LEU:HD21	2:V:38:TRP:HZ3	1.82	0.44
9:4:102:BCL:HHC	9:4:102:BCL:CBB	2.48	0.44
9:7:101:BCL:H62	9:7:101:BCL:H2	1.85	0.44
2:F:9:ARG:O	2:F:13:VAL:HG23	2.18	0.44
9:N:101:BCL:HMB1	9:N:101:BCL:CBB	2.47	0.44
9:V:101:BCL:HBB3	9:V:101:BCL:HMB1	2.00	0.44
9:6:101:BCL:H61	9:6:101:BCL:H41	1.84	0.44
3:C:241:THR:HG22	3:C:241:THR:O	2.18	0.44
2:H:17:LEU:O	2:H:21:VAL:HG23	2.18	0.44
2:P:26:ILE:O	2:P:30:VAL:HG23	2.18	0.44
2:T:31:LEU:HD13	2:T:38:TRP:CZ3	2.53	0.44
2:V:8:PHE:O	2:V:12:VAL:HG23	2.18	0.44
2:J:4:ARG:HG3	1:K:17:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:17:LEU:O	2:P:21:VAL:HG23	2.17	0.43
9:7:101:BCL:H111	9:7:101:BCL:H152	1.52	0.43
3:C:65:GLU:HB3	3:C:66:PRO:HD3	2.00	0.43
3:C:154:GLN:OE1	3:C:320:PRO:HG3	2.18	0.43
2:H:9:ARG:O	2:H:13:VAL:HG23	2.18	0.43
12:L:1005:BPB:H4	12:L:1005:BPB:H6	1.82	0.43
5:M:364:LEU:HD13	7:Y:28:TRP:HE3	1.83	0.43
1:O:37:LEU:O	1:O:41:VAL:HG23	2.17	0.43
9:B:101:BCL:H151	10:E:102:KGD:CBH	2.48	0.43
3:C:8:LEU:HD13	1:W:25:VAL:HG11	2.00	0.43
3:C:11:GLU:OE2	3:C:11:GLU:N	2.28	0.43
4:L:82:LEU:HD23	4:L:82:LEU:HA	1.86	0.43
12:L:1003:BPB:H44	12:L:1003:BPB:HBA	1.84	0.43
1:O:37:LEU:O	1:O:41:VAL:HG23	2.18	0.43
3:C:8:LEU:HD12	1:W:25:VAL:HG21	2.00	0.43
9:W:101:BCL:HBB2	9:W:101:BCL:HHC	1.99	0.43
9:F:101:BCL:HMB1	9:F:101:BCL:CBB	2.48	0.43
2:T:4:ARG:HH22	1:U:22:GLN:HE22	1.65	0.43
2:3:24:LEU:HD23	2:3:24:LEU:HA	1.89	0.43
1:O:12:ASP:HA	1:O:15:LYS:HD2	2.00	0.43
1:O:14:TRP:CE3	1:O:17:LEU:HD12	2.54	0.43
1:4:12:ASP:O	1:4:15:LYS:HG3	2.19	0.43
1:B:7:ASN:HA	1:B:20:ASN:HB2	2.01	0.43
3:C:58:ILE:HG13	3:C:59:TYR:CD2	2.53	0.43
9:K:101:BCL:H18	10:P:101:KGD:CBL	2.49	0.43
4:L:80:ILE:HD13	12:L:1003:BPB:H4A	1.99	0.43
5:M:396:ASP:OD2	5:M:417:VAL:HG12	2.19	0.43
1:U:7:ASN:OD1	1:U:15:LYS:HE2	2.18	0.43
1:2:53:TRP:CD1	1:2:54:ILE:HG13	2.54	0.43
2:7:31:LEU:HD13	2:7:38:TRP:CE3	2.54	0.43
11:C:402:HEM:HBB2	11:C:402:HEM:CMB	2.48	0.43
9:L:1002:BCL:H61	9:L:1002:BCL:H41	1.73	0.43
5:M:382:SER:HB3	5:M:451:THR:OG1	2.18	0.43
5:M:521:TYR:CE1	5:M:627:VAL:HG22	2.53	0.43
2:1:25:LEU:O	2:1:29:VAL:HG23	2.19	0.43
1:6:47:CYS:SG	9:6:101:BCL:HBC1	2.59	0.43
2:D:8:PHE:O	2:D:12:VAL:HG23	2.18	0.43
9:D:101:BCL:H152	9:D:101:BCL:H111	1.61	0.43
4:L:177:ALA:HB2	7:Y:9:MET:HG3	2.01	0.43
1:Q:17:LEU:HD13	9:Q:102:BCL:CMB	2.48	0.43
1:S:35:GLY:O	1:S:39:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:101:BCL:H62	9:3:101:BCL:H2	1.89	0.43
9:8:101:BCL:H61	9:8:101:BCL:H41	1.81	0.43
3:C:67:THR:CG2	3:C:70:ILE:HD12	2.47	0.43
2:H:10:THR:O	2:H:14:VAL:HG23	2.19	0.43
4:L:305:TRP:CB	5:M:410:ARG:HD3	2.46	0.43
3:C:155:ASN:O	3:C:159:LYS:HD2	2.19	0.42
1:E:48:TRP:CH2	1:E:52:PRO:HB3	2.53	0.42
4:L:311:GLY:O	4:L:314:VAL:HG12	2.18	0.42
5:M:505:ILE:HD12	12:M:704:BPB:ND	2.33	0.42
9:Q:101:BCL:HMB1	9:Q:101:BCL:CBB	2.47	0.42
2:9:32:SER:OG	5:M:399:ARG:HG3	2.19	0.42
3:C:19:ARG:HD3	6:X:25:MET:HE3	2.01	0.42
1:E:37:LEU:O	1:E:41:VAL:HG23	2.19	0.42
10:G:103:KGD:CAF	9:I:102:BCL:C5	2.96	0.42
9:6:102:BCL:H62	9:6:102:BCL:H41	1.80	0.42
9:D:102:BCL:H202	10:E:103:KGD:CAK	2.49	0.42
9:G:101:BCL:HMB1	9:G:101:BCL:CBB	2.48	0.42
1:K:47:CYS:HB3	9:K:101:BCL:HBC1	2.00	0.42
9:0:101:BCL:HBB1	9:7:101:BCL:HMC3	2.00	0.42
9:A:101:BCL:H111	9:A:101:BCL:H152	1.70	0.42
3:C:58:ILE:HA	3:C:311:GLN:HG3	2.01	0.42
9:D:101:BCL:H18	9:D:101:BCL:H151	1.89	0.42
2:H:7:GLU:OE1	2:H:7:GLU:HA	2.19	0.42
5:M:508:TRP:O	5:M:512:VAL:HG23	2.19	0.42
2:3:27:HIS:CE1	9:4:101:BCL:HMD1	2.54	0.42
9:V:101:BCL:H111	9:V:101:BCL:H152	1.59	0.42
9:V:101:BCL:H61	9:X:101:BCL:H101	2.02	0.42
2:R:8:PHE:O	2:R:12:VAL:HG23	2.19	0.42
2:V:38:TRP:HE1	6:X:6:MET:CG	2.29	0.42
9:X:101:BCL:H152	9:X:101:BCL:H18	1.84	0.42
9:3:101:BCL:HMB1	9:3:101:BCL:CBB	2.49	0.42
2:5:19:GLY:HA3	9:5:101:BCL:H42	2.02	0.42
1:B:42:ILE:O	1:B:45:VAL:HG12	2.20	0.42
3:C:82:ILE:HD11	3:C:103:SER:HB3	2.02	0.42
3:C:263:MET:HE1	11:C:405:HEM:C4D	2.55	0.42
9:D:102:BCL:H112	9:D:102:BCL:H71	1.70	0.42
9:J:101:BCL:HMB1	9:J:101:BCL:CBB	2.49	0.42
4:L:34:ILE:CD1	4:L:39:ILE:HD11	2.49	0.42
2:3:17:LEU:O	2:3:21:VAL:HG23	2.19	0.42
1:6:7:ASN:HA	1:6:20:ASN:HB2	2.02	0.42
2:D:39:LEU:HD23	2:D:39:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:102:BCL:CBB	9:I:102:BCL:HHC	2.50	0.42
2:N:25:LEU:O	2:N:29:VAL:HG23	2.19	0.42
1:S:19:ASN:OD1	1:S:20:ASN:N	2.47	0.42
9:V:101:BCL:HMD1	1:W:44:HIS:CE1	2.55	0.42
1:4:37:LEU:O	1:4:41:VAL:HG23	2.19	0.42
3:C:78:MET:O	3:C:82:ILE:HG12	2.20	0.42
2:F:25:LEU:O	2:F:29:VAL:HG23	2.20	0.42
4:L:74:ALA:HA	4:L:77:ILE:HG22	2.01	0.42
1:2:7:ASN:HA	1:2:20:ASN:CB	2.46	0.42
9:9:102:BCL:H62	9:9:102:BCL:H2	1.89	0.42
3:C:201:LEU:HD13	3:C:271:GLN:HB2	2.02	0.42
2:F:10:THR:O	2:F:14:VAL:HG23	2.20	0.42
4:L:197:SER:HA	9:L:1002:BCL:HBC1	2.01	0.42
2:T:15:SER:OG	9:U:102:BCL:HBC2	2.20	0.42
1:B:25:VAL:O	1:B:29:VAL:HG23	2.20	0.41
2:P:9:ARG:O	2:P:13:VAL:HG23	2.19	0.41
8:Z:21:ALA:HA	8:Z:25:VAL:HG23	2.01	0.41
1:O:7:ASN:CA	1:O:20:ASN:HD22	2.32	0.41
1:W:33:ILE:O	1:W:37:LEU:HG	2.20	0.41
9:4:101:BCL:HMB1	9:4:101:BCL:CBB	2.50	0.41
3:C:60:VAL:HG23	3:C:306:ALA:O	2.20	0.41
3:C:61:ASN:HB3	3:C:304:PRO:HB3	2.01	0.41
2:H:39:LEU:HD23	2:H:39:LEU:HA	1.83	0.41
4:L:39:ILE:HD12	5:M:569:GLN:OE1	2.20	0.41
5:M:417:VAL:HG23	5:M:417:VAL:O	2.21	0.41
7:Y:31:ASN:HB3	7:Y:32:PRO:HD3	2.03	0.41
9:5:101:BCL:CHD	9:6:101:BCL:HMD2	2.51	0.41
3:C:97:MET:SD	3:C:313:PRO:HB3	2.61	0.41
5:M:347:LEU:HD23	5:M:348:GLU:H	1.85	0.41
9:U:102:BCL:HHC	9:U:102:BCL:CBB	2.50	0.41
9:0:101:BCL:HMB1	9:0:101:BCL:CBB	2.49	0.41
1:2:7:ASN:OD1	1:2:15:LYS:HE2	2.21	0.41
9:4:101:BCL:H61	9:4:101:BCL:H41	1.80	0.41
1:B:17:LEU:HD13	9:B:102:BCL:CMB	2.50	0.41
4:L:234:LEU:HD21	5:M:590:ILE:HG13	2.02	0.41
4:L:308:VAL:HG21	5:M:406:ILE:HG22	2.02	0.41
9:0:101:BCL:CHB	9:7:101:BCL:HMB3	2.51	0.41
3:C:311:GLN:OE1	3:C:311:GLN:HA	2.20	0.41
1:I:37:LEU:HD23	1:I:37:LEU:HA	1.95	0.41
9:K:101:BCL:H162	10:P:101:KGD:CBN	2.50	0.41
4:L:156:VAL:HB	4:L:157:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:227:HIS:HD1	5:M:596:ALA:HB3	1.86	0.41
5:M:356:GLY:H	5:M:370:VAL:HG22	1.86	0.41
9:W:101:BCL:HHC	9:W:101:BCL:CBB	2.51	0.41
9:3:101:BCL:HMC3	9:6:101:BCL:HBB1	2.02	0.41
12:L:1003:BPB:H2	12:L:1003:BPB:H6	1.89	0.41
5:M:476:ALA:HB1	9:M:703:BCL:H92	2.03	0.41
5:M:479:LEU:HD12	5:M:479:LEU:O	2.19	0.41
2:N:10:THR:O	2:N:14:VAL:HG23	2.20	0.41
9:O:101:BCL:HMB1	9:O:101:BCL:CBB	2.50	0.41
9:R:101:BCL:H203	9:R:101:BCL:H162	1.95	0.41
1:O:42:ILE:O	1:O:45:VAL:HG12	2.20	0.41
1:B:29:VAL:O	1:B:33:ILE:HG13	2.21	0.41
3:C:138:LYS:CE	11:C:403:HEM:O1A	2.65	0.41
1:O:12:ASP:OD1	1:O:13:GLN:N	2.54	0.41
2:R:17:LEU:O	2:R:21:VAL:HG23	2.20	0.41
9:U:101:BCL:H61	9:U:101:BCL:H41	1.80	0.41
7:Y:9:MET:O	7:Y:13:VAL:HG23	2.21	0.41
1:6:47:CYS:CB	9:6:101:BCL:HBC1	2.51	0.41
2:9:17:LEU:O	2:9:21:VAL:HG23	2.20	0.41
1:B:9:LEU:HD12	1:B:20:ASN:OD1	2.21	0.41
3:C:297:HIS:HE1	11:C:405:HEM:NA	2.12	0.41
3:C:303:PRO:HA	3:C:304:PRO:HD3	2.00	0.41
9:E:101:BCL:H62	9:E:101:BCL:H41	1.89	0.41
1:I:29:VAL:O	1:I:33:ILE:HG13	2.21	0.41
13:L:1004:MQE:CBX	7:Y:18:LEU:HA	2.51	0.41
10:Q:103:KGD:CAF	9:S:102:BCL:H62	2.51	0.41
5:M:523:PRO:HA	5:M:526:MET:HE2	2.03	0.41
1:O:47:CYS:SG	9:O:101:BCL:HBC1	2.61	0.40
9:9:102:BCL:H111	9:9:102:BCL:H152	1.77	0.40
4:L:88:LEU:HD13	13:M:701:MQE:CCO	2.52	0.40
6:X:20:PHE:CB	9:X:101:BCL:H193	2.51	0.40
9:4:102:BCL:H62	9:4:102:BCL:H41	1.89	0.40
9:6:102:BCL:HHC	9:6:102:BCL:CBB	2.50	0.40
1:8:36:GLY:HA3	9:8:101:BCL:H62	2.02	0.40
2:A:17:LEU:HD11	5:M:381:ILE:HG12	2.03	0.40
10:C:406:KGD:CAK	7:Y:11:MET:HE1	2.52	0.40
1:I:41:VAL:O	1:I:45:VAL:HG23	2.21	0.40
9:I:102:BCL:HHC	9:I:102:BCL:HBB2	2.03	0.40
1:K:47:CYS:CB	9:K:101:BCL:HBC1	2.52	0.40
2:N:40:ARG:HG3	2:N:40:ARG:O	2.21	0.40
9:Q:102:BCL:HHC	9:Q:102:BCL:CBB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:31:LEU:HD11	2:V:39:LEU:HD12	2.03	0.40
1:2:19:ASN:OD1	1:2:20:ASN:N	2.49	0.40
1:4:39:ILE:HD13	1:4:39:ILE:HA	1.92	0.40
3:C:34:ALA:O	3:C:38:ILE:HG22	2.21	0.40
3:C:175:HIS:HE1	11:C:403:HEM:C1A	2.39	0.40
6:X:14:ILE:O	6:X:17:THR:HG22	2.21	0.40
1:0:33:ILE:O	1:0:37:LEU:HG	2.21	0.40
1:2:16:PRO:O	3:C:17:ARG:NH1	2.55	0.40
1:4:47:CYS:CB	9:4:101:BCL:HBC1	2.51	0.40
3:C:266:MET:O	3:C:270:ILE:HG13	2.22	0.40
2:D:9:ARG:O	2:D:13:VAL:HG12	2.21	0.40
2:D:38:TRP:CD1	1:G:54:ILE:HD13	2.56	0.40
4:L:64:ILE:HD12	4:L:69:VAL:HG21	2.03	0.40
1:2:29:VAL:O	1:2:33:ILE:HG13	2.21	0.40
3:C:258:ASN:O	3:C:262:ILE:HG12	2.22	0.40
9:I:101:BCL:HMB1	9:I:101:BCL:CBB	2.51	0.40
5:M:386:PHE:CE1	12:M:704:BPB:H19A	2.56	0.40
9:M:703:BCL:HAA2	9:M:703:BCL:HBD	2.04	0.40
8:Z:53:ASP:OD1	8:Z:55:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	47/55 (86%)	47 (100%)	0	0	100	100
1	2	47/55 (86%)	47 (100%)	0	0	100	100
1	4	47/55 (86%)	47 (100%)	0	0	100	100
1	6	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	8	47/55 (86%)	47 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	47/55 (86%)	47 (100%)	0	0	100	100
1	E	47/55 (86%)	47 (100%)	0	0	100	100
1	G	47/55 (86%)	47 (100%)	0	0	100	100
1	I	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	K	47/55 (86%)	47 (100%)	0	0	100	100
1	O	47/55 (86%)	47 (100%)	0	0	100	100
1	Q	47/55 (86%)	47 (100%)	0	0	100	100
1	S	47/55 (86%)	47 (100%)	0	0	100	100
1	U	47/55 (86%)	47 (100%)	0	0	100	100
1	W	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
2	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	3	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	5	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	7	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	9	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	A	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	D	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	H	36/42 (86%)	32 (89%)	4 (11%)	0	100	100
2	J	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	N	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	P	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	R	36/42 (86%)	32 (89%)	4 (11%)	0	100	100
2	T	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	V	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	C	313/320 (98%)	300 (96%)	13 (4%)	0	100	100
4	L	296/315 (94%)	284 (96%)	12 (4%)	0	100	100
5	M	304/307 (99%)	296 (97%)	7 (2%)	1 (0%)	37	68
6	X	24/32 (75%)	24 (100%)	0	0	100	100
7	Y	30/39 (77%)	30 (100%)	0	0	100	100
8	Z	45/63 (71%)	43 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2257/2531 (89%)	2178 (96%)	78 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	377	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/49 (88%)	43 (100%)	0	100	100
1	2	43/49 (88%)	43 (100%)	0	100	100
1	4	43/49 (88%)	41 (95%)	2 (5%)	22	52
1	6	43/49 (88%)	42 (98%)	1 (2%)	45	70
1	8	43/49 (88%)	43 (100%)	0	100	100
1	B	43/49 (88%)	43 (100%)	0	100	100
1	E	43/49 (88%)	43 (100%)	0	100	100
1	G	43/49 (88%)	43 (100%)	0	100	100
1	I	43/49 (88%)	43 (100%)	0	100	100
1	K	43/49 (88%)	43 (100%)	0	100	100
1	O	43/49 (88%)	43 (100%)	0	100	100
1	Q	43/49 (88%)	43 (100%)	0	100	100
1	S	43/49 (88%)	43 (100%)	0	100	100
1	U	43/49 (88%)	43 (100%)	0	100	100
1	W	43/49 (88%)	43 (100%)	0	100	100
2	1	33/37 (89%)	33 (100%)	0	100	100
2	3	33/37 (89%)	33 (100%)	0	100	100
2	5	33/37 (89%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	7	33/37 (89%)	33 (100%)	0	100	100
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	33 (100%)	0	100	100
2	D	33/37 (89%)	33 (100%)	0	100	100
2	F	33/37 (89%)	33 (100%)	0	100	100
2	H	33/37 (89%)	33 (100%)	0	100	100
2	J	33/37 (89%)	33 (100%)	0	100	100
2	N	33/37 (89%)	33 (100%)	0	100	100
2	P	33/37 (89%)	33 (100%)	0	100	100
2	R	33/37 (89%)	33 (100%)	0	100	100
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	33/37 (89%)	33 (100%)	0	100	100
3	C	257/262 (98%)	255 (99%)	2 (1%)	79	89
4	L	242/253 (96%)	242 (100%)	0	100	100
5	M	244/245 (100%)	243 (100%)	1 (0%)	89	94
6	X	23/28 (82%)	23 (100%)	0	100	100
7	Y	29/36 (81%)	29 (100%)	0	100	100
8	Z	36/50 (72%)	36 (100%)	0	100	100
All	All	1971/2164 (91%)	1965 (100%)	6 (0%)	90	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4	7	ASN
1	4	8	ASP
1	6	8	ASP
3	C	85	ASN
3	C	145	MET
5	M	493	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	85	ASN
3	C	154	GLN

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Mol	Chain	Res	Type
3	C	226	GLN
4	L	252	ASN
4	L	293	ASN
1	O	20	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 1 is monoatomic - leaving 91 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	$\# Z > 2$
9	BCL	B	102	-	64,74,74	1.27	5 (7%)	78,115,115	1.38	7 (8%)
10	KGD	T	102	-	41,41,41	1.05	1 (2%)	49,53,53	1.81	14 (28%)
9	BCL	8	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.47	8 (10%)
10	KGD	6	103	-	41,41,41	1.08	1 (2%)	49,53,53	2.01	14 (28%)
10	KGD	C	401	-	41,41,41	1.12	1 (2%)	49,53,53	2.13	15 (30%)
13	MQE	L	1004	-	69,69,69	0.29	0	84,87,87	0.46	1 (1%)
10	KGD	E	102	-	41,41,41	0.96	1 (2%)	49,53,53	1.76	13 (26%)
9	BCL	O	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	W	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	10 (12%)
10	KGD	C	406	-	41,41,41	2.49	12 (29%)	49,53,53	1.88	13 (26%)
9	BCL	S	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.50	9 (11%)
9	BCL	Q	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.47	8 (10%)
9	BCL	N	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.46	9 (11%)
10	KGD	3	102	-	41,41,41	1.02	1 (2%)	49,53,53	1.85	14 (28%)
12	BPB	L	1005	-	49,70,70	1.22	1 (2%)	47,101,101	1.19	5 (10%)
9	BCL	H	102	-	64,74,74	1.37	4 (6%)	78,115,115	1.37	8 (10%)
9	BCL	4	102	-	64,74,74	1.24	4 (6%)	78,115,115	1.44	9 (11%)
9	BCL	G	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.46	8 (10%)
9	BCL	D	102	-	64,74,74	1.26	5 (7%)	78,115,115	1.44	8 (10%)
9	BCL	D	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.43	9 (11%)
9	BCL	R	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.43	8 (10%)
9	BCL	6	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.40	9 (11%)
10	KGD	I	104	-	41,41,41	1.25	2 (4%)	49,53,53	2.16	12 (24%)
10	KGD	2	103	-	41,41,41	0.98	1 (2%)	49,53,53	1.76	12 (24%)
9	BCL	X	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.45	8 (10%)
10	KGD	4	103	-	41,41,41	0.97	1 (2%)	49,53,53	2.19	10 (20%)
9	BCL	M	703	-	64,74,74	1.27	7 (10%)	78,115,115	1.45	9 (11%)
9	BCL	E	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.43	10 (12%)
10	KGD	S	103	-	41,41,41	0.98	1 (2%)	49,53,53	1.91	15 (30%)
10	KGD	B	103	-	41,41,41	0.93	2 (4%)	49,53,53	2.11	13 (26%)
9	BCL	G	102	-	64,74,74	1.26	4 (6%)	78,115,115	1.41	8 (10%)
9	BCL	L	1001	-	64,74,74	1.28	4 (6%)	78,115,115	1.44	7 (8%)
10	KGD	8	103	-	41,41,41	1.06	1 (2%)	49,53,53	1.95	13 (26%)
9	BCL	9	102	-	64,74,74	1.28	4 (6%)	78,115,115	1.44	8 (10%)
10	KGD	P	103	-	41,41,41	0.99	2 (4%)	49,53,53	1.73	11 (22%)
9	BCL	A	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.45	10 (12%)
9	BCL	2	102	-	64,74,74	1.27	6 (9%)	78,115,115	1.44	8 (10%)
10	KGD	A	102	-	41,41,41	0.94	1 (2%)	49,53,53	1.62	11 (22%)
10	KGD	O	103	-	41,41,41	0.95	1 (2%)	49,53,53	1.89	12 (24%)
10	KGD	E	103	-	41,41,41	0.92	1 (2%)	49,53,53	1.87	13 (26%)
10	KGD	P	101	-	41,41,41	0.91	1 (2%)	49,53,53	1.65	12 (24%)
10	KGD	W	102	-	41,41,41	0.93	1 (2%)	49,53,53	1.70	12 (24%)
9	BCL	V	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.44	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	KGD	U	103	-	41,41,41	1.19	1 (2%)	49,53,53	1.98	12 (24%)
11	HEM	C	403	3	41,50,50	2.20	8 (19%)	45,82,82	2.24	16 (35%)
14	PGV	L	1007	-	44,44,50	0.51	0	47,50,56	0.55	0
10	KGD	G	103	-	41,41,41	0.92	1 (2%)	49,53,53	2.04	11 (22%)
9	BCL	0	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.45	8 (10%)
9	BCL	F	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.47	10 (12%)
9	BCL	3	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.46	8 (10%)
9	BCL	7	101	-	64,74,74	1.34	4 (6%)	78,115,115	1.39	8 (10%)
9	BCL	U	102	-	64,74,74	1.27	5 (7%)	78,115,115	1.40	9 (11%)
10	KGD	I	103	-	41,41,41	0.99	1 (2%)	49,53,53	1.72	13 (26%)
10	KGD	5	103	-	41,41,41	0.93	1 (2%)	49,53,53	1.74	13 (26%)
10	KGD	H	101	-	41,41,41	0.94	1 (2%)	49,53,53	1.73	12 (24%)
10	KGD	J	102	-	41,41,41	1.01	1 (2%)	49,53,53	1.82	14 (28%)
14	PGV	L	1006	-	31,31,50	0.59	0	34,37,56	0.59	0
11	HEM	C	405	3	41,50,50	1.50	3 (7%)	45,82,82	1.19	3 (6%)
12	BPB	M	704	-	49,70,70	1.25	1 (2%)	47,101,101	1.07	4 (8%)
9	BCL	4	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.47	9 (11%)
9	BCL	6	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.48	8 (10%)
14	PGV	P	104	-	34,34,50	0.58	0	37,40,56	0.54	0
9	BCL	I	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.46	10 (12%)
9	BCL	J	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.44	9 (11%)
10	KGD	Q	103	-	41,41,41	1.12	1 (2%)	49,53,53	1.89	14 (28%)
12	BPB	L	1003	-	49,70,70	1.23	1 (2%)	47,101,101	1.10	4 (8%)
13	MQE	M	701	-	69,69,69	0.29	0	84,87,87	0.49	1 (1%)
10	KGD	9	101	-	41,41,41	1.00	1 (2%)	49,53,53	1.71	10 (20%)
10	KGD	K	103	-	41,41,41	0.91	1 (2%)	49,53,53	1.91	10 (20%)
9	BCL	0	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.40	8 (10%)
13	MQE	M	705	-	25,25,69	0.43	0	31,34,87	0.87	2 (6%)
9	BCL	5	101	-	64,74,74	1.32	4 (6%)	78,115,115	1.41	9 (11%)
10	KGD	0	103	-	41,41,41	1.01	1 (2%)	49,53,53	1.69	10 (20%)
9	BCL	S	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.43	10 (12%)
9	BCL	K	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.52	9 (11%)
9	BCL	I	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.48	8 (10%)
11	HEM	C	404	3	41,50,50	1.45	4 (9%)	45,82,82	1.16	4 (8%)
9	BCL	U	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.46	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	K	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.42	10 (12%)
11	HEM	C	402	3	41,50,50	1.46	3 (7%)	45,82,82	1.14	2 (4%)
9	BCL	Q	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.41	9 (11%)
10	KGD	R	102	-	41,41,41	0.88	1 (2%)	49,53,53	1.62	8 (16%)
9	BCL	8	102	-	64,74,74	1.25	5 (7%)	78,115,115	1.44	10 (12%)
9	BCL	P	102	-	64,74,74	1.28	4 (6%)	78,115,115	1.44	8 (10%)
10	KGD	5	102	-	41,41,41	1.02	1 (2%)	49,53,53	1.71	11 (22%)
9	BCL	L	1002	-	64,74,74	1.30	3 (4%)	78,115,115	1.47	10 (12%)
9	BCL	O	102	-	64,74,74	1.25	5 (7%)	78,115,115	1.40	9 (11%)
9	BCL	2	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.44	8 (10%)
9	BCL	1	101	-	64,74,74	1.35	5 (7%)	78,115,115	1.38	9 (11%)
9	BCL	B	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.45	8 (10%)
9	BCL	T	101	-	64,74,74	1.28	4 (6%)	78,115,115	1.43	8 (10%)

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
9	BCL	B	102	-	-	7/37/137/137	-
10	KGD	T	102	-	-	6/36/56/56	0/1/1/1
9	BCL	8	101	-	-	7/37/137/137	-
10	KGD	6	103	-	-	3/36/56/56	0/1/1/1
10	KGD	C	401	-	-	5/36/56/56	0/1/1/1
13	MQE	L	1004	-	-	14/65/85/85	0/2/2/2
10	KGD	E	102	-	-	6/36/56/56	0/1/1/1
9	BCL	O	101	-	-	7/37/137/137	-
9	BCL	W	101	-	-	7/37/137/137	-
10	KGD	C	406	-	-	5/36/56/56	0/1/1/1
9	BCL	S	101	-	-	6/37/137/137	-
9	BCL	Q	101	-	-	7/37/137/137	-
9	BCL	N	101	-	-	5/37/137/137	-
10	KGD	3	102	-	-	6/36/56/56	0/1/1/1
12	BPB	L	1005	-	-	12/37/105/105	0/5/6/6
9	BCL	H	102	-	-	9/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	4	102	-	-	6/37/137/137	-
9	BCL	G	101	-	-	7/37/137/137	-
9	BCL	D	102	-	-	6/37/137/137	-
9	BCL	D	101	-	-	6/37/137/137	-
9	BCL	R	101	-	-	6/37/137/137	-
9	BCL	6	102	-	-	6/37/137/137	-
10	KGD	I	104	-	-	3/36/56/56	0/1/1/1
10	KGD	2	103	-	-	5/36/56/56	0/1/1/1
9	BCL	X	101	-	-	6/37/137/137	-
10	KGD	4	103	-	-	4/36/56/56	0/1/1/1
9	BCL	M	703	-	-	4/37/137/137	-
9	BCL	E	101	-	-	9/37/137/137	-
10	KGD	S	103	-	-	6/36/56/56	0/1/1/1
10	KGD	B	103	-	-	4/36/56/56	0/1/1/1
9	BCL	G	102	-	-	7/37/137/137	-
9	BCL	L	1001	-	-	6/37/137/137	-
10	KGD	8	103	-	-	6/36/56/56	0/1/1/1
9	BCL	9	102	-	-	6/37/137/137	-
10	KGD	P	103	-	-	6/36/56/56	0/1/1/1
9	BCL	A	101	-	-	5/37/137/137	-
9	BCL	2	102	-	-	6/37/137/137	-
10	KGD	A	102	-	-	5/36/56/56	0/1/1/1
10	KGD	O	103	-	-	2/36/56/56	0/1/1/1
10	KGD	E	103	-	-	1/36/56/56	0/1/1/1
10	KGD	P	101	-	-	8/36/56/56	0/1/1/1
10	KGD	W	102	-	-	4/36/56/56	0/1/1/1
9	BCL	V	101	-	-	8/37/137/137	-
10	KGD	U	103	-	-	7/36/56/56	0/1/1/1
11	HEM	C	403	3	-	8/12/54/54	-
14	PGV	L	1007	-	-	18/49/49/55	-
10	KGD	G	103	-	-	5/36/56/56	0/1/1/1
9	BCL	0	101	-	-	7/37/137/137	-
9	BCL	F	101	-	-	5/37/137/137	-
9	BCL	3	101	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	7	101	-	-	6/37/137/137	-
9	BCL	U	102	-	-	5/37/137/137	-
10	KGD	I	103	-	-	5/36/56/56	0/1/1/1
10	KGD	5	103	-	-	4/36/56/56	0/1/1/1
10	KGD	H	101	-	-	7/36/56/56	0/1/1/1
10	KGD	J	102	-	-	10/36/56/56	0/1/1/1
14	PGV	L	1006	-	-	10/36/36/55	-
11	HEM	C	405	3	-	2/12/54/54	-
12	BPB	M	704	-	-	17/37/105/105	0/5/6/6
9	BCL	4	101	-	-	5/37/137/137	-
9	BCL	6	101	-	-	9/37/137/137	-
14	PGV	P	104	-	-	10/39/39/55	-
9	BCL	I	102	-	-	8/37/137/137	-
9	BCL	J	101	-	-	4/37/137/137	-
10	KGD	Q	103	-	-	9/36/56/56	0/1/1/1
12	BPB	L	1003	-	-	13/37/105/105	0/5/6/6
13	MQE	M	701	-	-	12/65/85/85	0/2/2/2
10	KGD	9	101	-	-	4/36/56/56	0/1/1/1
10	KGD	K	103	-	-	6/36/56/56	0/1/1/1
9	BCL	0	102	-	-	7/37/137/137	-
13	MQE	M	705	-	-	1/13/33/85	0/2/2/2
9	BCL	5	101	-	-	6/37/137/137	-
10	KGD	0	103	-	-	3/36/56/56	0/1/1/1
9	BCL	S	102	-	-	6/37/137/137	-
9	BCL	K	101	-	-	6/37/137/137	-
9	BCL	I	101	-	-	9/37/137/137	-
11	HEM	C	404	3	-	8/12/54/54	-
9	BCL	U	101	-	-	6/37/137/137	-
9	BCL	K	102	-	-	9/37/137/137	-
11	HEM	C	402	3	-	6/12/54/54	-
9	BCL	Q	102	-	-	6/37/137/137	-
10	KGD	R	102	-	-	5/36/56/56	0/1/1/1
9	BCL	8	102	-	-	4/37/137/137	-
9	BCL	P	102	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	KGD	5	102	-	-	7/36/56/56	0/1/1/1
9	BCL	L	1002	-	-	9/37/137/137	-
9	BCL	O	102	-	-	9/37/137/137	-
9	BCL	2	101	-	-	6/37/137/137	-
9	BCL	1	101	-	-	6/37/137/137	-
9	BCL	B	101	-	-	7/37/137/137	-
9	BCL	T	101	-	-	4/37/137/137	-

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	406	KGD	CAE-CAI	-8.91	1.39	1.50
11	C	403	HEM	FE-NB	8.47	2.38	1.96
12	M	704	BPB	CAC-C3C	8.14	1.54	1.33
12	L	1003	BPB	CAC-C3C	8.04	1.53	1.33
12	L	1005	BPB	CAC-C3C	7.91	1.53	1.33
10	C	406	KGD	CAB-CAD	-7.17	1.43	1.53
9	H	102	BCL	C1B-NB	5.38	1.40	1.35
9	1	101	BCL	C1B-NB	5.36	1.40	1.35
9	7	101	BCL	C1B-NB	5.29	1.39	1.35
11	C	403	HEM	C4D-ND	-5.25	1.31	1.40
9	H	102	BCL	MG-NA	5.13	2.18	2.06
9	6	101	BCL	C1B-NB	5.12	1.39	1.35
9	L	1001	BCL	C1B-NB	5.11	1.39	1.35
9	P	102	BCL	C1B-NB	5.10	1.39	1.35
9	V	101	BCL	C1B-NB	5.07	1.39	1.35
9	M	703	BCL	MG-NA	5.07	2.18	2.06
9	L	1002	BCL	MG-NA	5.05	2.18	2.06
9	5	101	BCL	C1B-NB	5.05	1.39	1.35
9	I	101	BCL	C1B-NB	5.04	1.39	1.35
9	3	101	BCL	C1B-NB	5.04	1.39	1.35
9	X	101	BCL	C1B-NB	5.04	1.39	1.35
9	E	101	BCL	C1B-NB	5.02	1.39	1.35
9	7	101	BCL	MG-NA	5.02	2.18	2.06
9	5	101	BCL	MG-NA	5.01	2.18	2.06
9	2	101	BCL	C1B-NB	5.01	1.39	1.35
9	8	101	BCL	C1B-NB	5.01	1.39	1.35
9	D	102	BCL	C1B-NB	5.00	1.39	1.35
9	O	101	BCL	C1B-NB	5.00	1.39	1.35
9	9	102	BCL	C1B-NB	5.00	1.39	1.35
9	1	101	BCL	MG-NA	4.99	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	101	BCL	C1B-NB	4.98	1.39	1.35
9	A	101	BCL	C1B-NB	4.98	1.39	1.35
9	R	101	BCL	C1B-NB	4.98	1.39	1.35
9	0	101	BCL	C1B-NB	4.97	1.39	1.35
9	T	101	BCL	C1B-NB	4.97	1.39	1.35
9	B	101	BCL	C1B-NB	4.97	1.39	1.35
9	S	101	BCL	C1B-NB	4.97	1.39	1.35
9	J	101	BCL	C1B-NB	4.96	1.39	1.35
9	2	102	BCL	MG-NA	4.96	2.18	2.06
9	D	101	BCL	C1B-NB	4.96	1.39	1.35
9	U	102	BCL	MG-NA	4.95	2.18	2.06
9	K	101	BCL	C1B-NB	4.95	1.39	1.35
9	N	101	BCL	C1B-NB	4.95	1.39	1.35
9	K	102	BCL	C1B-NB	4.94	1.39	1.35
9	B	102	BCL	MG-NA	4.94	2.18	2.06
9	Q	101	BCL	C1B-NB	4.94	1.39	1.35
9	F	101	BCL	C1B-NB	4.93	1.39	1.35
9	U	102	BCL	C1B-NB	4.92	1.39	1.35
9	4	101	BCL	C1B-NB	4.91	1.39	1.35
9	B	102	BCL	C1B-NB	4.91	1.39	1.35
9	G	102	BCL	MG-NA	4.90	2.17	2.06
9	0	102	BCL	C1B-NB	4.90	1.39	1.35
9	S	102	BCL	C1B-NB	4.88	1.39	1.35
9	8	102	BCL	MG-NA	4.88	2.17	2.06
9	G	101	BCL	C1B-NB	4.88	1.39	1.35
9	W	101	BCL	MG-NA	4.87	2.17	2.06
9	L	1002	BCL	C1B-NB	4.86	1.39	1.35
9	T	101	BCL	MG-NA	4.85	2.17	2.06
9	D	101	BCL	MG-NA	4.84	2.17	2.06
9	6	102	BCL	C1B-NB	4.84	1.39	1.35
9	I	102	BCL	MG-NA	4.84	2.17	2.06
9	Q	102	BCL	C1B-NB	4.83	1.39	1.35
9	4	102	BCL	C1B-NB	4.83	1.39	1.35
9	W	101	BCL	C1B-NB	4.83	1.39	1.35
9	8	102	BCL	C1B-NB	4.83	1.39	1.35
9	F	101	BCL	MG-NA	4.82	2.17	2.06
9	9	102	BCL	MG-NA	4.82	2.17	2.06
9	I	102	BCL	C1B-NB	4.82	1.39	1.35
9	K	102	BCL	MG-NA	4.81	2.17	2.06
9	4	102	BCL	MG-NA	4.81	2.17	2.06
9	S	102	BCL	MG-NA	4.80	2.17	2.06
9	E	101	BCL	MG-NA	4.79	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	102	BCL	C1B-NB	4.79	1.39	1.35
9	L	1001	BCL	MG-NA	4.79	2.17	2.06
9	U	101	BCL	MG-NA	4.79	2.17	2.06
9	6	102	BCL	MG-NA	4.78	2.17	2.06
9	J	101	BCL	MG-NA	4.78	2.17	2.06
9	G	102	BCL	C1B-NB	4.78	1.39	1.35
9	2	102	BCL	C1B-NB	4.78	1.39	1.35
9	P	102	BCL	MG-NA	4.77	2.17	2.06
9	O	102	BCL	MG-NA	4.77	2.17	2.06
9	R	101	BCL	MG-NA	4.77	2.17	2.06
9	M	703	BCL	C1B-NB	4.76	1.39	1.35
9	I	101	BCL	MG-NA	4.76	2.17	2.06
9	V	101	BCL	MG-NA	4.75	2.17	2.06
9	8	101	BCL	MG-NA	4.75	2.17	2.06
10	C	406	KGD	CAC-CAE	-4.75	1.43	1.53
9	Q	101	BCL	MG-NA	4.74	2.17	2.06
9	0	102	BCL	MG-NA	4.74	2.17	2.06
9	B	101	BCL	MG-NA	4.74	2.17	2.06
9	G	101	BCL	MG-NA	4.73	2.17	2.06
9	N	101	BCL	MG-NA	4.73	2.17	2.06
9	3	101	BCL	MG-NA	4.72	2.17	2.06
9	A	101	BCL	MG-NA	4.72	2.17	2.06
9	D	102	BCL	MG-NA	4.72	2.17	2.06
9	K	101	BCL	MG-NA	4.71	2.17	2.06
9	S	101	BCL	MG-NA	4.71	2.17	2.06
9	Q	102	BCL	MG-NA	4.70	2.17	2.06
10	U	103	KGD	CAB-CAD	-4.70	1.47	1.53
9	X	101	BCL	MG-NA	4.66	2.17	2.06
9	6	101	BCL	MG-NA	4.66	2.17	2.06
11	C	403	HEM	C1B-NB	-4.65	1.32	1.40
9	0	101	BCL	MG-NA	4.65	2.17	2.06
9	4	101	BCL	MG-NA	4.64	2.17	2.06
9	2	101	BCL	MG-NA	4.63	2.17	2.06
9	O	101	BCL	MG-NA	4.62	2.17	2.06
11	C	405	HEM	C3C-C2C	-4.58	1.34	1.40
10	T	102	KGD	CAB-CAD	-4.49	1.47	1.53
10	I	104	KGD	CAB-CAD	-4.42	1.47	1.53
10	0	103	KGD	CAB-CAD	-4.35	1.47	1.53
10	5	102	KGD	CAB-CAD	-4.29	1.47	1.53
9	1	101	BCL	MG-NC	4.09	2.16	2.06
11	C	404	HEM	C3C-C2C	-4.09	1.34	1.40
9	H	102	BCL	MG-NC	4.08	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	103	KGD	CAB-CAD	-4.07	1.48	1.53
10	C	401	KGD	CAB-CAD	-4.06	1.48	1.53
11	C	402	HEM	C3C-C2C	-4.04	1.34	1.40
10	9	101	KGD	CAB-CAD	-4.03	1.48	1.53
9	7	101	BCL	MG-NC	4.01	2.15	2.06
10	2	103	KGD	CAB-CAD	-4.00	1.48	1.53
10	Q	103	KGD	CAB-CAD	-4.00	1.48	1.53
9	5	101	BCL	MG-NC	4.00	2.15	2.06
10	J	102	KGD	CAB-CAD	-3.94	1.48	1.53
11	C	402	HEM	C3C-CAC	3.85	1.55	1.47
11	C	404	HEM	C3C-CAC	3.80	1.55	1.47
10	6	103	KGD	CAB-CAD	-3.80	1.48	1.53
11	C	405	HEM	C3C-CAC	3.77	1.55	1.47
9	L	1002	BCL	MG-NC	3.73	2.15	2.06
10	C	406	KGD	CAI-CAH	-3.70	1.40	1.47
10	P	101	KGD	CAB-CAD	-3.69	1.48	1.53
10	A	102	KGD	CAB-CAD	-3.67	1.48	1.53
10	4	103	KGD	CAB-CAD	-3.64	1.48	1.53
10	3	102	KGD	CAB-CAD	-3.63	1.48	1.53
9	T	101	BCL	MG-NC	3.58	2.14	2.06
10	H	101	KGD	CAB-CAD	-3.57	1.48	1.53
9	F	101	BCL	MG-NC	3.56	2.14	2.06
9	9	102	BCL	MG-NC	3.56	2.14	2.06
9	3	101	BCL	MG-NC	3.53	2.14	2.06
9	P	102	BCL	MG-NC	3.52	2.14	2.06
9	V	101	BCL	MG-NC	3.52	2.14	2.06
9	L	1001	BCL	MG-NC	3.47	2.14	2.06
10	C	406	KGD	CBK-CBH	-3.46	1.43	1.50
10	O	103	KGD	CAB-CAD	-3.45	1.49	1.53
9	J	101	BCL	MG-NC	3.45	2.14	2.06
9	D	101	BCL	MG-NC	3.44	2.14	2.06
9	U	102	BCL	MG-NC	3.44	2.14	2.06
9	N	101	BCL	MG-NC	3.44	2.14	2.06
9	R	101	BCL	MG-NC	3.43	2.14	2.06
9	2	102	BCL	MG-NC	3.42	2.14	2.06
9	G	102	BCL	MG-NC	3.41	2.14	2.06
9	B	102	BCL	MG-NC	3.41	2.14	2.06
9	A	101	BCL	MG-NC	3.41	2.14	2.06
11	C	403	HEM	FE-ND	-3.40	1.80	1.96
9	W	101	BCL	MG-NC	3.38	2.14	2.06
9	E	101	BCL	MG-NC	3.37	2.14	2.06
10	5	103	KGD	CAB-CAD	-3.37	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	102	BCL	MG-NC	3.35	2.14	2.06
9	S	102	BCL	MG-NC	3.34	2.14	2.06
9	6	102	BCL	MG-NC	3.33	2.14	2.06
10	R	102	KGD	CAB-CAD	-3.31	1.49	1.53
9	U	101	BCL	MG-NC	3.31	2.14	2.06
9	O	102	BCL	MG-NC	3.31	2.14	2.06
9	Q	101	BCL	MG-NC	3.30	2.14	2.06
9	8	102	BCL	MG-NC	3.29	2.14	2.06
9	K	102	BCL	MG-NC	3.29	2.14	2.06
9	X	101	BCL	MG-NC	3.28	2.14	2.06
9	M	703	BCL	MG-NC	3.26	2.14	2.06
9	B	101	BCL	MG-NC	3.26	2.14	2.06
9	I	101	BCL	MG-NC	3.25	2.14	2.06
10	S	103	KGD	CAB-CAD	-3.24	1.49	1.53
9	0	102	BCL	MG-NC	3.23	2.14	2.06
9	K	101	BCL	MG-NC	3.23	2.13	2.06
9	G	101	BCL	MG-NC	3.22	2.13	2.06
9	O	101	BCL	MG-NC	3.22	2.13	2.06
9	8	101	BCL	MG-NC	3.22	2.13	2.06
11	C	403	HEM	C4B-NB	-3.22	1.32	1.38
9	2	101	BCL	MG-NC	3.20	2.13	2.06
9	4	102	BCL	MG-NC	3.20	2.13	2.06
9	D	102	BCL	MG-NC	3.19	2.13	2.06
9	Q	102	BCL	MG-NC	3.18	2.13	2.06
10	E	103	KGD	CAB-CAD	-3.18	1.49	1.53
9	S	101	BCL	MG-NC	3.17	2.13	2.06
10	K	103	KGD	CAB-CAD	-3.17	1.49	1.53
9	6	101	BCL	MG-NC	3.16	2.13	2.06
9	4	101	BCL	MG-NC	3.16	2.13	2.06
9	0	101	BCL	MG-NC	3.16	2.13	2.06
10	W	102	KGD	CAB-CAD	-3.15	1.49	1.53
11	C	402	HEM	CAB-C3B	3.11	1.55	1.47
10	8	103	KGD	CAB-CAD	-3.08	1.49	1.53
10	C	406	KGD	CBJ-CBH	-2.97	1.31	1.35
11	C	405	HEM	CAB-C3B	2.96	1.55	1.47
10	C	406	KGD	CBO-CBL	-2.91	1.44	1.50
11	C	404	HEM	CAB-C3B	2.86	1.55	1.47
10	E	102	KGD	CAB-CAD	-2.78	1.50	1.53
10	C	406	KGD	CAD-CAH	-2.70	1.32	1.35
10	P	103	KGD	CAE-CAI	-2.70	1.47	1.50
9	H	102	BCL	CHD-C1D	2.68	1.43	1.38
10	C	406	KGD	CAF-CAB	-2.62	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	103	KGD	CAB-CAD	-2.58	1.50	1.53
10	P	103	KGD	CAB-CAD	-2.50	1.50	1.53
9	7	101	BCL	CHD-C1D	2.49	1.43	1.38
9	1	101	BCL	CHD-C1D	2.49	1.43	1.38
9	4	101	BCL	CHD-C1D	2.46	1.43	1.38
9	X	101	BCL	CHD-C1D	2.46	1.43	1.38
9	I	101	BCL	CHD-C1D	2.45	1.43	1.38
9	B	101	BCL	CHD-C1D	2.45	1.43	1.38
9	2	101	BCL	CHD-C1D	2.44	1.43	1.38
9	O	101	BCL	CHD-C1D	2.44	1.43	1.38
9	8	101	BCL	CHD-C1D	2.44	1.43	1.38
9	K	101	BCL	CHD-C1D	2.43	1.43	1.38
9	G	101	BCL	CHD-C1D	2.42	1.43	1.38
9	5	101	BCL	CHD-C1D	2.42	1.43	1.38
9	S	101	BCL	CHD-C1D	2.42	1.43	1.38
9	6	101	BCL	CHD-C1D	2.40	1.43	1.38
9	L	1001	BCL	CHD-C1D	2.38	1.43	1.38
9	D	102	BCL	CHD-C1D	2.37	1.43	1.38
9	0	101	BCL	CHD-C1D	2.37	1.43	1.38
9	D	101	BCL	CHD-C1D	2.36	1.43	1.38
9	U	101	BCL	CHD-C1D	2.35	1.42	1.38
10	C	406	KGD	CAC-CAB	-2.34	1.48	1.54
11	C	403	HEM	C2C-C1C	-2.34	1.37	1.42
9	J	101	BCL	CHD-C1D	2.33	1.42	1.38
9	A	101	BCL	CHD-C1D	2.32	1.42	1.38
9	N	101	BCL	CHD-C1D	2.29	1.42	1.38
9	M	703	BCL	CHD-C1D	2.28	1.42	1.38
9	Q	101	BCL	CHD-C1D	2.27	1.42	1.38
9	9	102	BCL	CHD-C1D	2.27	1.42	1.38
9	F	101	BCL	CHD-C1D	2.27	1.42	1.38
9	T	101	BCL	CHD-C1D	2.27	1.42	1.38
9	B	102	BCL	CHD-C1D	2.27	1.42	1.38
9	2	102	BCL	CHD-C1D	2.26	1.42	1.38
9	P	102	BCL	CHD-C1D	2.25	1.42	1.38
10	C	406	KGD	CAK-CAH	-2.25	1.46	1.50
9	W	101	BCL	CHD-C1D	2.24	1.42	1.38
11	C	403	HEM	C1D-ND	-2.23	1.34	1.38
10	B	103	KGD	CAB-CAD	-2.23	1.50	1.53
9	3	101	BCL	CHD-C1D	2.23	1.42	1.38
9	G	102	BCL	CHD-C1D	2.20	1.42	1.38
9	O	102	BCL	CHD-C1D	2.19	1.42	1.38
9	0	102	BCL	CHD-C1D	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	BCL	C1D-ND	2.18	1.40	1.37
9	Q	102	BCL	CHD-C1D	2.18	1.42	1.38
9	E	101	BCL	C4B-NB	2.17	1.37	1.35
9	R	101	BCL	CHD-C1D	2.17	1.42	1.38
9	4	102	BCL	CHD-C1D	2.17	1.42	1.38
9	8	102	BCL	CHD-C1D	2.15	1.42	1.38
9	6	102	BCL	CHD-C1D	2.14	1.42	1.38
9	U	102	BCL	CHD-C1D	2.14	1.42	1.38
9	I	102	BCL	CHD-C1D	2.13	1.42	1.38
9	V	101	BCL	CHD-C1D	2.12	1.42	1.38
9	I	101	BCL	C3D-C4D	-2.11	1.39	1.44
9	8	102	BCL	C4B-NB	2.11	1.37	1.35
9	8	101	BCL	C3D-C4D	-2.10	1.39	1.44
10	C	406	KGD	CAU-CAR	-2.10	1.46	1.50
9	S	102	BCL	CHD-C1D	2.09	1.42	1.38
9	0	101	BCL	C1D-ND	2.09	1.40	1.37
11	C	403	HEM	C3C-C2C	-2.09	1.37	1.40
9	D	102	BCL	C1D-ND	2.08	1.40	1.37
9	8	101	BCL	C1D-ND	2.08	1.40	1.37
9	K	102	BCL	CHD-C1D	2.08	1.42	1.38
11	C	404	HEM	CMB-C2B	2.07	1.55	1.50
9	1	101	BCL	C1D-ND	2.07	1.40	1.37
9	G	101	BCL	C1D-ND	2.07	1.40	1.37
9	N	101	BCL	C1D-ND	2.06	1.40	1.37
9	6	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	2	101	BCL	C1D-ND	2.06	1.40	1.37
9	2	102	BCL	C1D-ND	2.06	1.40	1.37
9	M	703	BCL	C1D-ND	2.05	1.40	1.37
9	O	102	BCL	C3D-C4D	-2.05	1.39	1.44
10	I	104	KGD	CBJ-CBH	-2.05	1.33	1.35
9	M	703	BCL	C3D-C4D	-2.04	1.39	1.44
9	6	101	BCL	C1D-ND	2.04	1.40	1.37
9	U	102	BCL	C4B-NB	2.04	1.37	1.35
9	2	101	BCL	C3D-C4D	-2.03	1.39	1.44
9	M	703	BCL	C4B-NB	2.03	1.37	1.35
9	D	101	BCL	C4B-NB	2.03	1.37	1.35
9	E	101	BCL	CHD-C1D	2.03	1.42	1.38
9	B	102	BCL	C3D-C4D	-2.03	1.39	1.44
9	O	101	BCL	C1D-ND	2.02	1.40	1.37
9	S	101	BCL	C3D-C4D	-2.02	1.39	1.44
10	B	103	KGD	CAE-CAI	-2.01	1.48	1.50
9	W	101	BCL	C1D-ND	2.01	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	102	BCL	C4B-NB	2.01	1.37	1.35
9	A	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	Q	102	BCL	C3D-C4D	-2.00	1.39	1.44

All (825) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	103	KGD	CAP-CAO-CAM	-8.54	115.13	127.31
11	C	403	HEM	C4D-ND-C1D	6.67	111.96	105.07
10	B	103	KGD	CAP-CAO-CAM	-6.63	117.85	127.31
10	G	103	KGD	CAP-CAO-CAM	-6.42	118.14	127.31
10	B	103	KGD	CAJ-CAL-CAM	-6.36	116.63	126.23
10	I	104	KGD	CAP-CAO-CAM	-6.20	118.47	127.31
10	4	103	KGD	CAJ-CAL-CAM	-6.09	117.03	126.23
10	C	406	KGD	CBM-CBJ-CBH	-5.99	118.76	127.31
9	V	101	BCL	CHD-C1D-ND	-5.63	119.28	124.45
10	C	401	KGD	CAP-CAO-CAM	-5.50	119.47	127.31
9	D	101	BCL	CHD-C1D-ND	-5.48	119.42	124.45
9	B	102	BCL	C4D-CHA-C1A	5.45	127.88	121.25
10	I	104	KGD	CAJ-CAL-CAM	-5.44	118.01	126.23
9	W	101	BCL	C4D-CHA-C1A	5.41	127.83	121.25
9	I	101	BCL	C4D-CHA-C1A	5.38	127.80	121.25
9	R	101	BCL	CHD-C1D-ND	-5.35	119.54	124.45
9	8	101	BCL	C4D-CHA-C1A	5.35	127.75	121.25
9	G	102	BCL	C4D-CHA-C1A	5.33	127.74	121.25
9	U	101	BCL	C4D-CHA-C1A	5.33	127.73	121.25
9	A	101	BCL	CHD-C1D-ND	-5.32	119.56	124.45
9	X	101	BCL	C4D-CHA-C1A	5.31	127.72	121.25
9	Q	102	BCL	C4D-CHA-C1A	5.31	127.71	121.25
9	4	102	BCL	C4D-CHA-C1A	5.30	127.70	121.25
9	S	102	BCL	C4D-CHA-C1A	5.30	127.70	121.25
9	F	101	BCL	CHD-C1D-ND	-5.30	119.58	124.45
10	G	103	KGD	CAJ-CAL-CAM	-5.30	118.23	126.23
9	Q	101	BCL	C4D-CHA-C1A	5.29	127.69	121.25
9	8	102	BCL	C4D-CHA-C1A	5.28	127.67	121.25
9	D	102	BCL	C4D-CHA-C1A	5.27	127.67	121.25
9	U	102	BCL	C4D-CHA-C1A	5.27	127.66	121.25
9	T	101	BCL	CHD-C1D-ND	-5.26	119.62	124.45
9	L	1001	BCL	CHD-C1D-ND	-5.26	119.62	124.45
9	3	101	BCL	CHD-C1D-ND	-5.26	119.62	124.45
9	D	101	BCL	C4D-CHA-C1A	5.25	127.64	121.25
9	J	101	BCL	CHD-C1D-ND	-5.24	119.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	101	BCL	C4D-CHA-C1A	5.24	127.63	121.25
9	K	101	BCL	C4D-CHA-C1A	5.23	127.61	121.25
9	3	101	BCL	C4D-CHA-C1A	5.22	127.60	121.25
9	K	102	BCL	C4D-CHA-C1A	5.21	127.59	121.25
9	P	102	BCL	C4D-CHA-C1A	5.21	127.59	121.25
9	B	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
9	0	102	BCL	C4D-CHA-C1A	5.20	127.58	121.25
9	S	101	BCL	C4D-CHA-C1A	5.19	127.57	121.25
9	O	102	BCL	C4D-CHA-C1A	5.19	127.56	121.25
9	4	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
9	F	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
9	E	101	BCL	C4D-CHA-C1A	5.17	127.54	121.25
9	6	101	BCL	C4D-CHA-C1A	5.17	127.54	121.25
9	9	102	BCL	C4D-CHA-C1A	5.16	127.53	121.25
9	P	102	BCL	CHD-C1D-ND	-5.16	119.71	124.45
9	A	101	BCL	C4D-CHA-C1A	5.13	127.49	121.25
9	9	102	BCL	CHD-C1D-ND	-5.13	119.74	124.45
9	H	102	BCL	CHD-C1D-ND	-5.13	119.74	124.45
9	6	101	BCL	CHD-C1D-ND	-5.12	119.75	124.45
10	O	103	KGD	CAP-CAO-CAM	-5.12	120.00	127.31
9	2	102	BCL	C4D-CHA-C1A	5.12	127.48	121.25
9	G	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
9	N	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
10	I	104	KGD	CBG-CBI-CBL	-5.09	120.05	127.31
9	O	101	BCL	C4D-CHA-C1A	5.09	127.44	121.25
9	O	101	BCL	CHD-C1D-ND	-5.08	119.79	124.45
9	5	101	BCL	CHD-C1D-ND	-5.08	119.79	124.45
9	V	101	BCL	C4D-CHA-C1A	5.07	127.42	121.25
9	6	102	BCL	C4D-CHA-C1A	5.06	127.41	121.25
9	K	101	BCL	CHD-C1D-ND	-5.06	119.80	124.45
9	7	101	BCL	CHD-C1D-ND	-5.04	119.82	124.45
9	I	102	BCL	C4D-CHA-C1A	5.03	127.37	121.25
9	N	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
9	J	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
9	0	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
9	T	101	BCL	C4D-CHA-C1A	5.01	127.34	121.25
9	2	101	BCL	CHD-C1D-ND	-4.99	119.87	124.45
9	8	101	BCL	CHD-C1D-ND	-4.99	119.87	124.45
9	R	101	BCL	C4D-CHA-C1A	4.99	127.32	121.25
9	M	703	BCL	C4D-CHA-C1A	4.99	127.32	121.25
9	D	102	BCL	CHD-C1D-ND	-4.98	119.87	124.45
9	1	101	BCL	C4D-CHA-C1A	4.98	127.31	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	1002	BCL	CHD-C1D-ND	-4.98	119.88	124.45
9	5	101	BCL	C4D-CHA-C1A	4.97	127.29	121.25
9	W	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
9	S	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
9	M	703	BCL	CHD-C1D-ND	-4.95	119.90	124.45
9	X	101	BCL	CHD-C1D-ND	-4.95	119.91	124.45
9	G	101	BCL	CHD-C1D-ND	-4.94	119.91	124.45
9	1	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
9	Q	102	BCL	CHD-C1D-ND	-4.93	119.92	124.45
9	4	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
9	2	102	BCL	CHD-C1D-ND	-4.93	119.93	124.45
9	L	1001	BCL	C4D-CHA-C1A	4.92	127.24	121.25
9	L	1002	BCL	C4D-CHA-C1A	4.92	127.23	121.25
9	2	101	BCL	C4D-CHA-C1A	4.92	127.23	121.25
9	Q	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
10	5	103	KGD	CBG-CBI-CBL	-4.91	120.31	127.31
10	C	401	KGD	CBB-CAV-CAR	-4.90	120.31	127.31
9	E	101	BCL	CHD-C1D-ND	-4.89	119.96	124.45
9	0	102	BCL	CHD-C1D-ND	-4.89	119.96	124.45
9	S	102	BCL	CHD-C1D-ND	-4.88	119.97	124.45
9	I	101	BCL	CHD-C1D-ND	-4.88	119.97	124.45
9	B	101	BCL	CHD-C1D-ND	-4.87	119.98	124.45
9	G	102	BCL	CHD-C1D-ND	-4.87	119.98	124.45
10	6	103	KGD	CBB-CAV-CAR	-4.87	120.36	127.31
9	U	101	BCL	CHD-C1D-ND	-4.86	119.99	124.45
9	8	102	BCL	CHD-C1D-ND	-4.86	119.99	124.45
9	6	102	BCL	CHD-C1D-ND	-4.85	119.99	124.45
9	I	102	BCL	CHD-C1D-ND	-4.85	120.00	124.45
9	B	102	BCL	CHD-C1D-ND	-4.84	120.00	124.45
10	H	101	KGD	CBG-CBI-CBL	-4.83	120.41	127.31
10	C	401	KGD	CAJ-CAL-CAM	-4.82	118.95	126.23
10	4	103	KGD	CBG-CBI-CBL	-4.82	120.43	127.31
9	S	101	BCL	C1-C2-C3	-4.82	117.71	126.04
9	O	102	BCL	CHD-C1D-ND	-4.81	120.04	124.45
9	4	102	BCL	CHD-C1D-ND	-4.78	120.06	124.45
9	U	102	BCL	CHD-C1D-ND	-4.78	120.06	124.45
11	C	403	HEM	C1B-NB-C4B	4.76	109.99	105.07
11	C	403	HEM	CHD-C1D-ND	4.73	129.57	124.43
9	H	102	BCL	C4D-CHA-C1A	4.73	127.01	121.25
10	E	102	KGD	CBG-CBI-CBL	-4.70	120.60	127.31
9	K	102	BCL	CHD-C1D-ND	-4.69	120.14	124.45
10	T	102	KGD	CBG-CBI-CBL	-4.66	120.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	103	KGD	CBB-CAV-CAR	-4.66	120.66	127.31
10	U	103	KGD	CBB-CAV-CAR	-4.62	120.72	127.31
10	C	401	KGD	CBG-CBI-CBL	-4.62	120.72	127.31
10	I	103	KGD	CBG-CBI-CBL	-4.61	120.73	127.31
10	3	102	KGD	CBG-CBI-CBL	-4.60	120.74	127.31
12	L	1005	BPB	CBC-CAC-C3C	-4.59	114.53	126.70
9	7	101	BCL	C4D-CHA-C1A	4.58	126.83	121.25
10	G	103	KGD	CBG-CBI-CBL	-4.58	120.78	127.31
10	I	103	KGD	CAP-CAO-CAM	-4.58	120.78	127.31
10	K	103	KGD	CBG-CBI-CBL	-4.57	120.79	127.31
10	9	101	KGD	CBG-CBI-CBL	-4.57	120.79	127.31
9	6	101	BCL	C1-C2-C3	-4.55	118.17	126.04
10	O	103	KGD	CBG-CBI-CBL	-4.54	120.84	127.31
10	B	103	KGD	CBG-CBI-CBL	-4.51	120.88	127.31
10	Q	103	KGD	CAP-CAO-CAM	-4.50	120.89	127.31
10	E	103	KGD	CAJ-CAL-CAM	-4.50	119.44	126.23
10	K	103	KGD	CAP-CAO-CAM	-4.49	120.90	127.31
10	P	103	KGD	CBG-CBI-CBL	-4.48	120.91	127.31
10	K	103	KGD	CAJ-CAL-CAM	-4.48	119.47	126.23
12	L	1003	BPB	CBC-CAC-C3C	-4.46	114.86	126.70
9	K	101	BCL	C1-C2-C3	-4.46	118.33	126.04
10	8	103	KGD	CAJ-CAL-CAM	-4.43	119.55	126.23
10	6	103	KGD	CAP-CAO-CAM	-4.40	121.03	127.31
10	3	102	KGD	CBB-CAV-CAR	-4.40	121.03	127.31
10	K	103	KGD	CAE-CAI-CAH	-4.39	114.60	118.65
10	O	103	KGD	CAJ-CAL-CAM	-4.39	119.60	126.23
10	0	103	KGD	CAJ-CAL-CAM	-4.38	119.62	126.23
10	E	103	KGD	CAP-CAO-CAM	-4.37	121.07	127.31
10	U	103	KGD	CBG-CBB-CAV	-4.36	114.54	123.47
10	2	103	KGD	CBG-CBI-CBL	-4.34	121.12	127.31
9	O	101	BCL	C1-C2-C3	-4.32	118.57	126.04
10	6	103	KGD	CBG-CBI-CBL	-4.31	121.16	127.31
10	5	102	KGD	CBG-CBI-CBL	-4.28	121.20	127.31
10	E	103	KGD	CBG-CBI-CBL	-4.27	121.21	127.31
10	6	103	KGD	CAJ-CAL-CAM	-4.27	119.78	126.23
10	A	102	KGD	CBG-CBI-CBL	-4.24	121.26	127.31
9	I	101	BCL	C1-C2-C3	-4.23	118.73	126.04
12	M	704	BPB	CBC-CAC-C3C	-4.22	115.51	126.70
10	K	103	KGD	CBB-CAV-CAR	-4.20	121.31	127.31
9	G	101	BCL	C1-C2-C3	-4.17	118.83	126.04
10	W	102	KGD	CBG-CBI-CBL	-4.17	121.36	127.31
9	4	101	BCL	C1-C2-C3	-4.15	118.87	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	103	KGD	CBG-CBI-CBL	-4.14	121.40	127.31
10	5	102	KGD	CAP-CAO-CAM	-4.07	121.50	127.31
10	2	103	KGD	CAJ-CAL-CAM	-4.06	120.09	126.23
10	2	103	KGD	CAP-CAO-CAM	-4.03	121.56	127.31
10	E	102	KGD	CBB-CAV-CAR	-4.03	121.56	127.31
10	S	103	KGD	CBG-CBI-CBL	-4.02	121.57	127.31
10	R	102	KGD	CBG-CBI-CBL	-4.01	121.59	127.31
10	T	102	KGD	CBB-CAV-CAR	-4.00	121.60	127.31
10	J	102	KGD	CBG-CBI-CBL	-3.99	121.62	127.31
11	C	403	HEM	CAA-CBA-CGA	-3.97	102.62	113.76
10	8	103	KGD	CBG-CBI-CBL	-3.97	121.64	127.31
10	S	103	KGD	CAJ-CAL-CAM	-3.93	120.30	126.23
10	C	406	KGD	CAE-CAI-CAH	-3.91	115.05	118.65
10	3	102	KGD	CAP-CAO-CAM	-3.91	121.73	127.31
10	E	103	KGD	CBB-CAV-CAR	-3.88	121.77	127.31
10	9	101	KGD	CAJ-CAL-CAM	-3.87	120.39	126.23
10	J	102	KGD	CAJ-CAL-CAM	-3.84	120.44	126.23
10	J	102	KGD	CAP-CAO-CAM	-3.83	121.84	127.31
10	Q	103	KGD	CBG-CBI-CBL	-3.83	121.85	127.31
10	5	103	KGD	CAJ-CAL-CAM	-3.82	120.46	126.23
10	Q	103	KGD	CAJ-CAL-CAM	-3.79	120.51	126.23
9	X	101	BCL	CMB-C2B-C1B	-3.79	122.64	128.46
11	C	403	HEM	C3D-C4D-ND	-3.79	105.95	110.17
10	8	103	KGD	CAP-CAO-CAM	-3.78	121.91	127.31
9	M	703	BCL	CMB-C2B-C1B	-3.78	122.66	128.46
9	2	101	BCL	C1-C2-C3	-3.77	119.52	126.04
10	R	102	KGD	CAP-CAO-CAM	-3.77	121.93	127.31
10	P	101	KGD	CBG-CBI-CBL	-3.76	121.94	127.31
10	C	401	KGD	CBF-CBH-CBJ	-3.74	113.20	118.94
10	I	103	KGD	CAJ-CAL-CAM	-3.73	120.61	126.23
9	0	101	BCL	C1-C2-C3	-3.72	119.60	126.04
9	2	102	BCL	C4A-NA-C1A	3.72	108.38	106.71
10	S	103	KGD	CBG-CBB-CAV	-3.71	115.87	123.47
9	K	101	BCL	CMB-C2B-C1B	-3.71	122.77	128.46
10	I	104	KGD	CBB-CAV-CAR	-3.70	122.03	127.31
10	0	103	KGD	CAP-CAO-CAM	-3.68	122.06	127.31
9	8	101	BCL	C1-C2-C3	-3.66	119.71	126.04
10	3	102	KGD	CBM-CBJ-CBH	-3.64	122.11	127.31
10	U	103	KGD	CAJ-CAL-CAM	-3.64	120.73	126.23
10	Q	103	KGD	CAL-CAJ-CAD	-3.64	116.98	127.20
10	I	104	KGD	CBF-CBH-CBJ	-3.64	113.36	118.94
9	L	1001	BCL	C1D-ND-C4D	-3.62	103.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	101	BCL	C1D-ND-C4D	-3.62	103.77	106.33
10	8	103	KGD	CBB-CBG-CBI	-3.62	116.06	123.47
10	H	101	KGD	CAP-CAO-CAM	-3.60	122.17	127.31
10	W	102	KGD	CAP-CAO-CAM	-3.60	122.18	127.31
9	I	102	BCL	C4A-NA-C1A	3.59	108.32	106.71
9	R	101	BCL	C4A-NA-C1A	3.59	108.32	106.71
10	0	103	KGD	CBG-CBI-CBL	-3.58	122.20	127.31
9	Q	101	BCL	C1-C2-C3	-3.58	119.85	126.04
9	L	1002	BCL	CMB-C2B-C1B	-3.57	122.97	128.46
10	U	103	KGD	CAP-CAO-CAM	-3.57	122.21	127.31
10	P	101	KGD	CAP-CAO-CAM	-3.57	122.22	127.31
9	W	101	BCL	C1D-ND-C4D	-3.56	103.81	106.33
9	M	703	BCL	C4A-NA-C1A	3.56	108.31	106.71
9	Q	101	BCL	CMB-C2B-C1B	-3.55	123.01	128.46
9	G	101	BCL	CMB-C2B-C1B	-3.55	123.01	128.46
9	O	101	BCL	CMB-C2B-C1B	-3.54	123.02	128.46
9	N	101	BCL	CMB-C2B-C1B	-3.54	123.03	128.46
10	9	101	KGD	CAP-CAO-CAM	-3.54	122.26	127.31
9	F	101	BCL	CMB-C2B-C1B	-3.54	123.03	128.46
10	3	102	KGD	CAJ-CAL-CAM	-3.53	120.89	126.23
10	5	103	KGD	CAP-CAO-CAM	-3.53	122.27	127.31
10	A	102	KGD	CAP-CAO-CAM	-3.52	122.28	127.31
9	4	101	BCL	CMB-C2B-C1B	-3.52	123.05	128.46
10	G	103	KGD	CAE-CAI-CAH	-3.52	115.41	118.65
10	E	102	KGD	CAL-CAJ-CAD	-3.52	117.32	127.20
9	J	101	BCL	CMB-C2B-C1B	-3.51	123.07	128.46
10	P	103	KGD	CAJ-CAL-CAM	-3.51	120.93	126.23
9	N	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
10	O	103	KGD	CBB-CAV-CAR	-3.50	122.31	127.31
10	T	102	KGD	CAJ-CAL-CAM	-3.49	120.96	126.23
9	P	102	BCL	C1D-ND-C4D	-3.49	103.86	106.33
9	0	101	BCL	CMB-C2B-C1B	-3.49	123.10	128.46
9	X	101	BCL	CHA-C1A-NA	-3.48	118.42	126.40
9	3	101	BCL	CMB-C2B-C1B	-3.48	123.12	128.46
10	P	103	KGD	CAE-CAI-CAH	-3.47	115.45	118.65
9	I	101	BCL	CMB-C2B-C1B	-3.47	123.13	128.46
10	8	103	KGD	CAE-CAI-CAH	-3.46	115.46	118.65
9	S	101	BCL	CMB-C2B-C1B	-3.46	123.15	128.46
9	S	102	BCL	C1D-ND-C4D	-3.46	103.88	106.33
9	2	102	BCL	C1D-ND-C4D	-3.46	103.88	106.33
9	8	102	BCL	CMB-C2B-C1B	-3.45	123.16	128.46
10	R	102	KGD	CAJ-CAL-CAM	-3.45	121.03	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	101	BCL	C1D-ND-C4D	-3.44	103.89	106.33
10	C	406	KGD	CAP-CAO-CAM	-3.44	122.40	127.31
9	D	102	BCL	CMB-C2B-C1B	-3.44	123.18	128.46
9	Q	102	BCL	C1D-ND-C4D	-3.44	103.89	106.33
9	6	101	BCL	CMB-C2B-C1B	-3.43	123.19	128.46
9	9	102	BCL	C1D-ND-C4D	-3.43	103.90	106.33
9	9	102	BCL	C4A-NA-C1A	3.43	108.25	106.71
9	B	101	BCL	CMB-C2B-C1B	-3.43	123.20	128.46
10	6	103	KGD	CBF-CBH-CBJ	-3.42	113.69	118.94
9	U	101	BCL	CMB-C2B-C1B	-3.42	123.21	128.46
13	M	701	MQE	CAY-CAX-CBQ	-3.41	114.85	118.50
10	U	103	KGD	CAL-CAJ-CAD	-3.41	117.61	127.20
9	M	703	BCL	C1D-ND-C4D	-3.41	103.91	106.33
9	U	101	BCL	CHA-C1A-NA	-3.40	118.60	126.40
9	F	101	BCL	C1D-ND-C4D	-3.40	103.92	106.33
10	8	103	KGD	CAL-CAJ-CAD	-3.39	117.68	127.20
9	8	101	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
9	B	101	BCL	C1-C2-C3	-3.39	120.18	126.04
9	W	101	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
9	V	101	BCL	C4A-NA-C1A	3.39	108.23	106.71
9	P	102	BCL	CMB-C2B-C1B	-3.38	123.26	128.46
9	2	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
9	T	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
10	2	103	KGD	CAL-CAJ-CAD	-3.38	117.70	127.20
9	I	102	BCL	CMB-C2B-C1B	-3.38	123.27	128.46
10	W	102	KGD	CAL-CAJ-CAD	-3.37	117.72	127.20
9	2	101	BCL	CMB-C2B-C1B	-3.37	123.28	128.46
10	U	103	KGD	CBF-CBH-CBJ	-3.37	113.77	118.94
10	9	101	KGD	CBB-CAV-CAR	-3.37	122.50	127.31
10	5	103	KGD	CBB-CAV-CAR	-3.37	122.50	127.31
10	T	102	KGD	CAL-CAJ-CAD	-3.37	117.74	127.20
9	9	102	BCL	CMB-C2B-C1B	-3.37	123.29	128.46
9	D	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
9	E	101	BCL	CMB-C2B-C1B	-3.36	123.30	128.46
10	S	103	KGD	CAL-CAJ-CAD	-3.36	117.77	127.20
9	A	101	BCL	C1D-ND-C4D	-3.36	103.95	106.33
10	S	103	KGD	CBB-CAV-CAR	-3.36	122.52	127.31
10	S	103	KGD	CBF-CBH-CBJ	-3.35	113.80	118.94
9	E	101	BCL	C1D-ND-C4D	-3.35	103.95	106.33
9	N	101	BCL	C4A-NA-C1A	3.35	108.21	106.71
9	L	1001	BCL	CMB-C2B-C1B	-3.35	123.32	128.46
10	P	101	KGD	CAJ-CAL-CAM	-3.35	121.18	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	102	BCL	CMB-C2B-C1B	-3.35	123.32	128.46
9	L	1002	BCL	C1D-ND-C4D	-3.34	103.96	106.33
10	P	101	KGD	CBM-CBJ-CBH	-3.34	122.54	127.31
10	I	104	KGD	CBG-CBB-CAV	-3.34	116.64	123.47
10	5	102	KGD	CAJ-CAL-CAM	-3.33	121.20	126.23
9	0	102	BCL	C1D-ND-C4D	-3.33	103.97	106.33
10	C	406	KGD	CBB-CBG-CBI	-3.33	116.66	123.47
9	G	102	BCL	C1D-ND-C4D	-3.33	103.97	106.33
9	I	102	BCL	C1D-ND-C4D	-3.33	103.97	106.33
9	U	101	BCL	C1-C2-C3	-3.33	120.29	126.04
9	3	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
9	R	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
10	C	401	KGD	CAL-CAJ-CAD	-3.32	117.86	127.20
9	6	102	BCL	CMB-C2B-C1B	-3.31	123.37	128.46
10	J	102	KGD	CBM-CBJ-CBH	-3.31	122.58	127.31
9	5	101	BCL	C1D-ND-C4D	-3.30	103.99	106.33
9	6	102	BCL	C1D-ND-C4D	-3.30	103.99	106.33
9	Q	101	BCL	CHA-C1A-NA	-3.30	118.85	126.40
9	4	102	BCL	CMB-C2B-C1B	-3.29	123.41	128.46
9	M	703	BCL	CHA-C1A-NA	-3.29	118.87	126.40
9	A	101	BCL	C4A-NA-C1A	3.29	108.18	106.71
9	R	101	BCL	CMB-C2B-C1B	-3.28	123.42	128.46
9	U	102	BCL	CHA-C1A-NA	-3.28	118.89	126.40
10	T	102	KGD	CAP-CAO-CAM	-3.28	122.63	127.31
10	C	406	KGD	CAL-CAJ-CAD	-3.28	118.00	127.20
10	A	102	KGD	CAL-CAJ-CAD	-3.27	118.02	127.20
11	C	403	HEM	CHC-C4B-NB	3.27	127.98	124.43
9	J	101	BCL	C4A-NA-C1A	3.26	108.17	106.71
9	4	102	BCL	CHA-C1A-NA	-3.26	118.93	126.40
9	I	101	BCL	CHA-C1A-NA	-3.26	118.93	126.40
10	G	103	KGD	CBB-CAV-CAR	-3.26	122.66	127.31
9	D	102	BCL	CHA-C1A-NA	-3.26	118.94	126.40
9	5	101	BCL	CMB-C2B-C1B	-3.25	123.47	128.46
10	S	103	KGD	CAZ-CAW-CAS	3.25	120.73	115.27
9	B	101	BCL	CHA-C1A-NA	-3.24	118.97	126.40
9	U	102	BCL	CMB-C2B-C1B	-3.24	123.48	128.46
9	0	101	BCL	CHA-C1A-NA	-3.24	118.99	126.40
9	O	102	BCL	C1D-ND-C4D	-3.23	104.04	106.33
9	T	101	BCL	CMB-C2B-C1B	-3.23	123.50	128.46
10	H	101	KGD	CAJ-CAL-CAM	-3.23	121.36	126.23
10	9	101	KGD	CAE-CAC-CAB	-3.22	108.02	113.18
9	G	101	BCL	C1D-ND-C4D	-3.22	104.05	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	101	BCL	CMB-C2B-C1B	-3.21	123.52	128.46
9	8	102	BCL	C1D-ND-C4D	-3.21	104.05	106.33
10	5	102	KGD	CAL-CAJ-CAD	-3.21	118.18	127.20
9	4	101	BCL	CHA-C1A-NA	-3.21	119.05	126.40
10	6	103	KGD	CAL-CAJ-CAD	-3.20	118.21	127.20
9	S	101	BCL	CHA-C1A-NA	-3.20	119.06	126.40
10	P	103	KGD	CAP-CAO-CAM	-3.20	122.74	127.31
9	4	102	BCL	C1D-ND-C4D	-3.20	104.06	106.33
10	P	103	KGD	CAL-CAJ-CAD	-3.20	118.22	127.20
9	B	102	BCL	CHA-C1A-NA	-3.20	119.07	126.40
10	5	102	KGD	CAC-CAB-CAD	-3.20	105.56	110.48
9	K	102	BCL	C1D-ND-C4D	-3.19	104.07	106.33
9	W	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
9	I	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
9	7	101	BCL	CMB-C2B-C1B	-3.19	123.56	128.46
9	O	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
9	D	101	BCL	C4A-NA-C1A	3.19	108.14	106.71
9	F	101	BCL	C4A-NA-C1A	3.19	108.14	106.71
9	Q	102	BCL	CMB-C2B-C1B	-3.19	123.57	128.46
9	G	101	BCL	CHA-C1A-NA	-3.18	119.11	126.40
9	8	101	BCL	CHA-C1A-NA	-3.18	119.12	126.40
9	S	101	BCL	C1D-ND-C4D	-3.18	104.08	106.33
9	S	102	BCL	CMB-C2B-C1B	-3.18	123.58	128.46
9	Q	102	BCL	CHA-C1A-NA	-3.18	119.13	126.40
9	G	102	BCL	CHA-C1A-NA	-3.18	119.13	126.40
9	6	101	BCL	CHA-C1A-NA	-3.17	119.13	126.40
9	K	101	BCL	C1D-ND-C4D	-3.17	104.08	106.33
9	O	102	BCL	CMB-C2B-C1B	-3.17	123.59	128.46
9	K	102	BCL	CHA-C1A-NA	-3.17	119.14	126.40
10	J	102	KGD	CAC-CAB-CAD	-3.17	105.61	110.48
10	W	102	KGD	CBB-CAV-CAR	-3.16	122.80	127.31
10	J	102	KGD	CAL-CAJ-CAD	-3.16	118.32	127.20
9	B	102	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	K	101	BCL	CHA-C1A-NA	-3.16	119.16	126.40
10	H	101	KGD	CAL-CAJ-CAD	-3.16	118.33	127.20
9	O	101	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	U	102	BCL	C1D-ND-C4D	-3.15	104.09	106.33
9	0	102	BCL	CHA-C1A-NA	-3.15	119.19	126.40
10	T	102	KGD	CAC-CAB-CAD	-3.15	105.64	110.48
9	0	102	BCL	CMB-C2B-C1B	-3.14	123.63	128.46
9	D	102	BCL	C1D-ND-C4D	-3.13	104.11	106.33
9	Q	101	BCL	C1D-ND-C4D	-3.13	104.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	102	BCL	CMB-C2B-C1B	-3.13	123.65	128.46
9	L	1001	BCL	C2A-C1A-CHA	3.13	129.33	123.86
10	Q	103	KGD	CBG-CBB-CAV	-3.13	117.07	123.47
10	B	103	KGD	CBB-CAV-CAR	-3.13	122.85	127.31
9	2	101	BCL	CHA-C1A-NA	-3.13	119.24	126.40
10	3	102	KGD	CAL-CAJ-CAD	-3.12	118.43	127.20
9	B	102	BCL	CMB-C2B-C1B	-3.12	123.67	128.46
9	6	101	BCL	C1D-ND-C4D	-3.12	104.12	106.33
9	2	102	BCL	CMB-C2B-C1B	-3.12	123.67	128.46
9	O	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
10	8	103	KGD	CBF-CBH-CBJ	-3.12	114.16	118.94
9	1	101	BCL	C4A-NA-C1A	3.12	108.11	106.71
9	2	102	BCL	CHA-C1A-NA	-3.11	119.27	126.40
9	S	102	BCL	CHA-C1A-NA	-3.11	119.27	126.40
9	8	101	BCL	C1D-ND-C4D	-3.11	104.12	106.33
10	W	102	KGD	CAJ-CAL-CAM	-3.11	121.54	126.23
9	G	102	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
9	4	101	BCL	C1D-ND-C4D	-3.10	104.13	106.33
10	E	102	KGD	CAE-CAI-CAH	-3.10	115.79	118.65
10	P	101	KGD	CBB-CAV-CAR	-3.10	122.89	127.31
9	0	101	BCL	C1D-ND-C4D	-3.10	104.14	106.33
10	J	102	KGD	CBB-CAV-CAR	-3.09	122.90	127.31
9	G	102	BCL	C4A-NA-C1A	3.09	108.09	106.71
9	8	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
10	R	102	KGD	CAL-CAJ-CAD	-3.09	118.53	127.20
10	H	101	KGD	CBF-CBH-CBJ	-3.08	114.21	118.94
9	B	101	BCL	C1D-ND-C4D	-3.08	104.15	106.33
9	P	102	BCL	C4A-NA-C1A	3.08	108.09	106.71
9	H	102	BCL	CHA-C1A-NA	-3.07	119.36	126.40
9	6	102	BCL	CHA-C1A-NA	-3.07	119.38	126.40
9	T	101	BCL	C4A-NA-C1A	3.06	108.08	106.71
9	5	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
9	1	101	BCL	C1D-ND-C4D	-3.05	104.17	106.33
9	7	101	BCL	C1D-ND-C4D	-3.05	104.17	106.33
9	J	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40
9	U	101	BCL	C1D-ND-C4D	-3.04	104.18	106.33
9	D	101	BCL	CMB-C2B-C1B	-3.03	123.80	128.46
9	K	102	BCL	C4A-NA-C1A	3.03	108.07	106.71
10	O	103	KGD	CAL-CAJ-CAD	-3.03	118.69	127.20
9	L	1001	BCL	CHA-C1A-NA	-3.03	119.46	126.40
10	S	103	KGD	CAP-CAO-CAM	-3.03	122.98	127.31
9	1	101	BCL	CMB-C2B-C1B	-3.03	123.81	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	1002	BCL	C4A-NA-C1A	3.03	108.07	106.71
10	0	103	KGD	CAL-CAJ-CAD	-3.02	118.71	127.20
10	P	101	KGD	CAL-CAJ-CAD	-3.02	118.73	127.20
9	E	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
12	L	1003	BPB	CMB-C2B-C3B	3.02	130.32	124.68
9	H	102	BCL	C1D-ND-C4D	-3.02	104.19	106.33
9	1	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
9	I	101	BCL	C1D-ND-C4D	-3.01	104.20	106.33
10	P	103	KGD	CBB-CAV-CAR	-3.01	123.02	127.31
10	2	103	KGD	CAE-CAI-CAH	-3.01	115.88	118.65
10	9	101	KGD	CBM-CBJ-CBH	-3.01	123.02	127.31
9	V	101	BCL	CMB-C2B-C1B	-3.00	123.86	128.46
10	B	103	KGD	CBF-CBH-CBJ	-3.00	114.34	118.94
10	5	103	KGD	CAE-CAC-CAB	-3.00	108.37	113.18
10	Q	103	KGD	CAE-CAI-CAH	-2.99	115.89	118.65
10	I	103	KGD	CAL-CAJ-CAD	-2.98	118.82	127.20
9	X	101	BCL	C1D-ND-C4D	-2.98	104.22	106.33
9	7	101	BCL	C4A-NA-C1A	2.98	108.05	106.71
9	T	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
11	C	402	HEM	C3B-C2B-C1B	2.98	108.69	106.49
10	Q	103	KGD	CBF-CBH-CBJ	-2.97	114.38	118.94
9	L	1002	BCL	CHA-C1A-NA	-2.97	119.60	126.40
10	8	103	KGD	CAZ-CAW-CAS	2.97	120.27	115.27
9	N	101	BCL	CHA-C1A-NA	-2.96	119.61	126.40
10	0	103	KGD	CBG-CBB-CAV	-2.96	117.41	123.47
10	6	103	KGD	CAZ-CAW-CAS	2.96	120.25	115.27
10	0	103	KGD	CAE-CAI-CAH	-2.96	115.92	118.65
9	0	102	BCL	C4A-NA-C1A	2.96	108.03	106.71
11	C	405	HEM	CBB-CAB-C3B	-2.96	112.91	127.62
10	I	104	KGD	CAL-CAJ-CAD	-2.95	118.92	127.20
10	E	102	KGD	CAJ-CAL-CAM	-2.94	121.79	126.23
10	B	103	KGD	CAE-CAI-CAH	-2.94	115.94	118.65
10	C	406	KGD	CAJ-CAL-CAM	-2.94	121.80	126.23
10	E	102	KGD	CBM-CBJ-CBH	-2.94	123.12	127.31
9	O	102	BCL	C4A-NA-C1A	2.93	108.03	106.71
9	D	101	BCL	CHA-C1A-NA	-2.93	119.68	126.40
10	J	102	KGD	CBM-CBN-CBL	-2.93	118.18	126.42
9	F	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
9	X	101	BCL	C1-C2-C3	-2.93	120.97	126.04
9	4	102	BCL	C4A-NA-C1A	2.92	108.02	106.71
10	4	103	KGD	CBM-CBJ-CBH	-2.92	123.14	127.31
10	C	406	KGD	CBG-CBI-CBL	-2.92	123.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	103	KGD	CAZ-CAW-CAS	2.92	120.18	115.27
10	8	103	KGD	CAQ-CAR-CAV	-2.92	114.47	118.94
10	C	401	KGD	CAC-CAB-CAD	-2.92	105.99	110.48
9	V	101	BCL	CHA-C1A-NA	-2.90	119.75	126.40
10	S	103	KGD	CAE-CAI-CAH	-2.90	115.98	118.65
10	E	103	KGD	CAL-CAJ-CAD	-2.90	119.06	127.20
10	A	102	KGD	CAJ-CAL-CAM	-2.90	121.86	126.23
9	P	102	BCL	CHA-C1A-NA	-2.90	119.76	126.40
11	C	403	HEM	O2D-CGD-O1D	-2.90	116.08	123.30
9	3	101	BCL	C4A-NA-C1A	2.89	108.01	106.71
9	3	101	BCL	CHA-C1A-NA	-2.89	119.77	126.40
10	5	103	KGD	CAL-CAJ-CAD	-2.89	119.08	127.20
9	8	102	BCL	C4A-NA-C1A	2.89	108.00	106.71
9	7	101	BCL	CHA-C1A-NA	-2.89	119.79	126.40
9	A	101	BCL	CHA-C1A-NA	-2.89	119.79	126.40
9	R	101	BCL	CHA-C1A-NA	-2.88	119.79	126.40
10	4	103	KGD	CAL-CAM-CAO	2.88	123.37	118.94
10	G	103	KGD	CBF-CBH-CBJ	-2.88	114.52	118.94
10	I	104	KGD	CAE-CAC-CAB	-2.86	108.58	113.18
9	W	101	BCL	C4A-NA-C1A	2.86	107.99	106.71
9	9	102	BCL	CHA-C1A-NA	-2.86	119.85	126.40
10	C	401	KGD	CAZ-CAW-CAS	2.86	120.08	115.27
12	L	1005	BPB	C1A-C2A-C3A	-2.86	100.12	102.84
10	H	101	KGD	CBB-CAV-CAR	-2.85	123.24	127.31
10	G	103	KGD	CBG-CBB-CAV	-2.85	117.64	123.47
10	P	101	KGD	CAE-CAC-CAB	-2.84	108.61	113.18
10	C	406	KGD	CAC-CAE-CAI	-2.84	107.76	112.85
10	K	103	KGD	CAL-CAJ-CAD	-2.84	119.22	127.20
10	3	102	KGD	CBG-CBB-CAV	-2.84	117.66	123.47
10	5	103	KGD	CAE-CAI-CAH	-2.83	116.04	118.65
10	U	103	KGD	CAZ-CAW-CAS	2.83	120.04	115.27
10	W	102	KGD	CBM-CBJ-CBH	-2.83	123.27	127.31
9	S	102	BCL	C4A-NA-C1A	2.83	107.98	106.71
10	P	101	KGD	CAC-CAB-CAD	-2.81	106.15	110.48
10	U	103	KGD	CAC-CAB-CAD	-2.81	106.15	110.48
10	J	102	KGD	CAE-CAC-CAB	-2.81	108.67	113.18
10	9	101	KGD	CAC-CAB-CAD	-2.81	106.16	110.48
10	E	103	KGD	CAE-CAC-CAB	-2.81	108.68	113.18
10	Q	103	KGD	CBB-CAV-CAR	-2.80	123.31	127.31
10	R	102	KGD	CBB-CAV-CAR	-2.80	123.31	127.31
10	9	101	KGD	CAL-CAJ-CAD	-2.80	119.33	127.20
9	5	101	BCL	C4A-NA-C1A	2.80	107.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	104	KGD	CAC-CAB-CAD	-2.80	106.17	110.48
9	D	102	BCL	C1-C2-C3	-2.79	121.22	126.04
10	5	102	KGD	CAE-CAC-CAB	-2.79	108.70	113.18
10	6	103	KGD	CAE-CAC-CAB	-2.78	108.71	113.18
9	H	102	BCL	C4A-NA-C1A	2.77	107.95	106.71
10	E	103	KGD	CAE-CAI-CAH	-2.77	116.10	118.65
9	6	102	BCL	C4A-NA-C1A	2.76	107.95	106.71
10	G	103	KGD	CAZ-CAW-CAS	2.76	119.92	115.27
13	L	1004	MQE	CAY-CAX-CBQ	-2.76	115.54	118.50
11	C	403	HEM	CHA-C4D-ND	2.76	127.79	124.38
10	U	103	KGD	CAE-CAC-CAB	-2.76	108.76	113.18
12	L	1005	BPB	CMC-C2C-C1C	-2.75	109.73	114.36
10	U	103	KGD	CBJ-CBM-CBN	-2.75	114.65	123.22
10	I	103	KGD	CAC-CAB-CAD	-2.74	106.26	110.48
10	O	103	KGD	CAZ-CAW-CAS	2.74	119.88	115.27
10	C	401	KGD	CAE-CAI-CAH	-2.74	116.12	118.65
10	C	401	KGD	CAE-CAC-CAB	-2.73	108.79	113.18
10	I	103	KGD	CAE-CAC-CAB	-2.73	108.79	113.18
11	C	405	HEM	CBA-CAA-C2A	-2.73	107.96	112.62
10	2	103	KGD	CAZ-CAW-CAS	2.71	119.84	115.27
9	E	101	BCL	C4A-NA-C1A	2.71	107.93	106.71
9	B	101	BCL	C2A-C1A-CHA	2.71	128.60	123.86
10	5	103	KGD	CBM-CBJ-CBH	-2.71	123.44	127.31
9	S	101	BCL	C2A-C1A-CHA	2.71	128.59	123.86
9	X	101	BCL	CMB-C2B-C3B	2.70	129.74	124.68
10	3	102	KGD	CAE-CAC-CAB	-2.70	108.85	113.18
10	P	103	KGD	CBM-CBJ-CBH	-2.69	123.47	127.31
9	M	703	BCL	CMB-C2B-C3B	2.68	129.69	124.68
10	C	406	KGD	CAZ-CAW-CAS	2.68	119.78	115.27
10	O	103	KGD	CAE-CAC-CAB	-2.68	108.88	113.18
10	Q	103	KGD	CAE-CAC-CAB	-2.68	108.88	113.18
11	C	403	HEM	CBA-CAA-C2A	2.67	117.18	112.62
10	0	103	KGD	CBB-CAV-CAR	-2.67	123.50	127.31
10	C	406	KGD	CBM-CBN-CBL	-2.67	118.92	126.42
10	W	102	KGD	CAE-CAI-CAH	-2.66	116.19	118.65
10	B	103	KGD	CBG-CBB-CAV	-2.66	118.02	123.47
10	6	103	KGD	CAE-CAI-CAH	-2.65	116.21	118.65
10	3	102	KGD	CAE-CAI-CAH	-2.64	116.21	118.65
10	A	102	KGD	CAE-CAC-CAB	-2.64	108.94	113.18
10	6	103	KGD	CAC-CAB-CAD	-2.64	106.42	110.48
10	I	104	KGD	CAZ-CAW-CAS	2.63	119.70	115.27
10	T	102	KGD	CBM-CBJ-CBH	-2.63	123.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	101	BCL	CMB-C2B-C3B	2.62	129.58	124.68
10	4	103	KGD	CAN-CAM-CAL	-2.62	113.95	118.08
10	J	102	KGD	CBG-CBB-CAV	-2.62	118.11	123.47
10	O	103	KGD	CAE-CAI-CAH	-2.61	116.24	118.65
10	R	102	KGD	CBM-CBJ-CBH	-2.61	123.59	127.31
10	B	103	KGD	CAZ-CAW-CAS	2.60	119.64	115.27
10	E	102	KGD	CBE-CBF-CBH	-2.60	119.12	126.42
10	E	103	KGD	CAZ-CAW-CAS	2.59	119.63	115.27
10	H	101	KGD	CAE-CAC-CAB	-2.59	109.03	113.18
10	5	102	KGD	CBM-CBJ-CBH	-2.59	123.62	127.31
10	C	401	KGD	CBB-CBG-CBI	-2.58	118.18	123.47
10	2	103	KGD	CBB-CAV-CAR	-2.58	123.63	127.31
9	K	101	BCL	C2A-C1A-CHA	2.58	128.36	123.86
10	K	103	KGD	CAZ-CAW-CAS	2.58	119.60	115.27
9	F	101	BCL	CMB-C2B-C3B	2.57	129.49	124.68
10	H	101	KGD	CAC-CAB-CAD	-2.57	106.53	110.48
10	5	102	KGD	CBB-CAV-CAR	-2.56	123.66	127.31
10	B	103	KGD	CAE-CAC-CAB	-2.56	109.08	113.18
10	6	103	KGD	CBG-CBB-CAV	-2.55	118.25	123.47
10	S	103	KGD	CAE-CAC-CAB	-2.55	109.09	113.18
9	Q	102	BCL	C4A-NA-C1A	2.55	107.85	106.71
9	N	101	BCL	CMB-C2B-C3B	2.54	129.44	124.68
9	4	101	BCL	C2A-C1A-CHA	2.54	128.30	123.86
9	J	101	BCL	CMB-C2B-C3B	2.54	129.43	124.68
9	L	1002	BCL	CMB-C2B-C3B	2.54	129.43	124.68
9	Q	101	BCL	C2A-C1A-CHA	2.54	128.29	123.86
9	U	101	BCL	C2A-C1A-CHA	2.54	128.29	123.86
9	4	101	BCL	CMB-C2B-C3B	2.53	129.42	124.68
9	O	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
9	Q	101	BCL	CMB-C2B-C3B	2.52	129.40	124.68
10	2	103	KGD	CAE-CAC-CAB	-2.52	109.13	113.18
10	G	103	KGD	CAL-CAJ-CAD	-2.52	120.13	127.20
9	O	101	BCL	CMB-C2B-C3B	2.51	129.38	124.68
10	6	103	KGD	CAO-CAP-CAQ	-2.51	115.38	123.22
10	A	102	KGD	CAE-CAI-CAH	-2.51	116.34	118.65
10	E	103	KGD	CAC-CAB-CAD	-2.51	106.62	110.48
10	A	102	KGD	CBB-CAV-CAR	-2.51	123.73	127.31
10	E	102	KGD	CAP-CAO-CAM	-2.51	123.73	127.31
12	M	704	BPB	CMC-C2C-C1C	-2.51	110.15	114.36
9	3	101	BCL	C2A-C1A-CHA	2.50	128.23	123.86
9	G	101	BCL	CMB-C2B-C3B	2.50	129.36	124.68
10	A	102	KGD	CBG-CBB-CAV	-2.50	118.35	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	101	BCL	C2A-C1A-CHA	2.49	128.22	123.86
11	C	403	HEM	O2A-CGA-O1A	-2.49	117.09	123.30
9	3	101	BCL	CMB-C2B-C3B	2.49	129.33	124.68
10	3	102	KGD	CBE-CBF-CBH	-2.49	119.43	126.42
10	T	102	KGD	CAE-CAC-CAB	-2.48	109.19	113.18
9	8	101	BCL	C2A-C1A-CHA	2.48	128.20	123.86
10	C	406	KGD	CAN-CAM-CAL	-2.48	114.17	118.08
10	E	103	KGD	CBF-CBH-CBJ	-2.48	115.13	118.94
9	N	101	BCL	C2A-C1A-CHA	2.48	128.20	123.86
11	C	403	HEM	O2D-CGD-CBD	2.48	122.00	114.03
9	6	101	BCL	C2A-C1A-CHA	2.48	128.20	123.86
11	C	403	HEM	CBD-CAD-C3D	-2.48	105.74	112.63
9	0	101	BCL	CMB-C2B-C3B	2.47	129.30	124.68
10	4	103	KGD	CAP-CAQ-CAR	-2.47	119.48	126.42
10	J	102	KGD	CAZ-CAW-CAS	2.47	119.42	115.27
10	O	103	KGD	CBF-CBH-CBJ	-2.46	115.16	118.94
9	L	1001	BCL	CMB-C2B-C3B	2.46	129.28	124.68
10	3	102	KGD	CAC-CAB-CAD	-2.46	106.69	110.48
9	D	102	BCL	CMB-C2B-C3B	2.46	129.28	124.68
13	M	705	MQE	CCE-CBK-CBS	-2.45	112.20	116.27
12	L	1003	BPB	CMC-C2C-C1C	-2.45	110.24	114.36
9	B	101	BCL	CMB-C2B-C3B	2.45	129.27	124.68
10	I	104	KGD	CBJ-CBM-CBN	-2.45	115.57	123.22
10	H	101	KGD	CBM-CBN-CBL	-2.45	119.54	126.42
10	C	401	KGD	CBJ-CBM-CBN	-2.45	115.58	123.22
9	I	101	BCL	C2A-C1A-CHA	2.44	128.13	123.86
9	T	101	BCL	C2A-C1A-CHA	2.44	128.13	123.86
9	S	101	BCL	CMB-C2B-C3B	2.44	129.24	124.68
10	O	103	KGD	CAC-CAB-CAD	-2.44	106.73	110.48
9	P	102	BCL	CMB-C2B-C3B	2.43	129.22	124.68
9	9	102	BCL	C2A-C1A-CHA	2.43	128.10	123.86
10	5	103	KGD	CAC-CAB-CAD	-2.43	106.74	110.48
9	U	101	BCL	CMB-C2B-C3B	2.43	129.22	124.68
10	A	102	KGD	CAC-CAB-CAD	-2.42	106.75	110.48
9	2	101	BCL	C2A-C1A-CHA	2.42	128.09	123.86
10	B	103	KGD	CAK-CAH-CAI	-2.42	111.89	115.48
9	6	101	BCL	CMB-C2B-C3B	2.42	129.20	124.68
10	J	102	KGD	CAE-CAI-CAH	-2.42	116.42	118.65
10	G	103	KGD	CAE-CAC-CAB	-2.42	109.30	113.18
9	9	102	BCL	CMB-C2B-C3B	2.42	129.20	124.68
9	I	101	BCL	CMB-C2B-C3B	2.41	129.19	124.68
11	C	403	HEM	CMB-C2B-C1B	2.40	128.70	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	1005	BPB	CMB-C2B-C3B	2.40	129.18	124.68
12	M	704	BPB	CMB-C2B-C3B	2.39	129.16	124.68
9	G	101	BCL	C2A-C1A-CHA	2.39	128.04	123.86
10	H	101	KGD	CAZ-CAW-CAS	2.39	119.30	115.27
9	R	101	BCL	CMB-C2B-C3B	2.39	129.15	124.68
9	P	102	BCL	C2A-C1A-CHA	2.39	128.04	123.86
9	2	101	BCL	CMB-C2B-C3B	2.39	129.15	124.68
9	8	101	BCL	CMB-C2B-C3B	2.38	129.13	124.68
9	M	703	BCL	C2A-C1A-CHA	2.37	128.01	123.86
9	8	102	BCL	C1C-NC-C4C	2.37	107.77	106.71
9	D	101	BCL	C2A-C1A-CHA	2.37	128.00	123.86
10	I	104	KGD	CAE-CAI-CAH	-2.37	116.47	118.65
9	B	102	BCL	C4A-NA-C1A	2.36	107.77	106.71
9	S	102	BCL	C1-C2-C3	-2.36	121.95	126.04
9	U	102	BCL	C4A-NA-C1A	2.36	107.77	106.71
10	T	102	KGD	CBG-CBB-CAV	-2.36	118.64	123.47
9	2	102	BCL	C2A-C1A-CHA	2.36	127.98	123.86
9	7	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
9	6	102	BCL	C2A-C1A-CHA	2.35	127.96	123.86
9	D	102	BCL	C2A-C1A-CHA	2.35	127.96	123.86
9	O	102	BCL	C2A-C1A-CHA	2.35	127.96	123.86
10	P	103	KGD	CBM-CBN-CBL	-2.34	119.83	126.42
9	W	101	BCL	C1C-NC-C4C	2.34	107.76	106.71
10	9	101	KGD	CAE-CAI-CAH	-2.34	116.49	118.65
10	P	103	KGD	CAZ-CAW-CAS	2.34	119.21	115.27
10	U	103	KGD	CAE-CAI-CAH	-2.34	116.49	118.65
9	T	101	BCL	CMB-C2B-C3B	2.34	129.05	124.68
10	T	102	KGD	CAE-CAI-CAH	-2.33	116.51	118.65
11	C	402	HEM	CAA-CBA-CGA	-2.32	107.24	113.76
10	4	103	KGD	CAL-CAJ-CAD	-2.32	120.68	127.20
9	H	102	BCL	CMB-C2B-C3B	2.32	129.02	124.68
9	O	102	BCL	C1C-NC-C4C	2.32	107.75	106.71
12	L	1005	BPB	C1B-NB-C4B	2.32	111.85	107.09
9	F	101	BCL	C2A-C1A-CHA	2.32	127.91	123.86
11	C	403	HEM	C4A-C3A-C2A	2.32	108.61	107.00
9	5	101	BCL	CMB-C2B-C3B	2.32	129.01	124.68
9	A	101	BCL	CMB-C2B-C3B	2.32	129.01	124.68
10	H	101	KGD	CAE-CAI-CAH	-2.31	116.52	118.65
9	A	101	BCL	C2A-C1A-CHA	2.31	127.90	123.86
10	G	103	KGD	CAP-CAQ-CAR	-2.31	119.92	126.42
9	I	102	BCL	C2A-C1A-CHA	2.31	127.90	123.86
10	6	103	KGD	CBA-CBE-CBF	-2.31	116.01	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	102	KGD	CAZ-CAW-CAS	2.30	119.14	115.27
9	4	102	BCL	C2A-C1A-CHA	2.30	127.88	123.86
9	8	102	BCL	CMB-C2B-C3B	2.30	128.97	124.68
10	E	102	KGD	CBG-CBB-CAV	-2.29	118.78	123.47
10	R	102	KGD	CBG-CBB-CAV	-2.29	118.78	123.47
10	S	103	KGD	CAC-CAB-CAD	-2.29	106.95	110.48
10	E	103	KGD	CBM-CBJ-CBH	-2.29	124.04	127.31
9	5	101	BCL	C2A-C1A-CHA	2.28	127.85	123.86
9	1	101	BCL	C2A-C1A-CHA	2.28	127.85	123.86
9	J	101	BCL	C2A-C1A-CHA	2.28	127.85	123.86
9	6	102	BCL	C1C-NC-C4C	2.28	107.73	106.71
10	8	103	KGD	CAE-CAC-CAB	-2.27	109.53	113.18
10	B	103	KGD	CAP-CAQ-CAR	-2.27	120.03	126.42
10	E	102	KGD	CAN-CAM-CAO	2.27	126.11	122.92
9	E	101	BCL	C2A-C1A-CHA	2.27	127.83	123.86
10	T	102	KGD	CAZ-CAW-CAS	2.27	119.09	115.27
10	P	103	KGD	CBE-CBF-CBH	-2.27	120.05	126.42
9	K	102	BCL	C2A-C1A-CHA	2.26	127.82	123.86
9	R	101	BCL	C2A-C1A-CHA	2.26	127.80	123.86
13	M	705	MQE	CAY-CAX-CBQ	-2.25	116.09	118.50
10	E	103	KGD	CBG-CBB-CAV	-2.25	118.86	123.47
10	P	101	KGD	CBG-CBB-CAV	-2.25	118.86	123.47
10	4	103	KGD	CAZ-CAW-CAS	2.25	119.06	115.27
9	0	102	BCL	C2A-C1A-CHA	2.25	127.79	123.86
10	S	103	KGD	CBJ-CBM-CBN	-2.25	116.20	123.22
9	J	101	BCL	C1C-NC-C4C	2.24	107.71	106.71
9	I	102	BCL	CMB-C2B-C3B	2.24	128.87	124.68
10	T	102	KGD	CBF-CBH-CBJ	-2.24	115.51	118.94
10	P	101	KGD	CBM-CBN-CBL	-2.24	120.14	126.42
10	3	102	KGD	CAZ-CAW-CAS	2.23	119.03	115.27
9	W	101	BCL	C2A-C1A-CHA	2.23	127.76	123.86
12	M	704	BPB	C1B-NB-C4B	2.23	111.67	107.09
10	2	103	KGD	CBF-CBH-CBJ	-2.23	115.52	118.94
9	H	102	BCL	C2A-C1A-CHA	2.23	127.76	123.86
9	E	101	BCL	C1C-NC-C4C	2.23	107.71	106.71
11	C	403	HEM	CBB-CAB-C3B	-2.23	116.54	127.62
10	I	103	KGD	CBE-CBF-CBH	-2.23	120.17	126.42
10	E	102	KGD	CBM-CBN-CBL	-2.22	120.17	126.42
9	I	102	BCL	C1C-NC-C4C	2.22	107.71	106.71
9	W	101	BCL	CMB-C2B-C3B	2.22	128.84	124.68
10	Q	103	KGD	CBJ-CBM-CBN	-2.22	116.28	123.22
10	A	102	KGD	CBE-CBF-CBH	-2.22	120.18	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	102	BCL	C2A-C1A-CHA	2.22	127.74	123.86
10	Q	103	KGD	CAC-CAB-CAD	-2.22	107.07	110.48
9	7	101	BCL	CMB-C2B-C3B	2.22	128.82	124.68
10	W	102	KGD	CAZ-CAW-CAS	2.21	119.00	115.27
9	N	101	BCL	C1C-NC-C4C	2.21	107.70	106.71
10	S	103	KGD	CAP-CAQ-CAR	-2.21	120.22	126.42
12	L	1003	BPB	C1B-NB-C4B	2.20	111.62	107.09
10	W	102	KGD	CBG-CBB-CAV	-2.20	118.96	123.47
10	Q	103	KGD	CAP-CAQ-CAR	-2.20	120.23	126.42
10	H	101	KGD	CBG-CBB-CAV	-2.20	118.97	123.47
10	I	103	KGD	CAE-CAI-CAH	-2.20	116.62	118.65
10	K	103	KGD	CBF-CBH-CBJ	-2.20	115.57	118.94
10	8	103	KGD	CAC-CAB-CAD	-2.20	107.10	110.48
9	E	101	BCL	CMB-C2B-C3B	2.19	128.78	124.68
10	8	103	KGD	CAO-CAP-CAQ	-2.19	116.38	123.22
9	Q	102	BCL	C2A-C1A-CHA	2.19	127.69	123.86
10	O	103	KGD	CBM-CBJ-CBH	-2.19	124.19	127.31
9	6	102	BCL	CMB-C2B-C3B	2.19	128.77	124.68
11	C	403	HEM	C2D-C1D-ND	-2.19	107.26	109.88
9	S	102	BCL	C2A-C1A-CHA	2.18	127.68	123.86
11	C	405	HEM	C3B-C2B-C1B	2.18	108.11	106.49
9	V	101	BCL	C2A-C1A-CHA	2.18	127.67	123.86
11	C	404	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
10	P	101	KGD	CBE-CBF-CBH	-2.18	120.29	126.42
9	4	102	BCL	CMB-C2B-C3B	2.18	128.75	124.68
10	K	103	KGD	CBM-CBJ-CBH	-2.17	124.22	127.31
10	0	103	KGD	CBM-CBJ-CBH	-2.17	124.22	127.31
10	2	103	KGD	CBG-CBB-CAV	-2.16	119.04	123.47
9	U	102	BCL	C2A-C1A-CHA	2.16	127.64	123.86
10	0	103	KGD	CAZ-CAW-CAS	2.16	118.91	115.27
9	A	101	BCL	C1C-NC-C4C	2.15	107.67	106.71
10	5	103	KGD	CAP-CAQ-CAR	-2.15	120.39	126.42
10	W	102	KGD	CBE-CBF-CBH	-2.14	120.39	126.42
10	O	103	KGD	CBG-CBB-CAV	-2.14	119.08	123.47
9	F	101	BCL	C1C-NC-C4C	2.14	107.67	106.71
9	1	101	BCL	CMB-C2B-C3B	2.14	128.68	124.68
10	J	102	KGD	CBE-CBF-CBH	-2.14	120.40	126.42
10	A	102	KGD	CBM-CBJ-CBH	-2.14	124.26	127.31
10	0	103	KGD	CBF-CBH-CBJ	-2.14	115.66	118.94
10	2	103	KGD	CAC-CAB-CAD	-2.13	107.20	110.48
9	D	101	BCL	O2A-C1-C2	-2.13	103.03	108.64
9	S	102	BCL	C1C-NC-C4C	2.13	107.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	102	BCL	C1C-NC-C4C	2.13	107.66	106.71
9	Q	102	BCL	C1C-NC-C4C	2.13	107.66	106.71
10	S	103	KGD	CAN-CAM-CAO	2.13	125.90	122.92
10	T	102	KGD	CAP-CAQ-CAR	-2.12	120.45	126.42
10	P	101	KGD	CAE-CAI-CAH	-2.12	116.69	118.65
10	I	103	KGD	CBM-CBN-CBL	-2.12	120.45	126.42
9	U	102	BCL	CMB-C2B-C3B	2.12	128.64	124.68
9	S	102	BCL	CMB-C2B-C3B	2.12	128.64	124.68
9	V	101	BCL	CMB-C2B-C3B	2.12	128.64	124.68
9	Q	102	BCL	CMB-C2B-C3B	2.11	128.63	124.68
9	O	102	BCL	CMB-C2B-C3B	2.11	128.63	124.68
10	6	103	KGD	CBJ-CBM-CBN	-2.11	116.64	123.22
10	C	401	KGD	CAP-CAQ-CAR	-2.11	120.50	126.42
9	K	102	BCL	CMB-C2B-C3B	2.10	128.61	124.68
10	9	101	KGD	CBE-CBF-CBH	-2.10	120.51	126.42
10	5	103	KGD	CBG-CBB-CAV	-2.10	119.17	123.47
10	I	103	KGD	CBB-CBG-CBI	-2.10	119.17	123.47
9	E	101	BCL	OBB-CAB-CBB	-2.10	115.44	120.17
9	4	101	BCL	C17-C16-C15	2.10	122.88	113.24
9	L	1002	BCL	C2A-C1A-CHA	2.10	127.53	123.86
10	C	401	KGD	CBA-CBE-CBF	-2.09	116.68	123.22
10	B	103	KGD	CBM-CBJ-CBH	-2.09	124.32	127.31
9	K	101	BCL	C4A-NA-C1A	2.09	107.65	106.71
10	W	102	KGD	CAN-CAM-CAO	2.09	125.85	122.92
9	A	101	BCL	O2A-C1-C2	-2.09	103.14	108.64
10	I	103	KGD	CBM-CBJ-CBH	-2.09	124.33	127.31
9	0	102	BCL	CMB-C2B-C3B	2.09	128.58	124.68
10	I	103	KGD	CAZ-CAW-CAS	2.09	118.78	115.27
10	T	102	KGD	CBE-CBF-CBH	-2.09	120.56	126.42
10	5	102	KGD	CAZ-CAW-CAS	2.09	118.78	115.27
9	G	102	BCL	CMB-C2B-C3B	2.08	128.58	124.68
10	2	103	KGD	CBM-CBJ-CBH	-2.08	124.34	127.31
9	D	101	BCL	CMB-C2B-C3B	2.08	128.57	124.68
10	P	103	KGD	CAN-CAM-CAO	2.08	125.83	122.92
9	B	102	BCL	CMB-C2B-C3B	2.07	128.56	124.68
9	K	102	BCL	C1C-NC-C4C	2.07	107.64	106.71
9	1	101	BCL	O2A-C1-C2	-2.07	103.19	108.64
9	8	102	BCL	OBB-CAB-CBB	-2.07	115.51	120.17
9	M	703	BCL	OBB-CAB-CBB	-2.07	115.52	120.17
11	C	404	HEM	CBB-CAB-C3B	-2.06	117.35	127.62
9	I	102	BCL	OBB-CAB-CBB	-2.06	115.54	120.17
9	4	102	BCL	C1C-NC-C4C	2.05	107.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5	102	KGD	CBM-CBN-CBL	-2.05	120.65	126.42
9	L	1002	BCL	C6-C7-C8	-2.05	109.29	115.92
9	2	102	BCL	CMB-C2B-C3B	2.05	128.51	124.68
11	C	404	HEM	CMC-C2C-C3C	2.05	128.51	124.68
9	L	1002	BCL	C1C-NC-C4C	2.05	107.63	106.71
10	5	103	KGD	CBE-CBF-CBH	-2.04	120.67	126.42
9	X	101	BCL	OBb-CAB-CBB	-2.04	115.58	120.17
9	K	102	BCL	C1-C2-C3	-2.04	122.52	126.04
10	5	103	KGD	CBM-CBN-CBL	-2.04	120.70	126.42
10	R	102	KGD	CAZ-CAW-CAS	2.03	118.69	115.27
10	C	401	KGD	CBG-CBB-CAV	-2.03	119.31	123.47
10	B	103	KGD	CBJ-CBM-CBN	-2.03	116.88	123.22
10	5	102	KGD	CAE-CAI-CAH	-2.03	116.78	118.65
10	3	102	KGD	CAT-CAX-CAY	-2.03	120.81	127.75
10	C	406	KGD	CAN-CAM-CAO	2.03	125.76	122.92
10	8	103	KGD	CBJ-CBM-CBN	-2.03	116.89	123.22
9	S	101	BCL	C17-C16-C15	2.03	122.55	113.24
10	E	102	KGD	CAP-CAQ-CAR	-2.02	120.73	126.42
10	3	102	KGD	CBM-CBN-CBL	-2.02	120.73	126.42
10	C	406	KGD	CBB-CAV-CAR	-2.02	124.42	127.31
9	5	101	BCL	O2A-C1-C2	-2.02	103.33	108.64
10	S	103	KGD	CBA-CBE-CBF	-2.02	116.92	123.22
9	V	101	BCL	C1C-NC-C4C	2.02	107.61	106.71
10	W	102	KGD	CAT-CAX-CAY	-2.02	120.86	127.75
9	W	101	BCL	OBb-CAB-CBB	-2.01	115.64	120.17
10	J	102	KGD	CAP-CAQ-CAR	-2.01	120.77	126.42
9	G	102	BCL	C2A-C1A-CHA	2.01	127.37	123.86
10	K	103	KGD	CAC-CAB-CAD	-2.01	107.39	110.48
9	U	101	BCL	C17-C16-C15	2.01	122.46	113.24
10	I	103	KGD	CAQ-CAR-CAV	-2.01	115.86	118.94
11	C	404	HEM	CAD-CBD-CGD	-2.00	109.29	113.60
10	Q	103	KGD	CBM-CBJ-CBH	-2.00	124.45	127.31
10	E	103	KGD	CAP-CAQ-CAR	-2.00	120.79	126.42
9	F	101	BCL	O2A-C1-C2	-2.00	103.38	108.64

There are no chirality outliers.

All (598) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	4	101	BCL	C2-C3-C5-C6
9	4	101	BCL	C4-C3-C5-C6
9	4	102	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	4	102	BCL	C4-C3-C5-C6
9	5	101	BCL	CHA-CBD-CGD-O1D
9	5	101	BCL	CHA-CBD-CGD-O2D
9	6	102	BCL	C2-C3-C5-C6
9	6	102	BCL	C4-C3-C5-C6
9	8	101	BCL	C4-C3-C5-C6
9	8	102	BCL	C4-C3-C5-C6
9	9	102	BCL	CHA-CBD-CGD-O1D
9	9	102	BCL	CHA-CBD-CGD-O2D
9	B	101	BCL	C4-C3-C5-C6
9	B	102	BCL	C4C-C3C-CAC-CBC
9	D	101	BCL	CHA-CBD-CGD-O1D
9	D	101	BCL	CHA-CBD-CGD-O2D
9	G	101	BCL	C2-C3-C5-C6
9	G	101	BCL	C4-C3-C5-C6
9	G	102	BCL	C2C-C3C-CAC-CBC
9	G	102	BCL	C4C-C3C-CAC-CBC
9	I	101	BCL	C2-C3-C5-C6
9	I	101	BCL	C4-C3-C5-C6
9	I	102	BCL	C2C-C3C-CAC-CBC
9	I	102	BCL	C4C-C3C-CAC-CBC
9	J	101	BCL	CHA-CBD-CGD-O1D
9	J	101	BCL	CHA-CBD-CGD-O2D
9	K	102	BCL	C2-C3-C5-C6
9	K	102	BCL	C4-C3-C5-C6
9	M	703	BCL	C2-C3-C5-C6
9	M	703	BCL	C4-C3-C5-C6
9	O	102	BCL	C2C-C3C-CAC-CBC
9	O	102	BCL	C4C-C3C-CAC-CBC
9	P	102	BCL	CHA-CBD-CGD-O1D
9	P	102	BCL	CHA-CBD-CGD-O2D
9	Q	102	BCL	C4C-C3C-CAC-CBC
9	S	101	BCL	C2-C3-C5-C6
9	S	101	BCL	C4-C3-C5-C6
9	S	102	BCL	C2C-C3C-CAC-CBC
9	S	102	BCL	C4C-C3C-CAC-CBC
9	S	102	BCL	C2-C3-C5-C6
9	S	102	BCL	C4-C3-C5-C6
9	U	101	BCL	C2-C3-C5-C6
9	U	101	BCL	C4-C3-C5-C6
9	U	102	BCL	C4-C3-C5-C6
9	W	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	W	101	BCL	C4-C3-C5-C6
9	X	101	BCL	C2-C3-C5-C6
9	X	101	BCL	C4-C3-C5-C6
10	2	103	KGD	CBE-CBF-CBH-CBJ
10	2	103	KGD	CBE-CBF-CBH-CBK
10	3	102	KGD	CAJ-CAL-CAM-CAN
10	3	102	KGD	CBE-CBF-CBH-CBJ
10	3	102	KGD	CBE-CBF-CBH-CBK
10	4	103	KGD	CAJ-CAL-CAM-CAN
10	4	103	KGD	CAJ-CAL-CAM-CAO
10	4	103	KGD	CAW-CAS-CAT-CAX
10	5	102	KGD	CAJ-CAL-CAM-CAN
10	5	102	KGD	CAJ-CAL-CAM-CAO
10	5	102	KGD	CBE-CBF-CBH-CBJ
10	5	102	KGD	CBE-CBF-CBH-CBK
10	5	103	KGD	CBE-CBF-CBH-CBJ
10	5	103	KGD	CBE-CBF-CBH-CBK
10	6	103	KGD	CAW-CAS-CAT-CAX
10	6	103	KGD	CAT-CAS-CAW-CAZ
10	6	103	KGD	CAT-CAS-CAW-CBA
10	8	103	KGD	CAR-CAV-CBB-CBG
10	9	101	KGD	CAJ-CAL-CAM-CAN
10	9	101	KGD	CAJ-CAL-CAM-CAO
10	A	102	KGD	CAJ-CAL-CAM-CAN
10	A	102	KGD	CAJ-CAL-CAM-CAO
10	A	102	KGD	CBE-CBF-CBH-CBJ
10	A	102	KGD	CBE-CBF-CBH-CBK
10	B	103	KGD	CAW-CAS-CAT-CAX
10	B	103	KGD	CAT-CAS-CAW-CAZ
10	B	103	KGD	CAT-CAS-CAW-CBA
10	C	401	KGD	CAT-CAS-CAW-CAZ
10	C	401	KGD	CAT-CAS-CAW-CBA
10	C	406	KGD	CBE-CBF-CBH-CBJ
10	C	406	KGD	CBE-CBF-CBH-CBK
10	E	102	KGD	CAJ-CAL-CAM-CAN
10	E	102	KGD	CAJ-CAL-CAM-CAO
10	E	102	KGD	CBE-CBF-CBH-CBJ
10	E	102	KGD	CBE-CBF-CBH-CBK
10	G	103	KGD	CAW-CAS-CAT-CAX
10	G	103	KGD	CAT-CAS-CAW-CAZ
10	G	103	KGD	CAT-CAS-CAW-CBA
10	H	101	KGD	CAJ-CAL-CAM-CAN

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Mol	Chain	Res	Type	Atoms
10	H	101	KGD	CAJ-CAL-CAM-CAO
10	H	101	KGD	CAW-CAS-CAT-CAX
10	I	103	KGD	CAJ-CAL-CAM-CAN
10	I	103	KGD	CAJ-CAL-CAM-CAO
10	I	103	KGD	CBE-CBF-CBH-CBJ
10	I	103	KGD	CBE-CBF-CBH-CBK
10	I	104	KGD	CAW-CAS-CAT-CAX
10	I	104	KGD	CAT-CAS-CAW-CAZ
10	I	104	KGD	CAT-CAS-CAW-CBA
10	J	102	KGD	CAJ-CAL-CAM-CAN
10	J	102	KGD	CBI-CBL-CBN-CBM
10	J	102	KGD	CBO-CBL-CBN-CBM
10	P	101	KGD	CAJ-CAL-CAM-CAN
10	P	101	KGD	CAJ-CAL-CAM-CAO
10	P	101	KGD	CAW-CAS-CAT-CAX
10	P	101	KGD	CBE-CBF-CBH-CBJ
10	P	101	KGD	CBE-CBF-CBH-CBK
10	P	103	KGD	CAJ-CAL-CAM-CAN
10	P	103	KGD	CAJ-CAL-CAM-CAO
10	P	103	KGD	CBE-CBF-CBH-CBJ
10	P	103	KGD	CBE-CBF-CBH-CBK
10	Q	103	KGD	CAW-CAS-CAT-CAX
10	Q	103	KGD	CAT-CAS-CAW-CAZ
10	Q	103	KGD	CAT-CAS-CAW-CBA
10	Q	103	KGD	CBE-CBF-CBH-CBK
10	R	102	KGD	CAJ-CAL-CAM-CAN
10	R	102	KGD	CAJ-CAL-CAM-CAO
10	T	102	KGD	CAJ-CAL-CAM-CAN
10	T	102	KGD	CAJ-CAL-CAM-CAO
10	T	102	KGD	CBE-CBF-CBH-CBJ
10	T	102	KGD	CBE-CBF-CBH-CBK
10	U	103	KGD	CAW-CAS-CAT-CAX
10	W	102	KGD	CAJ-CAL-CAM-CAN
10	W	102	KGD	CAJ-CAL-CAM-CAO
10	W	102	KGD	CBE-CBF-CBH-CBJ
10	W	102	KGD	CBE-CBF-CBH-CBK
11	C	403	HEM	C2B-C3B-CAB-CBB
11	C	403	HEM	C4B-C3B-CAB-CBB
11	C	404	HEM	C1A-C2A-CAA-CBA
11	C	404	HEM	C3A-C2A-CAA-CBA
11	C	404	HEM	C2B-C3B-CAB-CBB
11	C	405	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	C	405	HEM	C4B-C3B-CAB-CBB
12	L	1003	BPB	C2C-C3C-CAC-CBC
12	L	1003	BPB	C4C-C3C-CAC-CBC
12	L	1005	BPB	O2A-C1-C2-C3
12	L	1005	BPB	C2C-C3C-CAC-CBC
12	L	1005	BPB	C4C-C3C-CAC-CBC
12	M	704	BPB	C2C-C3C-CAC-CBC
13	L	1004	MQE	CAM-CAG-CAW-CBH
13	L	1004	MQE	CAM-CAG-CAW-CBY
13	L	1004	MQE	CAZ-CAU-CBA-CBN
13	M	701	MQE	CAR-CAE-CAL-CBF
13	M	701	MQE	CAT-CAF-CAK-CBE
13	M	701	MQE	CAV-CAH-CAO-CBI
13	M	701	MQE	CAS-CAN-CBB-CBL
13	M	701	MQE	CAS-CAN-CBB-CCA
14	L	1006	PGV	C2-C1-O01-C02
14	L	1007	PGV	C04-C05-C06-O06
14	L	1007	PGV	C2-C1-O01-C02
14	P	104	PGV	C2-C1-O01-C02
14	L	1006	PGV	O02-C1-O01-C02
14	L	1007	PGV	O02-C1-O01-C02
14	P	104	PGV	O02-C1-O01-C02
9	2	101	BCL	C4-C3-C5-C6
9	6	101	BCL	C4-C3-C5-C6
9	K	101	BCL	C4-C3-C5-C6
9	O	101	BCL	C4-C3-C5-C6
9	Q	101	BCL	C4-C3-C5-C6
9	8	102	BCL	C2-C3-C5-C6
9	B	101	BCL	C2-C3-C5-C6
9	O	101	BCL	C2-C3-C5-C6
9	U	102	BCL	C2-C3-C5-C6
9	0	101	BCL	C4-C3-C5-C6
9	0	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C4-C3-C5-C6
9	B	102	BCL	C4-C3-C5-C6
9	D	102	BCL	C4-C3-C5-C6
9	E	101	BCL	C4-C3-C5-C6
9	G	102	BCL	C4-C3-C5-C6
9	I	102	BCL	C4-C3-C5-C6
9	O	102	BCL	C4-C3-C5-C6
9	Q	102	BCL	C4-C3-C5-C6
10	8	103	KGD	CAT-CAS-CAW-CAZ

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Mol	Chain	Res	Type	Atoms
10	S	103	KGD	CAT-CAS-CAW-CAZ
10	U	103	KGD	CAT-CAS-CAW-CAZ
13	M	701	MQE	CAM-CAG-CAW-CBY
9	0	102	BCL	C2-C3-C5-C6
9	2	102	BCL	C2-C3-C5-C6
9	8	101	BCL	C2-C3-C5-C6
9	B	102	BCL	C2-C3-C5-C6
9	D	102	BCL	C2-C3-C5-C6
9	E	101	BCL	C2-C3-C5-C6
9	G	102	BCL	C2-C3-C5-C6
9	I	102	BCL	C2-C3-C5-C6
9	O	102	BCL	C2-C3-C5-C6
9	Q	102	BCL	C2-C3-C5-C6
10	8	103	KGD	CAT-CAS-CAW-CBA
10	S	103	KGD	CAT-CAS-CAW-CBA
10	U	103	KGD	CAT-CAS-CAW-CBA
13	M	701	MQE	CAM-CAG-CAW-CBH
10	0	103	KGD	CAW-CAS-CAT-CAX
10	2	103	KGD	CAW-CAS-CAT-CAX
10	3	102	KGD	CAW-CAS-CAT-CAX
10	5	102	KGD	CAW-CAS-CAT-CAX
10	I	103	KGD	CAW-CAS-CAT-CAX
10	K	103	KGD	CAW-CAS-CAT-CAX
10	P	103	KGD	CAW-CAS-CAT-CAX
13	L	1004	MQE	CAP-CAC-CAI-CBD
13	L	1004	MQE	CAV-CAH-CAO-CBI
13	L	1004	MQE	CCC-CCD-CCI-CCM
12	L	1003	BPB	C8-C10-C11-C12
12	M	704	BPB	CBA-CGA-O2A-C1
14	P	104	PGV	C20-C19-O03-C01
12	M	704	BPB	C13-C15-C16-C17
12	M	704	BPB	O1A-CGA-O2A-C1
9	6	101	BCL	C2-C3-C5-C6
9	K	101	BCL	C2-C3-C5-C6
9	Q	101	BCL	C2-C3-C5-C6
12	L	1003	BPB	C6-C7-C8-C9
10	C	401	KGD	CAJ-CAL-CAM-CAN
10	K	103	KGD	CAJ-CAL-CAM-CAN
10	P	101	KGD	CBO-CBL-CBN-CBM
10	R	102	KGD	CBE-CBF-CBH-CBK
9	E	101	BCL	C13-C15-C16-C17
9	0	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	S	102	BCL	C12-C13-C15-C16
9	X	101	BCL	C11-C10-C8-C7
12	M	704	BPB	C2A-CAA-CBA-CGA
14	P	104	PGV	O04-C19-O03-C01
10	5	103	KGD	CAW-CAS-CAT-CAX
10	8	103	KGD	CAW-CAS-CAT-CAX
10	E	103	KGD	CAW-CAS-CAT-CAX
10	T	102	KGD	CAW-CAS-CAT-CAX
13	M	701	MQE	CAQ-CAD-CAJ-CBC
13	M	701	MQE	CAW-CAG-CAM-CBG
13	M	701	MQE	CBB-CAN-CAS-CBH
14	P	104	PGV	O12-C04-C05-O05
9	2	102	BCL	C10-C11-C12-C13
9	Q	102	BCL	C10-C11-C12-C13
12	L	1003	BPB	C10-C11-C12-C13
14	L	1006	PGV	C04-O12-P-O11
14	P	104	PGV	C03-O11-P-O12
14	P	104	PGV	O12-C04-C05-C06
9	L	1002	BCL	C4-C3-C5-C6
10	O	103	KGD	CAT-CAS-CAW-CAZ
9	2	101	BCL	C2-C3-C5-C6
9	W	101	BCL	C16-C17-C18-C20
9	L	1001	BCL	C13-C15-C16-C17
9	8	102	BCL	C16-C17-C18-C20
9	3	101	BCL	C4-C3-C5-C6
9	7	101	BCL	C4-C3-C5-C6
12	L	1005	BPB	C14-C13-C15-C16
9	L	1001	BCL	C2A-CAA-CBA-CGA
10	C	406	KGD	CAJ-CAL-CAM-CAN
10	H	101	KGD	CBE-CBF-CBH-CBK
10	C	406	KGD	CAJ-CAL-CAM-CAO
10	J	102	KGD	CAJ-CAL-CAM-CAO
10	K	103	KGD	CAJ-CAL-CAM-CAO
12	L	1005	BPB	C10-C11-C12-C13
14	L	1006	PGV	C3-C4-C5-C6
9	M	703	BCL	C5-C6-C7-C8
9	1	101	BCL	C4-C3-C5-C6
9	F	101	BCL	C4-C3-C5-C6
9	0	101	BCL	C2-C3-C5-C6
9	1	101	BCL	C2-C3-C5-C6
9	3	101	BCL	C2-C3-C5-C6
9	F	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	L	1003	BPB	C2-C3-C5-C6
12	L	1003	BPB	C2A-CAA-CBA-CGA
14	L	1007	PGV	O05-C05-C06-O06
9	W	101	BCL	C16-C17-C18-C19
9	8	102	BCL	C16-C17-C18-C19
10	2	103	KGD	CAB-CAD-CAJ-CAL
10	2	103	KGD	CAH-CAD-CAJ-CAL
10	B	103	KGD	CAH-CAD-CAJ-CAL
10	C	401	KGD	CAH-CAD-CAJ-CAL
10	C	406	KGD	CAH-CAD-CAJ-CAL
10	K	103	KGD	CAB-CAD-CAJ-CAL
10	Q	103	KGD	CAB-CAD-CAJ-CAL
10	Q	103	KGD	CAH-CAD-CAJ-CAL
10	U	103	KGD	CAB-CAD-CAJ-CAL
9	N	101	BCL	C4-C3-C5-C6
9	T	101	BCL	C4-C3-C5-C6
13	L	1004	MQE	CAL-CAE-CAR-CBV
9	5	101	BCL	C11-C10-C8-C7
9	6	102	BCL	C12-C13-C15-C16
9	7	101	BCL	C2-C3-C5-C6
9	L	1002	BCL	C11-C12-C13-C15
9	N	101	BCL	C2-C3-C5-C6
9	O	102	BCL	C12-C13-C15-C16
9	R	101	BCL	C2-C3-C5-C6
9	T	101	BCL	C2-C3-C5-C6
9	O	102	BCL	C13-C15-C16-C17
11	C	404	HEM	C4B-C3B-CAB-CBB
9	R	101	BCL	C4-C3-C5-C6
12	L	1003	BPB	C4-C3-C5-C6
9	A	101	BCL	C2-C3-C5-C6
9	L	1002	BCL	C2-C3-C5-C6
10	O	103	KGD	CAT-CAS-CAW-CBA
13	L	1004	MQE	CAL-CAE-CAR-CBD
9	5	101	BCL	C11-C10-C8-C9
9	O	102	BCL	C14-C13-C15-C16
9	S	102	BCL	C14-C13-C15-C16
10	Q	103	KGD	CBE-CBF-CBH-CBJ
14	L	1007	PGV	O12-C04-C05-C06
9	B	102	BCL	C2C-C3C-CAC-CBC
11	C	402	HEM	C2A-CAA-CBA-CGA
14	P	104	PGV	C25-C26-C27-C28
9	A	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	D	101	BCL	C4-C3-C5-C6
9	P	102	BCL	C4-C3-C5-C6
14	L	1007	PGV	C21-C22-C23-C24
12	L	1003	BPB	CHA-CBD-CGD-O1D
12	L	1003	BPB	CHA-CBD-CGD-O2D
13	L	1004	MQE	CAO-CAH-CAV-CBX
9	B	102	BCL	C12-C13-C15-C16
9	D	101	BCL	C2-C3-C5-C6
9	L	1002	BCL	C6-C7-C8-C10
9	P	102	BCL	C2-C3-C5-C6
9	6	102	BCL	C14-C13-C15-C16
9	B	102	BCL	C14-C13-C15-C16
10	9	101	KGD	CBE-CBF-CBH-CBK
10	J	102	KGD	CBE-CBF-CBH-CBK
10	P	101	KGD	CBI-CBL-CBN-CBM
10	R	102	KGD	CBE-CBF-CBH-CBJ
12	M	704	BPB	C16-C17-C18-C20
13	L	1004	MQE	CAO-CAH-CAV-CBF
14	L	1006	PGV	C05-C04-O12-P
12	M	704	BPB	C3A-C2A-CAA-CBA
9	V	101	BCL	C10-C11-C12-C13
14	L	1007	PGV	C7-C8-C9-C10
12	M	704	BPB	C16-C17-C18-C19
11	C	403	HEM	C4D-C3D-CAD-CBD
9	0	101	BCL	C2-C1-O2A-CGA
9	4	102	BCL	C2-C1-O2A-CGA
9	D	102	BCL	C2-C1-O2A-CGA
9	I	101	BCL	C2-C1-O2A-CGA
9	K	102	BCL	C2-C1-O2A-CGA
9	L	1001	BCL	C2-C1-O2A-CGA
9	Q	101	BCL	C2-C1-O2A-CGA
9	Q	102	BCL	C2-C1-O2A-CGA
9	W	101	BCL	C2-C1-O2A-CGA
9	G	102	BCL	C14-C13-C15-C16
9	L	1002	BCL	C11-C12-C13-C14
12	M	704	BPB	C14-C13-C15-C16
9	W	101	BCL	C10-C11-C12-C13
10	4	103	KGD	CAH-CAD-CAJ-CAL
10	8	103	KGD	CAH-CAD-CAJ-CAL
10	S	103	KGD	CAH-CAD-CAJ-CAL
10	U	103	KGD	CAH-CAD-CAJ-CAL
9	E	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
10	3	102	KGD	CAJ-CAL-CAM-CAO
10	9	101	KGD	CBE-CBF-CBH-CBJ
10	C	401	KGD	CAJ-CAL-CAM-CAO
10	H	101	KGD	CBE-CBF-CBH-CBJ
10	J	102	KGD	CBE-CBF-CBH-CBJ
9	U	102	BCL	C13-C15-C16-C17
14	L	1006	PGV	C01-C02-C03-O11
9	0	102	BCL	C12-C13-C15-C16
9	G	102	BCL	C12-C13-C15-C16
9	K	102	BCL	C12-C13-C15-C16
12	L	1003	BPB	C11-C10-C8-C7
12	M	704	BPB	C11-C10-C8-C7
10	U	103	KGD	CBB-CBG-CBI-CBL
9	2	102	BCL	C13-C15-C16-C17
9	6	101	BCL	CAD-CBD-CGD-O2D
9	O	102	BCL	CAD-CBD-CGD-O2D
9	S	101	BCL	CAD-CBD-CGD-O2D
9	U	101	BCL	CAD-CBD-CGD-O2D
9	U	102	BCL	CAD-CBD-CGD-O2D
12	L	1005	BPB	CAD-CBD-CGD-O2D
13	M	701	MQE	CBM-CBJ-CBO-CCB
9	3	101	BCL	CHA-CBD-CGD-O1D
9	6	101	BCL	CHA-CBD-CGD-O1D
9	L	1001	BCL	CHA-CBD-CGD-O1D
9	S	101	BCL	CHA-CBD-CGD-O1D
9	V	101	BCL	C4-C3-C5-C6
9	0	102	BCL	C14-C13-C15-C16
9	I	102	BCL	C14-C13-C15-C16
10	G	103	KGD	CAP-CAQ-CAR-CAV
13	M	701	MQE	CAF-CAK-CBE-CAQ
10	S	103	KGD	CBB-CBG-CBI-CBL
9	9	102	BCL	C4-C3-C5-C6
14	L	1006	PGV	C02-C03-O11-P
14	L	1007	PGV	C02-C03-O11-P
14	L	1006	PGV	C04-O12-P-O13
14	P	104	PGV	C03-O11-P-O13
9	I	102	BCL	C16-C17-C18-C19
9	K	102	BCL	C16-C17-C18-C19
14	L	1007	PGV	C22-C23-C24-C25
14	L	1007	PGV	C1-C2-C3-C4
9	8	101	BCL	C11-C10-C8-C7
9	H	102	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	I	102	BCL	C12-C13-C15-C16
9	Q	102	BCL	C2C-C3C-CAC-CBC
11	C	404	HEM	C2A-CAA-CBA-CGA
12	L	1003	BPB	C6-C7-C8-C10
12	L	1005	BPB	C11-C12-C13-C15
12	M	704	BPB	C12-C13-C15-C16
12	M	704	BPB	C4C-C3C-CAC-CBC
14	L	1006	PGV	O01-C02-C03-O11
10	Q	103	KGD	CBB-CBG-CBI-CBL
12	M	704	BPB	C15-C16-C17-C18
11	C	402	HEM	C1A-C2A-CAA-CBA
11	C	402	HEM	C3A-C2A-CAA-CBA
9	9	102	BCL	C2-C3-C5-C6
9	E	101	BCL	C14-C13-C15-C16
9	K	102	BCL	C14-C13-C15-C16
9	L	1002	BCL	C11-C10-C8-C9
9	X	101	BCL	C11-C10-C8-C9
12	L	1003	BPB	C11-C10-C8-C9
13	M	705	MQE	CBB-CAN-CAS-CBH
14	L	1006	PGV	C2-C3-C4-C5
9	V	101	BCL	C5-C6-C7-C8
9	6	101	BCL	C2-C1-O2A-CGA
9	B	101	BCL	C2-C1-O2A-CGA
9	B	102	BCL	C2-C1-O2A-CGA
9	O	102	BCL	C2-C1-O2A-CGA
9	U	102	BCL	C2-C1-O2A-CGA
9	I	102	BCL	C16-C17-C18-C20
9	K	102	BCL	C16-C17-C18-C20
10	U	103	KGD	CAR-CAV-CBB-CBG
10	K	103	KGD	CAT-CAS-CAW-CAZ
10	R	102	KGD	CAH-CAD-CAJ-CAL
10	S	103	KGD	CAB-CAD-CAJ-CAL
9	V	101	BCL	C2-C3-C5-C6
14	L	1007	PGV	C03-O11-P-O12
12	M	704	BPB	CHA-CBD-CGD-O2D
9	B	101	BCL	C11-C10-C8-C7
9	O	101	BCL	C11-C10-C8-C7
12	L	1005	BPB	C12-C13-C15-C16
9	H	102	BCL	C11-C10-C8-C9
9	L	1002	BCL	C6-C7-C8-C9
12	M	704	BPB	C11-C10-C8-C9
10	5	103	KGD	CAM-CAO-CAP-CAQ

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Mol	Chain	Res	Type	Atoms
10	E	102	KGD	CAM-CAO-CAP-CAQ
10	G	103	KGD	CAP-CAQ-CAR-CAU
11	C	403	HEM	C3D-CAD-CBD-CGD
11	C	404	HEM	CAA-CBA-CGA-O1A
9	I	101	BCL	C16-C17-C18-C19
10	P	103	KGD	CAW-CBA-CBE-CBF
9	4	102	BCL	C10-C11-C12-C13
9	E	101	BCL	C2-C1-O2A-CGA
11	C	403	HEM	C2A-CAA-CBA-CGA
9	I	101	BCL	C16-C17-C18-C20
12	M	704	BPB	O2A-C1-C2-C3
11	C	403	HEM	C2D-C3D-CAD-CBD
9	I	101	BCL	C11-C10-C8-C7
10	S	103	KGD	CAM-CAO-CAP-CAQ
11	C	403	HEM	CAA-CBA-CGA-O2A
14	L	1007	PGV	C13-C14-C15-C16
11	C	404	HEM	CAA-CBA-CGA-O2A
10	E	102	KGD	CAW-CBA-CBE-CBF
10	J	102	KGD	CAM-CAO-CAP-CAQ
9	M	703	BCL	CAA-CBA-CGA-O2A
10	H	101	KGD	CAT-CAS-CAW-CAZ
12	L	1005	BPB	C4-C3-C5-C6
9	0	102	BCL	C2-C1-O2A-CGA
9	2	101	BCL	C2-C1-O2A-CGA
9	4	101	BCL	C2-C1-O2A-CGA
9	6	102	BCL	C2-C1-O2A-CGA
9	8	101	BCL	C2-C1-O2A-CGA
9	G	101	BCL	C2-C1-O2A-CGA
9	U	101	BCL	C2-C1-O2A-CGA
12	L	1005	BPB	C6-C7-C8-C9
10	8	103	KGD	CAB-CAD-CAJ-CAL
10	0	103	KGD	CBB-CBG-CBI-CBL
10	T	102	KGD	CAM-CAO-CAP-CAQ
10	J	102	KGD	CAT-CAS-CAW-CAZ
13	L	1004	MQE	CAJ-CAD-CAQ-CBE
9	G	101	BCL	C15-C16-C17-C18
10	0	103	KGD	CAT-CAS-CAW-CAZ
13	L	1004	MQE	CAJ-CAD-CAQ-CBU
9	6	101	BCL	C11-C10-C8-C7
9	E	101	BCL	C12-C13-C15-C16
9	H	102	BCL	C2-C3-C5-C6
9	Q	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
11	C	403	HEM	CAA-CBA-CGA-O1A
9	L	1002	BCL	CAA-CBA-CGA-O2A
9	4	101	BCL	CAA-CBA-CGA-O2A
9	8	101	BCL	CAA-CBA-CGA-O2A
9	B	101	BCL	CAA-CBA-CGA-O2A
9	G	101	BCL	CAA-CBA-CGA-O2A
9	6	101	BCL	C13-C15-C16-C17
11	C	404	HEM	C4D-C3D-CAD-CBD
9	F	101	BCL	CAA-CBA-CGA-O2A
9	K	101	BCL	CAA-CBA-CGA-O2A
9	P	102	BCL	CAA-CBA-CGA-O2A
9	0	101	BCL	CAD-CBD-CGD-O2D
9	0	102	BCL	CAD-CBD-CGD-O2D
9	2	102	BCL	CAD-CBD-CGD-O2D
9	4	102	BCL	CAD-CBD-CGD-O2D
9	8	101	BCL	CAD-CBD-CGD-O2D
9	B	101	BCL	CAD-CBD-CGD-O2D
9	D	102	BCL	CAD-CBD-CGD-O2D
9	E	101	BCL	CAD-CBD-CGD-O2D
9	G	101	BCL	CAD-CBD-CGD-O2D
9	I	101	BCL	CAD-CBD-CGD-O2D
9	K	101	BCL	CAD-CBD-CGD-O2D
9	K	102	BCL	CAD-CBD-CGD-O2D
9	O	101	BCL	CAD-CBD-CGD-O2D
9	Q	101	BCL	CAD-CBD-CGD-O2D
9	W	101	BCL	CAD-CBD-CGD-O2D
9	O	101	BCL	C13-C15-C16-C17
9	D	101	BCL	CAA-CBA-CGA-O2A
10	K	103	KGD	CAT-CAS-CAW-CBA
9	0	101	BCL	CAA-CBA-CGA-O2A
9	7	101	BCL	CAA-CBA-CGA-O2A
9	A	101	BCL	CAA-CBA-CGA-O2A
9	N	101	BCL	CAA-CBA-CGA-O2A
9	O	101	BCL	CAA-CBA-CGA-O2A
9	R	101	BCL	CAA-CBA-CGA-O2A
10	5	102	KGD	CBI-CBL-CBN-CBM
9	2	101	BCL	CAA-CBA-CGA-O2A
9	3	101	BCL	CAA-CBA-CGA-O2A
9	5	101	BCL	CAA-CBA-CGA-O2A
9	9	102	BCL	CAA-CBA-CGA-O2A
9	D	102	BCL	CAA-CBA-CGA-O2A
9	H	102	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	Q	101	BCL	CAA-CBA-CGA-O2A
9	S	101	BCL	CAA-CBA-CGA-O2A
9	4	102	BCL	O2A-C1-C2-C3
9	E	101	BCL	O2A-C1-C2-C3
9	K	102	BCL	O2A-C1-C2-C3
9	J	101	BCL	CAA-CBA-CGA-O2A
9	T	101	BCL	CAA-CBA-CGA-O2A
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D
9	3	101	BCL	CHA-CBD-CGD-O2D
9	7	101	BCL	CHA-CBD-CGD-O1D
9	7	101	BCL	CHA-CBD-CGD-O2D
9	A	101	BCL	CHA-CBD-CGD-O2D
9	H	102	BCL	CHA-CBD-CGD-O1D
9	H	102	BCL	CHA-CBD-CGD-O2D
9	L	1001	BCL	CHA-CBD-CGD-O2D
9	R	101	BCL	CHA-CBD-CGD-O2D
9	V	101	BCL	CHA-CBD-CGD-O1D
9	V	101	BCL	CHA-CBD-CGD-O2D
9	X	101	BCL	CHA-CBD-CGD-O1D
9	X	101	BCL	CHA-CBD-CGD-O2D
10	P	101	KGD	CAT-CAS-CAW-CAZ
9	1	101	BCL	CAA-CBA-CGA-O2A
9	V	101	BCL	CAA-CBA-CGA-O2A
14	P	104	PGV	O03-C01-C02-O01
9	I	101	BCL	CAA-CBA-CGA-O2A
12	M	704	BPB	CHA-CBD-CGD-O1D
9	6	101	BCL	CAA-CBA-CGA-O2A
11	C	402	HEM	CAA-CBA-CGA-O1A
9	U	101	BCL	CAA-CBA-CGA-O2A
12	L	1005	BPB	C11-C12-C13-C14
10	Q	103	KGD	CAS-CAT-CAX-CAY
13	L	1004	MQE	CCD-CCI-CCM-CCN
9	N	101	BCL	CAA-CBA-CGA-O1A
9	4	101	BCL	CAA-CBA-CGA-O1A
9	7	101	BCL	CAA-CBA-CGA-O1A
9	A	101	BCL	CAA-CBA-CGA-O1A
9	S	101	BCL	CAA-CBA-CGA-O1A
9	I	101	BCL	CAA-CBA-CGA-O1A
9	2	102	BCL	C2-C1-O2A-CGA
9	G	102	BCL	C2-C1-O2A-CGA
9	5	101	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
9	8	101	BCL	CAA-CBA-CGA-O1A
9	B	101	BCL	CAA-CBA-CGA-O1A
9	G	101	BCL	CAA-CBA-CGA-O1A
9	K	101	BCL	CAA-CBA-CGA-O1A
9	T	101	BCL	CAA-CBA-CGA-O1A
11	C	402	HEM	CAD-CBD-CGD-O2D
9	H	102	BCL	C4-C3-C5-C6
9	1	101	BCL	CAA-CBA-CGA-O1A
14	L	1007	PGV	C03-O11-P-O13
9	K	101	BCL	C16-C17-C18-C19
10	J	102	KGD	CAS-CAT-CAX-CAY
9	F	101	BCL	CAA-CBA-CGA-O1A
9	L	1002	BCL	CAA-CBA-CGA-O1A
10	5	102	KGD	CAH-CAD-CAJ-CAL
10	A	102	KGD	CAH-CAD-CAJ-CAL
9	D	101	BCL	CAA-CBA-CGA-O1A
9	J	101	BCL	CAA-CBA-CGA-O1A
9	P	102	BCL	CAA-CBA-CGA-O1A
9	Q	101	BCL	CAA-CBA-CGA-O1A
9	3	101	BCL	CAA-CBA-CGA-O1A
9	D	102	BCL	CAA-CBA-CGA-O1A
9	H	102	BCL	CAA-CBA-CGA-O1A
9	O	101	BCL	CAA-CBA-CGA-O1A
9	R	101	BCL	CAA-CBA-CGA-O1A
9	V	101	BCL	CAA-CBA-CGA-O1A
9	2	101	BCL	CAA-CBA-CGA-O1A
9	9	102	BCL	CAA-CBA-CGA-O1A
10	3	102	KGD	CAW-CBA-CBE-CBF
10	J	102	KGD	CBH-CBJ-CBM-CBN
14	L	1007	PGV	C3-C4-C5-C6
9	2	101	BCL	CAD-CBD-CGD-O1D
9	H	102	BCL	CAD-CBD-CGD-O1D
14	L	1007	PGV	C01-C02-O01-C1
14	L	1007	PGV	C03-C02-O01-C1
9	0	101	BCL	CAA-CBA-CGA-O1A
14	L	1007	PGV	C14-C15-C16-C17
9	F	101	BCL	C11-C10-C8-C9
9	N	101	BCL	C5-C6-C7-C8
9	U	101	BCL	CAA-CBA-CGA-O1A
9	R	101	BCL	C15-C16-C17-C18
9	6	101	BCL	CAA-CBA-CGA-O1A
13	L	1004	MQE	CAS-CAN-CBB-CCA

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Mol	Chain	Res	Type	Atoms
9	0	101	BCL	C11-C10-C8-C7
9	L	1001	BCL	C3A-C2A-CAA-CBA
10	H	101	KGD	CAT-CAS-CAW-CBA
12	L	1005	BPB	C6-C7-C8-C10
11	C	402	HEM	CAA-CBA-CGA-O2A
14	L	1007	PGV	O12-C04-C05-O05
9	6	102	BCL	C13-C15-C16-C17

There are no ring outliers.

81 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	102	BCL	4	0
10	T	102	KGD	1	0
9	8	101	BCL	6	0
10	C	401	KGD	1	0
13	L	1004	MQE	2	0
10	E	102	KGD	6	0
9	O	101	BCL	7	0
9	W	101	BCL	4	0
10	C	406	KGD	5	0
9	S	101	BCL	3	0
9	Q	101	BCL	5	0
9	N	101	BCL	3	0
10	3	102	KGD	3	0
12	L	1005	BPB	9	0
9	H	102	BCL	2	0
9	4	102	BCL	6	0
9	G	101	BCL	7	0
9	D	102	BCL	7	0
9	D	101	BCL	5	0
9	R	101	BCL	5	0
9	6	102	BCL	5	0
10	I	104	KGD	4	0
10	2	103	KGD	1	0
9	X	101	BCL	12	0
10	4	103	KGD	1	0
9	M	703	BCL	8	0
9	E	101	BCL	3	0
10	S	103	KGD	1	0
9	G	102	BCL	4	0
9	L	1001	BCL	7	0

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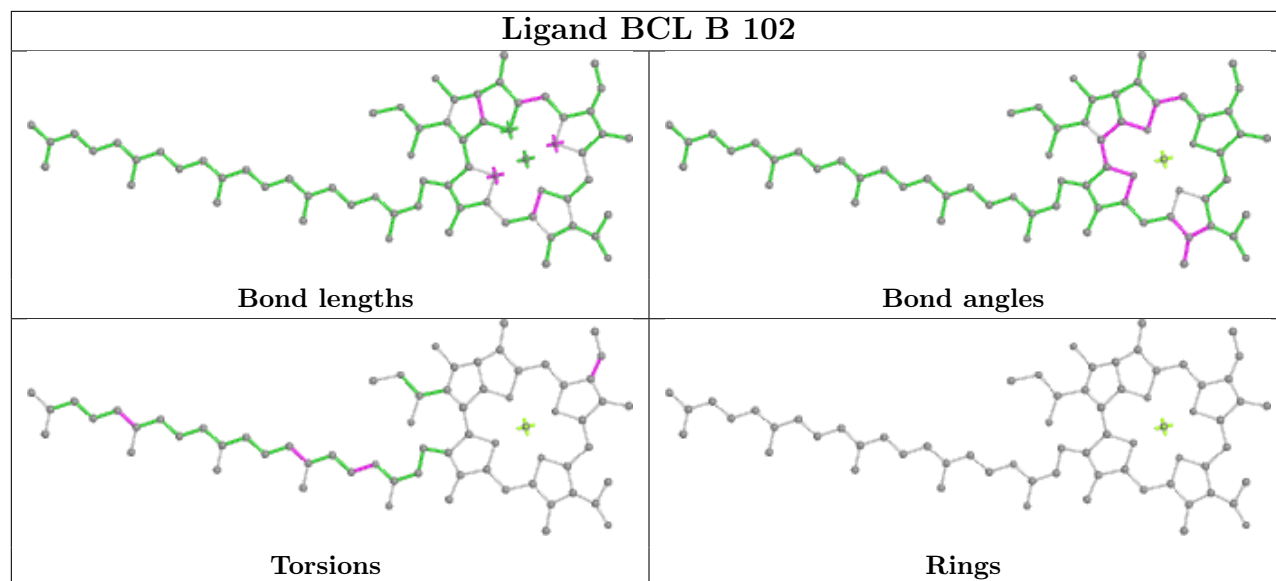
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	9	102	BCL	3	0
10	P	103	KGD	1	0
9	A	101	BCL	6	0
9	2	102	BCL	1	0
10	O	103	KGD	2	0
10	E	103	KGD	3	0
10	P	101	KGD	4	0
9	V	101	BCL	7	0
10	U	103	KGD	1	0
11	C	403	HEM	7	0
14	L	1007	PGV	1	0
10	G	103	KGD	3	0
9	0	101	BCL	7	0
9	F	101	BCL	4	0
9	3	101	BCL	5	0
9	7	101	BCL	6	0
9	U	102	BCL	6	0
10	I	103	KGD	2	0
10	5	103	KGD	1	0
10	J	102	KGD	1	0
14	L	1006	PGV	1	0
11	C	405	HEM	5	0
12	M	704	BPB	5	0
9	4	101	BCL	8	0
9	6	101	BCL	7	0
9	I	102	BCL	8	0
9	J	101	BCL	3	0
10	Q	103	KGD	2	0
12	L	1003	BPB	6	0
13	M	701	MQE	2	0
10	9	101	KGD	2	0
10	K	103	KGD	1	0
9	0	102	BCL	1	0
9	5	101	BCL	5	0
9	S	102	BCL	5	0
9	K	101	BCL	10	0
9	I	101	BCL	6	0
11	C	404	HEM	1	0
9	U	101	BCL	3	0
9	K	102	BCL	5	0
11	C	402	HEM	2	0
9	Q	102	BCL	4	0

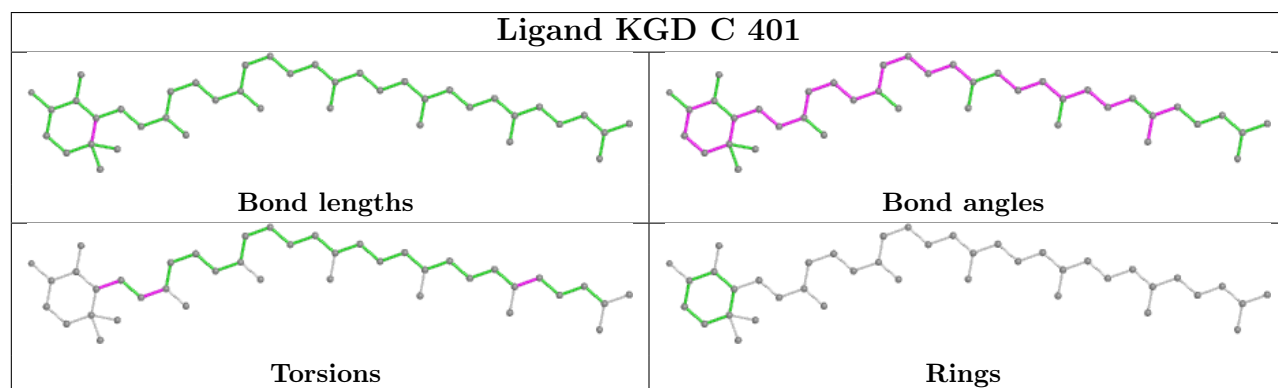
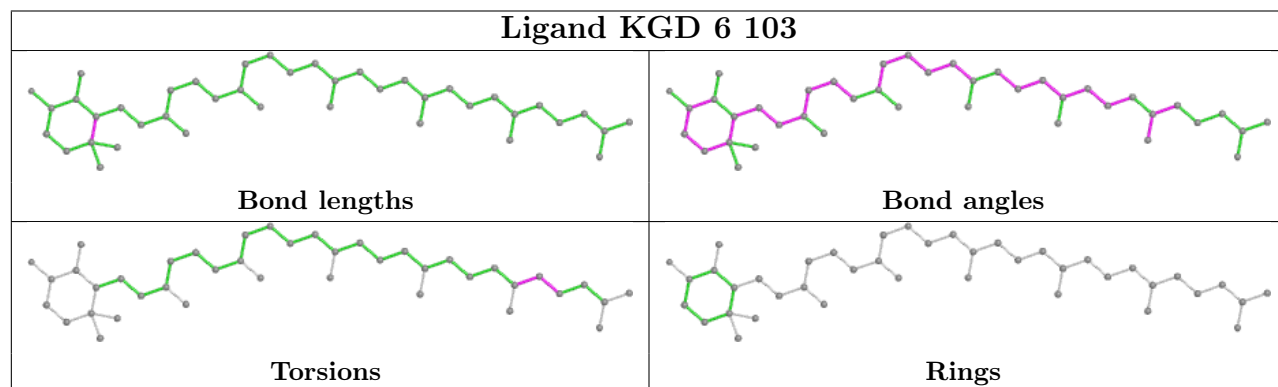
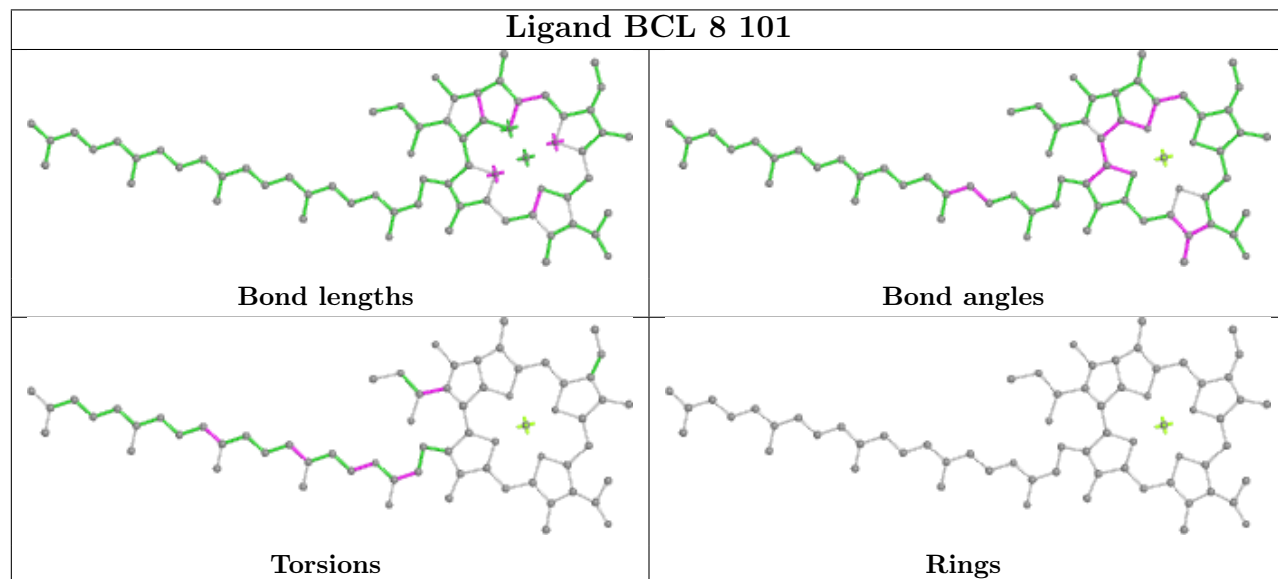
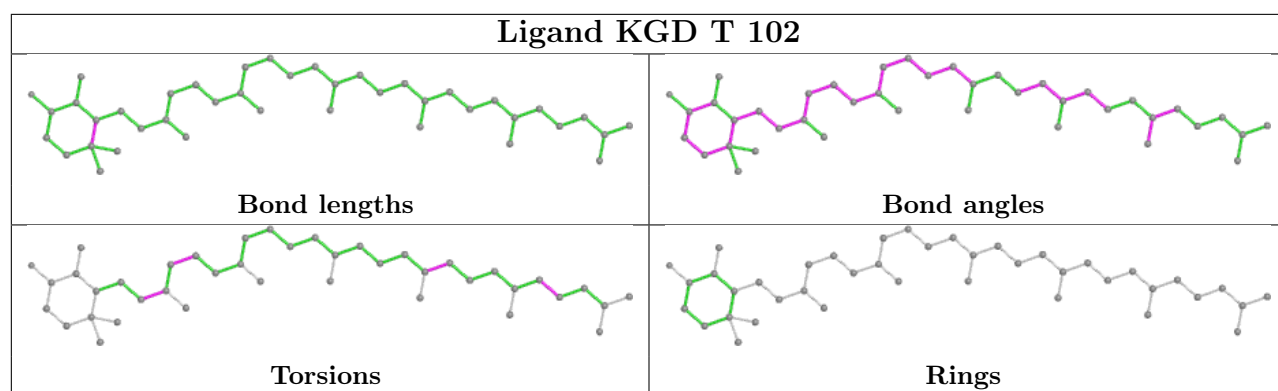
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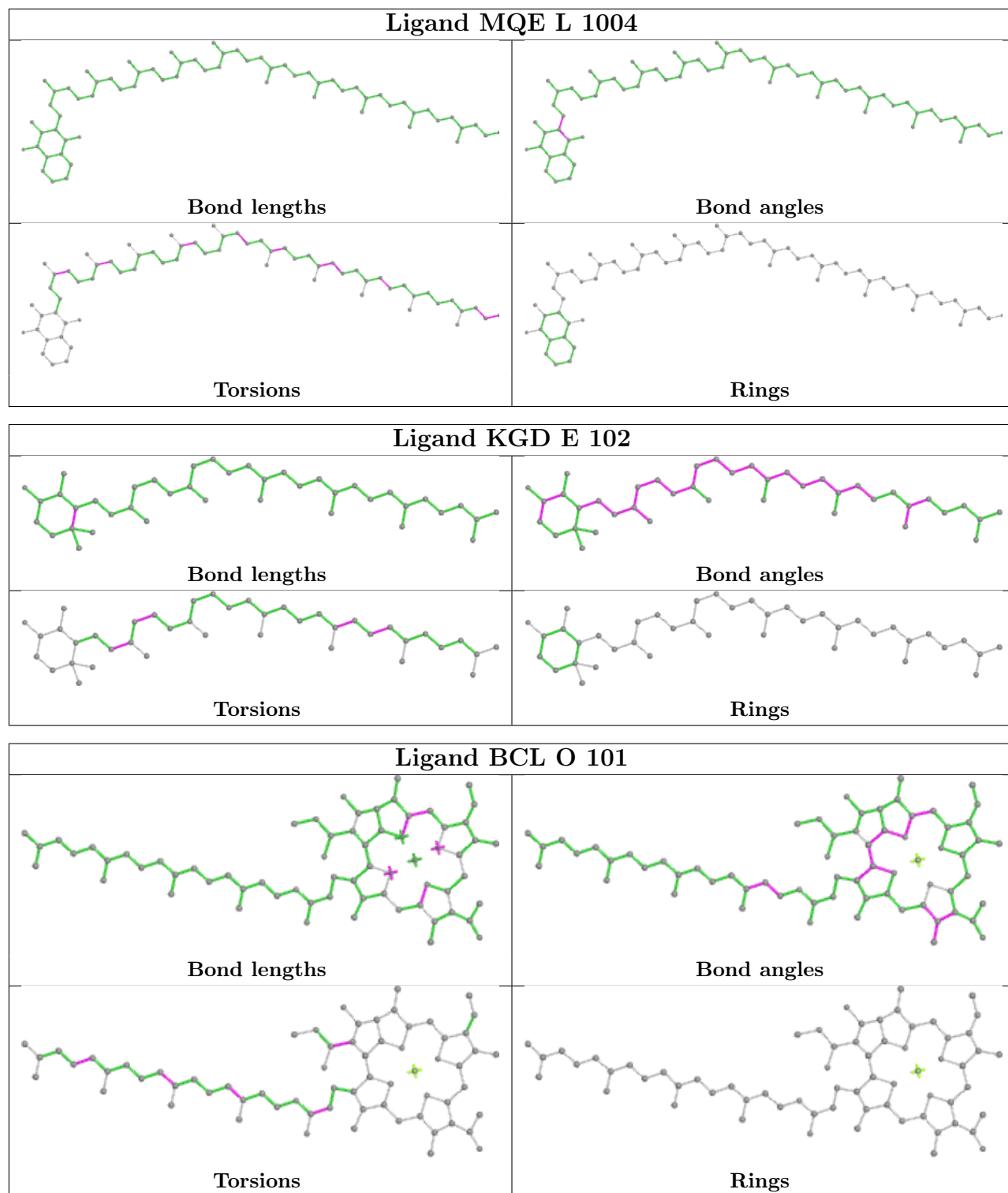
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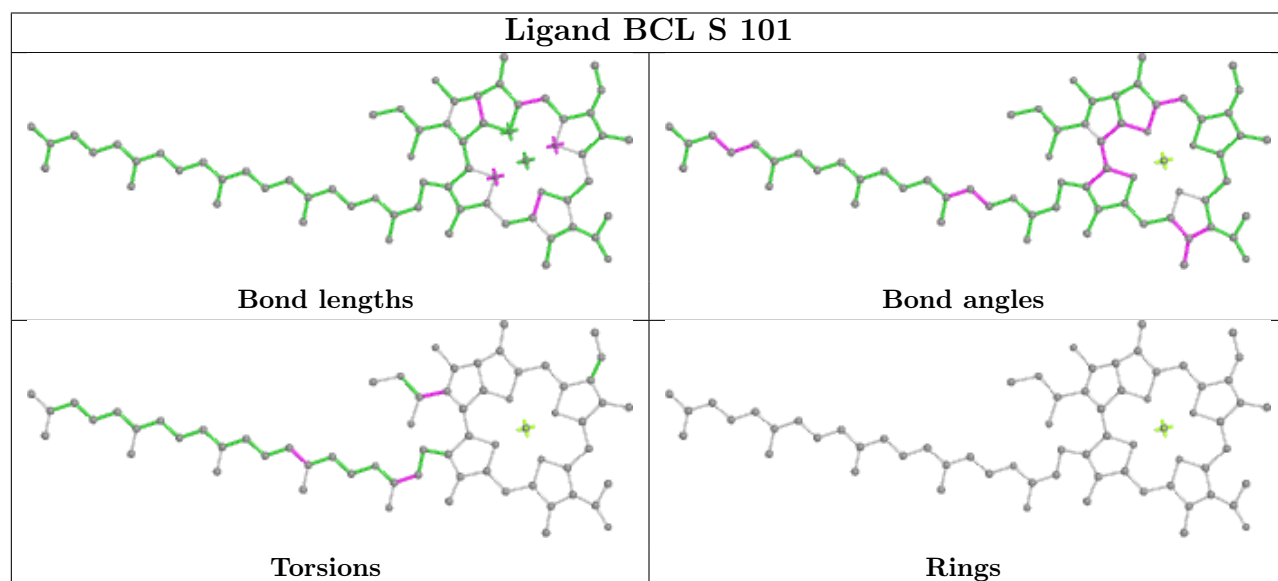
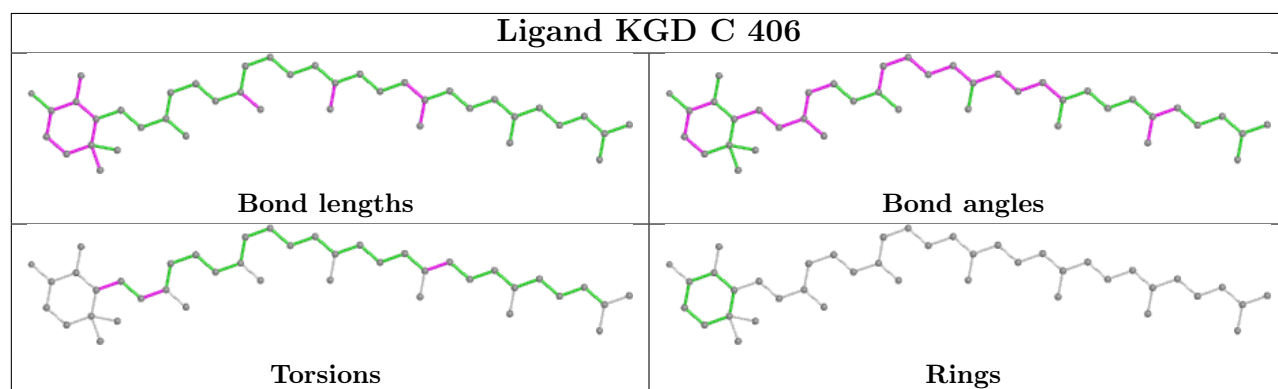
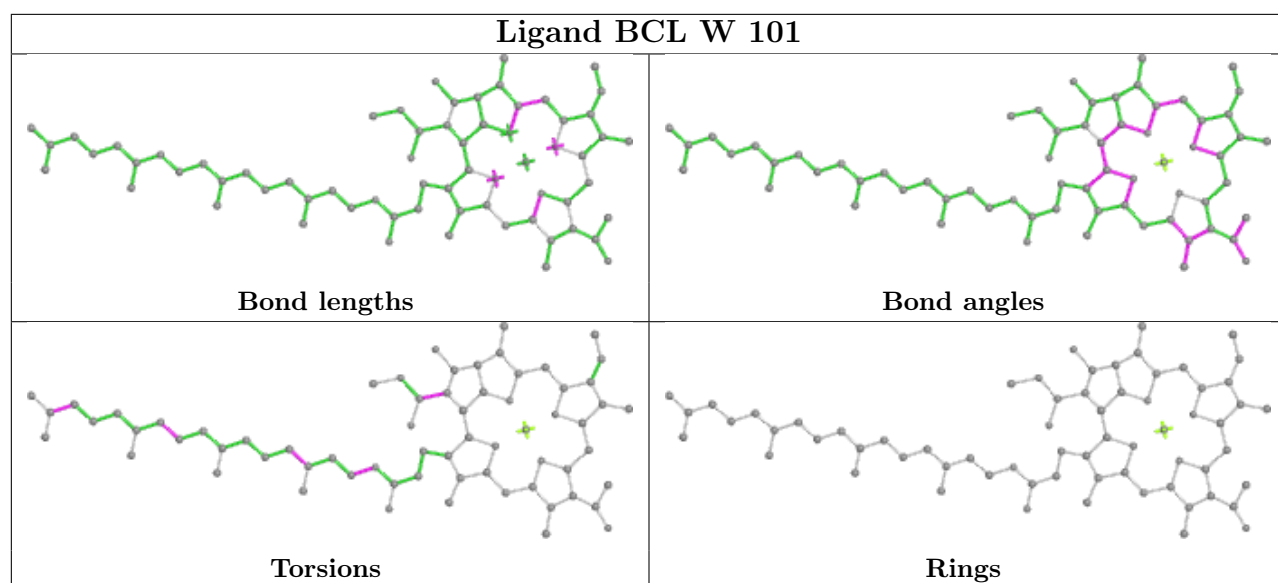
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	102	KGD	1	0
9	8	102	BCL	2	0
9	P	102	BCL	3	0
9	L	1002	BCL	8	0
9	O	102	BCL	4	0
9	2	101	BCL	5	0
9	1	101	BCL	4	0
9	B	101	BCL	5	0
9	T	101	BCL	3	0

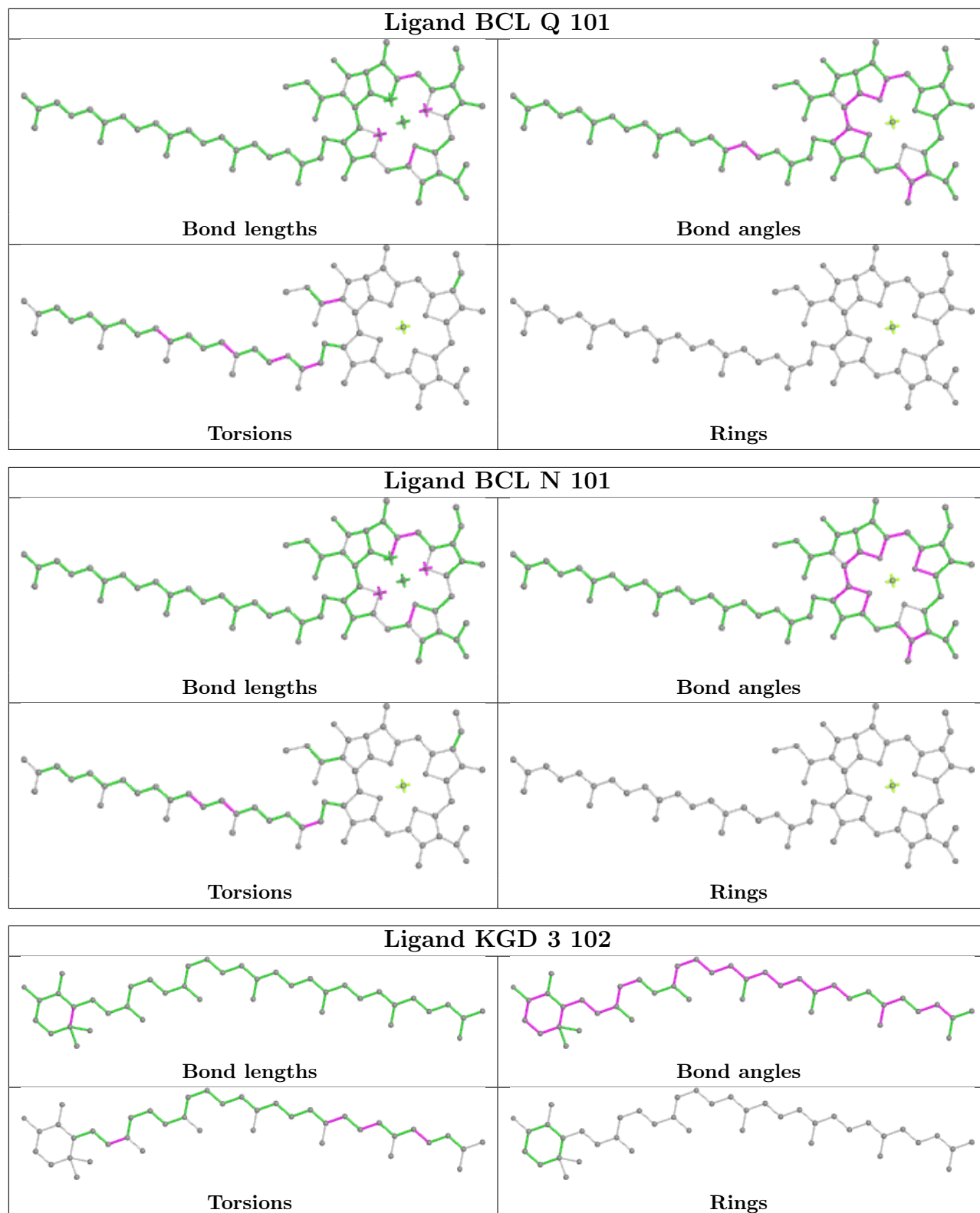
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

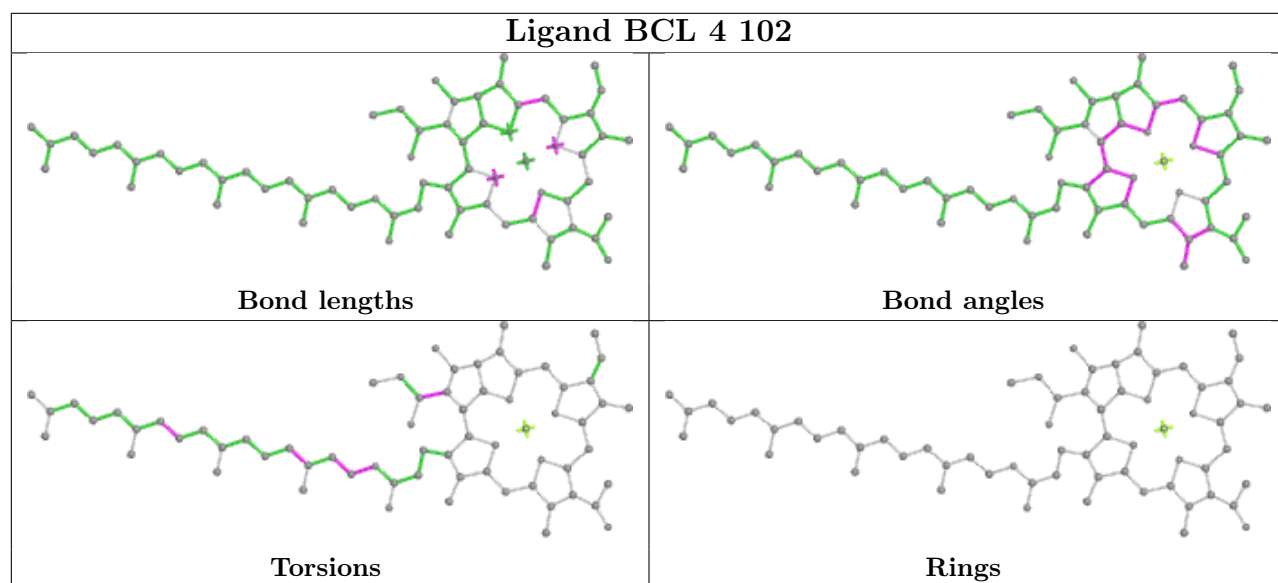
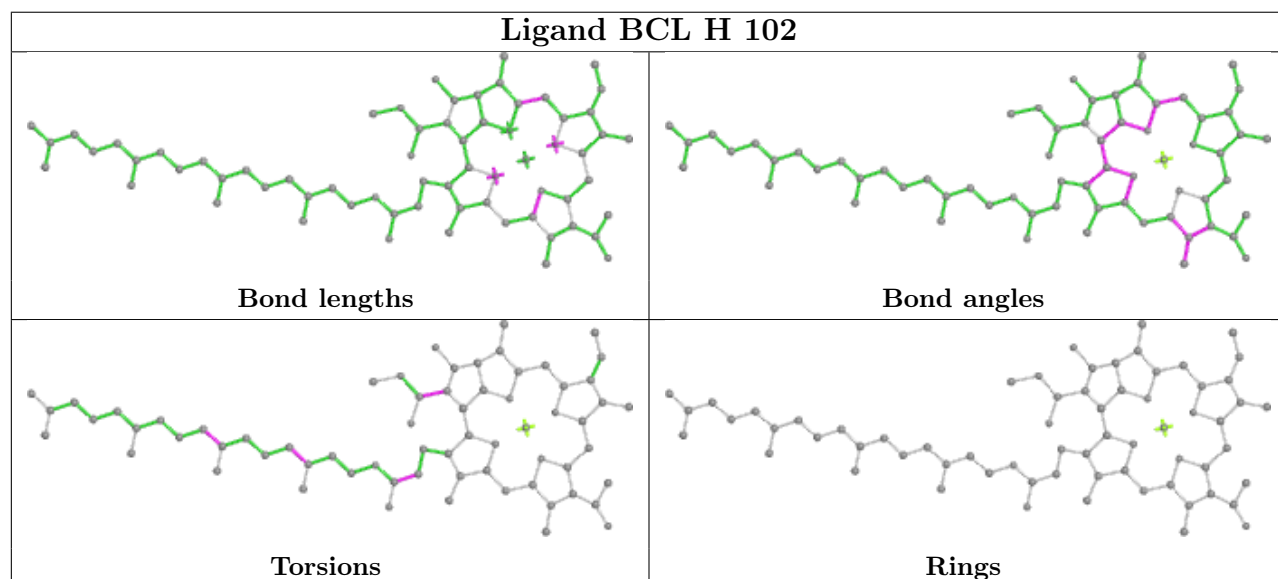
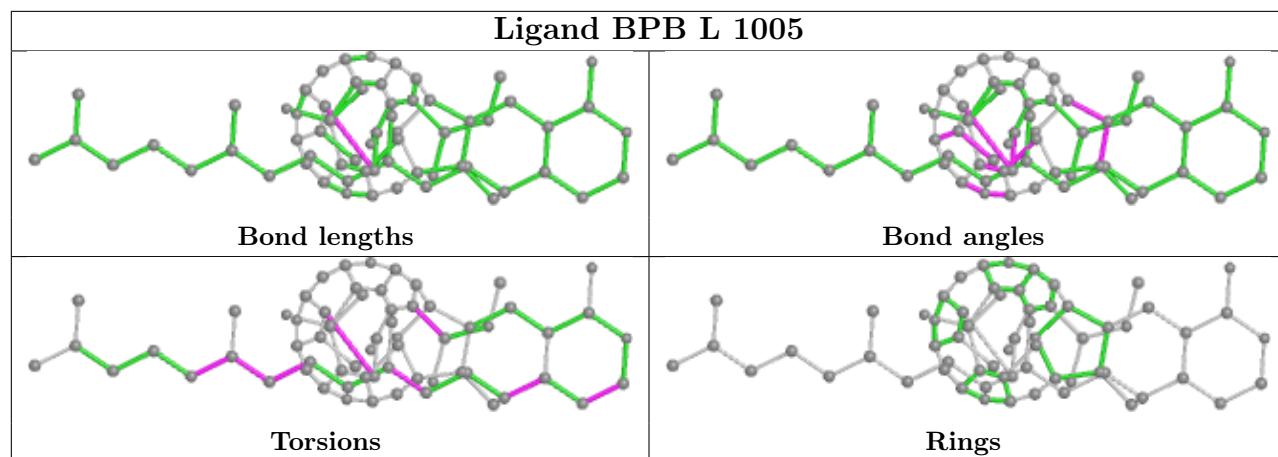


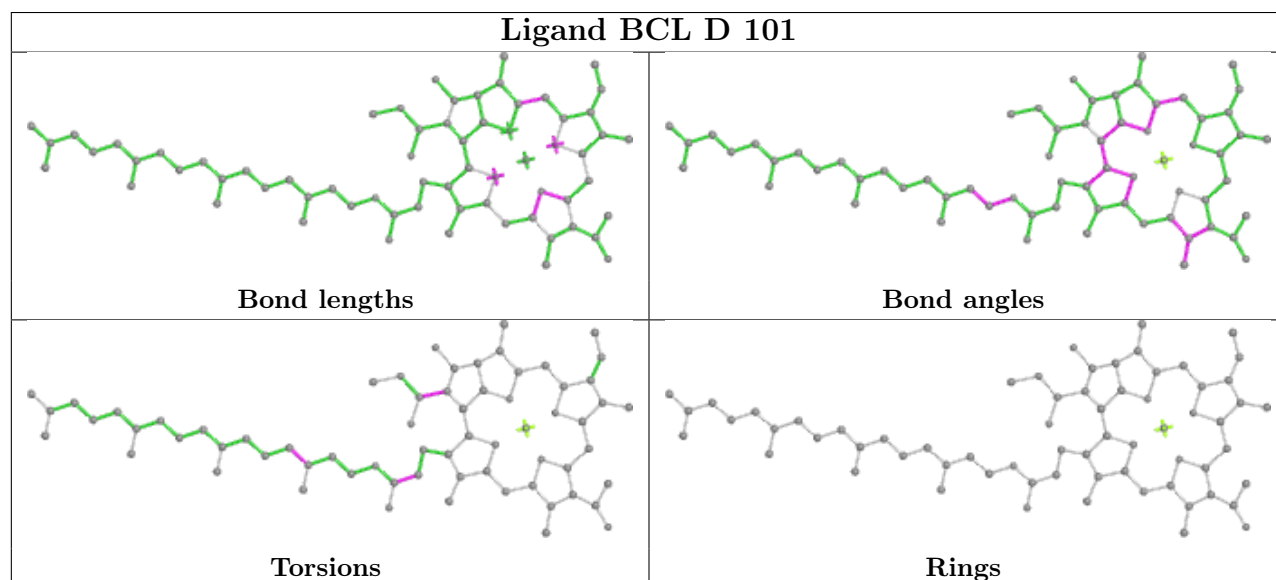
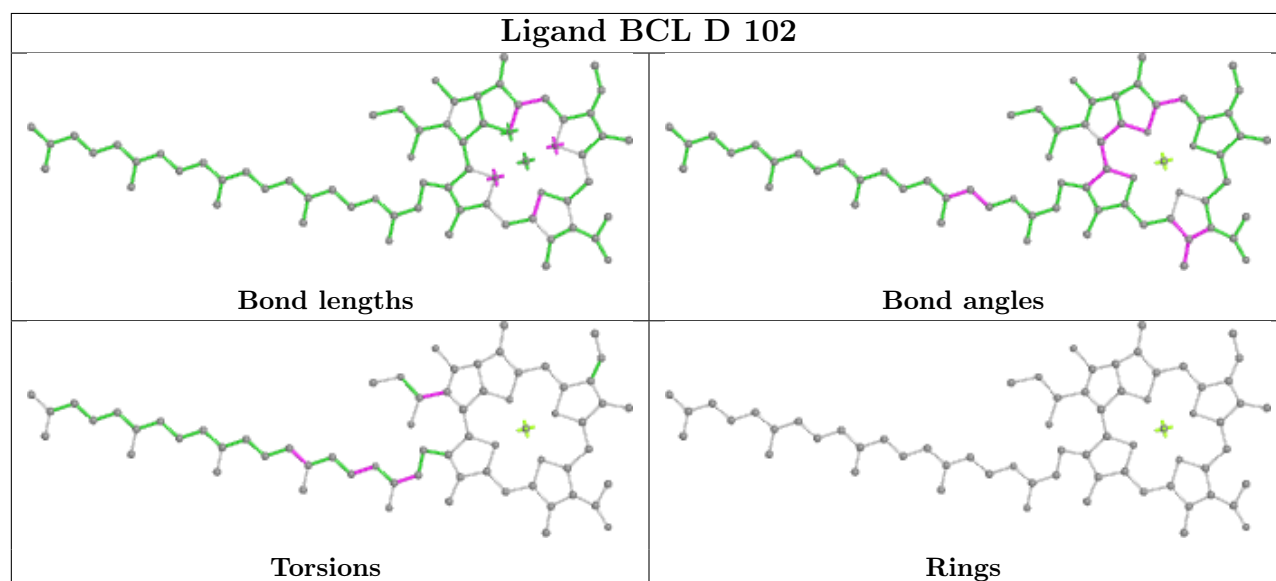
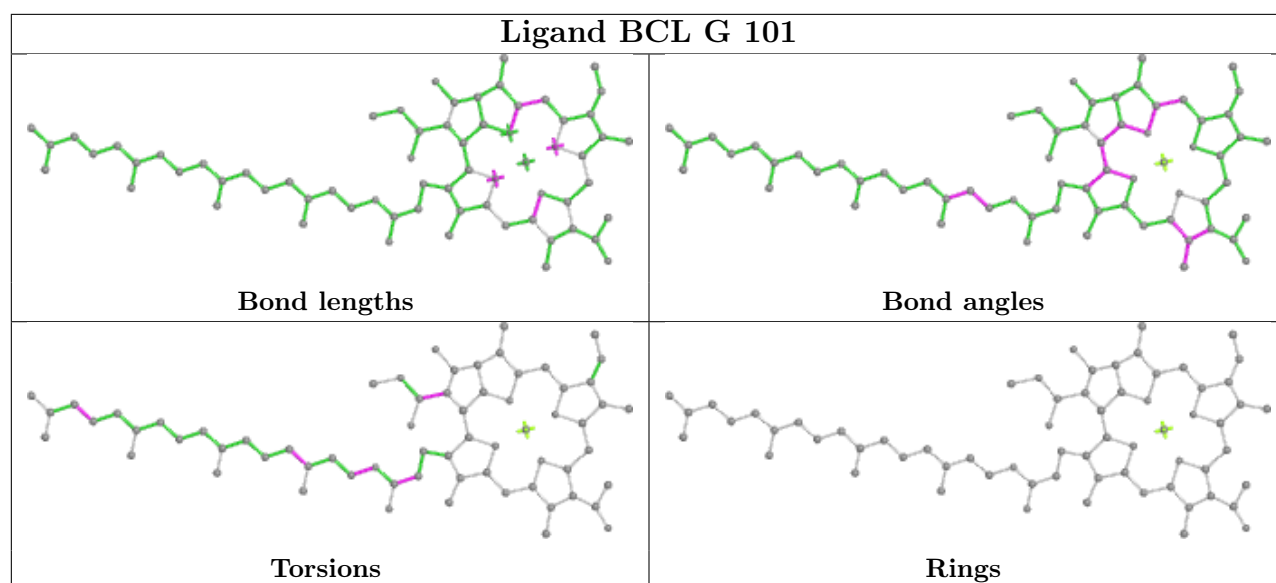


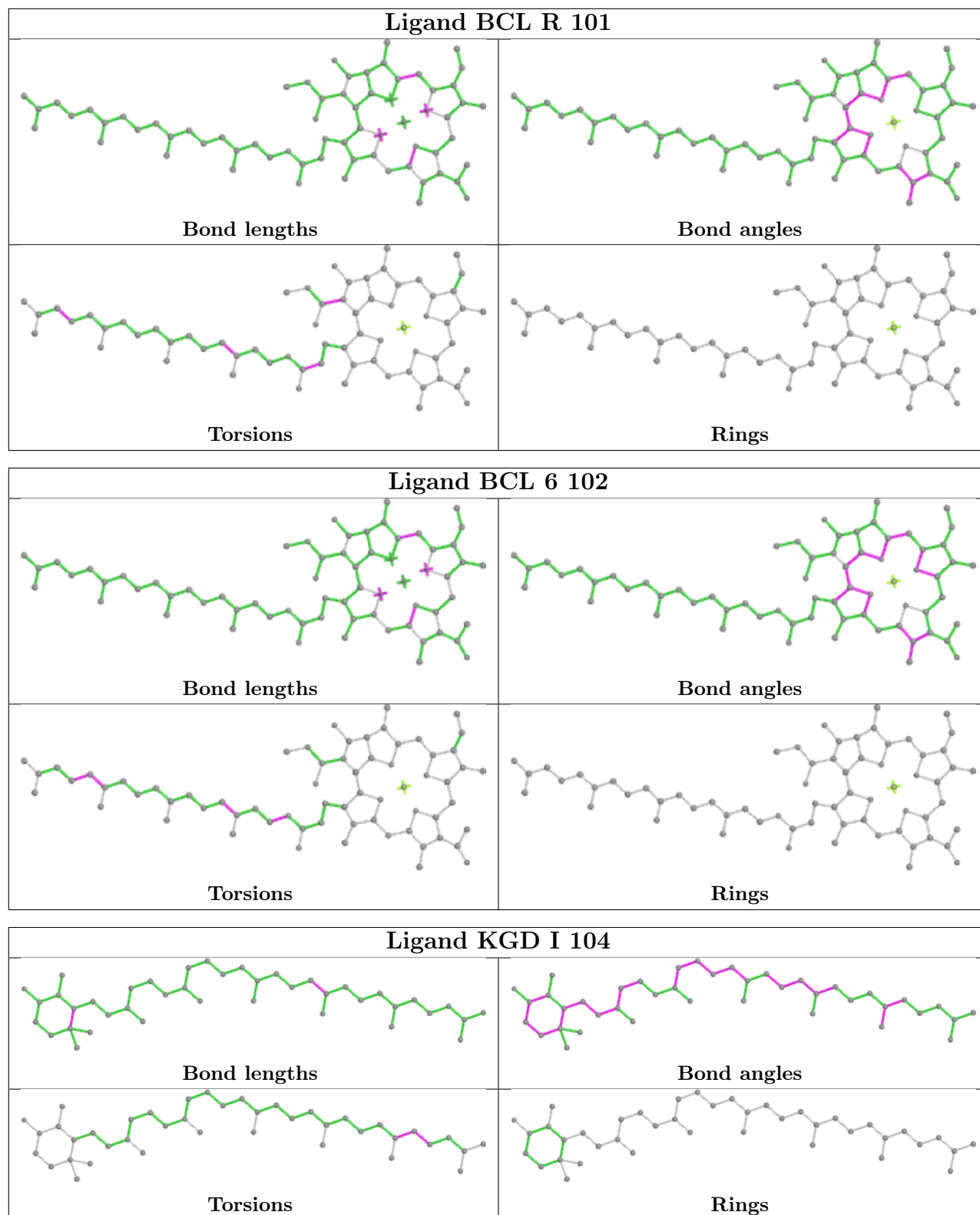


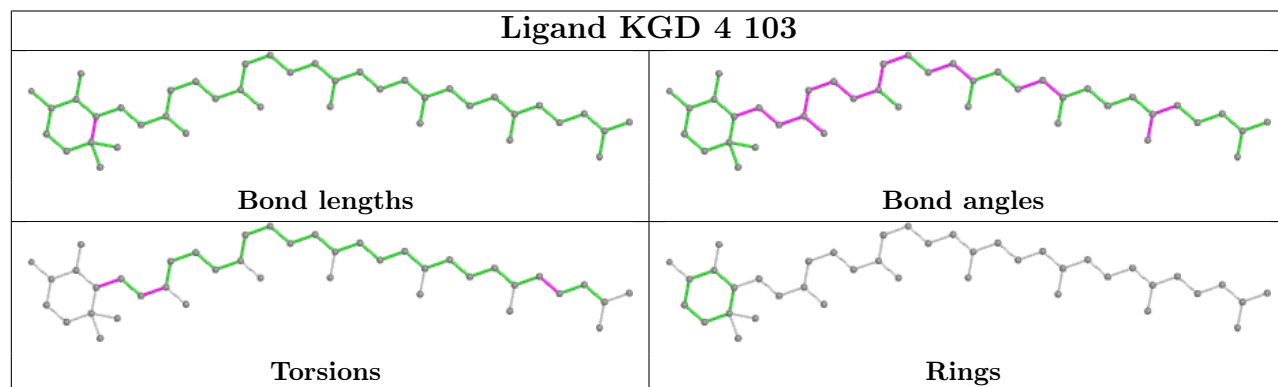
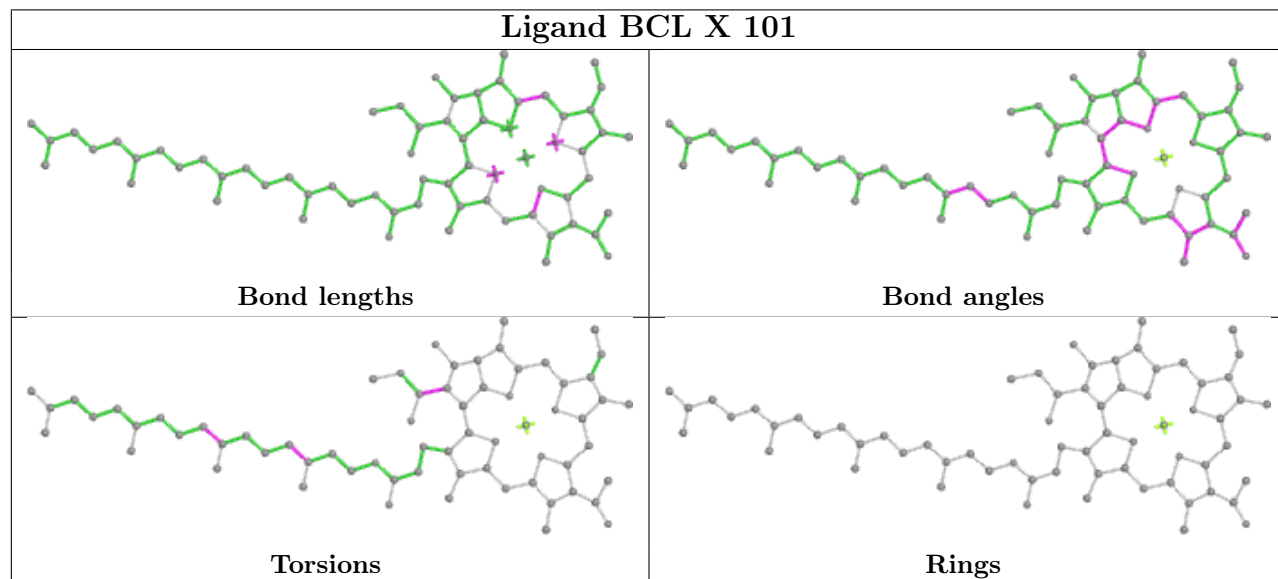
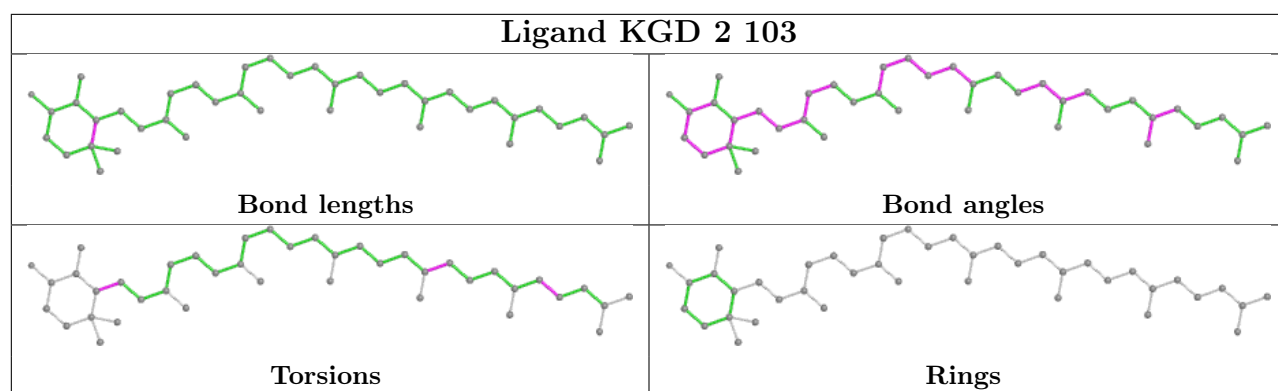


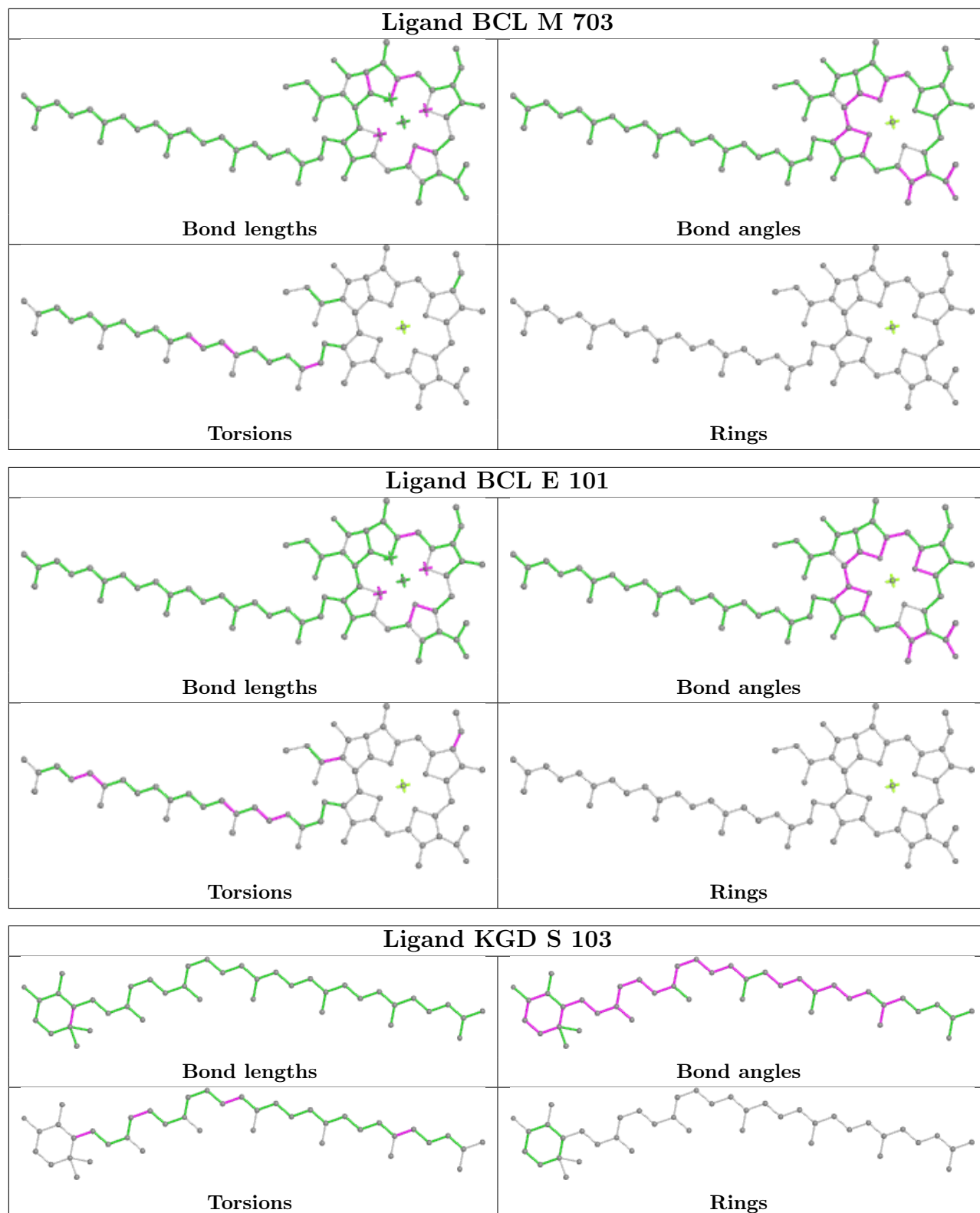


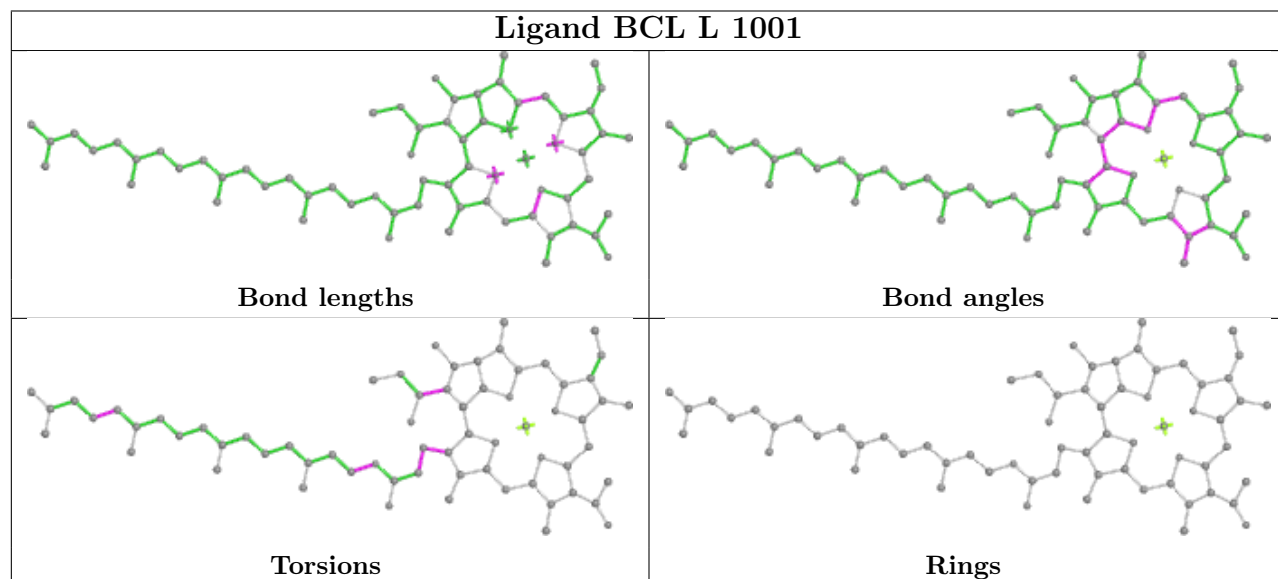
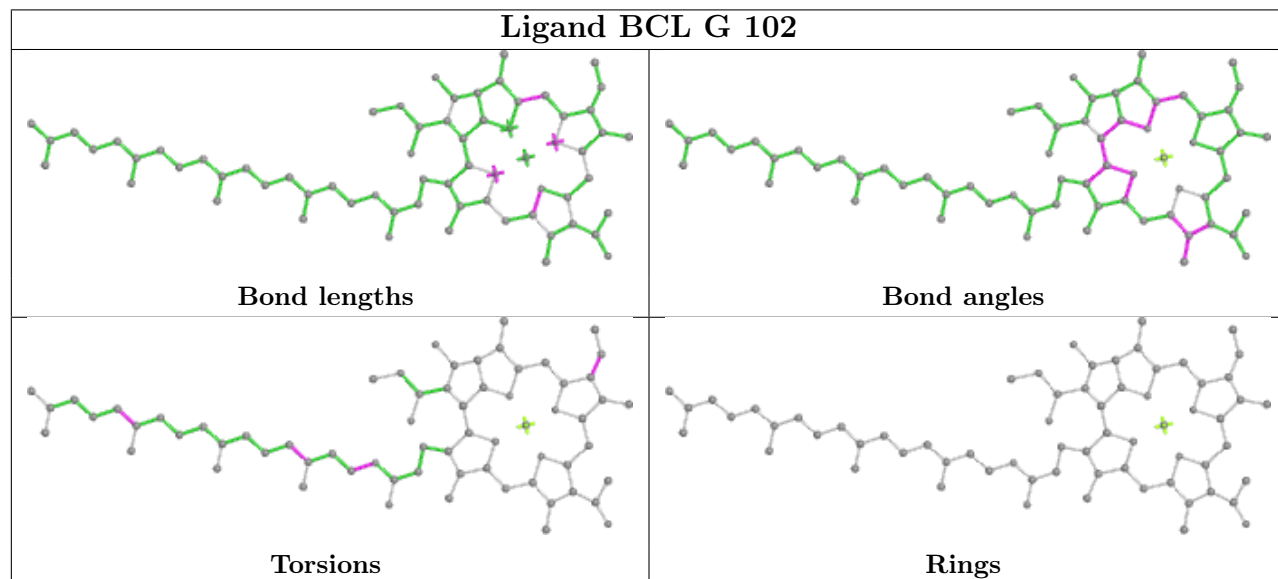
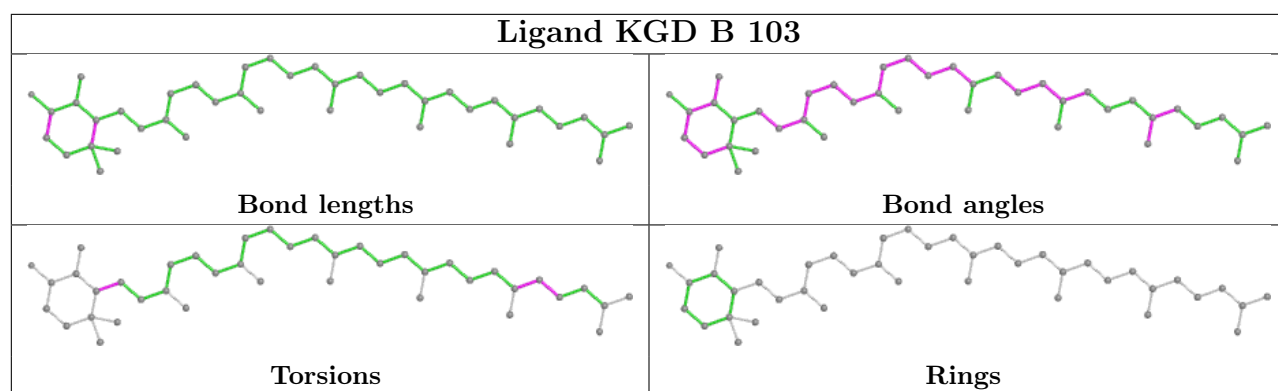


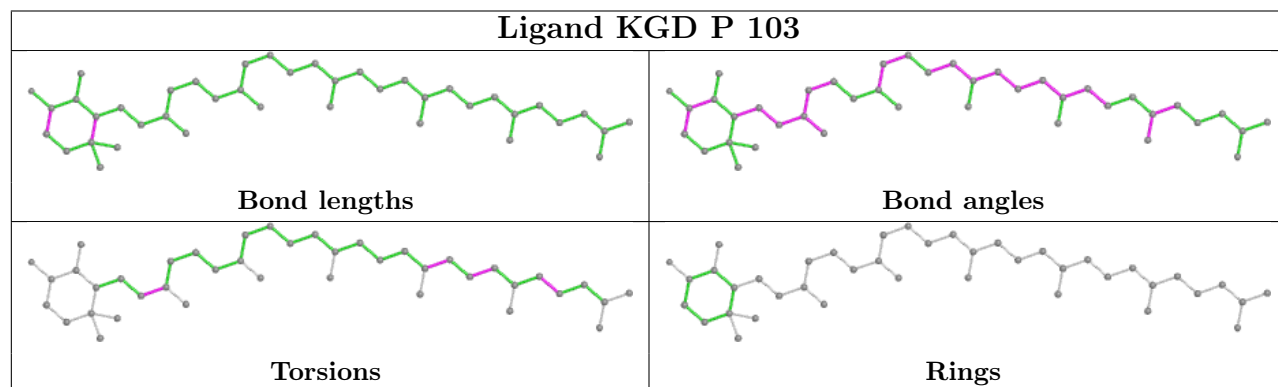
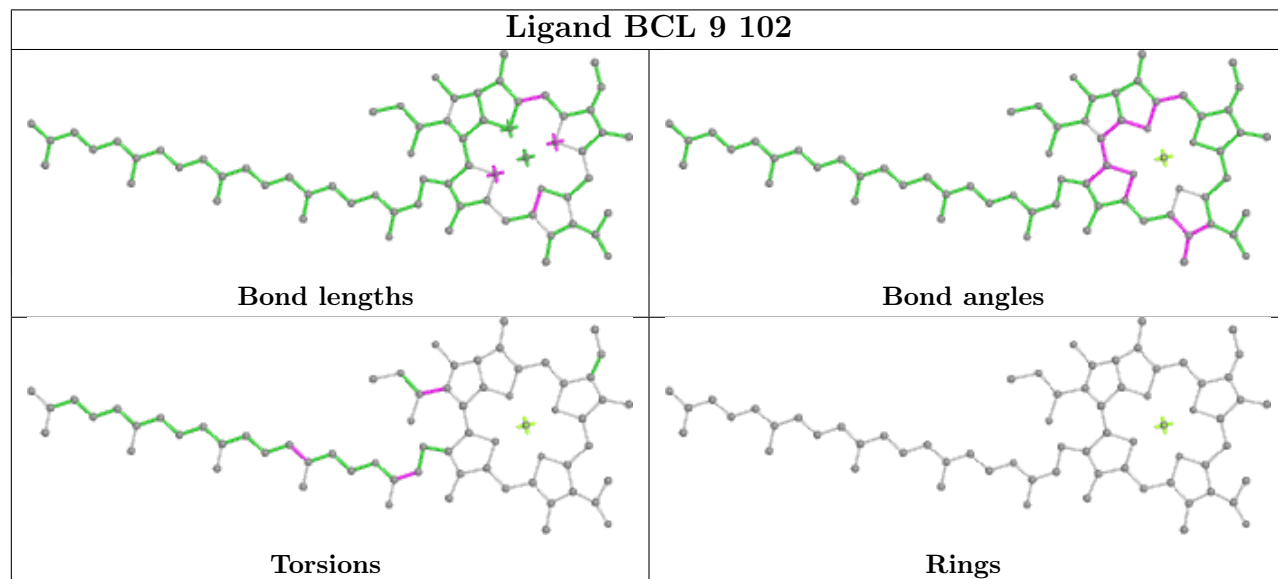
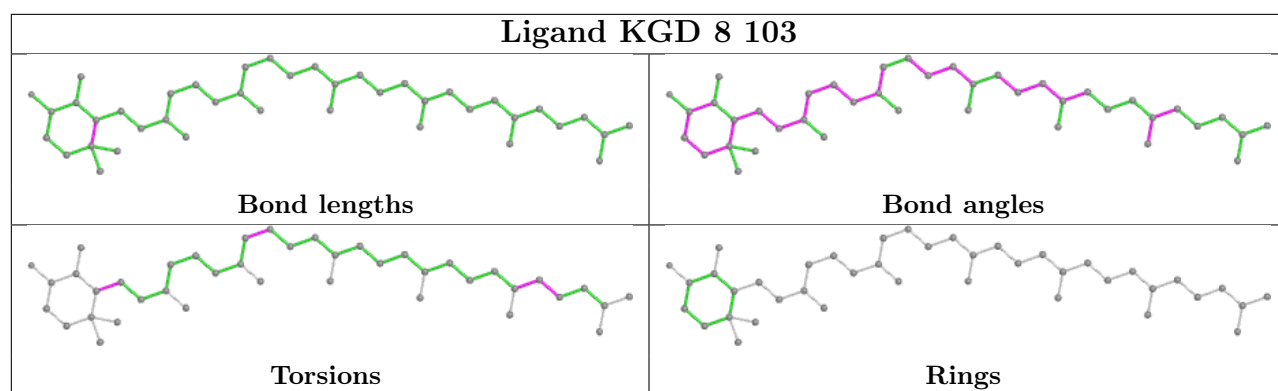


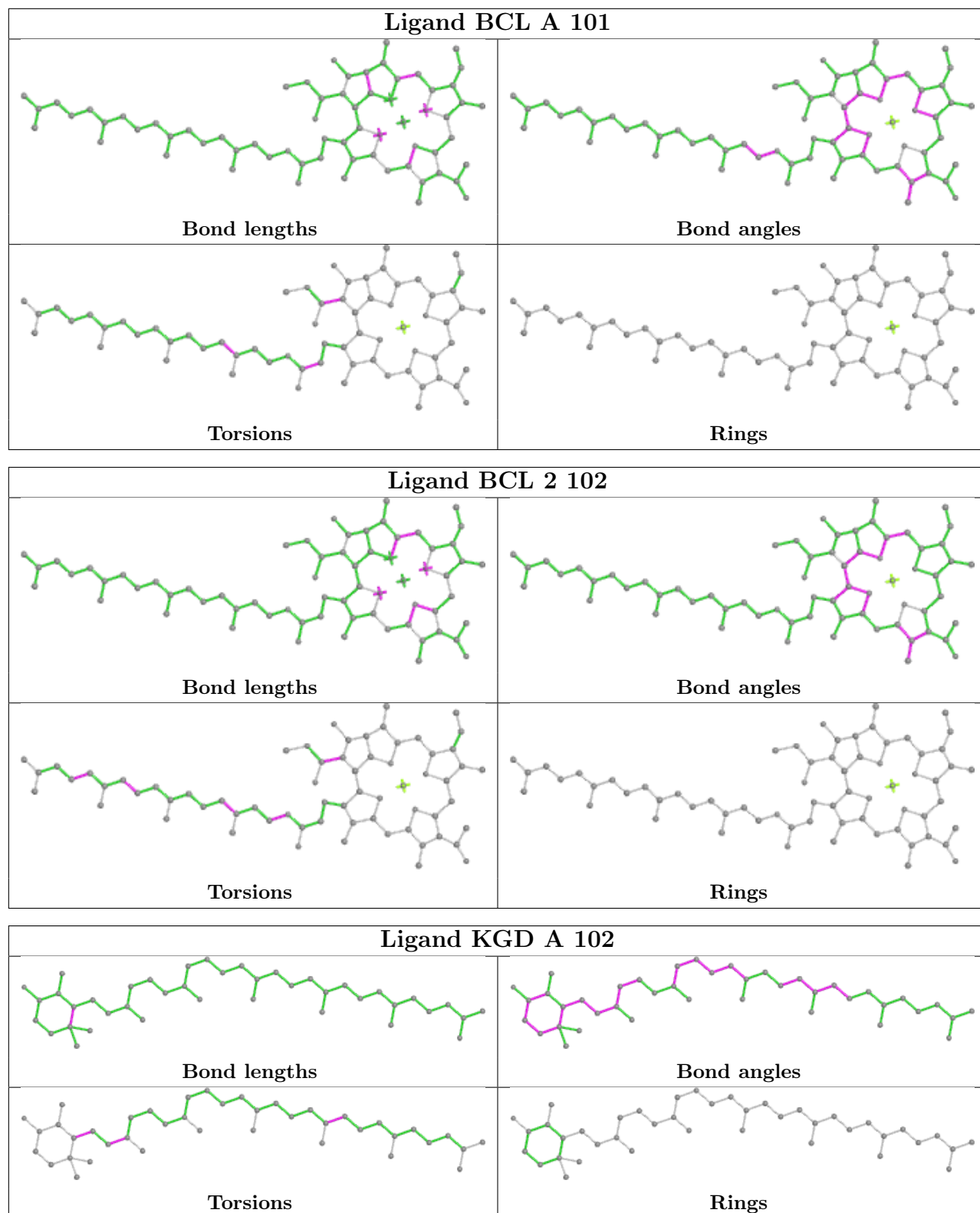


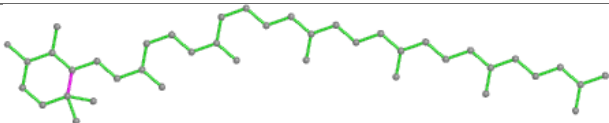
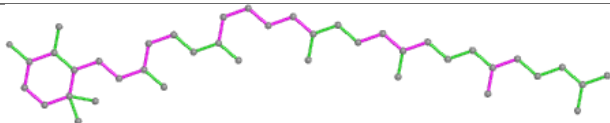
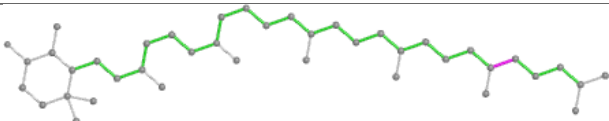
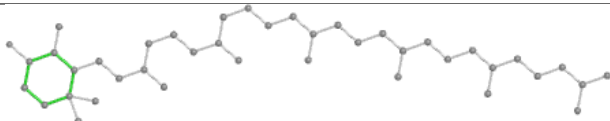


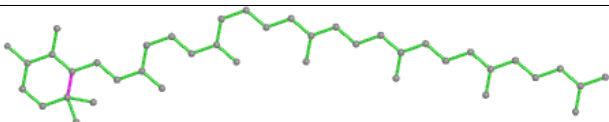
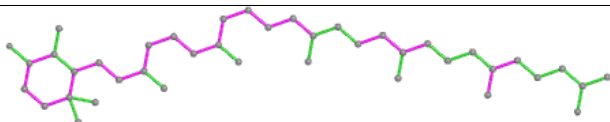
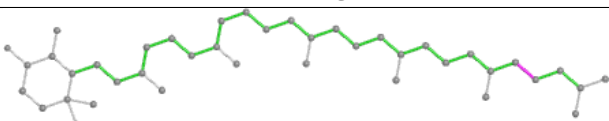
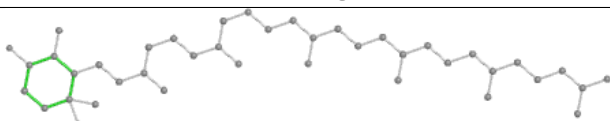


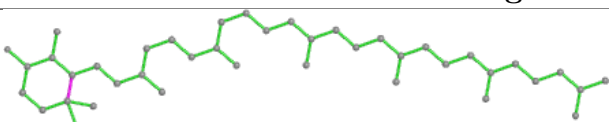
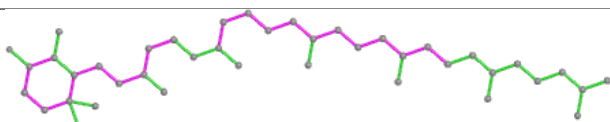
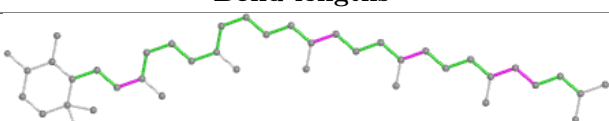



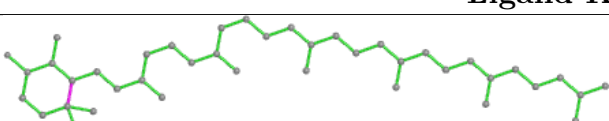
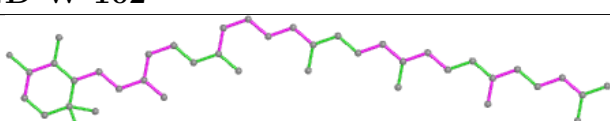
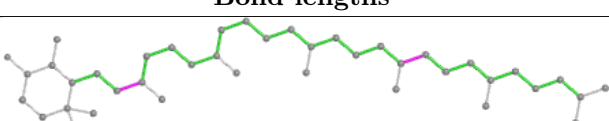
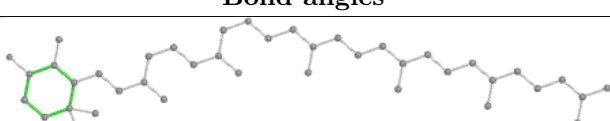


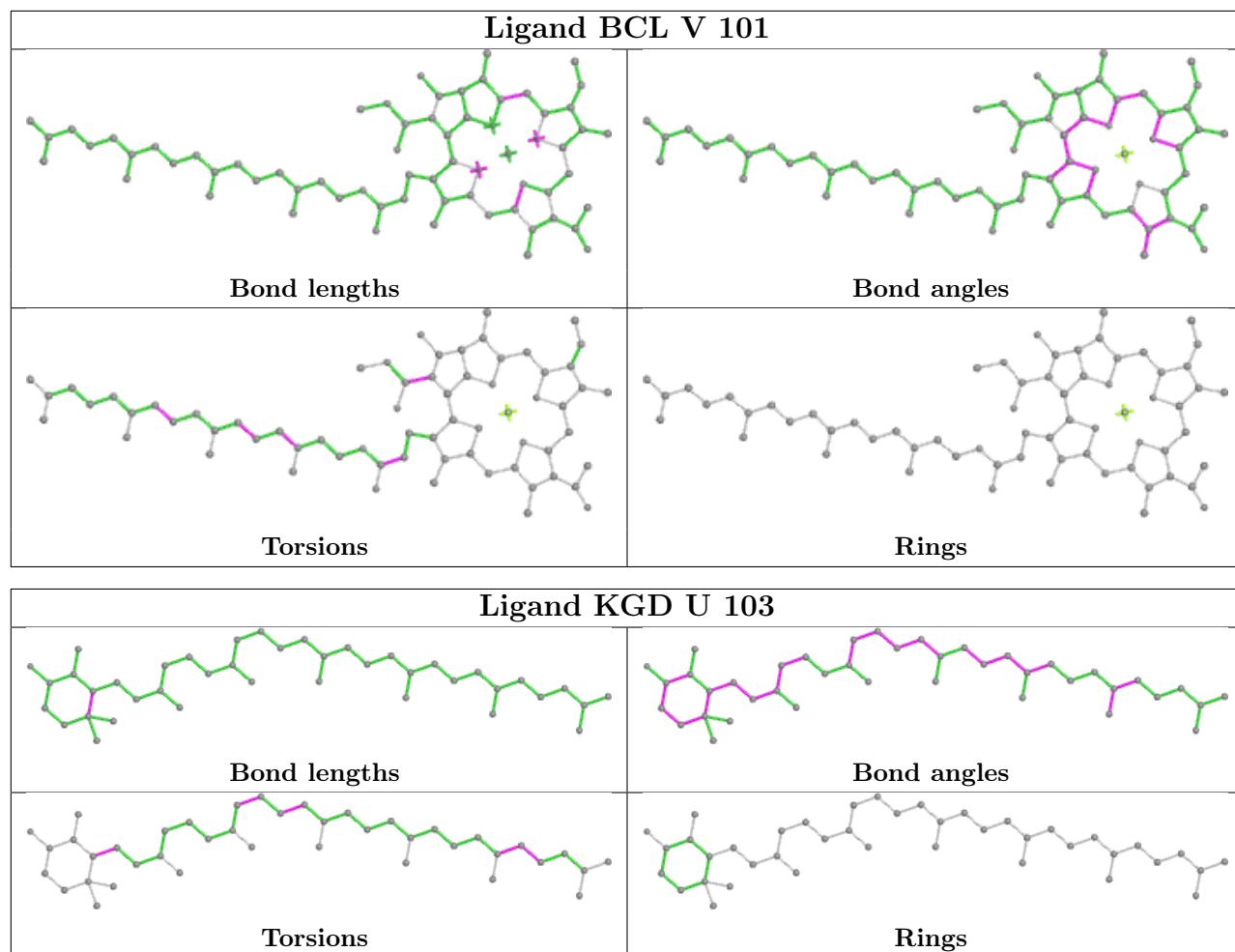


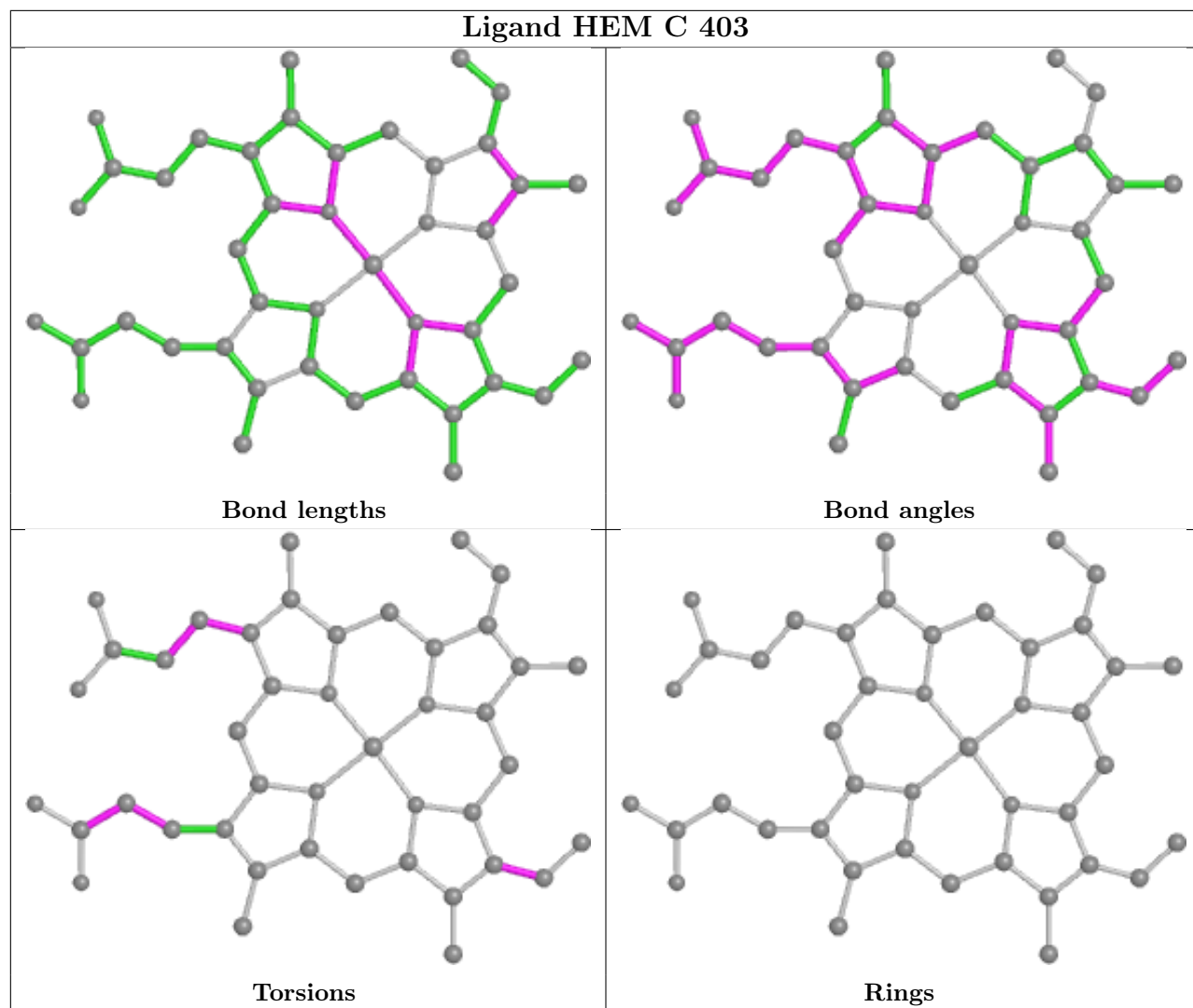
Ligand KGD O 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

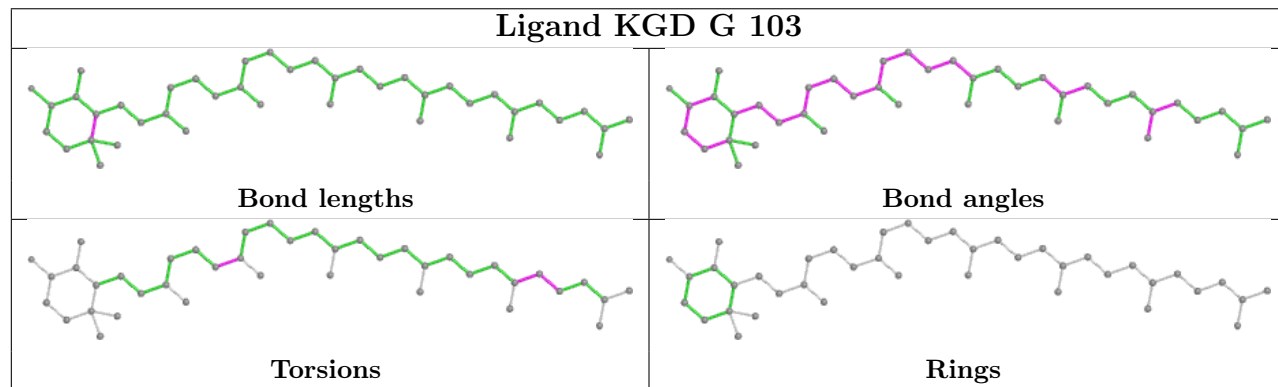
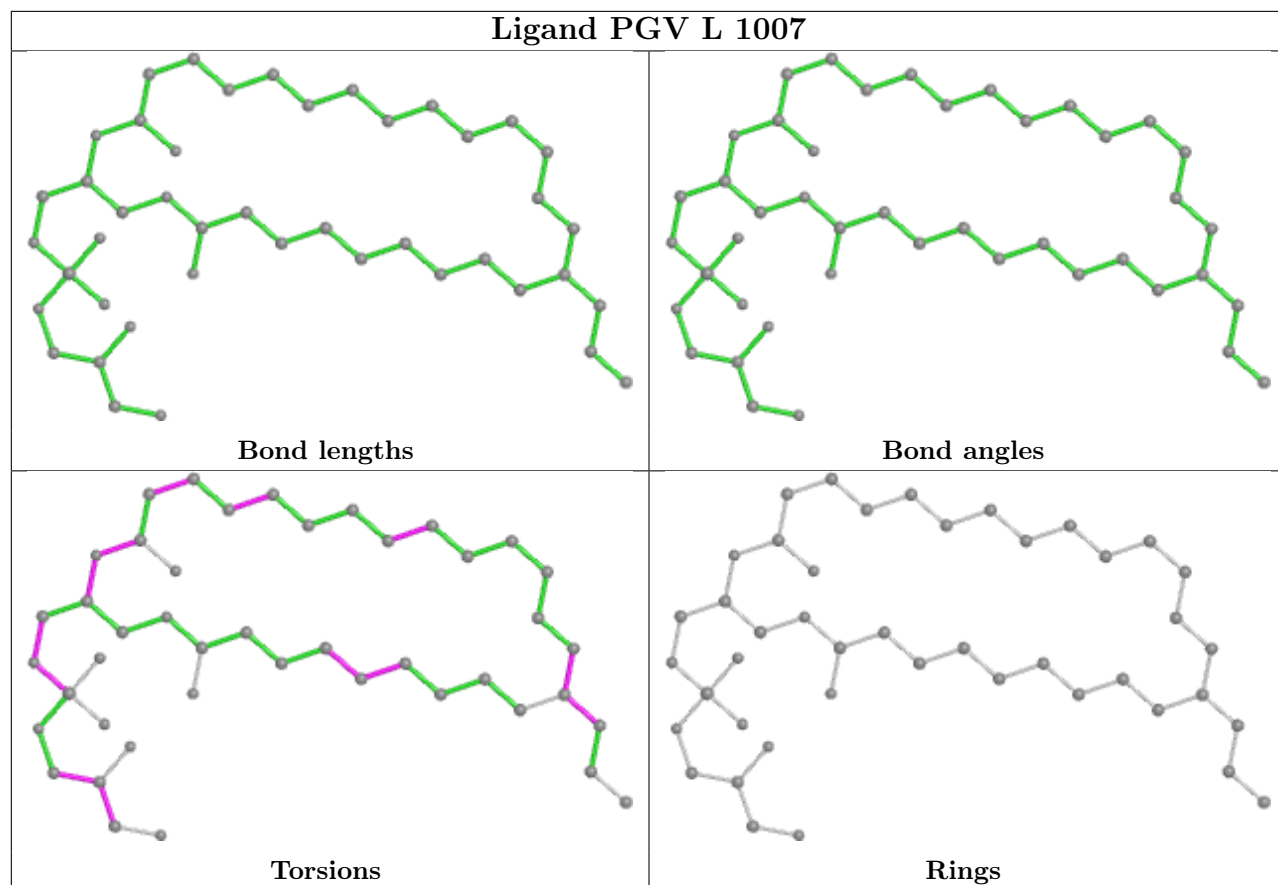
Ligand KGD E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

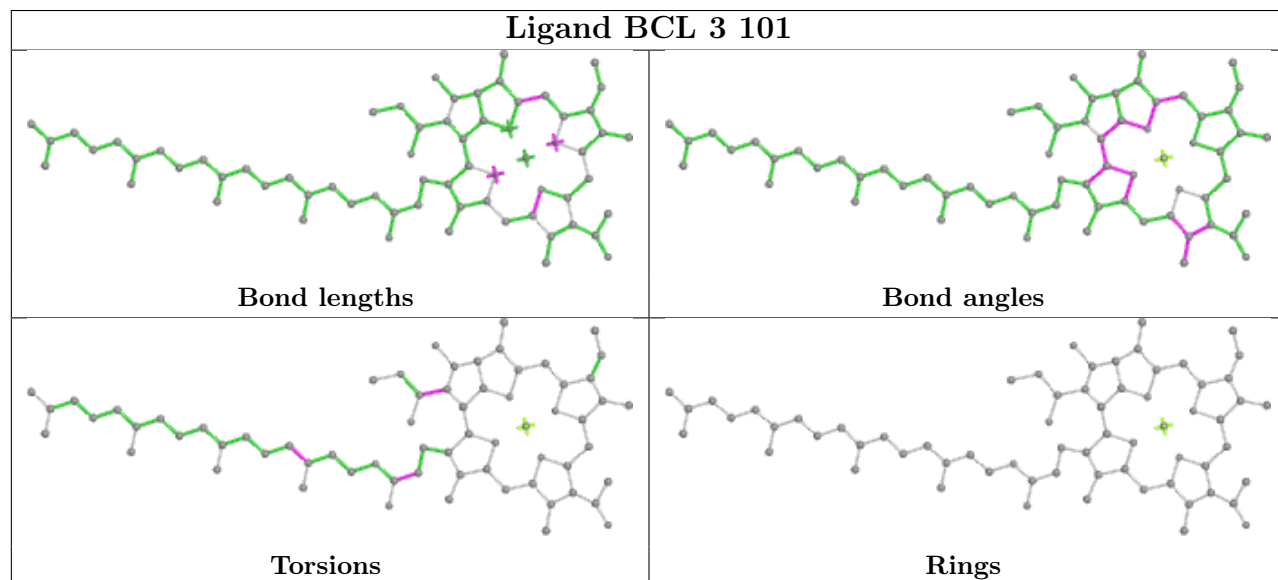
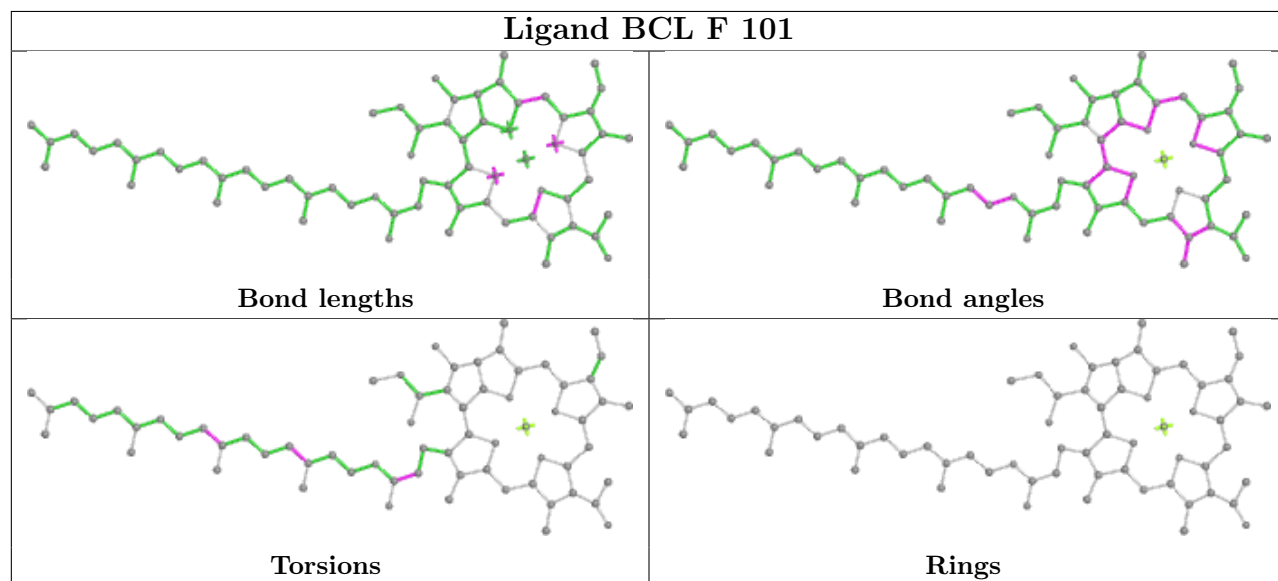
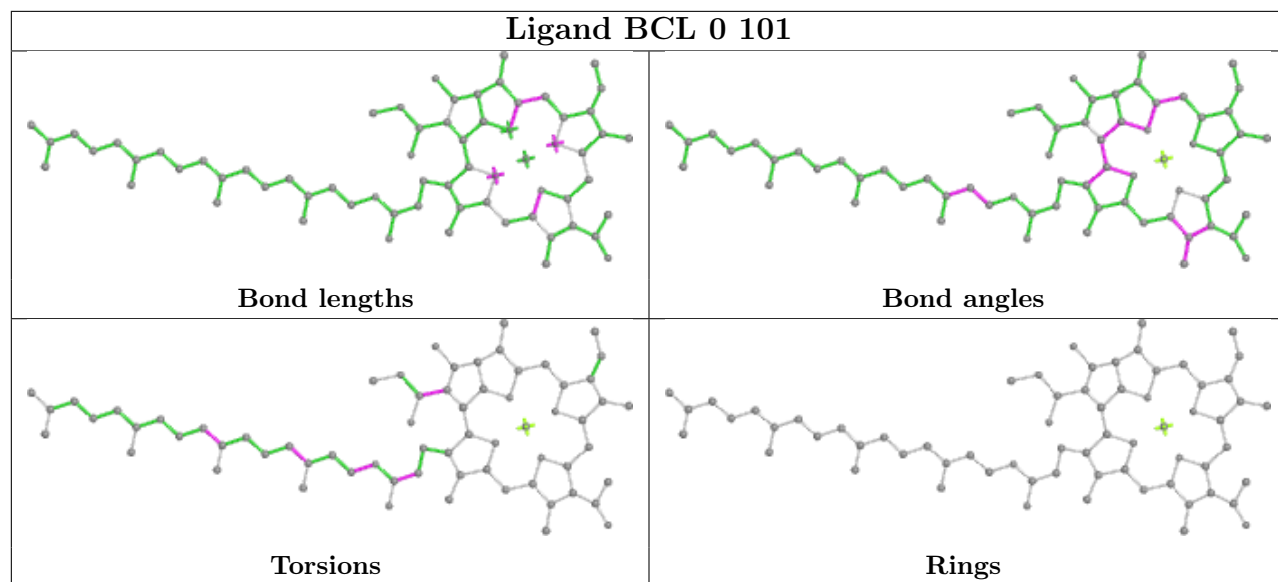
Ligand KGD P 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

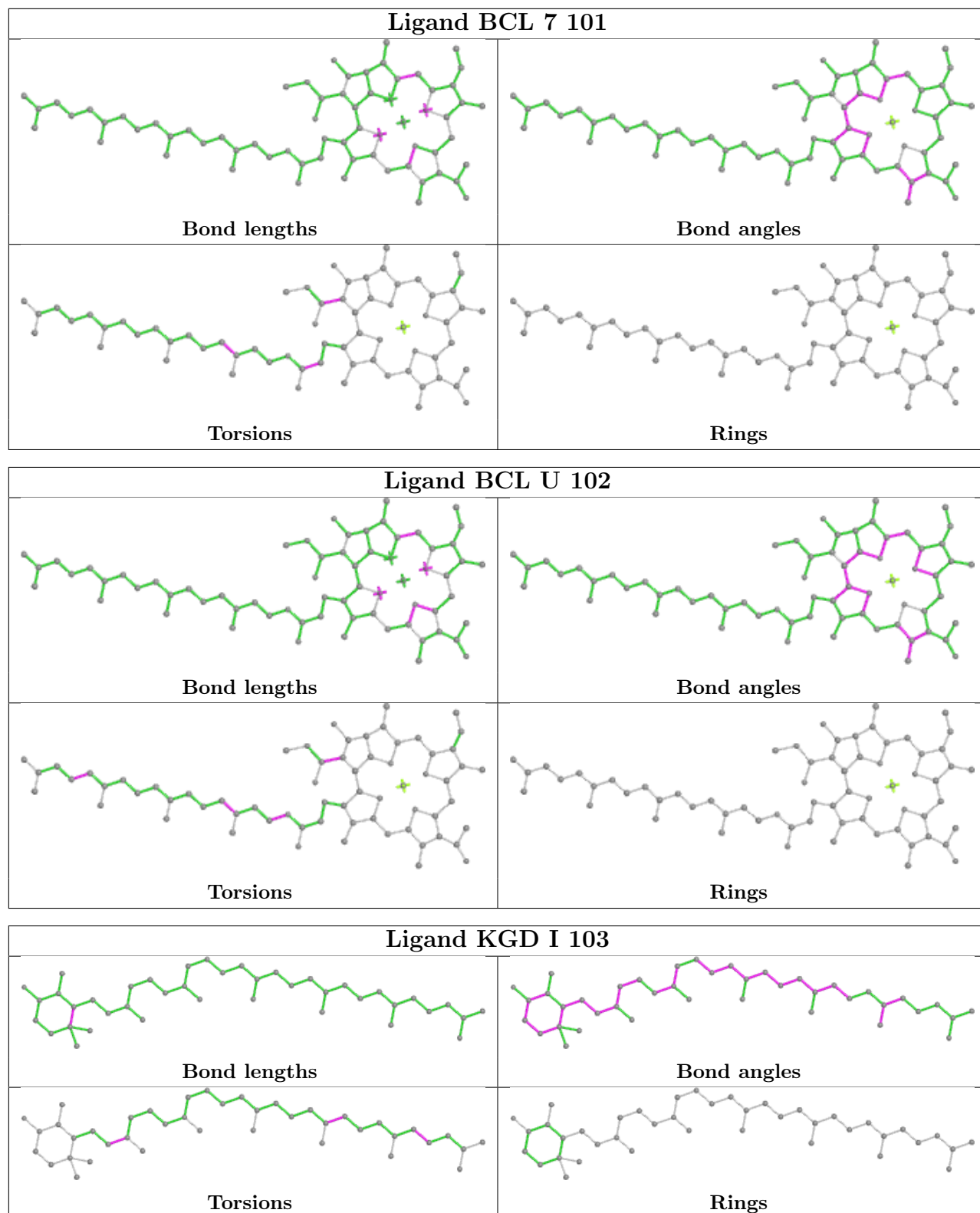
Ligand KGD W 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

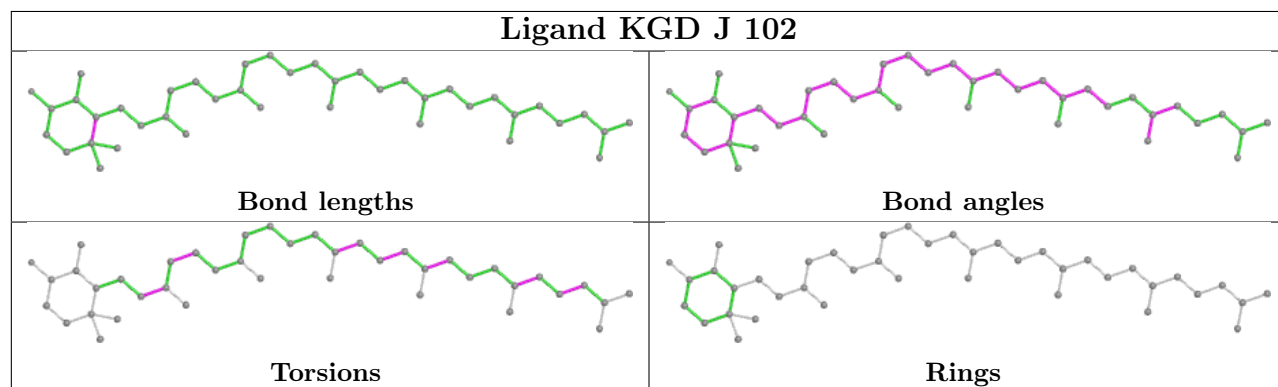
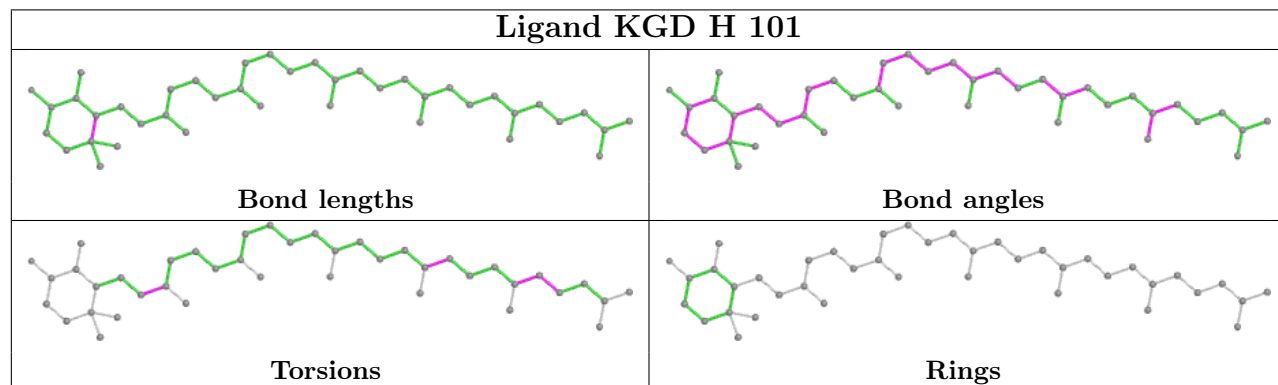
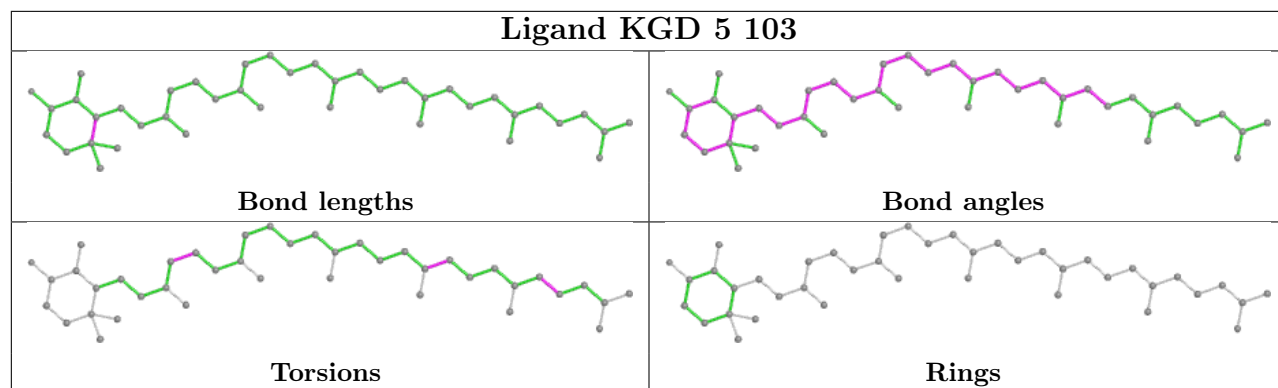


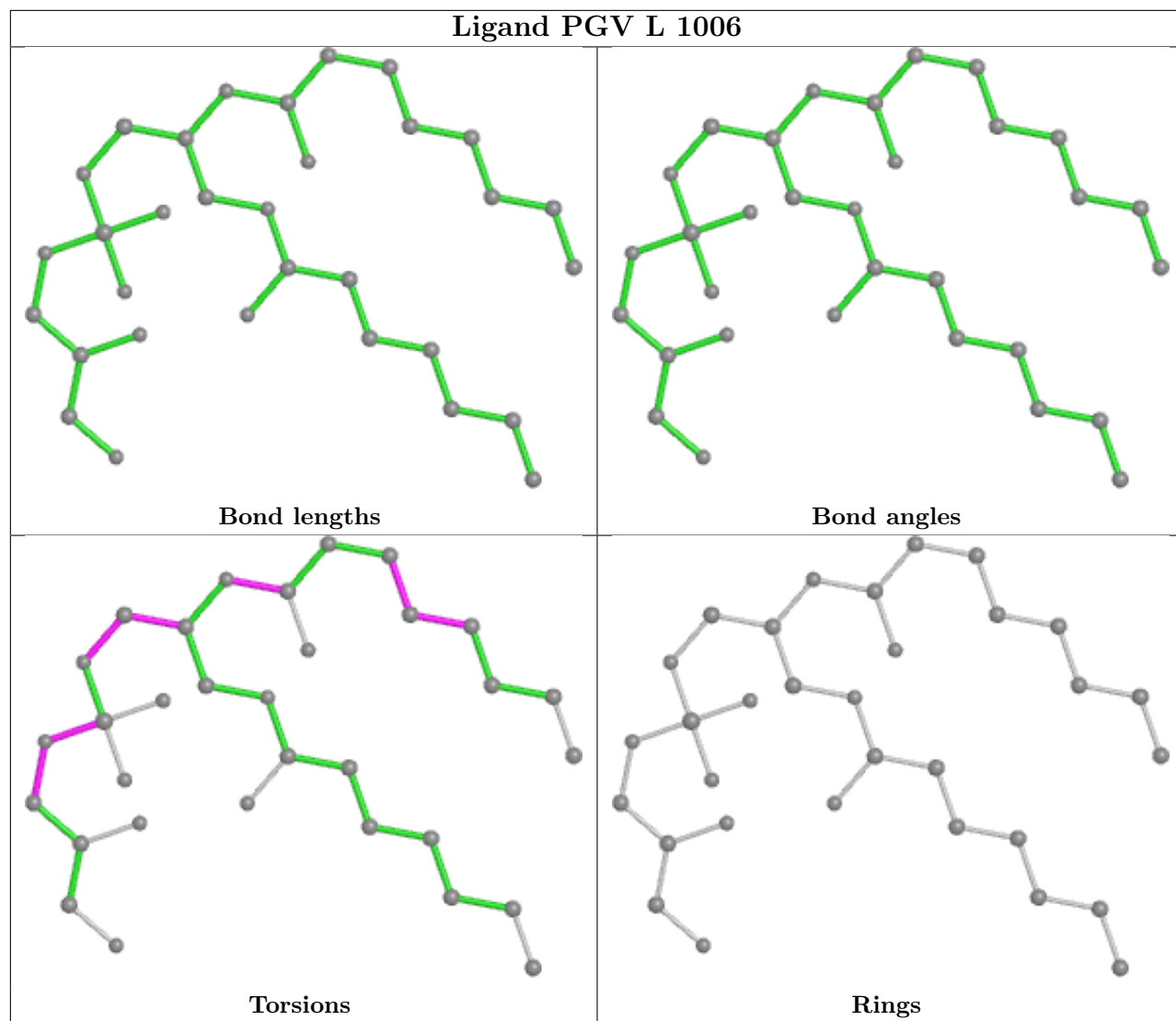


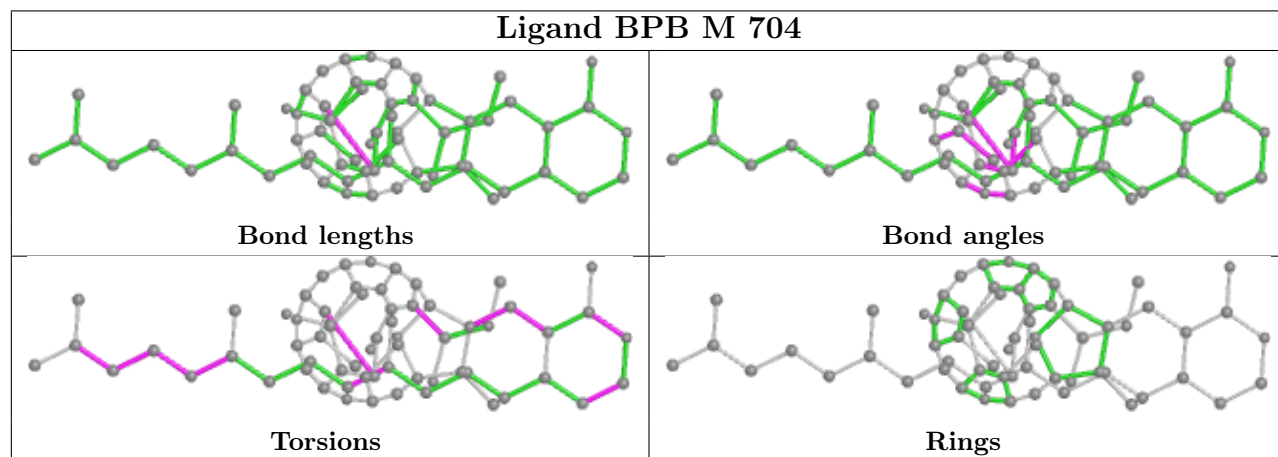
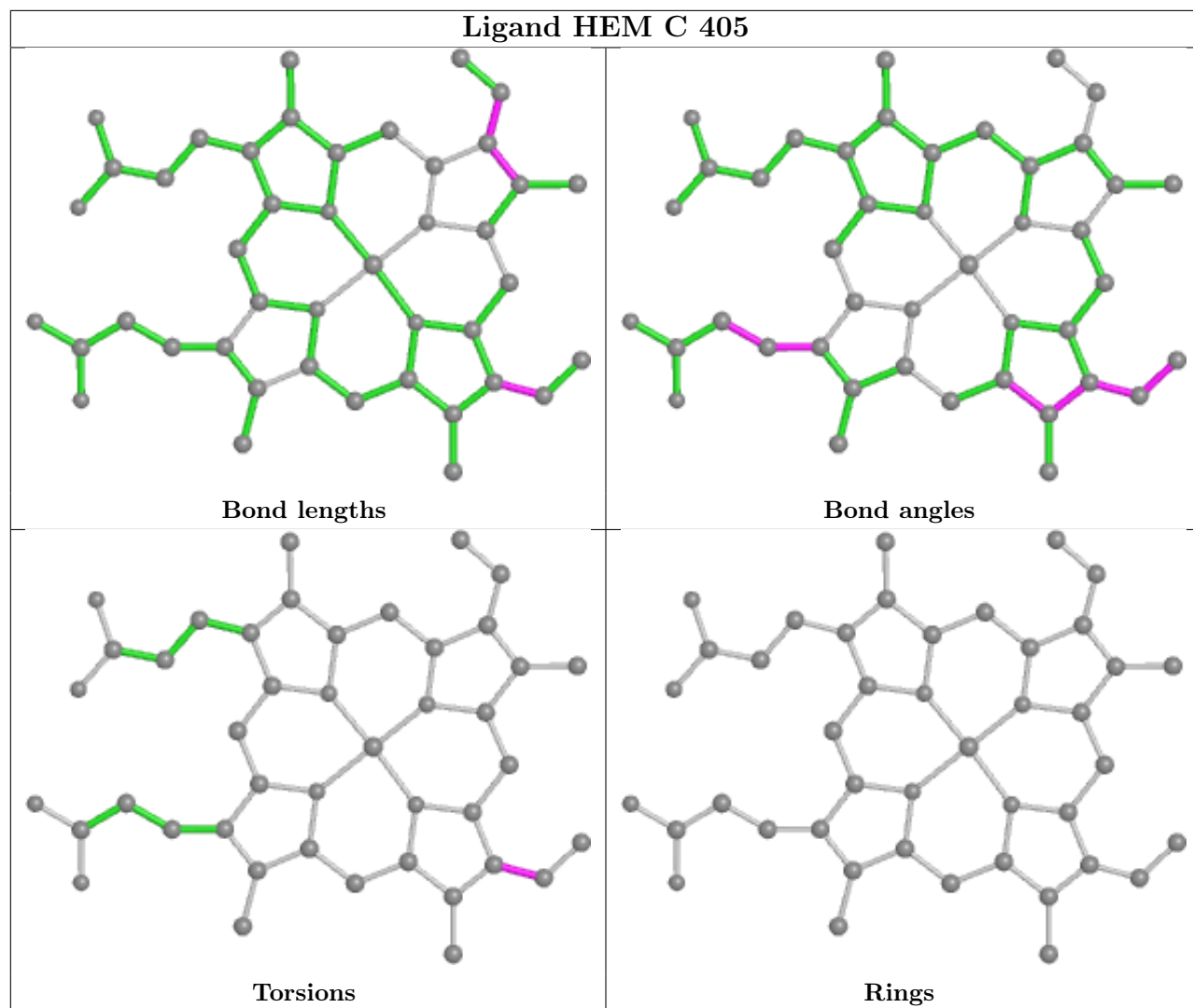


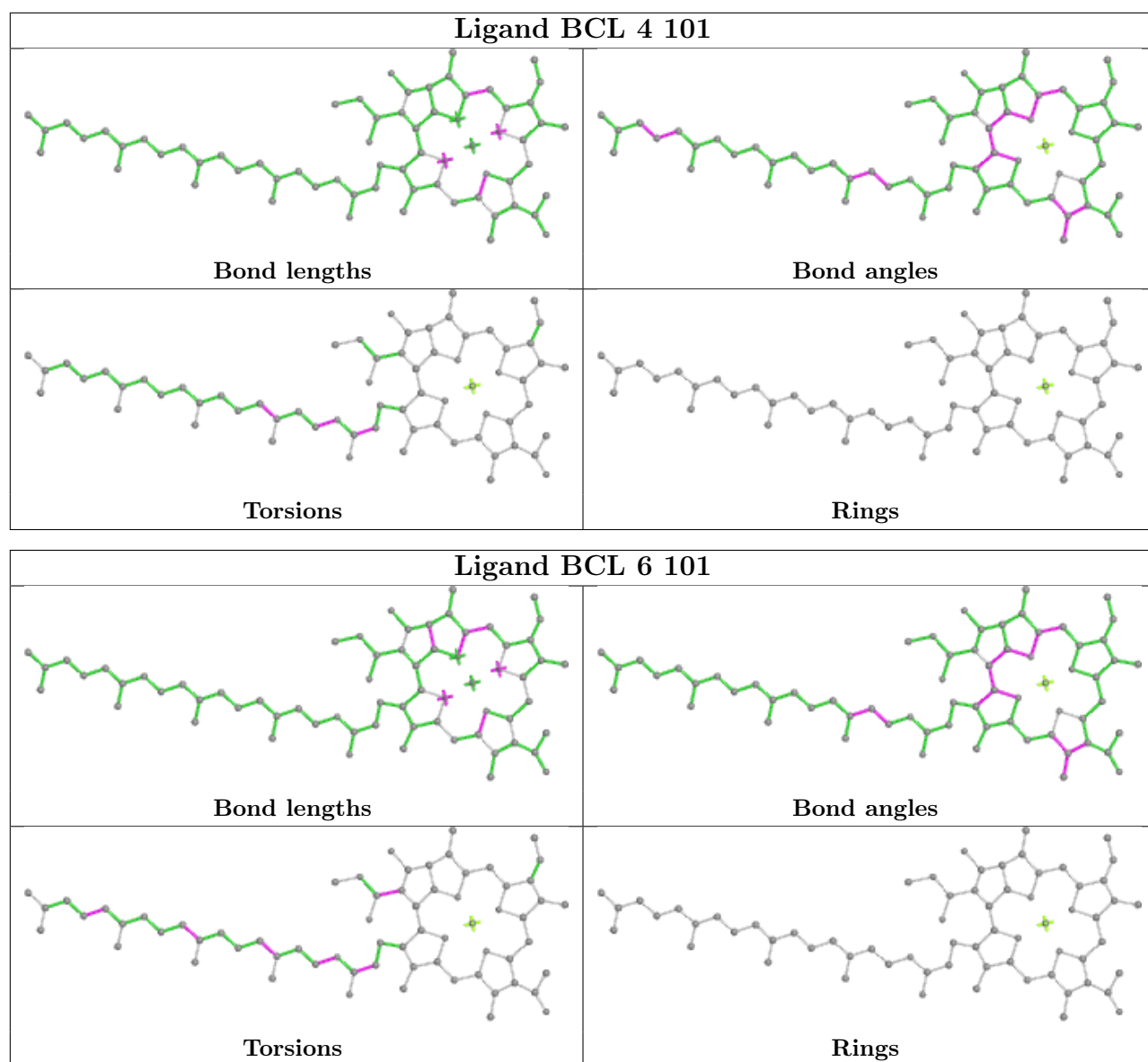


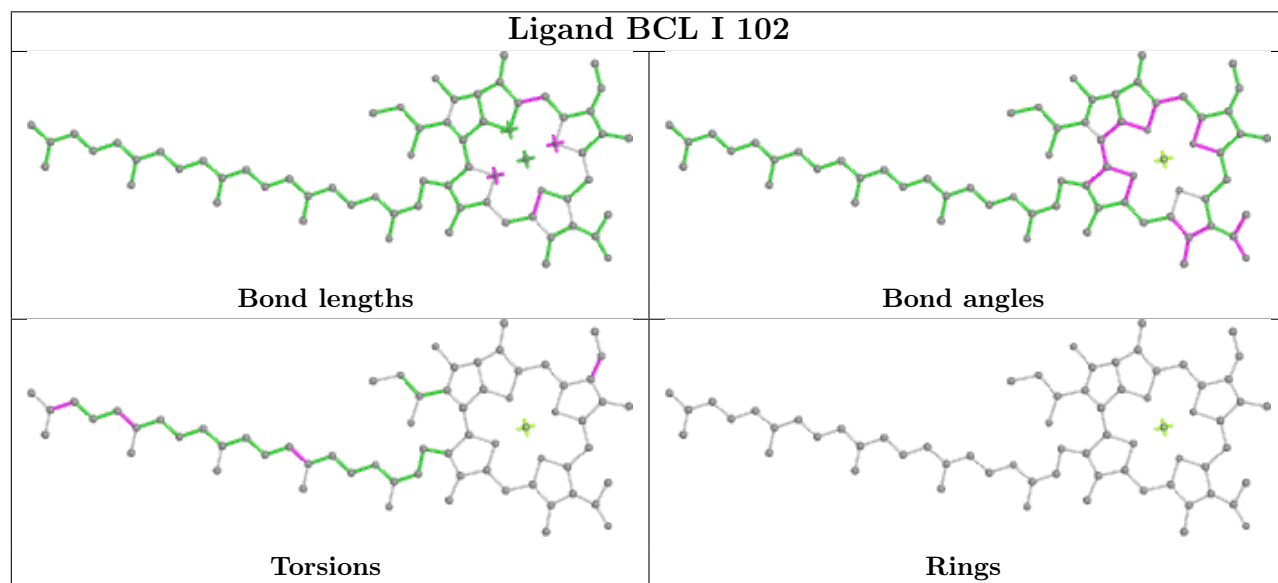
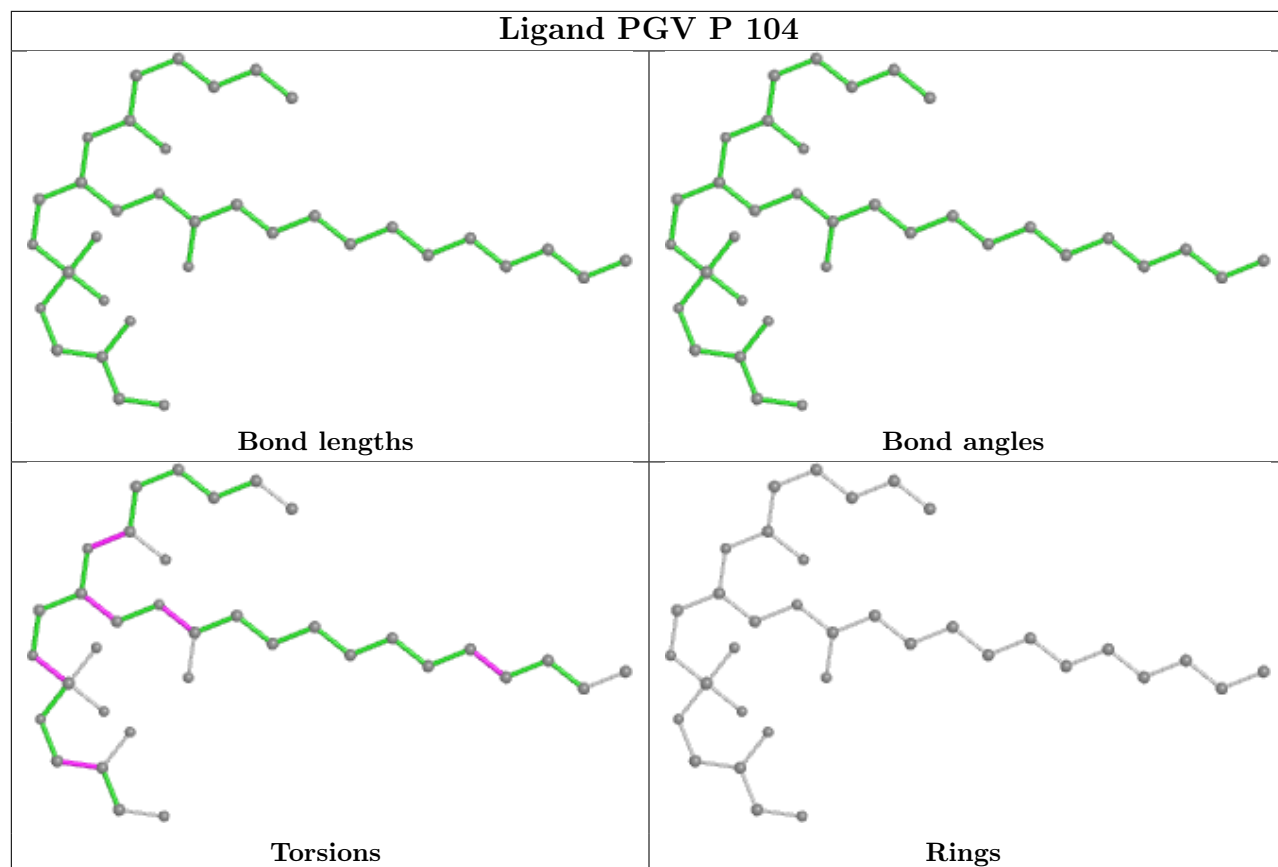


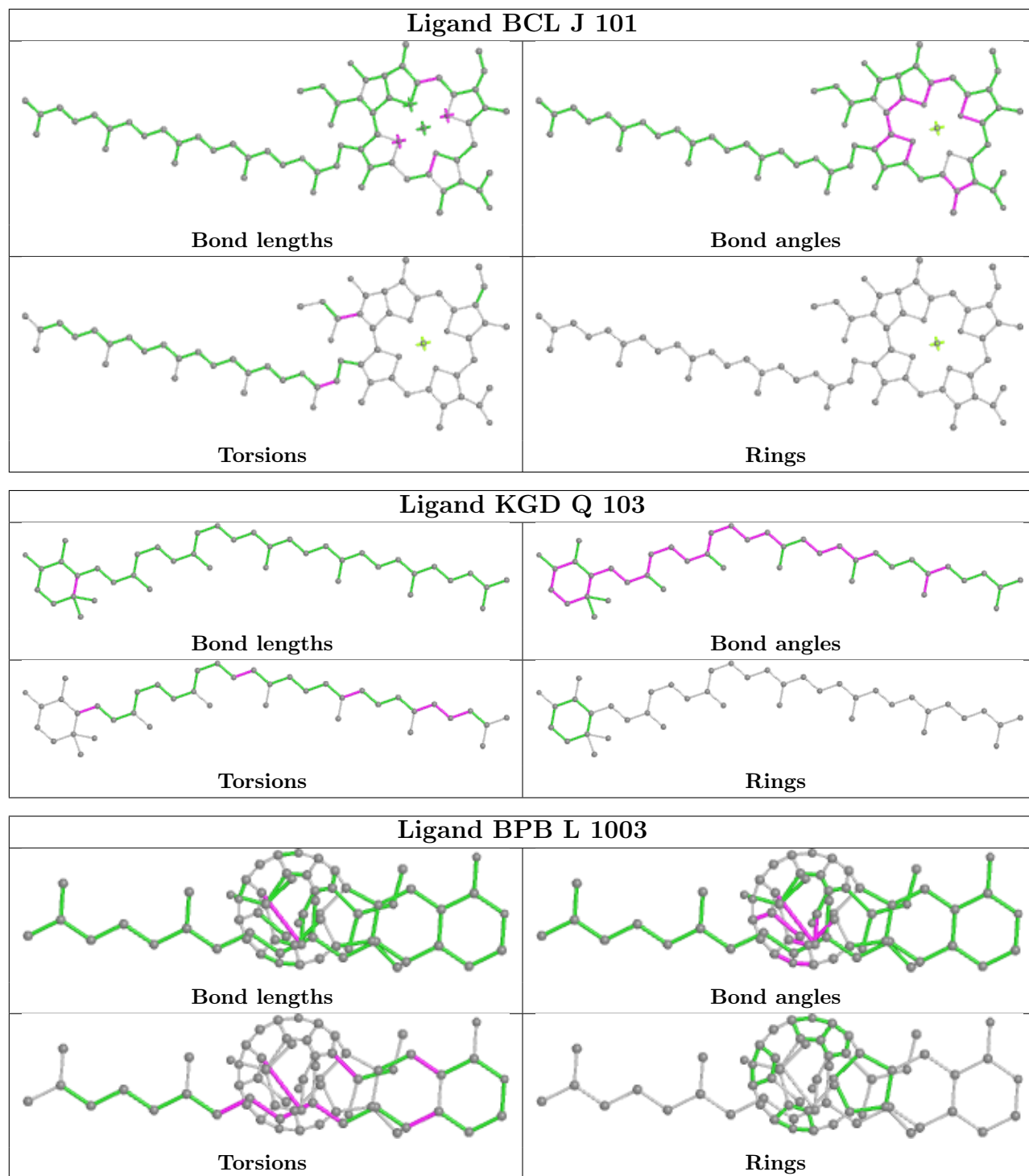


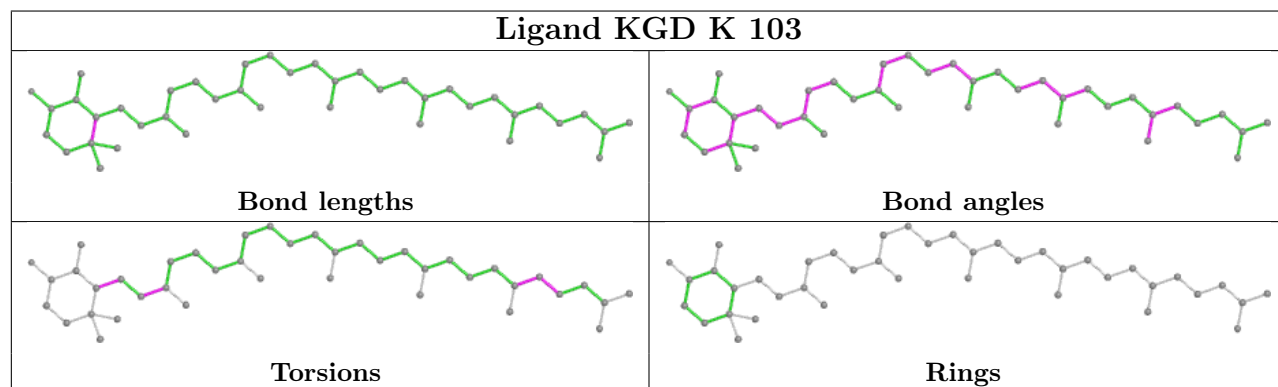
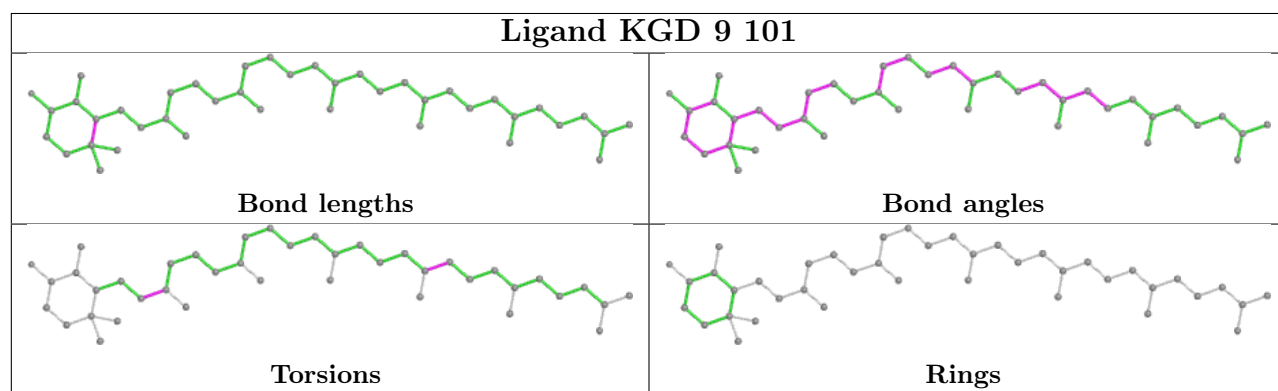
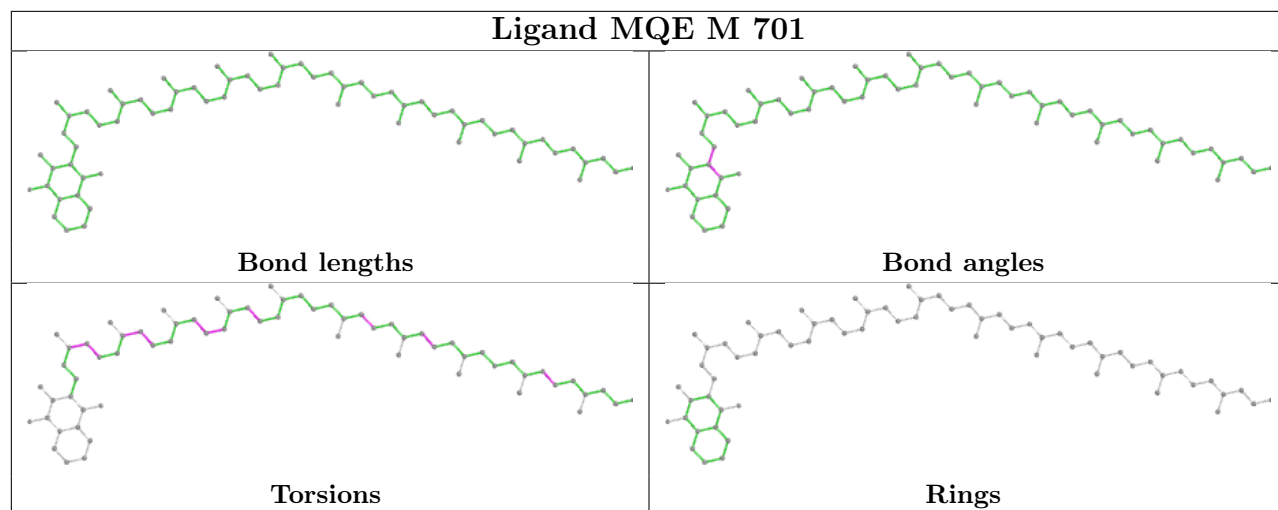


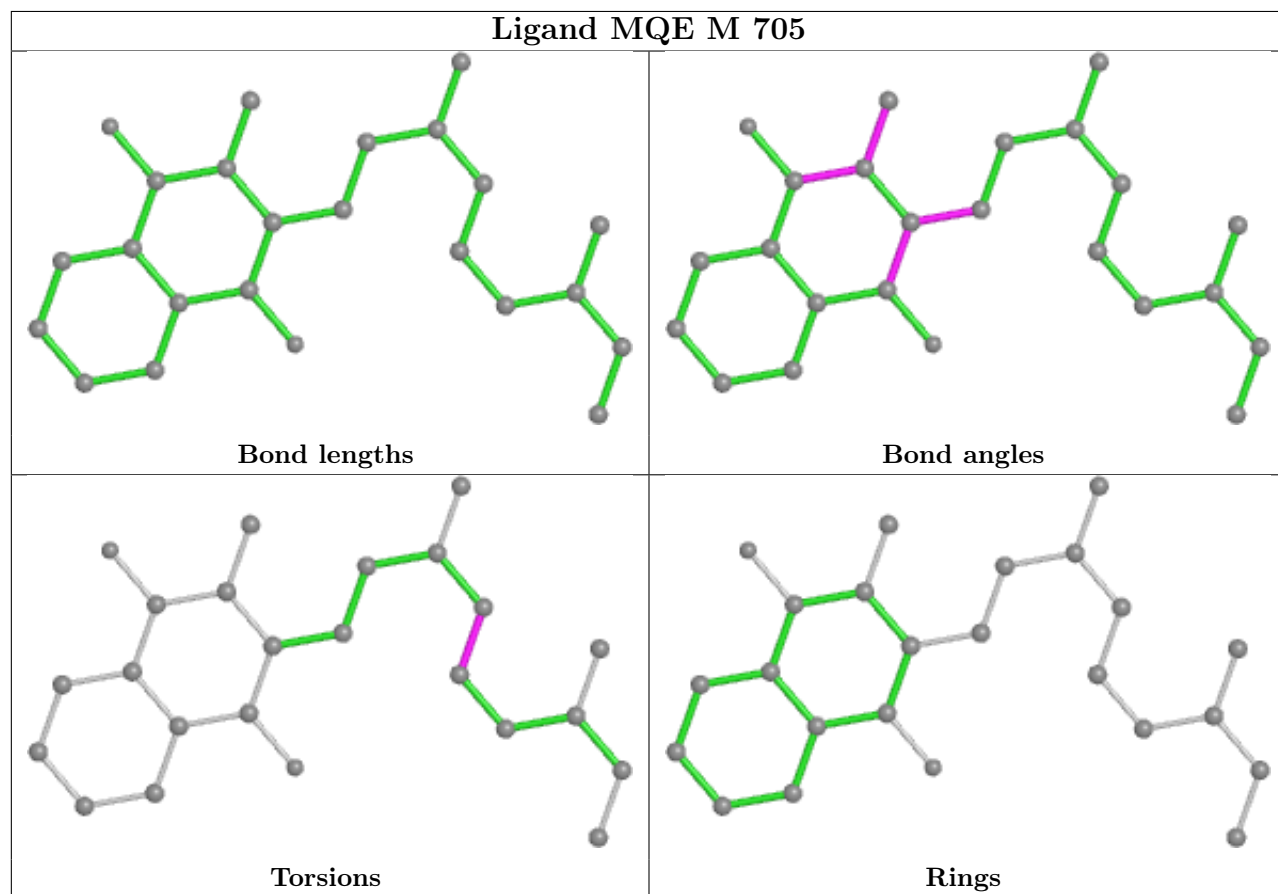
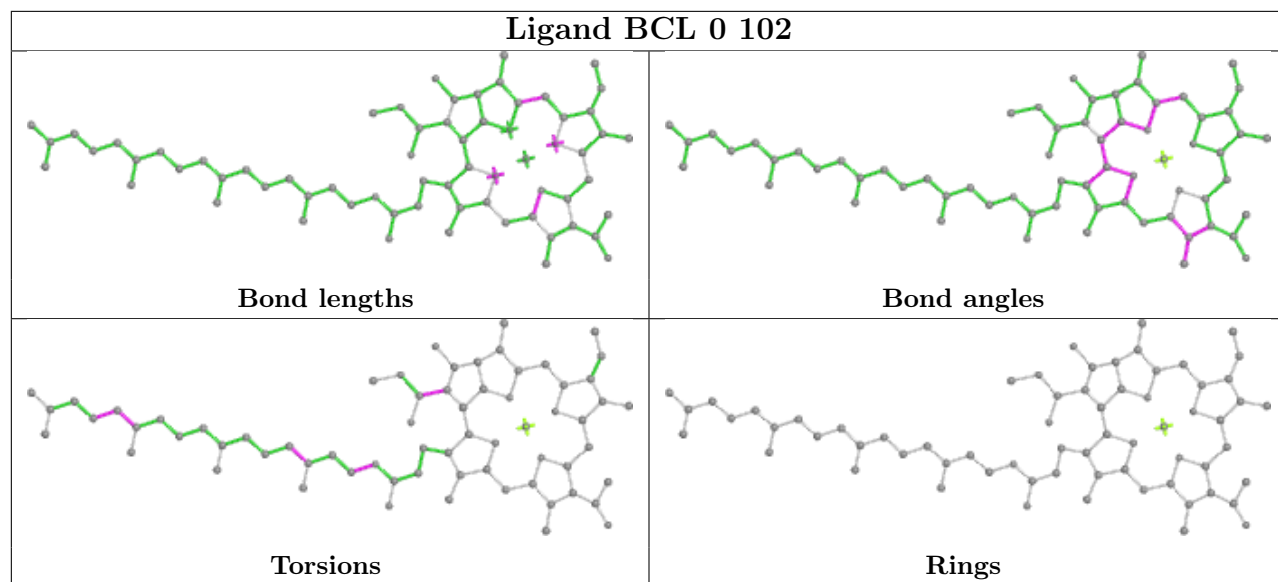


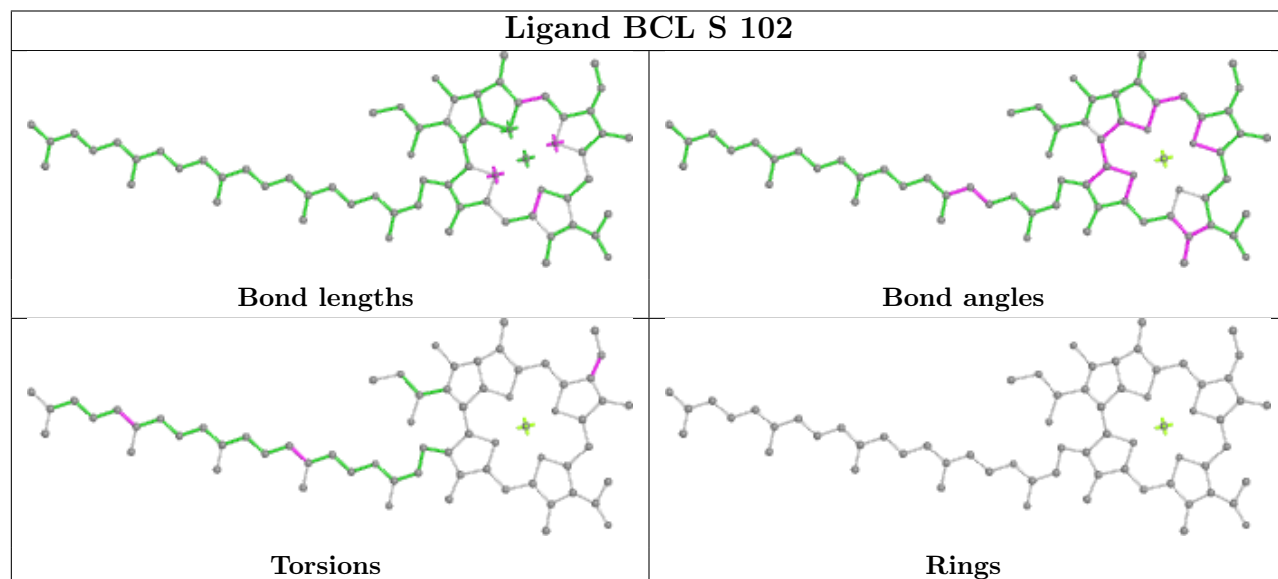
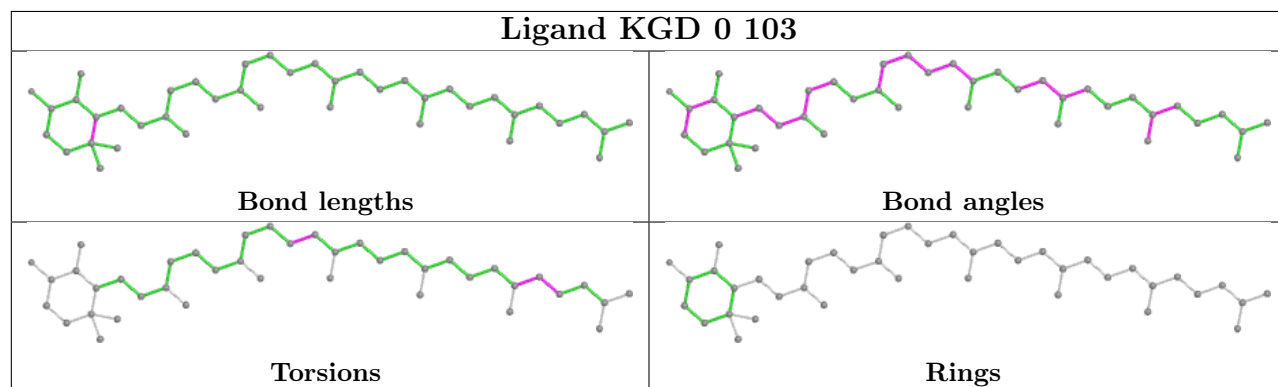
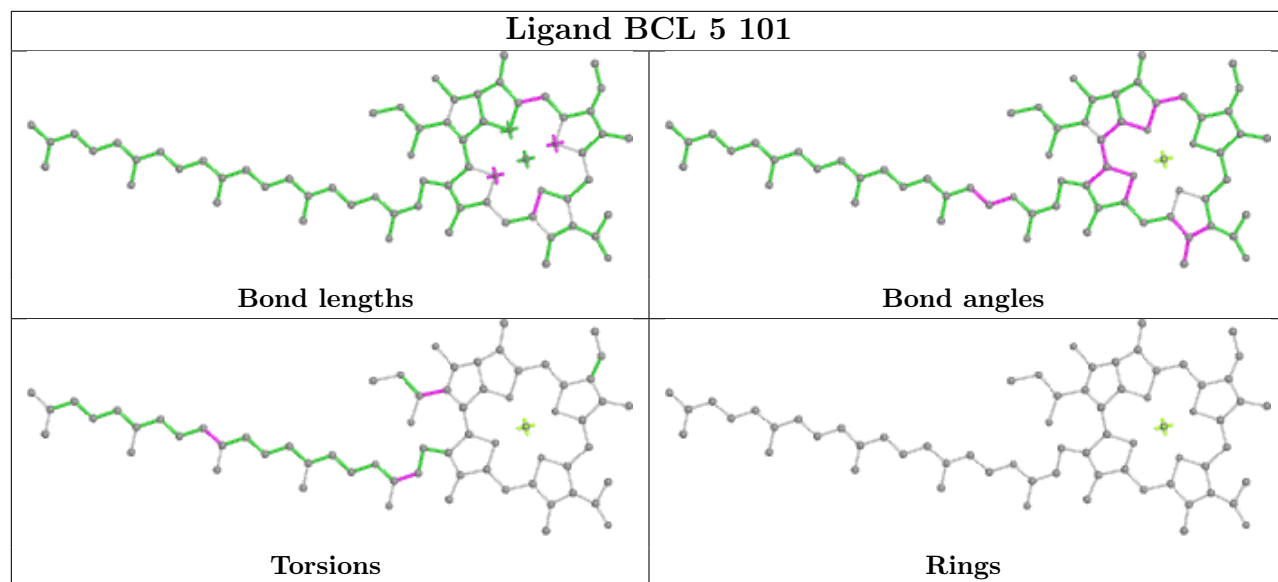


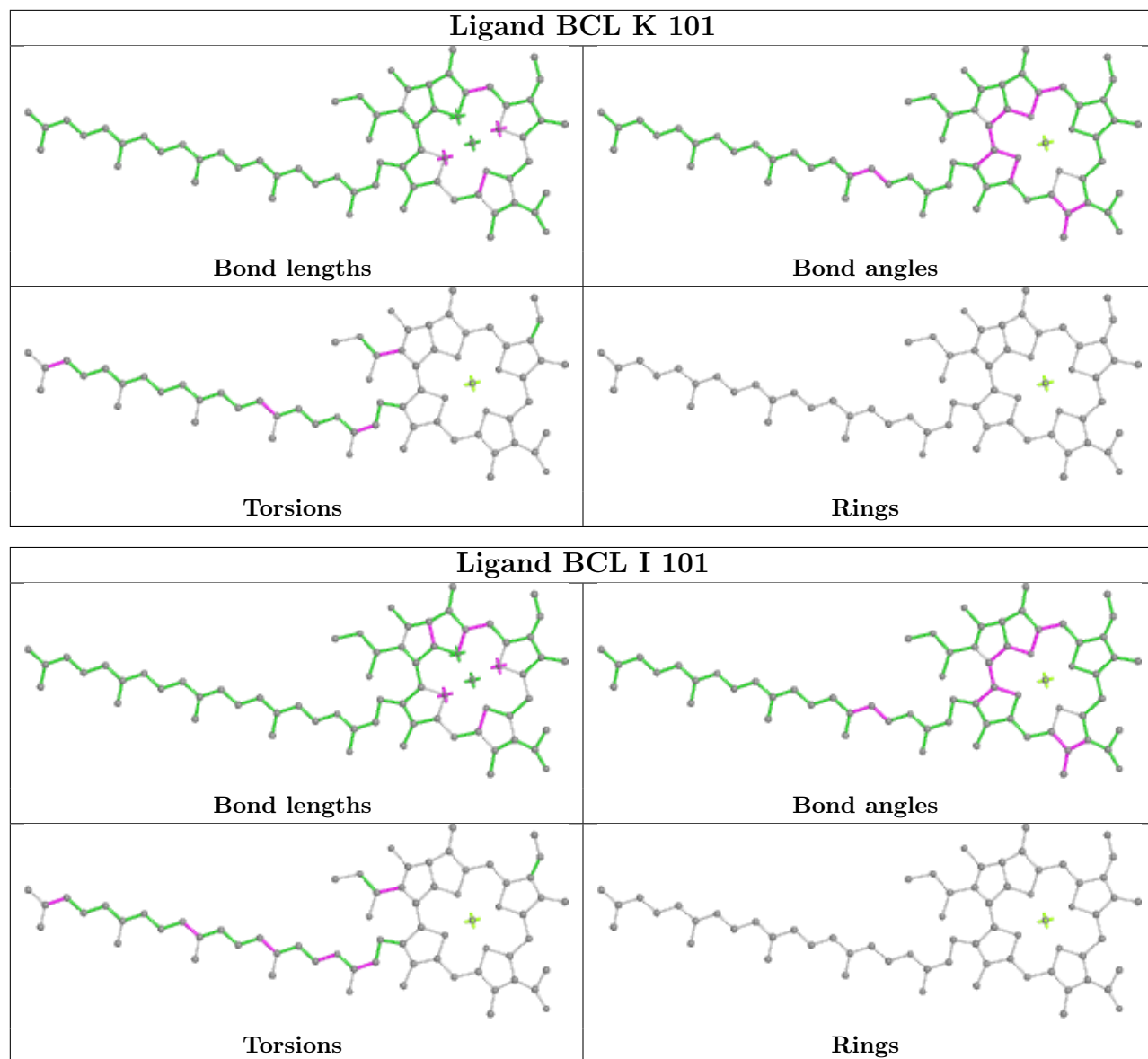


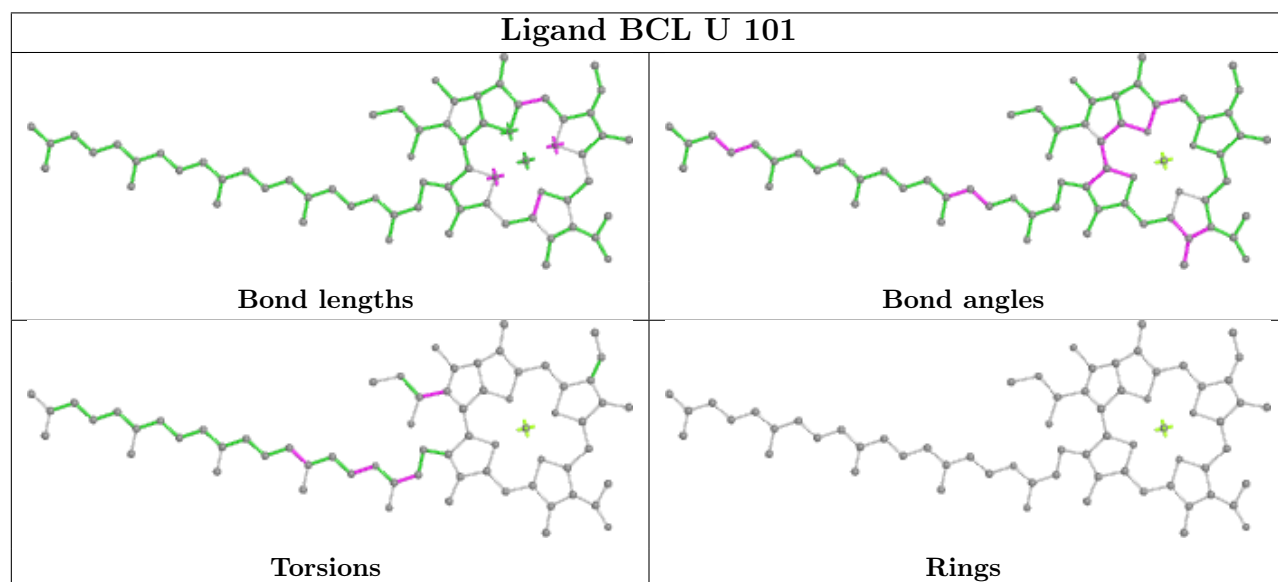
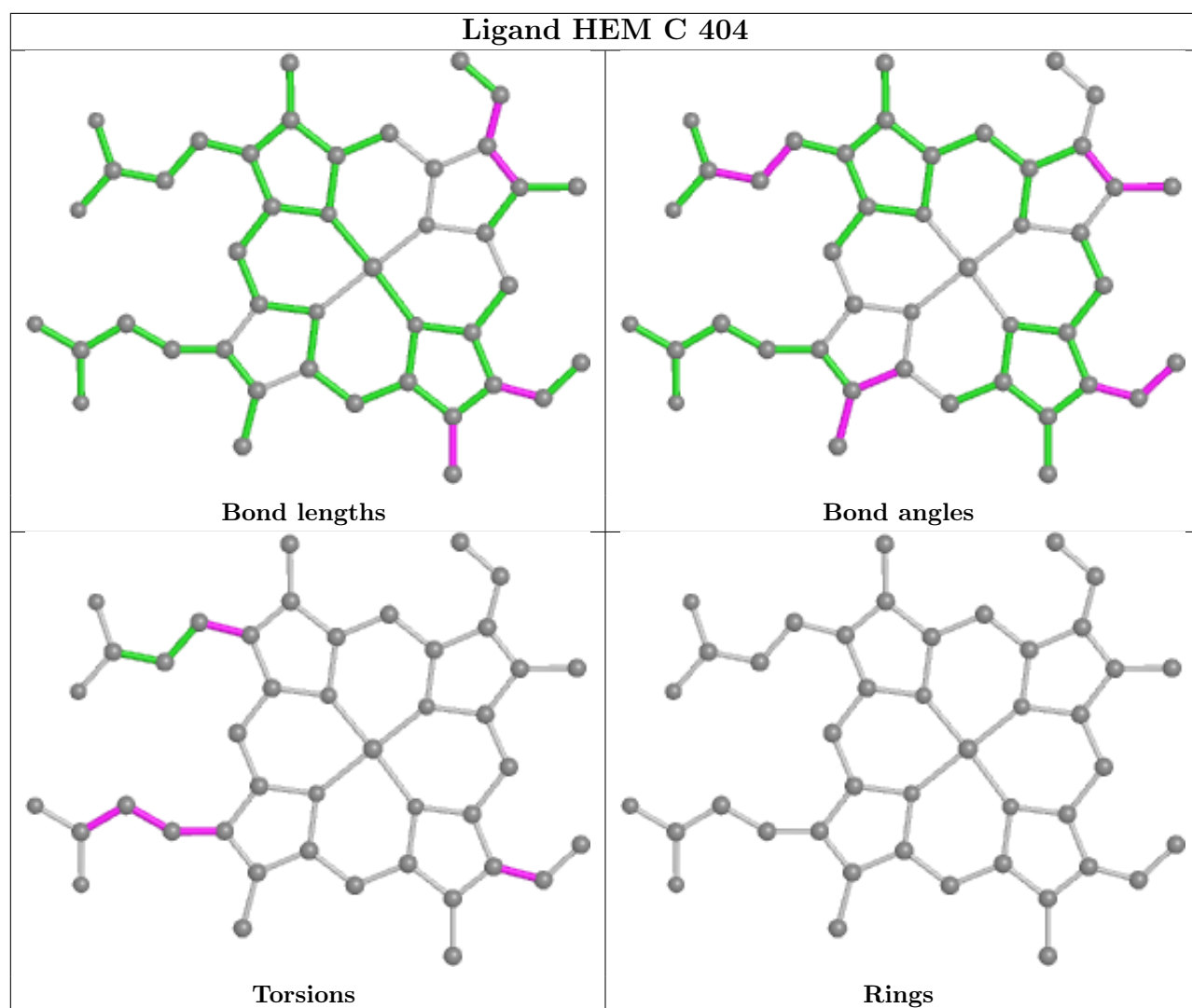


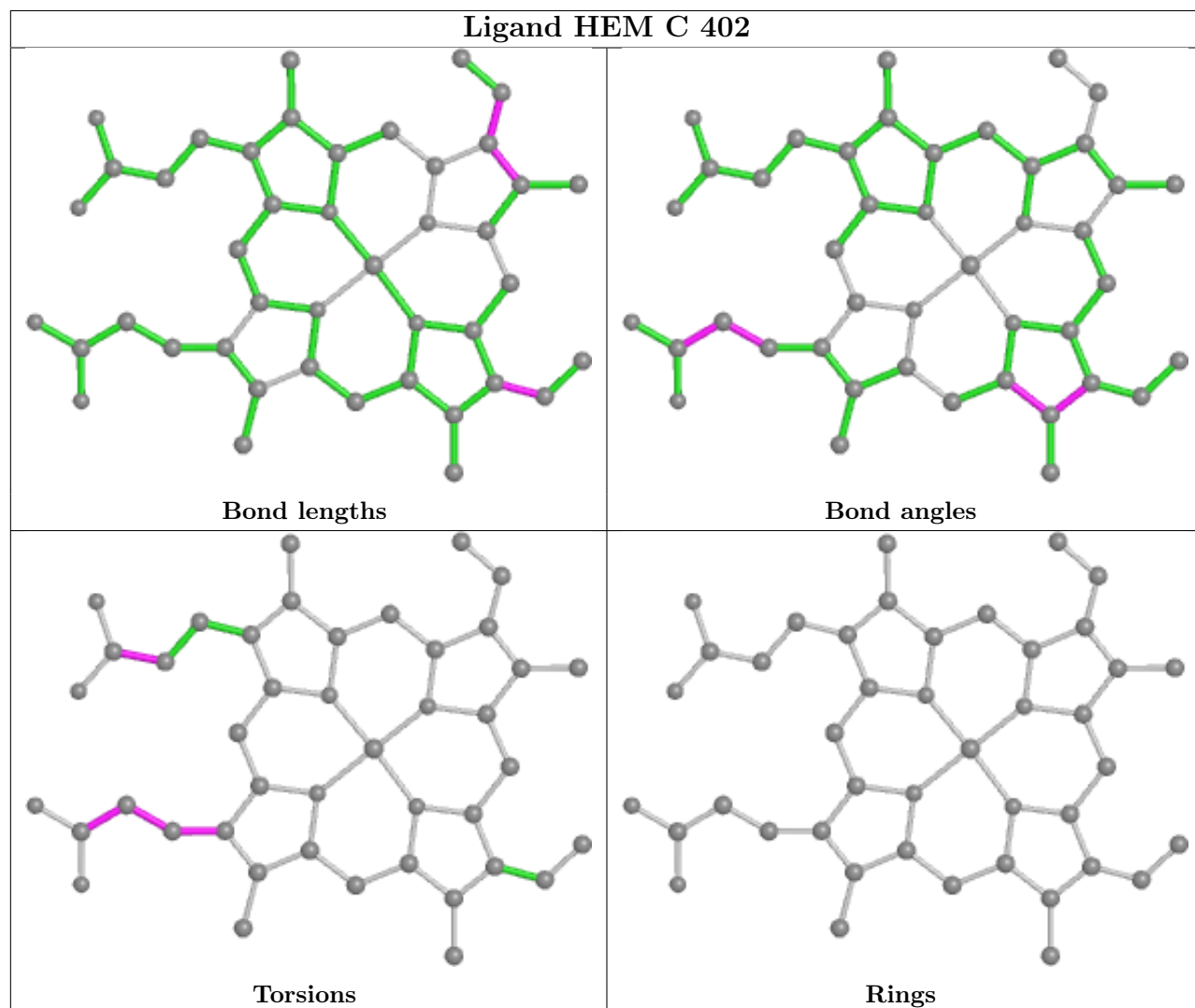
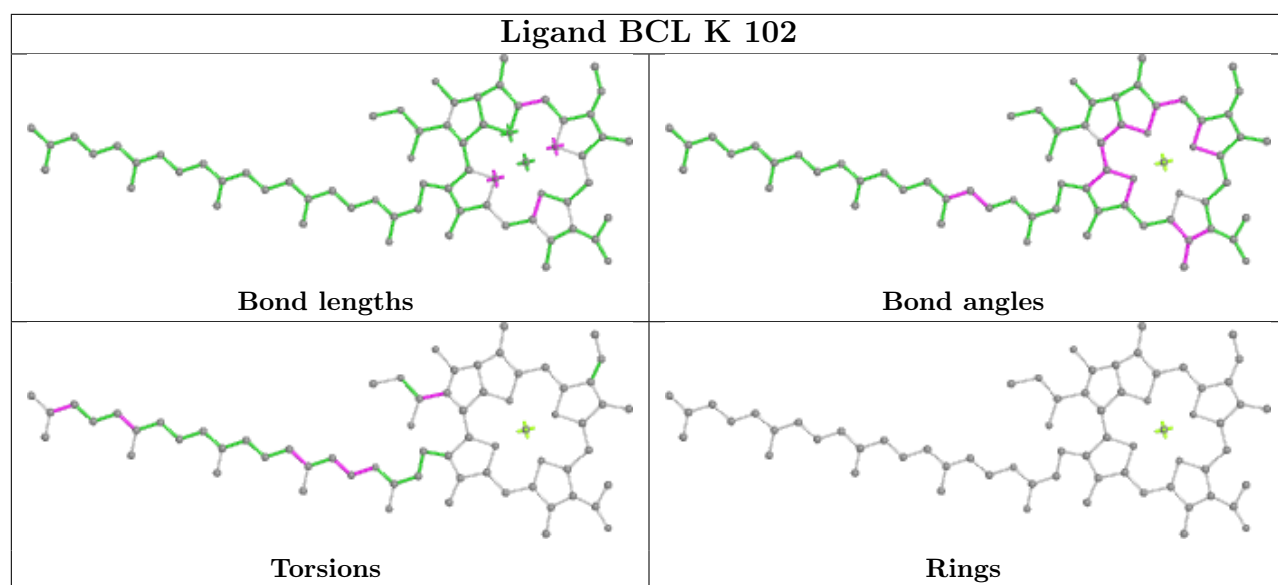


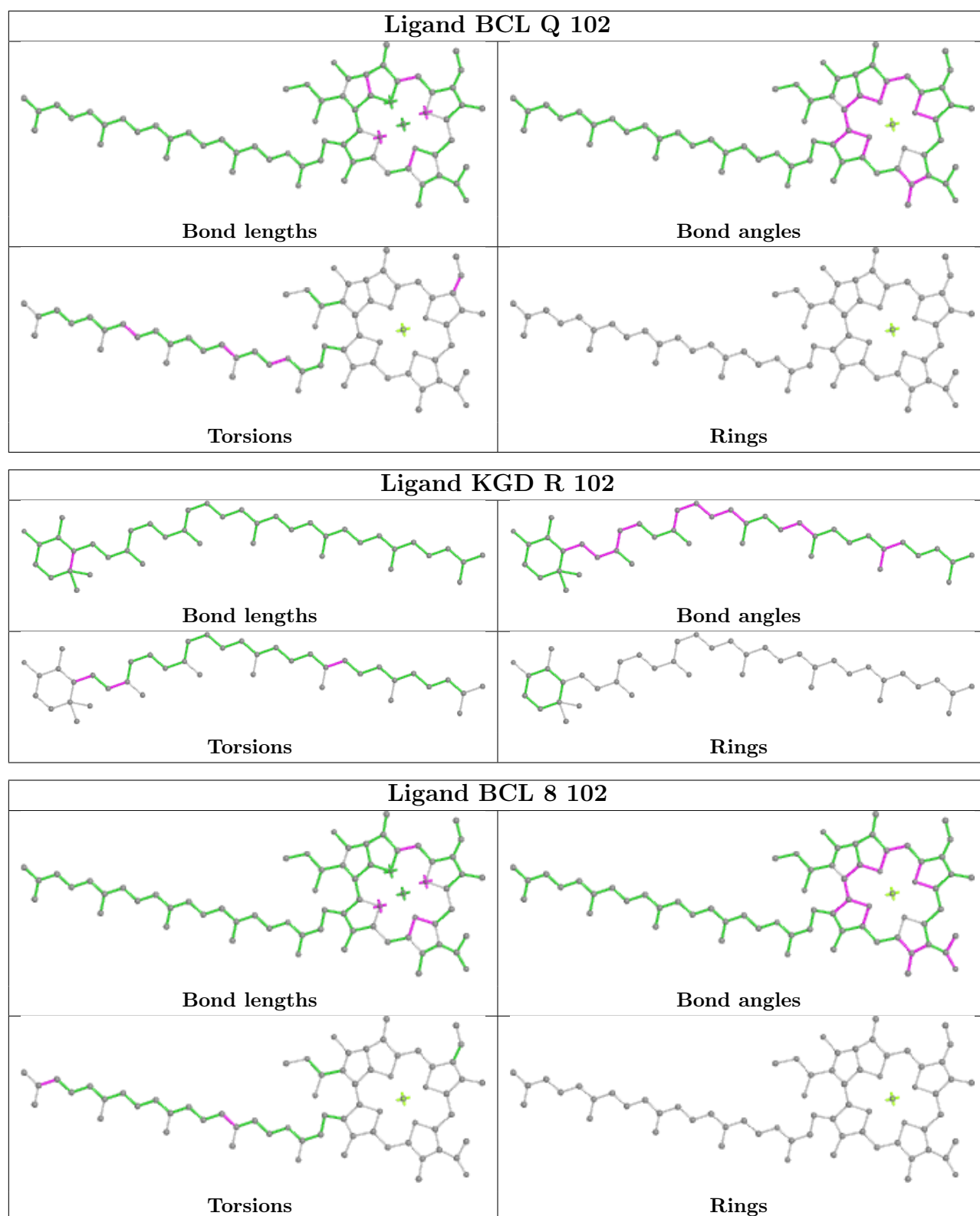


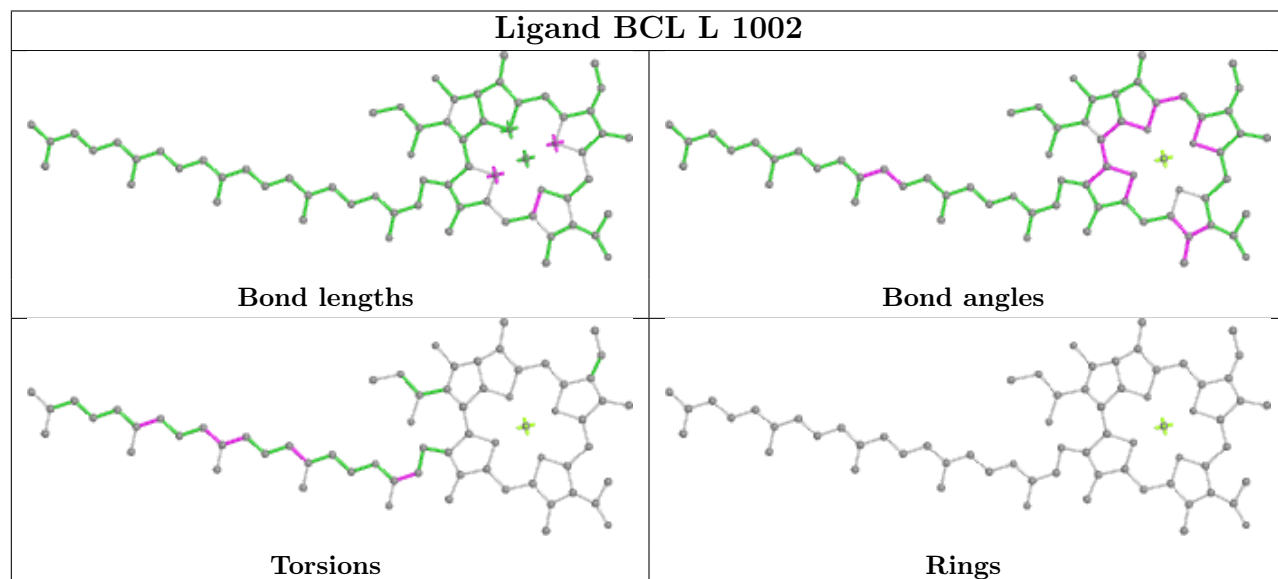
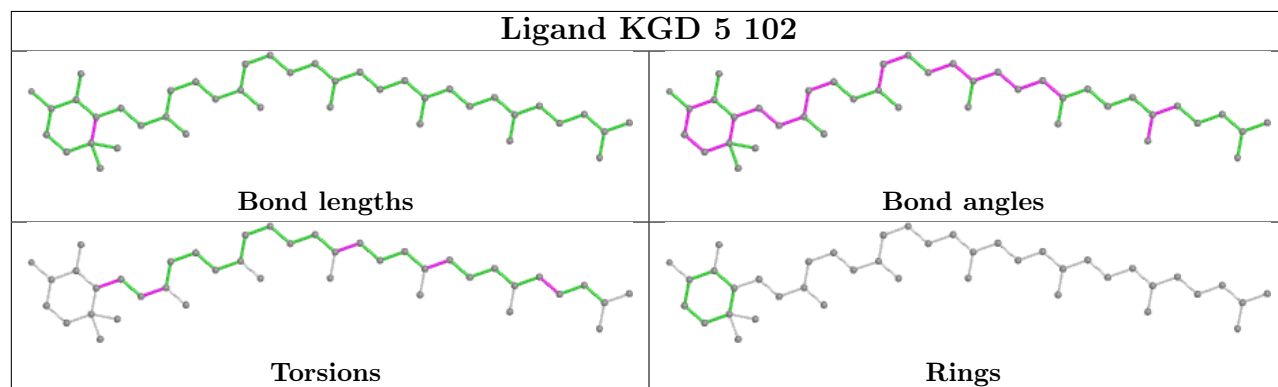
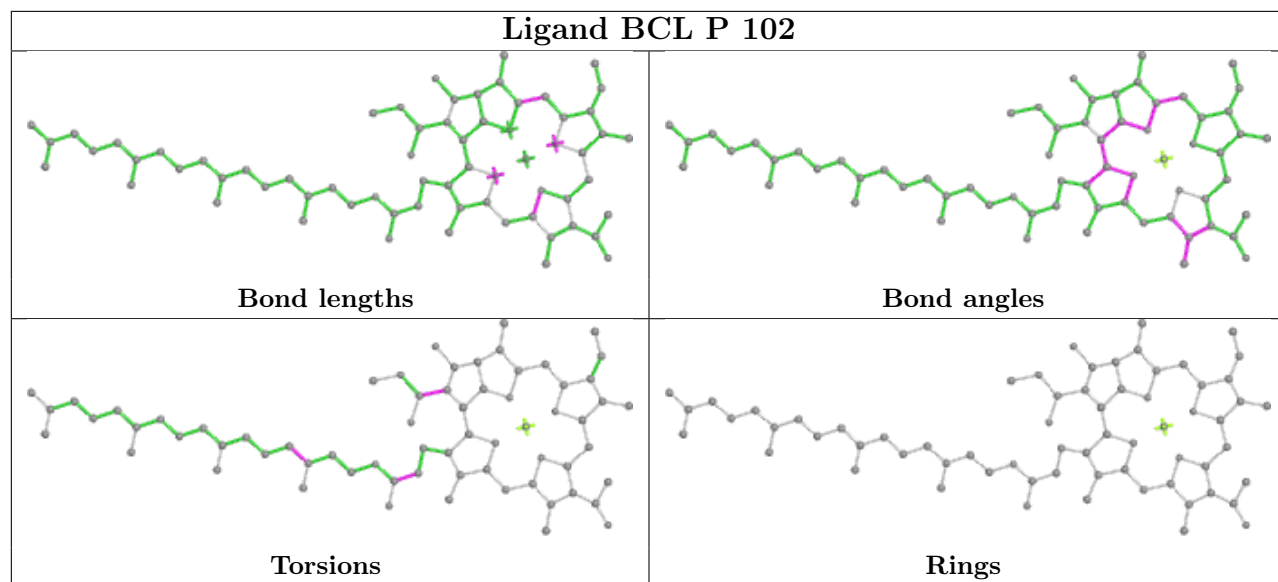


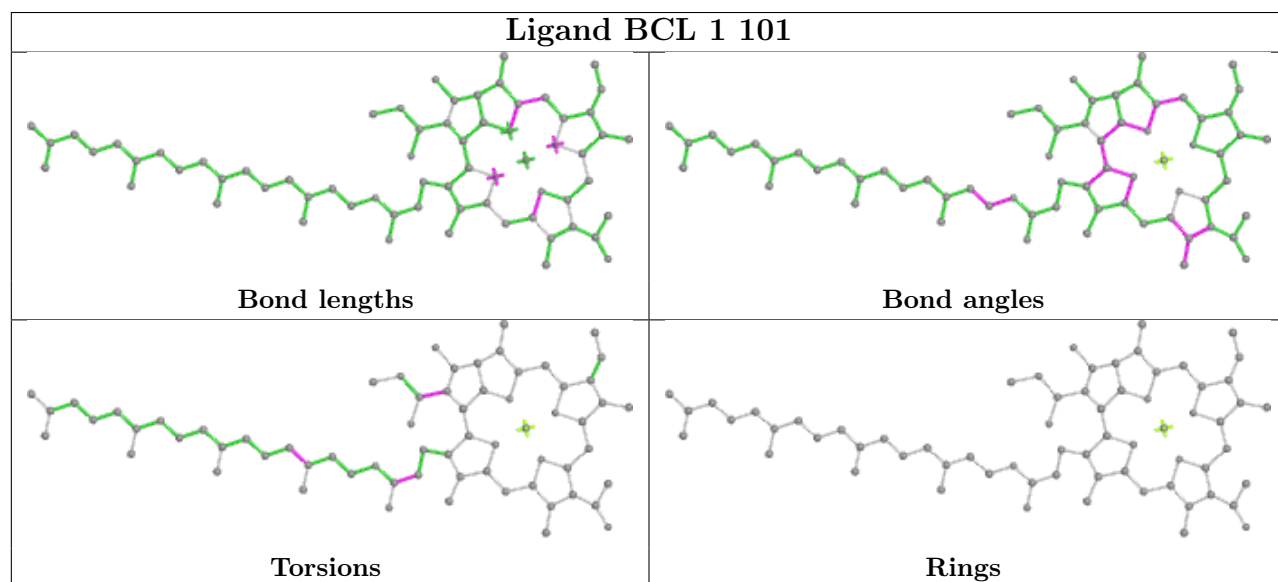
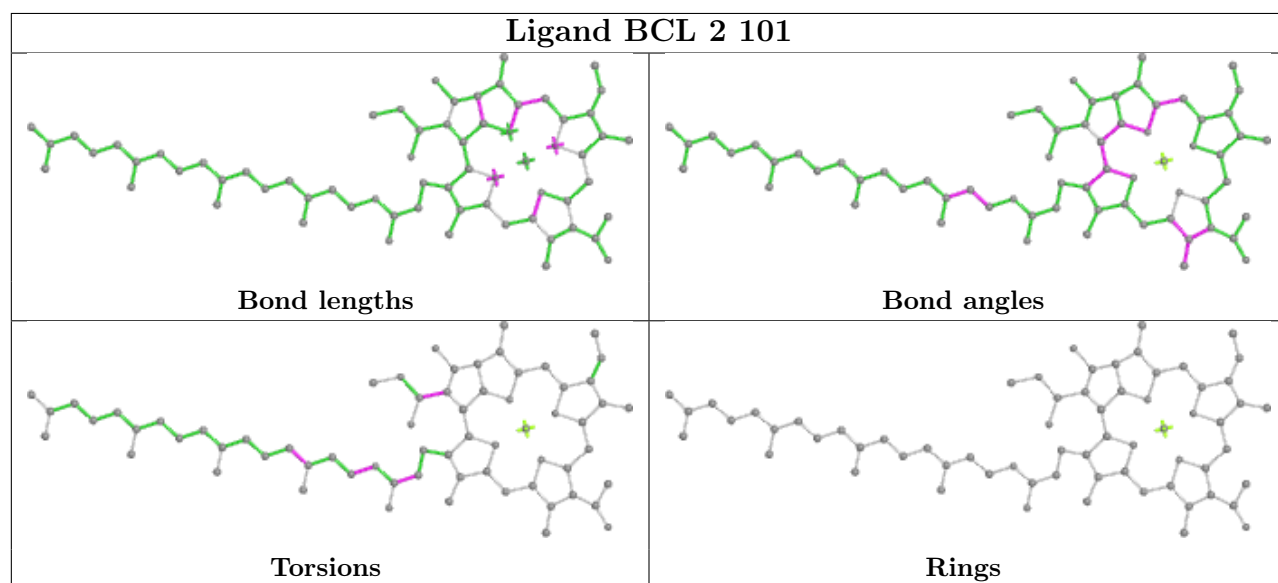
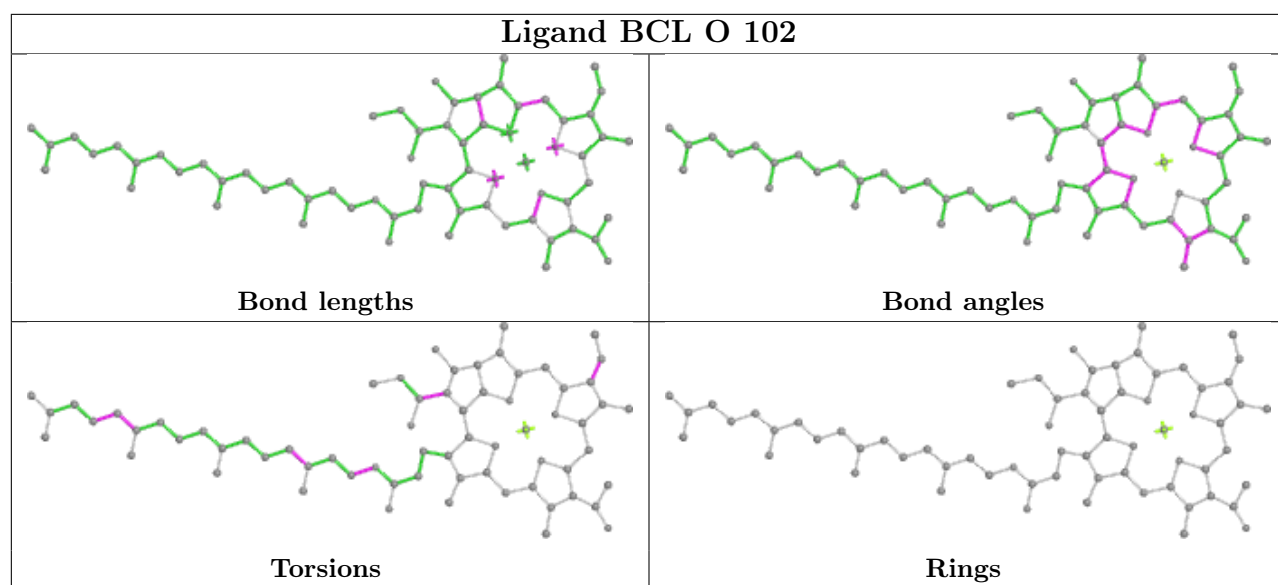


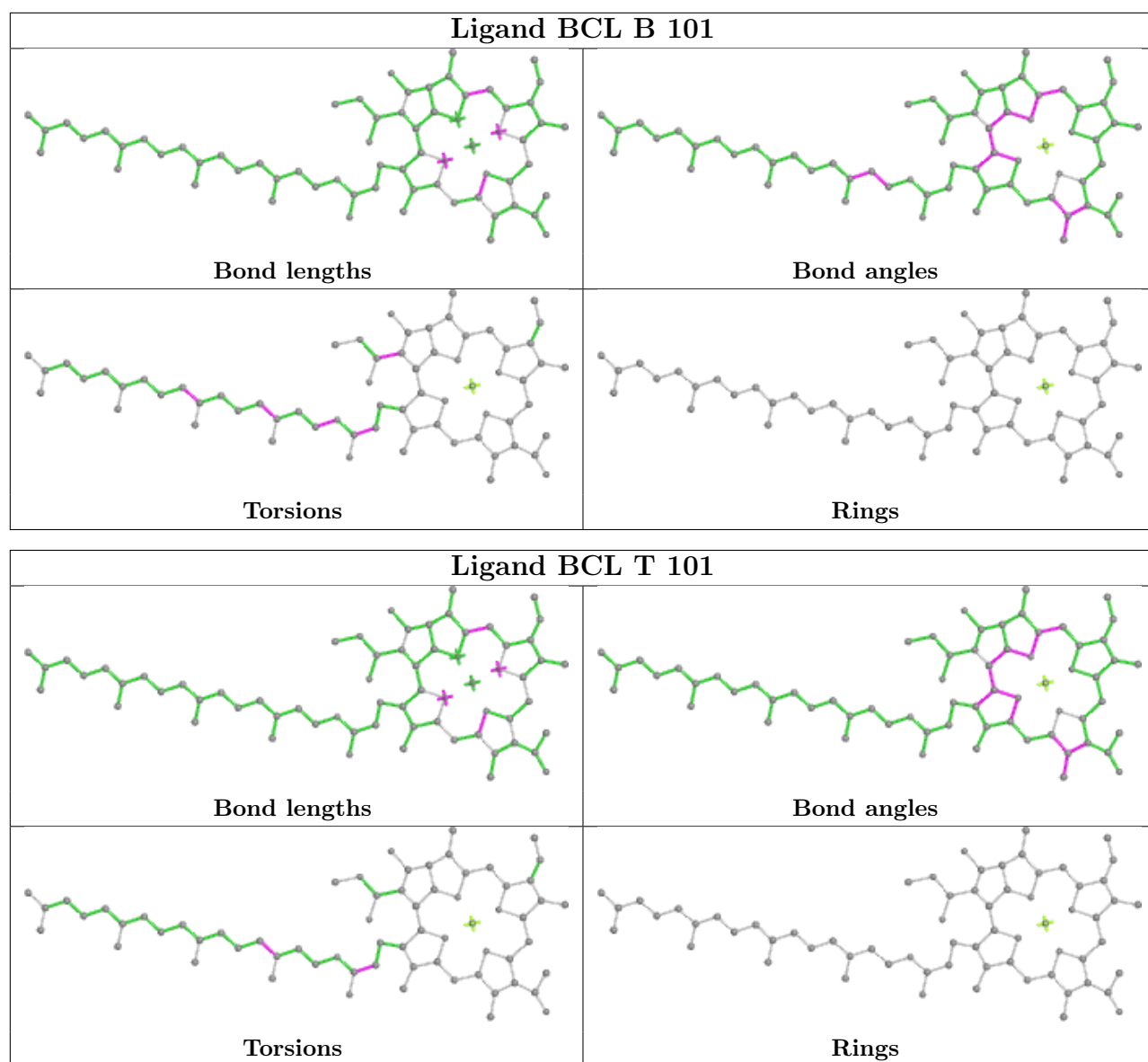












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

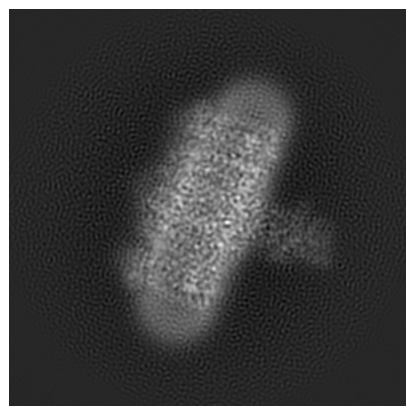
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35989. These allow visual inspection of the internal detail of the map and identification of artifacts.

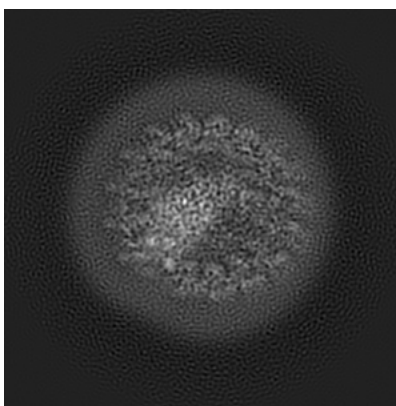
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

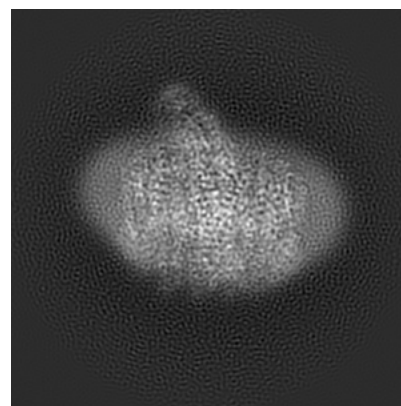
6.1.1 Primary map



X

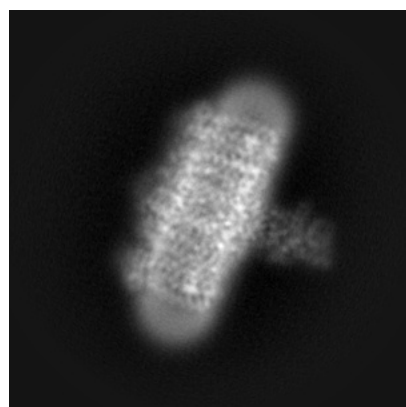


Y

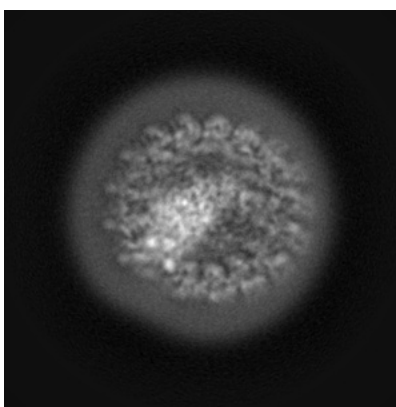


Z

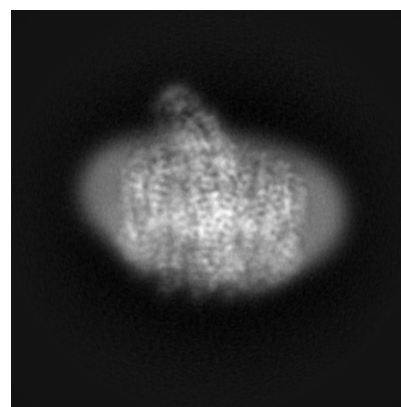
6.1.2 Raw map



X



Y

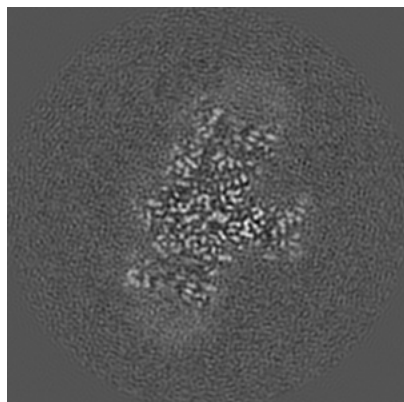


Z

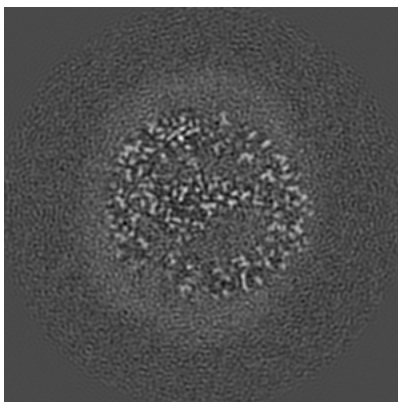
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

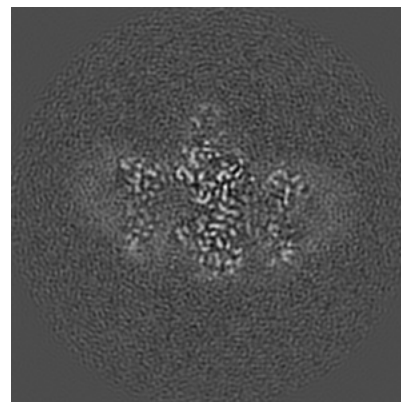
6.2.1 Primary map



X Index: 132

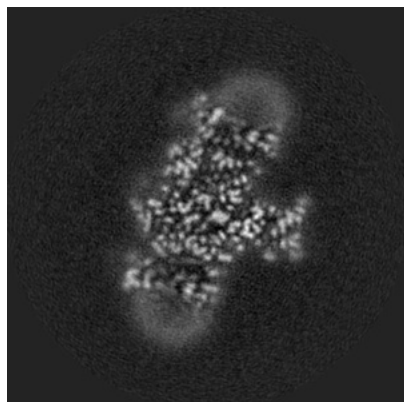


Y Index: 132

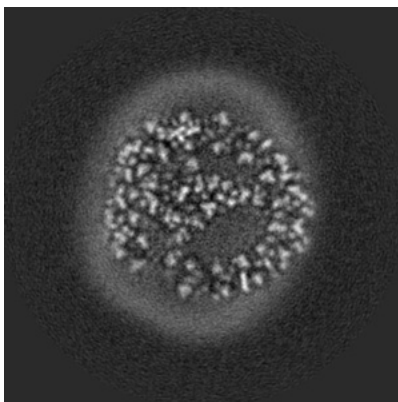


Z Index: 132

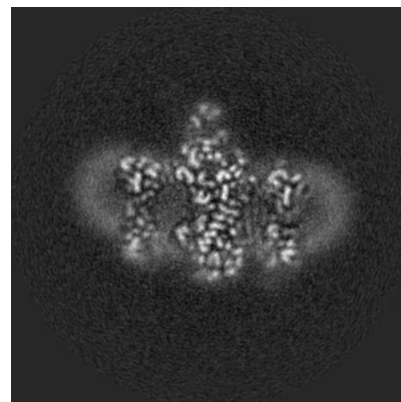
6.2.2 Raw map



X Index: 132



Y Index: 132

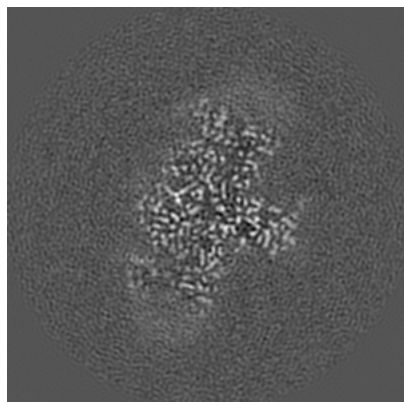


Z Index: 132

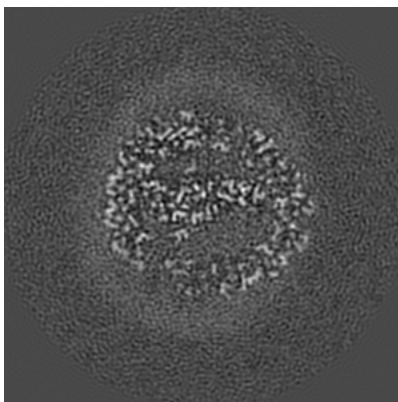
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

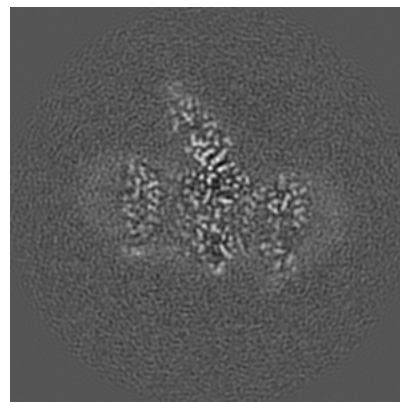
6.3.1 Primary map



X Index: 135

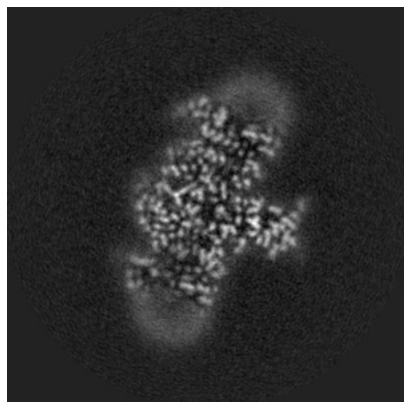


Y Index: 130

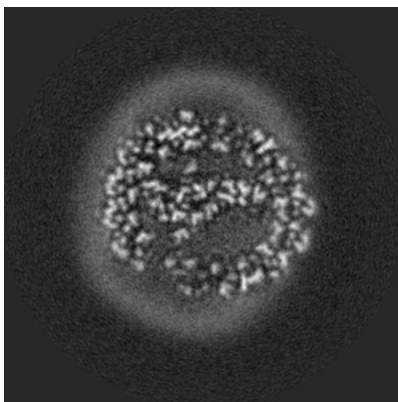


Z Index: 121

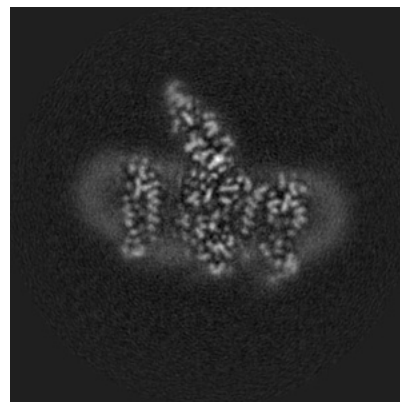
6.3.2 Raw map



X Index: 135



Y Index: 130

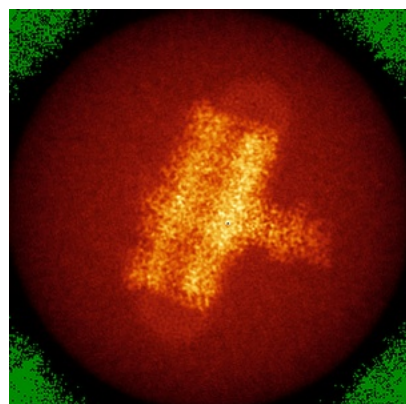


Z Index: 122

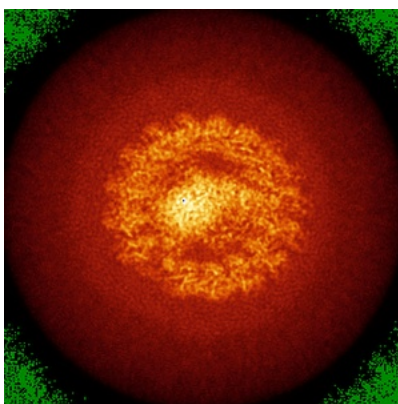
The images above show the largest variance slices of the map in three orthogonal directions.

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

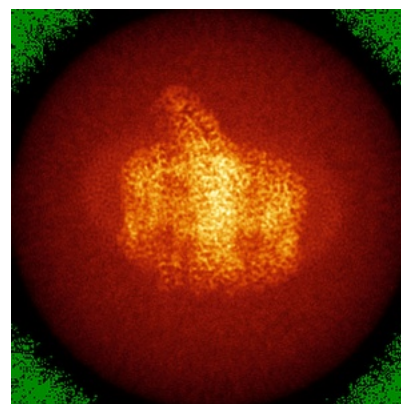
6.4.1 Primary map



X

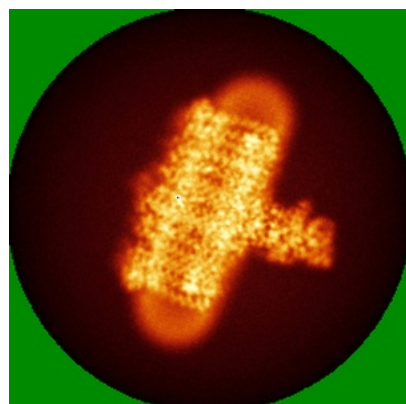


Y

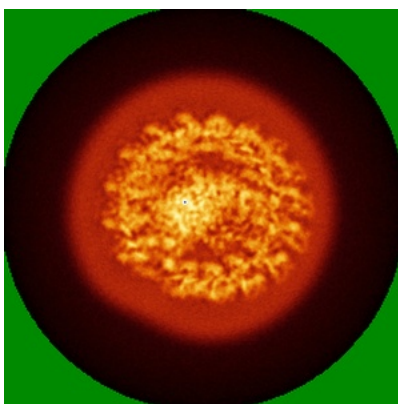


Z

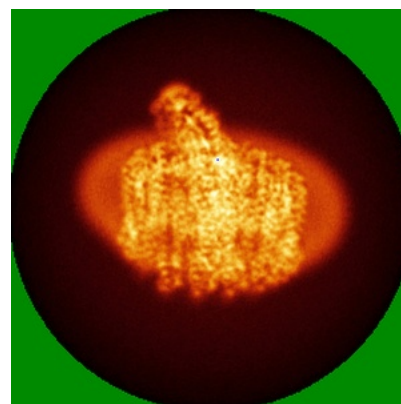
6.4.2 Raw map



X



Y

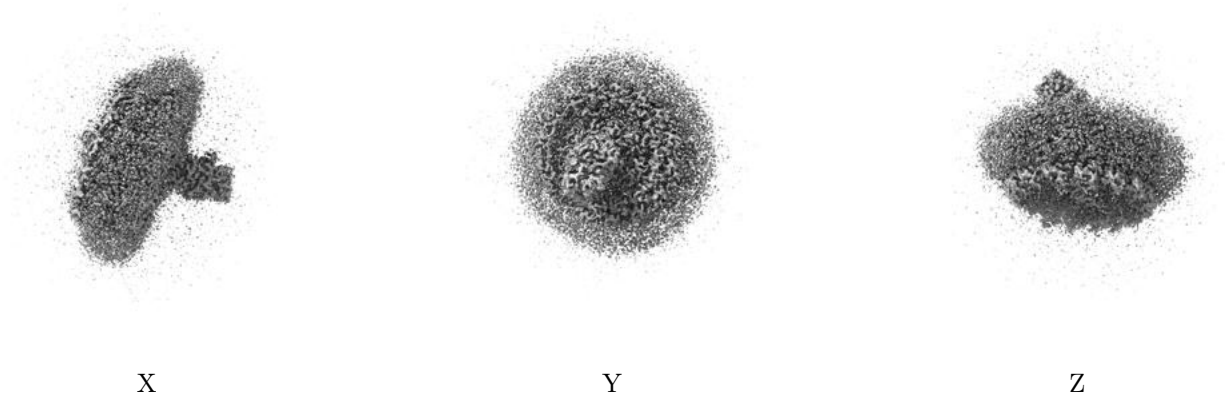


Z

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

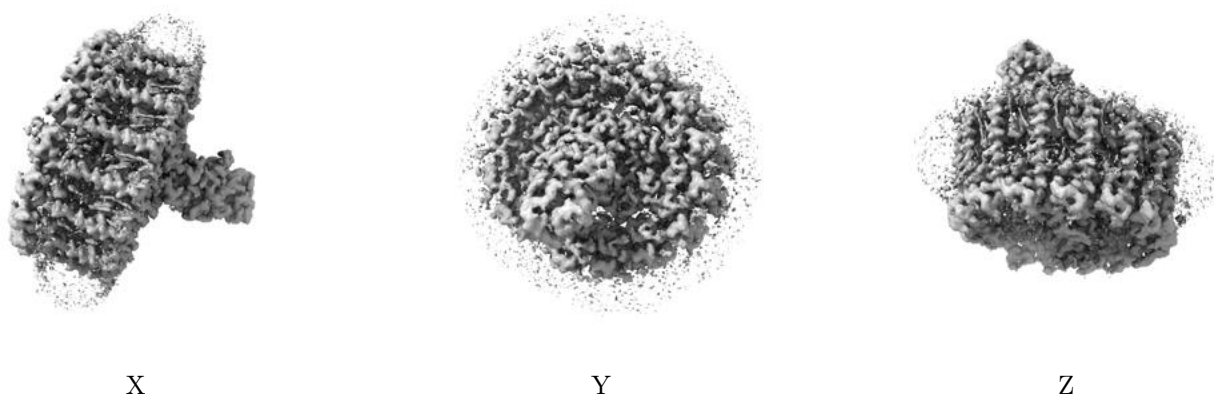
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

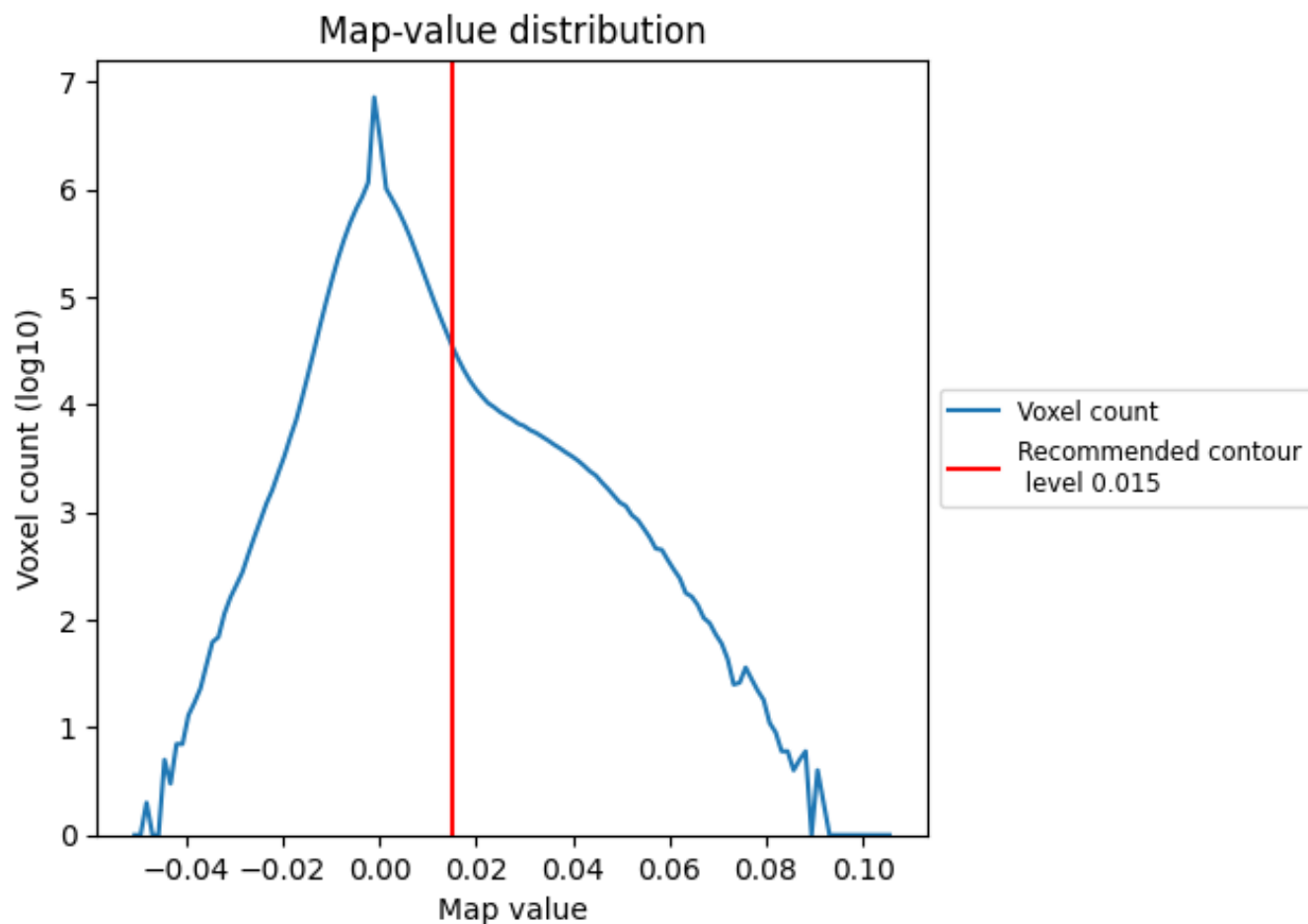
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

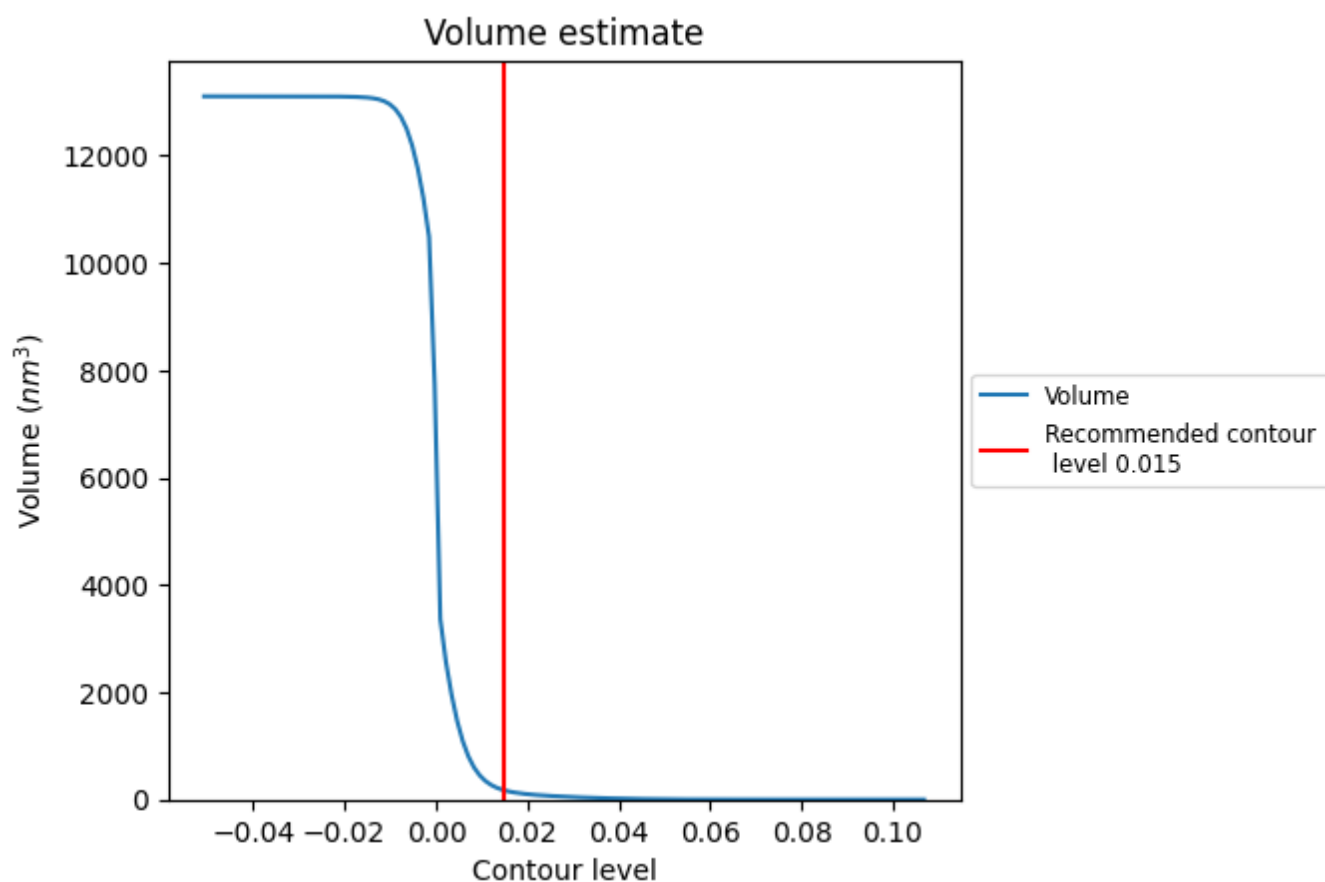
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

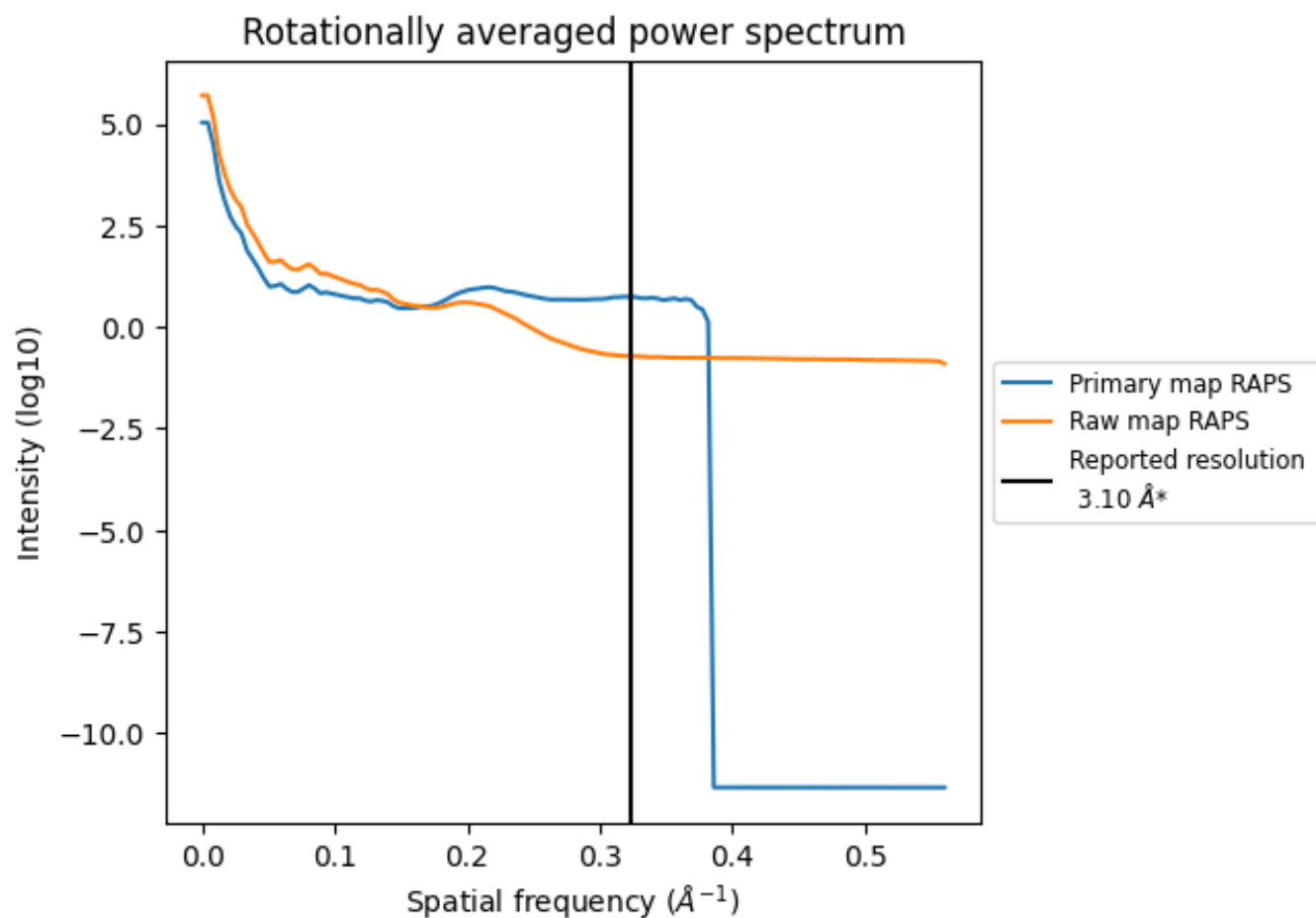
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 156 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

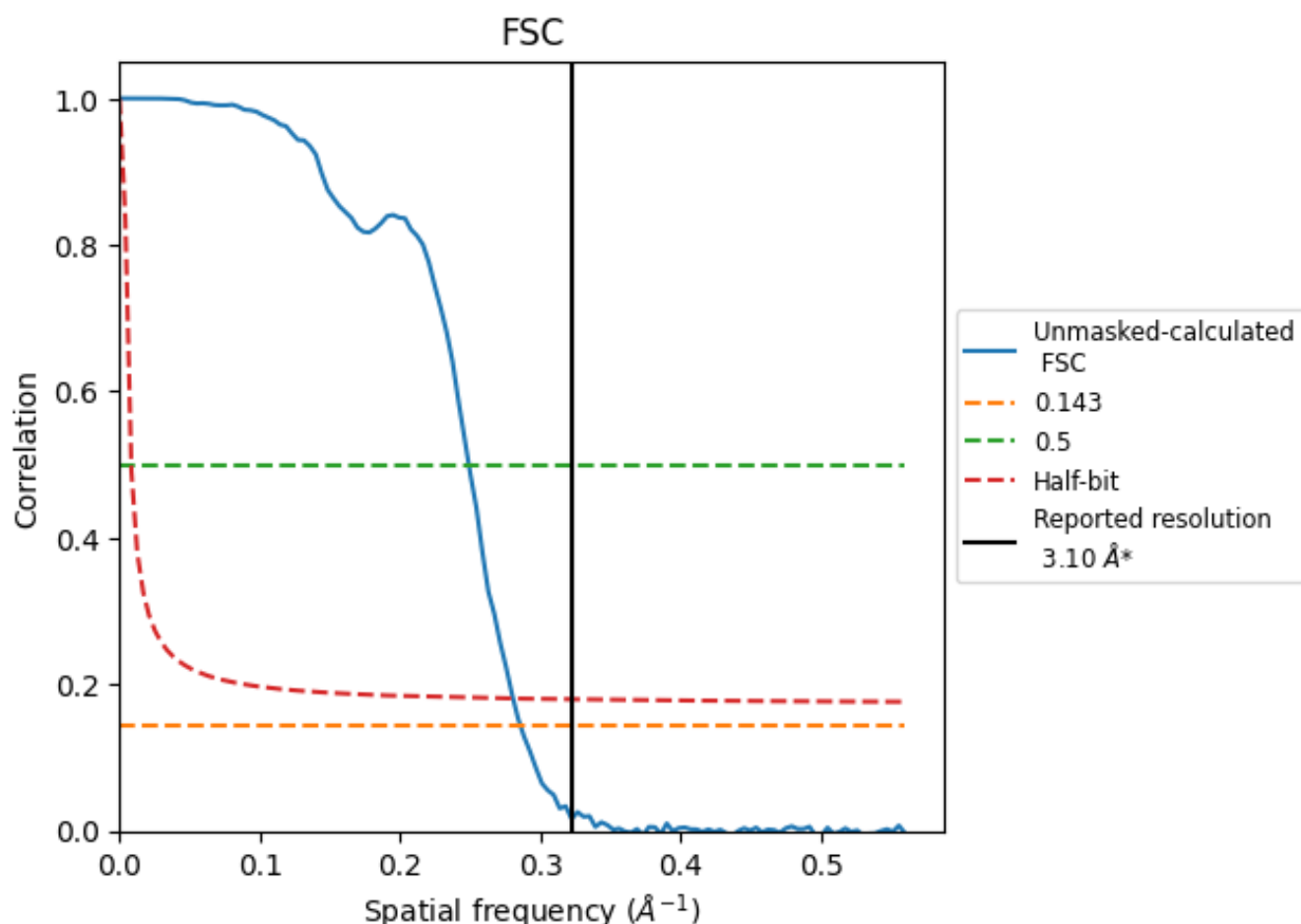


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

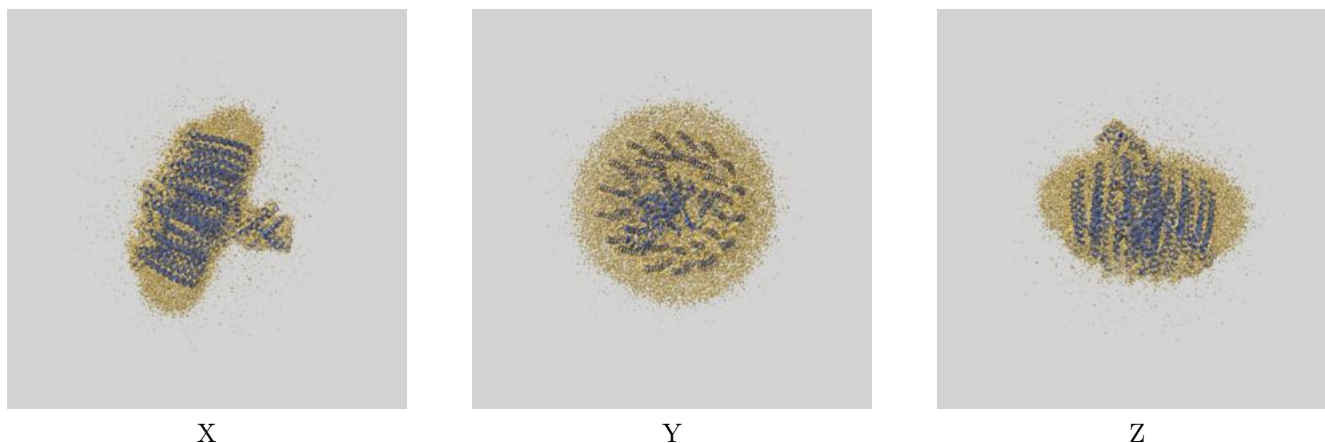
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	4.01	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

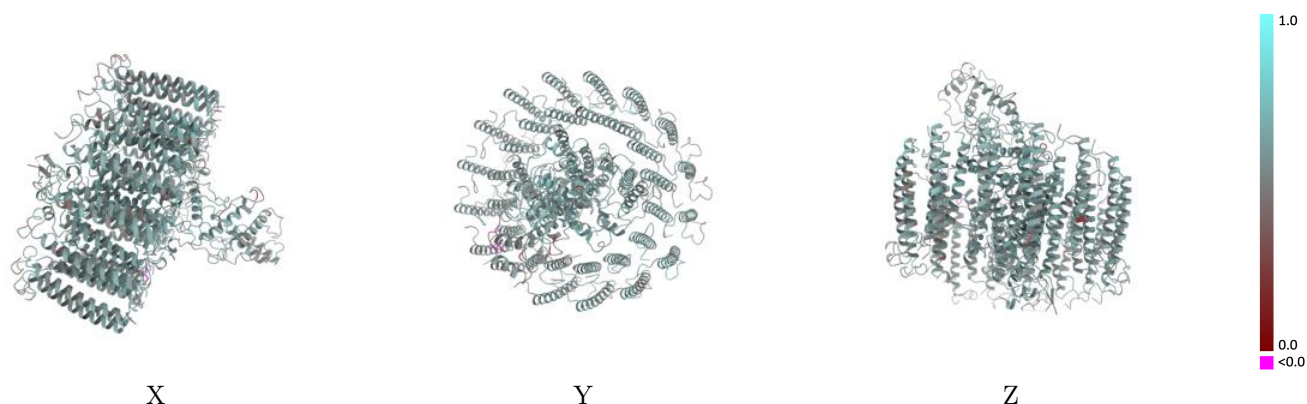
This section contains information regarding the fit between EMDB map EMD-35989 and PDB model 8J5P. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



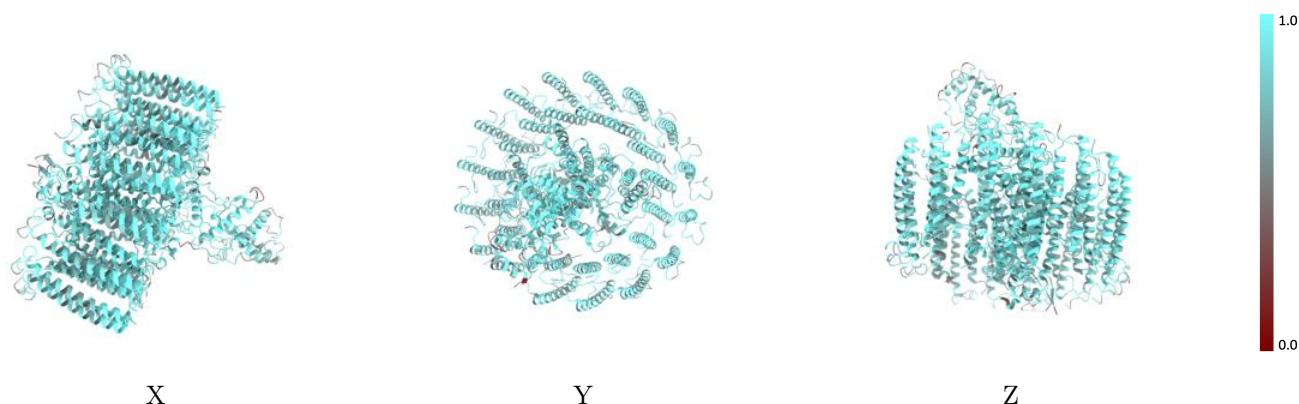
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



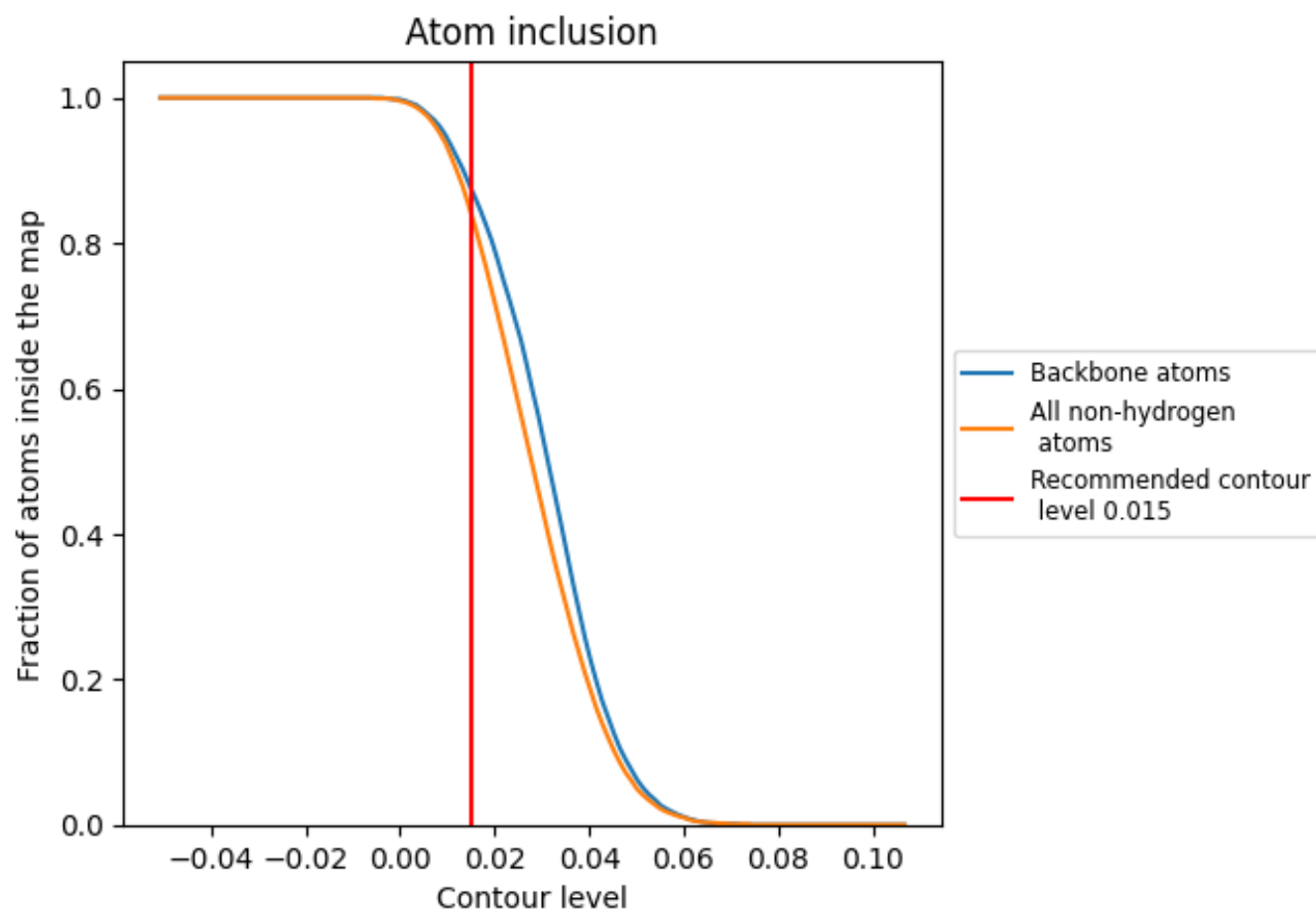
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5620
0	 0.8150	 0.5480
1	 0.8200	 0.5580
2	 0.7650	 0.5150
3	 0.8880	 0.5780
4	 0.8080	 0.5450
5	 0.8680	 0.5680
6	 0.8080	 0.5500
7	 0.8730	 0.5860
8	 0.8130	 0.5530
9	 0.8960	 0.5720
A	 0.8660	 0.5830
B	 0.8080	 0.5420
C	 0.8380	 0.5550
D	 0.8270	 0.5580
E	 0.8010	 0.5300
F	 0.8680	 0.5820
G	 0.8100	 0.5390
H	 0.8660	 0.5710
I	 0.8240	 0.5530
J	 0.8680	 0.5850
K	 0.7920	 0.5480
L	 0.8780	 0.5860
M	 0.9040	 0.5990
N	 0.8700	 0.5850
O	 0.8470	 0.5600
P	 0.8650	 0.5870
Q	 0.8220	 0.5490
R	 0.8780	 0.5830
S	 0.8220	 0.5510
T	 0.8550	 0.5740
U	 0.7970	 0.5380
V	 0.6700	 0.4510
W	 0.7880	 0.5080
X	 0.7120	 0.4940



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Chain	Atom inclusion	Q-score
Y	 0.8320	 0.5550
Z	 0.8480	 0.5780