



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:25 PM JST

PDB ID : 8J5O / pdb_00008j5o
EMDB ID : EMD-35988
Title : Cryo-EM structure of native RC-LH complex from *Roseiflexus castenholzii* at 100lux
Authors : Xu, X.; Xin, J.
Deposited on : 2023-04-24
Resolution : 2.90 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:

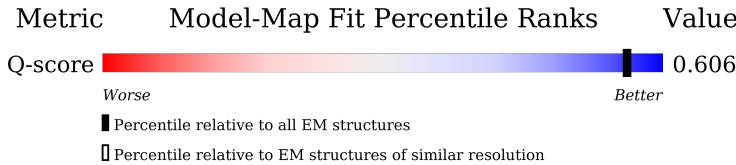
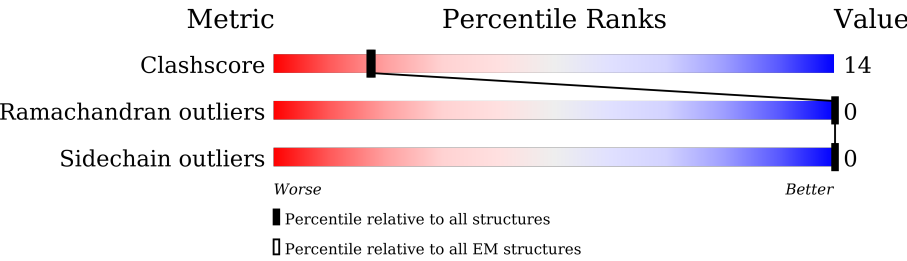
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	62% 27% 11%
1	2	55	78% 11% 11%
1	4	55	69% 20% 11%
1	6	55	65% 24% 11%

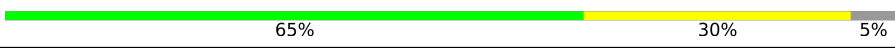
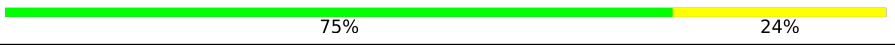
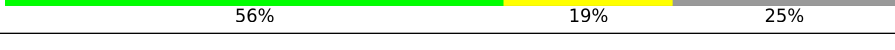
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Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	1	42	
2	3	42	
2	5	42	
2	7	42	
2	9	42	
2	A	42	
2	D	42	
2	F	42	
2	H	42	
2	J	42	
2	N	42	
2	P	42	
2	R	42	
2	T	42	

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Mol	Chain	Length	Quality of chain
2	V	42	
3	C	320	
4	L	315	
5	M	307	
6	X	32	
7	Y	39	
8	Z	63	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23692 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	34	Total	C	N	O	S	0	0
			266	178	44	43	1		
2	3	37	Total	C	N	O	S	0	0
			295	198	50	46	1		
2	5	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	7	37	Total	C	N	O	S	0	0
			295	198	50	46	1		
2	9	37	Total	C	N	O	S	0	0
			295	198	50	46	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	37	Total	C	N	O	S	0	0
			295	198	50	46	1		
2	H	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	J	37	Total	C	N	O	S	0	0
			295	198	50	46	1		
2	N	37	Total	C	N	O	S	0	0
			295	198	50	46	1		
2	P	37	Total	C	N	O	S	0	0
			295	198	50	46	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	37	Total	C	N	O	S	0	0
			295	198	50	46	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	299	Total	C	N	O	S	0	0
			2364	1583	380	393	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		

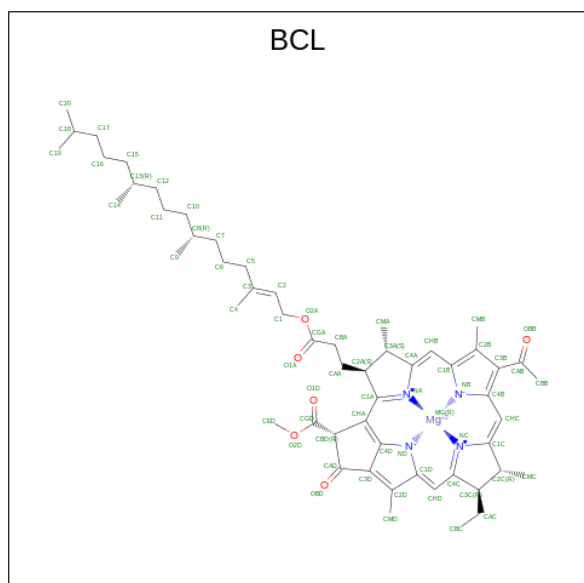
- Molecule 7 is a protein called Subunit Y.

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 (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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	E	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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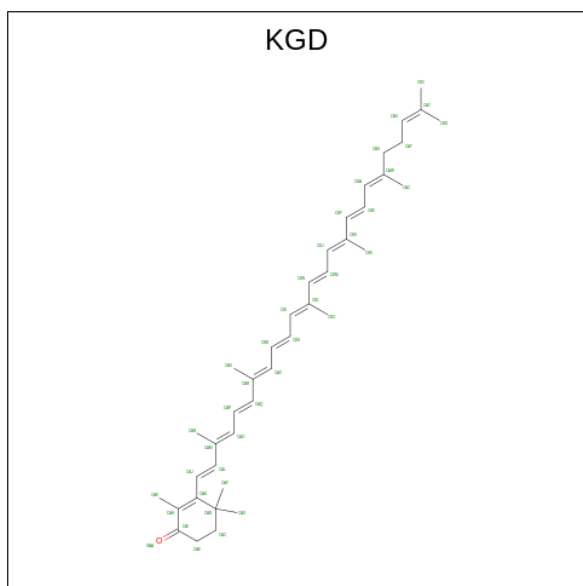
Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	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	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is beta,psi-caroten-4-one (CCD ID: KGD) (formula: C₄₀H₅₄O).



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

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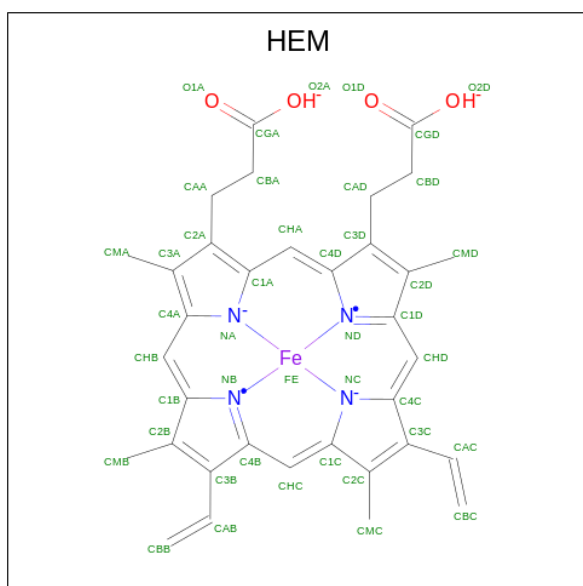
Mol	Chain	Residues	Atoms			AltConf
10	5	1	Total 41	C 40	O 1	0
10	6	1	Total 41	C 40	O 1	0
10	7	1	Total 41	C 40	O 1	0
10	8	1	Total 41	C 40	O 1	0
10	A	1	Total 41	C 40	O 1	0
10	B	1	Total 41	C 40	O 1	0
10	C	1	Total 41	C 40	O 1	0
10	C	1	Total 41	C 40	O 1	0
10	D	1	Total 41	C 40	O 1	0
10	D	1	Total 41	C 40	O 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	J	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	Q	1	Total 41	C 40	O 1	0
10	R	1	Total 41	C 40	O 1	0

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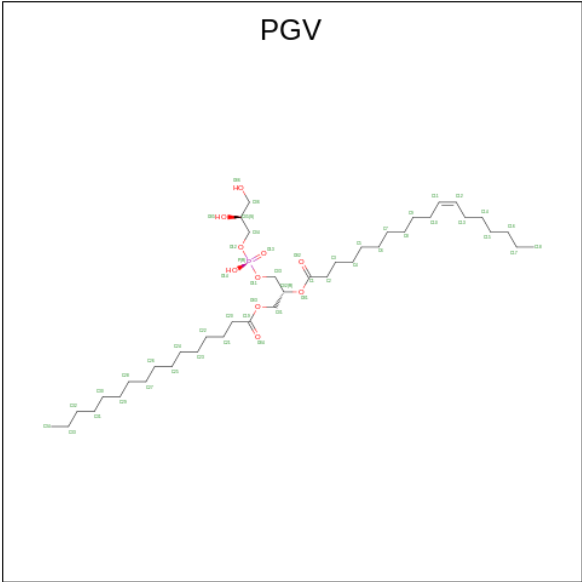
Mol	Chain	Residues	Atoms			AltConf
10	S	1	Total	C	O	0
			41	40	1	
10	S	1	Total	C	O	0
			41	40	1	
10	U	1	Total	C	O	0
			41	40	1	

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



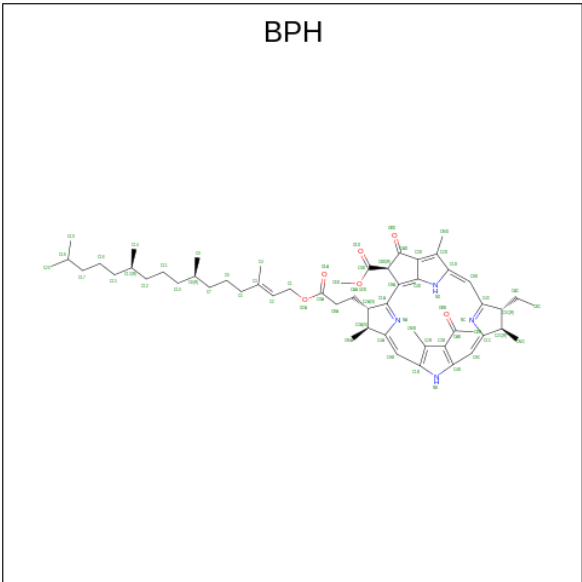
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	C	1	45	34	10	1	0
12	L	1	30	19	10	1	0
12	L	1	42	31	10	1	0
12	L	1	35	24	10	1	0

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

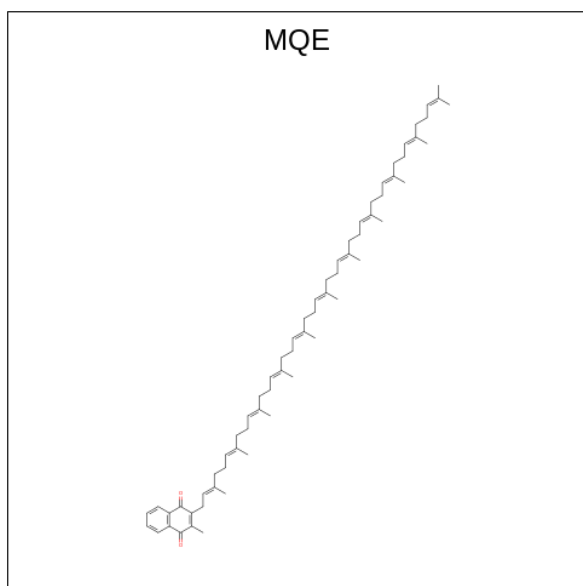


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			65	55	4	6	
13	L	1	Total	C	N	O	0
			65	55	4	6	
13	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

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



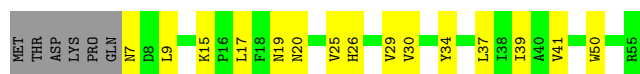
Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	C	O	0
			68	66	2	
15	M	1	Total	C	O	0
			68	66	2	
15	M	1	Total	C	O	0
			24	22	2	

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

Chain B:  75% 15% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain E:  65% 24% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain G:  69% 20% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain I:  69% 20% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain K:  71% 18% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain O:  64% 25% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain Q:  65% 24% 11%



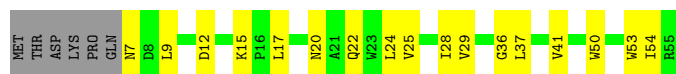
- Molecule 1: Beta subunit of light-harvesting 1

Chain S:  64% 25% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain U:  58% 31% 11%



- Molecule 1: Beta subunit of light-harvesting 1

Chain W:  62% 27% 11%



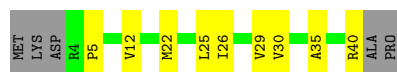
- Molecule 2: Alpha subunit of light-harvesting 1

Chain 1:  67% 14% 19%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 3:  67% 21% 12%



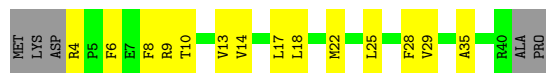
- Molecule 2: Alpha subunit of light-harvesting 1

Chain 5:  55% 36% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 7:  55% 33% 12%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:  71% 17% 12%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain A:  62% 29% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain D:  52% 38% 10%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain F:  62% 26% 12%



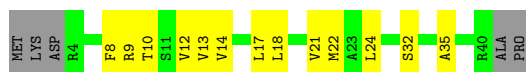
- Molecule 2: Alpha subunit of light-harvesting 1

Chain H:  71% 19% 10%



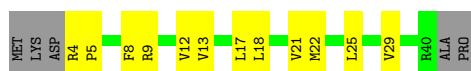
- Molecule 2: Alpha subunit of light-harvesting 1

Chain J:  57% 31% 12%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain N:  60% 29% 12%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain P:  81% 7% 12%



- Molecule 2: Alpha subunit of light-harvesting 1

Chain R:  62% 29% 10%



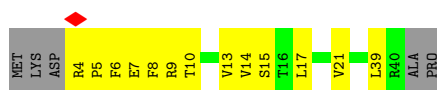
- Molecule 2: Alpha subunit of light-harvesting 1

Chain T:  71% 19% 10%



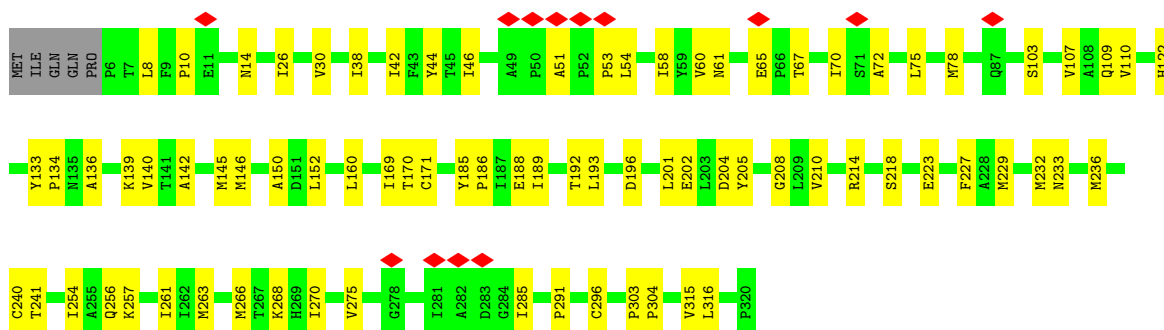
- Molecule 2: Alpha subunit of light-harvesting 1

Chain V:  57% 31% 12%



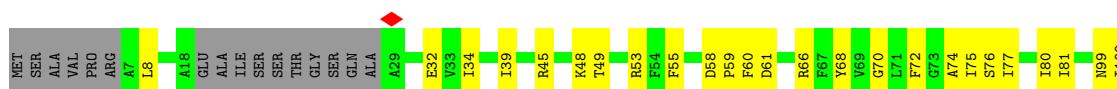
- Molecule 3: MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN

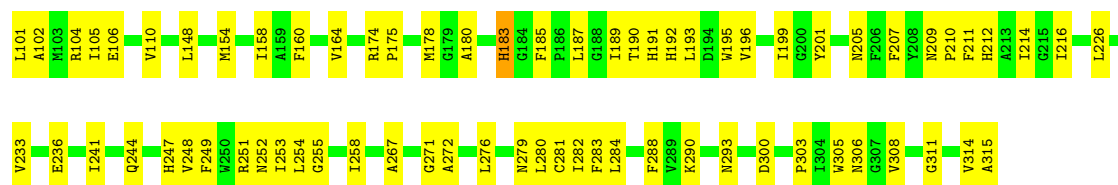
Chain C:  74% 25% 1%



- Molecule 4: Reaction center protein L chain

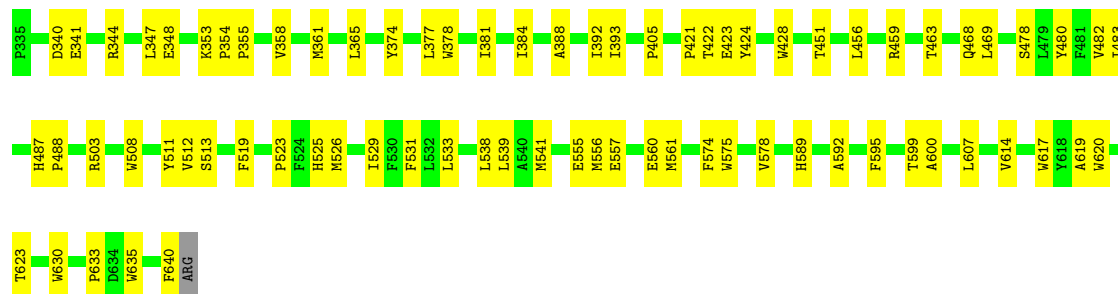
Chain L:  65% 30% 5%





• Molecule 5: Reaction center protein M chain

Chain M: 75% 24%



• Molecule 6: Subunit X

Chain X: 69% 12% 19%



• Molecule 7: Subunit Y

Chain Y: 56% 23% 18%



• Molecule 8: Subunit Z

Chain Z: 56% 19% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	322595	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	0.237	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	235.752, 235.752, 235.752	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.893, 0.893, 0.893	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/423	0.28	0/585
1	2	0.14	0/423	0.25	0/585
1	4	0.16	0/423	0.28	0/585
1	6	0.13	0/423	0.25	0/585
1	8	0.17	0/423	0.29	0/585
1	B	0.16	0/423	0.28	0/585
1	E	0.23	0/423	0.35	0/585
1	G	0.22	0/423	0.33	0/585
1	I	0.12	0/423	0.26	0/585
1	K	0.12	0/423	0.22	0/585
1	O	0.14	0/423	0.25	0/585
1	Q	0.12	0/423	0.27	0/585
1	S	0.12	0/423	0.27	0/585
1	U	0.13	0/423	0.30	0/585
1	W	0.14	0/423	0.29	0/585
2	1	0.19	0/271	0.40	0/368
2	3	0.14	0/302	0.29	0/410
2	5	0.11	0/307	0.24	0/417
2	7	0.11	0/302	0.24	0/410
2	9	0.13	0/302	0.26	0/410
2	A	0.14	0/307	0.28	0/417
2	D	0.12	0/307	0.27	0/417
2	F	0.12	0/302	0.26	0/410
2	H	0.11	0/307	0.25	0/417
2	J	0.13	0/302	0.28	0/410
2	N	0.10	0/302	0.23	0/410
2	P	0.13	0/302	0.23	0/410
2	R	0.12	0/307	0.23	0/417
2	T	0.13	0/307	0.27	0/417
2	V	0.13	0/302	0.24	0/410
3	C	0.14	0/2469	0.33	0/3371
4	L	0.24	0/2448	0.48	3/3342 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.19	0/2597	0.37	0/3566
6	X	0.11	0/211	0.23	0/285
7	Y	0.39	0/268	0.47	1/370 (0.3%)
8	Z	0.14	0/374	0.36	0/513
All	All	0.17	0/19241	0.33	4/26372 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	185	PHE	N-CA-C	8.98	121.06	109.93
4	L	183	HIS	N-CA-CB	-5.47	102.27	110.91
4	L	308	VAL	N-CA-C	5.44	118.12	112.90
7	Y	2	ASN	N-CA-C	-5.10	100.85	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	407	0	407	12	0
1	2	407	0	407	4	0
1	4	407	0	407	8	0
1	6	407	0	407	11	0
1	8	407	0	407	8	0
1	B	407	0	407	5	0
1	E	407	0	407	9	0
1	G	407	0	407	8	0
1	I	407	0	407	6	0
1	K	407	0	407	7	0
1	O	407	0	407	12	0
1	Q	407	0	407	11	0
1	S	407	0	407	14	0
1	U	407	0	407	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	407	0	407	10	0
2	1	266	0	282	4	0
2	3	295	0	311	8	0
2	5	300	0	316	10	0
2	7	295	0	311	14	0
2	9	295	0	311	11	0
2	A	300	0	316	21	0
2	D	300	0	316	17	0
2	F	295	0	311	10	0
2	H	300	0	316	12	0
2	J	295	0	311	13	0
2	N	295	0	311	12	0
2	P	295	0	311	2	0
2	R	300	0	316	14	0
2	T	300	0	316	10	0
2	V	295	0	311	15	0
3	C	2404	0	2360	66	0
4	L	2364	0	2324	79	0
5	M	2488	0	2373	67	0
6	X	206	0	224	2	0
7	Y	259	0	272	12	0
8	Z	362	0	366	13	0
9	0	132	0	148	11	0
9	1	66	0	74	0	0
9	2	132	0	148	3	0
9	3	66	0	74	5	0
9	4	132	0	148	11	0
9	5	66	0	74	1	0
9	6	132	0	148	12	0
9	7	66	0	74	3	0
9	8	132	0	148	9	0
9	9	66	0	74	5	0
9	A	66	0	74	7	0
9	B	132	0	148	10	0
9	D	66	0	74	3	0
9	E	132	0	148	11	0
9	F	132	0	148	2	0
9	G	66	0	74	4	0
9	H	66	0	74	1	0
9	I	132	0	148	10	0
9	J	66	0	74	2	0
9	K	132	0	148	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	132	0	148	6	0
9	M	66	0	74	4	0
9	N	66	0	74	5	0
9	O	132	0	148	12	0
9	P	66	0	74	4	0
9	Q	132	0	148	9	0
9	R	66	0	74	5	0
9	S	132	0	148	17	0
9	T	66	0	74	8	0
9	U	132	0	148	14	0
9	V	66	0	74	3	0
9	W	132	0	148	8	0
10	0	82	0	0	1	0
10	1	82	0	0	2	0
10	2	41	0	0	3	0
10	4	41	0	0	3	0
10	5	41	0	0	1	0
10	6	41	0	0	4	0
10	7	41	0	0	1	0
10	8	41	0	0	1	0
10	A	41	0	0	2	0
10	B	41	0	0	4	0
10	C	82	0	0	3	0
10	D	82	0	0	10	0
10	E	41	0	0	3	0
10	G	41	0	0	5	0
10	H	41	0	0	2	0
10	I	41	0	0	3	0
10	J	82	0	0	3	0
10	K	41	0	0	2	0
10	O	41	0	0	1	0
10	P	41	0	0	3	0
10	Q	41	0	0	1	0
10	R	41	0	0	1	0
10	S	82	0	0	8	0
10	U	41	0	0	9	0
11	C	172	0	120	13	0
12	C	45	0	61	2	0
12	L	107	0	122	2	0
13	L	130	0	152	12	0
13	M	65	0	76	4	0
14	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	68	0	0	1	0
15	M	92	0	0	5	0
All	All	23692	0	22773	636	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 14.

All (636) 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)
10:U:103:KGD:CAF	9:W:102:BCL:H62	1.72	1.19
4:L:211:PHE:HB2	4:L:281:CYS:HB3	1.28	1.07
10:S:104:KGD:CAG	9:U:102:BCL:H62	1.85	1.06
10:H:102:KGD:CAE	9:K:102:BCL:HBB3	1.94	0.98
4:L:8:LEU:HB3	8:Z:50:LEU:HD11	1.46	0.96
5:M:358:VAL:HG21	5:M:361:MET:HE2	1.52	0.92
2:V:13:VAL:HG13	9:V:101:BCL:H193	1.51	0.90
10:U:103:KGD:CAU	9:W:102:BCL:H193	2.02	0.88
10:S:104:KGD:CAG	9:U:102:BCL:C6	2.51	0.87
10:6:103:KGD:CAF	9:8:102:BCL:H62	2.05	0.86
2:A:17:LEU:HD23	5:M:384:ILE:HD12	1.58	0.84
2:7:13:VAL:HG22	9:7:101:BCL:H193	1.60	0.83
4:L:253:ILE:HD13	5:M:456:LEU:HD23	1.60	0.83
10:U:103:KGD:CAU	9:W:102:BCL:H202	2.09	0.83
1:U:22:GLN:HG2	2:V:5:PRO:HG3	1.63	0.81
7:Y:14:LEU:HA	7:Y:17:PHE:HD2	1.47	0.80
10:D:102:KGD:OAA	2:F:6:PHE:CD2	2.37	0.78
1:2:39:ILE:HD11	9:4:102:BCL:H122	1.66	0.77
2:3:12:VAL:HG12	9:3:101:BCL:H192	1.67	0.76
10:U:103:KGD:CAF	9:W:102:BCL:C6	2.60	0.75
2:A:40:ARG:HE	2:A:41:ALA:H	1.34	0.75
2:R:4:ARG:HG3	1:S:17:LEU:HD23	1.68	0.75
8:Z:53:ASP:HB3	8:Z:56:LYS:HG2	1.68	0.75
10:C:505:KGD:CBI	9:U:101:BCL:H201	2.16	0.75
2:H:22:MET:HE2	2:H:22:MET:HA	1.67	0.75
4:L:280:LEU:HB2	7:Y:17:PHE:HZ	1.52	0.74
1:S:12:ASP:HA	1:S:15:LYS:HD2	1.68	0.74
2:H:4:ARG:HH22	1:I:22:GLN:HE22	1.35	0.73
5:M:482:VAL:HG12	5:M:607:LEU:HD22	1.71	0.73
9:M:702:BCL:H201	13:M:703:BPH:H102	1.71	0.73
9:O:101:BCL:H202	10:O:103:KGD:CAK	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:17:LEU:HD21	5:M:381:ILE:HA	1.71	0.72
10:P:102:KGD:CAF	9:R:101:BCL:H13	2.20	0.71
4:L:300:ASP:HA	4:L:305:TRP:HE1	1.56	0.71
2:9:13:VAL:HG22	9:9:101:BCL:H193	1.71	0.71
4:L:254:LEU:HD21	13:L:1006:BPH:HED3	1.71	0.71
1:B:26:HIS:O	1:B:30:VAL:HG23	1.92	0.70
3:C:275:VAL:HG21	3:C:291:PRO:HD3	1.74	0.70
10:G:102:KGD:CAF	9:I:102:BCL:H51	2.22	0.69
2:V:4:ARG:HH21	2:V:8:PHE:H	1.40	0.69
10:1:102:KGD:CAZ	3:C:38:ILE:HB	2.23	0.69
2:N:13:VAL:HG22	9:N:101:BCL:H193	1.74	0.69
10:K:103:KGD:CAU	9:O:102:BCL:H192	2.23	0.69
10:I:103:KGD:CAG	9:K:102:BCL:H62	2.23	0.69
2:A:4:ARG:NH1	2:A:6:PHE:O	2.27	0.68
10:S:104:KGD:CAG	9:U:102:BCL:C5	2.71	0.68
1:S:39:ILE:HD11	9:U:102:BCL:H122	1.74	0.68
4:L:192:HIS:O	4:L:196:VAL:HG23	1.94	0.68
3:C:54:LEU:HD22	3:C:61:ASN:HA	1.75	0.68
4:L:154:MET:O	4:L:158:ILE:HG13	1.94	0.67
4:L:207:PHE:CE1	9:L:1002:BCL:HMC2	2.29	0.67
3:C:185:TYR:HA	3:C:189:ILE:HD11	1.76	0.67
3:C:232:MET:HE2	11:C:503:HEM:CBC	2.25	0.67
9:5:101:BCL:H43	9:6:101:BCL:H52	1.76	0.67
2:H:4:ARG:NH2	2:H:7:GLU:OE1	2.27	0.67
4:L:160:PHE:O	4:L:164:VAL:HG23	1.94	0.67
4:L:212:HIS:O	4:L:216:ILE:HG13	1.95	0.66
9:0:102:BCL:H122	1:8:39:ILE:HD11	1.78	0.66
2:3:40:ARG:H	1:6:55:ARG:HH22	1.44	0.66
2:A:4:ARG:HH12	2:A:7:GLU:HA	1.60	0.66
2:N:4:ARG:HB3	1:O:17:LEU:HD23	1.78	0.66
2:T:4:ARG:NH1	1:U:17:LEU:O	2.29	0.66
3:C:78:MET:HE2	11:C:501:HEM:HMB3	1.77	0.66
2:D:22:MET:HE2	10:D:102:KGD:CBE	2.26	0.65
1:S:37:LEU:HD12	9:S:101:BCL:H12	1.77	0.65
1:6:37:LEU:HD22	9:6:101:BCL:H12	1.78	0.65
2:J:8:PHE:O	2:J:12:VAL:HG23	1.96	0.65
1:W:19:ASN:OD1	1:W:20:ASN:N	2.29	0.65
3:C:232:MET:HE2	11:C:503:HEM:HBC2	1.79	0.65
1:O:37:LEU:HD23	9:O:101:BCL:H12	1.79	0.65
1:2:11:PRO:O	1:2:15:LYS:HG3	1.97	0.64
12:L:1008:PGV:H232	7:Y:18:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:103:KGD:CAF	9:8:102:BCL:C6	2.74	0.64
3:C:205:TYR:HE2	3:C:268:LYS:HB2	1.62	0.64
10:4:103:KGD:CAG	9:6:102:BCL:C3D	2.76	0.64
2:R:37:ASN:HA	2:R:41:ALA:HA	1.80	0.64
2:H:31:LEU:HD22	2:H:38:TRP:CE3	2.33	0.64
9:T:101:BCL:O1D	10:U:103:KGD:CBO	2.46	0.64
3:C:169:ILE:CD1	3:C:266:MET:HE1	2.28	0.64
3:C:233:ASN:HD21	3:C:240:CYS:HA	1.63	0.64
2:V:9:ARG:O	2:V:13:VAL:HG23	1.98	0.64
3:C:152:LEU:HB3	3:C:266:MET:HE3	1.81	0.63
3:C:8:LEU:O	2:V:9:ARG:NH2	2.32	0.63
2:V:17:LEU:O	2:V:21:VAL:HG23	1.98	0.63
10:D:103:KGD:OAA	2:H:6:PHE:HD2	1.81	0.63
5:M:340:ASP:O	5:M:344:ARG:HG3	1.98	0.63
5:M:388:ALA:O	5:M:392:ILE:HG13	1.99	0.63
10:S:104:KGD:CAG	9:U:102:BCL:H51	2.29	0.63
5:M:556:MET:O	5:M:560:GLU:HG2	1.98	0.63
3:C:109:GLN:OE1	3:C:170:THR:HG21	1.97	0.63
1:G:25:VAL:O	1:G:29:VAL:HG23	1.99	0.63
1:K:12:ASP:HA	1:K:15:LYS:HE2	1.79	0.63
1:Q:22:GLN:HG2	2:R:5:PRO:HG3	1.81	0.63
9:U:101:BCL:H152	9:U:101:BCL:H102	1.80	0.63
1:U:7:ASN:HA	1:U:20:ASN:HB2	1.80	0.62
2:H:40:ARG:HB2	2:J:35:ALA:HB2	1.81	0.62
2:7:10:THR:O	2:7:14:VAL:HG23	1.99	0.62
1:E:35:GLY:O	1:E:39:ILE:HG12	1.99	0.62
9:P:101:BCL:H43	9:Q:101:BCL:H52	1.82	0.62
10:H:102:KGD:CAE	9:K:102:BCL:CBB	2.75	0.62
1:U:24:LEU:O	1:U:28:ILE:HG13	1.99	0.62
5:M:456:LEU:HD22	5:M:469:LEU:HD23	1.81	0.62
2:5:17:LEU:O	2:5:21:VAL:HG23	2.00	0.62
1:I:37:LEU:O	1:I:41:VAL:HG23	1.99	0.62
3:C:170:THR:HG22	3:C:171:CYS:H	1.63	0.62
10:G:102:KGD:CAF	9:I:102:BCL:C5	2.78	0.61
1:W:25:VAL:O	1:W:29:VAL:HG23	1.99	0.61
5:M:574:PHE:O	5:M:578:VAL:HG23	2.01	0.61
2:R:13:VAL:HG22	9:R:101:BCL:H193	1.82	0.61
9:O:101:BCL:H102	9:O:101:BCL:H152	1.83	0.61
2:D:37:ASN:HA	2:D:41:ALA:HA	1.83	0.61
2:J:10:THR:O	2:J:14:VAL:HG23	2.00	0.61
1:O:19:ASN:OD1	1:O:20:ASN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:ILE:HG21	3:C:109:GLN:HE22	1.66	0.61
9:Q:101:BCL:H142	10:S:103:KGD:CAQ	2.30	0.60
2:D:9:ARG:O	2:D:13:VAL:HG23	2.02	0.60
10:G:102:KGD:CAF	9:I:102:BCL:H62	2.31	0.60
1:8:24:LEU:O	1:8:28:ILE:HG13	2.01	0.60
1:K:19:ASN:HB3	1:K:22:GLN:HG3	1.82	0.60
13:L:1006:BPH:HBC1	5:M:600:ALA:HB2	1.83	0.60
9:T:101:BCL:H193	2:V:6:PHE:CE1	2.36	0.60
7:Y:9:MET:O	7:Y:13:VAL:HG23	2.02	0.60
3:C:263:MET:HG3	11:C:504:HEM:C4A	2.36	0.60
1:G:27:ASP:OD2	1:G:31:LYS:NZ	2.34	0.60
4:L:290:LYS:HE2	5:M:640:PHE:CE2	2.37	0.60
3:C:192:THR:HA	12:C:507:PGV:O14	2.02	0.60
2:D:10:THR:O	2:D:14:VAL:HG23	2.01	0.60
4:L:209:ASN:ND2	4:L:281:CYS:HB2	2.17	0.60
1:Q:39:ILE:HD11	9:S:102:BCL:H122	1.83	0.60
1:O:24:LEU:O	1:O:28:ILE:HG13	2.01	0.60
4:L:45:ARG:HB3	4:L:48:LYS:HZ1	1.67	0.59
4:L:311:GLY:O	4:L:314:VAL:HG12	2.01	0.59
2:F:4:ARG:HH22	1:G:22:GLN:HE22	1.50	0.59
1:B:25:VAL:O	1:B:29:VAL:HG23	2.03	0.59
13:L:1006:BPH:H13	13:L:1006:BPH:H7C2	1.84	0.59
5:M:607:LEU:HD12	9:M:702:BCL:OBD	2.02	0.59
4:L:236:GLU:HB2	4:L:241:ILE:HD11	1.84	0.59
2:9:25:LEU:O	2:9:29:VAL:HG23	2.02	0.59
4:L:226:LEU:HG	5:M:592:ALA:HB1	1.85	0.59
9:O:101:BCL:H101	9:9:101:BCL:H92	1.85	0.59
5:M:555:GLU:HG2	5:M:556:MET:HE2	1.85	0.59
4:L:209:ASN:HD21	4:L:281:CYS:HB2	1.68	0.58
1:W:50:TRP:CD1	1:W:51:THR:HG23	2.39	0.58
2:A:17:LEU:HD23	5:M:384:ILE:CD1	2.33	0.58
3:C:58:ILE:HG21	3:C:109:GLN:NE2	2.18	0.58
4:L:45:ARG:HB3	4:L:48:LYS:NZ	2.18	0.58
4:L:258:ILE:HD11	5:M:365:LEU:HD13	1.84	0.58
1:8:19:ASN:OD1	1:8:20:ASN:N	2.37	0.58
12:C:507:PGV:C12	13:M:703:BPH:HED1	2.34	0.58
1:E:26:HIS:O	1:E:30:VAL:HG23	2.04	0.58
2:9:9:ARG:HG3	2:A:6:PHE:CZ	2.39	0.58
5:M:348:GLU:OE2	5:M:374:TYR:OH	2.22	0.57
1:I:11:PRO:O	1:I:15:LYS:HG3	2.05	0.57
5:M:423:GLU:HG3	5:M:424:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:20:TYR:HA	8:Z:24:PHE:HD2	1.70	0.57
1:K:18:PHE:HE2	9:K:102:BCL:HMA1	1.69	0.57
13:L:1006:BPH:HBB3	13:L:1006:BPH:HHC	1.86	0.57
2:7:4:ARG:HH22	1:8:22:GLN:HE22	1.53	0.57
2:A:38:TRP:CZ2	9:A:101:BCL:HHC	2.40	0.57
3:C:254:ILE:HG22	3:C:256:GLN:OE1	2.05	0.57
2:A:19:GLY:HA3	9:A:101:BCL:H42	1.85	0.57
1:U:9:LEU:HB2	1:U:20:ASN:OD1	2.05	0.57
2:H:4:ARG:HD2	2:H:6:PHE:O	2.04	0.57
9:E:101:BCL:H151	9:E:101:BCL:H192	1.87	0.56
1:8:11:PRO:O	1:8:15:LYS:HG3	2.06	0.56
2:P:38:TRP:CZ2	9:P:101:BCL:HHC	2.40	0.56
1:6:33:ILE:O	1:6:37:LEU:HD23	2.06	0.56
3:C:136:ALA:O	3:C:140:VAL:HG23	2.05	0.56
9:L:1002:BCL:H52	13:L:1003:BPH:HBB2	1.87	0.56
4:L:174:ARG:O	4:L:178:MET:HG3	2.05	0.56
2:T:9:ARG:O	2:T:13:VAL:HG23	2.05	0.56
1:S:41:VAL:O	1:S:45:VAL:HG23	2.04	0.56
10:U:103:KGD:CAU	9:W:102:BCL:C19	2.81	0.56
4:L:110:VAL:HG13	4:L:180:ALA:HB1	1.87	0.56
2:N:13:VAL:HA	9:N:101:BCL:H192	1.87	0.56
9:E:101:BCL:HHC	9:E:101:BCL:HBB2	1.88	0.56
2:J:18:LEU:O	2:J:22:MET:HG2	2.06	0.56
4:L:174:ARG:HB3	4:L:175:PRO:HD3	1.88	0.55
2:N:18:LEU:O	2:N:22:MET:HG2	2.06	0.55
3:C:10:PRO:O	3:C:14:ASN:HB2	2.05	0.55
4:L:32:GLU:HG3	4:L:34:ILE:HG13	1.88	0.55
3:C:201:LEU:HA	3:C:205:TYR:OH	2.06	0.55
2:A:4:ARG:NH1	2:A:7:GLU:HA	2.22	0.55
1:O:26:HIS:O	1:O:30:VAL:HG23	2.07	0.55
1:W:9:LEU:HB2	1:W:20:ASN:OD1	2.07	0.55
7:Y:5:VAL:O	7:Y:9:MET:HG2	2.07	0.55
1:6:11:PRO:O	1:6:15:LYS:HG3	2.07	0.55
5:M:468:GLN:N	5:M:468:GLN:OE1	2.39	0.55
1:O:41:VAL:O	1:O:45:VAL:HG23	2.07	0.55
9:O:102:BCL:HHC	9:O:102:BCL:HBB2	1.89	0.55
2:3:22:MET:HE2	2:3:22:MET:HA	1.89	0.55
2:5:4:ARG:HH21	2:5:7:GLU:HG3	1.70	0.55
2:5:40:ARG:HB2	2:7:35:ALA:HB2	1.88	0.54
1:O:37:LEU:O	1:O:41:VAL:HG23	2.07	0.54
1:E:11:PRO:O	1:E:15:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:37:LEU:CD1	9:S:101:BCL:H12	2.37	0.54
9:S:102:BCL:HHC	9:S:102:BCL:HBB2	1.89	0.54
9:I:101:BCL:H151	9:I:101:BCL:H192	1.89	0.54
9:I:102:BCL:HHC	9:I:102:BCL:HBB2	1.88	0.54
10:I:103:KGD:CAG	9:K:102:BCL:C6	2.85	0.54
2:T:4:ARG:HB3	1:U:17:LEU:HD23	1.88	0.54
7:Y:11:MET:O	7:Y:15:VAL:HG23	2.07	0.54
2:D:4:ARG:NH2	2:D:7:GLU:OE2	2.25	0.54
9:Q:102:BCL:HBB2	9:Q:102:BCL:HHC	1.90	0.54
2:1:8:PHE:O	2:1:12:VAL:HG23	2.07	0.53
2:7:13:VAL:O	2:7:17:LEU:HD23	2.08	0.53
4:L:60:PHE:O	4:L:70:GLY:HA2	2.07	0.53
1:0:17:LEU:HD23	2:9:4:ARG:HB3	1.90	0.53
4:L:55:PHE:CD1	9:T:101:BCL:H191	2.43	0.53
4:L:104:ARG:HD2	4:L:106:GLU:OE2	2.09	0.53
3:C:205:TYR:OH	3:C:268:LYS:HG3	2.08	0.53
1:6:9:LEU:HB2	1:6:20:ASN:OD1	2.08	0.53
9:K:101:BCL:HBC3	9:K:101:BCL:HHD	1.91	0.53
3:C:210:VAL:O	3:C:214:ARG:NH1	2.41	0.53
4:L:253:ILE:HD11	5:M:459:ARG:HB2	1.90	0.53
9:L:1001:BCL:O1A	5:M:533:LEU:HD12	2.07	0.53
9:0:102:BCL:HHC	9:0:102:BCL:HBB2	1.91	0.53
10:G:102:KGD:CAF	9:I:102:BCL:C6	2.87	0.53
2:J:9:ARG:HD3	2:N:5:PRO:O	2.09	0.53
5:M:541:MET:HE3	5:M:575:TRP:CH2	2.44	0.53
8:Z:25:VAL:HB	8:Z:26:PRO:HD3	1.89	0.53
1:O:31:LYS:HB2	9:Q:102:BCL:H42	1.89	0.53
1:0:50:TRP:CE3	10:0:104:KGD:CAZ	2.92	0.53
2:A:7:GLU:OE1	2:A:9:ARG:NH2	2.42	0.53
9:6:102:BCL:HBB2	9:6:102:BCL:HHC	1.91	0.53
8:Z:20:TYR:HA	8:Z:24:PHE:CD2	2.44	0.53
2:F:9:ARG:HG3	2:H:6:PHE:CZ	2.43	0.53
4:L:110:VAL:HG13	4:L:180:ALA:CB	2.39	0.53
2:D:9:ARG:HD2	2:F:5:PRO:O	2.08	0.52
2:F:9:ARG:O	2:F:13:VAL:HG23	2.08	0.52
10:J:103:KGD:CAK	10:J:103:KGD:CAL	2.85	0.52
2:R:22:MET:HB3	9:S:101:BCL:HED1	1.91	0.52
1:Q:12:ASP:HA	1:Q:15:LYS:HE2	1.91	0.52
3:C:110:VAL:HG13	11:C:501:HEM:HBC2	1.90	0.52
5:M:377:LEU:HD23	5:M:377:LEU:O	2.10	0.52
7:Y:14:LEU:HA	7:Y:17:PHE:CD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:487:HIS:HB3	5:M:488:PRO:HD3	1.90	0.52
5:M:614:VAL:HG11	5:M:617:TRP:CE3	2.44	0.52
4:L:59:PRO:HA	2:T:10:THR:HG23	1.92	0.52
9:G:101:BCL:HHC	9:G:101:BCL:HBB2	1.91	0.52
2:3:12:VAL:CG1	9:3:101:BCL:H192	2.38	0.52
3:C:44:TYR:HE2	7:Y:4:ILE:HD11	1.74	0.52
4:L:105:ILE:HD13	4:L:187:LEU:O	2.09	0.52
9:B:101:BCL:H151	9:B:101:BCL:H192	1.91	0.52
4:L:207:PHE:CD1	9:L:1002:BCL:HMC2	2.45	0.52
5:M:421:PRO:HD2	5:M:424:TYR:OH	2.09	0.52
5:M:523:PRO:HA	5:M:526:MET:HE3	1.92	0.52
4:L:271:GLY:O	13:L:1003:BPH:HBC1	2.10	0.51
3:C:65:GLU:O	3:C:67:THR:HG23	2.10	0.51
10:D:102:KGD:CAK	10:D:102:KGD:CAL	2.87	0.51
4:L:189:ILE:HG22	4:L:190:THR:HG23	1.91	0.51
4:L:244:GLN:O	4:L:248:VAL:HG23	2.10	0.51
9:O:101:BCL:H151	9:O:101:BCL:H192	1.91	0.51
2:A:4:ARG:HD3	1:B:17:LEU:HA	1.93	0.51
4:L:252:ASN:OD1	5:M:459:ARG:NH2	2.44	0.51
5:M:620:TRP:CZ2	8:Z:19:GLY:HA2	2.46	0.51
1:S:34:TYR:O	1:S:38:ILE:HG12	2.09	0.51
10:2:103:KGD:CAG	9:4:102:BCL:H62	2.40	0.51
9:4:101:BCL:H151	9:4:101:BCL:H192	1.92	0.51
10:4:103:KGD:CAG	9:6:102:BCL:CAD	2.89	0.51
3:C:170:THR:HG22	3:C:171:CYS:N	2.26	0.51
5:M:353:LYS:O	5:M:355:PRO:HD3	2.10	0.51
1:S:19:ASN:OD1	1:S:20:ASN:N	2.43	0.51
13:M:703:BPH:H141	15:M:704:MQE:CCA	2.41	0.51
1:U:37:LEU:O	1:U:41:VAL:HG23	2.10	0.51
1:0:7:ASN:O	1:0:15:LYS:HE2	2.11	0.51
2:A:12:VAL:HG11	10:A:102:KGD:CAK	2.41	0.51
9:L:1001:BCL:HED2	5:M:526:MET:SD	2.51	0.51
9:U:102:BCL:HBC3	9:U:102:BCL:HHD	1.93	0.51
1:2:8:ASP:OD1	1:2:9:LEU:N	2.43	0.51
9:4:102:BCL:HBB2	9:4:102:BCL:HHC	1.92	0.51
9:E:101:BCL:H102	9:E:101:BCL:H152	1.93	0.51
2:A:40:ARG:NH1	2:D:34:GLY:O	2.44	0.51
8:Z:26:PRO:O	8:Z:30:VAL:HG23	2.11	0.51
2:A:9:ARG:O	2:A:13:VAL:HG23	2.11	0.50
10:U:103:KGD:CAU	9:W:102:BCL:C20	2.86	0.50
10:A:102:KGD:CAK	10:A:102:KGD:CAL	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:102:KGD:OAA	2:F:6:PHE:HD2	1.93	0.50
15:M:701:MQE:CBA	2:R:17:LEU:HD12	2.42	0.50
2:R:9:ARG:O	2:R:13:VAL:HG23	2.11	0.50
1:Q:19:ASN:OD1	1:Q:20:ASN:N	2.44	0.50
9:Q:101:BCL:C20	1:S:37:LEU:HD11	2.42	0.50
2:J:9:ARG:O	2:J:13:VAL:HG23	2.12	0.50
1:O:34:TYR:OH	9:O:102:BCL:OBD	2.26	0.50
9:S:102:BCL:H13	10:S:103:KGD:CAP	2.42	0.50
2:7:9:ARG:HG3	2:9:6:PHE:CE1	2.47	0.50
9:B:101:BCL:H13	10:B:103:KGD:CAQ	2.41	0.50
1:6:34:TYR:OH	9:6:102:BCL:OBD	2.24	0.50
3:C:186:PRO:HB2	3:C:188:GLU:OE1	2.12	0.50
1:4:24:LEU:HD12	1:6:17:LEU:HD11	1.94	0.50
10:E:103:KGD:CAF	9:G:101:BCL:H62	2.42	0.50
4:L:59:PRO:HB3	2:T:10:THR:HG23	1.94	0.50
5:M:525:HIS:CE1	5:M:529:ILE:HD11	2.47	0.50
4:L:72:PHE:HA	4:L:75:ILE:HD12	1.94	0.49
4:L:226:LEU:HD13	5:M:539:LEU:HB2	1.94	0.49
4:L:267:ALA:HB1	5:M:539:LEU:HG	1.93	0.49
1:U:50:TRP:CE3	10:U:103:KGD:CAZ	2.96	0.49
4:L:290:LYS:HE2	5:M:640:PHE:CD2	2.47	0.49
3:C:160:LEU:HD12	11:C:504:HEM:HBD1	1.92	0.49
5:M:358:VAL:HG11	5:M:361:MET:HG3	1.93	0.49
5:M:393:ILE:HG21	15:M:704:MQE:CCE	2.42	0.49
5:M:619:ALA:O	5:M:623:THR:HG23	2.13	0.49
1:K:11:PRO:O	1:K:15:LYS:HG3	2.13	0.49
1:4:31:LYS:HB2	9:6:102:BCL:H42	1.95	0.49
3:C:150:ALA:HB2	3:C:316:LEU:HD23	1.93	0.49
2:F:10:THR:O	2:F:14:VAL:HG13	2.12	0.49
5:M:538:LEU:HD22	5:M:595:PHE:CE2	2.47	0.49
9:3:101:BCL:H112	9:6:102:BCL:HBC1	1.94	0.49
10:P:102:KGD:CBN	9:Q:101:BCL:H162	2.43	0.49
2:T:22:MET:HE3	2:T:22:MET:HA	1.93	0.49
3:C:60:VAL:O	3:C:304:PRO:HA	2.12	0.49
3:C:218:SER:HB3	5:M:422:THR:OG1	2.11	0.49
1:O:37:LEU:HD23	9:O:101:BCL:C1	2.42	0.49
10:2:103:KGD:CAG	9:4:102:BCL:H51	2.42	0.49
1:B:8:ASP:OD1	1:B:9:LEU:N	2.46	0.49
9:M:702:BCL:H92	9:M:702:BCL:H52	1.95	0.49
1:O:39:ILE:HD11	9:Q:102:BCL:H122	1.94	0.49
3:C:110:VAL:CG1	11:C:501:HEM:HBC2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:VAL:HG11	10:D:102:KGD:CAK	2.43	0.48
9:F:102:BCL:H151	9:F:102:BCL:H192	1.95	0.48
1:W:37:LEU:O	1:W:41:VAL:HG23	2.13	0.48
1:6:19:ASN:OD1	1:6:20:ASN:N	2.45	0.48
1:6:26:HIS:O	1:6:30:VAL:HG23	2.13	0.48
9:B:101:BCL:H152	9:B:101:BCL:H102	1.94	0.48
9:S:101:BCL:HBC3	9:S:101:BCL:HHD	1.95	0.48
2:A:15:SER:OG	9:B:102:BCL:HBC2	2.14	0.48
2:F:4:ARG:NH1	1:G:17:LEU:O	2.44	0.48
4:L:53:ARG:NH2	4:L:148:LEU:HD11	2.28	0.48
4:L:76:SER:O	4:L:80:ILE:HG13	2.14	0.48
9:B:102:BCL:HHC	9:B:102:BCL:HBB2	1.95	0.48
4:L:314:VAL:HG22	4:L:315:ALA:N	2.28	0.48
5:M:353:LYS:HB2	5:M:354:PRO:HD3	1.95	0.48
5:M:480:TYR:HB2	9:M:702:BCL:H62	1.95	0.48
3:C:263:MET:HG3	11:C:504:HEM:CHB	2.44	0.48
2:F:25:LEU:O	2:F:29:VAL:HG23	2.13	0.48
9:W:101:BCL:HHD	9:W:101:BCL:HBC3	1.95	0.48
6:X:14:ILE:O	6:X:18:LEU:HG	2.14	0.48
10:6:103:KGD:CAK	10:6:103:KGD:CAL	2.91	0.48
1:E:19:ASN:OD1	1:E:20:ASN:N	2.47	0.48
2:P:8:PHE:O	2:P:12:VAL:HG23	2.13	0.48
1:4:53:TRP:CD1	1:4:54:ILE:HG13	2.49	0.48
3:C:232:MET:HE3	11:C:504:HEM:CMB	2.43	0.48
4:L:254:LEU:HD21	13:L:1006:BPH:CED	2.40	0.48
1:O:26:HIS:O	1:O:30:VAL:HG23	2.14	0.48
1:Q:31:LYS:HB2	9:S:102:BCL:H42	1.95	0.48
2:V:13:VAL:O	2:V:17:LEU:HG	2.13	0.48
1:8:34:TYR:OH	9:8:102:BCL:OBD	2.23	0.48
5:M:630:TRP:NE1	5:M:633:PRO:HG3	2.28	0.47
9:T:101:BCL:H92	9:U:101:BCL:H101	1.96	0.47
1:I:27:ASP:OD1	1:I:31:LYS:HE2	2.14	0.47
1:Q:9:LEU:HB2	1:Q:20:ASN:OD1	2.14	0.47
1:0:37:LEU:O	1:0:41:VAL:HG23	2.15	0.47
9:0:101:BCL:H192	9:0:101:BCL:H151	1.96	0.47
10:5:102:KGD:CAK	10:5:102:KGD:CAL	2.92	0.47
4:L:254:LEU:CD2	13:L:1006:BPH:H151	2.44	0.47
4:L:283:PHE:CZ	7:Y:9:MET:HB2	2.48	0.47
1:4:37:LEU:O	1:4:41:VAL:HG23	2.15	0.47
3:C:42:ILE:O	3:C:46:ILE:HG12	2.15	0.47
3:C:152:LEU:HD13	3:C:266:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:MET:HG3	11:C:504:HEM:C1B	2.49	0.47
4:L:58:ASP:HB3	4:L:61:ASP:HB2	1.97	0.47
2:R:17:LEU:O	2:R:21:VAL:HG23	2.13	0.47
2:7:9:ARG:O	2:7:13:VAL:HG23	2.14	0.47
4:L:100:ILE:HG13	4:L:101:LEU:CD1	2.45	0.47
4:L:251:ARG:O	4:L:255:GLY:HA2	2.15	0.47
1:S:37:LEU:O	1:S:41:VAL:HG23	2.15	0.47
1:K:19:ASN:OD1	1:K:20:ASN:N	2.48	0.47
4:L:253:ILE:HG22	4:L:254:LEU:HG	1.95	0.47
1:G:39:ILE:HD11	9:I:102:BCL:H152	1.96	0.47
1:I:25:VAL:O	1:I:29:VAL:HG23	2.15	0.47
2:N:13:VAL:HG22	9:N:101:BCL:C19	2.44	0.47
1:U:36:GLY:HA3	9:U:101:BCL:H41	1.96	0.47
7:Y:2:ASN:ND2	7:Y:5:VAL:HG23	2.30	0.47
3:C:257:LYS:O	3:C:261:ILE:HG12	2.14	0.47
1:E:37:LEU:O	1:E:41:VAL:HG23	2.15	0.47
9:8:101:BCL:H152	9:8:101:BCL:H102	1.97	0.47
1:G:11:PRO:O	1:G:15:LYS:HG3	2.15	0.47
4:L:279:ASN:HA	4:L:282:ILE:HG22	1.98	0.47
9:A:101:BCL:H193	2:D:6:PHE:CE2	2.50	0.46
3:C:122:HIS:HB3	3:C:139:LYS:HD2	1.95	0.46
2:5:10:THR:O	2:5:14:VAL:HG23	2.15	0.46
9:K:102:BCL:H151	9:K:102:BCL:H18	1.72	0.46
5:M:358:VAL:CG2	5:M:361:MET:HE2	2.34	0.46
9:0:102:BCL:H51	10:8:103:KGD:CAF	2.45	0.46
10:E:103:KGD:CAU	9:G:101:BCL:H162	2.45	0.46
2:D:8:PHE:O	2:D:12:VAL:HG23	2.15	0.46
2:J:32:SER:HB2	8:Z:20:TYR:HE2	1.79	0.46
1:U:28:ILE:HD11	1:W:14:TRP:CH2	2.51	0.46
15:L:1005:MQE:CBI	7:Y:14:LEU:HD23	2.45	0.46
2:5:9:ARG:O	2:5:13:VAL:HG23	2.16	0.46
4:L:180:ALA:HB3	4:L:183:HIS:CE1	2.50	0.46
2:5:8:PHE:O	2:5:12:VAL:HG23	2.16	0.46
1:8:8:ASP:OD1	1:8:9:LEU:N	2.48	0.46
3:C:152:LEU:HD13	3:C:266:MET:HE2	1.97	0.46
9:E:102:BCL:H101	9:E:102:BCL:H152	1.96	0.46
4:L:55:PHE:HD1	9:T:101:BCL:H191	1.80	0.46
5:M:483:ILE:HG12	5:M:607:LEU:CD1	2.46	0.46
2:N:25:LEU:O	2:N:29:VAL:HG23	2.16	0.46
9:6:101:BCL:H151	9:6:101:BCL:H192	1.98	0.46
9:3:101:BCL:H93	9:4:101:BCL:H101	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4:ARG:NH1	1:6:17:LEU:O	2.49	0.46
2:A:17:LEU:CD2	5:M:381:ILE:HA	2.45	0.46
10:B:103:KGD:CAK	10:B:103:KGD:CAL	2.92	0.46
1:Q:39:ILE:CD1	9:S:102:BCL:H122	2.45	0.46
1:S:36:GLY:HA3	9:S:101:BCL:H62	1.98	0.46
9:S:101:BCL:H61	9:S:101:BCL:H41	1.84	0.46
2:D:4:ARG:HH22	1:E:22:GLN:HE22	1.64	0.46
9:F:102:BCL:H61	9:F:102:BCL:H41	1.80	0.46
1:K:25:VAL:O	1:K:29:VAL:HG23	2.16	0.46
5:M:341:GLU:HA	5:M:344:ARG:NH1	2.31	0.46
1:4:7:ASN:O	1:4:15:LYS:HE3	2.16	0.45
2:5:25:LEU:O	2:5:29:VAL:HG23	2.16	0.45
2:5:37:ASN:HA	2:5:41:ALA:HA	1.98	0.45
9:S:101:BCL:H152	9:S:101:BCL:H102	1.99	0.45
2:V:4:ARG:HB2	1:W:17:LEU:HD23	1.97	0.45
9:W:101:BCL:H61	9:W:101:BCL:H41	1.79	0.45
1:I:19:ASN:OD1	1:I:20:ASN:N	2.49	0.45
5:M:378:TRP:HE3	5:M:451:THR:HG23	1.81	0.45
9:P:101:BCL:HMC3	9:S:101:BCL:HBB1	1.98	0.45
10:R:102:KGD:CAK	10:R:102:KGD:CAL	2.91	0.45
3:C:204:ASP:O	3:C:208:GLY:N	2.49	0.45
10:C:505:KGD:CAK	10:C:505:KGD:CAL	2.90	0.45
9:E:102:BCL:H62	9:E:102:BCL:H41	1.82	0.45
10:E:103:KGD:CAK	10:E:103:KGD:CAL	2.94	0.45
13:L:1003:BPH:H3A	13:L:1003:BPH:HBA1	1.50	0.45
1:Q:11:PRO:O	1:Q:15:LYS:HG3	2.17	0.45
9:2:102:BCL:HHC	9:2:102:BCL:HBB2	1.99	0.45
2:H:40:ARG:HB2	2:J:35:ALA:CB	2.44	0.45
2:R:13:VAL:HG22	9:R:101:BCL:C19	2.44	0.45
1:S:12:ASP:HA	1:S:15:LYS:CD	2.44	0.45
4:L:193:LEU:HD21	9:L:1001:BCL:C2D	2.47	0.45
2:F:17:LEU:O	2:F:21:VAL:HG23	2.16	0.45
1:G:12:ASP:HA	1:G:15:LYS:HD2	1.98	0.45
4:L:284:LEU:HD12	4:L:288:PHE:HB2	1.98	0.45
2:D:28:PHE:HE2	5:M:428:TRP:HE1	1.64	0.45
4:L:49:THR:HG21	4:L:68:TYR:OH	2.17	0.45
13:L:1006:BPH:H161	13:L:1006:BPH:HMA1	1.99	0.45
9:U:102:BCL:H62	9:U:102:BCL:H41	1.82	0.45
10:1:102:KGD:CAE	9:4:102:BCL:HBB3	2.48	0.45
9:2:102:BCL:H62	9:2:102:BCL:H41	1.82	0.45
2:9:13:VAL:HG22	9:9:101:BCL:C19	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:103:KGD:CBJ	9:E:101:BCL:H143	2.47	0.45
4:L:249:PHE:HB2	5:M:463:THR:HG21	1.98	0.45
9:N:101:BCL:HMB3	9:N:101:BCL:HBB3	1.98	0.45
9:I:102:BCL:H62	9:I:102:BCL:H41	1.85	0.44
1:O:7:ASN:ND2	1:O:15:LYS:HD2	2.33	0.44
9:B:101:BCL:H61	9:B:101:BCL:H41	1.83	0.44
5:M:513:SER:HA	5:M:519:PHE:CE2	2.53	0.44
2:R:12:VAL:HG12	9:R:101:BCL:H192	2.00	0.44
2:V:10:THR:O	2:V:14:VAL:HG23	2.17	0.44
9:O:101:BCL:H141	9:O:101:BCL:H162	1.76	0.44
3:C:205:TYR:CE2	3:C:268:LYS:HB2	2.48	0.44
10:D:103:KGD:CAL	10:D:103:KGD:CAK	2.94	0.44
15:M:701:MQE:CBN	2:R:17:LEU:HD12	2.46	0.44
2:A:9:ARG:HD3	2:D:5:PRO:O	2.17	0.44
3:C:122:HIS:HA	3:C:133:TYR:CE2	2.52	0.44
4:L:247:HIS:HB3	4:L:251:ARG:NH1	2.32	0.44
1:O:34:TYR:OH	9:O:102:BCL:OBD	2.29	0.44
2:1:40:ARG:HG2	2:3:35:ALA:CB	2.47	0.44
1:6:37:LEU:O	1:6:41:VAL:HG23	2.18	0.44
2:9:9:ARG:HG3	2:A:6:PHE:CE1	2.53	0.44
3:C:103:SER:O	3:C:107:VAL:HG23	2.18	0.44
2:J:17:LEU:O	2:J:21:VAL:HG23	2.18	0.44
4:L:276:LEU:HB3	7:Y:17:PHE:CE1	2.52	0.44
3:C:266:MET:O	3:C:270:ILE:HG13	2.18	0.44
4:L:74:ALA:O	4:L:77:ILE:HG22	2.18	0.44
10:D:103:KGD:CBH	9:E:101:BCL:H143	2.48	0.44
4:L:39:ILE:HD12	4:L:39:ILE:H	1.82	0.44
4:L:81:ILE:CG2	2:R:21:VAL:HG11	2.47	0.44
4:L:205:ASN:HB2	4:L:293:ASN:OD1	2.18	0.44
2:3:26:ILE:O	2:3:30:VAL:HG23	2.18	0.43
2:7:25:LEU:O	2:7:29:VAL:HG23	2.18	0.43
10:K:103:KGD:CAK	10:K:103:KGD:CAL	2.95	0.43
9:O:101:BCL:H61	9:O:101:BCL:H41	1.81	0.43
2:D:4:ARG:NH1	1:E:17:LEU:O	2.48	0.43
2:D:13:VAL:HA	9:D:101:BCL:H193	2.00	0.43
4:L:195:TRP:O	4:L:199:ILE:HG12	2.19	0.43
2:N:8:PHE:O	2:N:12:VAL:HG23	2.18	0.43
1:B:34:TYR:OH	9:B:102:BCL:OBD	2.29	0.43
10:B:103:KGD:CAP	9:E:102:BCL:H142	2.47	0.43
4:L:236:GLU:HB2	4:L:241:ILE:CD1	2.46	0.43
9:R:101:BCL:H18	9:R:101:BCL:H151	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:103:KGD:CAF	9:6:102:BCL:H51	2.48	0.43
5:M:347:LEU:O	5:M:348:GLU:HB2	2.18	0.43
1:0:39:ILE:HD11	9:B:102:BCL:H122	2.01	0.43
9:9:101:BCL:H122	9:9:101:BCL:H72	2.00	0.43
4:L:81:ILE:HG21	2:R:21:VAL:HG11	2.00	0.43
2:1:9:ARG:NH1	2:3:5:PRO:O	2.50	0.43
3:C:196:ASP:OD1	3:C:196:ASP:N	2.48	0.43
4:L:66:ARG:HD2	12:L:1009:PGV:H02	1.99	0.43
9:S:102:BCL:H62	10:S:103:KGD:CAF	2.48	0.43
9:2:102:BCL:HBC3	9:2:102:BCL:HHD	2.00	0.43
5:M:513:SER:HA	5:M:519:PHE:CD2	2.54	0.43
2:V:4:ARG:NH2	2:V:7:GLU:OE1	2.51	0.43
9:4:102:BCL:H62	9:4:102:BCL:H41	1.86	0.43
2:N:13:VAL:HA	9:N:101:BCL:C19	2.48	0.43
9:0:101:BCL:H101	9:9:101:BCL:C9	2.48	0.43
2:9:4:ARG:HD2	2:9:6:PHE:O	2.19	0.43
2:N:17:LEU:O	2:N:21:VAL:HG23	2.19	0.43
9:4:101:BCL:HBB2	9:4:101:BCL:HMB3	2.01	0.43
3:C:142:ALA:O	3:C:146:MET:HG3	2.18	0.43
3:C:241:THR:O	5:M:635:TRP:HZ2	2.01	0.43
10:P:102:KGD:CAL	10:P:102:KGD:CAK	2.96	0.43
2:V:13:VAL:HG13	9:V:101:BCL:C19	2.37	0.43
8:Z:53:ASP:H	8:Z:56:LYS:HE3	1.84	0.43
9:6:102:BCL:H62	9:6:102:BCL:H41	1.90	0.42
2:7:13:VAL:HA	9:7:101:BCL:C19	2.49	0.42
3:C:70:ILE:HG21	3:C:75:LEU:HG	2.01	0.42
3:C:315:VAL:HG13	3:C:316:LEU:HG	2.01	0.42
4:L:272:ALA:O	4:L:276:LEU:HG	2.19	0.42
2:1:10:THR:O	2:1:14:VAL:HG23	2.19	0.42
2:7:8:PHE:HD2	2:9:5:PRO:HG3	1.85	0.42
9:8:101:BCL:H141	9:8:101:BCL:H162	1.76	0.42
9:8:101:BCL:H151	9:8:101:BCL:H192	2.01	0.42
2:A:12:VAL:HG12	9:A:101:BCL:H192	2.01	0.42
3:C:229:MET:HB3	11:C:503:HEM:C4B	2.54	0.42
9:K:101:BCL:H152	9:K:101:BCL:H102	2.01	0.42
4:L:99:ASN:OD1	4:L:102:ALA:HB3	2.19	0.42
2:R:25:LEU:O	2:R:29:VAL:HG23	2.19	0.42
9:6:101:BCL:H152	9:6:101:BCL:H102	2.00	0.42
5:M:557:GLU:O	5:M:561:MET:HG3	2.18	0.42
9:O:101:BCL:HBB2	9:O:101:BCL:HMB3	2.02	0.42
10:B:103:KGD:CAE	9:E:102:BCL:H43	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:THR:HB	5:M:635:TRP:CZ2	2.55	0.42
9:J:101:BCL:H18	9:J:101:BCL:H151	1.76	0.42
4:L:233:VAL:HG11	5:M:589:HIS:CD2	2.55	0.42
9:J:101:BCL:HBB2	10:J:103:KGD:CBD	2.49	0.42
4:L:211:PHE:CB	4:L:281:CYS:HB3	2.21	0.42
9:T:101:BCL:H142	2:V:15:SER:OG	2.19	0.42
8:Z:39:ARG:NH1	8:Z:43:LYS:HE3	2.33	0.42
1:E:41:VAL:O	1:E:45:VAL:HG23	2.19	0.42
13:M:703:BPH:H202	15:M:704:MQE:OAB	2.20	0.42
9:U:101:BCL:H41	9:U:101:BCL:H62	1.87	0.42
10:2:103:KGD:CAG	9:4:102:BCL:C5	2.97	0.42
9:A:101:BCL:HMB1	9:A:101:BCL:HBB3	2.01	0.42
3:C:70:ILE:HG22	3:C:72:ALA:H	1.84	0.42
3:C:193:LEU:HD22	3:C:227:PHE:CD1	2.54	0.42
3:C:223:GLU:HG3	5:M:511:TYR:OH	2.20	0.42
2:H:40:ARG:CB	2:J:35:ALA:HB2	2.49	0.42
1:K:50:TRP:CH2	1:O:54:ILE:HG23	2.55	0.42
9:K:101:BCL:HBB2	9:K:101:BCL:HMB3	2.02	0.42
4:L:279:ASN:O	4:L:282:ILE:HG22	2.19	0.42
5:M:478:SER:O	5:M:482:VAL:HG23	2.19	0.42
1:W:10:VAL:HG13	1:W:11:PRO:HD2	2.00	0.42
9:0:101:BCL:HBB2	9:0:101:BCL:HMB3	2.02	0.42
2:7:18:LEU:O	2:7:22:MET:HG2	2.20	0.42
3:C:133:TYR:HB2	3:C:134:PRO:HD2	2.02	0.42
3:C:236:MET:HE1	11:C:504:HEM:HMA3	2.02	0.42
10:C:505:KGD:CBL	9:U:101:BCL:H201	2.50	0.42
9:D:101:BCL:H18	9:D:101:BCL:H151	1.93	0.42
5:M:503:ARG:O	5:M:503:ARG:HG2	2.19	0.42
2:V:4:ARG:CB	1:W:17:LEU:HD23	2.49	0.42
2:9:9:ARG:O	2:9:13:VAL:HG23	2.20	0.42
2:H:15:SER:OG	9:I:102:BCL:HBC2	2.20	0.42
4:L:303:PRO:HA	4:L:306:ASN:ND2	2.34	0.42
9:O:102:BCL:H192	9:O:102:BCL:H162	1.81	0.42
1:2:21:ALA:HB1	1:4:17:LEU:HD21	2.01	0.42
3:C:169:ILE:HD13	11:C:504:HEM:CBC	2.50	0.42
9:H:101:BCL:H111	9:H:101:BCL:H152	1.88	0.42
9:0:102:BCL:H62	9:0:102:BCL:H41	1.87	0.41
2:5:9:ARG:HG3	2:7:6:PHE:CZ	2.55	0.41
2:7:28:PHE:HB3	5:M:405:PRO:HD3	2.01	0.41
5:M:358:VAL:CG1	5:M:361:MET:HG3	2.50	0.41
2:N:9:ARG:O	2:N:13:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:22:MET:HE2	10:7:102:KGD:CBE	2.50	0.41
2:D:4:ARG:HB2	1:E:17:LEU:HD23	2.01	0.41
13:L:1003:BPH:O1A	13:L:1003:BPH:H4C3	2.19	0.41
1:Q:37:LEU:O	1:Q:41:VAL:HG23	2.20	0.41
2:3:25:LEU:O	2:3:29:VAL:HG23	2.20	0.41
9:8:102:BCL:HBB2	9:8:102:BCL:HMB3	2.01	0.41
1:U:25:VAL:O	1:U:29:VAL:HG23	2.20	0.41
2:V:39:LEU:HD21	9:V:101:BCL:HMC1	2.02	0.41
1:0:17:LEU:CD2	2:9:4:ARG:HB3	2.49	0.41
1:4:34:TYR:OH	9:4:102:BCL:OBD	2.28	0.41
3:C:26:ILE:O	3:C:30:VAL:HG23	2.21	0.41
4:L:210:PRO:O	4:L:214:ILE:HG13	2.20	0.41
9:Q:101:BCL:HBB2	9:Q:101:BCL:HMB3	2.02	0.41
2:T:13:VAL:HG22	9:T:101:BCL:C19	2.51	0.41
9:B:102:BCL:HHC	9:B:102:BCL:CBB	2.49	0.41
4:L:32:GLU:O	8:Z:50:LEU:HA	2.20	0.41
1:Q:33:ILE:O	1:Q:37:LEU:HG	2.20	0.41
1:U:53:TRP:CD1	1:U:54:ILE:HG13	2.56	0.41
10:U:103:KGD:CAL	10:U:103:KGD:CAK	2.97	0.41
10:6:103:KGD:CAF	9:8:102:BCL:C5	2.99	0.41
2:A:12:VAL:HG12	9:A:101:BCL:C19	2.50	0.41
9:K:101:BCL:H192	9:K:101:BCL:H151	2.02	0.41
1:S:26:HIS:O	1:S:30:VAL:HG23	2.21	0.41
9:3:101:BCL:H72	9:3:101:BCL:H122	2.03	0.41
3:C:51:ALA:O	3:C:53:PRO:HD3	2.20	0.41
3:C:202:GLU:N	3:C:202:GLU:OE1	2.54	0.41
2:J:22:MET:CB	9:K:101:BCL:HED1	2.50	0.41
13:L:1003:BPH:OBB	5:M:533:LEU:HD13	2.20	0.41
5:M:508:TRP:O	5:M:512:VAL:HG23	2.21	0.41
1:S:34:TYR:OH	9:S:102:BCL:OBD	2.27	0.41
1:U:12:ASP:HA	1:U:15:LYS:NZ	2.36	0.41
3:C:145:MET:HE2	3:C:285:ILE:HD12	2.03	0.41
3:C:296:CYS:O	3:C:303:PRO:HB3	2.21	0.41
9:O:102:BCL:H62	9:O:102:BCL:H41	1.86	0.41
1:0:25:VAL:O	1:0:29:VAL:HG23	2.21	0.41
9:7:101:BCL:HBB3	9:7:101:BCL:HMB1	2.03	0.41
9:B:101:BCL:HMB3	9:B:101:BCL:HBB2	2.03	0.41
9:D:101:BCL:H111	9:D:101:BCL:H152	1.74	0.41
10:D:103:KGD:OAA	2:H:6:PHE:CD2	2.70	0.41
9:E:101:BCL:H61	9:E:101:BCL:H41	1.90	0.41
10:G:102:KGD:CAL	10:G:102:KGD:CAK	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:103:KGD:CAL	10:I:103:KGD:CAK	2.99	0.41
4:L:104:ARG:HG3	4:L:191:HIS:NE2	2.35	0.41
4:L:178:MET:HE2	4:L:178:MET:HB3	1.97	0.41
5:M:531:PHE:HB3	5:M:599:THR:OG1	2.21	0.41
1:O:25:VAL:O	1:O:29:VAL:HG23	2.20	0.41
1:Q:34:TYR:OH	9:Q:102:BCL:OBD	2.33	0.41
9:S:102:BCL:HBC3	9:S:102:BCL:HHD	2.01	0.41
9:O:101:BCL:H61	9:O:101:BCL:H41	1.82	0.41
9:E:101:BCL:HHC	9:E:101:BCL:CBB	2.51	0.41
9:I:101:BCL:H152	9:I:101:BCL:H102	2.03	0.41
9:P:101:BCL:H13	10:Q:103:KGD:CAG	2.51	0.41
9:U:101:BCL:H152	9:U:101:BCL:C10	2.48	0.41
8:Z:53:ASP:OD2	8:Z:55:ALA:HB3	2.21	0.41
9:A:101:BCL:H151	9:A:101:BCL:H18	1.90	0.40
9:S:101:BCL:H202	10:S:104:KGD:CAN	2.50	0.40
1:W:53:TRP:CD1	1:W:54:ILE:HG13	2.56	0.40
2:D:40:ARG:HA	1:G:55:ARG:HH22	1.86	0.40
5:M:483:ILE:HG12	5:M:607:LEU:HD13	2.03	0.40
9:8:102:BCL:H62	9:8:102:BCL:H41	1.88	0.40
9:G:101:BCL:HHC	9:G:101:BCL:CBB	2.51	0.40
1:O:9:LEU:HD13	1:O:20:ASN:HD21	1.84	0.40
1:8:53:TRP:CD1	1:8:54:ILE:HG13	2.57	0.40
3:C:240:CYS:HB3	4:L:201:TYR:O	2.22	0.40
2:J:9:ARG:HG2	2:N:5:PRO:HB3	2.02	0.40
2:T:13:VAL:HG22	9:T:101:BCL:H192	2.02	0.40
2:T:18:LEU:O	2:T:22:MET:HG2	2.21	0.40
6:X:17:THR:O	6:X:21:LEU:HG	2.22	0.40
8:Z:53:ASP:HB3	8:Z:56:LYS:HE3	2.03	0.40
1:4:27:ASP:OD2	1:4:31:LYS:HE3	2.21	0.40
2:J:24:LEU:HD23	10:J:103:KGD:CAZ	2.52	0.40
2:T:17:LEU:O	2:T:21:VAL:HG23	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%)	46 (98%)	1 (2%)	0	100	100
1	6	47/55 (86%)	47 (100%)	0	0	100	100
1	8	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	B	47/55 (86%)	46 (98%)	1 (2%)	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%)	47 (100%)	0	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	32/42 (76%)	30 (94%)	2 (6%)	0	100	100
2	3	35/42 (83%)	33 (94%)	2 (6%)	0	100	100
2	5	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	7	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	9	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	A	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	D	36/42 (86%)	32 (89%)	4 (11%)	0	100	100
2	F	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	H	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	J	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	N	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	P	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	R	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	T	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	V	35/42 (83%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	313/320 (98%)	296 (95%)	17 (5%)	0	100	100
4	L	295/315 (94%)	283 (96%)	12 (4%)	0	100	100
5	M	304/307 (99%)	293 (96%)	11 (4%)	0	100	100
6	X	24/32 (75%)	23 (96%)	1 (4%)	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
All	All	2244/2531 (89%)	2172 (97%)	72 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/49 (88%)	43 (100%)	0	100	100
1	2	43/49 (88%)	43 (100%)	0	100	100
1	4	43/49 (88%)	43 (100%)	0	100	100
1	6	43/49 (88%)	43 (100%)	0	100	100
1	8	43/49 (88%)	43 (100%)	0	100	100
1	B	43/49 (88%)	43 (100%)	0	100	100
1	E	43/49 (88%)	43 (100%)	0	100	100
1	G	43/49 (88%)	43 (100%)	0	100	100
1	I	43/49 (88%)	43 (100%)	0	100	100
1	K	43/49 (88%)	43 (100%)	0	100	100
1	O	43/49 (88%)	43 (100%)	0	100	100
1	Q	43/49 (88%)	43 (100%)	0	100	100
1	S	43/49 (88%)	43 (100%)	0	100	100
1	U	43/49 (88%)	43 (100%)	0	100	100
1	W	43/49 (88%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	30/37 (81%)	30 (100%)	0	100	100
2	3	33/37 (89%)	33 (100%)	0	100	100
2	5	33/37 (89%)	33 (100%)	0	100	100
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%)	257 (100%)	0	100	100
4	L	241/253 (95%)	241 (100%)	0	100	100
5	M	244/245 (100%)	244 (100%)	0	100	100
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	1967/2164 (91%)	1967 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	20	ASN
2	3	27	HIS
2	A	27	HIS
3	C	85	ASN
3	C	176	ASN
3	C	225	ASN

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Mol	Chain	Res	Type
3	C	226	GLN
1	I	22	GLN
4	L	183	HIS
5	M	404	ASN
5	M	582	ASN
2	P	27	HIS
2	P	37	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 93 ligands modelled in this entry, 1 is monoatomic - leaving 92 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	N	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.39	7 (8%)
10	KGD	1	102	-	41,41,41	1.25	1 (2%)	49,53,53	2.03	15 (30%)
9	BCL	S	102	1	69,74,74	1.11	5 (7%)	83,115,115	1.37	9 (10%)
10	KGD	A	102	-	41,41,41	1.00	2 (4%)	49,53,53	1.49	10 (20%)
10	KGD	7	102	-	41,41,41	1.05	3 (7%)	49,53,53	1.62	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	KGD	H	102	-	41,41,41	1.04	1 (2%)	49,53,53	1.68	7 (14%)
9	BCL	U	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
9	BCL	F	101	2	69,74,74	1.13	6 (8%)	83,115,115	1.39	8 (9%)
13	BPH	L	1006	-	59,70,70	1.00	3 (5%)	61,101,101	1.42	6 (9%)
10	KGD	J	103	-	41,41,41	2.15	15 (36%)	49,53,53	1.34	6 (12%)
15	MQE	M	704	-	25,25,69	0.49	0	31,34,87	0.94	2 (6%)
9	BCL	L	1002	4	69,74,74	1.14	5 (7%)	83,115,115	1.34	8 (9%)
12	PGV	L	1007	-	29,29,50	0.61	0	32,35,56	0.59	0
10	KGD	E	103	-	41,41,41	1.05	1 (2%)	49,53,53	1.73	11 (22%)
9	BCL	U	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.36	8 (9%)
10	KGD	P	102	-	41,41,41	1.01	1 (2%)	49,53,53	1.50	10 (20%)
9	BCL	K	102	1	69,74,74	1.80	19 (27%)	83,115,115	2.42	23 (27%)
10	KGD	0	103	-	41,41,41	1.03	1 (2%)	49,53,53	1.56	8 (16%)
9	BCL	G	101	1	69,74,74	1.12	4 (5%)	83,115,115	1.39	10 (12%)
9	BCL	8	102	1	69,74,74	1.10	6 (8%)	83,115,115	1.41	8 (9%)
9	BCL	2	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	7 (8%)
9	BCL	H	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.41	8 (9%)
9	BCL	V	101	2	69,74,74	1.16	5 (7%)	83,115,115	1.39	7 (8%)
10	KGD	1	103	-	41,41,41	1.17	3 (7%)	49,53,53	1.81	14 (28%)
10	KGD	G	102	-	41,41,41	0.99	2 (4%)	49,53,53	1.93	8 (16%)
11	HEM	C	504	3	50,50,50	1.24	3 (6%)	66,82,82	1.10	2 (3%)
9	BCL	B	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.35	9 (10%)
9	BCL	L	1001	4	69,74,74	1.15	5 (7%)	83,115,115	1.42	6 (7%)
10	KGD	8	103	-	41,41,41	1.16	4 (9%)	49,53,53	1.85	13 (26%)
9	BCL	3	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.37	8 (9%)
9	BCL	4	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	8 (9%)
10	KGD	C	505	-	41,41,41	0.96	1 (2%)	49,53,53	1.57	10 (20%)
9	BCL	I	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.42	11 (13%)
9	BCL	7	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.38	7 (8%)
10	KGD	I	103	-	41,41,41	1.21	1 (2%)	49,53,53	2.21	15 (30%)
9	BCL	5	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.42	9 (10%)
9	BCL	E	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	9 (10%)
15	MQE	M	701	-	69,69,69	0.31	0	84,87,87	0.61	2 (2%)
10	KGD	Q	103	-	41,41,41	1.01	2 (4%)	49,53,53	1.61	10 (20%)
9	BCL	0	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	8	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.41	9 (10%)
11	HEM	C	503	3	50,50,50	1.22	5 (10%)	66,82,82	1.09	5 (7%)
10	KGD	D	103	-	41,41,41	0.91	1 (2%)	49,53,53	1.60	12 (24%)
9	BCL	R	101	2	69,74,74	1.13	6 (8%)	83,115,115	1.38	7 (8%)
9	BCL	T	101	2	69,74,74	1.13	5 (7%)	83,115,115	1.37	8 (9%)
9	BCL	W	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.36	7 (8%)
10	KGD	0	104	-	41,41,41	1.10	1 (2%)	49,53,53	1.46	7 (14%)
9	BCL	6	102	1	69,74,74	1.13	4 (5%)	83,115,115	1.37	9 (10%)
9	BCL	B	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.35	9 (10%)
9	BCL	4	102	1	69,74,74	1.10	4 (5%)	83,115,115	1.39	10 (12%)
9	BCL	6	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.42	9 (10%)
9	BCL	0	102	1	69,74,74	1.11	4 (5%)	83,115,115	1.35	8 (9%)
12	PGV	C	507	-	44,44,50	0.51	0	47,50,56	0.69	1 (2%)
10	KGD	K	103	-	41,41,41	1.03	1 (2%)	49,53,53	1.80	9 (18%)
13	BPH	M	703	-	59,70,70	1.00	3 (5%)	61,101,101	1.36	4 (6%)
13	BPH	L	1003	-	59,70,70	1.01	2 (3%)	61,101,101	1.46	7 (11%)
9	BCL	P	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.32	7 (8%)
9	BCL	I	102	1	69,74,74	1.11	5 (7%)	83,115,115	1.36	9 (10%)
9	BCL	A	101	2	69,74,74	1.13	4 (5%)	83,115,115	1.35	7 (8%)
9	BCL	K	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
11	HEM	C	501	3	50,50,50	1.21	4 (8%)	66,82,82	1.11	5 (7%)
9	BCL	J	101	2	69,74,74	1.13	5 (7%)	83,115,115	1.40	7 (8%)
10	KGD	U	103	-	41,41,41	1.26	3 (7%)	49,53,53	1.96	15 (30%)
11	HEM	C	502	3	50,50,50	1.30	4 (8%)	66,82,82	1.15	5 (7%)
10	KGD	S	103	-	41,41,41	1.17	1 (2%)	49,53,53	1.77	10 (20%)
9	BCL	S	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.37	8 (9%)
9	BCL	F	102	1	69,74,74	1.14	5 (7%)	83,115,115	1.39	10 (12%)
10	KGD	J	102	-	41,41,41	1.12	1 (2%)	49,53,53	1.66	12 (24%)
9	BCL	O	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.37	9 (10%)
9	BCL	W	102	1	69,74,74	1.79	18 (26%)	83,115,115	2.46	25 (30%)
9	BCL	2	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.35	7 (8%)
9	BCL	D	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.38	7 (8%)
9	BCL	M	702	5	69,74,74	1.15	5 (7%)	83,115,115	1.43	8 (9%)
10	KGD	O	103	-	41,41,41	0.99	1 (2%)	49,53,53	1.68	10 (20%)
9	BCL	E	102	1	69,74,74	1.10	5 (7%)	83,115,115	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	KGD	5	102	-	41,41,41	1.12	1 (2%)	49,53,53	1.61	9 (18%)
10	KGD	2	103	-	41,41,41	0.95	2 (4%)	49,53,53	1.58	10 (20%)
9	BCL	9	101	2	69,74,74	1.14	4 (5%)	83,115,115	1.41	7 (8%)
10	KGD	R	102	-	41,41,41	1.15	1 (2%)	49,53,53	1.76	11 (22%)
12	PGV	L	1008	-	41,41,50	0.54	0	44,47,56	0.52	0
10	KGD	C	506	-	41,41,41	1.47	6 (14%)	49,53,53	1.59	7 (14%)
15	MQE	L	1005	-	69,69,69	0.30	0	84,87,87	0.48	1 (1%)
9	BCL	Q	101	1	69,74,74	1.10	5 (7%)	83,115,115	1.34	7 (8%)
10	KGD	B	103	-	41,41,41	1.16	2 (4%)	49,53,53	2.18	11 (22%)
9	BCL	Q	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
9	BCL	1	101	2	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
10	KGD	D	102	-	41,41,41	0.95	1 (2%)	49,53,53	1.48	9 (18%)
10	KGD	6	103	-	41,41,41	1.24	2 (4%)	49,53,53	1.99	12 (24%)
12	PGV	L	1009	-	34,34,50	0.57	0	37,40,56	0.54	0
10	KGD	S	104	-	41,41,41	1.10	1 (2%)	49,53,53	1.72	14 (28%)
10	KGD	4	103	-	41,41,41	1.46	2 (4%)	49,53,53	2.06	9 (18%)
9	BCL	O	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.54	9 (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	N	101	2	-	6/41/137/137	-
10	KGD	1	102	-	-	5/36/56/56	0/1/1/1
9	BCL	S	102	1	-	4/41/137/137	-
10	KGD	A	102	-	-	3/36/56/56	0/1/1/1
10	KGD	7	102	-	-	4/36/56/56	0/1/1/1
10	KGD	H	102	-	-	3/36/56/56	0/1/1/1
9	BCL	U	102	1	-	4/41/137/137	-
9	BCL	F	101	2	-	4/41/137/137	-
13	BPH	L	1006	-	-	16/37/105/105	0/5/6/6
10	KGD	J	103	-	-	4/36/56/56	0/1/1/1
15	MQE	M	704	-	-	2/13/33/85	0/2/2/2
9	BCL	L	1002	4	-	5/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGV	L	1007	-	-	12/34/34/55	-
10	KGD	E	103	-	-	5/36/56/56	0/1/1/1
9	BCL	U	101	1	-	9/41/137/137	-
10	KGD	P	102	-	-	2/36/56/56	0/1/1/1
9	BCL	K	102	1	-	22/41/137/137	-
10	KGD	O	103	-	-	0/36/56/56	0/1/1/1
9	BCL	G	101	1	-	4/41/137/137	-
9	BCL	8	102	1	-	3/41/137/137	-
9	BCL	2	101	1	-	4/41/137/137	-
9	BCL	H	101	2	-	3/41/137/137	-
9	BCL	V	101	2	-	4/41/137/137	-
10	KGD	1	103	-	-	4/36/56/56	0/1/1/1
10	KGD	G	102	-	-	7/36/56/56	0/1/1/1
11	HEM	C	504	3	-	6/14/54/54	-
9	BCL	B	101	1	-	4/41/137/137	-
9	BCL	L	1001	4	-	3/41/137/137	-
10	KGD	8	103	-	-	4/36/56/56	0/1/1/1
9	BCL	3	101	2	-	4/41/137/137	-
9	BCL	4	101	1	-	7/41/137/137	-
10	KGD	C	505	-	-	4/36/56/56	0/1/1/1
9	BCL	I	101	1	-	6/41/137/137	-
9	BCL	7	101	2	-	7/41/137/137	-
10	KGD	I	103	-	-	4/36/56/56	0/1/1/1
9	BCL	5	101	2	-	7/41/137/137	-
9	BCL	E	101	1	-	8/41/137/137	-
15	MQE	M	701	-	-	19/65/85/85	0/2/2/2
10	KGD	Q	103	-	-	4/36/56/56	0/1/1/1
9	BCL	O	101	1	-	4/41/137/137	-
9	BCL	8	101	1	-	2/41/137/137	-
11	HEM	C	503	3	-	9/14/54/54	-
10	KGD	D	103	-	-	3/36/56/56	0/1/1/1
9	BCL	R	101	2	-	7/41/137/137	-
9	BCL	T	101	2	-	4/41/137/137	-
9	BCL	W	101	1	-	4/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	KGD	0	104	-	-	4/36/56/56	0/1/1/1
9	BCL	6	102	1	-	2/41/137/137	-
9	BCL	B	102	1	-	3/41/137/137	-
9	BCL	4	102	1	-	2/41/137/137	-
9	BCL	6	101	1	-	7/41/137/137	-
9	BCL	0	102	1	-	2/41/137/137	-
12	PGV	C	507	-	-	18/49/49/55	-
10	KGD	K	103	-	-	7/36/56/56	0/1/1/1
13	BPH	M	703	-	-	20/37/105/105	0/5/6/6
13	BPH	L	1003	-	-	18/37/105/105	0/5/6/6
9	BCL	P	101	2	-	3/41/137/137	-
9	BCL	I	102	1	-	4/41/137/137	-
9	BCL	A	101	2	-	5/41/137/137	-
9	BCL	K	101	1	-	7/41/137/137	-
11	HEM	C	501	3	-	4/14/54/54	-
9	BCL	J	101	2	-	7/41/137/137	-
10	KGD	U	103	-	-	4/36/56/56	0/1/1/1
11	HEM	C	502	3	-	7/14/54/54	-
10	KGD	S	103	-	-	12/36/56/56	0/1/1/1
9	BCL	S	101	1	-	5/41/137/137	-
9	BCL	F	102	1	-	2/41/137/137	-
10	KGD	J	102	-	-	6/36/56/56	0/1/1/1
9	BCL	O	102	1	-	4/41/137/137	-
9	BCL	W	102	1	-	18/41/137/137	-
9	BCL	2	102	1	-	10/41/137/137	-
9	BCL	D	101	2	-	6/41/137/137	-
9	BCL	M	702	5	-	4/41/137/137	-
10	KGD	O	103	-	-	4/36/56/56	0/1/1/1
9	BCL	E	102	1	-	6/41/137/137	-
10	KGD	5	102	-	-	4/36/56/56	0/1/1/1
10	KGD	2	103	-	-	8/36/56/56	0/1/1/1
9	BCL	9	101	2	-	7/41/137/137	-
10	KGD	R	102	-	-	4/36/56/56	0/1/1/1
12	PGV	L	1008	-	-	18/46/46/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	KGD	C	506	-	-	6/36/56/56	0/1/1/1
15	MQE	L	1005	-	-	9/65/85/85	0/2/2/2
9	BCL	Q	101	1	-	5/41/137/137	-
10	KGD	B	103	-	-	9/36/56/56	0/1/1/1
9	BCL	Q	102	1	-	4/41/137/137	-
9	BCL	1	101	2	-	8/41/137/137	-
10	KGD	D	102	-	-	6/36/56/56	0/1/1/1
10	KGD	6	103	-	-	6/36/56/56	0/1/1/1
12	PGV	L	1009	-	-	15/39/39/55	-
10	KGD	S	104	-	-	7/36/56/56	0/1/1/1
10	KGD	4	103	-	-	3/36/56/56	0/1/1/1
9	BCL	O	101	1	-	6/41/137/137	-

All (349) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	103	KGD	CAG-CAB	-5.70	1.42	1.53
10	4	103	KGD	CAB-CAD	-5.55	1.46	1.53
9	L	1001	BCL	MG-NA	5.08	2.18	2.06
9	M	702	BCL	MG-NA	5.07	2.18	2.06
9	W	102	BCL	O2D-CGD	5.02	1.45	1.33
9	V	101	BCL	MG-NA	5.01	2.18	2.06
9	P	101	BCL	MG-NA	4.94	2.18	2.06
9	H	101	BCL	MG-NA	4.92	2.17	2.06
9	T	101	BCL	MG-NA	4.90	2.17	2.06
9	6	102	BCL	MG-NA	4.89	2.17	2.06
9	U	102	BCL	MG-NA	4.88	2.17	2.06
9	W	101	BCL	MG-NA	4.87	2.17	2.06
9	L	1002	BCL	MG-NA	4.87	2.17	2.06
9	F	102	BCL	MG-NA	4.85	2.17	2.06
9	K	102	BCL	C3D-C4D	-4.85	1.33	1.44
9	9	101	BCL	MG-NA	4.85	2.17	2.06
9	A	101	BCL	MG-NA	4.85	2.17	2.06
10	R	102	KGD	CAB-CAD	-4.84	1.47	1.53
9	U	101	BCL	MG-NA	4.82	2.17	2.06
10	5	102	KGD	CAB-CAD	-4.82	1.47	1.53
9	3	101	BCL	MG-NA	4.82	2.17	2.06
9	G	101	BCL	MG-NA	4.82	2.17	2.06
9	2	102	BCL	MG-NA	4.81	2.17	2.06
9	B	101	BCL	MG-NA	4.81	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	BCL	MG-NA	4.81	2.17	2.06
9	1	101	BCL	MG-NA	4.80	2.17	2.06
9	O	101	BCL	MG-NA	4.80	2.17	2.06
9	K	101	BCL	MG-NA	4.80	2.17	2.06
9	B	102	BCL	MG-NA	4.80	2.17	2.06
9	Q	101	BCL	MG-NA	4.80	2.17	2.06
9	7	101	BCL	MG-NA	4.79	2.17	2.06
9	O	102	BCL	MG-NA	4.78	2.17	2.06
9	K	102	BCL	O2D-CGD	4.78	1.44	1.33
9	R	101	BCL	MG-NA	4.78	2.17	2.06
9	N	101	BCL	MG-NA	4.78	2.17	2.06
9	0	101	BCL	MG-NA	4.76	2.17	2.06
9	E	102	BCL	MG-NA	4.76	2.17	2.06
9	8	101	BCL	MG-NA	4.75	2.17	2.06
9	S	101	BCL	MG-NA	4.74	2.17	2.06
9	4	101	BCL	MG-NA	4.74	2.17	2.06
9	J	101	BCL	MG-NA	4.74	2.17	2.06
9	S	102	BCL	MG-NA	4.73	2.17	2.06
9	Q	102	BCL	MG-NA	4.73	2.17	2.06
10	J	103	KGD	CAZ-CAW	-4.72	1.38	1.50
9	5	101	BCL	MG-NA	4.71	2.17	2.06
9	I	101	BCL	MG-NA	4.71	2.17	2.06
9	6	101	BCL	MG-NA	4.70	2.17	2.06
9	0	102	BCL	MG-NA	4.69	2.17	2.06
10	J	103	KGD	CAF-CAB	-4.69	1.44	1.53
9	W	102	BCL	C3D-C4D	-4.68	1.33	1.44
13	L	1003	BPH	C1B-C2B	4.68	1.44	1.39
9	D	101	BCL	MG-NA	4.68	2.17	2.06
9	2	101	BCL	MG-NA	4.65	2.17	2.06
9	E	101	BCL	MG-NA	4.65	2.17	2.06
13	M	703	BPH	C1B-C2B	4.63	1.44	1.39
9	I	102	BCL	MG-NA	4.62	2.17	2.06
9	4	102	BCL	MG-NA	4.60	2.17	2.06
9	8	102	BCL	MG-NA	4.56	2.17	2.06
10	U	103	KGD	CAB-CAD	-4.53	1.47	1.53
9	W	102	BCL	O2A-CGA	4.51	1.46	1.33
13	L	1006	BPH	C1B-C2B	4.47	1.44	1.39
10	0	104	KGD	CAB-CAD	-4.46	1.47	1.53
9	K	102	BCL	O2A-CGA	4.43	1.46	1.33
10	6	103	KGD	CAB-CAD	-4.36	1.47	1.53
10	J	103	KGD	CBD-CAY	-4.34	1.38	1.50
10	H	102	KGD	CAB-CAD	-4.30	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	103	KGD	CAN-CAM	-4.26	1.42	1.50
10	I	103	KGD	CAB-CAD	-4.23	1.48	1.53
10	S	104	KGD	CAB-CAD	-4.20	1.48	1.53
10	J	102	KGD	CAB-CAD	-4.17	1.48	1.53
10	1	102	KGD	CAB-CAD	-4.10	1.48	1.53
10	C	506	KGD	CBK-CBH	-4.04	1.42	1.50
10	C	506	KGD	CAG-CAB	-3.96	1.46	1.53
10	O	103	KGD	CAB-CAD	-3.92	1.48	1.53
13	L	1003	BPH	C4D-ND	-3.85	1.33	1.38
13	L	1006	BPH	C4D-ND	-3.82	1.33	1.38
9	V	101	BCL	MG-NC	3.80	2.15	2.06
9	K	102	BCL	CHD-C1D	3.78	1.45	1.38
10	0	103	KGD	CAB-CAD	-3.77	1.48	1.53
9	P	101	BCL	MG-NC	3.77	2.15	2.06
10	B	103	KGD	CAE-CAI	-3.76	1.45	1.50
13	M	703	BPH	C4D-ND	-3.76	1.33	1.38
9	K	102	BCL	C3B-C4B	3.71	1.48	1.41
9	3	101	BCL	MG-NC	3.70	2.15	2.06
9	W	102	BCL	CHD-C1D	3.69	1.45	1.38
9	L	1001	BCL	MG-NC	3.65	2.14	2.06
9	1	101	BCL	MG-NC	3.62	2.14	2.06
10	J	103	KGD	CBK-CBH	-3.62	1.43	1.50
9	T	101	BCL	MG-NC	3.61	2.14	2.06
10	E	103	KGD	CAB-CAD	-3.59	1.48	1.53
9	A	101	BCL	MG-NC	3.58	2.14	2.06
9	H	101	BCL	MG-NC	3.54	2.14	2.06
10	K	103	KGD	CAB-CAD	-3.53	1.48	1.53
9	W	101	BCL	MG-NC	3.51	2.14	2.06
9	J	101	BCL	MG-NC	3.50	2.14	2.06
9	9	101	BCL	MG-NC	3.50	2.14	2.06
9	7	101	BCL	MG-NC	3.50	2.14	2.06
9	D	101	BCL	MG-NC	3.48	2.14	2.06
10	J	103	KGD	CAS-CAW	-3.46	1.44	1.51
9	K	102	BCL	CHB-C1B	3.46	1.47	1.39
9	5	101	BCL	MG-NC	3.45	2.14	2.06
9	L	1002	BCL	MG-NC	3.43	2.14	2.06
9	W	102	BCL	C3B-C4B	3.43	1.47	1.41
9	N	101	BCL	MG-NC	3.42	2.14	2.06
9	U	102	BCL	MG-NC	3.40	2.14	2.06
10	S	103	KGD	CAB-CAD	-3.40	1.49	1.53
9	B	101	BCL	MG-NC	3.40	2.14	2.06
9	R	101	BCL	MG-NC	3.40	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	102	BCL	MG-NC	3.40	2.14	2.06
9	S	102	BCL	MG-NC	3.39	2.14	2.06
9	F	101	BCL	MG-NC	3.39	2.14	2.06
9	K	101	BCL	MG-NC	3.38	2.14	2.06
9	S	101	BCL	MG-NC	3.38	2.14	2.06
9	0	101	BCL	MG-NC	3.37	2.14	2.06
9	2	102	BCL	MG-NC	3.36	2.14	2.06
9	G	101	BCL	MG-NC	3.35	2.14	2.06
10	1	103	KGD	CAB-CAD	-3.35	1.49	1.53
9	U	101	BCL	MG-NC	3.35	2.14	2.06
9	F	102	BCL	MG-NC	3.34	2.14	2.06
9	B	102	BCL	MG-NC	3.34	2.14	2.06
9	W	102	BCL	C4B-NB	-3.30	1.33	1.37
9	W	102	BCL	CHB-C1B	3.30	1.46	1.39
9	M	702	BCL	MG-NC	3.29	2.14	2.06
9	O	101	BCL	MG-NC	3.29	2.14	2.06
9	W	102	BCL	OBD-CAD	3.28	1.28	1.22
10	J	103	KGD	CAE-CAI	-3.26	1.46	1.50
9	6	101	BCL	MG-NC	3.26	2.14	2.06
9	0	102	BCL	MG-NC	3.26	2.14	2.06
9	Q	102	BCL	MG-NC	3.26	2.14	2.06
9	O	102	BCL	MG-NC	3.24	2.14	2.06
9	E	102	BCL	MG-NC	3.24	2.14	2.06
9	I	101	BCL	MG-NC	3.23	2.13	2.06
9	2	101	BCL	MG-NC	3.22	2.13	2.06
9	4	101	BCL	MG-NC	3.21	2.13	2.06
9	Q	101	BCL	MG-NC	3.21	2.13	2.06
9	E	101	BCL	MG-NC	3.20	2.13	2.06
9	8	101	BCL	MG-NC	3.20	2.13	2.06
10	1	103	KGD	CAE-CAI	-3.19	1.46	1.50
9	I	102	BCL	MG-NC	3.13	2.13	2.06
9	8	102	BCL	MG-NC	3.13	2.13	2.06
10	C	506	KGD	CAE-CAI	-3.12	1.46	1.50
10	J	103	KGD	OAA-CAI	-3.10	1.16	1.23
10	2	103	KGD	CAB-CAD	-3.10	1.49	1.53
9	W	102	BCL	CHC-C4B	3.08	1.46	1.39
9	K	102	BCL	C4B-NB	-3.08	1.34	1.37
9	K	102	BCL	OBD-CAD	3.06	1.27	1.22
9	K	102	BCL	CHC-C4B	3.06	1.46	1.39
10	U	103	KGD	CAF-CAB	-3.04	1.47	1.53
9	4	102	BCL	MG-NC	2.99	2.13	2.06
10	7	102	KGD	CAB-CAD	-2.99	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	501	HEM	CAC-C3C	2.97	1.55	1.47
11	C	504	HEM	CAB-C3B	2.96	1.55	1.47
11	C	502	HEM	CAC-C3C	2.96	1.55	1.47
10	J	103	KGD	CAU-CAR	-2.95	1.44	1.50
9	B	102	BCL	C3B-C4B	2.94	1.46	1.41
9	W	102	BCL	C3D-C2D	2.94	1.47	1.39
11	C	504	HEM	CAC-C3C	2.94	1.55	1.47
11	C	503	HEM	CAC-C3C	2.91	1.55	1.47
9	6	102	BCL	C3B-C4B	2.90	1.46	1.41
11	C	502	HEM	CAB-C3B	2.90	1.55	1.47
9	4	102	BCL	C3B-C4B	2.89	1.46	1.41
9	O	102	BCL	C3B-C4B	2.85	1.46	1.41
9	G	101	BCL	C3B-C4B	2.85	1.46	1.41
9	E	101	BCL	C3B-C4B	2.83	1.46	1.41
11	C	501	HEM	CAB-C3B	2.83	1.55	1.47
9	0	102	BCL	C3B-C4B	2.82	1.46	1.41
9	W	102	BCL	CHD-C4C	2.82	1.47	1.39
9	K	102	BCL	C1B-NB	-2.82	1.34	1.37
9	L	1002	BCL	C3B-C4B	2.81	1.46	1.41
9	I	102	BCL	C3B-C4B	2.80	1.46	1.41
9	K	102	BCL	C3D-C2D	2.80	1.46	1.39
9	K	102	BCL	C1D-ND	-2.79	1.34	1.37
10	J	103	KGD	CAC-CAB	-2.79	1.47	1.54
9	Q	102	BCL	C3B-C4B	2.78	1.46	1.41
9	K	102	BCL	CHD-C4C	2.77	1.47	1.39
11	C	504	HEM	C1B-NB	-2.76	1.35	1.40
9	W	102	BCL	C1B-NB	-2.76	1.34	1.37
9	W	102	BCL	C1D-ND	-2.74	1.34	1.37
9	H	101	BCL	C3B-C4B	2.72	1.46	1.41
10	P	102	KGD	CAB-CAD	-2.70	1.50	1.53
11	C	503	HEM	CAB-C3B	2.70	1.54	1.47
10	B	103	KGD	CAB-CAD	-2.70	1.50	1.53
9	S	102	BCL	C3B-C4B	2.69	1.46	1.41
9	S	101	BCL	C3B-C4B	2.69	1.46	1.41
9	I	101	BCL	C3B-C4B	2.68	1.46	1.41
9	F	102	BCL	C3B-C4B	2.68	1.46	1.41
9	M	702	BCL	C3B-C4B	2.66	1.46	1.41
9	3	101	BCL	C3B-C4B	2.65	1.46	1.41
9	F	101	BCL	C3B-C4B	2.65	1.46	1.41
9	4	101	BCL	C3B-C4B	2.65	1.46	1.41
9	8	101	BCL	C3B-C4B	2.64	1.46	1.41
10	A	102	KGD	CAE-CAI	-2.64	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	506	KGD	CAS-CAW	-2.63	1.45	1.51
9	A	101	BCL	C3B-C4B	2.62	1.45	1.41
10	A	102	KGD	CAB-CAD	-2.61	1.50	1.53
9	6	101	BCL	C3B-C4B	2.60	1.45	1.41
10	G	102	KGD	CAE-CAI	-2.59	1.47	1.50
9	0	101	BCL	C3B-C4B	2.59	1.45	1.41
9	K	102	BCL	MG-NA	-2.57	2.00	2.06
9	O	101	BCL	C3B-C4B	2.57	1.45	1.41
9	U	101	BCL	C3B-C4B	2.56	1.45	1.41
9	2	101	BCL	C3B-C4B	2.55	1.45	1.41
9	V	101	BCL	C3B-C4B	2.55	1.45	1.41
9	K	101	BCL	C3B-C4B	2.55	1.45	1.41
9	U	102	BCL	C3B-C4B	2.54	1.45	1.41
9	W	102	BCL	C1D-C2D	2.54	1.50	1.45
9	1	101	BCL	C3B-C4B	2.53	1.45	1.41
9	L	1001	BCL	C3B-C4B	2.52	1.45	1.41
11	C	502	HEM	C4A-NA	-2.52	1.34	1.39
9	J	101	BCL	C3B-C4B	2.52	1.45	1.41
9	T	101	BCL	C3B-C4B	2.52	1.45	1.41
9	K	102	BCL	C1B-C2B	2.50	1.49	1.43
9	2	101	BCL	CHD-C1D	2.50	1.43	1.38
9	R	101	BCL	C3B-C4B	2.49	1.45	1.41
9	K	102	BCL	C1D-C2D	2.47	1.50	1.45
9	8	102	BCL	C3B-C4B	2.47	1.45	1.41
9	9	101	BCL	C3B-C4B	2.46	1.45	1.41
10	D	103	KGD	CAB-CAD	-2.46	1.50	1.53
9	W	101	BCL	C3B-C4B	2.46	1.45	1.41
9	D	101	BCL	C3B-C4B	2.45	1.45	1.41
9	L	1001	BCL	CHD-C1D	2.44	1.43	1.38
10	C	506	KGD	CAK-CAH	-2.44	1.45	1.50
9	W	102	BCL	MG-NA	-2.44	2.00	2.06
9	B	101	BCL	CHD-C1D	2.43	1.43	1.38
9	0	101	BCL	CHD-C1D	2.42	1.43	1.38
9	B	101	BCL	C3B-C4B	2.42	1.45	1.41
9	Q	101	BCL	C3B-C4B	2.42	1.45	1.41
10	U	103	KGD	CBK-CBH	-2.42	1.45	1.50
10	D	102	KGD	CAE-CAI	-2.41	1.47	1.50
10	C	506	KGD	OAA-CAI	-2.41	1.18	1.23
9	8	101	BCL	CHD-C1D	2.41	1.43	1.38
9	6	101	BCL	CHD-C1D	2.41	1.43	1.38
9	O	101	BCL	CHD-C1D	2.40	1.43	1.38
9	U	101	BCL	CHD-C1D	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	102	BCL	C3B-C4B	2.40	1.45	1.41
9	E	101	BCL	CHD-C1D	2.39	1.43	1.38
9	2	102	BCL	CHD-C1D	2.38	1.43	1.38
9	E	102	BCL	CHD-C1D	2.38	1.43	1.38
9	N	101	BCL	CHD-C1D	2.38	1.43	1.38
9	4	101	BCL	CHD-C1D	2.36	1.43	1.38
9	N	101	BCL	C3B-C4B	2.36	1.45	1.41
9	J	101	BCL	CHD-C1D	2.35	1.42	1.38
9	I	101	BCL	CHD-C1D	2.34	1.42	1.38
9	R	101	BCL	CHD-C1D	2.34	1.42	1.38
9	Q	101	BCL	CHD-C1D	2.34	1.42	1.38
9	F	102	BCL	CHD-C1D	2.32	1.42	1.38
10	G	102	KGD	CAB-CAD	-2.32	1.50	1.53
9	5	101	BCL	C3B-C4B	2.32	1.45	1.41
9	S	102	BCL	CHD-C1D	2.32	1.42	1.38
9	9	101	BCL	CHD-C1D	2.32	1.42	1.38
9	O	102	BCL	CHD-C1D	2.31	1.42	1.38
9	7	101	BCL	CHD-C1D	2.31	1.42	1.38
9	E	102	BCL	C3B-C4B	2.30	1.45	1.41
13	L	1006	BPH	C3B-C4B	2.30	1.45	1.41
10	7	102	KGD	CAE-CAI	-2.29	1.47	1.50
9	G	101	BCL	CHD-C1D	2.28	1.42	1.38
9	D	101	BCL	CHD-C1D	2.28	1.42	1.38
10	J	103	KGD	CAK-CAH	-2.28	1.46	1.50
9	F	101	BCL	CHD-C1D	2.28	1.42	1.38
9	P	101	BCL	CHD-C1D	2.27	1.42	1.38
9	W	101	BCL	CHD-C1D	2.27	1.42	1.38
9	W	102	BCL	C1B-C2B	2.27	1.48	1.43
10	8	103	KGD	CAS-CAW	-2.27	1.46	1.51
9	S	101	BCL	CHD-C1D	2.27	1.42	1.38
10	Q	103	KGD	CAB-CAD	-2.26	1.50	1.53
9	5	101	BCL	CHD-C1D	2.26	1.42	1.38
9	A	101	BCL	CHD-C1D	2.26	1.42	1.38
9	H	101	BCL	CHD-C1D	2.26	1.42	1.38
9	U	102	BCL	CHD-C1D	2.25	1.42	1.38
13	M	703	BPH	C3B-C4B	2.25	1.45	1.41
9	8	102	BCL	CHD-C1D	2.25	1.42	1.38
9	M	702	BCL	CHD-C1D	2.24	1.42	1.38
10	J	103	KGD	CAB-CAD	-2.24	1.50	1.53
9	T	101	BCL	CHD-C1D	2.24	1.42	1.38
9	1	101	BCL	CHD-C1D	2.23	1.42	1.38
9	W	102	BCL	MG-NC	-2.23	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	101	BCL	C3B-C4B	2.23	1.45	1.41
9	K	102	BCL	MG-NC	-2.21	2.01	2.06
9	I	102	BCL	CHD-C1D	2.20	1.42	1.38
9	K	101	BCL	CHD-C1D	2.20	1.42	1.38
9	3	101	BCL	CHD-C1D	2.20	1.42	1.38
9	6	102	BCL	CHD-C1D	2.19	1.42	1.38
10	J	103	KGD	CBO-CBL	-2.18	1.46	1.50
9	M	702	BCL	C3D-C4D	-2.17	1.39	1.44
9	P	101	BCL	C3B-C4B	2.17	1.45	1.41
9	B	102	BCL	CHD-C1D	2.16	1.42	1.38
10	J	103	KGD	CAT-CAX	-2.15	1.43	1.50
9	K	102	BCL	CHC-C1C	-2.15	1.32	1.37
9	V	101	BCL	CHD-C1D	2.15	1.42	1.38
9	Q	102	BCL	CHD-C1D	2.15	1.42	1.38
10	C	505	KGD	CAB-CAD	-2.15	1.50	1.53
9	0	102	BCL	CHD-C1D	2.14	1.42	1.38
10	Q	103	KGD	CAE-CAI	-2.13	1.48	1.50
10	7	102	KGD	CAC-CAB	-2.12	1.49	1.54
9	U	101	BCL	C3D-C4D	-2.10	1.39	1.44
11	C	502	HEM	C2A-C3A	-2.10	1.33	1.38
9	4	102	BCL	CHD-C1D	2.10	1.42	1.38
10	6	103	KGD	CAF-CAB	-2.09	1.49	1.53
9	8	102	BCL	C1D-ND	2.09	1.40	1.37
10	8	103	KGD	CAE-CAI	-2.08	1.48	1.50
11	C	501	HEM	CMC-C2C	2.08	1.55	1.50
9	S	101	BCL	C3D-C4D	-2.07	1.39	1.44
9	2	102	BCL	C3D-C4D	-2.07	1.39	1.44
9	4	101	BCL	C3D-C4D	-2.07	1.39	1.44
9	J	101	BCL	C1D-ND	2.06	1.40	1.37
9	I	102	BCL	C3D-C4D	-2.06	1.39	1.44
9	E	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	O	102	BCL	C3D-C4D	-2.06	1.39	1.44
9	L	1002	BCL	CHD-C1D	2.06	1.42	1.38
9	2	101	BCL	C3D-C4D	-2.06	1.39	1.44
9	W	102	BCL	CHC-C1C	-2.05	1.32	1.37
10	8	103	KGD	CBJ-CBH	-2.05	1.33	1.35
9	3	101	BCL	C3D-C4D	-2.05	1.39	1.44
9	1	101	BCL	C3D-C4D	-2.05	1.39	1.44
9	B	101	BCL	C3D-C4D	-2.04	1.39	1.44
9	I	101	BCL	C3D-C4D	-2.04	1.39	1.44
10	8	103	KGD	CAB-CAD	-2.04	1.51	1.53
9	F	102	BCL	C3D-C4D	-2.04	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	1001	BCL	C3D-C4D	-2.04	1.39	1.44
11	C	503	HEM	CMC-C2C	2.04	1.55	1.50
9	L	1002	BCL	C1D-C2D	-2.04	1.41	1.45
9	Q	101	BCL	C3D-C4D	-2.04	1.39	1.44
11	C	503	HEM	CMB-C2B	2.03	1.55	1.50
9	K	101	BCL	C3D-C4D	-2.03	1.39	1.44
9	E	102	BCL	C3D-C4D	-2.03	1.39	1.44
9	O	101	BCL	C3D-C4D	-2.03	1.39	1.44
10	1	103	KGD	CAS-CAW	-2.03	1.47	1.51
9	P	101	BCL	C3D-C4D	-2.03	1.39	1.44
9	U	102	BCL	C3D-C4D	-2.03	1.39	1.44
9	V	101	BCL	C3D-C4D	-2.02	1.39	1.44
10	2	103	KGD	CAE-CAI	-2.02	1.48	1.50
9	S	102	BCL	C3D-C4D	-2.02	1.39	1.44
9	F	101	BCL	C1D-ND	2.02	1.40	1.37
9	0	101	BCL	C3D-C4D	-2.02	1.39	1.44
9	W	101	BCL	C3D-C4D	-2.02	1.39	1.44
9	H	101	BCL	C1D-ND	2.02	1.40	1.37
9	Q	102	BCL	C3D-C4D	-2.01	1.39	1.44
10	J	103	KGD	CAS-CAT	-2.01	1.46	1.53
9	B	102	BCL	C3D-C4D	-2.01	1.39	1.44
9	T	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	F	101	BCL	C3D-C4D	-2.01	1.39	1.44
9	K	102	BCL	C4D-CHA	2.01	1.45	1.38
9	R	101	BCL	C1D-ND	2.01	1.40	1.37
9	8	102	BCL	C3D-C4D	-2.00	1.39	1.44
9	8	101	BCL	C3D-C4D	-2.00	1.39	1.44
9	R	101	BCL	C3D-C4D	-2.00	1.39	1.44
11	C	501	HEM	CMA-C3A	2.00	1.55	1.50
11	C	503	HEM	CMA-C3A	2.00	1.55	1.50
9	6	101	BCL	C3D-C4D	-2.00	1.39	1.44

All (774) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	102	BCL	C2B-C1B-NB	8.94	116.22	110.23
9	K	102	BCL	CHD-C1D-ND	-8.35	116.78	124.45
9	W	102	BCL	CHD-C1D-ND	-8.28	116.85	124.45
9	K	102	BCL	CMD-C2D-C1D	8.20	139.17	124.71
9	K	102	BCL	C2B-C1B-NB	7.90	115.53	110.23
9	W	102	BCL	CMD-C2D-C1D	7.83	138.52	124.71
10	B	103	KGD	CAJ-CAL-CAM	-7.59	114.76	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	103	KGD	CAP-CAO-CAM	-7.58	116.50	127.31
13	L	1006	BPH	C4D-CHA-CBD	-7.37	105.18	108.52
13	L	1003	BPH	C4D-CHA-CBD	-7.36	105.19	108.52
13	M	703	BPH	C4D-CHA-CBD	-7.01	105.34	108.52
10	4	103	KGD	CAJ-CAL-CAM	-6.56	116.32	126.23
10	I	103	KGD	CAJ-CAL-CAM	-6.53	116.37	126.23
10	G	102	KGD	CAJ-CAL-CAM	-6.52	116.39	126.23
10	B	103	KGD	CAP-CAO-CAM	-6.42	118.15	127.31
10	I	103	KGD	CAP-CAO-CAM	-6.35	118.25	127.31
9	O	101	BCL	C1-C2-C3	-6.24	115.26	126.04
10	I	103	KGD	CBG-CBI-CBL	-5.60	119.31	127.31
9	W	102	BCL	O2D-CGD-CBD	5.60	121.22	111.27
10	C	506	KGD	CAJ-CAL-CAM	-5.57	117.82	126.23
9	L	1001	BCL	CHD-C1D-ND	-5.53	119.37	124.45
9	2	101	BCL	C4D-CHA-C1A	5.44	127.87	121.25
10	G	102	KGD	CAP-CAO-CAM	-5.39	119.62	127.31
9	8	102	BCL	C4D-CHA-C1A	5.39	127.81	121.25
9	F	102	BCL	C4D-CHA-C1A	5.37	127.79	121.25
9	V	101	BCL	CHD-C1D-ND	-5.37	119.52	124.45
10	6	103	KGD	CAJ-CAL-CAM	-5.37	118.12	126.23
9	K	102	BCL	CHB-C1B-NB	-5.34	118.61	124.26
9	0	101	BCL	C4D-CHA-C1A	5.33	127.74	121.25
9	E	101	BCL	C4D-CHA-C1A	5.33	127.73	121.25
9	W	101	BCL	C4D-CHA-C1A	5.33	127.73	121.25
9	4	101	BCL	C4D-CHA-C1A	5.32	127.73	121.25
9	5	101	BCL	CHD-C1D-ND	-5.31	119.57	124.45
9	8	101	BCL	C4D-CHA-C1A	5.30	127.70	121.25
9	S	101	BCL	C4D-CHA-C1A	5.29	127.69	121.25
9	6	101	BCL	C4D-CHA-C1A	5.29	127.69	121.25
9	Q	102	BCL	C4D-CHA-C1A	5.28	127.68	121.25
9	G	101	BCL	C4D-CHA-C1A	5.28	127.68	121.25
9	S	102	BCL	C4D-CHA-C1A	5.27	127.66	121.25
9	Q	101	BCL	C4D-CHA-C1A	5.26	127.65	121.25
9	6	102	BCL	C4D-CHA-C1A	5.23	127.62	121.25
9	U	102	BCL	C4D-CHA-C1A	5.23	127.62	121.25
9	K	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
9	N	101	BCL	C4D-CHA-C1A	5.19	127.57	121.25
9	I	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
9	D	101	BCL	C4D-CHA-C1A	5.18	127.56	121.25
9	O	102	BCL	C4D-CHA-C1A	5.18	127.56	121.25
10	J	103	KGD	CAJ-CAL-CAM	-5.18	118.41	126.23
9	9	101	BCL	C4D-CHA-C1A	5.17	127.54	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	101	BCL	CHD-C1D-ND	-5.17	119.70	124.45
9	5	101	BCL	C4D-CHA-C1A	5.17	127.54	121.25
9	B	102	BCL	C4D-CHA-C1A	5.17	127.53	121.25
9	0	102	BCL	C4D-CHA-C1A	5.16	127.53	121.25
9	B	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
9	1	101	BCL	CHD-C1D-ND	-5.15	119.72	124.45
9	8	102	BCL	CHD-C1D-ND	-5.14	119.73	124.45
9	7	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
10	1	102	KGD	CAP-CAO-CAM	-5.11	120.02	127.31
9	A	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
9	F	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
9	O	101	BCL	C4D-CHA-C1A	5.11	127.46	121.25
9	H	101	BCL	C4D-CHA-C1A	5.10	127.46	121.25
9	N	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
9	K	102	BCL	O2D-CGD-CBD	5.09	120.31	111.27
9	S	101	BCL	CHD-C1D-ND	-5.08	119.79	124.45
9	U	101	BCL	CHD-C1D-ND	-5.08	119.79	124.45
9	4	102	BCL	C4D-CHA-C1A	5.08	127.43	121.25
9	3	101	BCL	CHD-C1D-ND	-5.07	119.79	124.45
9	J	101	BCL	CHD-C1D-ND	-5.07	119.80	124.45
9	2	101	BCL	CHD-C1D-ND	-5.07	119.80	124.45
9	D	101	BCL	CHD-C1D-ND	-5.06	119.80	124.45
9	8	101	BCL	CHD-C1D-ND	-5.06	119.81	124.45
9	S	102	BCL	CHD-C1D-ND	-5.06	119.81	124.45
9	E	101	BCL	CHD-C1D-ND	-5.05	119.81	124.45
9	J	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
9	Q	102	BCL	CHD-C1D-ND	-5.05	119.81	124.45
9	1	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
9	U	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
9	I	102	BCL	C4D-CHA-C1A	5.05	127.39	121.25
9	I	101	BCL	CHD-C1D-ND	-5.04	119.82	124.45
10	H	102	KGD	CAJ-CAL-CAM	-5.03	118.63	126.23
9	0	102	BCL	CHD-C1D-ND	-5.03	119.83	124.45
9	0	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
9	6	102	BCL	CHD-C1D-ND	-5.02	119.84	124.45
9	K	102	BCL	C3D-C2D-C1D	-5.02	98.99	105.83
9	6	101	BCL	CHD-C1D-ND	-5.01	119.85	124.45
9	T	101	BCL	CHD-C1D-ND	-5.01	119.85	124.45
9	7	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
9	4	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
9	W	101	BCL	CHD-C1D-ND	-4.99	119.86	124.45
9	P	101	BCL	CHD-C1D-ND	-4.99	119.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	101	BCL	CHD-C1D-ND	-4.99	119.87	124.45
9	Q	101	BCL	CHD-C1D-ND	-4.98	119.87	124.45
9	F	102	BCL	CHD-C1D-ND	-4.98	119.88	124.45
10	U	103	KGD	CBG-CBI-CBL	-4.97	120.22	127.31
9	E	102	BCL	CHD-C1D-ND	-4.96	119.89	124.45
9	G	101	BCL	CHD-C1D-ND	-4.96	119.89	124.45
9	2	102	BCL	C4D-CHA-C1A	4.95	127.27	121.25
9	9	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
9	K	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
9	V	101	BCL	C4D-CHA-C1A	4.93	127.25	121.25
9	R	101	BCL	CHD-C1D-ND	-4.92	119.93	124.45
9	I	102	BCL	CHD-C1D-ND	-4.92	119.93	124.45
9	O	102	BCL	CHD-C1D-ND	-4.89	119.96	124.45
9	F	101	BCL	CHD-C1D-ND	-4.88	119.97	124.45
9	U	102	BCL	CHD-C1D-ND	-4.88	119.97	124.45
9	B	101	BCL	CHD-C1D-ND	-4.87	119.97	124.45
9	M	702	BCL	C4D-CHA-C1A	4.87	127.18	121.25
9	M	702	BCL	CHD-C1D-ND	-4.87	119.98	124.45
9	E	102	BCL	C4D-CHA-C1A	4.86	127.16	121.25
9	B	102	BCL	CHD-C1D-ND	-4.85	120.00	124.45
9	2	102	BCL	CHD-C1D-ND	-4.84	120.00	124.45
9	R	101	BCL	C4D-CHA-C1A	4.83	127.13	121.25
9	W	102	BCL	C3D-C2D-C1D	-4.82	99.25	105.83
9	4	102	BCL	CHD-C1D-ND	-4.81	120.03	124.45
9	L	1002	BCL	CHD-C1D-ND	-4.79	120.06	124.45
9	A	101	BCL	C4D-CHA-C1A	4.77	127.05	121.25
10	0	103	KGD	CAJ-CAL-CAM	-4.76	119.05	126.23
10	1	102	KGD	CAJ-CAL-CAM	-4.76	119.05	126.23
9	L	1001	BCL	C4D-CHA-C1A	4.75	127.03	121.25
9	T	101	BCL	C4D-CHA-C1A	4.74	127.02	121.25
9	P	101	BCL	C4D-CHA-C1A	4.69	126.96	121.25
10	U	103	KGD	CBB-CAV-CAR	-4.67	120.64	127.31
9	3	101	BCL	C4D-CHA-C1A	4.65	126.91	121.25
10	1	103	KGD	CBB-CAV-CAR	-4.63	120.70	127.31
9	K	102	BCL	CHC-C4B-NB	-4.62	119.37	124.26
9	L	1002	BCL	C4D-CHA-C1A	4.59	126.83	121.25
10	6	103	KGD	CBG-CBI-CBL	-4.57	120.79	127.31
10	7	102	KGD	CBG-CBI-CBL	-4.56	120.80	127.31
10	K	103	KGD	CBB-CAV-CAR	-4.53	120.84	127.31
10	4	103	KGD	CBG-CBI-CBL	-4.43	120.99	127.31
9	W	102	BCL	CHB-C1B-NB	-4.42	119.58	124.26
10	8	103	KGD	CAJ-CAL-CAM	-4.42	119.56	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	103	KGD	CBB-CAV-CAR	-4.42	121.00	127.31
10	R	102	KGD	CBB-CAV-CAR	-4.41	121.02	127.31
9	W	102	BCL	C2D-C1D-ND	4.37	113.32	110.10
10	U	103	KGD	CAJ-CAL-CAM	-4.35	119.66	126.23
10	B	103	KGD	CBG-CBI-CBL	-4.34	121.11	127.31
10	1	103	KGD	CBG-CBI-CBL	-4.32	121.15	127.31
10	A	102	KGD	CBG-CBI-CBL	-4.28	121.20	127.31
10	R	102	KGD	CBG-CBI-CBL	-4.27	121.22	127.31
9	K	102	BCL	C2D-C1D-ND	4.26	113.24	110.10
10	7	102	KGD	CAJ-CAL-CAM	-4.25	119.81	126.23
10	E	103	KGD	CBG-CBI-CBL	-4.25	121.25	127.31
13	M	703	BPH	C2B-C1B-NB	-4.23	106.60	109.53
10	1	103	KGD	CAJ-CAL-CAM	-4.23	119.85	126.23
13	L	1006	BPH	C2B-C1B-NB	-4.21	106.62	109.53
10	O	103	KGD	CAJ-CAL-CAM	-4.21	119.88	126.23
10	Q	103	KGD	CBG-CBI-CBL	-4.18	121.34	127.31
10	H	102	KGD	CAP-CAO-CAM	-4.18	121.34	127.31
13	L	1003	BPH	C2B-C1B-NB	-4.15	106.66	109.53
10	S	103	KGD	CAL-CAJ-CAD	-4.15	115.56	127.20
10	K	103	KGD	CAE-CAI-CAH	-4.14	114.83	118.65
10	K	103	KGD	CBG-CBI-CBL	-4.13	121.42	127.31
10	1	102	KGD	CBG-CBI-CBL	-4.09	121.47	127.31
10	C	505	KGD	CBG-CBI-CBL	-4.06	121.51	127.31
10	E	103	KGD	CAJ-CAL-CAM	-4.05	120.11	126.23
10	J	102	KGD	CAJ-CAL-CAM	-4.03	120.14	126.23
10	B	103	KGD	CAE-CAI-CAH	-4.02	114.94	118.65
10	5	102	KGD	CBG-CBI-CBL	-4.01	121.59	127.31
10	I	103	KGD	CBF-CBH-CBJ	-4.01	112.79	118.94
10	O	103	KGD	CAP-CAO-CAM	-3.99	121.61	127.31
10	8	103	KGD	CAE-CAI-CAH	-3.98	114.98	118.65
10	P	102	KGD	CBG-CBI-CBL	-3.95	121.68	127.31
10	1	102	KGD	CBF-CBH-CBJ	-3.95	112.89	118.94
10	E	103	KGD	CAP-CAO-CAM	-3.95	121.68	127.31
10	D	103	KGD	CAJ-CAL-CAM	-3.94	120.28	126.23
9	6	101	BCL	C1-C2-C3	-3.93	119.24	126.04
10	U	103	KGD	CBG-CBB-CAV	-3.93	115.42	123.47
9	W	102	BCL	C1-C2-C3	-3.91	119.28	126.04
9	W	102	BCL	CHD-C4C-NC	3.89	129.40	125.08
10	P	102	KGD	CAJ-CAL-CAM	-3.89	120.36	126.23
10	6	103	KGD	CBF-CBH-CBJ	-3.87	113.00	118.94
10	1	102	KGD	CBB-CAV-CAR	-3.87	121.79	127.31
10	D	103	KGD	CBG-CBI-CBL	-3.86	121.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	103	KGD	CBB-CAV-CAR	-3.85	121.82	127.31
10	O	103	KGD	CBG-CBI-CBL	-3.84	121.83	127.31
9	M	702	BCL	C4A-NA-C1A	3.83	108.43	106.71
10	S	103	KGD	CAP-CAO-CAM	-3.79	121.90	127.31
10	G	102	KGD	CBG-CBI-CBL	-3.79	121.90	127.31
9	W	102	BCL	CHC-C4B-NB	-3.79	120.25	124.26
10	K	103	KGD	CAJ-CAL-CAM	-3.78	120.52	126.23
10	Q	103	KGD	CAJ-CAL-CAM	-3.77	120.54	126.23
10	J	102	KGD	CBG-CBI-CBL	-3.77	121.93	127.31
10	6	103	KGD	CAP-CAO-CAM	-3.77	121.94	127.31
10	D	102	KGD	CBG-CBI-CBL	-3.77	121.94	127.31
10	S	104	KGD	CAJ-CAL-CAM	-3.72	120.61	126.23
10	C	506	KGD	CAP-CAO-CAM	-3.72	122.01	127.31
10	2	103	KGD	CAP-CAO-CAM	-3.69	122.04	127.31
9	K	102	BCL	CHD-C4C-NC	3.69	129.18	125.08
10	E	103	KGD	CBB-CAV-CAR	-3.64	122.11	127.31
10	C	506	KGD	CAE-CAI-CAH	-3.64	115.30	118.65
9	9	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
9	8	102	BCL	C1D-ND-C4D	-3.62	103.76	106.33
9	Q	102	BCL	C1D-ND-C4D	-3.62	103.76	106.33
10	5	102	KGD	CAJ-CAL-CAM	-3.61	120.78	126.23
9	H	101	BCL	C4A-NA-C1A	3.60	108.32	106.71
10	8	103	KGD	CBG-CBI-CBL	-3.60	122.18	127.31
9	L	1002	BCL	C1D-ND-C4D	-3.59	103.78	106.33
10	0	103	KGD	CBG-CBI-CBL	-3.59	122.19	127.31
9	L	1001	BCL	C1D-ND-C4D	-3.57	103.80	106.33
10	H	102	KGD	CBG-CBI-CBL	-3.57	122.22	127.31
9	8	102	BCL	C4A-NA-C1A	3.56	108.31	106.71
9	3	101	BCL	C4A-NA-C1A	3.55	108.30	106.71
9	F	101	BCL	C4A-NA-C1A	3.55	108.30	106.71
9	7	101	BCL	C1D-ND-C4D	-3.55	103.81	106.33
10	G	102	KGD	CAE-CAI-CAH	-3.54	115.39	118.65
9	9	101	BCL	C1D-ND-C4D	-3.52	103.83	106.33
10	5	102	KGD	CAP-CAO-CAM	-3.50	122.31	127.31
10	S	104	KGD	CBG-CBI-CBL	-3.50	122.31	127.31
10	2	103	KGD	CBG-CBI-CBL	-3.49	122.32	127.31
9	5	101	BCL	C1D-ND-C4D	-3.49	103.85	106.33
12	C	507	PGV	C02-O01-C1	3.49	126.38	117.79
10	R	102	KGD	CAJ-CAL-CAM	-3.48	120.97	126.23
10	2	103	KGD	CAL-CAJ-CAD	-3.48	117.44	127.20
9	S	102	BCL	C1D-ND-C4D	-3.47	103.87	106.33
11	C	504	HEM	CBB-CAB-C3B	-3.46	110.39	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	103	KGD	CBF-CBH-CBJ	-3.45	113.64	118.94
9	V	101	BCL	C1D-ND-C4D	-3.45	103.88	106.33
9	L	1001	BCL	C2A-C1A-CHA	3.45	129.89	123.86
9	N	101	BCL	C1D-ND-C4D	-3.44	103.89	106.33
10	U	103	KGD	CBF-CBH-CBJ	-3.43	113.69	118.94
10	C	505	KGD	CAJ-CAL-CAM	-3.42	121.07	126.23
10	8	103	KGD	CBB-CBG-CBI	-3.42	116.48	123.47
9	R	101	BCL	C1D-ND-C4D	-3.41	103.91	106.33
10	Q	103	KGD	CAE-CAI-CAH	-3.39	115.52	118.65
9	0	102	BCL	C1D-ND-C4D	-3.39	103.92	106.33
9	D	101	BCL	C1D-ND-C4D	-3.39	103.93	106.33
9	E	102	BCL	C4A-NA-C1A	3.38	108.23	106.71
9	T	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
9	J	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
9	G	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
9	2	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
9	U	101	BCL	CHA-C1A-NA	-3.36	118.70	126.40
9	F	101	BCL	C1D-ND-C4D	-3.35	103.95	106.33
10	0	104	KGD	CAJ-CAL-CAM	-3.35	121.17	126.23
9	1	101	BCL	C1D-ND-C4D	-3.34	103.96	106.33
9	H	101	BCL	C1D-ND-C4D	-3.34	103.96	106.33
9	M	702	BCL	CHA-C1A-NA	-3.34	118.75	126.40
9	J	101	BCL	C4A-NA-C1A	3.33	108.20	106.71
10	0	104	KGD	CAP-CAO-CAM	-3.33	122.56	127.31
9	U	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
10	1	103	KGD	CAE-CAI-CAH	-3.32	115.59	118.65
9	P	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
9	A	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
9	U	102	BCL	C1D-ND-C4D	-3.31	103.98	106.33
9	5	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
9	O	101	BCL	C1D-ND-C4D	-3.30	103.99	106.33
10	R	102	KGD	CAC-CAB-CAD	-3.30	105.41	110.48
9	6	102	BCL	C1D-ND-C4D	-3.30	103.99	106.33
9	K	102	BCL	C3C-C4C-CHD	-3.29	116.35	123.39
9	4	101	BCL	C1D-ND-C4D	-3.29	104.00	106.33
9	E	101	BCL	CHA-C1A-NA	-3.29	118.87	126.40
9	E	102	BCL	C1D-ND-C4D	-3.28	104.01	106.33
10	S	103	KGD	CBG-CBI-CBL	-3.27	122.64	127.31
9	0	101	BCL	CHA-C1A-NA	-3.26	118.93	126.40
9	2	101	BCL	CHA-C1A-NA	-3.26	118.93	126.40
9	O	102	BCL	C1D-ND-C4D	-3.25	104.03	106.33
10	C	505	KGD	CAP-CAO-CAM	-3.25	122.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	101	BCL	CHA-C1A-NA	-3.25	118.95	126.40
10	5	102	KGD	CAC-CAB-CAD	-3.25	105.48	110.48
9	7	101	BCL	C4A-NA-C1A	3.24	108.16	106.71
9	T	101	BCL	C4A-NA-C1A	3.24	108.16	106.71
9	8	101	BCL	CHA-C1A-NA	-3.23	119.01	126.40
9	N	101	BCL	C4A-NA-C1A	3.22	108.16	106.71
9	8	102	BCL	CHA-C1A-NA	-3.22	119.02	126.40
9	M	702	BCL	C1D-ND-C4D	-3.22	104.05	106.33
10	J	102	KGD	CAC-CAB-CAD	-3.22	105.52	110.48
9	F	102	BCL	CHA-C1A-NA	-3.22	119.03	126.40
9	I	102	BCL	C1D-ND-C4D	-3.21	104.06	106.33
11	C	504	HEM	CBC-CAC-C3C	-3.21	111.66	127.62
10	Q	103	KGD	CAL-CAJ-CAD	-3.21	118.19	127.20
9	B	102	BCL	C1D-ND-C4D	-3.21	104.06	106.33
9	4	102	BCL	C1D-ND-C4D	-3.20	104.06	106.33
9	S	101	BCL	CHA-C1A-NA	-3.20	119.07	126.40
9	3	101	BCL	C1D-ND-C4D	-3.20	104.06	106.33
9	Q	101	BCL	CHA-C1A-NA	-3.20	119.07	126.40
10	C	505	KGD	CAL-CAJ-CAD	-3.20	118.22	127.20
9	K	102	BCL	C1-C2-C3	-3.19	120.53	126.04
10	S	104	KGD	CAL-CAJ-CAD	-3.19	118.25	127.20
9	S	101	BCL	C1D-ND-C4D	-3.19	104.07	106.33
9	I	101	BCL	C1D-ND-C4D	-3.18	104.07	106.33
9	R	101	BCL	C4A-NA-C1A	3.18	108.13	106.71
9	2	102	BCL	C1D-ND-C4D	-3.18	104.08	106.33
10	S	103	KGD	CAE-CAI-CAH	-3.17	115.73	118.65
9	6	102	BCL	CHA-C1A-NA	-3.17	119.14	126.40
9	I	101	BCL	CHA-C1A-NA	-3.17	119.14	126.40
9	K	101	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	F	102	BCL	C1D-ND-C4D	-3.16	104.09	106.33
9	L	1002	BCL	C4A-NA-C1A	3.16	108.12	106.71
9	L	1001	BCL	CHA-C1A-NA	-3.15	119.19	126.40
9	2	102	BCL	CHA-C1A-NA	-3.15	119.19	126.40
9	O	102	BCL	CHA-C1A-NA	-3.15	119.19	126.40
9	W	101	BCL	C1D-ND-C4D	-3.15	104.10	106.33
9	S	102	BCL	CHA-C1A-NA	-3.15	119.19	126.40
9	6	101	BCL	C1D-ND-C4D	-3.15	104.10	106.33
10	I	103	KGD	CBG-CBB-CAV	-3.14	117.04	123.47
10	S	104	KGD	CBG-CBB-CAV	-3.14	117.04	123.47
10	1	102	KGD	CAL-CAJ-CAD	-3.14	118.39	127.20
9	4	102	BCL	CHA-C1A-NA	-3.14	119.21	126.40
9	4	101	BCL	CHA-C1A-NA	-3.14	119.22	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	102	BCL	CHA-C1A-NA	-3.14	119.22	126.40
9	I	102	BCL	CHA-C1A-NA	-3.14	119.22	126.40
9	8	101	BCL	C1D-ND-C4D	-3.13	104.11	106.33
10	0	103	KGD	CAC-CAB-CAD	-3.13	105.66	110.48
9	G	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
10	S	104	KGD	CAZ-CAW-CAS	3.13	120.53	115.27
10	7	102	KGD	CAE-CAC-CAB	-3.13	108.16	113.18
9	B	101	BCL	C1D-ND-C4D	-3.12	104.12	106.33
9	E	102	BCL	CHA-C1A-NA	-3.12	119.25	126.40
9	B	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
10	D	102	KGD	CAL-CAJ-CAD	-3.12	118.44	127.20
9	O	102	BCL	C4A-NA-C1A	3.12	108.11	106.71
9	K	102	BCL	C4A-NA-C1A	3.12	108.11	106.71
9	V	101	BCL	C4A-NA-C1A	3.12	108.11	106.71
9	K	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
9	0	101	BCL	C1D-ND-C4D	-3.11	104.13	106.33
10	R	102	KGD	CAL-CAJ-CAD	-3.11	118.47	127.20
10	S	104	KGD	CBB-CAV-CAR	-3.11	122.88	127.31
10	0	103	KGD	CAP-CAO-CAM	-3.11	122.88	127.31
9	6	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
9	W	102	BCL	O2D-CGD-O1D	-3.10	117.78	123.84
9	I	101	BCL	C1-C2-C3	-3.09	120.70	126.04
9	B	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
9	W	102	BCL	C1D-ND-C4D	-3.09	104.14	106.33
9	P	101	BCL	CHA-C1A-NA	-3.09	119.33	126.40
9	W	102	BCL	C3C-C4C-CHD	-3.09	116.80	123.39
11	C	502	HEM	CBC-CAC-C3C	-3.08	112.30	127.62
9	Q	102	BCL	CHA-C1A-NA	-3.08	119.35	126.40
9	Q	101	BCL	C1D-ND-C4D	-3.07	104.15	106.33
9	O	101	BCL	CHA-C1A-NA	-3.07	119.36	126.40
15	M	701	MQE	CAY-CAX-CBQ	-3.07	115.22	118.50
10	7	102	KGD	CBB-CAV-CAR	-3.06	122.95	127.31
10	I	103	KGD	CAE-CAC-CAB	-3.05	108.28	113.18
10	0	104	KGD	CAL-CAJ-CAD	-3.05	118.63	127.20
10	8	103	KGD	CBF-CBH-CBJ	-3.04	114.27	118.94
10	0	103	KGD	CAE-CAC-CAB	-3.04	108.30	113.18
10	A	102	KGD	CAJ-CAL-CAM	-3.04	121.65	126.23
10	2	103	KGD	CAE-CAI-CAH	-3.03	115.85	118.65
10	R	102	KGD	CBG-CBB-CAV	-3.03	117.27	123.47
10	S	104	KGD	CAE-CAI-CAH	-3.03	115.86	118.65
9	E	101	BCL	C1D-ND-C4D	-3.03	104.18	106.33
9	0	102	BCL	CHA-C1A-NA	-3.03	119.47	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	102	KGD	CBM-CBJ-CBH	-3.02	123.01	127.31
9	S	101	BCL	C1-C2-C3	-3.01	120.83	126.04
10	1	103	KGD	CBM-CBJ-CBH	-3.01	123.01	127.31
9	W	102	BCL	O2A-CGA-CBA	3.01	121.35	111.91
10	D	102	KGD	CAE-CAI-CAH	-3.01	115.88	118.65
9	K	102	BCL	CMB-C2B-C1B	3.00	129.94	125.37
9	7	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40
9	1	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
9	O	101	BCL	C4A-NA-C1A	2.99	108.05	106.71
9	2	102	BCL	C4A-NA-C1A	2.99	108.05	106.71
10	J	103	KGD	CAN-CAM-CAL	-2.99	113.37	118.08
9	U	102	BCL	C4A-NA-C1A	2.98	108.05	106.71
9	2	102	BCL	C2A-C1A-CHA	2.97	129.05	123.86
9	A	101	BCL	C4A-NA-C1A	2.96	108.04	106.71
9	W	102	BCL	C3D-C4D-ND	2.96	115.03	110.24
10	1	102	KGD	CAC-CAB-CAD	-2.96	105.92	110.48
10	J	103	KGD	CAC-CAB-CAD	-2.95	105.93	110.48
10	8	103	KGD	CAL-CAJ-CAD	-2.95	118.92	127.20
9	T	101	BCL	CHA-C1A-NA	-2.95	119.65	126.40
9	R	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
10	S	103	KGD	CAZ-CAW-CAS	2.94	120.21	115.27
10	O	103	KGD	CBB-CAV-CAR	-2.93	123.12	127.31
10	S	103	KGD	CBG-CBB-CAV	-2.93	117.47	123.47
10	S	103	KGD	CBF-CBH-CBJ	-2.93	114.44	118.94
9	A	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
9	V	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
10	J	102	KGD	CAL-CAJ-CAD	-2.93	118.98	127.20
10	1	103	KGD	CAE-CAC-CAB	-2.92	108.49	113.18
9	D	101	BCL	CHA-C1A-NA	-2.92	119.71	126.40
10	0	104	KGD	CBG-CBB-CAV	-2.92	117.50	123.47
9	3	101	BCL	CHA-C1A-NA	-2.92	119.72	126.40
10	J	102	KGD	CBM-CBN-CBL	-2.91	118.23	126.42
9	N	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
10	4	103	KGD	CBM-CBJ-CBH	-2.91	123.16	127.31
9	H	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
9	4	102	BCL	C4A-NA-C1A	2.90	108.01	106.71
9	I	102	BCL	C4A-NA-C1A	2.90	108.01	106.71
9	9	101	BCL	CHA-C1A-NA	-2.90	119.75	126.40
10	J	102	KGD	CAP-CAO-CAM	-2.90	123.17	127.31
9	D	101	BCL	C4A-NA-C1A	2.90	108.01	106.71
9	F	102	BCL	C1-C2-C3	-2.90	121.03	126.04
10	U	103	KGD	CAP-CAO-CAM	-2.89	123.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	BCL	CHA-C1A-NA	-2.89	119.78	126.40
10	6	103	KGD	CAZ-CAW-CAS	2.89	120.13	115.27
9	1	101	BCL	C4A-NA-C1A	2.89	108.00	106.71
9	K	102	BCL	O2D-CGD-O1D	-2.88	118.20	123.84
11	C	503	HEM	CBB-CAB-C3B	-2.88	113.30	127.62
9	J	101	BCL	CHA-C1A-NA	-2.87	119.82	126.40
9	5	101	BCL	CHA-C1A-NA	-2.87	119.83	126.40
15	M	704	MQE	CCE-CBK-CBS	-2.87	111.52	116.27
10	R	102	KGD	CAP-CAO-CAM	-2.86	123.23	127.31
9	2	101	BCL	C1-C2-C3	-2.85	121.11	126.04
10	K	103	KGD	CAL-CAJ-CAD	-2.85	119.20	127.20
9	0	101	BCL	C17-C16-C15	2.84	126.30	113.24
10	6	103	KGD	CAE-CAC-CAB	-2.84	108.62	113.18
9	8	101	BCL	C17-C16-C15	2.83	126.24	113.24
9	O	101	BCL	C2A-C1A-CHA	2.82	128.79	123.86
10	H	102	KGD	CAE-CAC-CAB	-2.82	108.65	113.18
9	8	101	BCL	C1-C2-C3	-2.82	121.17	126.04
10	D	102	KGD	CAJ-CAL-CAM	-2.81	121.99	126.23
10	I	103	KGD	CAZ-CAW-CAS	2.81	119.99	115.27
9	K	102	BCL	C1D-ND-C4D	-2.80	104.35	106.33
10	O	103	KGD	CAL-CAJ-CAD	-2.79	119.37	127.20
13	L	1003	BPH	CMB-C2B-C3B	2.79	129.89	124.68
10	8	103	KGD	CAQ-CAR-CAV	-2.78	114.67	118.94
10	H	102	KGD	CAC-CAB-CAD	-2.77	106.21	110.48
15	L	1005	MQE	CAY-CAX-CBQ	-2.77	115.54	118.50
9	E	101	BCL	C1-C2-C3	-2.76	121.27	126.04
10	D	103	KGD	CBF-CBH-CBJ	-2.75	114.72	118.94
9	K	102	BCL	C3D-C4D-ND	2.75	114.69	110.24
10	R	102	KGD	CBF-CBH-CBJ	-2.75	114.72	118.94
10	U	103	KGD	CBJ-CBM-CBN	-2.75	114.64	123.22
9	5	101	BCL	C1-C2-C3	-2.75	121.29	126.04
9	0	101	BCL	C1-C2-C3	-2.74	121.30	126.04
10	8	103	KGD	CAZ-CAW-CAS	2.74	119.89	115.27
11	C	501	HEM	CBC-CAC-C3C	-2.74	113.98	127.62
10	6	103	KGD	CBA-CBE-CBF	-2.74	114.66	123.22
10	U	103	KGD	CAL-CAJ-CAD	-2.74	119.51	127.20
10	S	103	KGD	CBB-CAV-CAR	-2.74	123.40	127.31
9	7	101	BCL	C2A-C1A-CHA	2.74	128.65	123.86
10	1	102	KGD	CBK-CBH-CBJ	2.74	126.76	122.92
10	5	102	KGD	CAL-CAJ-CAD	-2.73	119.53	127.20
10	K	103	KGD	CAP-CAO-CAM	-2.73	123.41	127.31
10	1	103	KGD	CBG-CBB-CAV	-2.73	117.89	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	101	BCL	C4A-NA-C1A	2.72	107.93	106.71
9	I	102	BCL	C2A-C1A-CHA	2.72	128.62	123.86
10	B	103	KGD	CBG-CBB-CAV	-2.72	117.91	123.47
11	C	501	HEM	CBB-CAB-C3B	-2.72	114.11	127.62
9	L	1002	BCL	CHA-C1A-NA	-2.71	120.18	126.40
10	S	104	KGD	CBF-CBH-CBJ	-2.71	114.78	118.94
10	7	102	KGD	CAC-CAB-CAD	-2.71	106.31	110.48
10	2	103	KGD	CAJ-CAL-CAM	-2.71	122.14	126.23
9	G	101	BCL	C4A-NA-C1A	2.70	107.92	106.71
10	C	506	KGD	CBG-CBI-CBL	-2.70	123.45	127.31
10	U	103	KGD	CAZ-CAW-CAS	2.70	119.81	115.27
9	F	101	BCL	C2A-C1A-CHA	2.70	128.58	123.86
10	1	102	KGD	CAZ-CAW-CAS	2.70	119.81	115.27
10	A	102	KGD	CAE-CAI-CAH	-2.69	116.17	118.65
10	0	104	KGD	CAE-CAI-CAH	-2.69	116.17	118.65
10	O	103	KGD	CAZ-CAW-CAS	2.69	119.79	115.27
10	C	505	KGD	CAE-CAI-CAH	-2.69	116.17	118.65
9	A	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
9	4	102	BCL	C1C-NC-C4C	2.68	107.91	106.71
9	Q	102	BCL	C4A-NA-C1A	2.68	107.91	106.71
10	I	103	KGD	CBJ-CBM-CBN	-2.68	114.85	123.22
10	P	102	KGD	CAL-CAJ-CAD	-2.68	119.67	127.20
10	U	103	KGD	CAE-CAC-CAB	-2.68	108.88	113.18
10	B	103	KGD	CBB-CAV-CAR	-2.67	123.50	127.31
9	I	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
9	1	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
10	1	103	KGD	CAL-CAJ-CAD	-2.64	119.78	127.20
10	D	103	KGD	CAZ-CAW-CAS	2.64	119.72	115.27
9	K	101	BCL	C17-C16-C15	2.64	125.36	113.24
9	4	102	BCL	CHC-C4B-NB	-2.64	121.46	124.26
10	8	103	KGD	CAP-CAO-CAM	-2.64	123.55	127.31
9	K	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
9	D	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
9	I	102	BCL	CHC-C4B-NB	-2.63	121.48	124.26
10	I	103	KGD	CAC-CAB-CAD	-2.63	106.44	110.48
9	B	101	BCL	C1-C2-C3	-2.63	121.50	126.04
10	D	103	KGD	CAE-CAI-CAH	-2.63	116.23	118.65
9	H	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
9	B	102	BCL	CHC-C4B-NB	-2.62	121.48	124.26
9	R	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
9	B	102	BCL	C4A-NA-C1A	2.62	107.88	106.71
10	7	102	KGD	CAP-CAO-CAM	-2.61	123.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	4	102	BCL	C2A-C1A-CHA	2.61	128.43	123.86
9	N	101	BCL	C2A-C1A-CHA	2.61	128.42	123.86
9	6	101	BCL	C17-C16-C15	2.60	125.20	113.24
9	S	102	BCL	CHC-C4B-NB	-2.60	121.50	124.26
10	S	103	KGD	CAP-CAQ-CAR	-2.60	119.10	126.42
10	A	102	KGD	CAL-CAJ-CAD	-2.59	119.92	127.20
9	5	101	BCL	C2A-C1A-CHA	2.59	128.39	123.86
9	Q	102	BCL	CHC-C4B-NB	-2.59	121.52	124.26
11	C	502	HEM	C2A-C1A-NA	-2.58	107.26	110.15
10	I	103	KGD	CBK-CBH-CBJ	2.58	126.54	122.92
9	O	102	BCL	CHC-C4B-NB	-2.58	121.52	124.26
9	4	101	BCL	C4A-NA-C1A	2.58	107.87	106.71
10	G	102	KGD	CAZ-CAW-CAS	2.58	119.61	115.27
9	0	102	BCL	CHC-C4B-NB	-2.58	121.53	124.26
10	E	103	KGD	CBF-CBH-CBJ	-2.58	114.99	118.94
10	2	103	KGD	CAZ-CAW-CAS	2.58	119.60	115.27
10	1	102	KGD	CAE-CAC-CAB	-2.57	109.05	113.18
10	D	103	KGD	CBB-CAV-CAR	-2.57	123.64	127.31
9	G	101	BCL	CHC-C4B-NB	-2.57	121.53	124.26
10	G	102	KGD	CBF-CBH-CBJ	-2.57	115.00	118.94
9	T	101	BCL	C2A-C1A-CHA	2.56	128.34	123.86
10	I	103	KGD	CBB-CAV-CAR	-2.56	123.65	127.31
9	K	102	BCL	C4B-C3B-C2B	-2.56	104.24	108.36
9	U	101	BCL	C2A-C1A-CHA	2.56	128.34	123.86
9	3	101	BCL	C2A-C1A-CHA	2.56	128.33	123.86
9	Q	101	BCL	C2A-C1A-CHA	2.56	128.33	123.86
9	0	102	BCL	C4A-NA-C1A	2.55	107.85	106.71
9	6	102	BCL	C4A-NA-C1A	2.55	107.85	106.71
9	9	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86
11	C	503	HEM	CBC-CAC-C3C	-2.55	114.92	127.62
9	J	101	BCL	C2A-C1A-CHA	2.55	128.31	123.86
11	C	501	HEM	C3B-C2B-C1B	2.54	108.37	106.49
10	K	103	KGD	CBM-CBJ-CBH	-2.54	123.68	127.31
9	6	102	BCL	CHC-C4B-NB	-2.54	121.57	124.26
10	4	103	KGD	CAL-CAM-CAO	2.54	122.83	118.94
10	E	103	KGD	CAE-CAC-CAB	-2.53	109.12	113.18
10	D	103	KGD	CAL-CAJ-CAD	-2.53	120.10	127.20
10	D	103	KGD	CAP-CAO-CAM	-2.53	123.70	127.31
10	J	103	KGD	CBG-CBI-CBL	-2.53	123.71	127.31
10	K	103	KGD	CAZ-CAW-CAS	2.52	119.51	115.27
9	1	101	BCL	CHC-C4B-NB	-2.52	121.59	124.26
9	W	102	BCL	C4B-C3B-C2B	-2.52	104.31	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	102	KGD	CAE-CAC-CAB	-2.52	109.14	113.18
9	M	702	BCL	CHC-C4B-NB	-2.51	121.60	124.26
10	U	103	KGD	CBA-CBE-CBF	-2.51	115.38	123.22
10	C	506	KGD	CBG-CBB-CAV	-2.51	118.34	123.47
9	K	102	BCL	CMD-C2D-C3D	-2.51	121.84	127.61
13	M	703	BPH	CMB-C2B-C3B	2.50	129.36	124.68
10	1	102	KGD	CBJ-CBM-CBN	-2.50	115.41	123.22
11	C	502	HEM	CBB-CAB-C3B	-2.50	115.17	127.62
10	E	103	KGD	CAL-CAJ-CAD	-2.50	120.19	127.20
9	0	101	BCL	C2A-C1A-CHA	2.49	128.21	123.86
10	B	103	KGD	CAZ-CAW-CAS	2.48	119.44	115.27
9	T	101	BCL	CHC-C4B-NB	-2.48	121.63	124.26
10	1	102	KGD	CAE-CAI-CAH	-2.48	116.37	118.65
10	Q	103	KGD	CAP-CAO-CAM	-2.48	123.77	127.31
9	2	102	BCL	CHC-C4B-NB	-2.48	121.63	124.26
10	D	102	KGD	CAP-CAO-CAM	-2.47	123.78	127.31
9	6	101	BCL	C2A-C1A-CHA	2.47	128.18	123.86
10	A	102	KGD	CAE-CAC-CAB	-2.47	109.22	113.18
10	P	102	KGD	CBB-CAV-CAR	-2.47	123.79	127.31
10	0	104	KGD	CBG-CBI-CBL	-2.46	123.79	127.31
9	M	702	BCL	C2A-C1A-CHA	2.46	128.16	123.86
9	0	102	BCL	C2A-C1A-CHA	2.46	128.16	123.86
9	B	102	BCL	C2A-C1A-CHA	2.45	128.15	123.86
10	4	103	KGD	CAP-CAQ-CAR	-2.45	119.53	126.42
10	4	103	KGD	CAE-CAC-CAB	-2.45	109.25	113.18
10	U	103	KGD	CAC-CAB-CAD	-2.45	106.72	110.48
10	J	102	KGD	CBG-CBB-CAV	-2.45	118.46	123.47
10	2	103	KGD	CAE-CAC-CAB	-2.44	109.26	113.18
9	4	101	BCL	C17-C16-C15	2.44	124.46	113.24
9	B	101	BCL	C17-C16-C15	2.43	124.39	113.24
10	O	103	KGD	CAE-CAC-CAB	-2.42	109.29	113.18
10	J	102	KGD	CBB-CAV-CAR	-2.42	123.86	127.31
10	Q	103	KGD	CBM-CBJ-CBH	-2.41	123.87	127.31
9	O	102	BCL	C2A-C1A-CHA	2.41	128.07	123.86
10	1	103	KGD	CAC-CAB-CAD	-2.40	106.78	110.48
10	G	102	KGD	CBB-CAV-CAR	-2.40	123.88	127.31
9	8	102	BCL	C2A-C1A-CHA	2.40	128.06	123.86
10	7	102	KGD	CAE-CAI-CAH	-2.40	116.44	118.65
10	2	103	KGD	CBB-CAV-CAR	-2.40	123.89	127.31
9	V	101	BCL	CHC-C4B-NB	-2.39	121.72	124.26
10	1	102	KGD	CBA-CBE-CBF	-2.39	115.77	123.22
10	1	103	KGD	OAA-CAI-CAH	2.39	123.08	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5	102	KGD	CAE-CAI-CAH	-2.38	116.46	118.65
9	F	101	BCL	CHC-C4B-NB	-2.38	121.74	124.26
9	E	101	BCL	C2A-C1A-CHA	2.38	128.02	123.86
9	E	101	BCL	CHC-C4B-NB	-2.38	121.74	124.26
9	E	102	BCL	C2A-C1A-CHA	2.37	128.01	123.86
10	C	505	KGD	CBB-CAV-CAR	-2.37	123.92	127.31
10	H	102	KGD	CAZ-CAW-CAS	2.37	119.26	115.27
9	J	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
9	2	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
9	3	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
9	B	101	BCL	C2A-C1A-CHA	2.36	127.99	123.86
9	U	102	BCL	C2A-C1A-CHA	2.36	127.98	123.86
9	L	1001	BCL	CHC-C4B-NB	-2.36	121.76	124.26
9	G	101	BCL	C2A-C1A-CHA	2.36	127.98	123.86
9	4	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
9	F	102	BCL	C17-C16-C15	2.35	124.03	113.24
9	H	101	BCL	CHC-C4B-NB	-2.35	121.77	124.26
10	A	102	KGD	CAP-CAO-CAM	-2.35	123.96	127.31
10	O	103	KGD	CBM-CBJ-CBH	-2.35	123.96	127.31
10	6	103	KGD	CAE-CAI-CAH	-2.35	116.49	118.65
10	E	103	KGD	CAE-CAI-CAH	-2.35	116.49	118.65
10	H	102	KGD	CAE-CAI-CAH	-2.35	116.49	118.65
9	6	102	BCL	C2A-C1A-CHA	2.34	127.96	123.86
10	C	505	KGD	CAT-CAX-CAY	-2.34	119.75	127.75
9	W	102	BCL	CMD-C2D-C3D	-2.34	122.24	127.61
10	1	102	KGD	CBB-CBG-CBI	-2.33	118.69	123.47
9	E	102	BCL	CHC-C4B-NB	-2.33	121.79	124.26
11	C	502	HEM	CAA-CBA-CGA	-2.33	108.60	113.60
10	S	104	KGD	CAE-CAC-CAB	-2.32	109.45	113.18
9	U	101	BCL	CHC-C4B-NB	-2.32	121.80	124.26
10	I	103	KGD	CAE-CAI-CAH	-2.32	116.51	118.65
9	U	102	BCL	CHC-C4B-NB	-2.32	121.80	124.26
10	E	103	KGD	CAZ-CAW-CAS	2.32	119.17	115.27
9	V	101	BCL	C2A-C1A-CHA	2.32	127.91	123.86
10	4	103	KGD	CAN-CAM-CAL	-2.32	114.43	118.08
9	A	101	BCL	CHC-C4B-NB	-2.32	121.81	124.26
10	G	102	KGD	CBG-CBB-CAV	-2.31	118.74	123.47
10	P	102	KGD	CAP-CAO-CAM	-2.31	124.02	127.31
9	R	101	BCL	CHC-C4B-NB	-2.31	121.81	124.26
13	L	1006	BPH	CMB-C2B-C3B	2.30	128.99	124.68
10	1	103	KGD	CAP-CAO-CAM	-2.30	124.03	127.31
9	9	101	BCL	CHC-C4B-NB	-2.30	121.82	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	102	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
9	8	102	BCL	CHC-C4B-NB	-2.29	121.83	124.26
9	I	101	BCL	C11-C10-C8	-2.29	108.51	115.92
9	I	102	BCL	C1C-NC-C4C	2.29	107.74	106.71
10	S	104	KGD	CAN-CAM-CAO	2.29	126.13	122.92
9	W	101	BCL	CHC-C4B-NB	-2.29	121.83	124.26
10	0	103	KGD	CAL-CAJ-CAD	-2.29	120.77	127.20
10	S	104	KGD	CBJ-CBM-CBN	-2.28	116.09	123.22
10	S	103	KGD	CBM-CBJ-CBH	-2.28	124.05	127.31
9	S	102	BCL	C2A-C1A-CHA	2.28	127.85	123.86
10	U	103	KGD	CAF-CAB-CAD	-2.28	106.60	110.30
10	I	103	KGD	CAT-CAX-CAY	-2.28	119.96	127.75
9	8	101	BCL	C2A-C1A-CHA	2.28	127.84	123.86
9	E	101	BCL	CAB-C3B-C2B	-2.27	124.93	128.34
10	J	102	KGD	CAE-CAC-CAB	-2.27	109.53	113.18
13	L	1003	BPH	C1A-C2A-C3A	-2.27	100.68	102.84
9	K	102	BCL	C4-C3-C5	2.27	119.09	115.27
9	S	101	BCL	C2A-C1A-CHA	2.27	127.83	123.86
9	B	102	BCL	CAB-C3B-C2B	-2.27	124.94	128.34
9	8	101	BCL	CHC-C4B-NB	-2.27	121.86	124.26
9	W	102	BCL	C4A-NA-C1A	2.27	107.72	106.71
11	C	503	HEM	CAA-CBA-CGA	-2.26	108.73	113.60
9	D	101	BCL	CHC-C4B-NB	-2.26	121.86	124.26
10	Q	103	KGD	CAN-CAM-CAO	2.26	126.09	122.92
9	S	102	BCL	C4A-NA-C1A	2.26	107.72	106.71
9	S	101	BCL	CHC-C4B-NB	-2.26	121.86	124.26
15	M	701	MQE	CAO-CBI-CAZ	2.26	133.10	127.66
9	K	102	BCL	O2A-CGA-CBA	2.26	119.00	111.91
9	E	101	BCL	C11-C10-C8	-2.25	108.64	115.92
10	B	103	KGD	OAA-CAI-CAH	2.25	122.96	120.96
10	8	103	KGD	CBA-CBE-CBF	-2.25	116.19	123.22
9	I	101	BCL	CHC-C4B-NB	-2.25	121.88	124.26
9	K	101	BCL	C2A-C1A-CHA	2.25	127.79	123.86
9	P	101	BCL	C2A-C1A-CHA	2.25	127.79	123.86
10	5	102	KGD	CAE-CAC-CAB	-2.25	109.57	113.18
9	W	102	BCL	C11-C10-C8	-2.25	108.66	115.92
9	Q	102	BCL	C2A-C1A-CHA	2.24	127.78	123.86
10	2	103	KGD	CBF-CBH-CBJ	-2.24	115.50	118.94
9	0	102	BCL	CAB-C3B-C2B	-2.24	124.98	128.34
10	J	103	KGD	CAK-CAH-CAI	-2.24	112.16	115.48
10	1	103	KGD	CBE-CBF-CBH	-2.24	120.13	126.42
10	J	102	KGD	CAZ-CAW-CAS	2.24	119.03	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2	103	KGD	OAA-CAI-CAH	2.24	122.94	120.96
10	P	102	KGD	CBG-CBB-CAV	-2.23	118.91	123.47
9	I	101	BCL	C17-C16-C15	2.23	123.47	113.24
9	F	102	BCL	CHC-C4B-NB	-2.23	121.90	124.26
9	4	102	BCL	CAB-C3B-C2B	-2.23	125.00	128.34
9	L	1002	BCL	CHC-C4B-NB	-2.23	121.90	124.26
9	F	102	BCL	C2A-C1A-CHA	2.23	127.75	123.86
10	0	103	KGD	CAE-CAI-CAH	-2.22	116.61	118.65
9	U	101	BCL	C4A-NA-C1A	2.22	107.70	106.71
9	W	101	BCL	C2A-C1A-CHA	2.21	127.73	123.86
10	R	102	KGD	CAN-CAM-CAO	2.21	126.02	122.92
10	7	102	KGD	CAL-CAJ-CAD	-2.21	120.99	127.20
10	I	103	KGD	CBA-CBE-CBF	-2.21	116.32	123.22
10	C	506	KGD	CAQ-CAR-CAV	-2.21	115.55	118.94
10	D	103	KGD	CBG-CBB-CAV	-2.21	118.95	123.47
10	5	102	KGD	CBF-CBH-CBJ	-2.21	115.55	118.94
10	P	102	KGD	CAE-CAC-CAB	-2.20	109.64	113.18
9	4	101	BCL	CHC-C4B-NB	-2.20	121.92	124.26
9	0	101	BCL	CHC-C4B-NB	-2.19	121.94	124.26
10	Q	103	KGD	CAZ-CAW-CAS	2.19	118.95	115.27
9	O	101	BCL	CHC-C4B-NB	-2.19	121.94	124.26
9	K	102	BCL	C1-O2A-CGA	2.19	122.18	116.44
9	B	101	BCL	C4A-NA-C1A	2.18	107.69	106.71
9	Q	101	BCL	C4A-NA-C1A	2.18	107.69	106.71
9	K	101	BCL	CHC-C4B-NB	-2.18	121.95	124.26
9	6	101	BCL	CHC-C4B-NB	-2.18	121.95	124.26
9	K	102	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
10	A	102	KGD	CBG-CBB-CAV	-2.17	119.04	123.47
9	W	101	BCL	C4A-NA-C1A	2.16	107.68	106.71
10	K	103	KGD	CAC-CAB-CAD	-2.16	107.15	110.48
13	L	1003	BPH	C2D-C1D-ND	-2.16	108.03	109.53
9	W	102	BCL	CHC-C1C-NC	2.16	127.49	124.51
10	J	102	KGD	CAE-CAI-CAH	-2.15	116.67	118.65
10	A	102	KGD	CAC-CAB-CAD	-2.15	107.17	110.48
10	D	102	KGD	CBM-CBN-CBL	-2.15	120.37	126.42
9	O	102	BCL	C1C-NC-C4C	2.15	107.67	106.71
9	6	101	BCL	C4A-NA-C1A	2.14	107.67	106.71
9	K	102	BCL	CHD-C1D-C2D	2.14	129.97	125.48
9	W	102	BCL	CMB-C2B-C1B	2.14	128.62	125.37
10	Q	103	KGD	CBB-CAV-CAR	-2.14	124.26	127.31
11	C	501	HEM	CHB-C1B-NB	2.14	127.01	124.37
9	Q	102	BCL	CAB-C3B-C2B	-2.13	125.14	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	102	KGD	CAC-CAB-CAD	-2.13	107.20	110.48
11	C	502	HEM	CHB-C1B-NB	2.13	127.00	124.37
10	C	505	KGD	CBE-CBF-CBH	-2.13	120.43	126.42
9	6	102	BCL	CAB-C3B-C2B	-2.13	125.15	128.34
10	1	103	KGD	CAT-CAX-CAY	-2.12	120.49	127.75
10	O	103	KGD	CBF-CBH-CBJ	-2.12	115.69	118.94
9	5	101	BCL	CHC-C4B-NB	-2.12	122.01	124.26
9	N	101	BCL	CHC-C4B-NB	-2.11	122.02	124.26
9	G	101	BCL	CAB-C3B-C2B	-2.11	125.17	128.34
10	7	102	KGD	CBM-CBJ-CBH	-2.11	124.29	127.31
9	8	102	BCL	C1C-NC-C4C	2.11	107.66	106.71
10	R	102	KGD	CAE-CAI-CAH	-2.11	116.71	118.65
10	D	103	KGD	CAC-CAB-CAD	-2.11	107.23	110.48
9	Q	101	BCL	CHC-C4B-NB	-2.11	122.03	124.26
10	S	104	KGD	CAC-CAB-CAD	-2.11	107.24	110.48
10	C	506	KGD	CAN-CAM-CAL	-2.11	114.76	118.08
9	5	101	BCL	C1C-NC-C4C	2.11	107.65	106.71
13	L	1003	BPH	C1C-C2C-C3C	-2.10	100.84	102.84
10	D	102	KGD	CBB-CAV-CAR	-2.10	124.31	127.31
10	6	103	KGD	CBJ-CBM-CBN	-2.10	116.66	123.22
10	7	102	KGD	CBG-CBB-CAV	-2.10	119.17	123.47
13	L	1003	BPH	C4C-C3C-C2C	-2.10	100.84	102.84
10	1	103	KGD	CAN-CAM-CAO	2.09	125.86	122.92
10	B	103	KGD	CBA-CBE-CBF	-2.09	116.70	123.22
10	A	102	KGD	CBB-CAV-CAR	-2.09	124.33	127.31
9	S	102	BCL	CAB-C3B-C2B	-2.09	125.22	128.34
10	D	103	KGD	CAE-CAC-CAB	-2.08	109.83	113.18
10	D	102	KGD	CAN-CAM-CAO	2.08	125.84	122.92
10	S	104	KGD	CAP-CAQ-CAR	-2.08	120.56	126.42
9	M	702	BCL	C4B-C3B-C2B	-2.08	105.01	108.36
10	0	104	KGD	CAZ-CAW-CAS	2.08	118.77	115.27
9	S	102	BCL	C1C-NC-C4C	2.08	107.64	106.71
10	U	103	KGD	CAO-CAP-CAQ	-2.08	116.73	123.22
9	H	101	BCL	C4B-C3B-C2B	-2.08	105.02	108.36
10	O	103	KGD	CAE-CAI-CAH	-2.07	116.74	118.65
9	P	101	BCL	CHC-C4B-NB	-2.07	122.06	124.26
10	E	103	KGD	CAC-CAB-CAD	-2.07	107.29	110.48
13	L	1006	BPH	CMC-C2C-C1C	-2.07	109.84	114.38
10	U	103	KGD	CAN-CAM-CAO	2.07	125.82	122.92
9	L	1002	BCL	C2A-C1A-CHA	2.07	127.47	123.86
10	5	102	KGD	CBM-CBJ-CBH	-2.07	124.36	127.31
10	8	103	KGD	OAA-CAI-CAH	2.06	122.79	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	704	MQE	CAY-CAX-CBQ	-2.06	116.29	118.50
11	C	503	HEM	CAD-CBD-CGD	-2.06	109.16	113.60
9	W	102	BCL	CHD-C1D-C2D	2.06	129.81	125.48
10	B	103	KGD	CAN-CAM-CAL	-2.06	114.83	118.08
9	S	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
10	J	103	KGD	CAL-CAJ-CAD	-2.06	121.43	127.20
13	M	703	BPH	C2D-C1D-ND	-2.06	108.11	109.53
9	3	101	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
10	Q	103	KGD	CBE-CBF-CBH	-2.05	120.65	126.42
9	7	101	BCL	CHC-C4B-NB	-2.05	122.08	124.26
9	B	101	BCL	CHC-C4B-NB	-2.05	122.08	124.26
10	6	103	KGD	CBK-CBH-CBJ	2.05	125.80	122.92
9	O	101	BCL	C17-C16-C15	2.05	122.67	113.24
10	8	103	KGD	CAO-CAP-CAQ	-2.05	116.81	123.22
10	C	505	KGD	CBG-CBB-CAV	-2.05	119.27	123.47
9	I	101	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
10	C	505	KGD	CAN-CAM-CAO	2.05	125.80	122.92
10	D	103	KGD	CBM-CBN-CBL	-2.05	120.65	126.42
9	G	101	BCL	C1C-NC-C4C	2.05	107.63	106.71
13	L	1006	BPH	C1B-NB-C4B	2.05	112.00	108.83
10	D	102	KGD	CAZ-CAW-CAS	2.05	118.72	115.27
10	P	102	KGD	CBF-CBH-CBJ	-2.05	115.80	118.94
9	W	102	BCL	C4-C3-C5	2.05	118.71	115.27
9	F	102	BCL	C4B-C3B-C2B	-2.04	105.07	108.36
9	F	101	BCL	C4B-C3B-C2B	-2.04	105.08	108.36
10	E	103	KGD	CBJ-CBM-CBN	-2.04	116.85	123.22
10	1	102	KGD	CBD-CAY-CBC	2.04	119.11	114.60
9	O	102	BCL	CAB-C3B-C2B	-2.04	125.29	128.34
9	I	102	BCL	CAB-C3B-C2B	-2.04	125.29	128.34
9	F	102	BCL	C4A-NA-C1A	2.03	107.62	106.71
11	C	503	HEM	C4D-ND-C1D	2.03	107.17	105.07
9	B	102	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
9	I	101	BCL	C4A-NA-C1A	2.03	107.62	106.71
13	L	1006	BPH	C2D-C1D-ND	-2.03	108.12	109.53
10	A	102	KGD	CBF-CBH-CBJ	-2.03	115.83	118.94
9	4	102	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
9	1	101	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
9	2	101	BCL	C2A-C1A-CHA	2.03	127.40	123.86
10	0	103	KGD	CBM-CBJ-CBH	-2.02	124.42	127.31
10	S	104	KGD	CBA-CBE-CBF	-2.02	116.90	123.22
10	6	103	KGD	CBD-CAY-CBC	2.02	119.07	114.60
9	U	102	BCL	C1C-NC-C4C	2.02	107.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	103	KGD	CBD-CAY-CBC	2.02	119.07	114.60
9	T	101	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
9	6	102	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
9	W	102	BCL	CHC-C4B-C3B	-2.02	125.17	132.35
9	G	101	BCL	C4B-C3B-C2B	-2.01	105.12	108.36
10	P	102	KGD	CAN-CAM-CAO	2.01	125.74	122.92
9	U	101	BCL	C4B-C3B-C2B	-2.01	105.13	108.36
9	L	1002	BCL	C4B-C3B-C2B	-2.01	105.13	108.36
9	8	101	BCL	C4B-C3B-C2B	-2.01	105.13	108.36
11	C	501	HEM	CMB-C2B-C1B	-2.00	121.99	125.04
10	8	103	KGD	CBD-CAY-CBC	2.00	119.03	114.60

There are no chirality outliers.

All (585) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C2-C3-C5-C6
9	2	102	BCL	C4-C3-C5-C6
9	4	101	BCL	C2-C3-C5-C6
9	4	101	BCL	C4-C3-C5-C6
9	4	102	BCL	C4-C3-C5-C6
9	6	101	BCL	C4-C3-C5-C6
9	6	102	BCL	C4-C3-C5-C6
9	8	102	BCL	C2-C3-C5-C6
9	8	102	BCL	C4-C3-C5-C6
9	9	101	BCL	CHA-CBD-CGD-O1D
9	9	101	BCL	CHA-CBD-CGD-O2D
9	A	101	BCL	CHA-CBD-CGD-O1D
9	A	101	BCL	CHA-CBD-CGD-O2D
9	E	102	BCL	O2A-C1-C2-C3
9	E	102	BCL	C2-C3-C5-C6
9	E	102	BCL	C4-C3-C5-C6
9	I	102	BCL	C2-C3-C5-C6
9	I	102	BCL	C4-C3-C5-C6
9	K	101	BCL	C2-C3-C5-C6
9	K	101	BCL	C4-C3-C5-C6
9	K	102	BCL	C2B-C3B-CAB-OB
9	K	102	BCL	C2B-C3B-CAB-CB
9	K	102	BCL	C4B-C3B-CAB-CB
9	K	102	BCL	C2C-C3C-CAC-CB
9	K	102	BCL	C4C-C3C-CAC-CB

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Mol	Chain	Res	Type	Atoms
9	K	102	BCL	C4-C3-C5-C6
9	L	1002	BCL	C2-C3-C5-C6
9	L	1002	BCL	C4-C3-C5-C6
9	M	702	BCL	C2-C3-C5-C6
9	M	702	BCL	C4-C3-C5-C6
9	O	102	BCL	C2-C3-C5-C6
9	O	102	BCL	C4-C3-C5-C6
9	P	101	BCL	CHA-CBD-CGD-O1D
9	P	101	BCL	CHA-CBD-CGD-O2D
9	Q	101	BCL	C2-C3-C5-C6
9	Q	101	BCL	C4-C3-C5-C6
9	R	101	BCL	CHA-CBD-CGD-O1D
9	R	101	BCL	CHA-CBD-CGD-O2D
9	S	101	BCL	C2-C3-C5-C6
9	S	101	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	C2-C3-C5-C6
9	U	102	BCL	C4-C3-C5-C6
9	W	101	BCL	C2-C3-C5-C6
9	W	101	BCL	C4-C3-C5-C6
10	2	103	KGD	CAH-CAD-CAJ-CAL
10	2	103	KGD	CAJ-CAL-CAM-CAN
10	2	103	KGD	CAJ-CAL-CAM-CAO
10	4	103	KGD	CAW-CAS-CAT-CAX
10	6	103	KGD	CAJ-CAL-CAM-CAN
10	6	103	KGD	CAJ-CAL-CAM-CAO
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	B	103	KGD	CAH-CAD-CAJ-CAL
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	505	KGD	CBE-CBF-CBH-CBJ
10	C	505	KGD	CBE-CBF-CBH-CBK
10	C	506	KGD	CAJ-CAL-CAM-CAN
10	C	506	KGD	CAJ-CAL-CAM-CAO
10	D	103	KGD	CAW-CAS-CAT-CAX
10	G	102	KGD	CAP-CAQ-CAR-CAU
10	G	102	KGD	CAP-CAQ-CAR-CAV
10	G	102	KGD	CAW-CAS-CAT-CAX

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Mol	Chain	Res	Type	Atoms
10	G	102	KGD	CAT-CAS-CAW-CAZ
10	G	102	KGD	CAT-CAS-CAW-CBA
10	H	102	KGD	CAJ-CAL-CAM-CAN
10	I	103	KGD	CAW-CAS-CAT-CAX
10	I	103	KGD	CAT-CAS-CAW-CAZ
10	J	102	KGD	CBI-CBL-CBN-CBM
10	J	102	KGD	CBO-CBL-CBN-CBM
10	J	103	KGD	CAW-CAS-CAT-CAX
10	K	103	KGD	CAH-CAD-CAJ-CAL
10	K	103	KGD	CAJ-CAL-CAM-CAN
10	K	103	KGD	CAJ-CAL-CAM-CAO
10	P	102	KGD	CBE-CBF-CBH-CBJ
10	P	102	KGD	CBE-CBF-CBH-CBK
10	Q	103	KGD	CBE-CBF-CBH-CBJ
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	S	103	KGD	CAB-CAD-CAJ-CAL
10	S	103	KGD	CAH-CAD-CAJ-CAL
10	S	103	KGD	CAJ-CAL-CAM-CAN
10	S	103	KGD	CAJ-CAL-CAM-CAO
10	S	103	KGD	CAP-CAQ-CAR-CAU
10	S	103	KGD	CAP-CAQ-CAR-CAV
10	S	103	KGD	CAW-CAS-CAT-CAX
10	U	103	KGD	CAW-CAS-CAT-CAX
11	C	501	HEM	C2B-C3B-CAB-CBB
11	C	501	HEM	C2C-C3C-CAC-CBC
11	C	501	HEM	C4C-C3C-CAC-CBC
11	C	502	HEM	C2B-C3B-CAB-CBB
11	C	502	HEM	C4B-C3B-CAB-CBB
11	C	502	HEM	C2C-C3C-CAC-CBC
11	C	502	HEM	C4C-C3C-CAC-CBC
11	C	503	HEM	C2C-C3C-CAC-CBC
11	C	504	HEM	C2B-C3B-CAB-CBB
11	C	504	HEM	C4B-C3B-CAB-CBB
11	C	504	HEM	C2C-C3C-CAC-CBC
11	C	504	HEM	C4C-C3C-CAC-CBC
12	C	507	PGV	C04-O12-P-O13
12	C	507	PGV	C04-O12-P-O14
12	C	507	PGV	O12-C04-C05-C06
12	C	507	PGV	C2-C1-O01-C02
12	L	1007	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
12	L	1007	PGV	C04-O12-P-O13
12	L	1007	PGV	C04-O12-P-O14
12	L	1007	PGV	O01-C02-C03-O11
12	L	1008	PGV	C03-O11-P-O14
12	L	1008	PGV	O12-C04-C05-O05
12	L	1008	PGV	C05-C04-O12-P
12	L	1009	PGV	C03-O11-P-O12
12	L	1009	PGV	C04-O12-P-O13
13	L	1003	BPH	C4C-C3C-CAC-CBC
13	L	1003	BPH	C2C-C3C-CAC-CBC
13	L	1003	BPH	C3A-C2A-CAA-CBA
13	L	1003	BPH	C1A-C2A-CAA-CBA
13	L	1003	BPH	C2A-CAA-CBA-CGA
13	L	1006	BPH	CHA-CBD-CGD-O1D
13	L	1006	BPH	CHA-CBD-CGD-O2D
13	L	1006	BPH	C4C-C3C-CAC-CBC
13	L	1006	BPH	C2C-C3C-CAC-CBC
13	M	703	BPH	C3A-C2A-CAA-CBA
15	L	1005	MQE	CAM-CAG-CAW-CBY
15	M	701	MQE	CAW-CAG-CAM-CBG
15	M	701	MQE	CAV-CAH-CAO-CBI
15	M	701	MQE	CAO-CAH-CAV-CBX
15	M	701	MQE	CAH-CAO-CBI-CAZ
15	M	701	MQE	CCB-CCC-CCD-CCI
15	M	701	MQE	CCL-CCC-CCD-CCI
12	L	1009	PGV	O04-C19-O03-C01
12	C	507	PGV	O02-C1-O01-C02
9	0	101	BCL	C4-C3-C5-C6
9	F	102	BCL	C4-C3-C5-C6
10	S	103	KGD	CAT-CAS-CAW-CAZ
9	0	102	BCL	C2-C3-C5-C6
9	4	102	BCL	C2-C3-C5-C6
9	6	101	BCL	C2-C3-C5-C6
9	F	102	BCL	C2-C3-C5-C6
9	K	102	BCL	C2-C3-C5-C6
10	I	103	KGD	CAT-CAS-CAW-CBA
10	S	103	KGD	CAT-CAS-CAW-CBA
15	L	1005	MQE	CAM-CAG-CAW-CBH
13	M	703	BPH	C2A-CAA-CBA-CGA
9	W	102	BCL	C3-C5-C6-C7
12	L	1009	PGV	C20-C19-O03-C01
10	8	103	KGD	CAR-CAV-CBB-CBG

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Mol	Chain	Res	Type	Atoms
12	C	507	PGV	O12-C04-C05-O05
9	8	101	BCL	C4-C3-C5-C6
9	B	101	BCL	C4-C3-C5-C6
9	B	102	BCL	C4-C3-C5-C6
9	G	101	BCL	C4-C3-C5-C6
9	Q	102	BCL	C4-C3-C5-C6
9	S	102	BCL	C4-C3-C5-C6
10	8	103	KGD	CAT-CAS-CAW-CAZ
10	S	104	KGD	CAT-CAS-CAW-CAZ
10	U	103	KGD	CAT-CAS-CAW-CAZ
15	M	701	MQE	CAK-CAF-CAT-CBW
9	6	102	BCL	C2-C3-C5-C6
9	8	101	BCL	C2-C3-C5-C6
9	B	101	BCL	C2-C3-C5-C6
9	B	102	BCL	C2-C3-C5-C6
9	G	101	BCL	C2-C3-C5-C6
9	Q	102	BCL	C2-C3-C5-C6
9	S	102	BCL	C2-C3-C5-C6
10	8	103	KGD	CAT-CAS-CAW-CBA
10	S	104	KGD	CAT-CAS-CAW-CBA
10	U	103	KGD	CAT-CAS-CAW-CBA
15	M	701	MQE	CAK-CAF-CAT-CBG
15	M	701	MQE	CAO-CAH-CAV-CBF
10	0	104	KGD	CAW-CAS-CAT-CAX
10	1	103	KGD	CAW-CAS-CAT-CAX
10	2	103	KGD	CAW-CAS-CAT-CAX
10	8	103	KGD	CAW-CAS-CAT-CAX
10	K	103	KGD	CAW-CAS-CAT-CAX
10	Q	103	KGD	CAW-CAS-CAT-CAX
15	L	1005	MQE	CAP-CAC-CAI-CBD
15	L	1005	MQE	CAV-CAH-CAO-CBI
15	L	1005	MQE	CCC-CCD-CCI-CCM
15	M	701	MQE	CAQ-CAD-CAJ-CBC
15	M	701	MQE	CAR-CAE-CAL-CBF
12	L	1008	PGV	O12-C04-C05-C06
9	W	102	BCL	CBA-CGA-O2A-C1
9	K	102	BCL	C8-C10-C11-C12
12	L	1008	PGV	O03-C01-C02-O01
9	0	101	BCL	C2-C3-C5-C6
9	K	102	BCL	C11-C10-C8-C9
9	P	101	BCL	C6-C7-C8-C9
13	M	703	BPH	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	L	1003	BPH	C10-C11-C12-C13
9	O	101	BCL	C2A-CAA-CBA-CGA
10	1	103	KGD	CBE-CBF-CBH-CBK
10	4	103	KGD	CAJ-CAL-CAM-CAN
10	A	102	KGD	CBE-CBF-CBH-CBK
10	C	506	KGD	CBE-CBF-CBH-CBK
10	D	102	KGD	CBO-CBL-CBN-CBM
13	L	1006	BPH	C8-C10-C11-C12
12	L	1008	PGV	C20-C19-O03-C01
13	M	703	BPH	C13-C15-C16-C17
9	W	102	BCL	C11-C10-C8-C7
9	W	102	BCL	O1A-CGA-O2A-C1
10	C	506	KGD	CAW-CAS-CAT-CAX
10	E	103	KGD	CAW-CAS-CAT-CAX
15	M	704	MQE	CBB-CAN-CAS-CBH
12	L	1008	PGV	O04-C19-O03-C01
10	2	103	KGD	CAS-CAT-CAX-CAY
12	C	507	PGV	C03-O11-P-O12
12	C	507	PGV	C04-O12-P-O11
12	L	1008	PGV	C03-O11-P-O12
13	M	703	BPH	CBA-CGA-O2A-C1
9	O	101	BCL	C4-C3-C5-C6
10	K	103	KGD	CAT-CAS-CAW-CAZ
9	K	102	BCL	C5-C6-C7-C8
12	L	1008	PGV	C2-C1-O01-C02
12	C	507	PGV	C01-C02-O01-C1
12	C	507	PGV	C4-C5-C6-C7
12	C	507	PGV	C22-C23-C24-C25
9	K	102	BCL	C4B-C3B-CAB-OB
9	1	101	BCL	C11-C10-C8-C9
9	4	101	BCL	C11-C12-C13-C14
9	7	101	BCL	C11-C10-C8-C9
12	L	1008	PGV	C5-C6-C7-C8
9	W	102	BCL	C5-C6-C7-C8
12	L	1009	PGV	C04-C05-C06-O06
10	4	103	KGD	CAJ-CAL-CAM-CAO
12	L	1008	PGV	O02-C1-O01-C02
12	L	1008	PGV	C21-C22-C23-C24
10	S	104	KGD	CAM-CAO-CAP-CAQ
13	M	703	BPH	O1A-CGA-O2A-C1
9	I	102	BCL	O2A-C1-C2-C3
9	O	102	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	U	102	BCL	O2A-C1-C2-C3
13	L	1006	BPH	O2A-C1-C2-C3
15	M	701	MQE	CAS-CAN-CBB-CCA
15	M	701	MQE	CAS-CAN-CBB-CBL
12	L	1009	PGV	O05-C05-C06-O06
10	0	104	KGD	CAH-CAD-CAJ-CAL
10	2	103	KGD	CAB-CAD-CAJ-CAL
10	6	103	KGD	CAH-CAD-CAJ-CAL
10	B	103	KGD	CAB-CAD-CAJ-CAL
10	C	505	KGD	CAB-CAD-CAJ-CAL
10	C	506	KGD	CAB-CAD-CAJ-CAL
10	E	103	KGD	CAH-CAD-CAJ-CAL
10	G	102	KGD	CAH-CAD-CAJ-CAL
10	I	103	KGD	CAH-CAD-CAJ-CAL
10	K	103	KGD	CAB-CAD-CAJ-CAL
10	S	104	KGD	CAH-CAD-CAJ-CAL
13	L	1006	BPH	C5-C6-C7-C8
9	5	101	BCL	C4-C3-C5-C6
9	D	101	BCL	C4-C3-C5-C6
9	1	101	BCL	C11-C10-C8-C7
9	4	101	BCL	C11-C12-C13-C15
9	5	101	BCL	C2-C3-C5-C6
9	7	101	BCL	C11-C10-C8-C7
15	M	701	MQE	CAL-CAE-CAR-CBD
12	L	1007	PGV	O02-C1-O01-C02
12	L	1007	PGV	C2-C1-O01-C02
12	L	1009	PGV	C2-C1-O01-C02
11	C	501	HEM	C4B-C3B-CAB-CBB
11	C	503	HEM	C4C-C3C-CAC-CBC
12	L	1009	PGV	O02-C1-O01-C02
12	L	1009	PGV	C5-C6-C7-C8
9	I	101	BCL	C4-C3-C5-C6
10	2	103	KGD	CAT-CAS-CAW-CAZ
15	M	701	MQE	CAL-CAE-CAR-CBV
9	D	101	BCL	C2-C3-C5-C6
9	O	101	BCL	C2-C3-C5-C6
10	K	103	KGD	CAT-CAS-CAW-CBA
9	K	102	BCL	C6-C7-C8-C9
13	L	1003	BPH	C11-C10-C8-C9
13	L	1006	BPH	C11-C12-C13-C14
10	1	102	KGD	CAJ-CAL-CAM-CAN
10	5	102	KGD	CBE-CBF-CBH-CBK

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Mol	Chain	Res	Type	Atoms
10	1	103	KGD	CBE-CBF-CBH-CBJ
10	D	102	KGD	CBI-CBL-CBN-CBM
13	M	703	BPH	C16-C17-C18-C20
10	S	103	KGD	CAS-CAT-CAX-CAY
9	W	102	BCL	C10-C11-C12-C13
12	L	1007	PGV	C01-C02-C03-O11
9	K	102	BCL	C3-C5-C6-C7
13	L	1006	BPH	C10-C11-C12-C13
10	H	102	KGD	CAW-CAS-CAT-CAX
10	2	103	KGD	CAT-CAS-CAW-CBA
9	W	102	BCL	C15-C16-C17-C18
9	2	102	BCL	C4B-C3B-CAB-OB
9	2	102	BCL	C4B-C3B-CAB-CB
13	M	703	BPH	CHA-CBD-CGD-O1D
13	M	703	BPH	CHA-CBD-CGD-O2D
9	K	102	BCL	C6-C7-C8-C10
9	K	102	BCL	C11-C10-C8-C7
9	N	101	BCL	C11-C10-C8-C7
9	V	101	BCL	C11-C10-C8-C7
13	L	1003	BPH	C11-C10-C8-C7
13	L	1006	BPH	C11-C12-C13-C15
13	M	703	BPH	C6-C7-C8-C10
13	M	703	BPH	C12-C13-C15-C16
9	J	101	BCL	C11-C10-C8-C9
9	V	101	BCL	C11-C10-C8-C9
13	L	1003	BPH	C6-C7-C8-C9
13	L	1006	BPH	C6-C7-C8-C9
13	L	1006	BPH	C14-C13-C15-C16
13	M	703	BPH	C6-C7-C8-C9
13	M	703	BPH	C14-C13-C15-C16
12	L	1007	PGV	C21-C22-C23-C24
10	H	102	KGD	CAJ-CAL-CAM-CAO
12	L	1008	PGV	C6-C7-C8-C9
13	L	1003	BPH	CBA-CGA-O2A-C1
9	2	102	BCL	C2B-C3B-CAB-CB
12	L	1008	PGV	O03-C01-C02-C03
12	L	1009	PGV	O03-C01-C02-C03
9	E	101	BCL	C4-C3-C5-C6
10	1	102	KGD	CAT-CAS-CAW-CAZ
13	M	703	BPH	C16-C17-C18-C19
9	M	702	BCL	C5-C6-C7-C8
10	R	102	KGD	CAW-CAS-CAT-CAX

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Mol	Chain	Res	Type	Atoms
15	M	701	MQE	CCC-CCD-CCI-CCM
9	2	101	BCL	C2-C1-O2A-CGA
9	B	102	BCL	C2-C1-O2A-CGA
9	O	102	BCL	C2-C1-O2A-CGA
9	7	101	BCL	C6-C7-C8-C9
9	J	101	BCL	C6-C7-C8-C9
10	1	102	KGD	CAH-CAD-CAJ-CAL
10	G	102	KGD	CAB-CAD-CAJ-CAL
10	S	104	KGD	CAB-CAD-CAJ-CAL
9	0	101	BCL	C4C-C3C-CAC-CBC
10	5	102	KGD	CBE-CBF-CBH-CBJ
10	A	102	KGD	CBE-CBF-CBH-CBJ
10	B	103	KGD	CAJ-CAL-CAM-CAO
12	L	1007	PGV	C1-C2-C3-C4
12	C	507	PGV	C01-C02-C03-O11
13	L	1003	BPH	C4-C3-C5-C6
9	J	101	BCL	C11-C10-C8-C7
13	L	1006	BPH	C6-C7-C8-C10
11	C	503	HEM	C3A-C2A-CAA-CBA
9	L	1001	BCL	C2A-CAA-CBA-CGA
9	0	101	BCL	CAD-CBD-CGD-O2D
9	E	101	BCL	CAD-CBD-CGD-O2D
9	O	101	BCL	CAD-CBD-CGD-O2D
9	U	101	BCL	CAD-CBD-CGD-O2D
11	C	503	HEM	C2B-C3B-CAB-CBB
10	D	103	KGD	CAT-CAS-CAW-CAZ
12	L	1007	PGV	C3-C4-C5-C6
9	I	101	BCL	C2-C3-C5-C6
12	L	1009	PGV	C05-C04-O12-P
9	E	101	BCL	CHA-CBD-CGD-O1D
12	L	1009	PGV	O03-C01-C02-O01
13	L	1003	BPH	O1A-CGA-O2A-C1
9	W	102	BCL	C4B-C3B-CAB-OB
9	W	102	BCL	C4-C3-C5-C6
12	L	1008	PGV	C2-C3-C4-C5
10	B	103	KGD	CAJ-CAL-CAM-CAN
10	B	103	KGD	CAP-CAQ-CAR-CAU
10	7	102	KGD	CBE-CBF-CBH-CBJ
9	K	102	BCL	C1A-C2A-CAA-CBA
12	L	1008	PGV	C04-O12-P-O11
12	C	507	PGV	C03-O11-P-O13
12	L	1009	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
13	L	1006	BPH	C4-C3-C5-C6
9	R	101	BCL	C11-C10-C8-C7
10	U	103	KGD	CAR-CAV-CBB-CBG
9	2	102	BCL	C2B-C3B-CAB-OB
9	N	101	BCL	C11-C10-C8-C9
13	M	703	BPH	C11-C12-C13-C14
10	7	102	KGD	CAW-CAS-CAT-CAX
12	L	1008	PGV	C11-C10-C9-C8
9	W	102	BCL	C2-C3-C5-C6
13	L	1003	BPH	C2-C3-C5-C6
15	M	704	MQE	CBQ-CAX-CAY-CBL
9	2	102	BCL	C2-C1-O2A-CGA
9	I	101	BCL	C2-C1-O2A-CGA
9	I	102	BCL	C2-C1-O2A-CGA
9	K	101	BCL	C2-C1-O2A-CGA
9	K	102	BCL	C2-C1-O2A-CGA
9	U	102	BCL	C2-C1-O2A-CGA
10	S	103	KGD	CBB-CBG-CBI-CBL
15	L	1005	MQE	CAO-CAH-CAV-CBX
10	D	103	KGD	CAT-CAS-CAW-CBA
9	K	102	BCL	CBD-CGD-O2D-CED
12	L	1009	PGV	C04-O12-P-O11
12	C	507	PGV	C1-C2-C3-C4
9	W	102	BCL	C4B-C3B-CAB-CBB
13	L	1003	BPH	CHA-CBD-CGD-O1D
13	L	1003	BPH	CHA-CBD-CGD-O2D
9	R	101	BCL	C11-C10-C8-C9
9	W	102	BCL	C11-C10-C8-C9
10	0	104	KGD	CBB-CBG-CBI-CBL
11	C	503	HEM	C1A-C2A-CAA-CBA
12	C	507	PGV	C19-C20-C21-C22
12	L	1007	PGV	C02-C03-O11-P
10	1	102	KGD	CAJ-CAL-CAM-CAO
10	C	506	KGD	CBE-CBF-CBH-CBJ
9	K	102	BCL	C15-C16-C17-C18
9	E	101	BCL	C2-C3-C5-C6
10	1	102	KGD	CAT-CAS-CAW-CBA
10	D	102	KGD	CBH-CBJ-CBM-CBN
13	M	703	BPH	C15-C16-C17-C18
9	4	101	BCL	C2-C1-O2A-CGA
9	E	102	BCL	C2-C1-O2A-CGA
9	Q	101	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	K	102	BCL	C16-C17-C18-C19
9	E	102	BCL	C11-C12-C13-C14
9	T	101	BCL	C6-C7-C8-C9
12	C	507	PGV	C14-C15-C16-C17
9	8	102	BCL	O2A-C1-C2-C3
10	7	102	KGD	CBE-CBF-CBH-CBK
10	D	102	KGD	CBE-CBF-CBH-CBK
10	O	103	KGD	CAP-CAQ-CAR-CAU
10	B	103	KGD	CAP-CAQ-CAR-CAV
10	J	103	KGD	CAT-CAS-CAW-CAZ
10	O	103	KGD	CAT-CAS-CAW-CAZ
9	W	102	BCL	C1A-C2A-CAA-CBA
13	M	703	BPH	C11-C10-C8-C7
10	J	102	KGD	CAM-CAO-CAP-CAQ
11	C	503	HEM	C2A-CAA-CBA-CGA
10	C	505	KGD	CAW-CBA-CBE-CBF
10	E	103	KGD	CAW-CBA-CBE-CBF
10	J	102	KGD	CBH-CBJ-CBM-CBN
11	C	502	HEM	CAA-CBA-CGA-O2A
9	L	1002	BCL	C10-C11-C12-C13
15	L	1005	MQE	CAR-CAE-CAL-CBF
9	U	101	BCL	C2-C1-O2A-CGA
9	9	101	BCL	C11-C10-C8-C9
12	C	507	PGV	C13-C14-C15-C16
11	C	503	HEM	CAA-CBA-CGA-O1A
10	7	102	KGD	CAM-CAO-CAP-CAQ
10	Q	103	KGD	CAW-CBA-CBE-CBF
10	S	104	KGD	CBB-CBG-CBI-CBL
9	E	101	BCL	C4C-C3C-CAC-CBC
9	K	101	BCL	C4C-C3C-CAC-CBC
9	S	101	BCL	C4C-C3C-CAC-CBC
9	U	101	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C4C-C3C-CAC-CBC
10	D	102	KGD	CBE-CBF-CBH-CBJ
15	L	1005	MQE	CAO-CAH-CAV-CBF
11	C	502	HEM	CAA-CBA-CGA-O1A
9	9	101	BCL	C4-C3-C5-C6
13	L	1006	BPH	C12-C13-C15-C16
9	W	102	BCL	C8-C10-C11-C12
9	I	101	BCL	CAA-CBA-CGA-O2A
10	0	104	KGD	CAT-CAS-CAW-CAZ
10	J	103	KGD	CAT-CAS-CAW-CBA

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Mol	Chain	Res	Type	Atoms
13	L	1006	BPH	C2-C3-C5-C6
9	A	101	BCL	CAA-CBA-CGA-O2A
9	Q	102	BCL	CAA-CBA-CGA-O2A
9	1	101	BCL	C6-C7-C8-C9
9	E	102	BCL	C11-C10-C8-C9
9	R	101	BCL	C6-C7-C8-C9
9	W	102	BCL	C6-C7-C8-C9
9	9	101	BCL	CAA-CBA-CGA-O2A
9	D	101	BCL	CAA-CBA-CGA-O2A
9	H	101	BCL	CAA-CBA-CGA-O2A
12	C	507	PGV	C11-C12-C13-C14
9	6	101	BCL	CAD-CBD-CGD-O2D
9	I	101	BCL	CAD-CBD-CGD-O2D
9	K	101	BCL	CAD-CBD-CGD-O2D
9	S	101	BCL	CAD-CBD-CGD-O2D
9	W	101	BCL	CAD-CBD-CGD-O2D
13	M	703	BPH	C3-C5-C6-C7
9	E	101	BCL	C2B-C3B-CAB-CBB
9	2	101	BCL	CAA-CBA-CGA-O2A
9	G	101	BCL	CAA-CBA-CGA-O2A
9	L	1002	BCL	CAA-CBA-CGA-O2A
9	R	101	BCL	CAA-CBA-CGA-O2A
9	F	101	BCL	CAA-CBA-CGA-O2A
9	K	101	BCL	CAA-CBA-CGA-O2A
10	5	102	KGD	CBI-CBL-CBN-CBM
10	D	102	KGD	CAJ-CAL-CAM-CAO
10	O	103	KGD	CAP-CAQ-CAR-CAV
10	R	102	KGD	CBE-CBF-CBH-CBJ
10	S	104	KGD	CAP-CAQ-CAR-CAV
15	M	701	MQE	CAF-CAK-CBE-CAQ
13	L	1003	BPH	C8-C10-C11-C12
9	1	101	BCL	CAA-CBA-CGA-O2A
9	3	101	BCL	CAA-CBA-CGA-O2A
9	T	101	BCL	CAA-CBA-CGA-O2A
11	C	503	HEM	C4B-C3B-CAB-CBB
9	J	101	BCL	CAA-CBA-CGA-O2A
9	Q	101	BCL	CAA-CBA-CGA-O2A
9	S	102	BCL	CAA-CBA-CGA-O2A
13	M	703	BPH	CAA-CBA-CGA-O2A
12	L	1008	PGV	C11-C12-C13-C14
9	1	101	BCL	CHA-CBD-CGD-O1D
9	1	101	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	2	101	BCL	CHA-CBD-CGD-O2D
9	2	102	BCL	CHA-CBD-CGD-O1D
9	2	102	BCL	CHA-CBD-CGD-O2D
9	3	101	BCL	CHA-CBD-CGD-O1D
9	3	101	BCL	CHA-CBD-CGD-O2D
9	5	101	BCL	CHA-CBD-CGD-O1D
9	5	101	BCL	CHA-CBD-CGD-O2D
9	7	101	BCL	CHA-CBD-CGD-O1D
9	7	101	BCL	CHA-CBD-CGD-O2D
9	D	101	BCL	CHA-CBD-CGD-O1D
9	D	101	BCL	CHA-CBD-CGD-O2D
9	F	101	BCL	CHA-CBD-CGD-O1D
9	F	101	BCL	CHA-CBD-CGD-O2D
9	H	101	BCL	CHA-CBD-CGD-O2D
9	J	101	BCL	CHA-CBD-CGD-O1D
9	J	101	BCL	CHA-CBD-CGD-O2D
9	L	1001	BCL	CHA-CBD-CGD-O1D
9	L	1001	BCL	CHA-CBD-CGD-O2D
9	S	101	BCL	CHA-CBD-CGD-O2D
9	U	101	BCL	CHA-CBD-CGD-O2D
9	W	102	BCL	CHA-CBD-CGD-O1D
9	W	102	BCL	CHA-CBD-CGD-O2D
9	4	101	BCL	CAA-CBA-CGA-O2A
9	5	101	BCL	CAA-CBA-CGA-O2A
9	7	101	BCL	CAA-CBA-CGA-O2A
13	L	1003	BPH	CAA-CBA-CGA-O2A
9	6	101	BCL	CAA-CBA-CGA-O2A
9	M	702	BCL	CAA-CBA-CGA-O2A
9	U	101	BCL	CAA-CBA-CGA-O2A
9	N	101	BCL	C15-C16-C17-C18
9	N	101	BCL	CAA-CBA-CGA-O2A
9	O	101	BCL	CAA-CBA-CGA-O2A
9	V	101	BCL	CAA-CBA-CGA-O2A
10	J	102	KGD	CAT-CAS-CAW-CAZ
9	K	102	BCL	C16-C17-C18-C20
9	6	101	BCL	C11-C12-C13-C14
9	A	101	BCL	C6-C7-C8-C9
9	D	101	BCL	CAA-CBA-CGA-O1A
9	H	101	BCL	CAA-CBA-CGA-O1A
15	M	701	MQE	CBM-CBJ-CBO-CCB
11	C	504	HEM	CAA-CBA-CGA-O2A
9	T	101	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
10	A	102	KGD	CAS-CAT-CAX-CAY
9	K	101	BCL	CAA-CBA-CGA-O1A
15	M	701	MQE	CBA-CAU-CAZ-CBZ
11	C	503	HEM	CAA-CBA-CGA-O2A
9	Q	102	BCL	CAA-CBA-CGA-O1A
9	K	102	BCL	O1D-CGD-O2D-CED
10	J	102	KGD	CAS-CAT-CAX-CAY
9	2	101	BCL	CAA-CBA-CGA-O1A
9	4	101	BCL	CAA-CBA-CGA-O1A
9	L	1002	BCL	CAA-CBA-CGA-O1A
9	R	101	BCL	CAA-CBA-CGA-O1A
9	A	101	BCL	CAA-CBA-CGA-O1A
9	U	101	BCL	CAA-CBA-CGA-O1A
9	V	101	BCL	CAA-CBA-CGA-O1A
9	9	101	BCL	CAA-CBA-CGA-O1A
9	I	101	BCL	CAA-CBA-CGA-O1A
9	Q	101	BCL	CAA-CBA-CGA-O1A
9	S	102	BCL	CAA-CBA-CGA-O1A
13	L	1003	BPH	CAA-CBA-CGA-O1A
10	E	103	KGD	CAB-CAD-CAJ-CAL
10	J	103	KGD	CAB-CAD-CAJ-CAL
9	7	101	BCL	CAA-CBA-CGA-O1A
9	F	101	BCL	CAA-CBA-CGA-O1A
9	J	101	BCL	CAA-CBA-CGA-O1A
12	L	1009	PGV	O01-C1-C2-C3
12	L	1007	PGV	C20-C21-C22-C23
9	3	101	BCL	CAA-CBA-CGA-O1A
9	5	101	BCL	CAA-CBA-CGA-O1A
9	N	101	BCL	CAA-CBA-CGA-O1A
9	T	101	BCL	C4-C3-C5-C6
15	L	1005	MQE	CAI-CAC-CAP-CBT
9	1	101	BCL	CAD-CBD-CGD-O1D
9	2	102	BCL	CAD-CBD-CGD-O1D
9	1	101	BCL	CAA-CBA-CGA-O1A
9	G	101	BCL	CAA-CBA-CGA-O1A
9	B	101	BCL	CAA-CBA-CGA-O2A
11	C	504	HEM	CAA-CBA-CGA-O1A
9	6	101	BCL	CAA-CBA-CGA-O1A
13	M	703	BPH	CAA-CBA-CGA-O1A
9	6	101	BCL	C11-C12-C13-C15
9	9	101	BCL	C11-C10-C8-C7
9	W	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
10	O	103	KGD	CAT-CAS-CAW-CBA
10	E	103	KGD	CAJ-CAL-CAM-CAO
10	S	103	KGD	CBE-CBF-CBH-CBJ
10	1	103	KGD	CAR-CAV-CBB-CBG
9	E	101	BCL	C2B-C3B-CAB-OBB
9	E	101	BCL	CAA-CBA-CGA-O2A
9	5	101	BCL	C8-C10-C11-C12
9	B	101	BCL	CAA-CBA-CGA-O1A
9	O	101	BCL	CAA-CBA-CGA-O1A
10	5	102	KGD	CAW-CAS-CAT-CAX
9	U	101	BCL	C10-C11-C12-C13
9	N	101	BCL	C4-C3-C5-C6
11	C	502	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

83 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	101	BCL	5	0
10	1	102	KGD	2	0
9	S	102	BCL	8	0
10	A	102	KGD	2	0
10	7	102	KGD	1	0
10	H	102	KGD	2	0
9	U	102	BCL	7	0
13	L	1006	BPH	7	0
10	J	103	KGD	3	0
15	M	704	MQE	3	0
9	L	1002	BCL	3	0
10	E	103	KGD	3	0
9	U	101	BCL	7	0
10	P	102	KGD	3	0
9	K	102	BCL	6	0
9	G	101	BCL	4	0
9	8	102	BCL	6	0
9	H	101	BCL	1	0
9	V	101	BCL	3	0
10	G	102	KGD	5	0
11	C	504	HEM	7	0
9	B	101	BCL	5	0
9	L	1001	BCL	3	0
10	8	103	KGD	1	0

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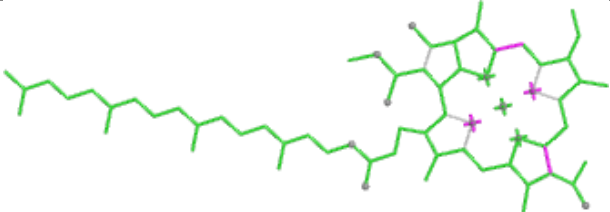
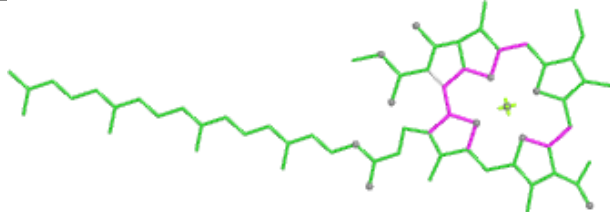
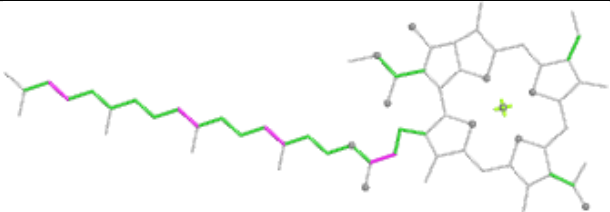
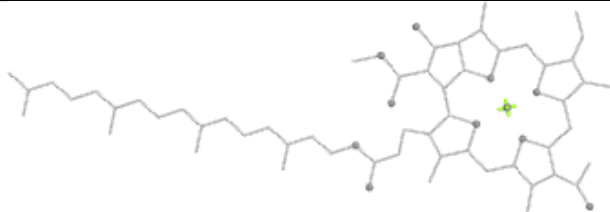
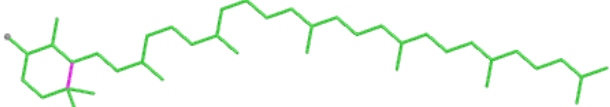
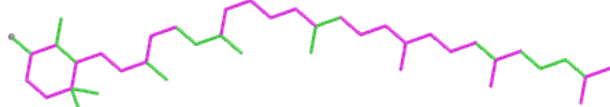
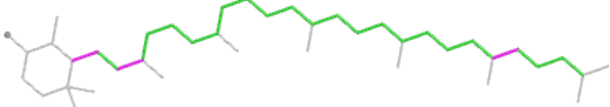
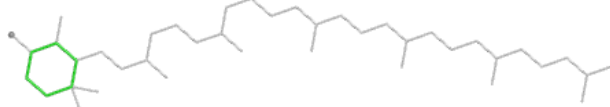
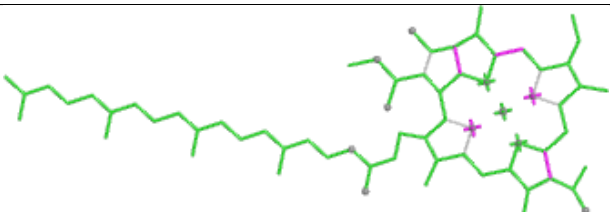
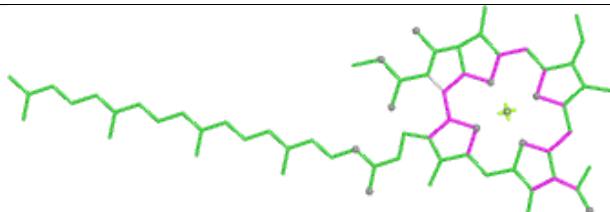
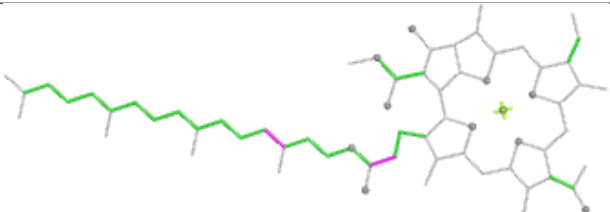
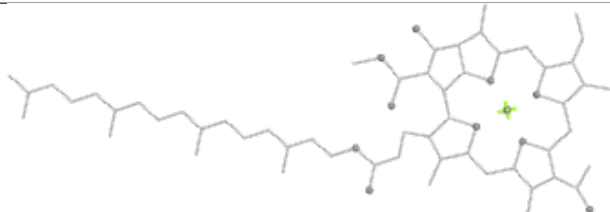
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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9	4	101	BCL	3	0
10	C	505	KGD	3	0
9	I	101	BCL	2	0
9	7	101	BCL	3	0
10	I	103	KGD	3	0
9	5	101	BCL	1	0
9	E	101	BCL	7	0
15	M	701	MQE	2	0
10	Q	103	KGD	1	0
9	0	101	BCL	6	0
9	8	101	BCL	3	0
11	C	503	HEM	3	0
10	D	103	KGD	5	0
9	R	101	BCL	5	0
9	T	101	BCL	8	0
9	W	101	BCL	2	0
10	0	104	KGD	1	0
9	6	102	BCL	8	0
9	B	102	BCL	5	0
9	4	102	BCL	8	0
9	6	101	BCL	4	0
9	0	102	BCL	5	0
12	C	507	PGV	2	0
10	K	103	KGD	2	0
13	M	703	BPH	4	0
13	L	1003	BPH	5	0
9	P	101	BCL	4	0
9	I	102	BCL	8	0
9	A	101	BCL	7	0
9	K	101	BCL	5	0
11	C	501	HEM	3	0
9	J	101	BCL	2	0
10	U	103	KGD	9	0
10	S	103	KGD	3	0
9	S	101	BCL	9	0
9	F	102	BCL	2	0
9	O	102	BCL	5	0
9	W	102	BCL	6	0
9	2	102	BCL	3	0
9	D	101	BCL	3	0
9	M	702	BCL	4	0

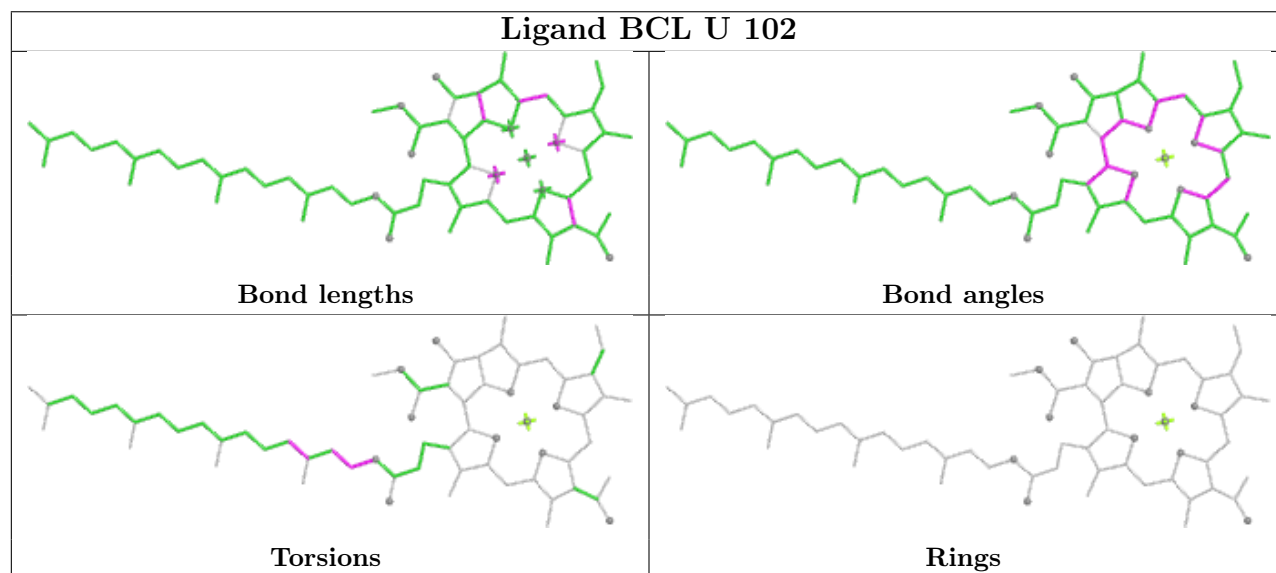
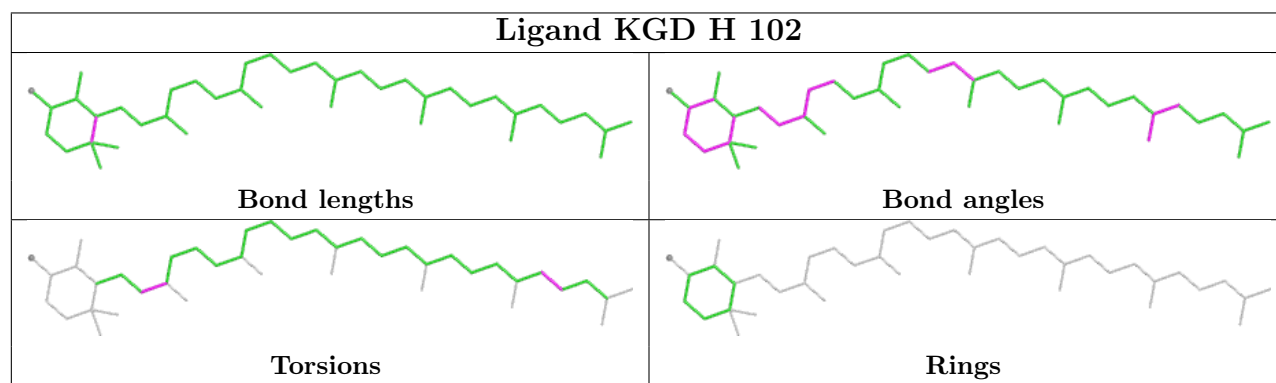
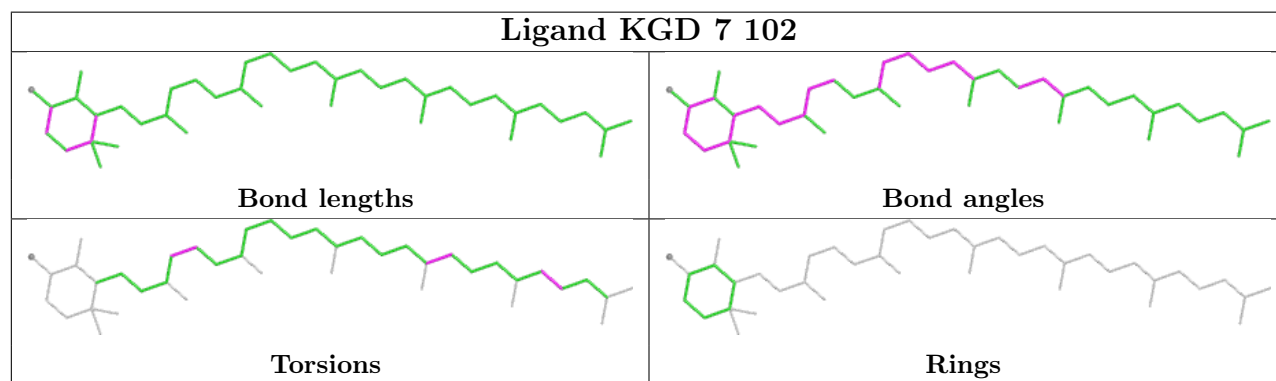
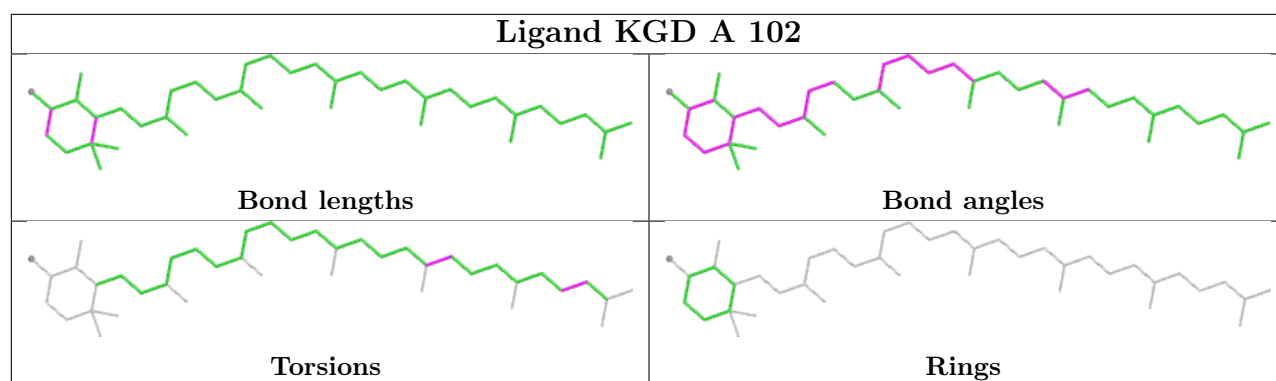
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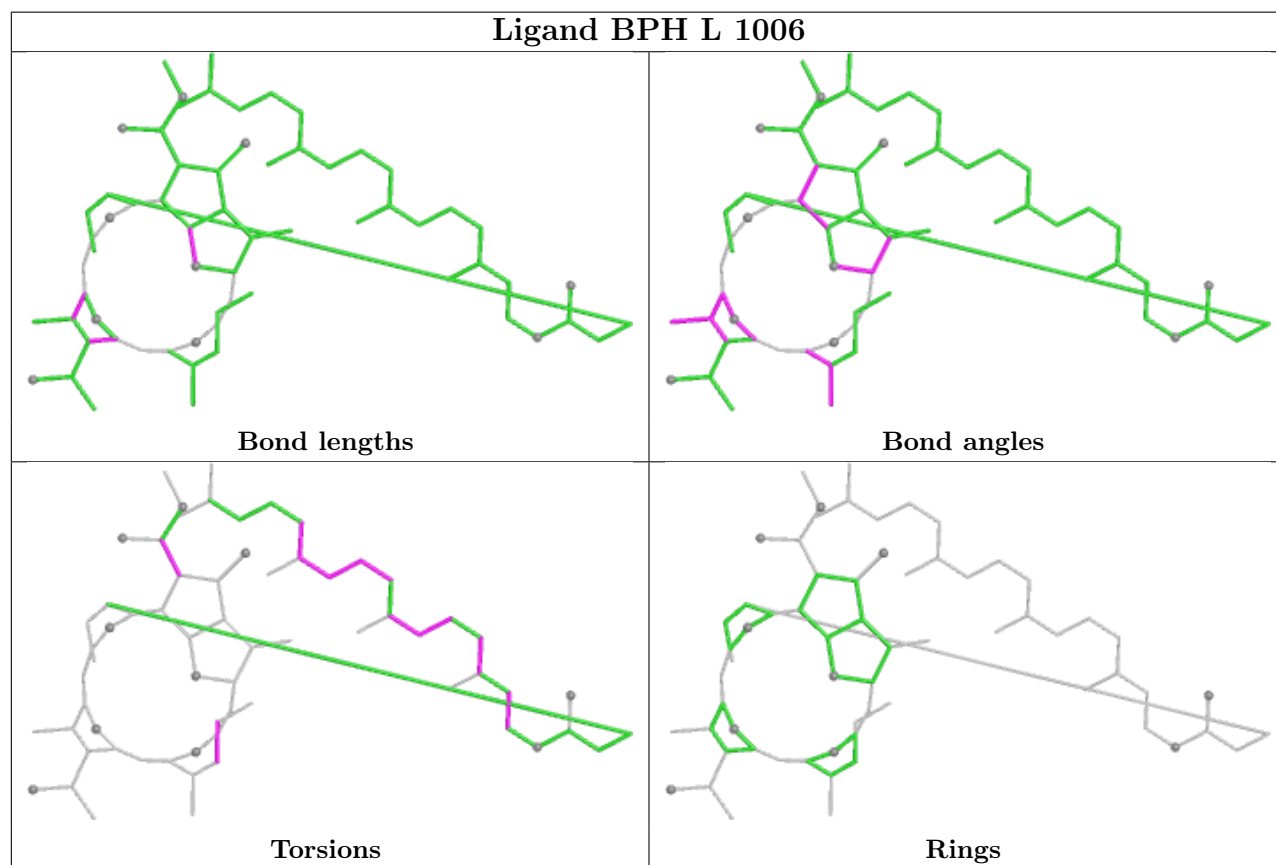
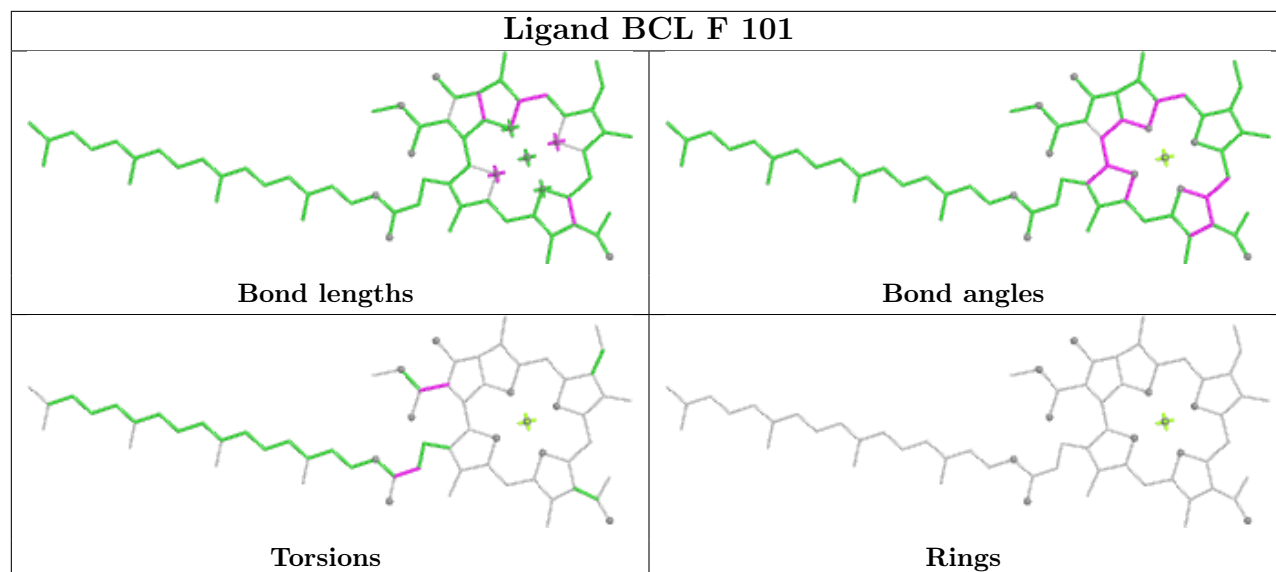
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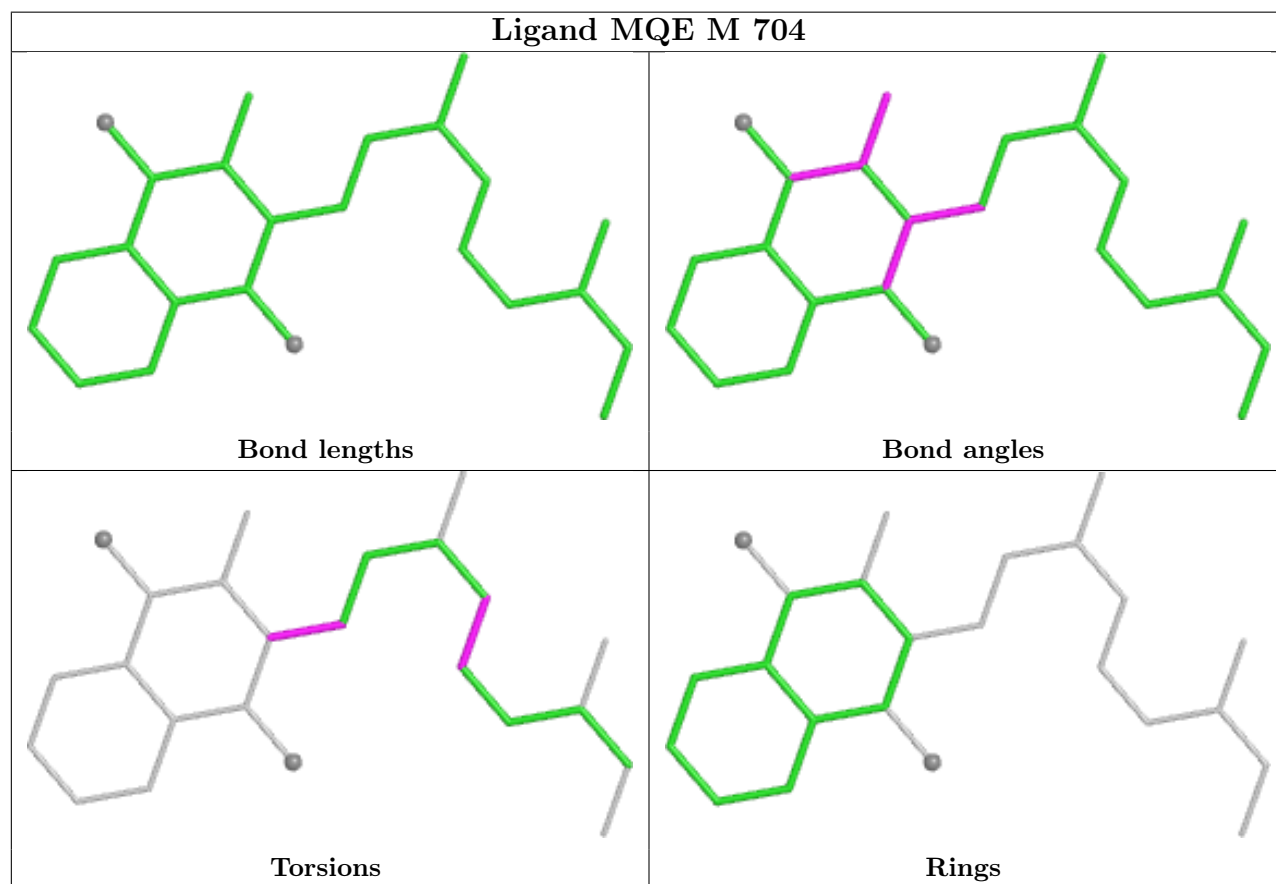
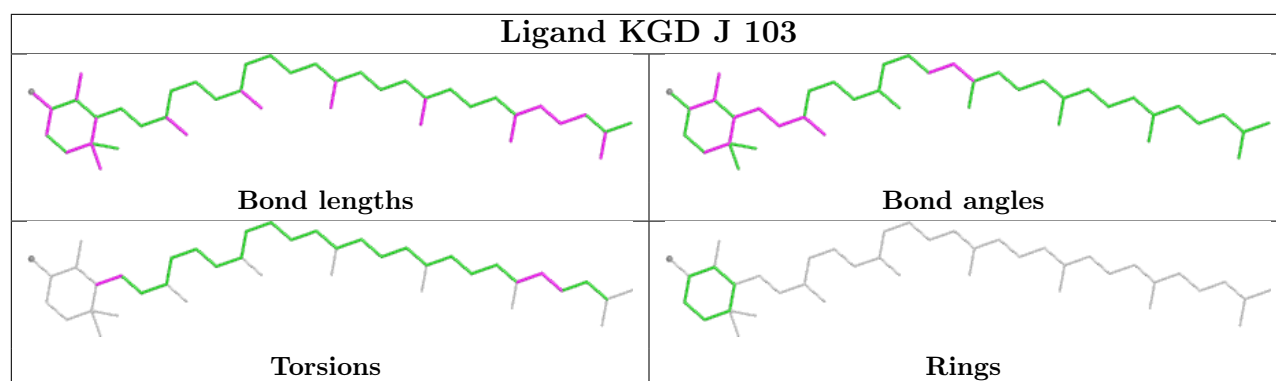
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	O	103	KGD	1	0
9	E	102	BCL	4	0
10	5	102	KGD	1	0
10	2	103	KGD	3	0
9	9	101	BCL	5	0
10	R	102	KGD	1	0
12	L	1008	PGV	1	0
15	L	1005	MQE	1	0
9	Q	101	BCL	5	0
10	B	103	KGD	4	0
9	Q	102	BCL	4	0
10	D	102	KGD	5	0
10	6	103	KGD	4	0
12	L	1009	PGV	1	0
10	S	104	KGD	5	0
10	4	103	KGD	3	0
9	O	101	BCL	7	0

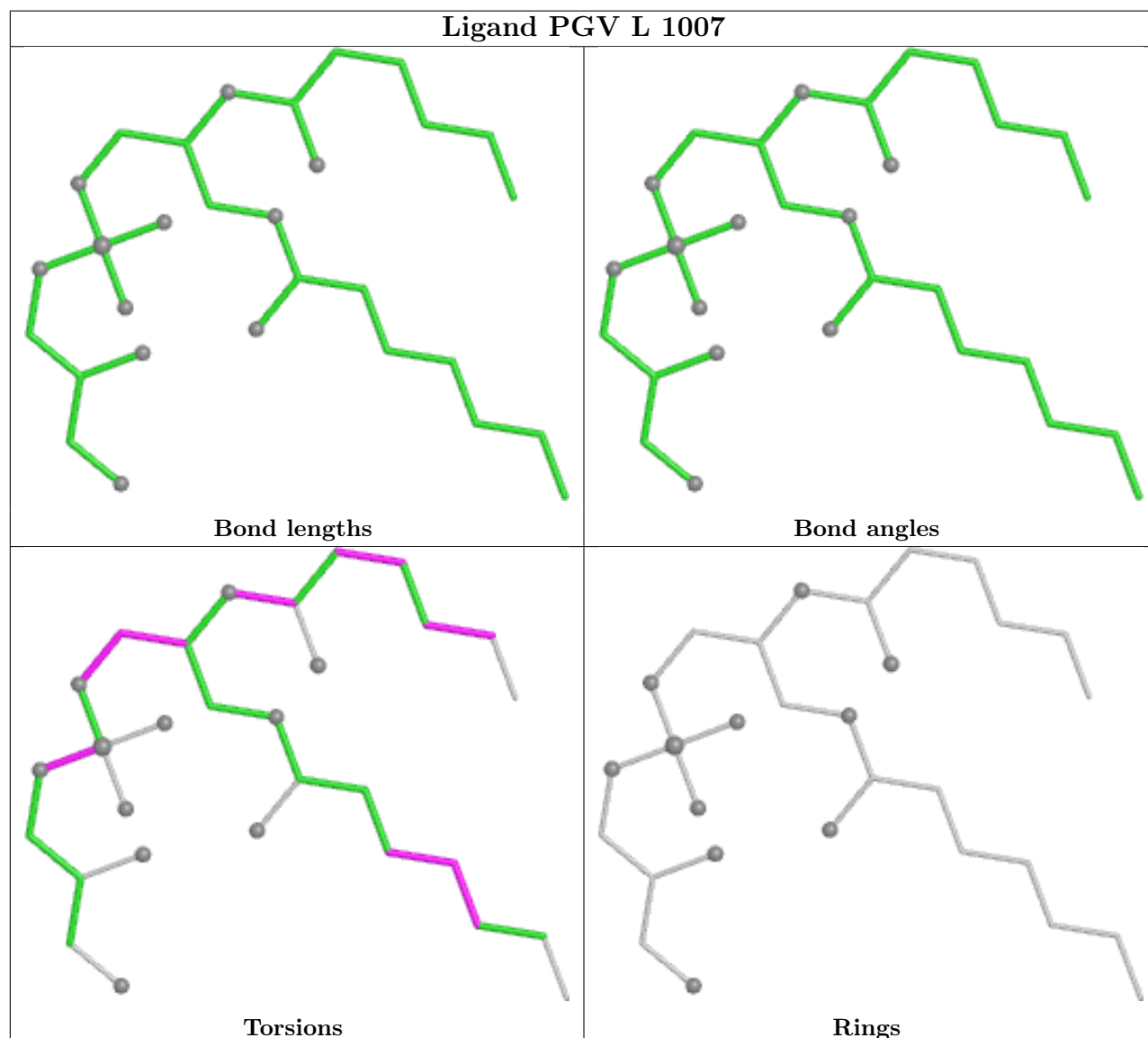
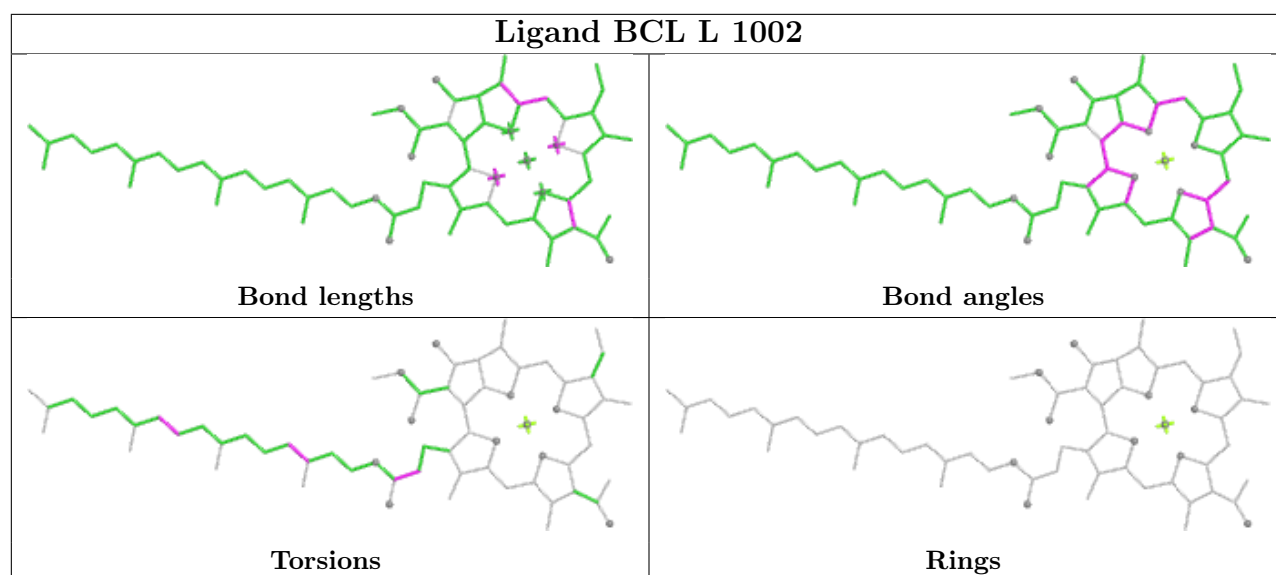
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

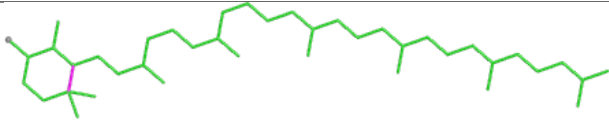
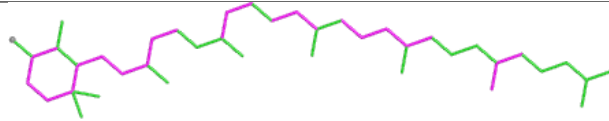
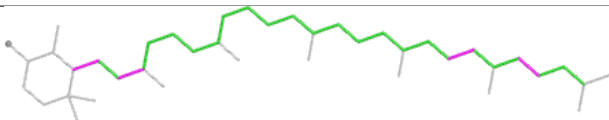
Ligand BCL N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand KGD 1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL S 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

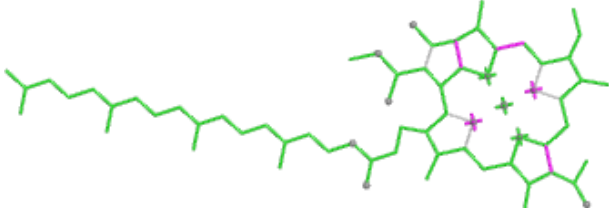
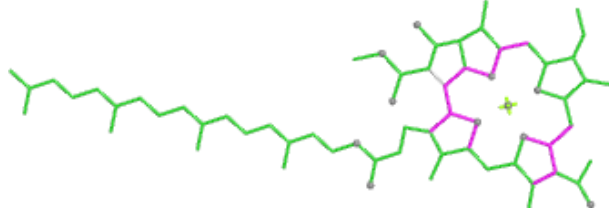
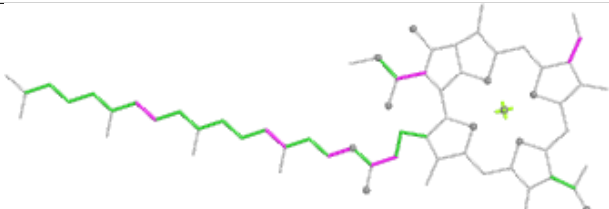
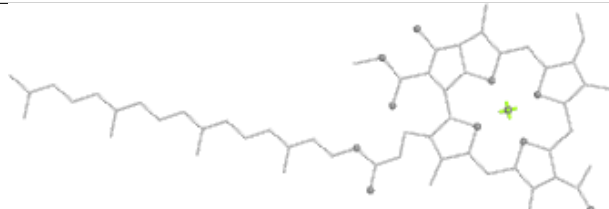


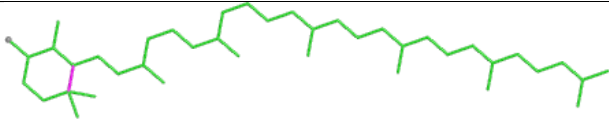
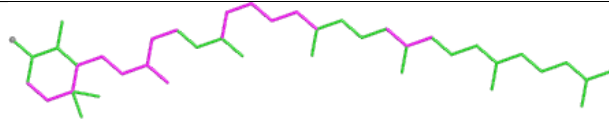
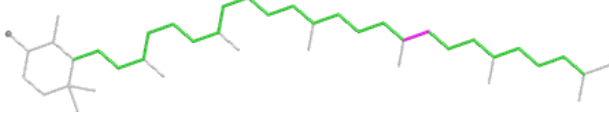
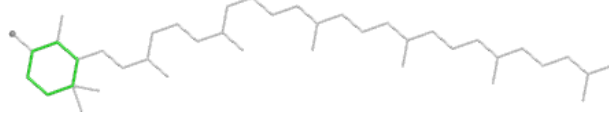


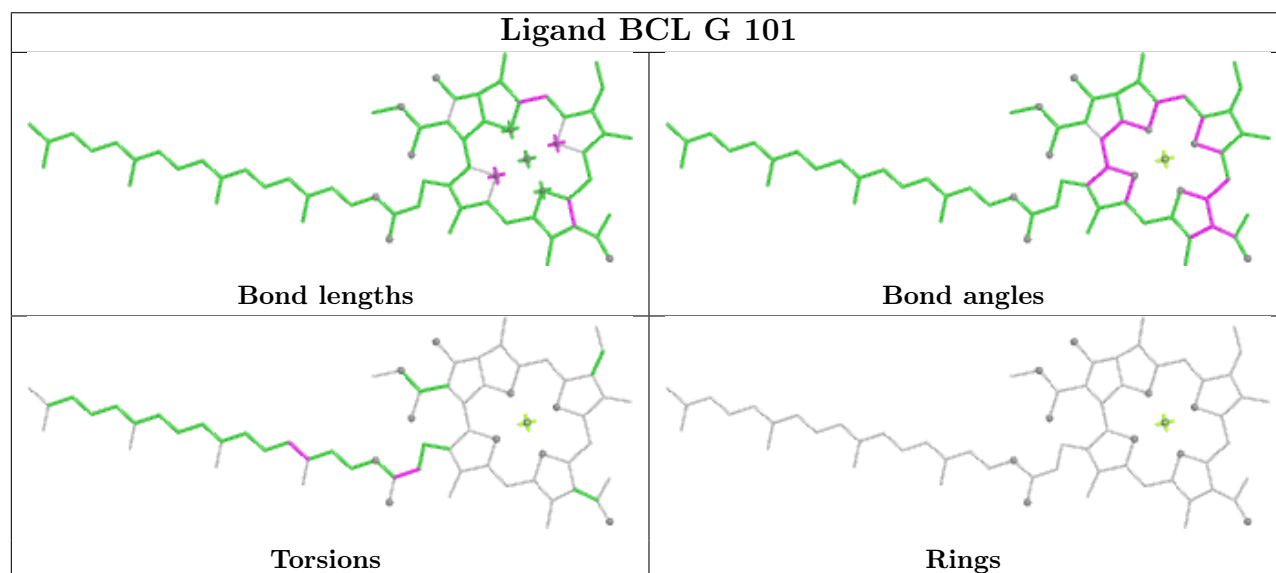
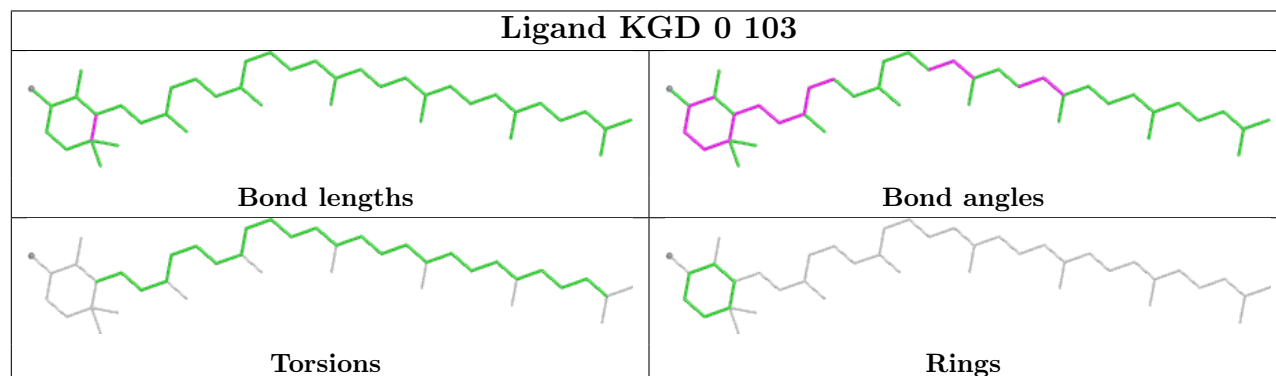
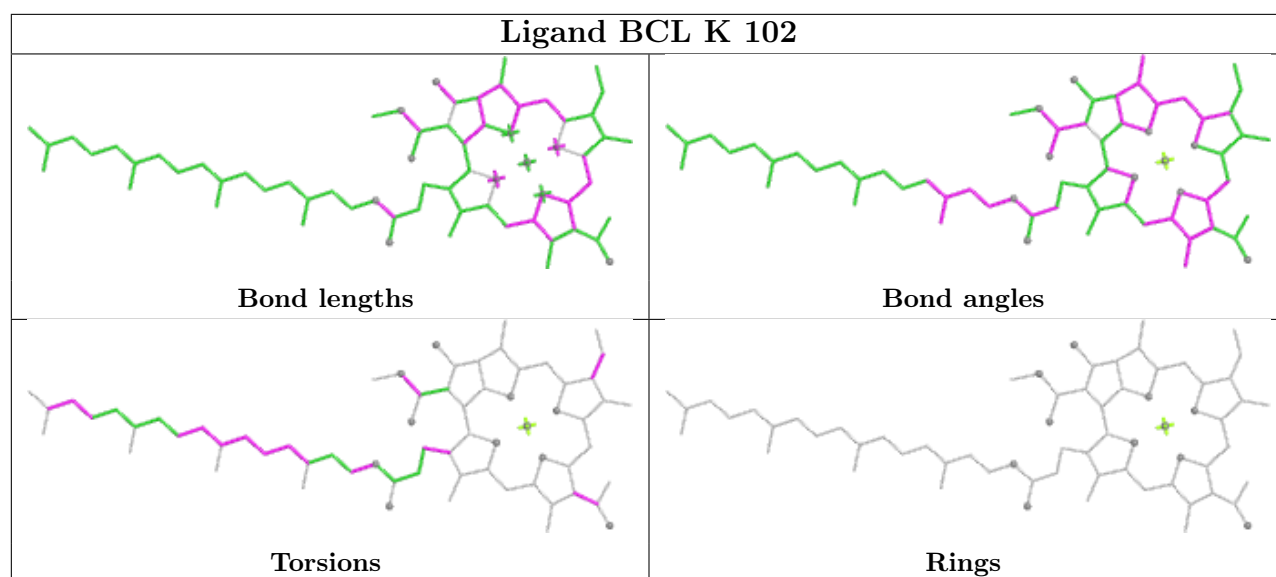


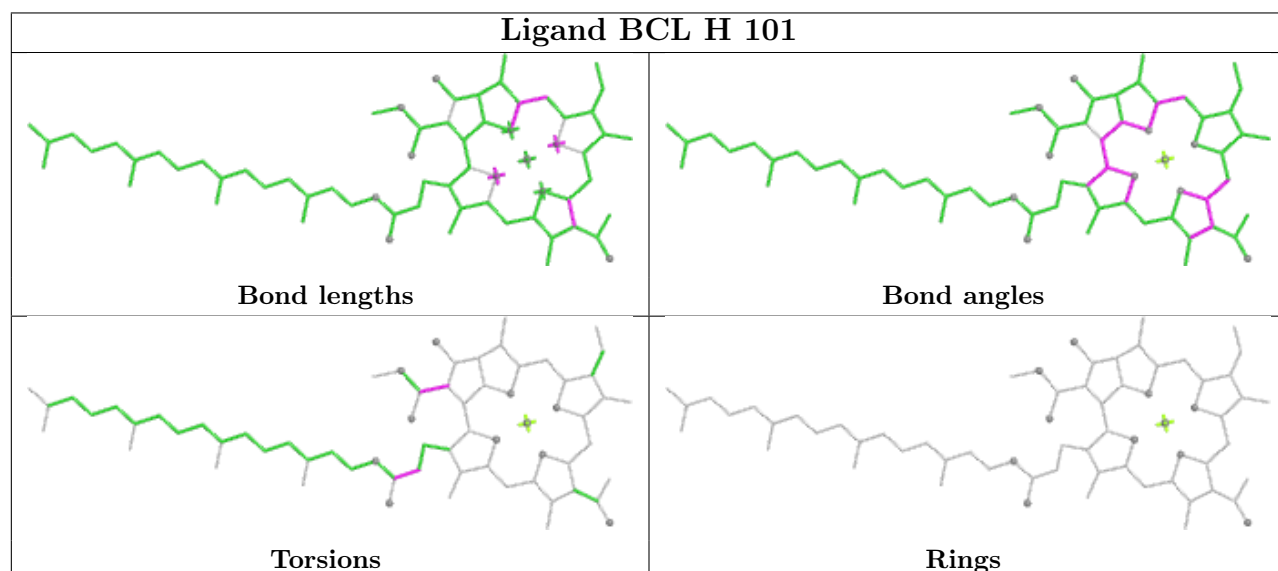
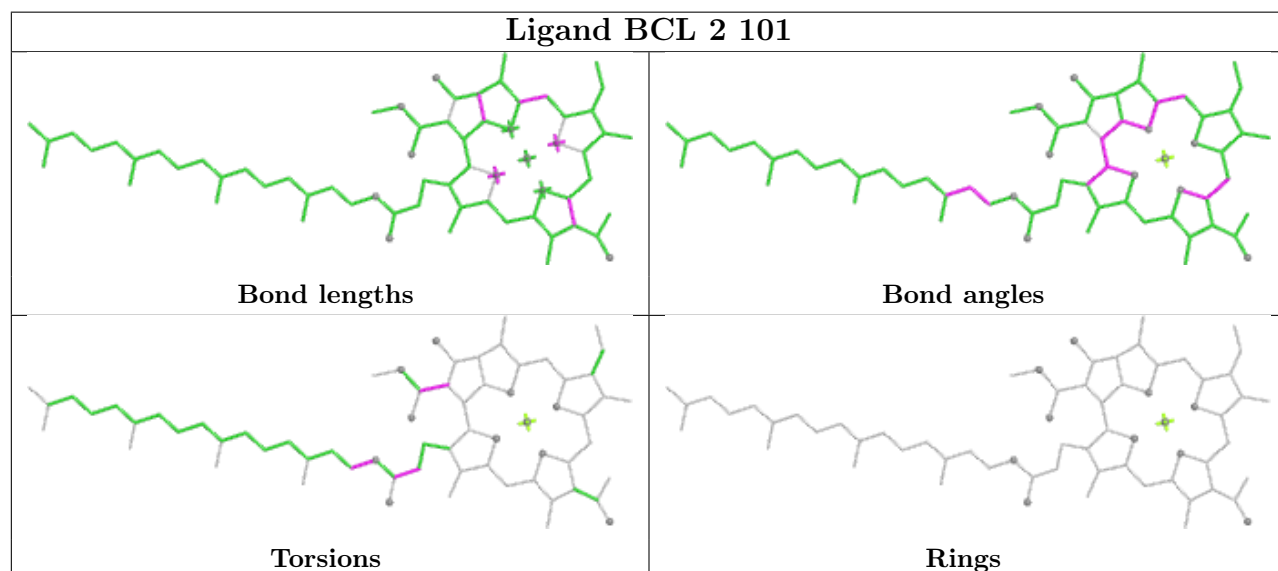
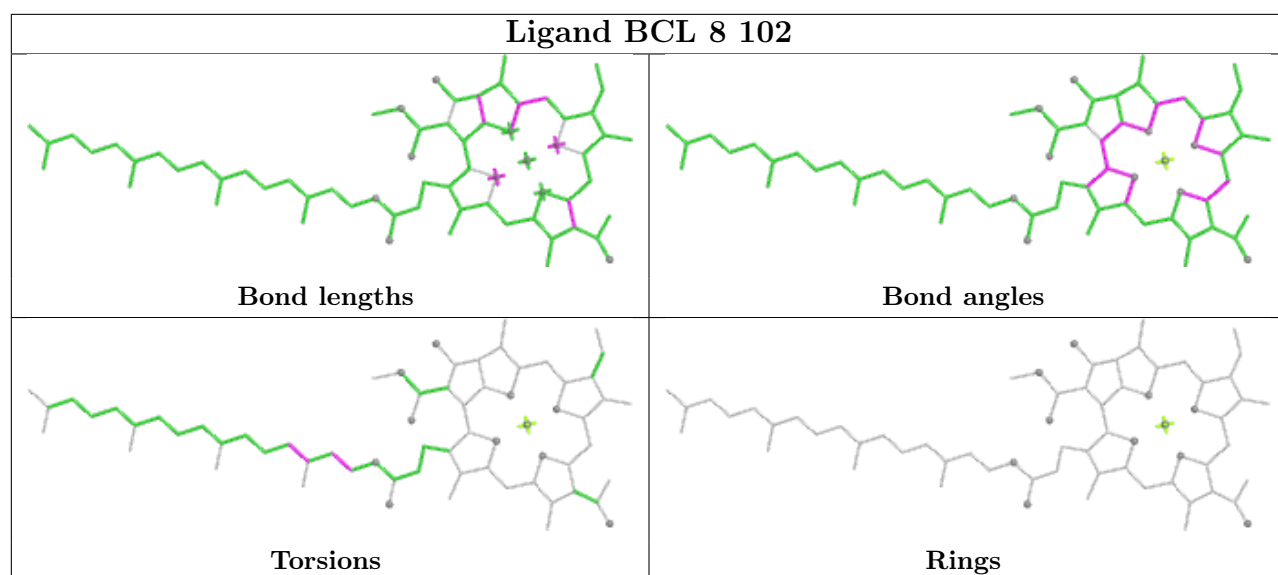


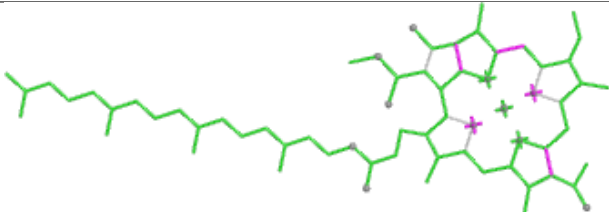
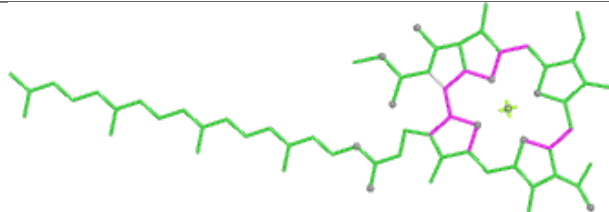
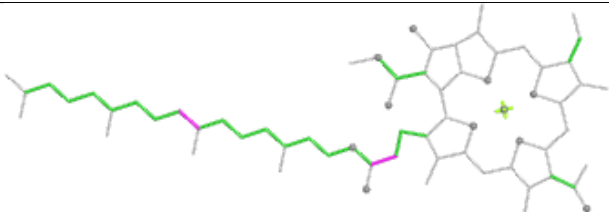
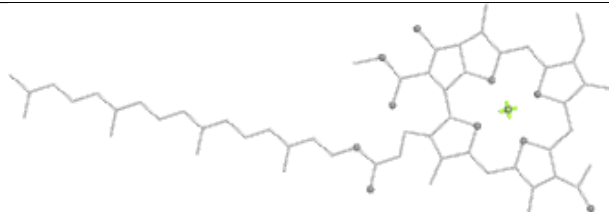
Ligand KGD E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

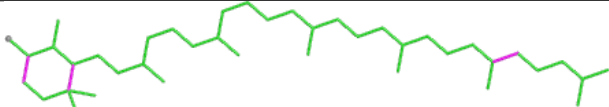
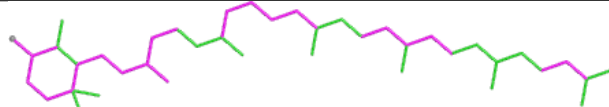
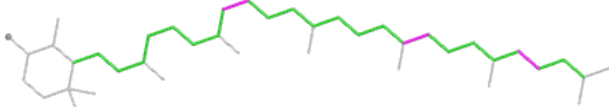
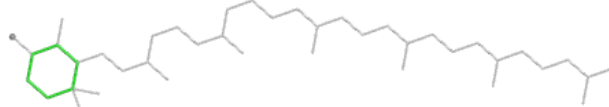
Ligand BCL U 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

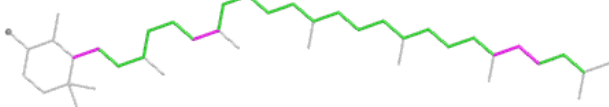
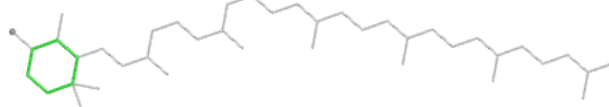
Ligand KGD P 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

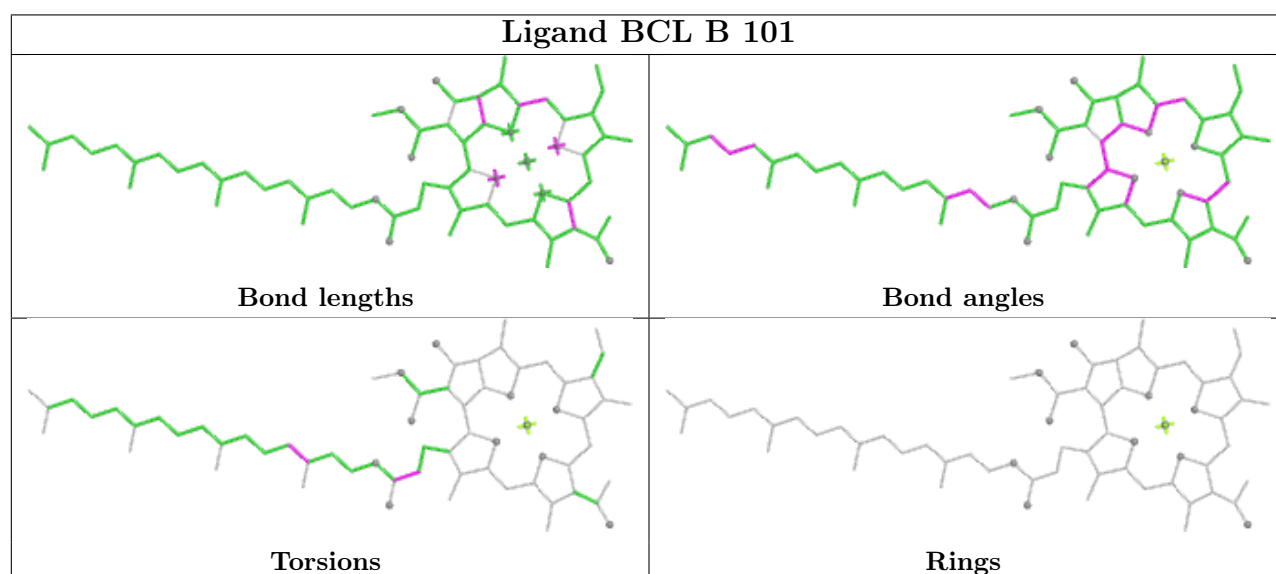
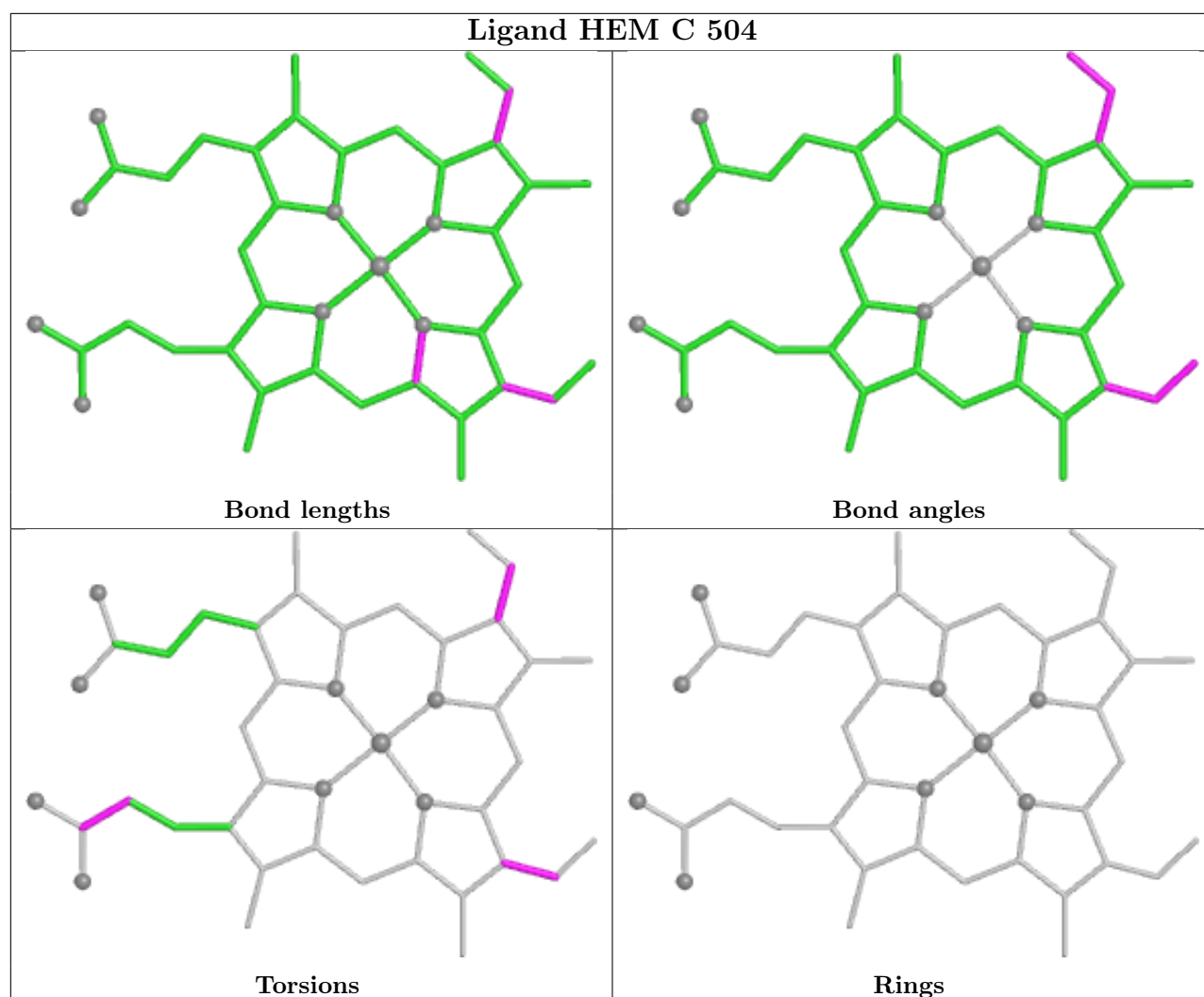


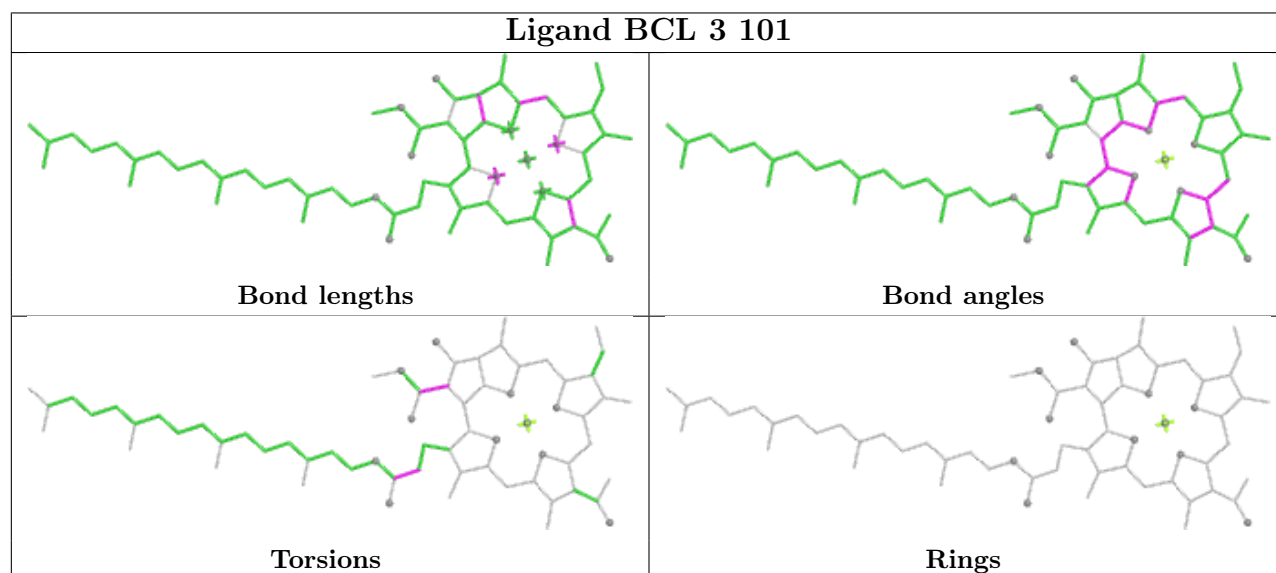
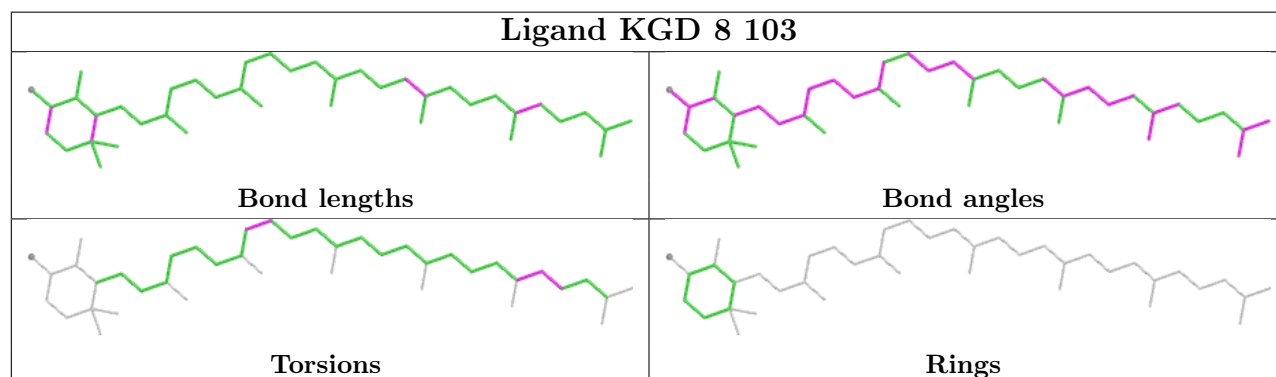
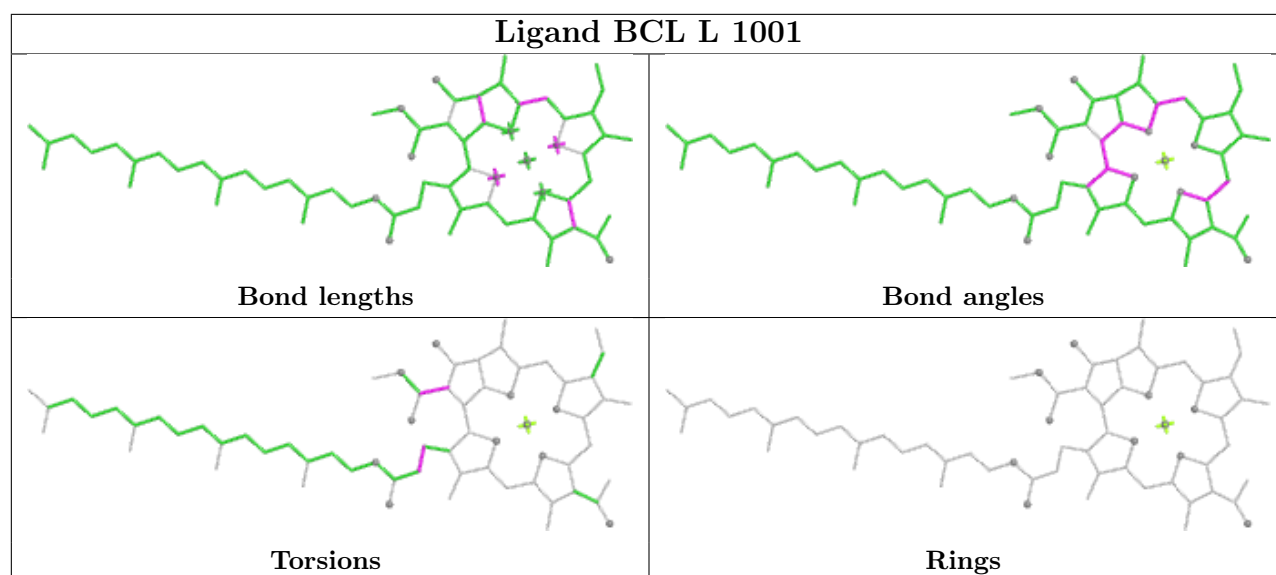


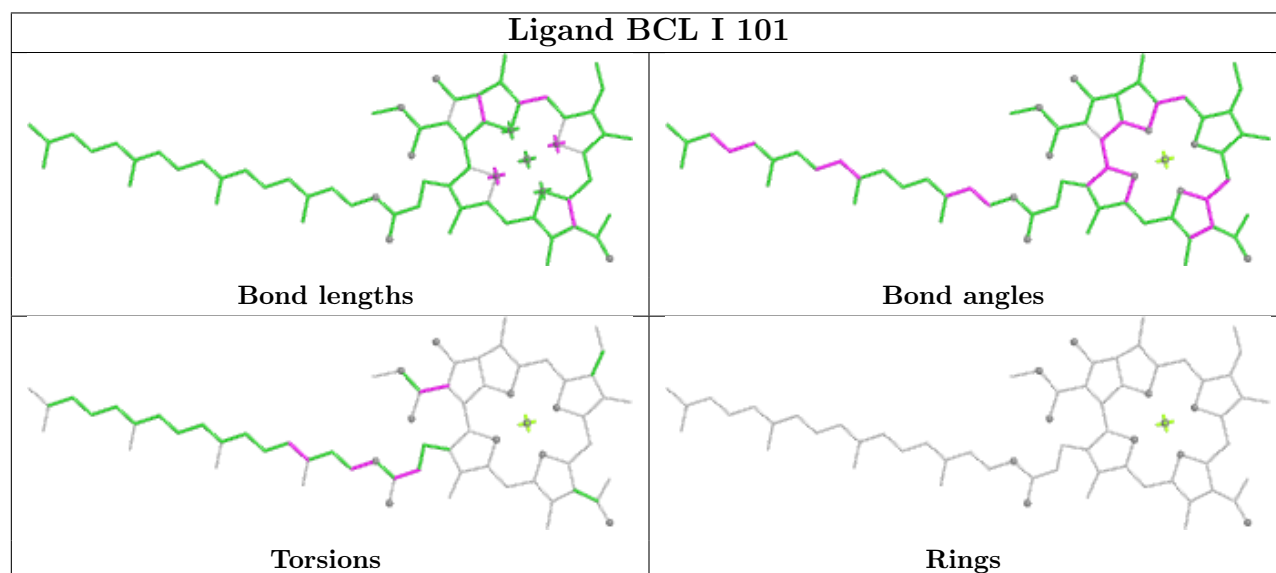
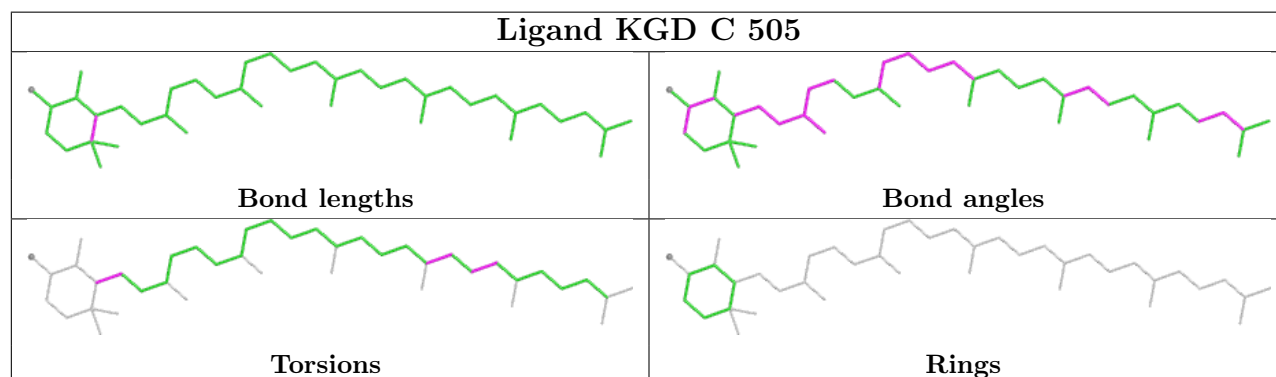
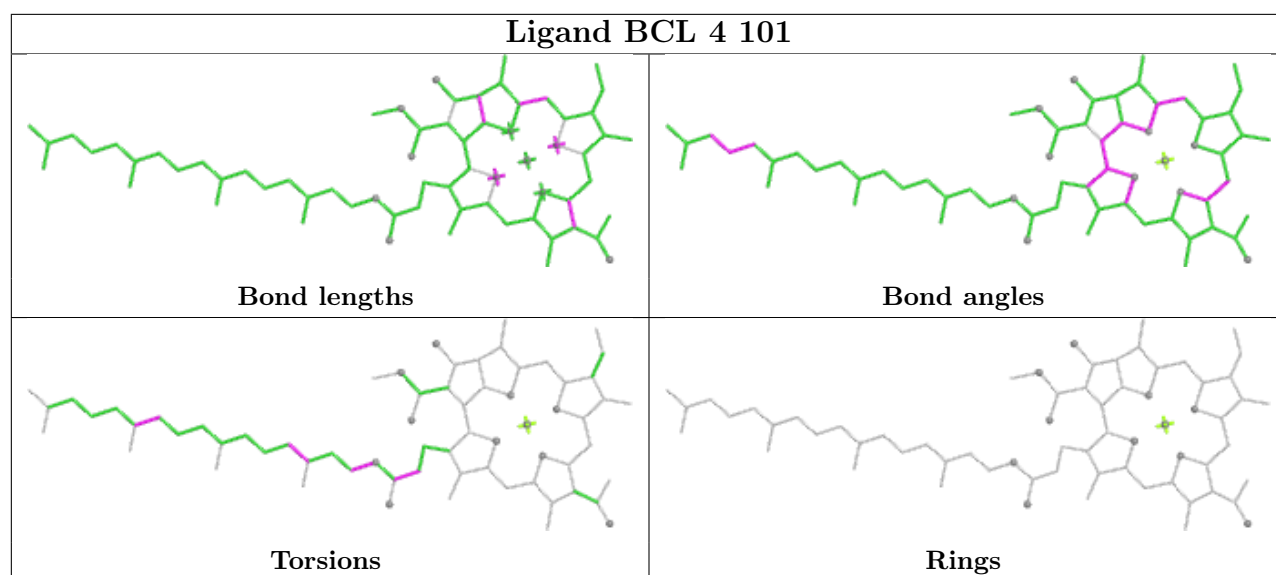
Ligand BCL V 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

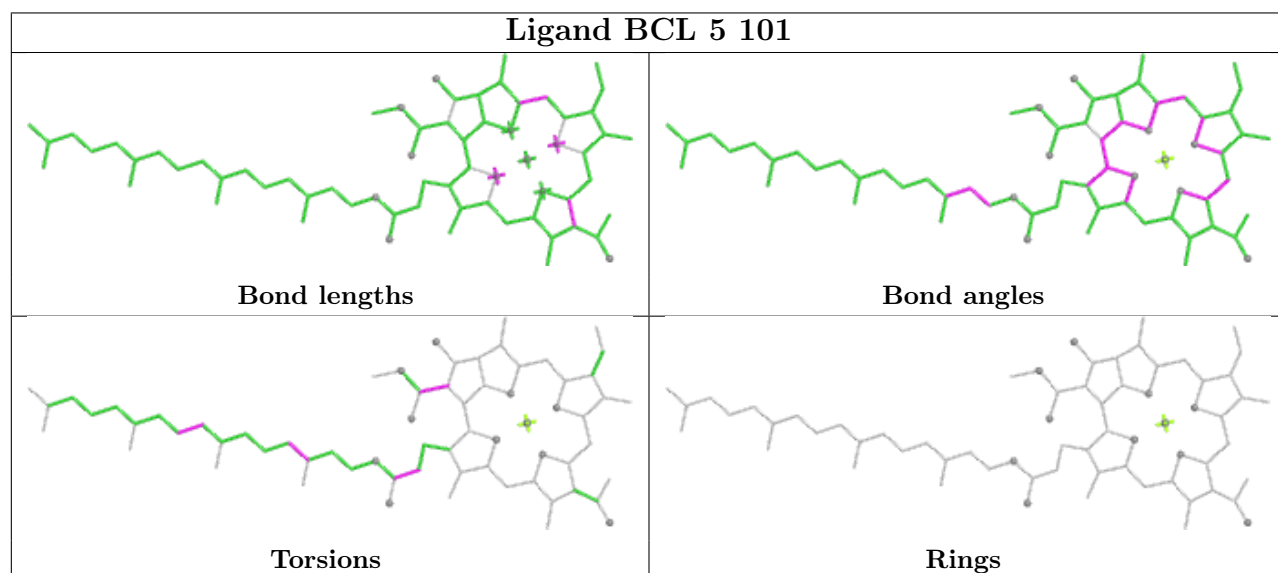
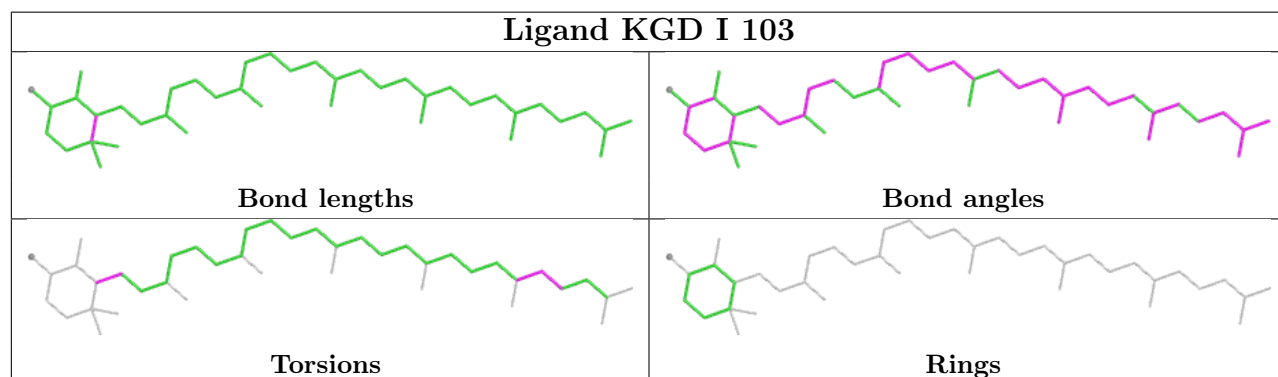
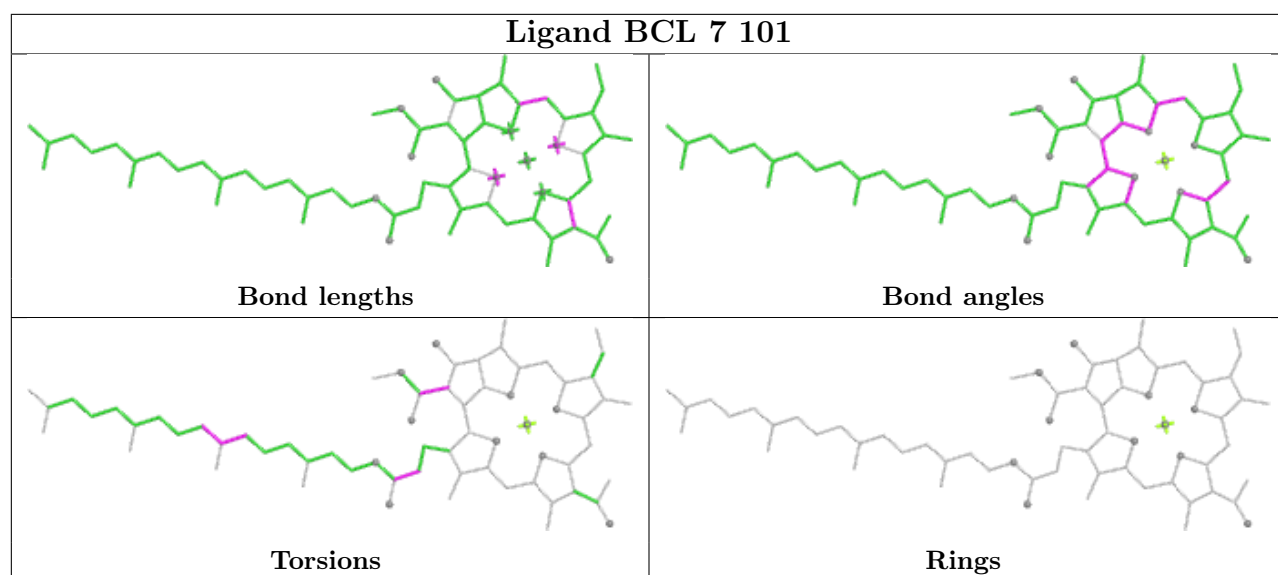
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Bond lengths	Bond angles
	
Torsions	Rings

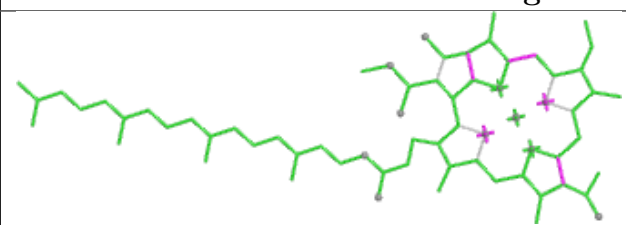
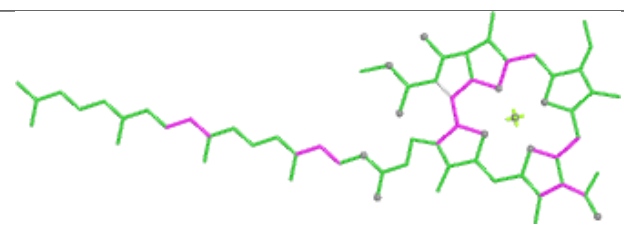
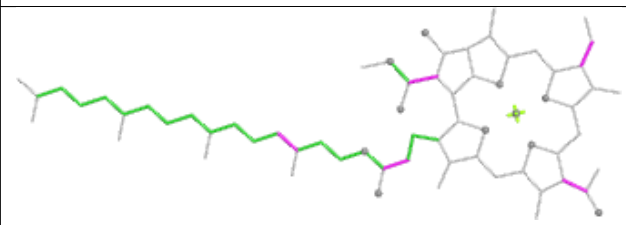
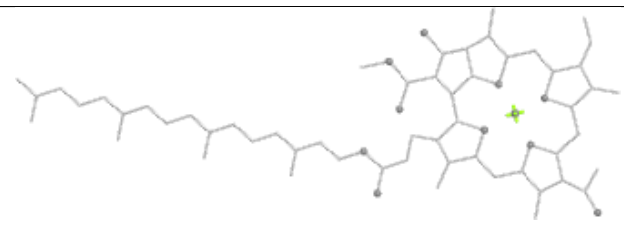
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Bond lengths	Bond angles
	
Torsions	Rings

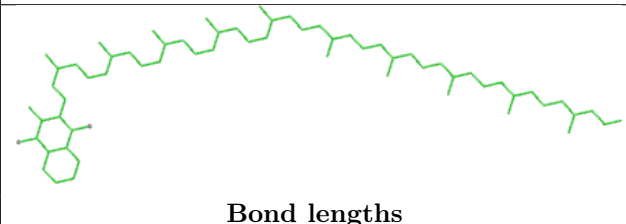
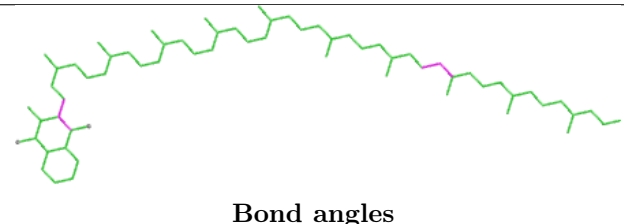
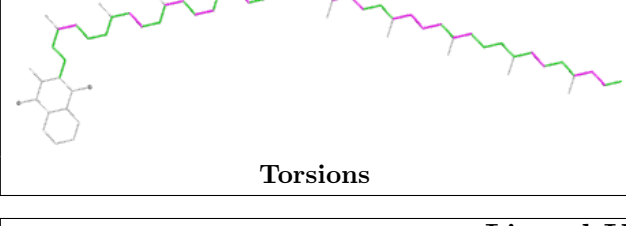


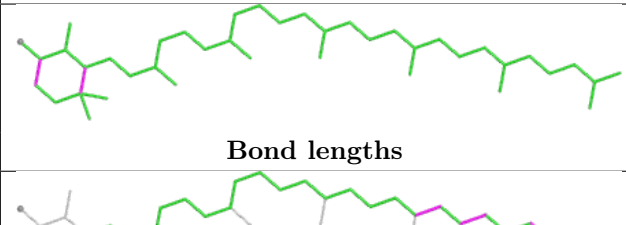
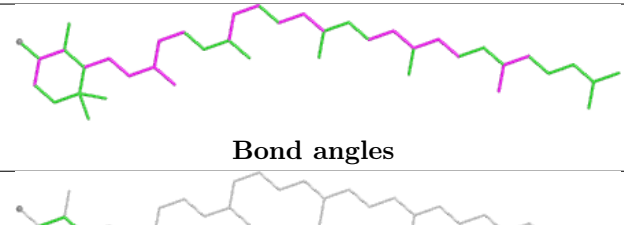
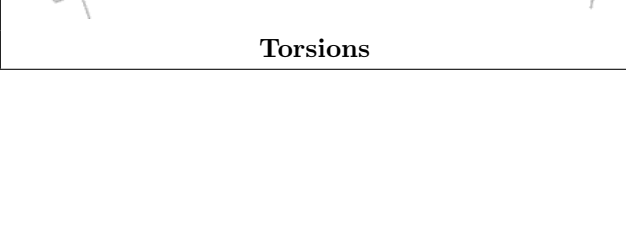
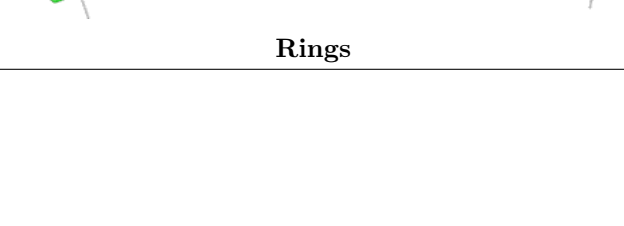


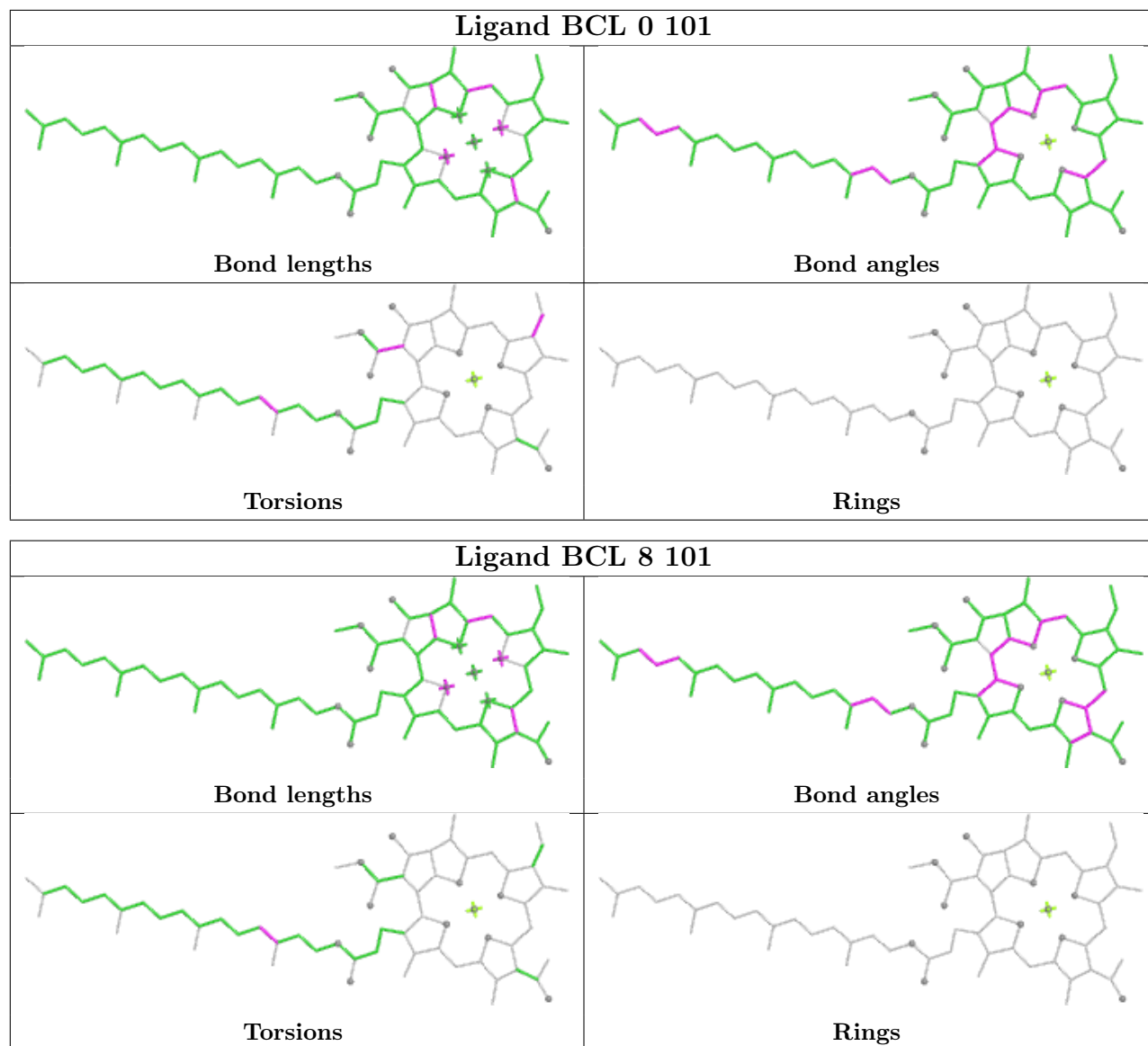


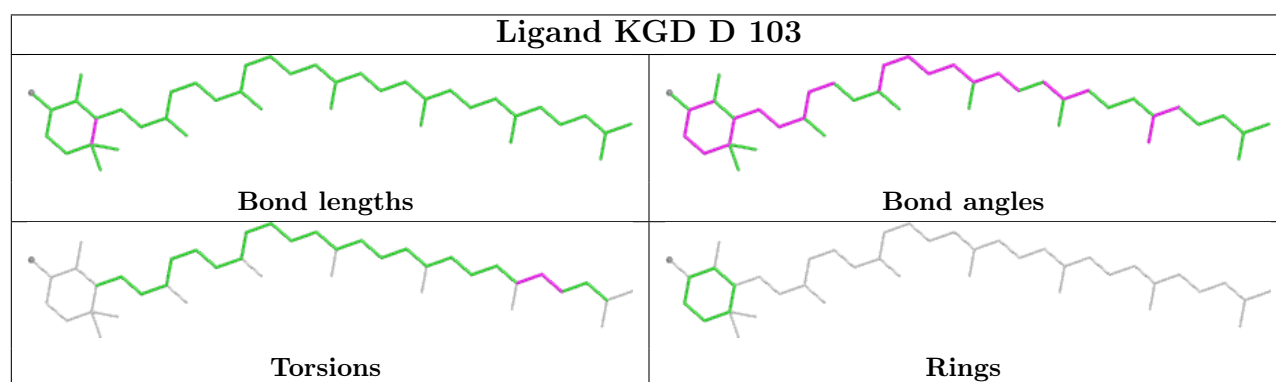
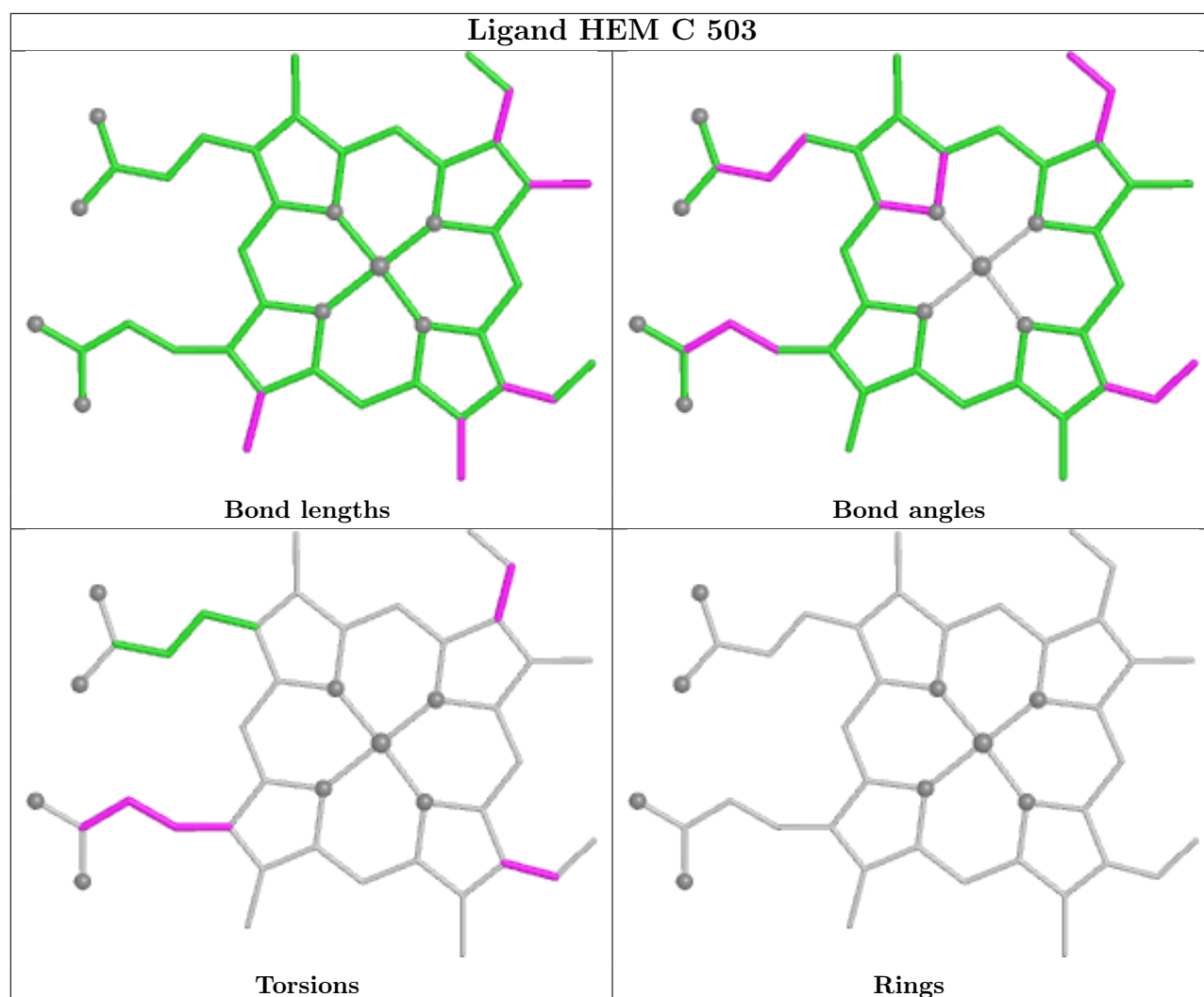


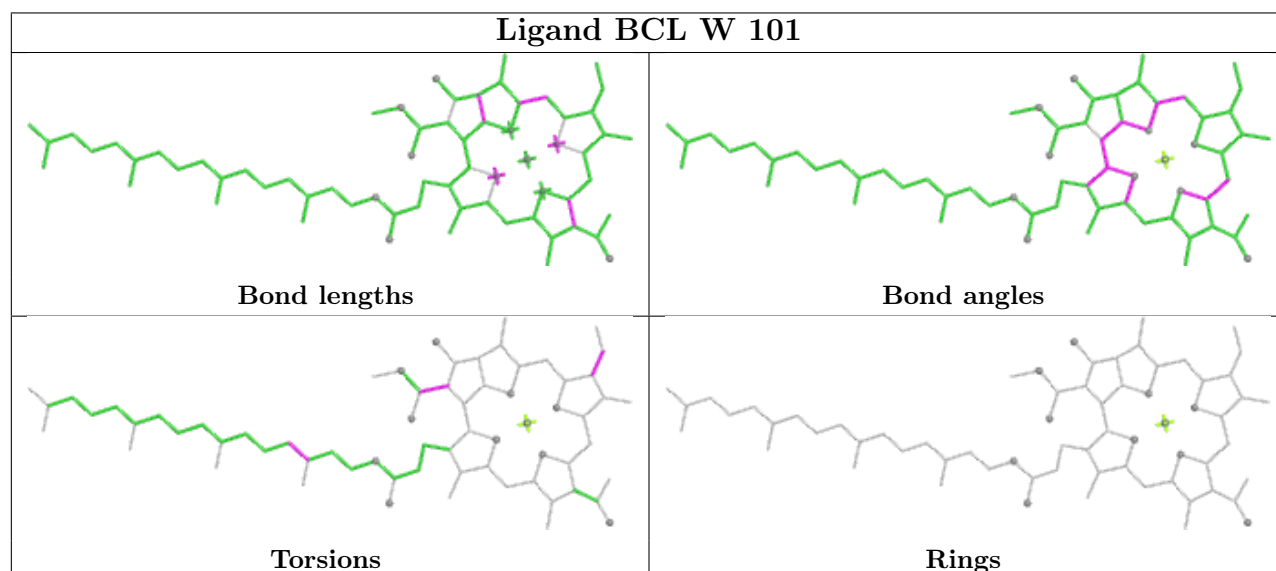
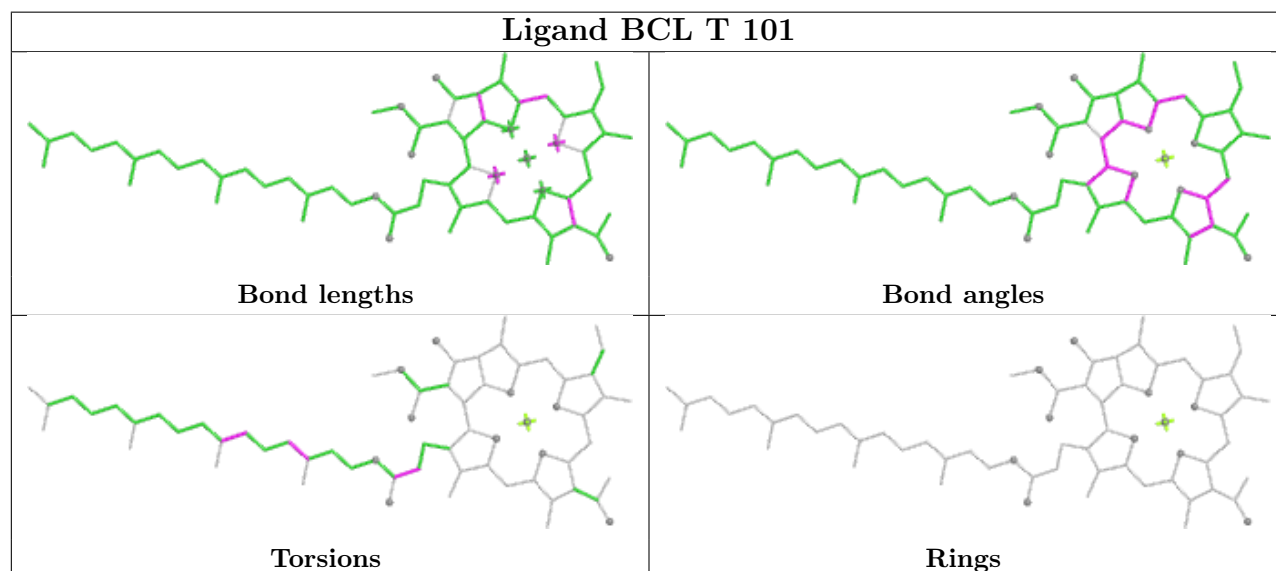
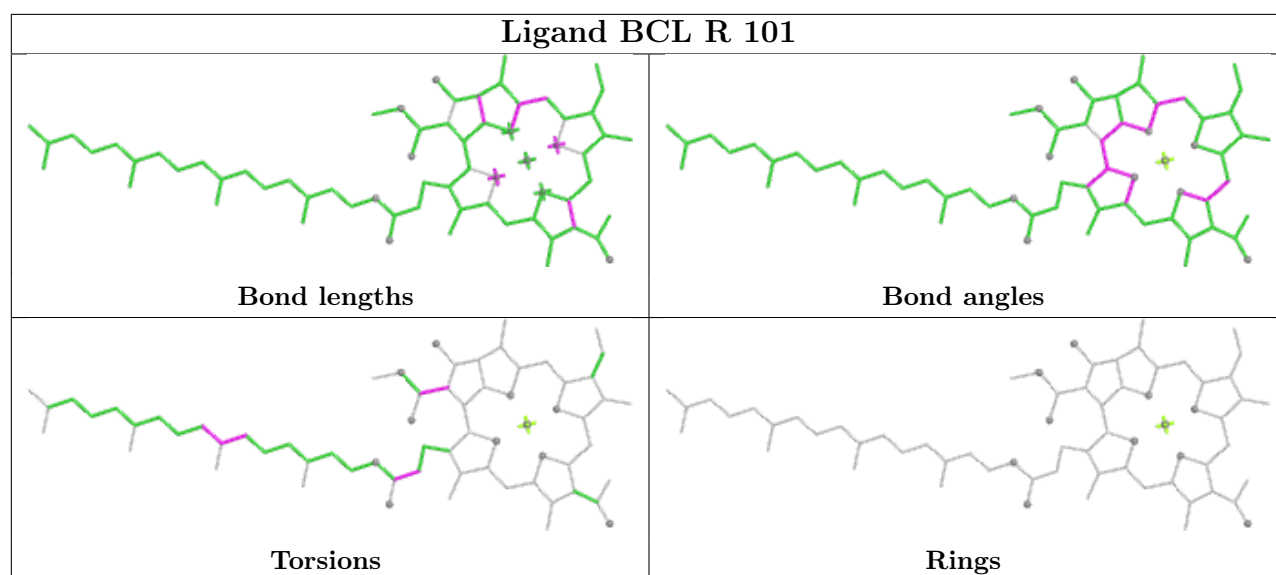
Ligand BCL E 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

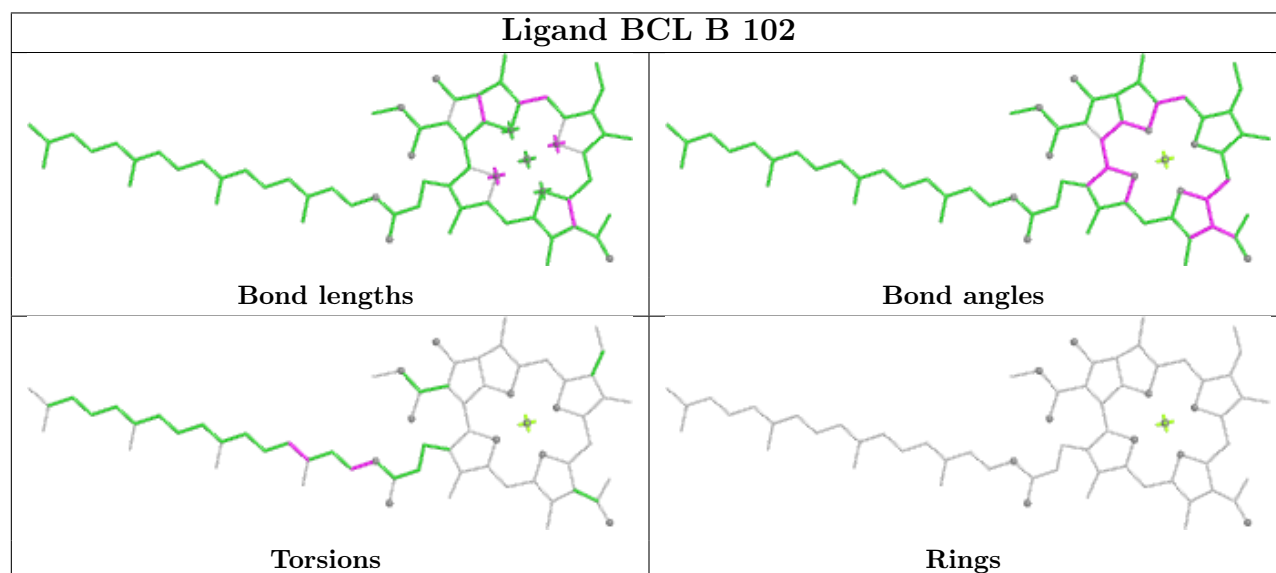
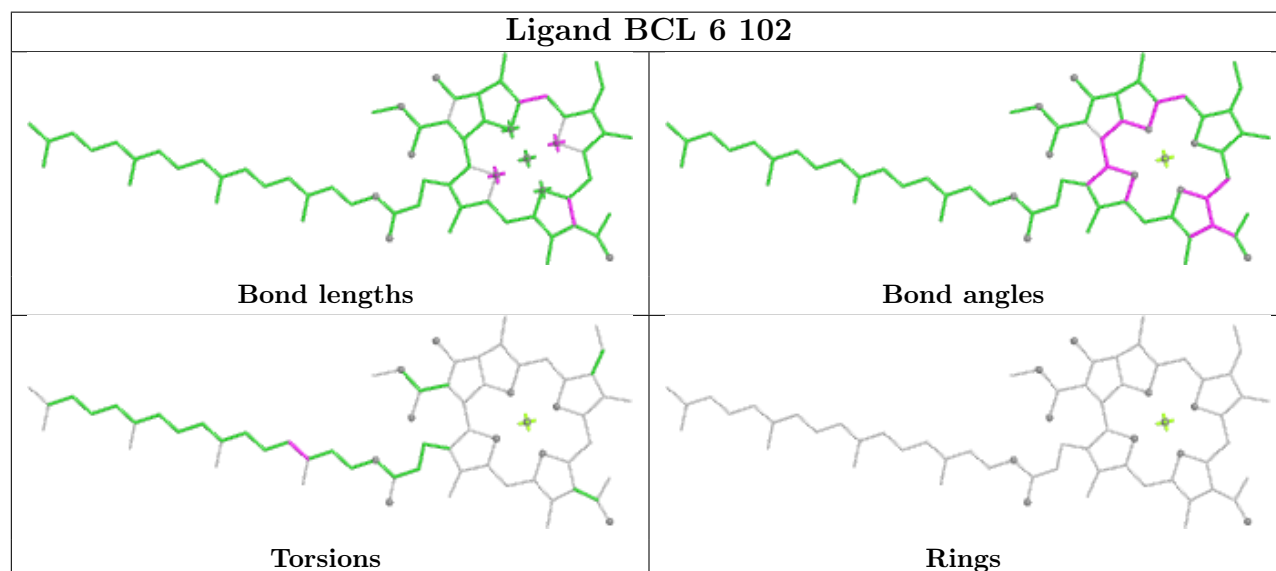
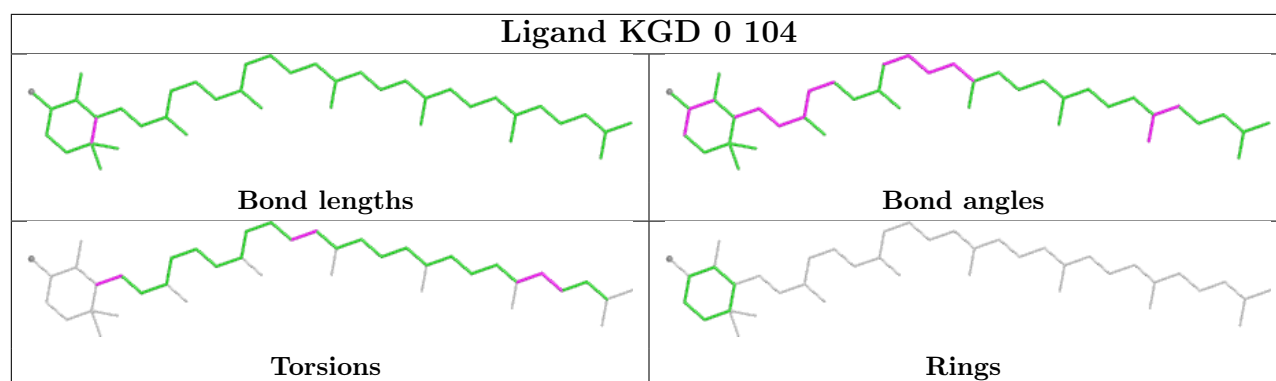
Ligand MQE M 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

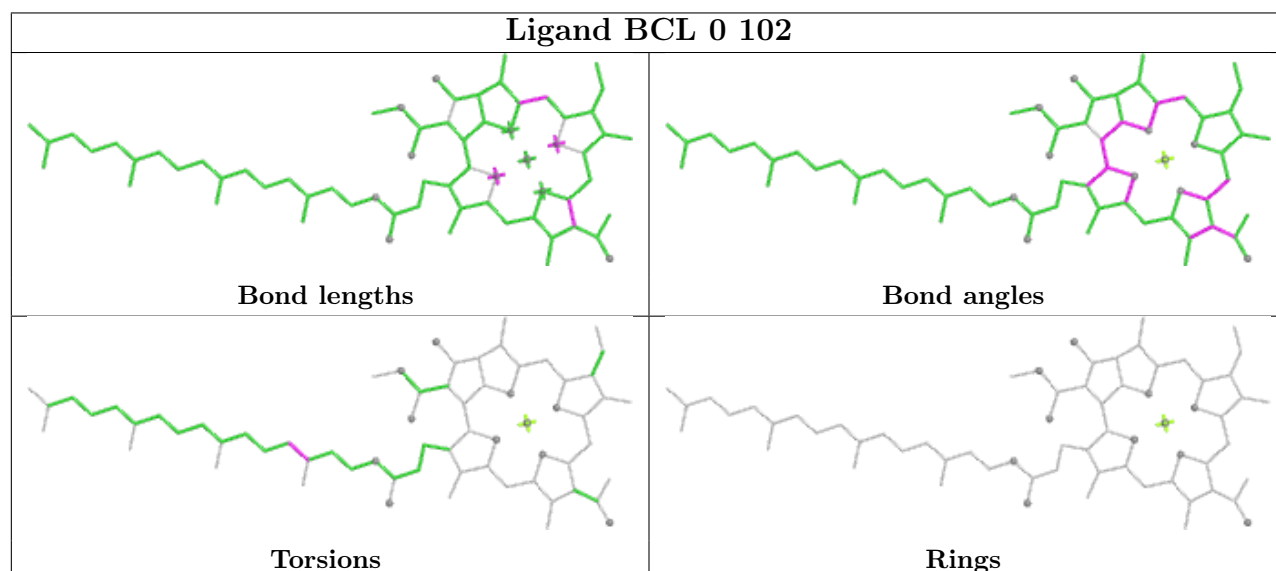
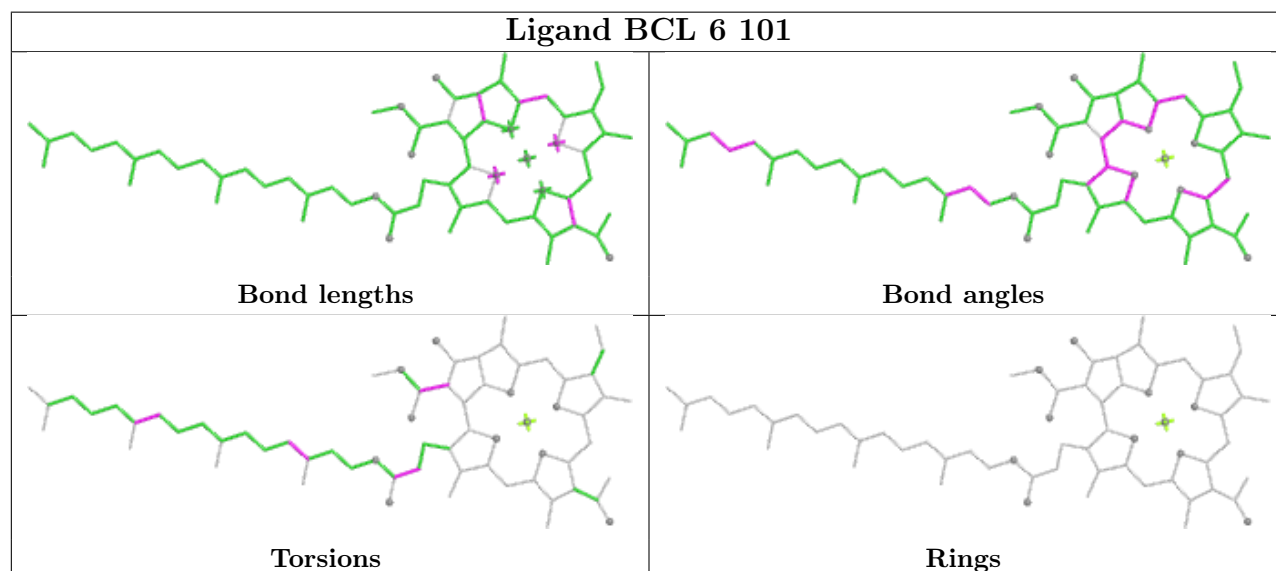
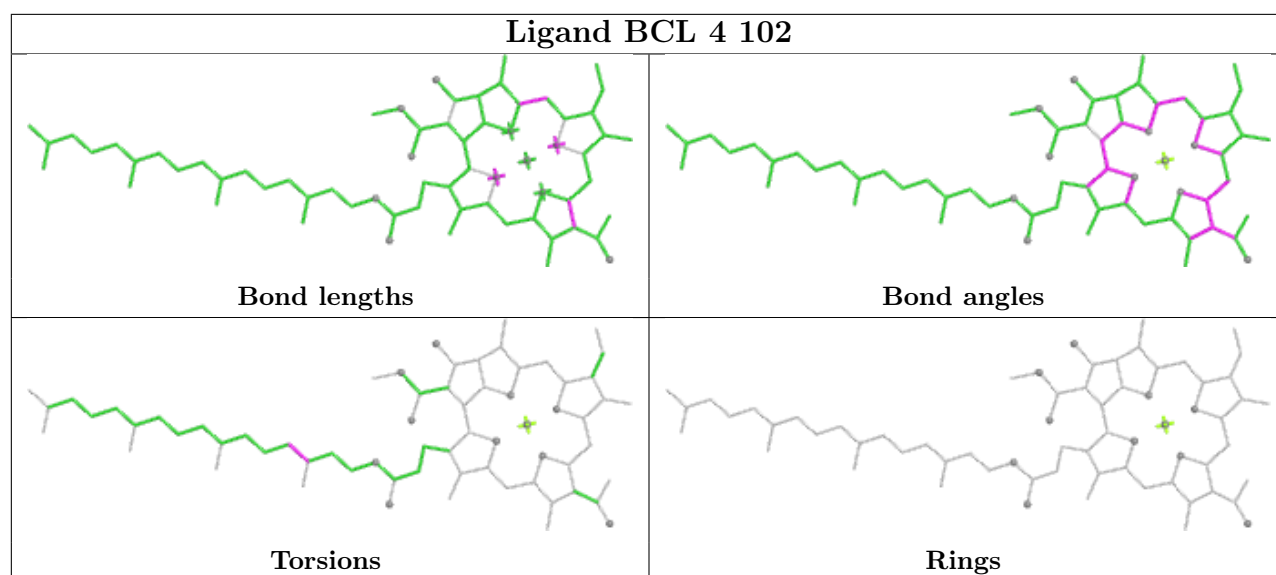
Ligand KGD Q 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

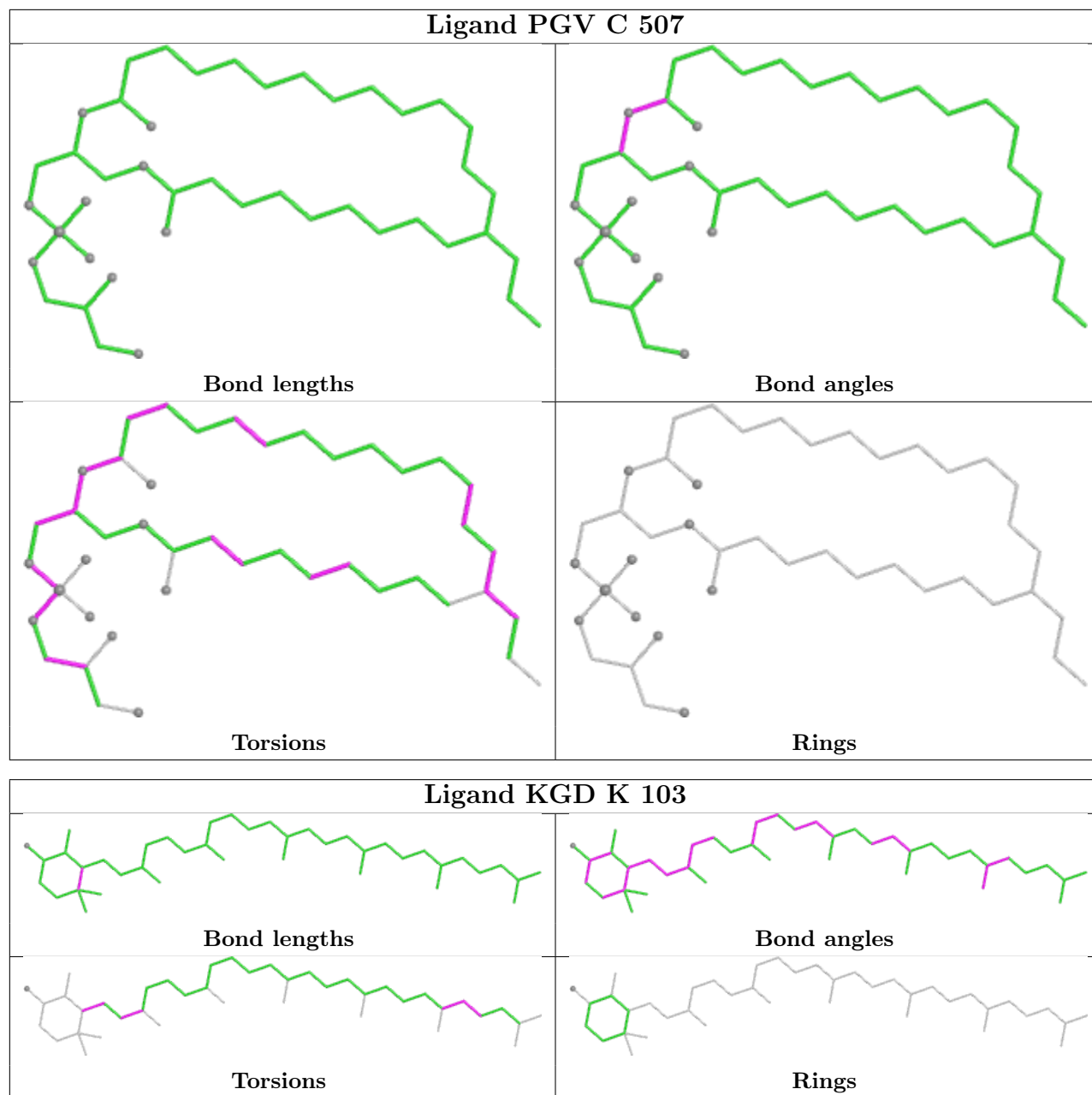


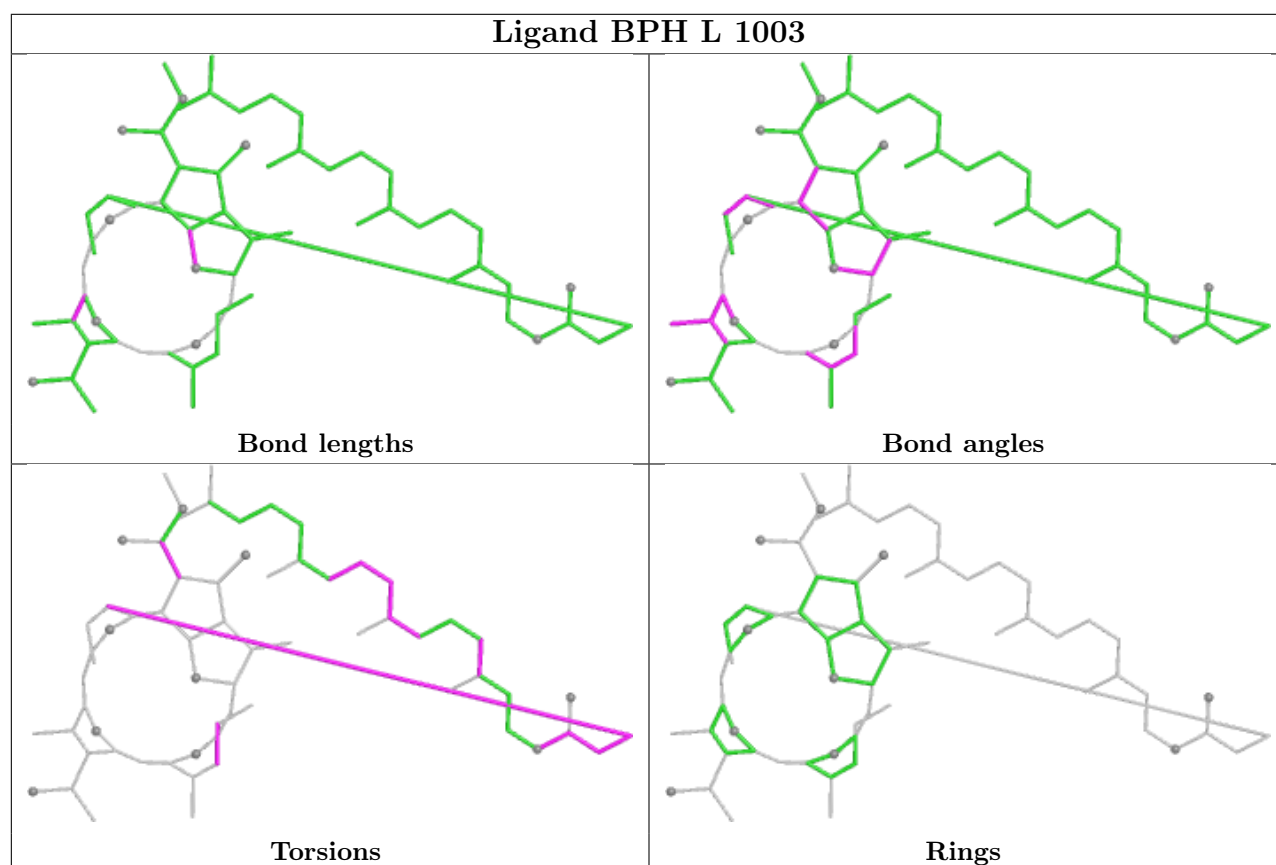
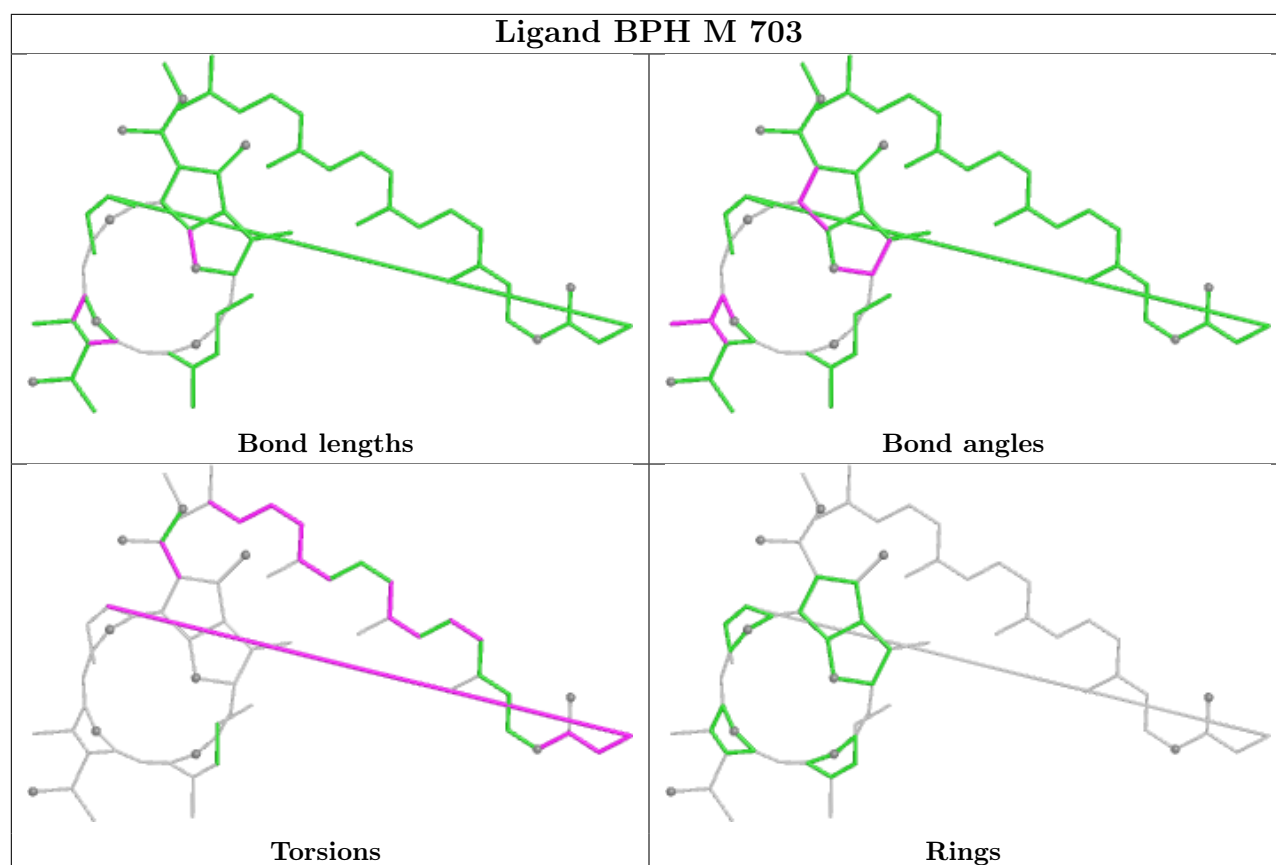


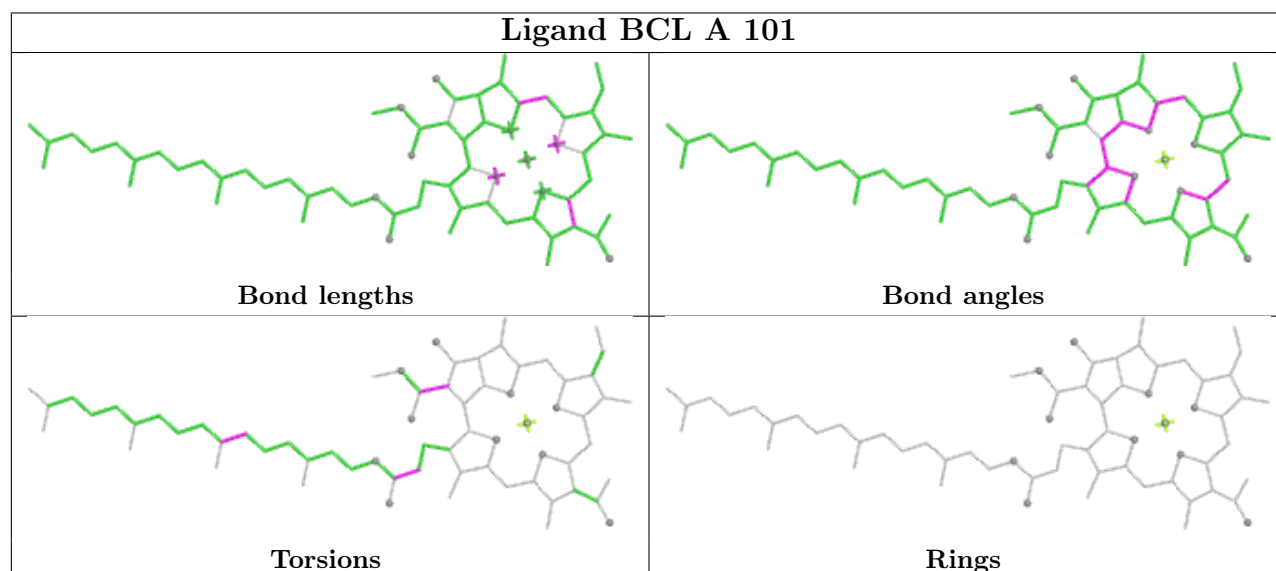
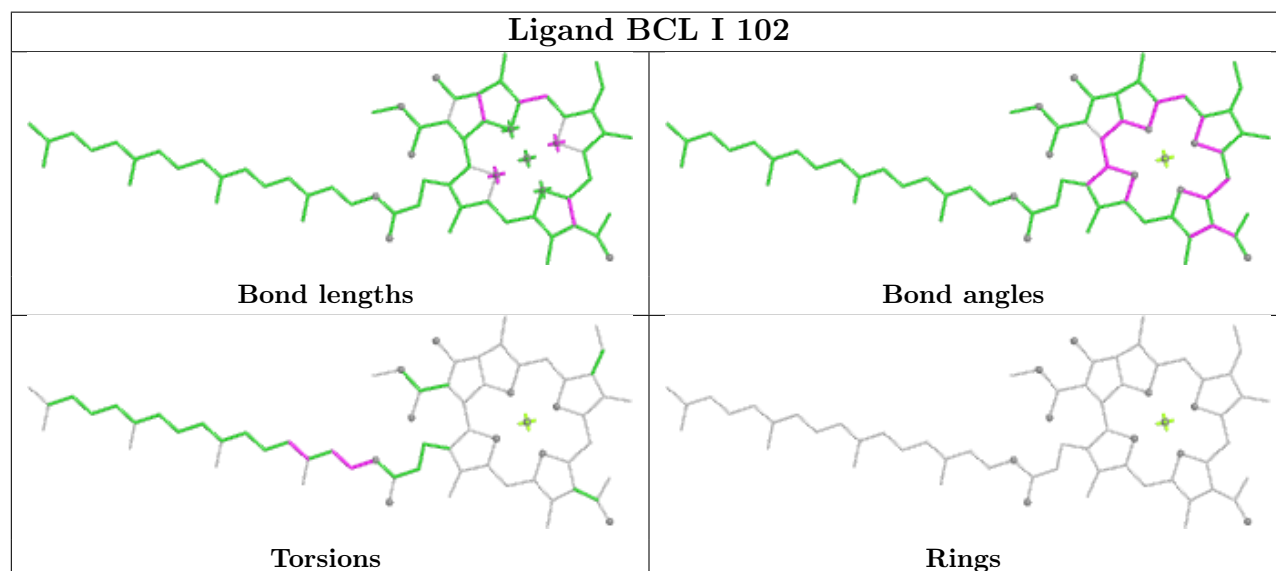
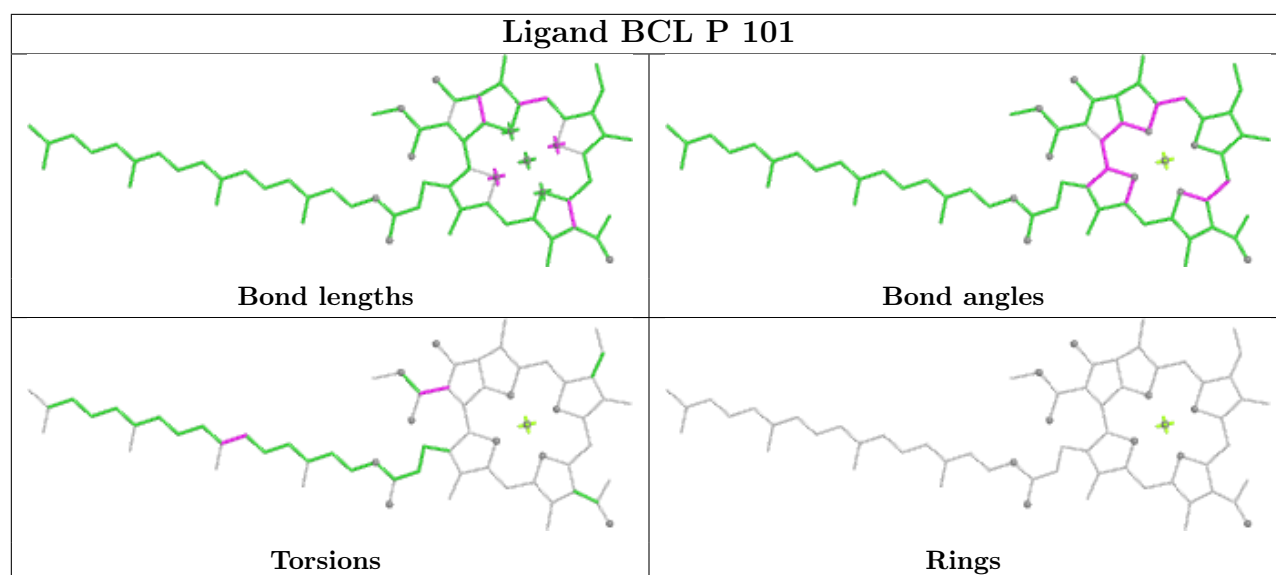


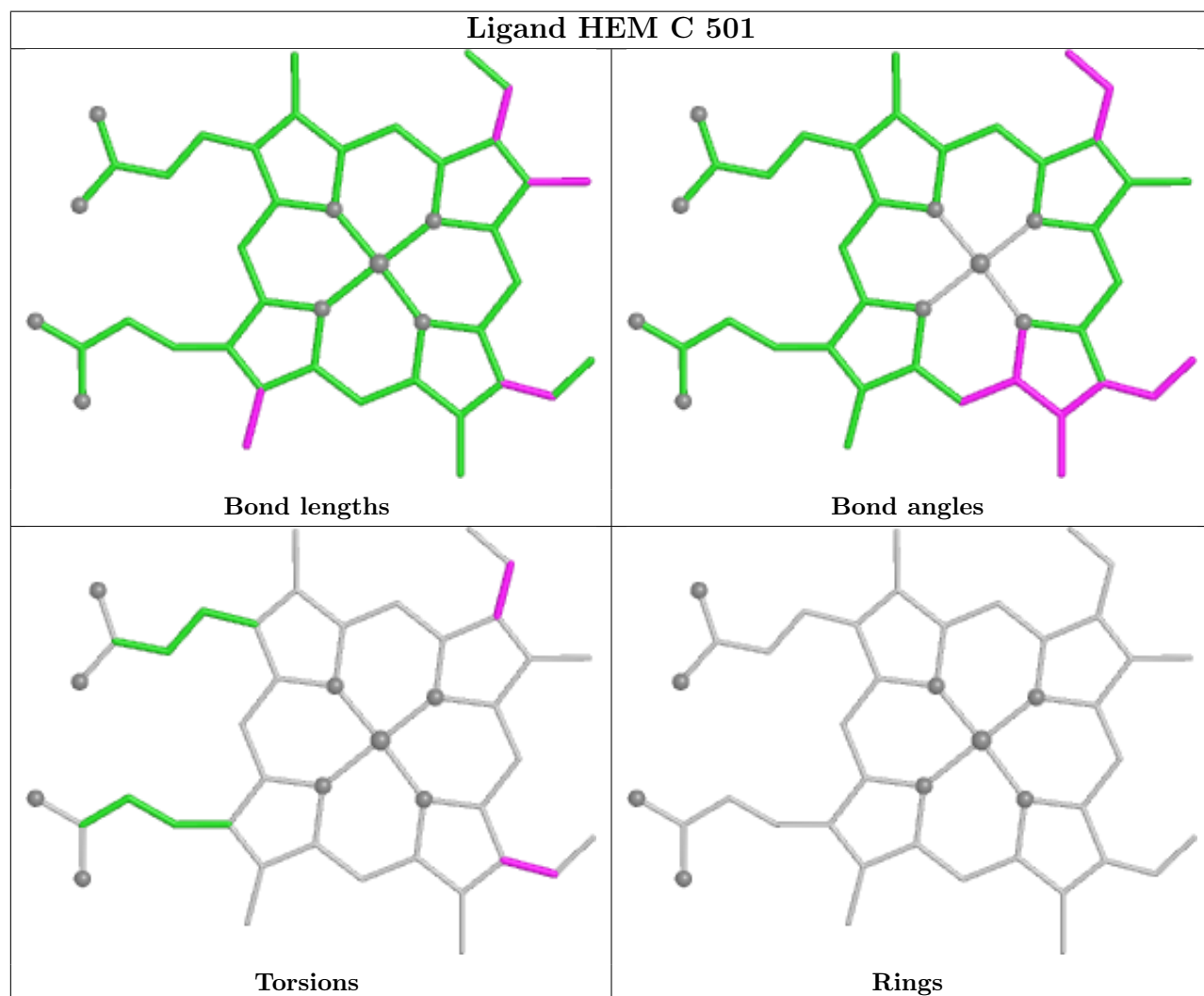
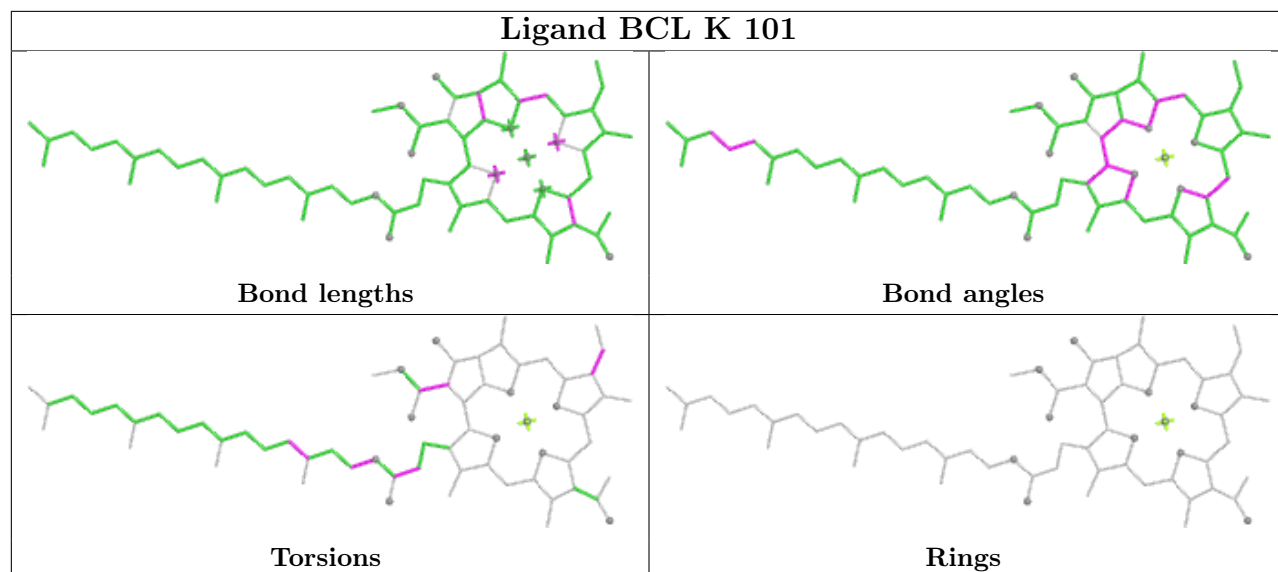


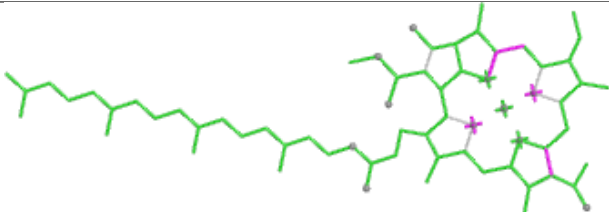
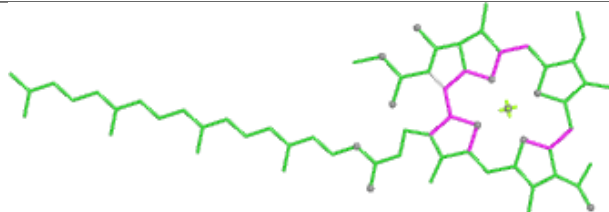
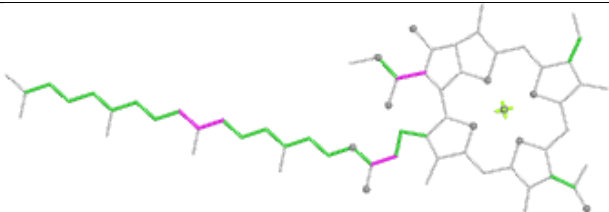
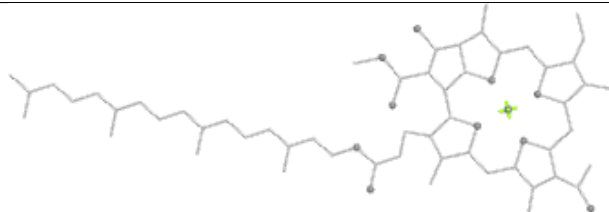


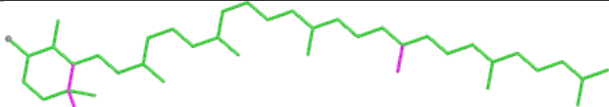
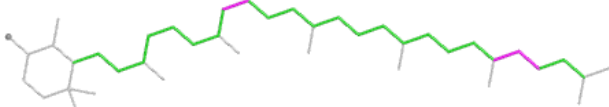
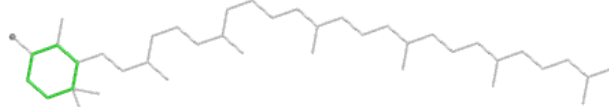


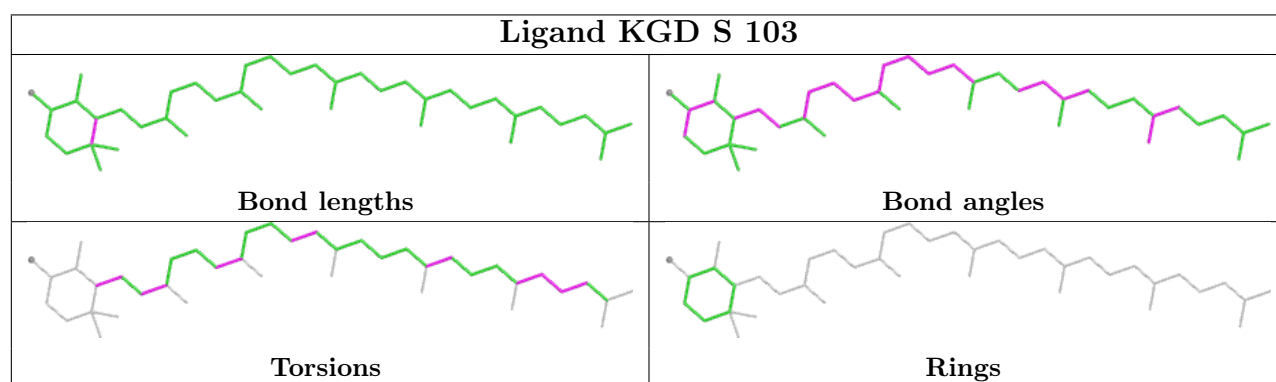
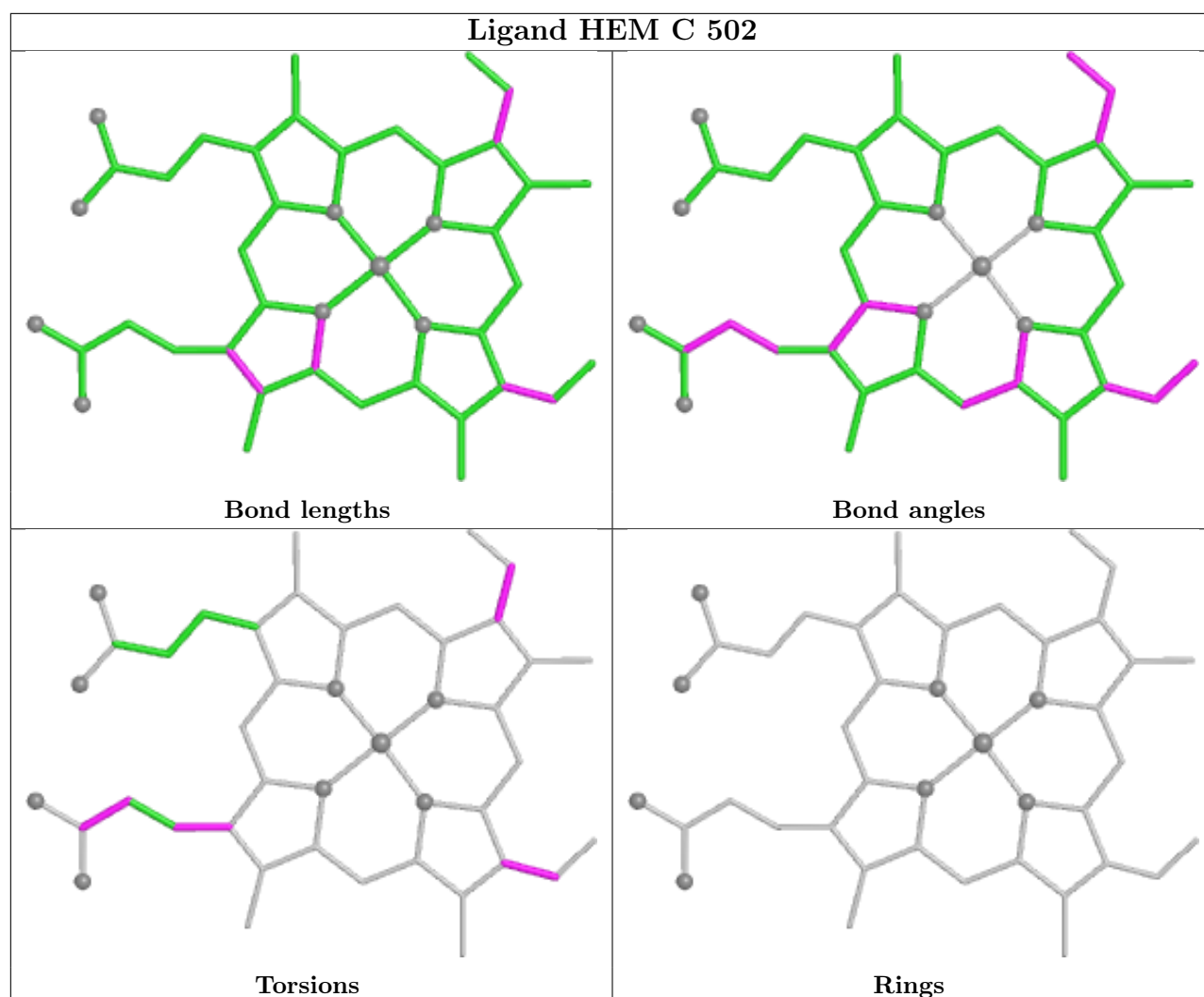


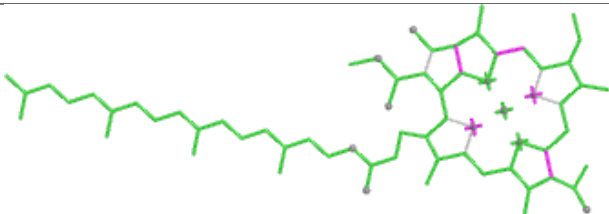
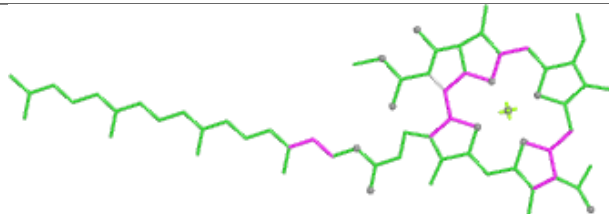
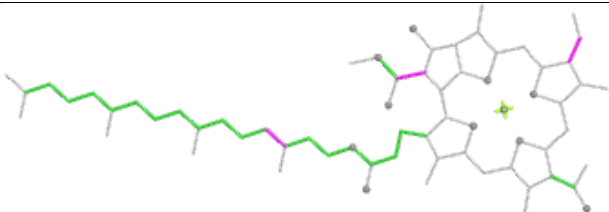
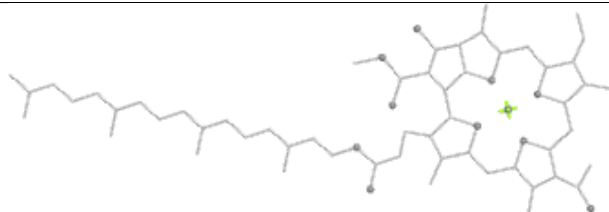


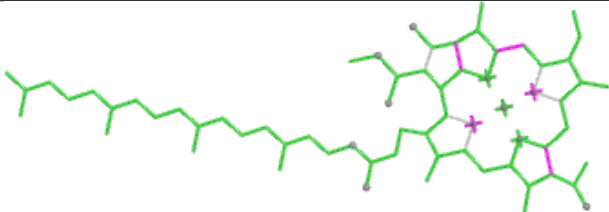
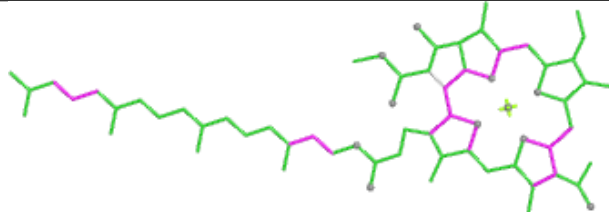
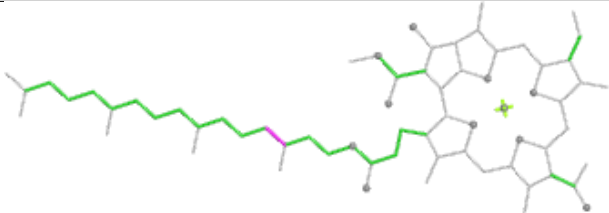
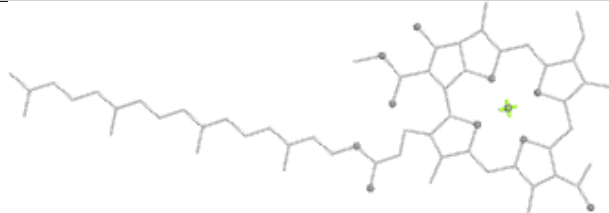


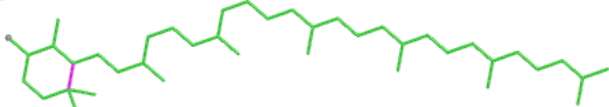
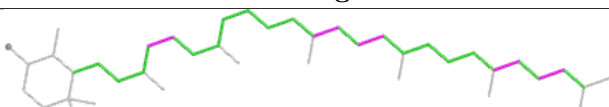
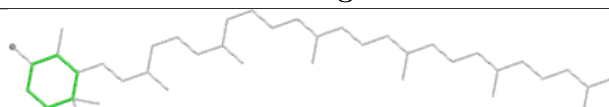
Ligand BCL J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

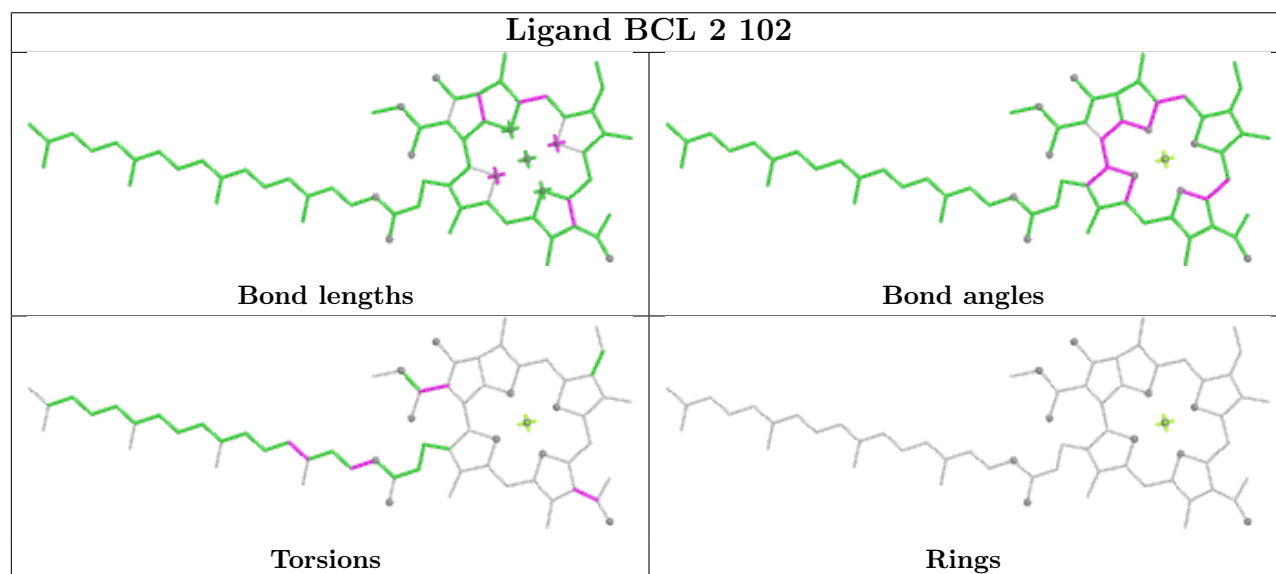
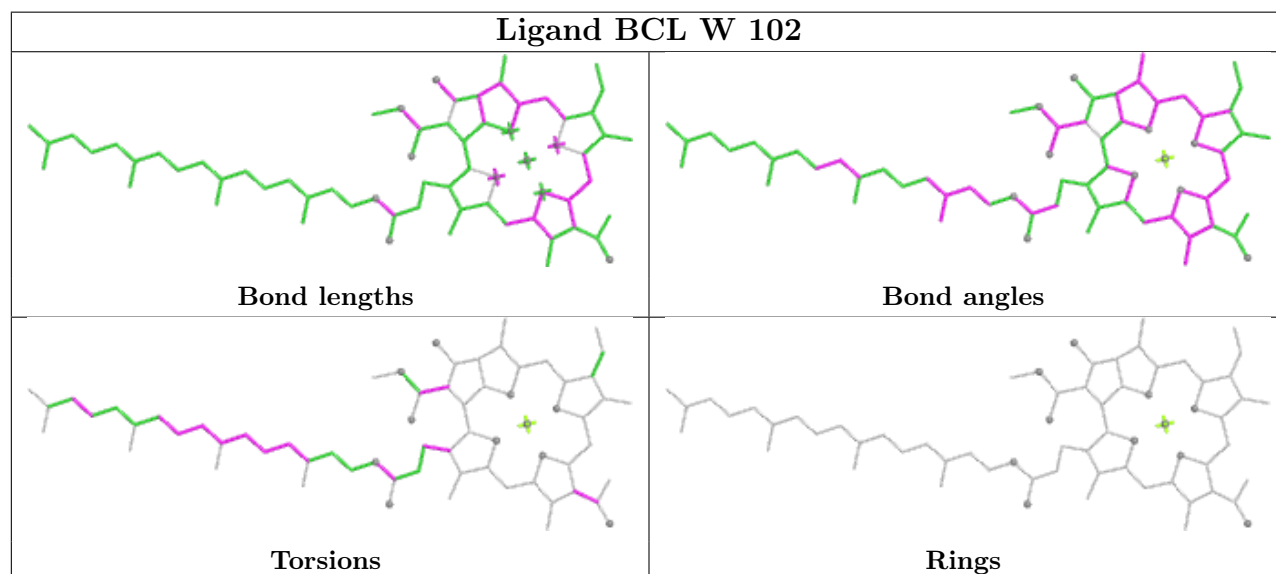
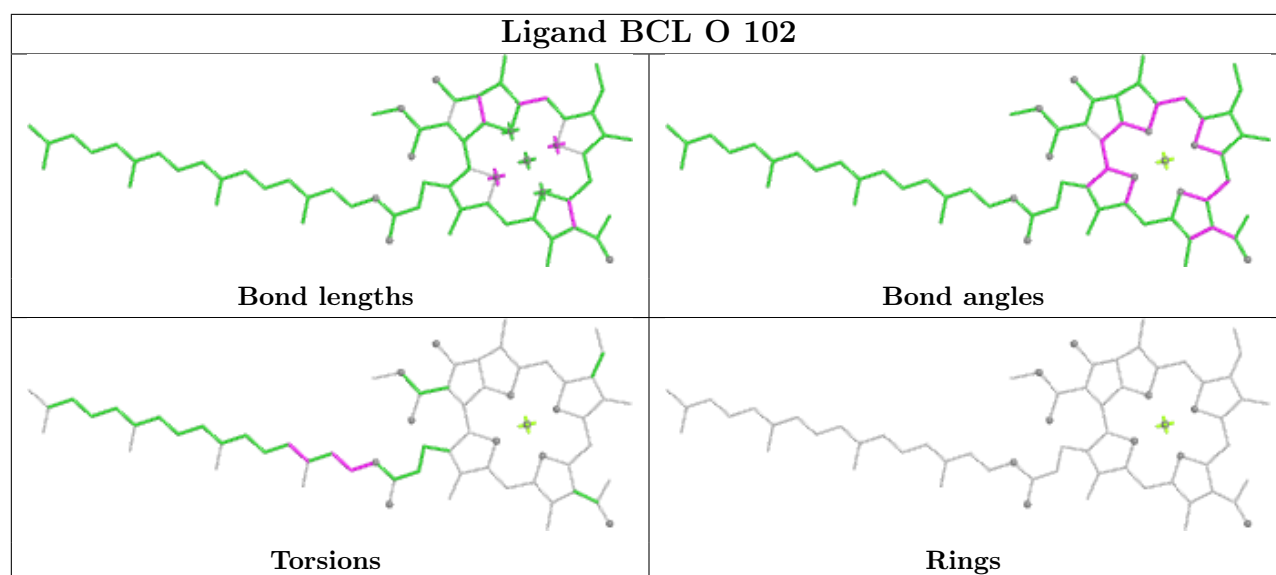
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Bond lengths	Bond angles
	
Torsions	Rings

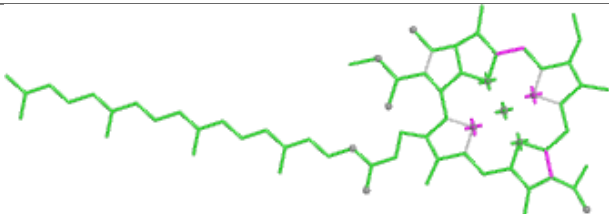
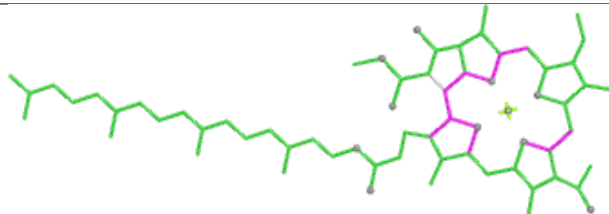
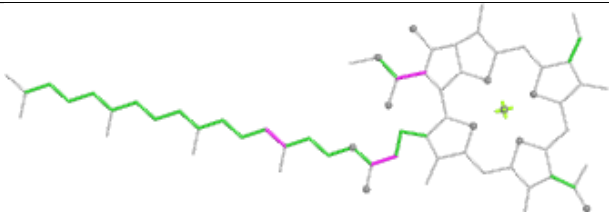
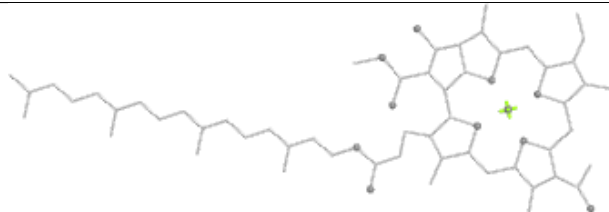


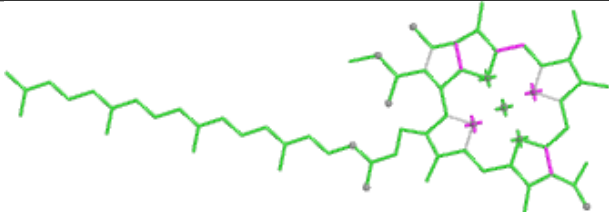
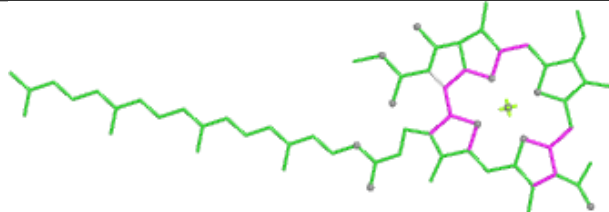
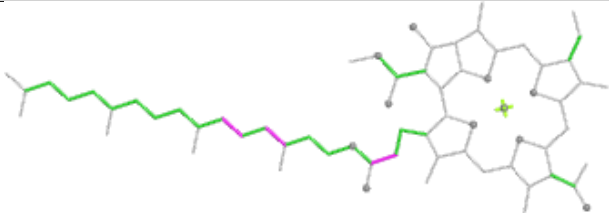
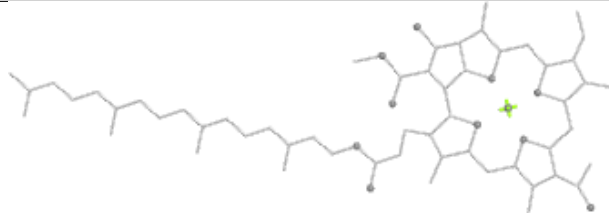
Ligand BCL S 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

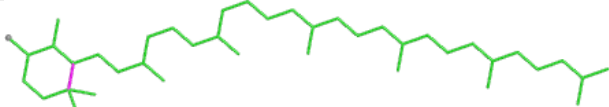
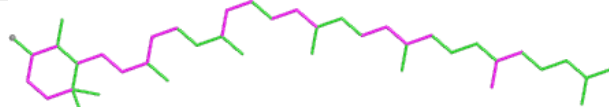
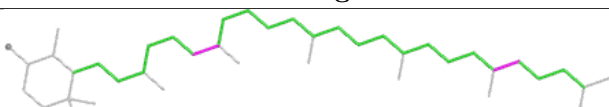
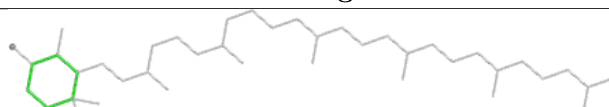
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Bond lengths	Bond angles
	
Torsions	Rings

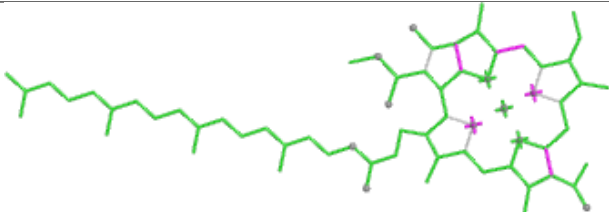
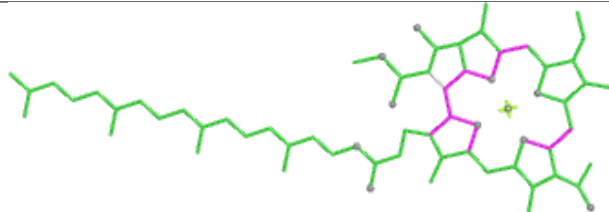
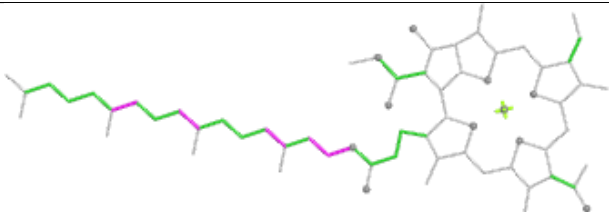
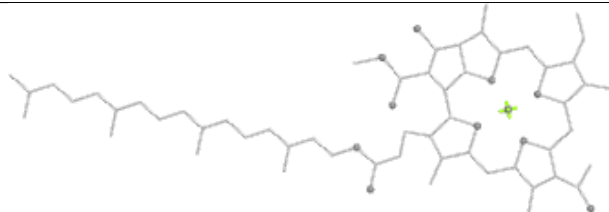
Ligand KGD J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

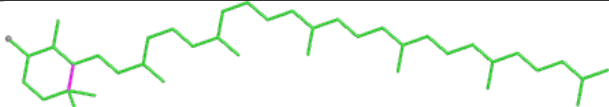
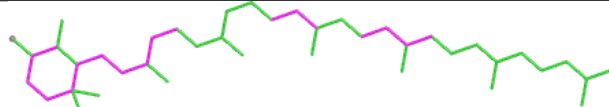
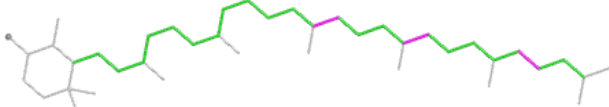
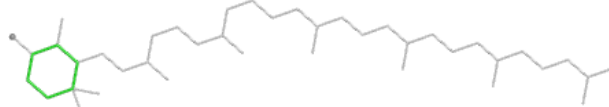


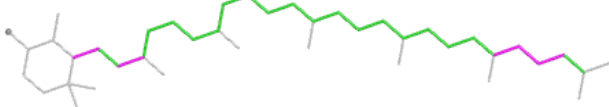
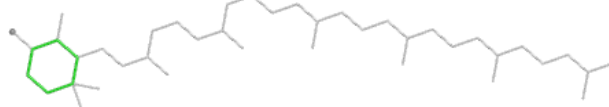
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Bond lengths	Bond angles
	
Torsions	Rings

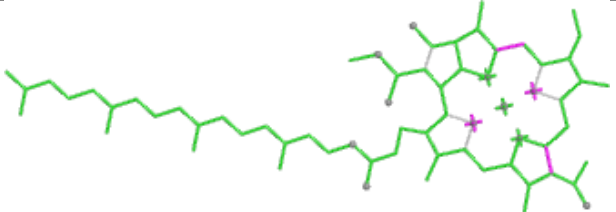
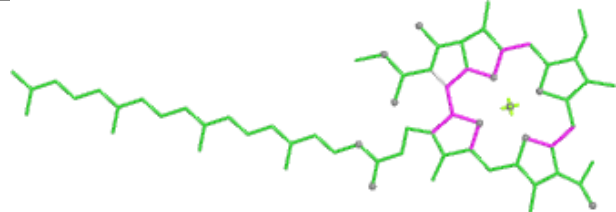
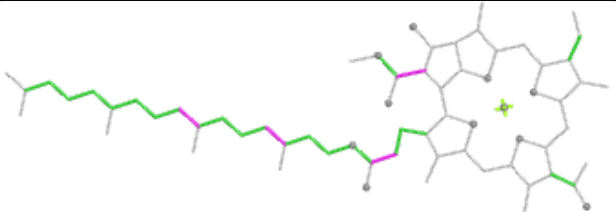
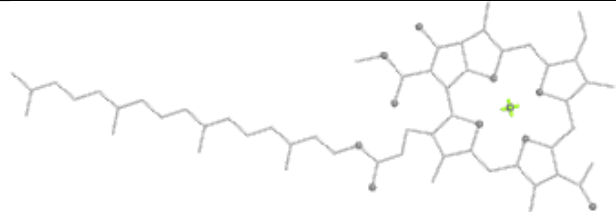
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Bond lengths	Bond angles
	
Torsions	Rings

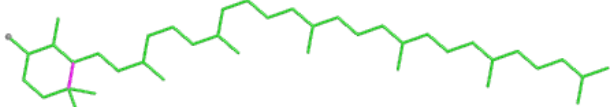
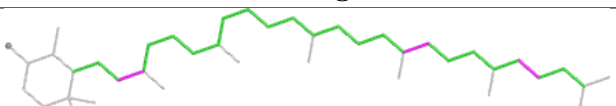
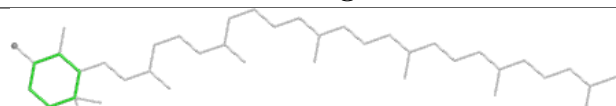
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Bond lengths	Bond angles
	
Torsions	Rings

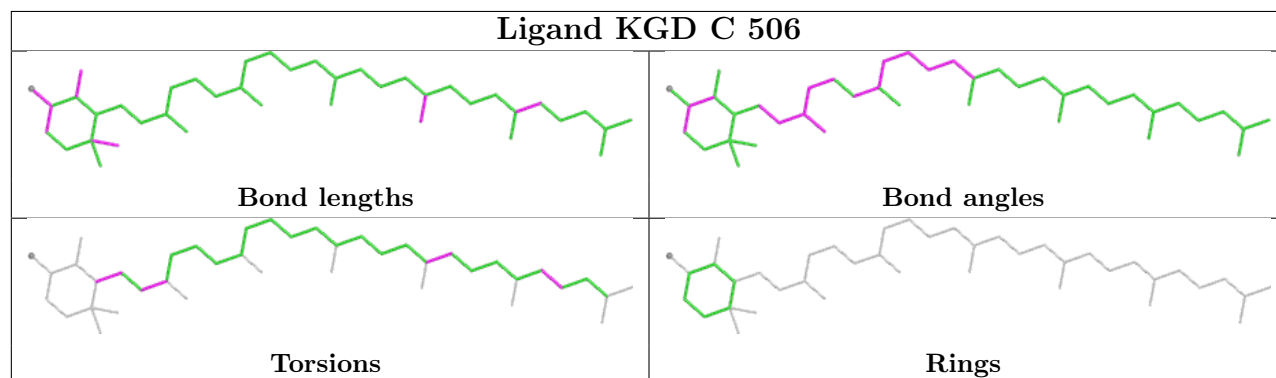
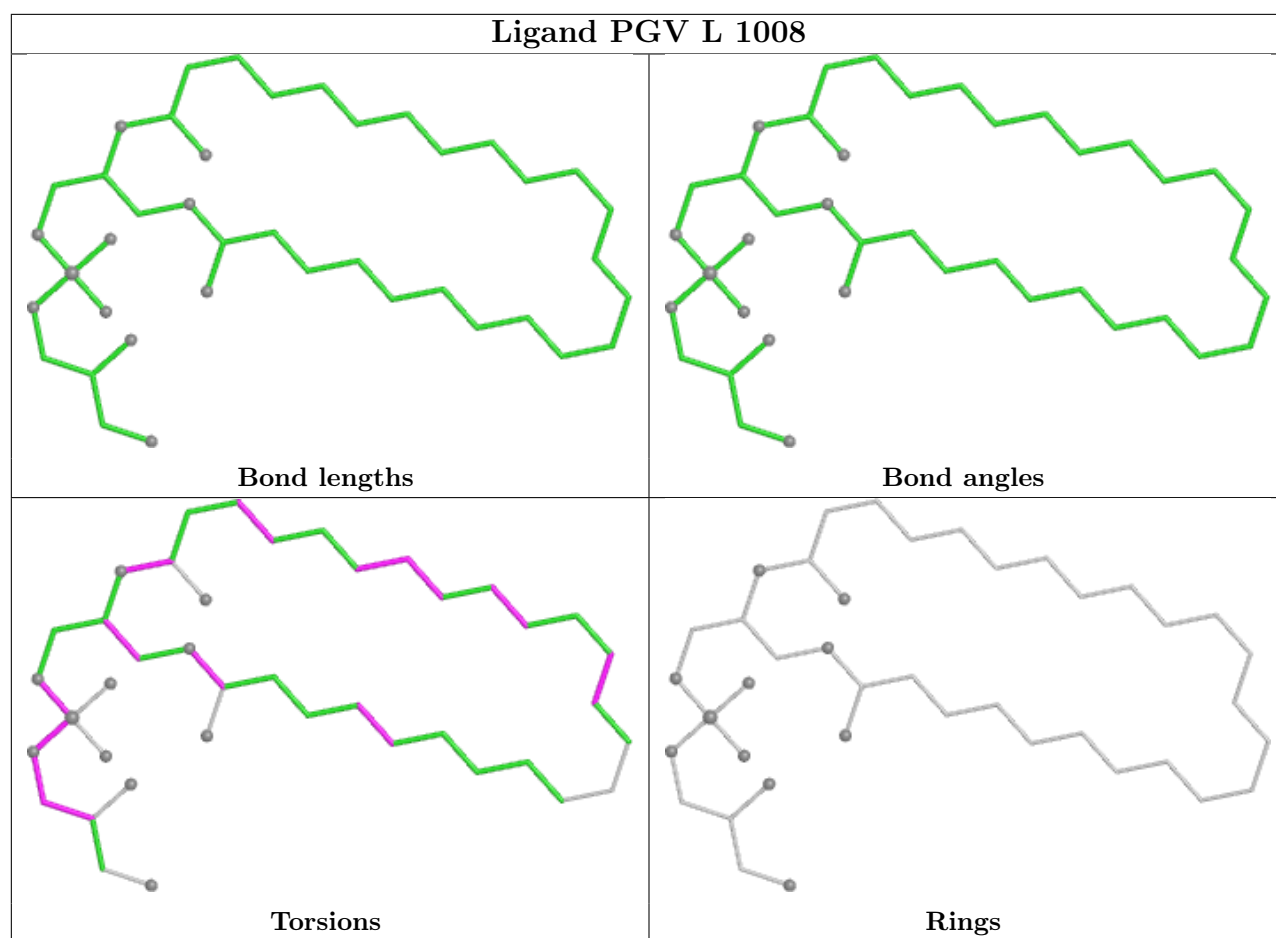
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Bond lengths	Bond angles
	
Torsions	Rings

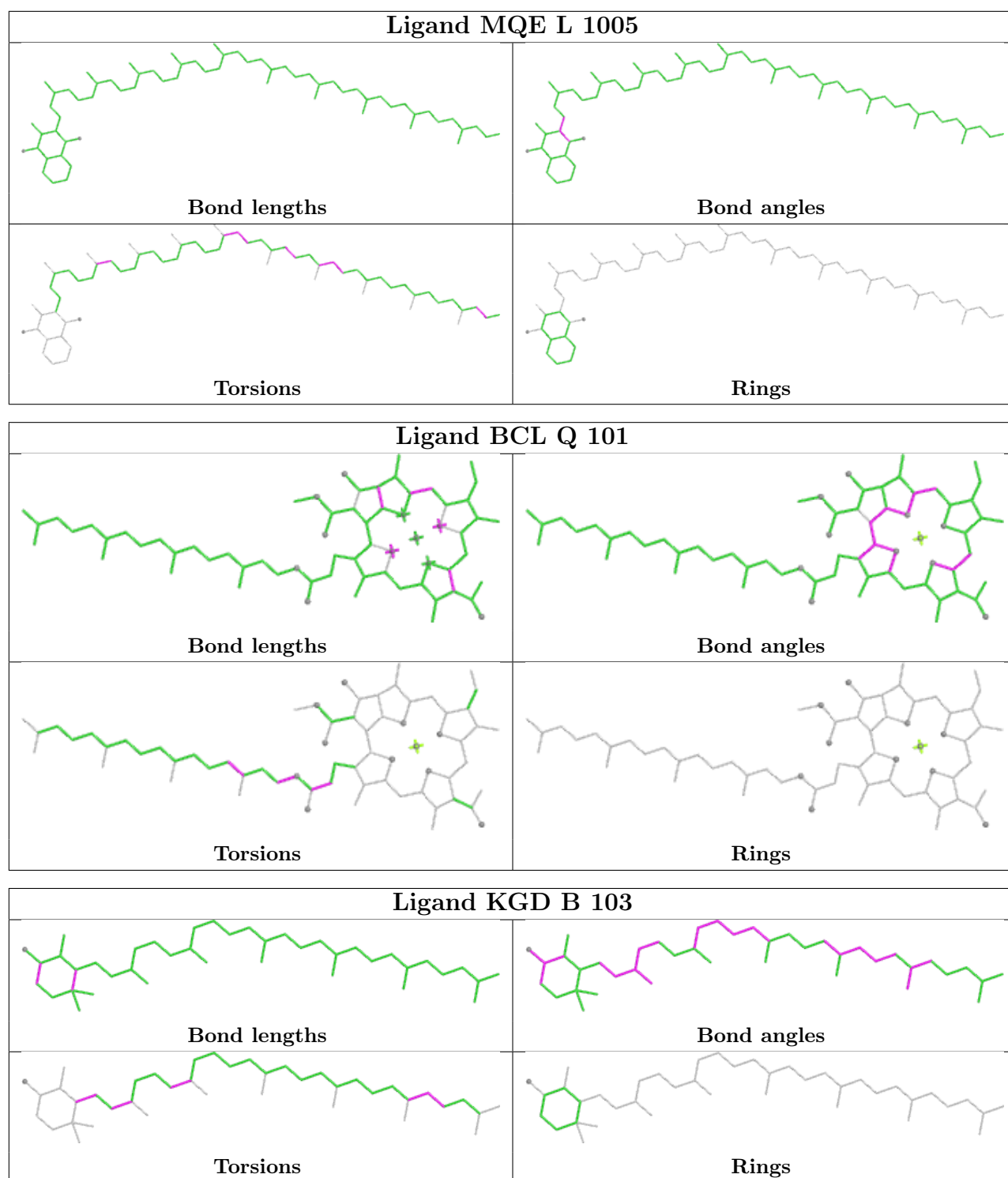
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Bond lengths	Bond angles
	
Torsions	Rings

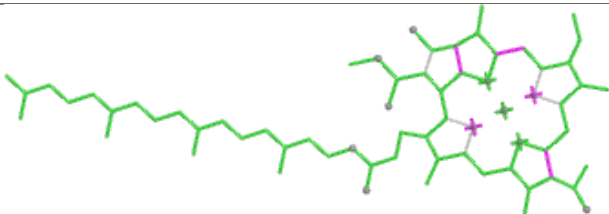
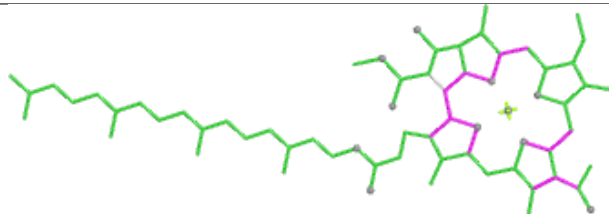
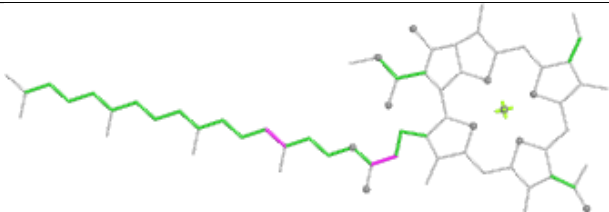
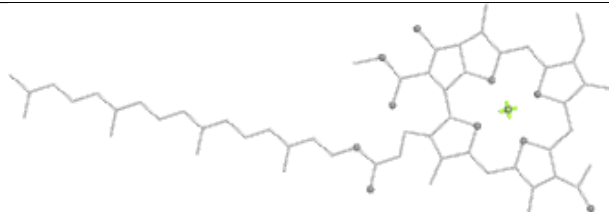
Ligand KGD 2 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

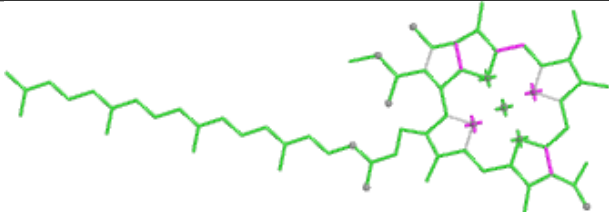
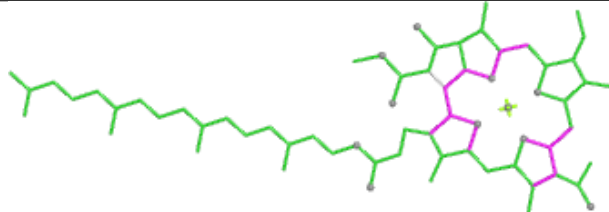
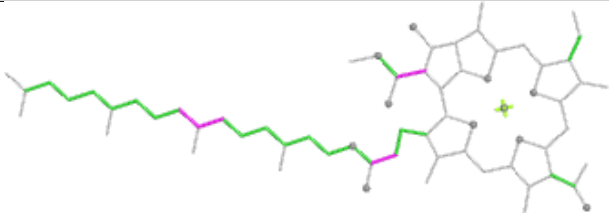
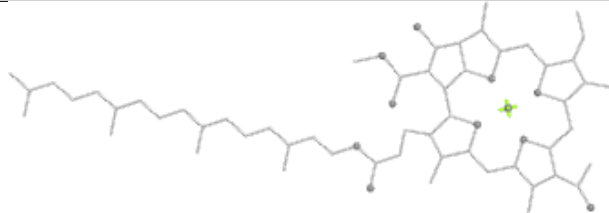
Ligand BCL 9 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

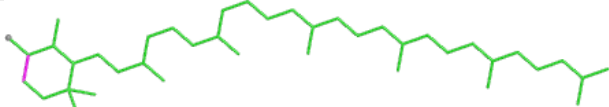
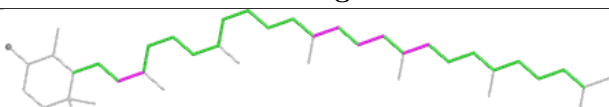
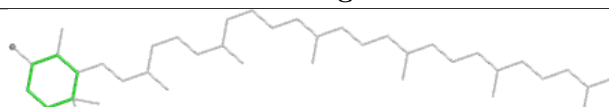
Ligand KGD R 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

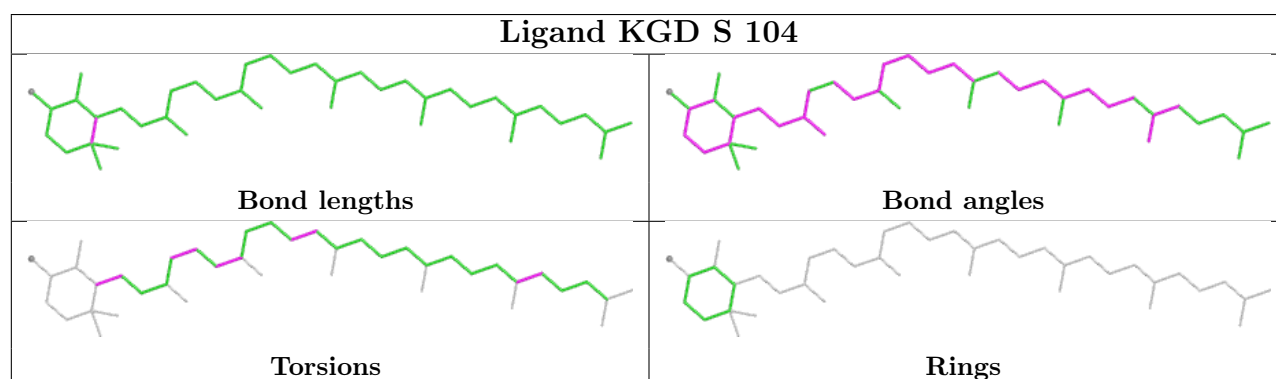
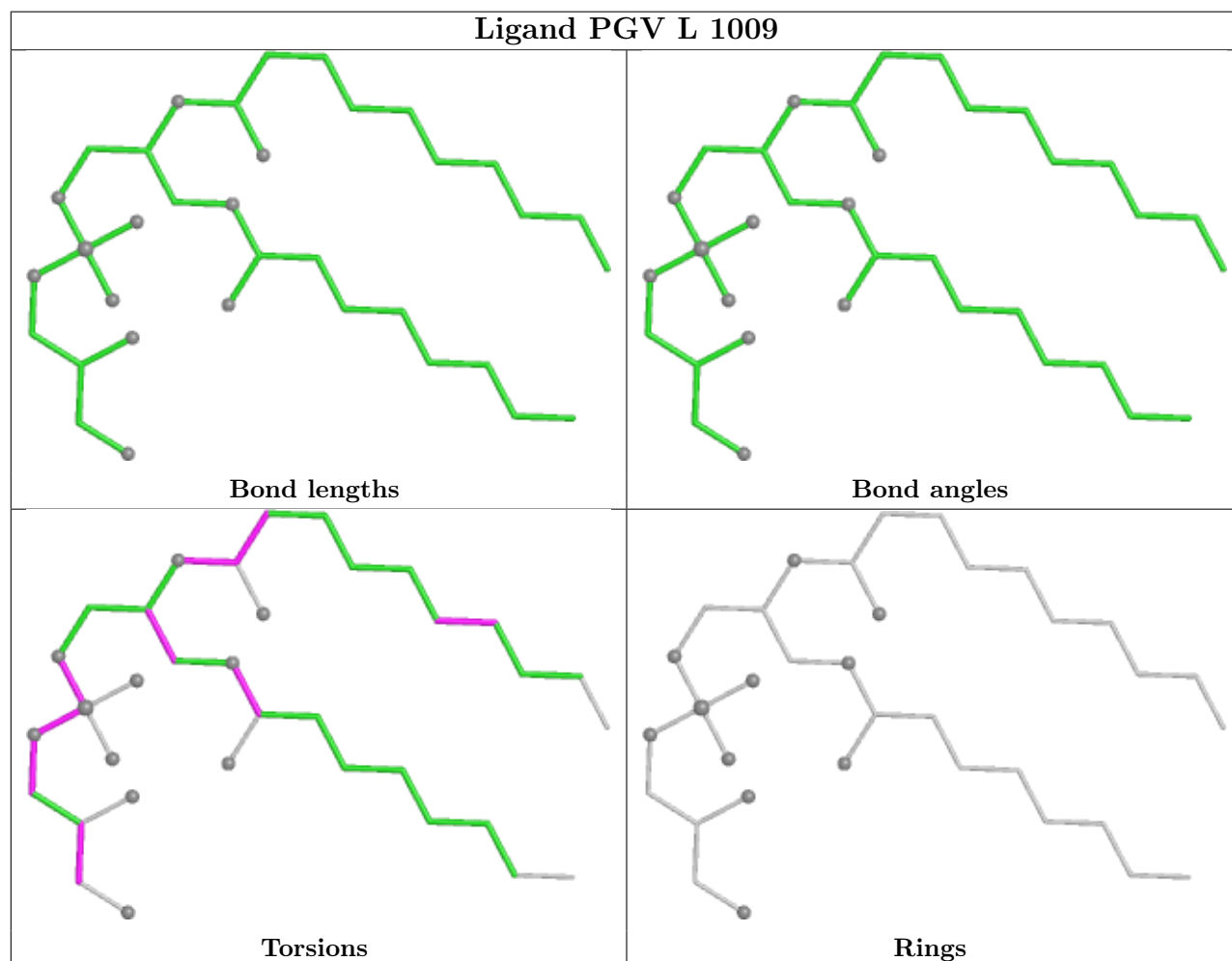
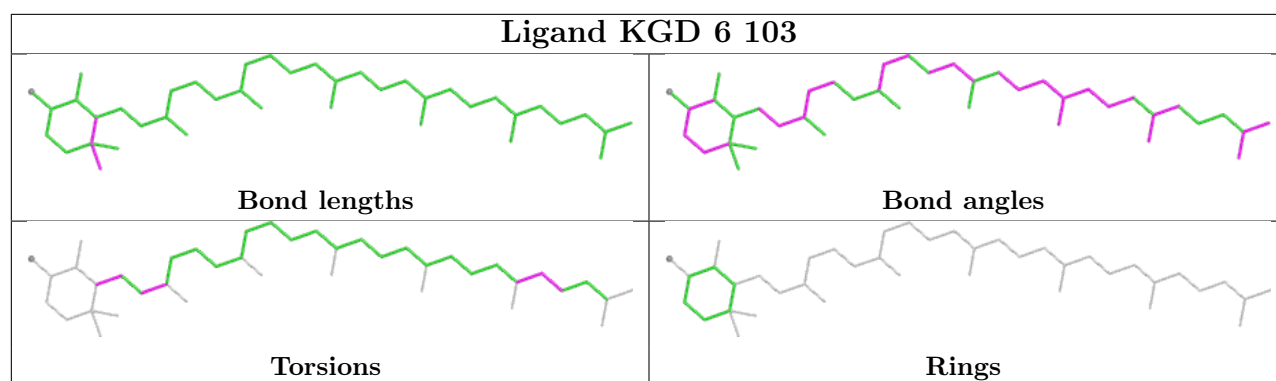


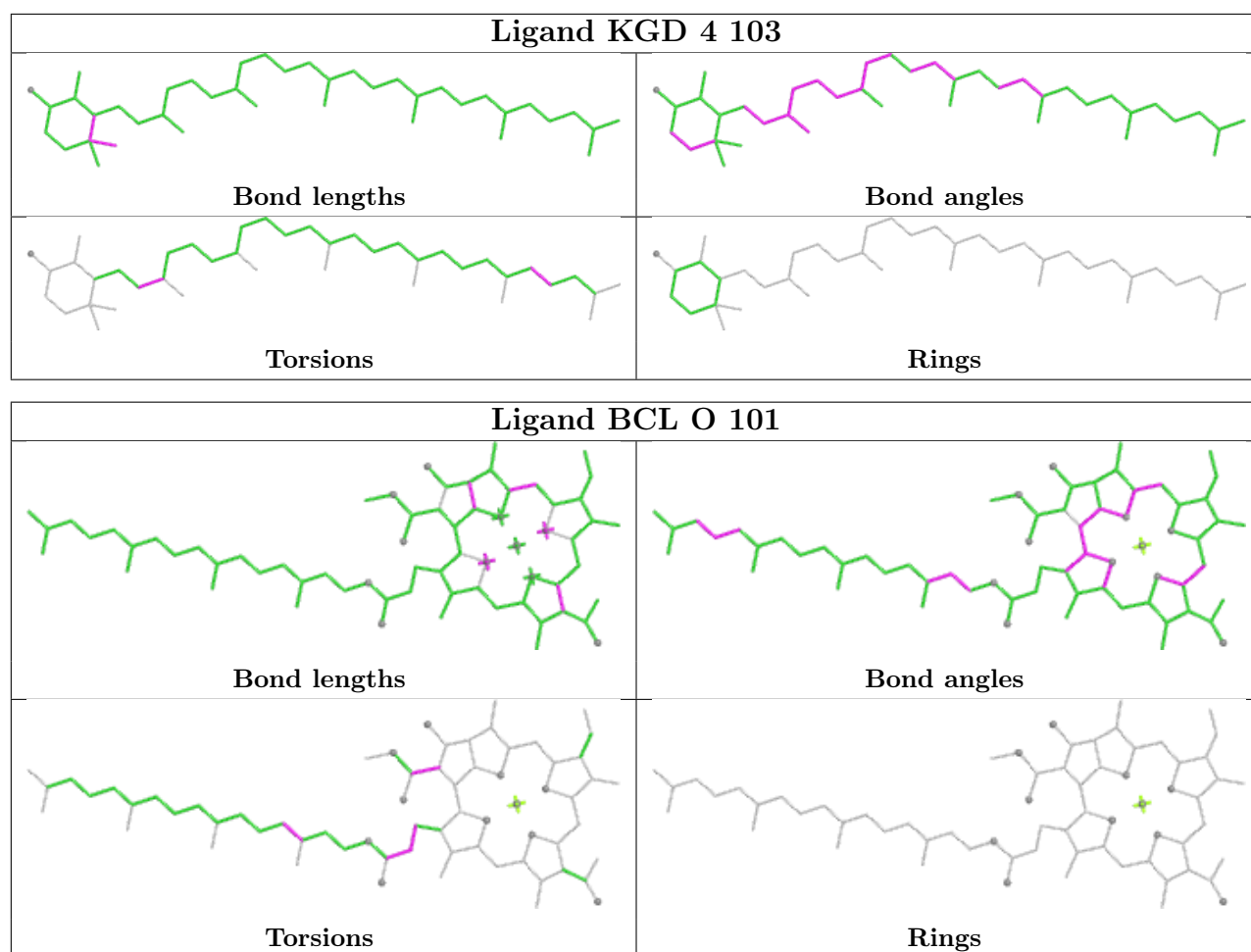


Ligand BCL Q 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL 1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand KGD D 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.

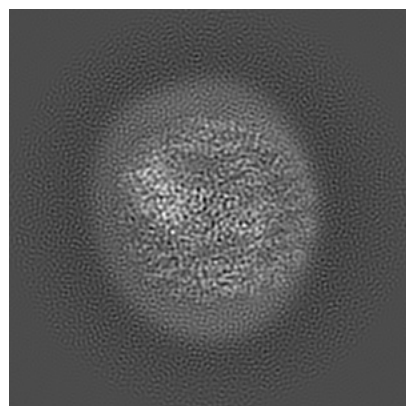
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35988. These allow visual inspection of the internal detail of the map and identification of artifacts.

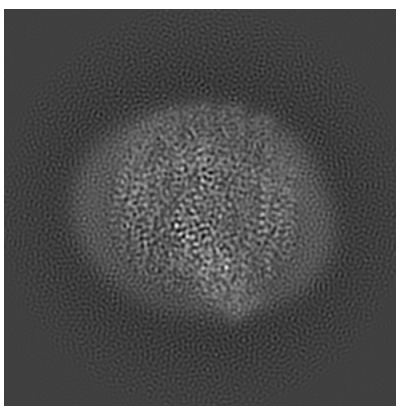
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

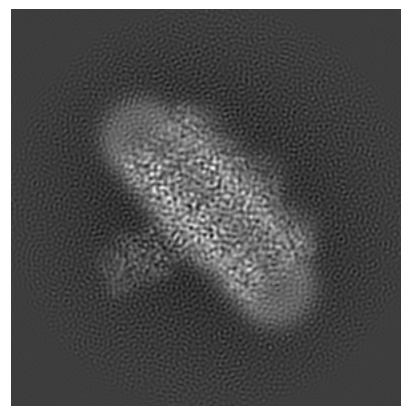
6.1.1 Primary map



X

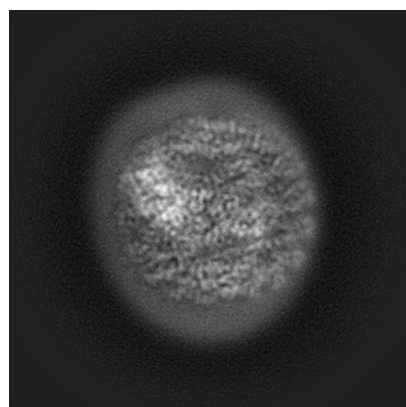


Y

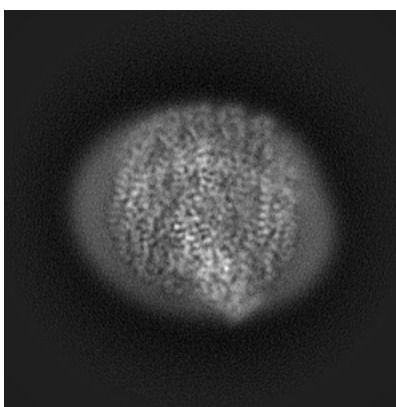


Z

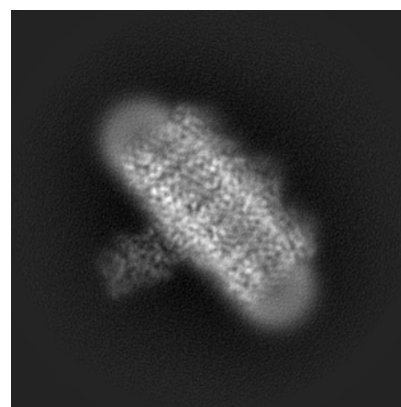
6.1.2 Raw map



X



Y

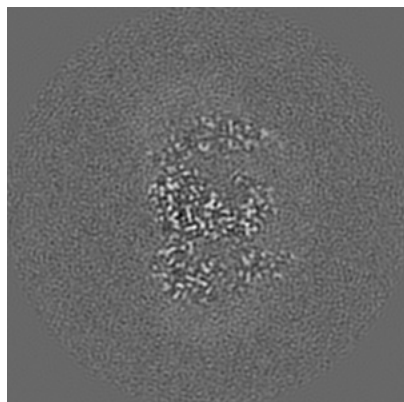


Z

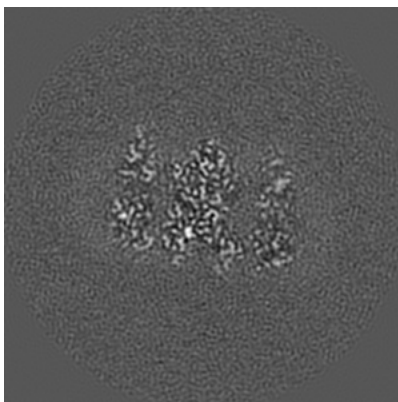
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

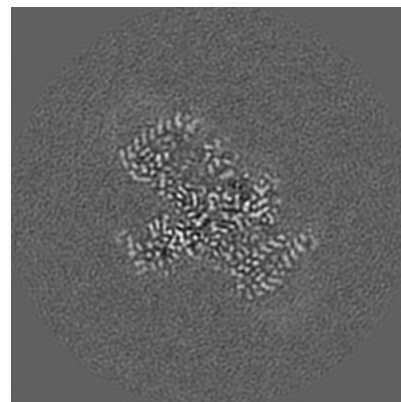
6.2.1 Primary map



X Index: 132

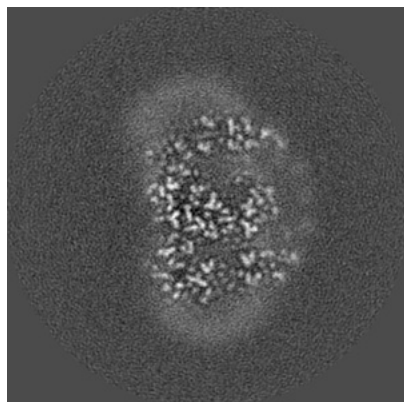


Y Index: 132

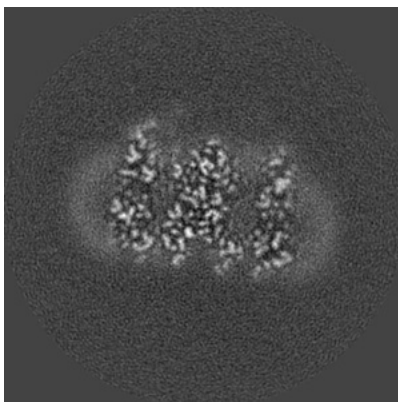


Z Index: 132

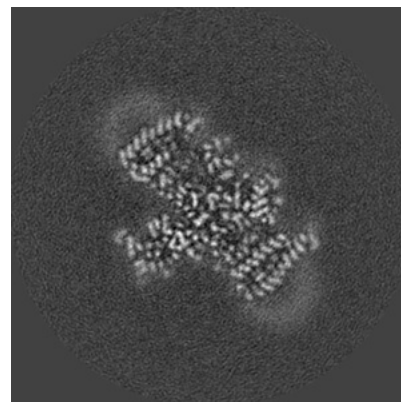
6.2.2 Raw map



X Index: 132



Y Index: 132

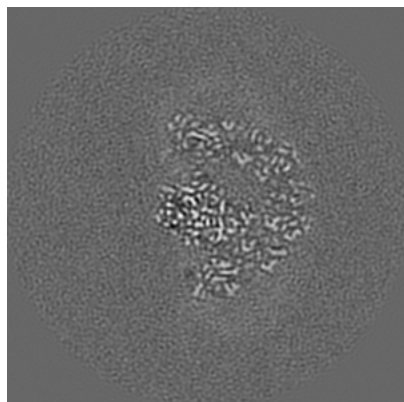


Z Index: 132

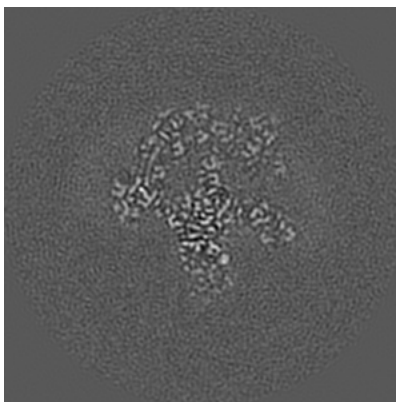
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

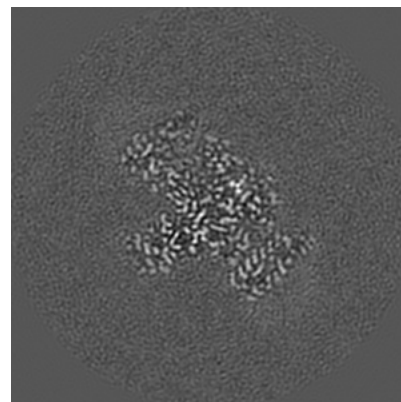
6.3.1 Primary map



X Index: 114

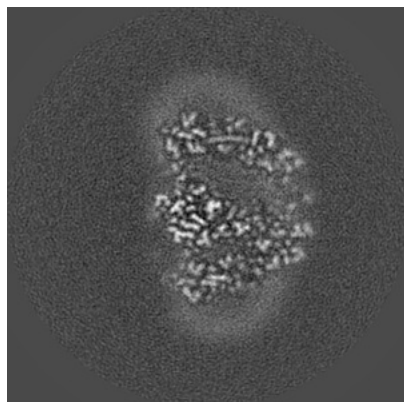


Y Index: 112

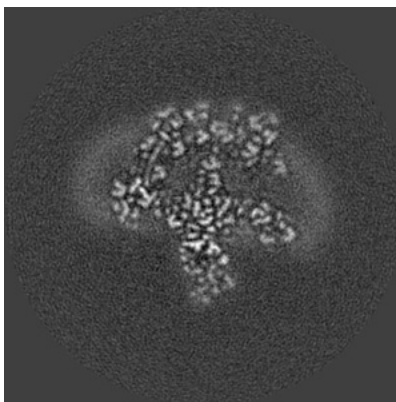


Z Index: 130

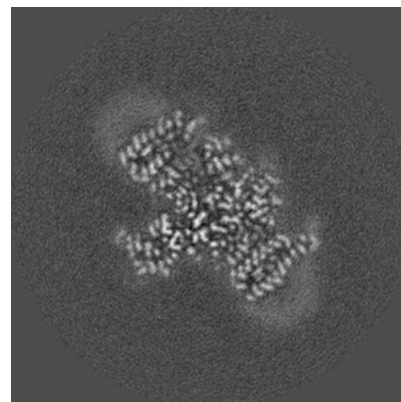
6.3.2 Raw map



X Index: 121



Y Index: 112

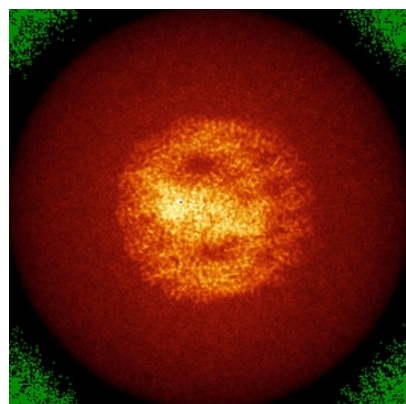


Z Index: 131

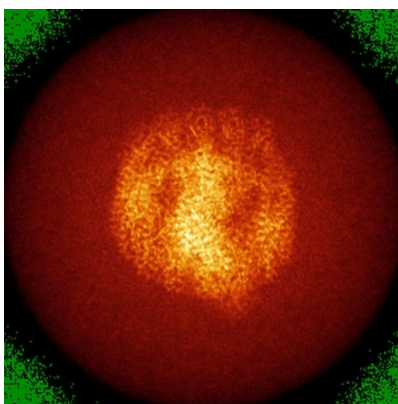
The images above show the largest variance slices of the map in three orthogonal directions.

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

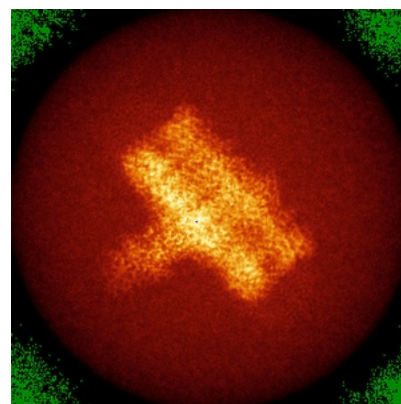
6.4.1 Primary map



X

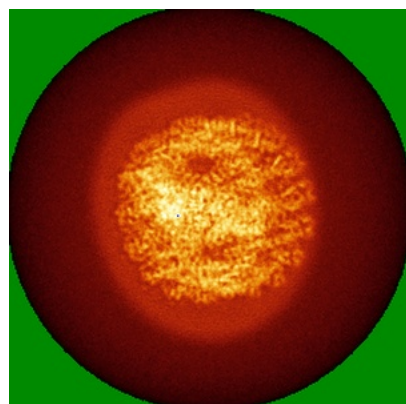


Y

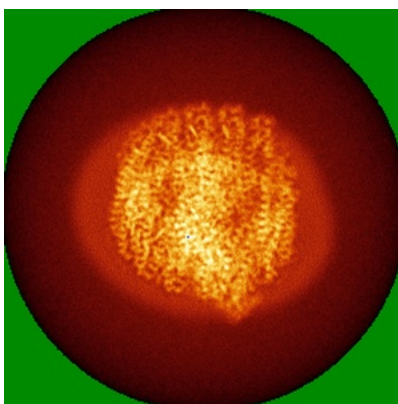


Z

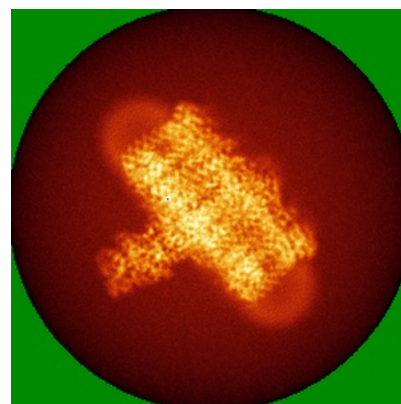
6.4.2 Raw map



X



Y

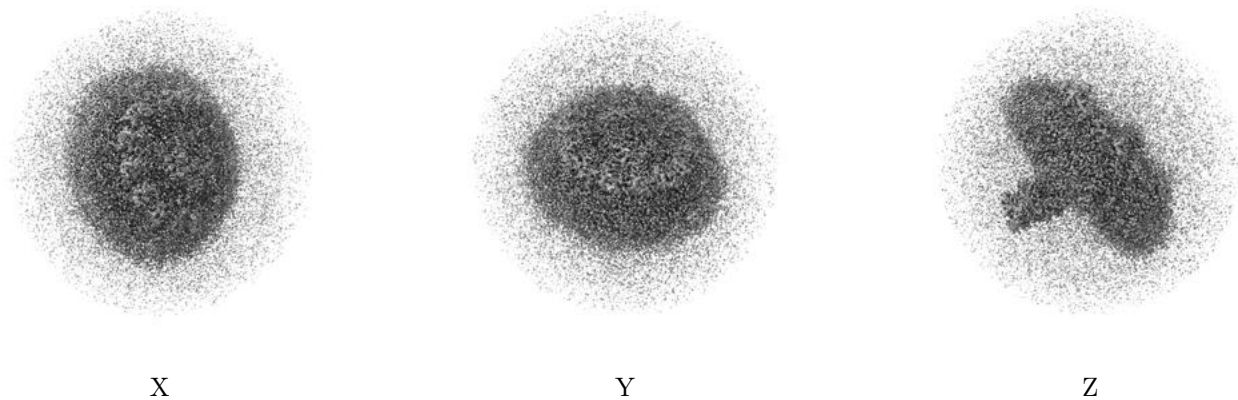


Z

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.

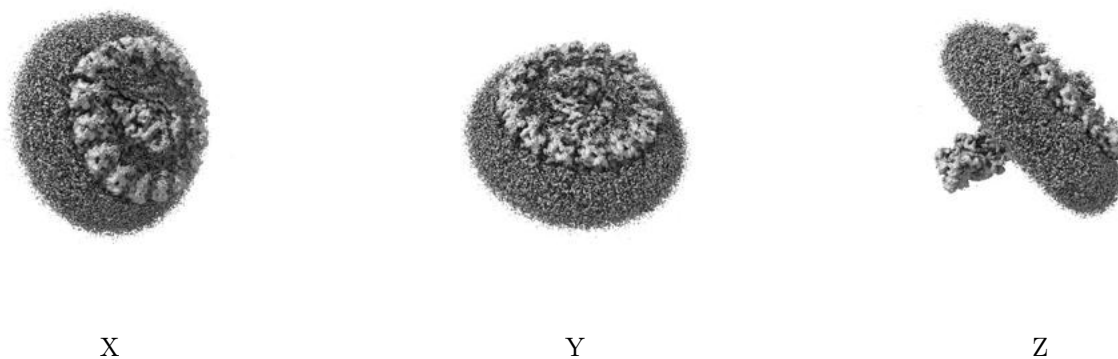
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

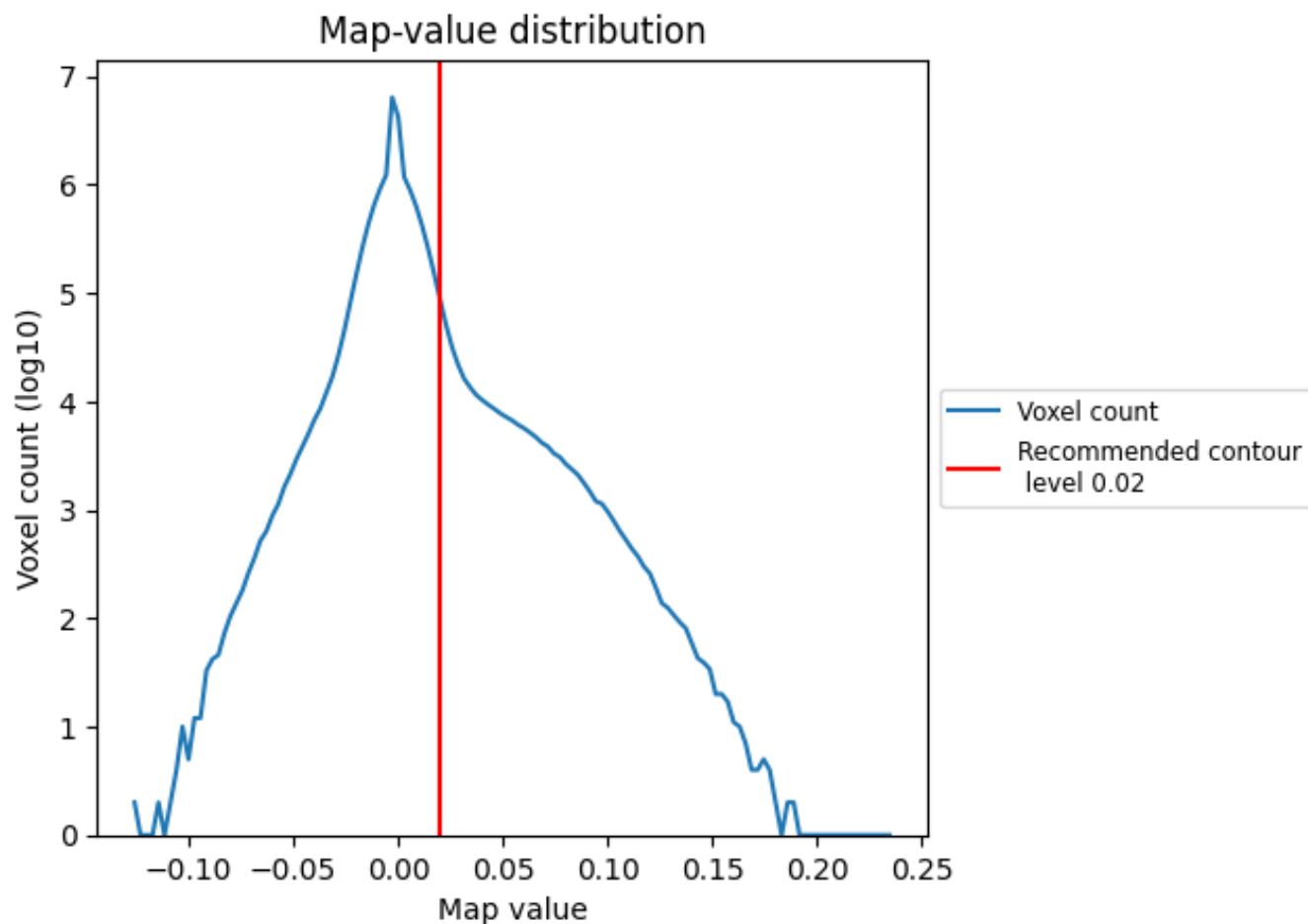
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

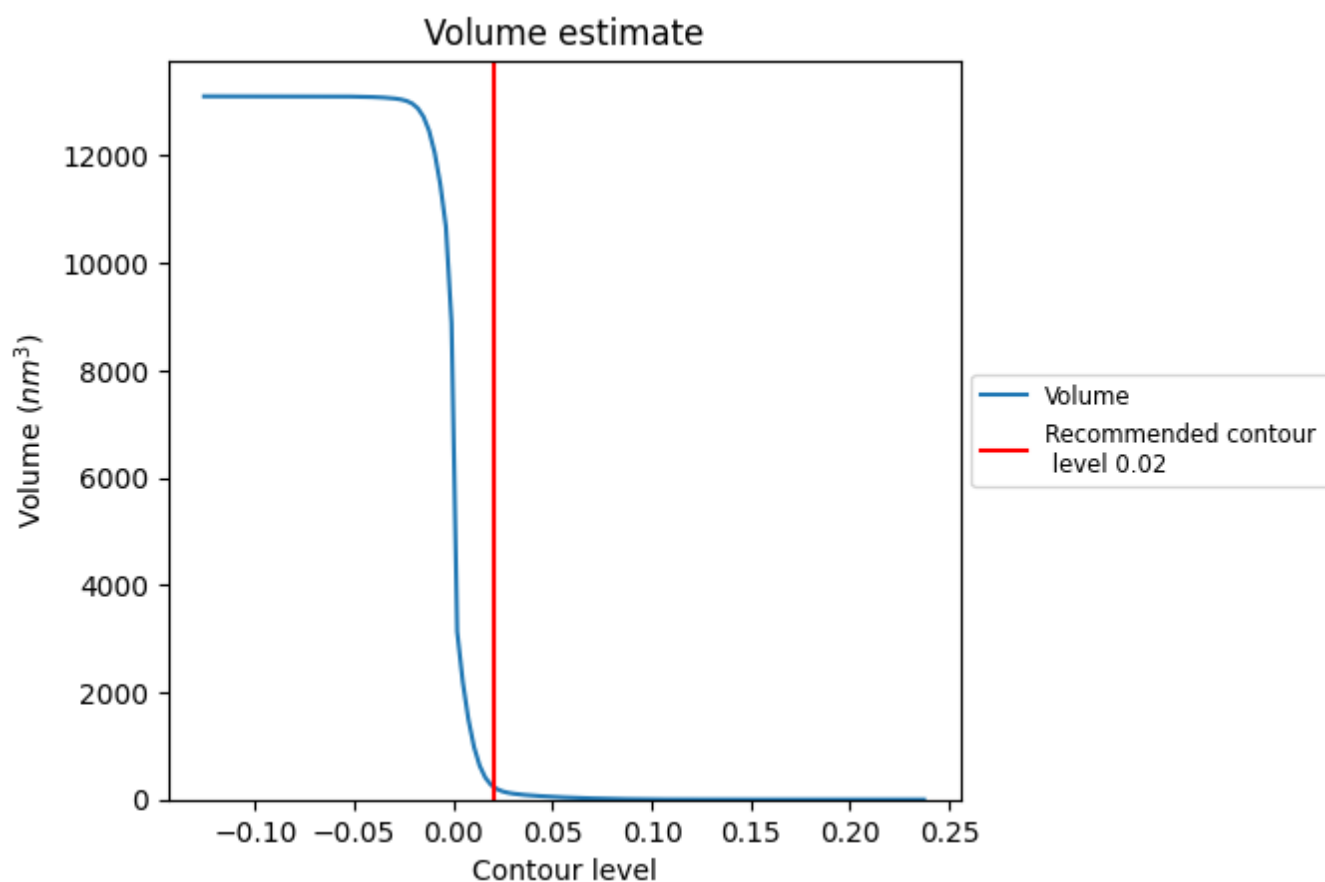
This section contains the results of statistical analysis of the map.

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.

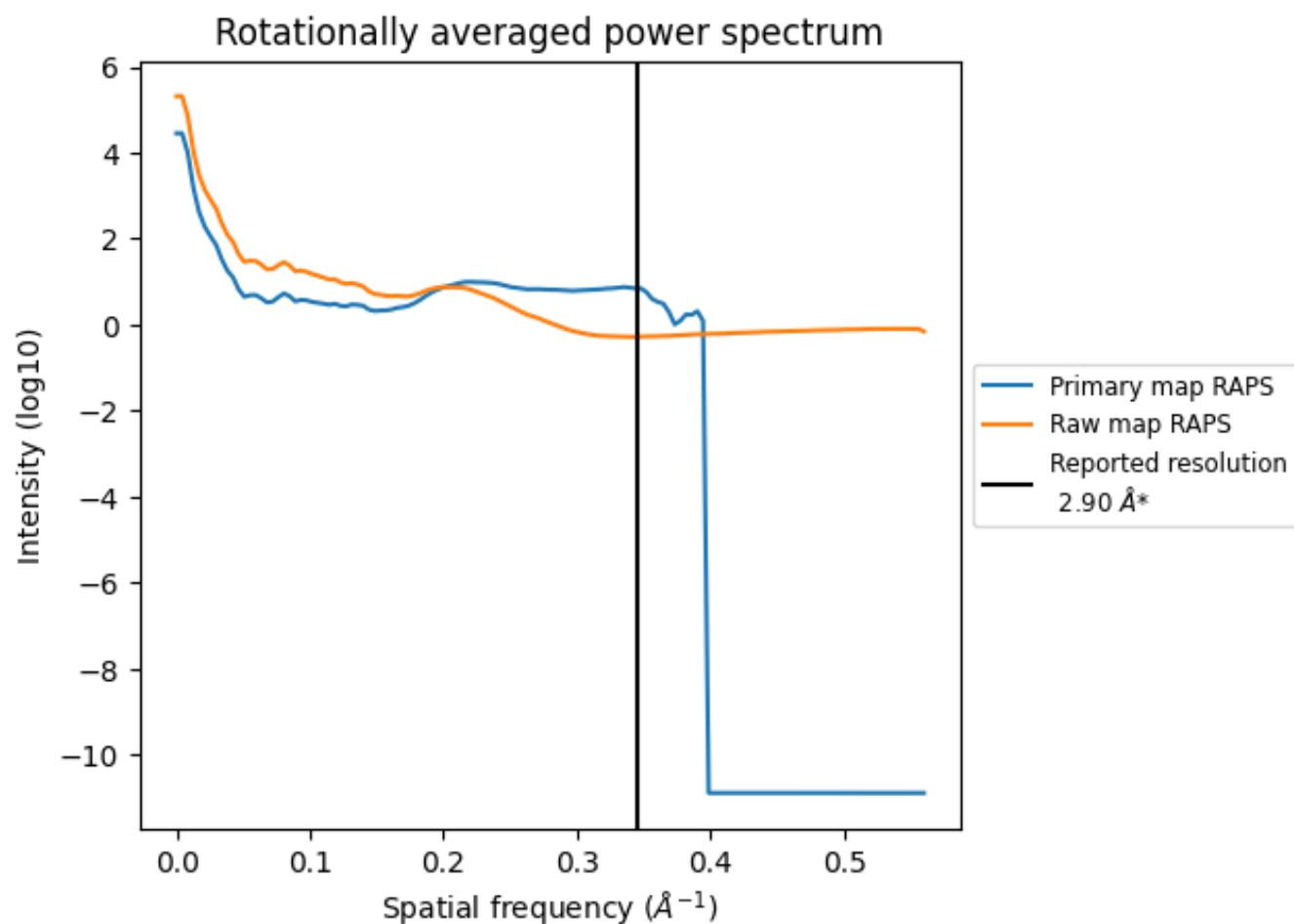
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

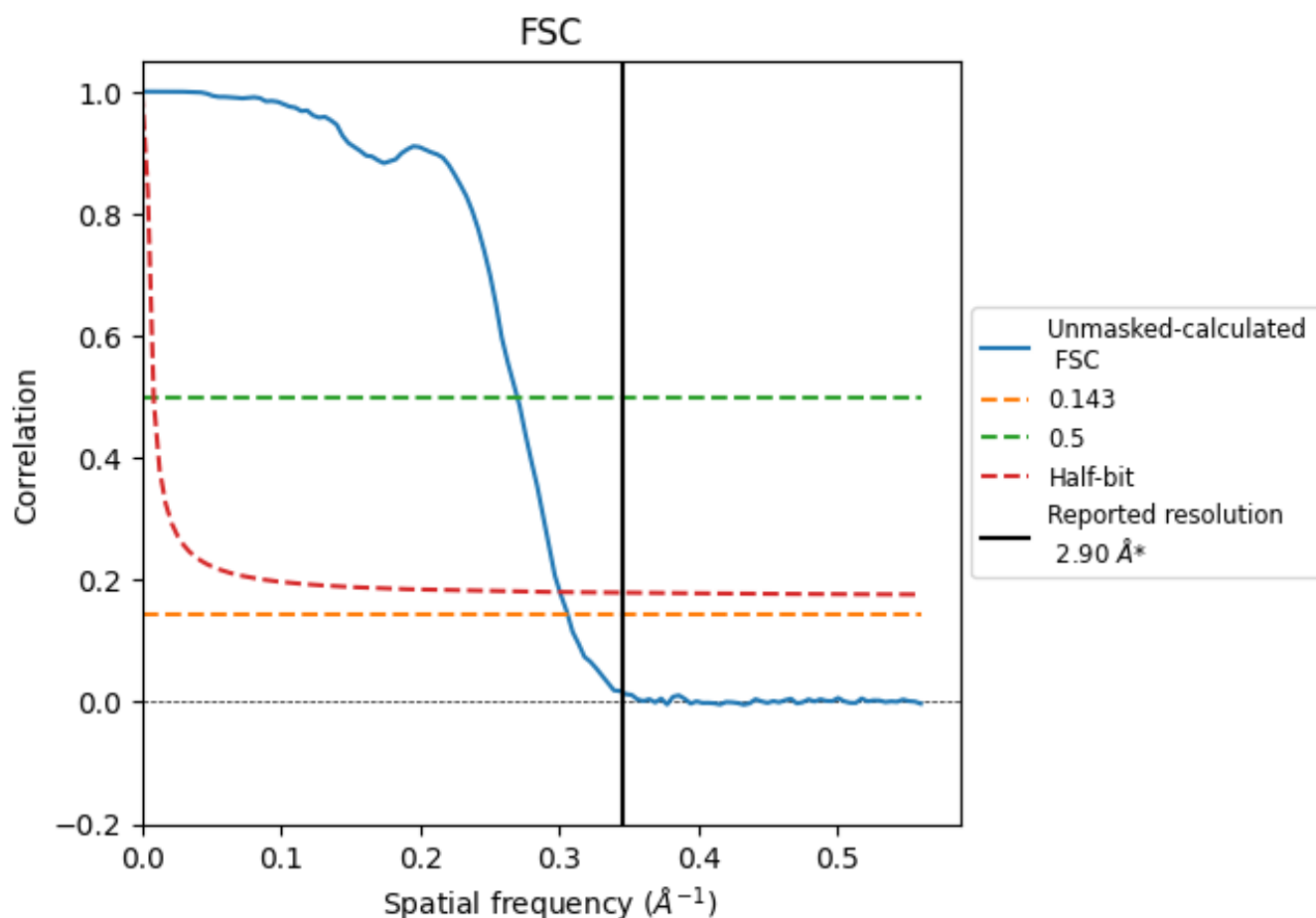


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

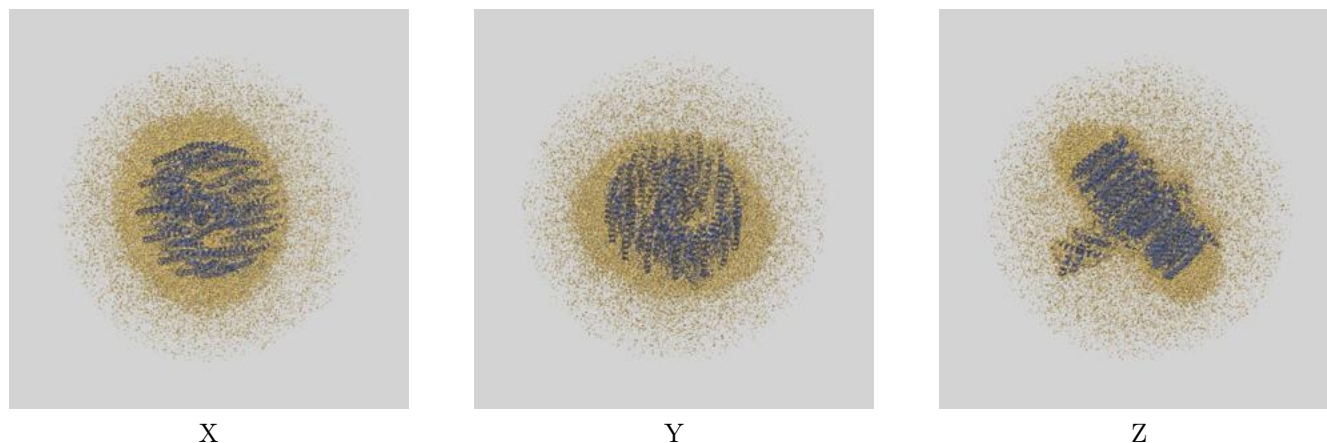
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	3.71	3.33

*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 3.27 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

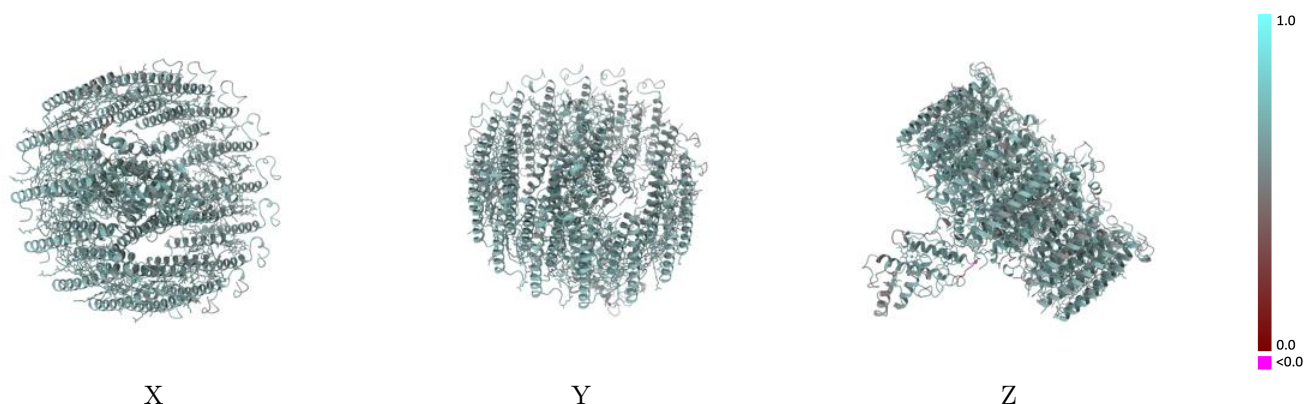
This section contains information regarding the fit between EMDB map EMD-35988 and PDB model 8J5O. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



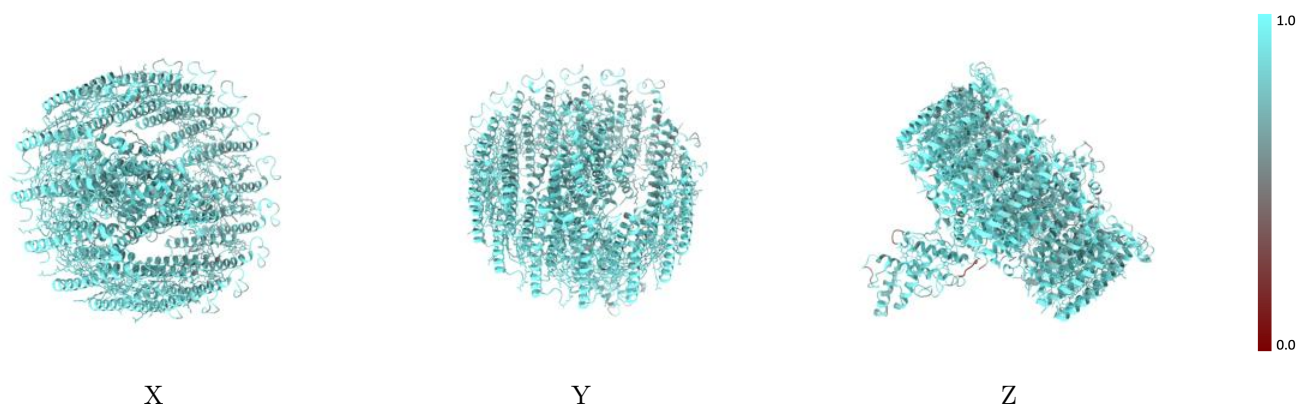
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



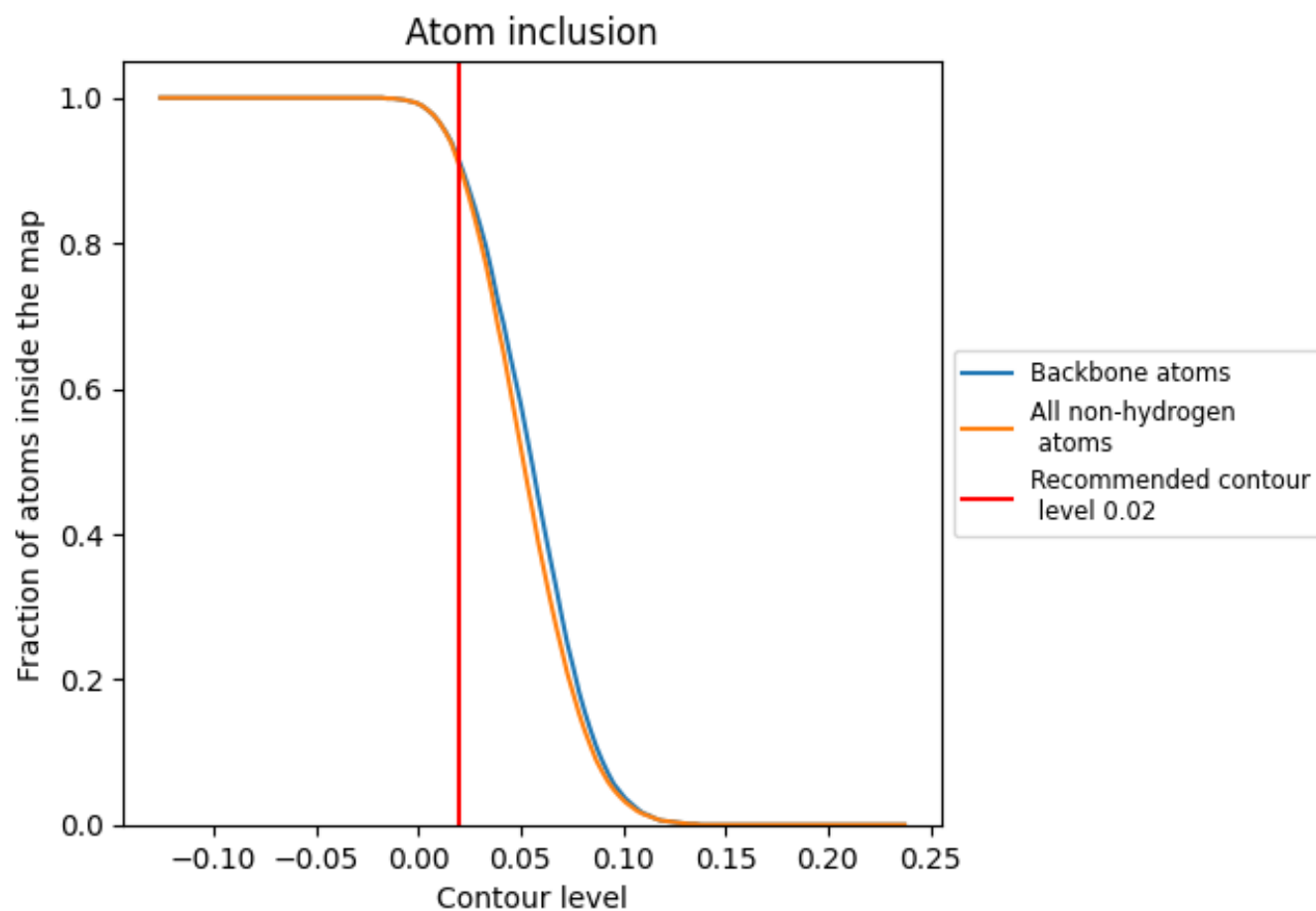
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.6060
0	 0.9020	 0.6030
1	 0.9280	 0.6150
2	 0.8430	 0.5720
3	 0.9310	 0.6140
4	 0.8840	 0.5870
5	 0.9210	 0.6170
6	 0.8840	 0.5900
7	 0.9410	 0.6260
8	 0.8770	 0.5930
9	 0.9290	 0.6160
A	 0.9260	 0.6060
B	 0.9060	 0.6130
C	 0.8830	 0.5860
D	 0.9450	 0.6270
E	 0.8970	 0.6070
F	 0.9220	 0.6160
G	 0.8820	 0.5920
H	 0.9360	 0.6220
I	 0.8990	 0.5920
J	 0.9440	 0.6350
K	 0.8950	 0.6070
L	 0.9180	 0.6160
M	 0.9460	 0.6290
N	 0.9510	 0.6250
O	 0.9070	 0.6010
P	 0.9460	 0.6200
Q	 0.9000	 0.6030
R	 0.9260	 0.6190
S	 0.8980	 0.6130
T	 0.9210	 0.6020
U	 0.8830	 0.5990
V	 0.8740	 0.5730
W	 0.8510	 0.5720
X	 0.7460	 0.5500



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Chain	Atom inclusion	Q-score
Y	 0.9060	 0.5970
Z	 0.8930	 0.5980