



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:40 AM UTC

PDB ID : 1EYS / pdb_00001eys
Title : CRYSTAL STRUCTURE OF PHOTOSYNTHETIC REACTION CENTER FROM A THERMOPHILIC BACTERIUM, THERMOCHROMATIUM TEPIDUM
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Deposited on : 2000-05-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

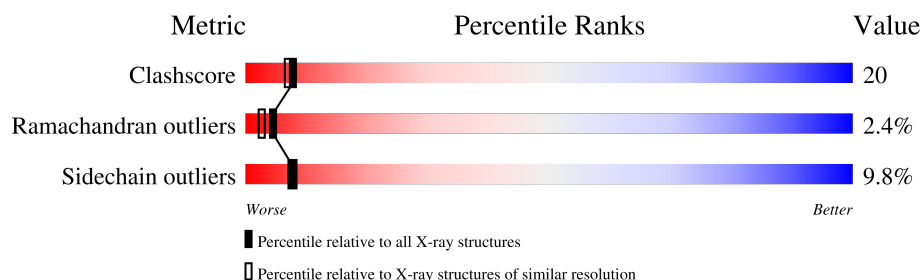
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	382	
2	L	280	
3	M	324	
4	H	259	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BPH	L	606	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	310	Total	C	N	O	S	0	0	0
			2402	1514	421	451	16			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2233	1501	361	361	10			

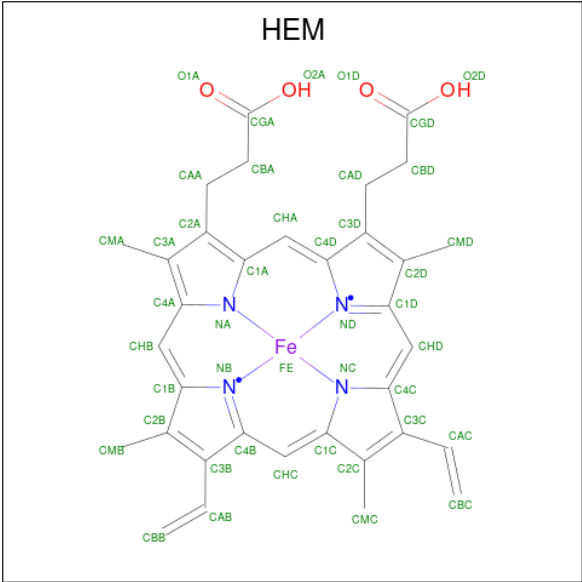
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	0	0
			2537	1705	413	409	10			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

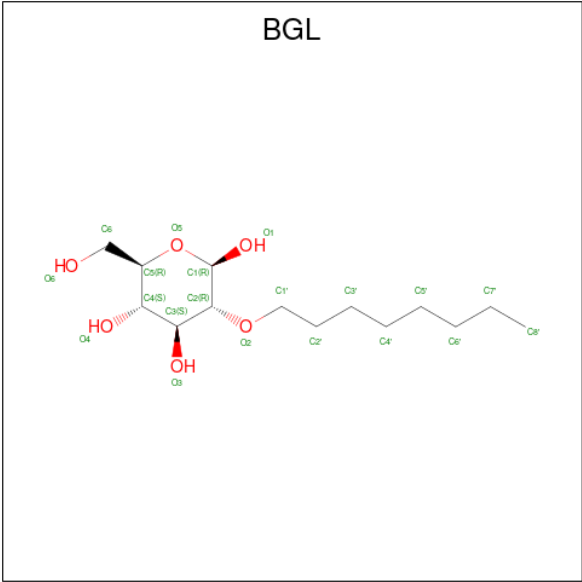
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	238	Total	C	N	O	S	0	0	0
			1837	1187	309	336	5			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



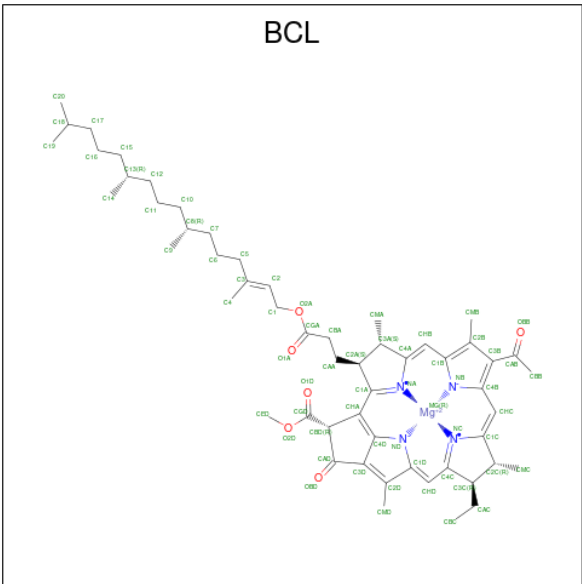
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



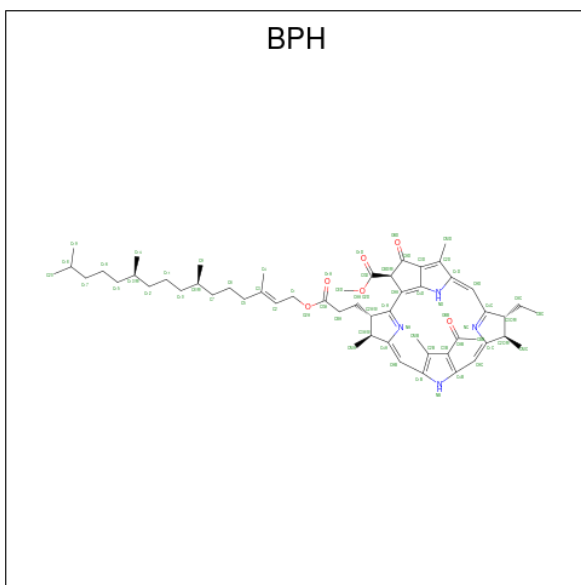
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			20	14	6		
6	L	1	Total	C	O	0	0
			20	14	6		
6	L	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



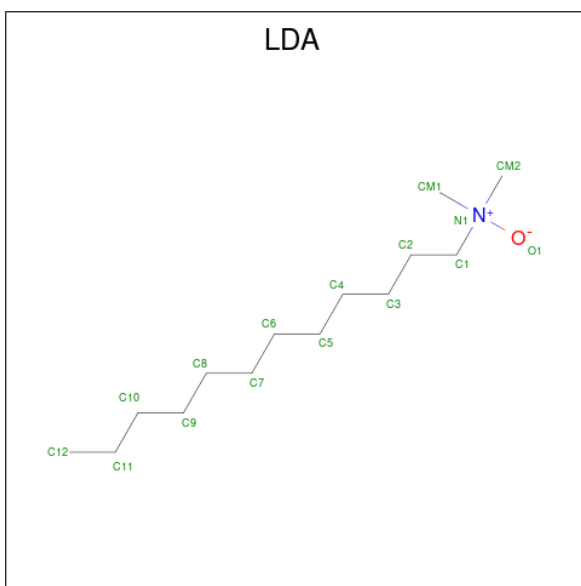
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

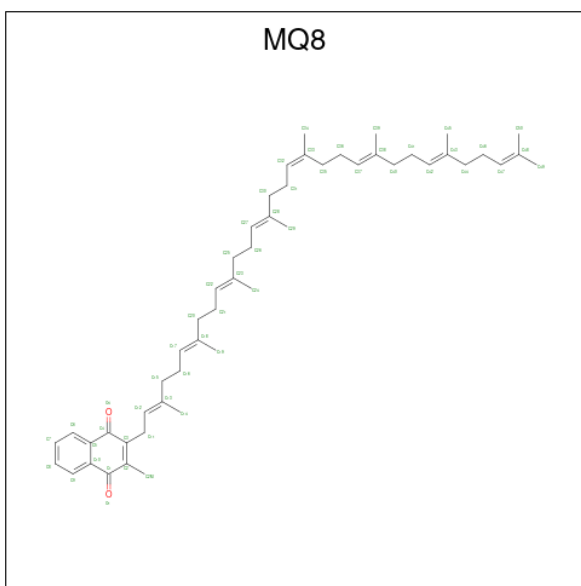


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

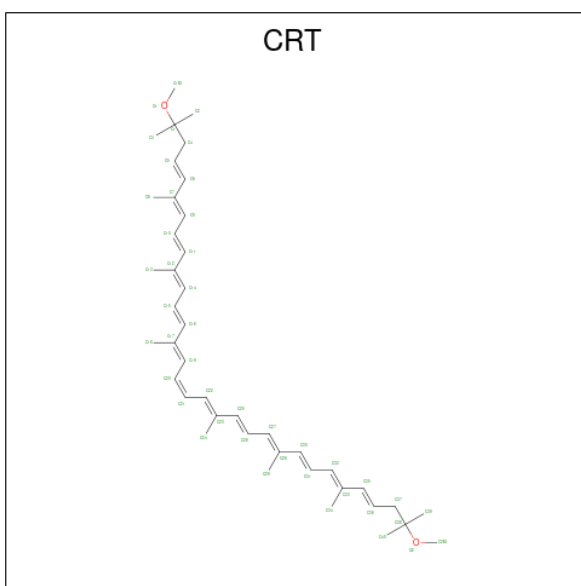
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



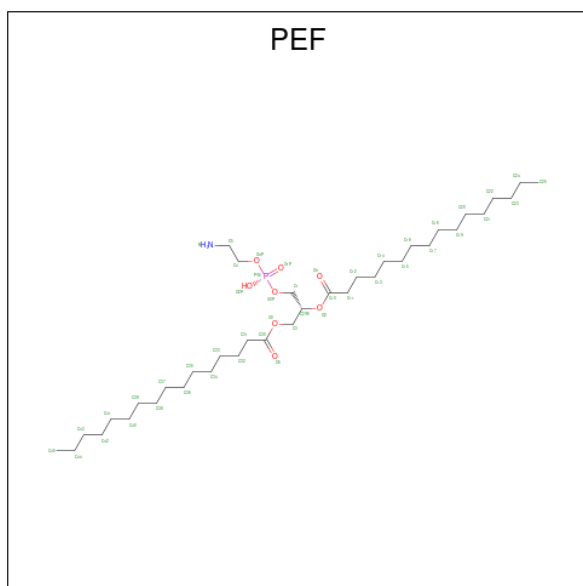
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 12 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			44	42	2		

- Molecule 13 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	H	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 14 is water.

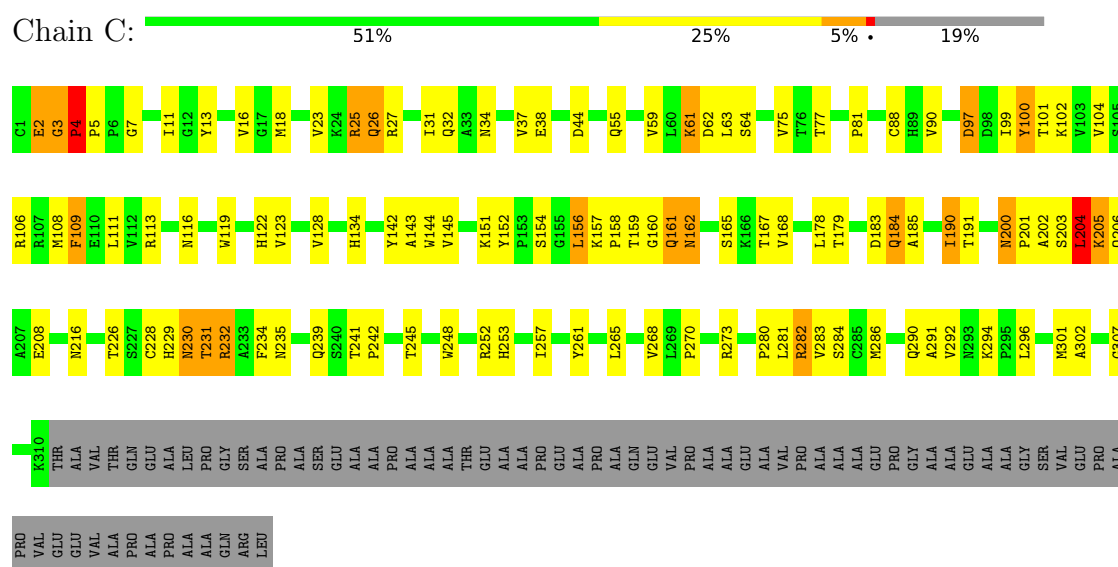
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	94	Total	O	0	0
			94	94		
14	L	37	Total	O	0	0
			37	37		
14	M	35	Total	O	0	0
			35	35		
14	H	22	Total	O	0	0
			22	22		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

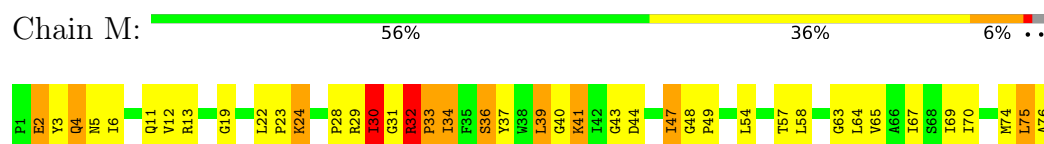
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

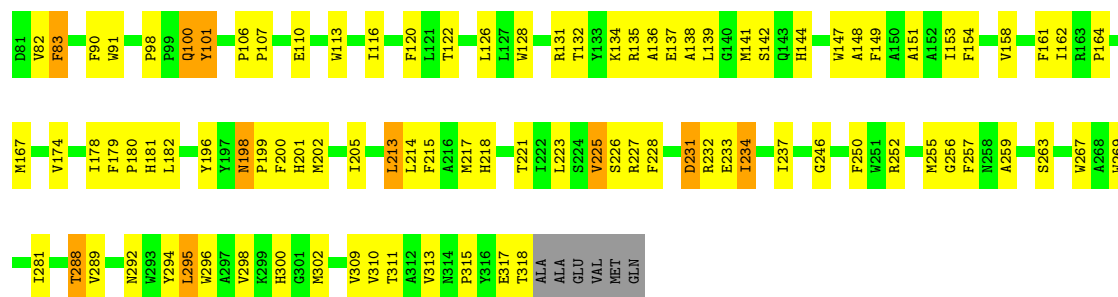


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



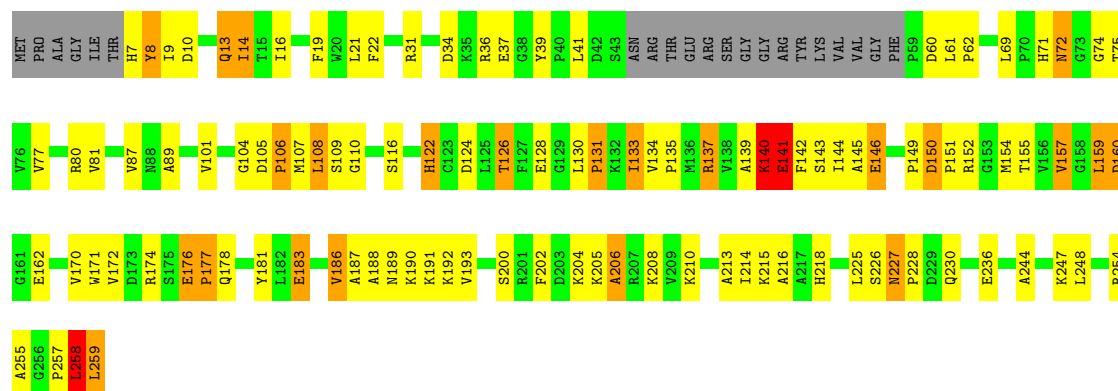
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER





• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H: 50% 32% 9% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.30Å 196.60Å 84.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ8, LDA, BCL, FE, BPH, PEF, BGL, CRT, HEM

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	C	0.69	0/2471	1.09	22/3374 (0.7%)
2	L	0.68	0/2320	0.99	14/3170 (0.4%)
3	M	0.67	0/2637	1.04	14/3610 (0.4%)
4	H	0.60	0/1890	1.12	14/2576 (0.5%)
All	All	0.66	0/9318	1.06	64/12730 (0.5%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	109	SER	N-CA-C	8.85	121.73	111.11
3	M	39	LEU	N-CA-C	-8.56	101.95	111.28
1	C	44	ASP	N-CA-C	-8.43	97.66	110.30
4	H	254	ARG	N-CA-C	-8.03	102.22	110.97
4	H	8	TYR	N-CA-C	-7.97	104.04	113.21
1	C	143	ALA	N-CA-C	-7.95	98.76	110.52
3	M	47	ILE	N-CA-C	-7.72	95.95	107.37
1	C	230	ASN	N-CA-C	-7.25	92.55	107.70
2	L	236	ALA	N-CA-C	7.12	119.94	111.33
1	C	134	HIS	N-CA-C	6.88	118.86	111.36
1	C	178	LEU	N-CA-C	6.75	121.76	112.04
4	H	141	GLU	N-CA-C	6.64	118.21	110.97
1	C	3	GLY	N-CA-C	6.64	125.88	112.34
2	L	171	GLN	N-CA-C	-6.60	104.48	112.54
1	C	116	ASN	N-CA-C	6.59	119.46	111.82
4	H	258	LEU	N-CA-C	-6.58	107.12	114.62
2	L	252	SER	N-CA-C	-6.50	104.27	111.36
1	C	109	PHE	N-CA-C	-6.45	104.11	112.23
4	H	124	ASP	N-CA-C	-6.26	101.67	110.50
2	L	16	LEU	N-CA-C	-6.18	105.64	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	139	ALA	N-CA-C	-6.12	102.94	110.65
3	M	48	GLY	CA-C-N	6.12	127.49	119.84
3	M	48	GLY	C-N-CA	6.12	127.49	119.84
4	H	74	GLY	N-CA-C	-6.08	102.60	110.38
2	L	69	LEU	N-CA-C	6.06	118.68	111.71
3	M	48	GLY	N-CA-C	6.01	124.61	112.34
3	M	201	HIS	N-CA-C	-5.97	104.35	111.69
1	C	154	SER	N-CA-C	-5.96	100.29	109.76
1	C	7	GLY	N-CA-C	-5.93	104.07	112.37
2	L	35	GLY	N-CA-C	-5.89	105.03	113.86
1	C	55	GLN	N-CA-C	5.87	120.57	113.41
2	L	238	HIS	N-CA-C	-5.86	104.85	112.23
1	C	3	GLY	CA-C-N	5.83	126.39	120.38
1	C	3	GLY	C-N-CA	5.83	126.39	120.38
3	M	32	ARG	CA-C-N	5.70	126.97	119.84
3	M	32	ARG	C-N-CA	5.70	126.97	119.84
3	M	267	TRP	N-CA-C	-5.67	105.19	111.36
3	M	24	LYS	N-CA-C	5.65	117.67	108.63
1	C	90	VAL	N-CA-C	-5.63	102.08	107.76
4	H	110	GLY	N-CA-C	-5.61	105.16	114.48
3	M	281	ILE	N-CA-C	-5.61	104.90	110.62
3	M	101	TYR	N-CA-C	5.61	120.19	113.23
1	C	167	THR	N-CA-C	5.53	120.02	113.28
2	L	225	ARG	N-CA-C	-5.49	105.70	112.90
4	H	176	GLU	CA-C-N	5.49	126.71	119.84
4	H	176	GLU	C-N-CA	5.49	126.71	119.84
3	M	83	PHE	N-CA-C	-5.43	104.78	111.40
4	H	60	ASP	N-CA-C	-5.42	101.40	109.96
1	C	302	ALA	N-CA-C	5.42	117.88	111.33
2	L	227	ILE	N-CA-C	5.38	115.58	110.42
1	C	97	ASP	N-CA-C	-5.35	105.20	112.26
2	L	3	LEU	N-CA-C	-5.34	103.44	110.43
2	L	27	GLY	N-CA-C	-5.32	101.49	112.34
1	C	184	GLN	N-CA-C	-5.30	101.52	109.79
4	H	126	THR	N-CA-C	-5.29	103.63	110.19
3	M	3	TYR	N-CA-C	-5.26	102.82	110.24
1	C	232	ARG	N-CA-C	-5.23	106.40	112.89
1	C	100	TYR	N-CA-C	5.17	118.36	111.75
1	C	161	GLN	N-CA-C	-5.13	106.56	114.16
2	L	44	LEU	N-CA-C	-5.13	105.87	111.82
2	L	279	LEU	N-CA-C	-5.12	105.69	112.34
2	L	30	TYR	N-CA-C	-5.08	101.42	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	LEU	N-CA-C	-5.06	105.95	111.82
4	H	150	ASP	N-CA-C	-5.02	101.99	109.42

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	C	2402	0	2323	82	0
2	L	2233	0	2195	92	0
3	M	2537	0	2511	133	0
4	H	1837	0	1831	87	0
5	C	172	0	120	5	0
6	L	60	0	84	9	0
6	M	60	0	84	1	0
7	L	132	0	148	14	0
7	M	132	0	148	16	0
8	L	65	0	75	7	0
8	M	65	0	75	4	0
9	L	16	0	31	2	0
10	M	1	0	0	0	0
11	M	53	0	72	1	0
12	M	44	0	60	2	0
13	H	47	0	73	7	0
14	C	94	0	0	0	0
14	H	22	0	0	1	0
14	L	37	0	0	0	0
14	M	35	0	0	1	0
All	All	10044	0	9830	391	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 20.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:69:ILE:HD13	3:M:116:ILE:HG23	1.36	1.06
4:H:7:HIS:HB3	4:H:9:ILE:HG12	1.40	1.00
4:H:151:PRO:HA	4:H:154:MET:SD	2.07	0.94
3:M:33:PRO:HG3	3:M:49:PRO:HD3	1.52	0.92
6:L:704:BGL:H1	3:M:302:MET:HE2	1.53	0.90
2:L:86:ALA:H	2:L:95:GLN:HE22	1.06	0.90
4:H:9:ILE:HA	4:H:13:GLN:HE22	1.37	0.89
4:H:105:ASP:HB3	4:H:108:LEU:HD23	1.53	0.88
4:H:215:LYS:H	4:H:218:HIS:HD2	1.22	0.86
4:H:7:HIS:CG	4:H:8:TYR:H	1.97	0.83
3:M:75:LEU:HD22	3:M:80:TRP:HA	1.61	0.81
2:L:249:ALA:HB2	8:L:606:BPH:HBC3	1.65	0.77
3:M:107:PRO:HG2	3:M:110:GLU:HB2	1.65	0.76
4:H:186:VAL:HG23	4:H:191:LYS:O	1.86	0.75
11:M:608:MQ8:H252	13:H:708:PEF:H362	1.69	0.75
1:C:27:ARG:O	1:C:31:ILE:HG13	1.87	0.74
4:H:189:ASN:ND2	4:H:191:LYS:HB2	2.03	0.74
1:C:203:SER:H	1:C:206:GLN:NE2	1.86	0.73
4:H:189:ASN:HD22	4:H:191:LYS:HD2	1.53	0.73
7:L:602:BCL:HAA2	7:L:604:BCL:HBC1	1.69	0.73
3:M:131:ARG:HG3	3:M:131:ARG:HH11	1.54	0.72
4:H:9:ILE:HA	4:H:13:GLN:NE2	2.05	0.72
4:H:134:VAL:HG22	4:H:174:ARG:HD2	1.70	0.72
1:C:88:CYS:HA	1:C:101:THR:OG1	1.89	0.71
3:M:198:ASN:C	3:M:198:ASN:HD22	1.96	0.71
2:L:183:LEU:HG	6:L:701:BGL:O6	1.91	0.70
7:L:604:BCL:HBB3	8:L:606:BPH:H141	1.73	0.70
3:M:22:LEU:HD21	3:M:29:ARG:HH12	1.57	0.70
3:M:30:ILE:HG13	3:M:31:GLY:N	2.07	0.70
3:M:69:ILE:HD13	3:M:116:ILE:CG2	2.18	0.70
2:L:117:ARG:HH12	4:H:258:LEU:CD1	2.04	0.69
4:H:171:TRP:HE1	4:H:183:GLU:HG3	1.57	0.69
3:M:75:LEU:HD13	3:M:80:TRP:CE3	2.28	0.69
1:C:161:GLN:O	1:C:162:ASN:HB2	1.94	0.68
7:M:601:BCL:HMB1	7:M:601:BCL:HBB2	1.75	0.67
1:C:4:PRO:HD3	2:L:261:PRO:O	1.93	0.67
3:M:113:TRP:O	3:M:116:ILE:HG22	1.94	0.67
3:M:213:LEU:HD22	3:M:217:MET:SD	2.35	0.67
3:M:40:GLY:HA2	3:M:43:GLY:O	1.95	0.66
1:C:200:ASN:C	1:C:200:ASN:HD22	2.03	0.66
2:L:117:ARG:HH12	4:H:258:LEU:HD13	1.60	0.66
1:C:161:GLN:HB2	1:C:184:GLN:HB3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:54:LEU:O	3:M:57:THR:HG22	1.95	0.65
3:M:11:GLN:OE1	3:M:13:ARG:NH2	2.30	0.65
4:H:10:ASP:H	4:H:13:GLN:HE21	1.44	0.64
4:H:215:LYS:HB2	4:H:218:HIS:CD2	2.32	0.64
4:H:162:GLU:HB2	4:H:216:ALA:CB	2.28	0.64
4:H:134:VAL:HG21	4:H:174:ARG:NH1	2.13	0.64
2:L:210:ARG:NE	2:L:211:GLY:H	1.95	0.64
2:L:183:LEU:HA	6:L:701:BGL:H62	1.78	0.64
3:M:292:ASN:ND2	3:M:295:LEU:HD22	2.11	0.64
2:L:17:ILE:HB	4:H:259:LEU:HG	1.78	0.63
1:C:161:GLN:HG3	1:C:185:ALA:H	1.64	0.63
3:M:154:PHE:O	3:M:158:VAL:HG23	1.98	0.63
2:L:215:LYS:HD2	2:L:219:HIS:ND1	2.13	0.63
2:L:76:PRO:HB2	2:L:151:GLY:HA2	1.81	0.63
2:L:70:TRP:CE2	6:L:703:BGL:H2'1	2.33	0.63
2:L:200:SER:HG	3:M:269:TRP:CD1	2.16	0.62
2:L:207:ASN:N	2:L:207:ASN:HD22	1.96	0.62
2:L:227:ILE:HD11	3:M:135:ARG:HB2	1.82	0.62
4:H:7:HIS:C	4:H:9:ILE:H	2.07	0.62
3:M:232:ARG:HH22	4:H:236:GLU:CD	2.08	0.62
2:L:143:ARG:HB3	2:L:144:PRO:HD3	1.82	0.61
4:H:133:ILE:HD11	4:H:181:TYR:HD2	1.65	0.61
1:C:142:TYR:CD1	1:C:290:GLN:HG2	2.36	0.61
1:C:37:VAL:O	1:C:301:MET:HE3	2.01	0.61
2:L:178:ASN:O	2:L:182:MET:HG3	2.01	0.60
2:L:16:LEU:HG	2:L:114:GLU:HG2	1.83	0.60
7:L:604:BCL:HMB1	7:L:604:BCL:HBB2	1.83	0.60
1:C:242:PRO:HD3	3:M:311:THR:O	2.01	0.60
3:M:288:THR:HG22	3:M:289:VAL:HG23	1.82	0.60
4:H:7:HIS:CD2	4:H:8:TYR:H	2.18	0.60
3:M:11:GLN:NE2	3:M:41:LYS:HD2	2.17	0.59
3:M:128:TRP:O	3:M:131:ARG:HB3	2.02	0.59
4:H:150:ASP:OD1	4:H:152:ARG:HB2	2.02	0.59
2:L:69:LEU:HB2	6:L:703:BGL:H1'1	1.84	0.59
1:C:235:ASN:H	1:C:235:ASN:HD22	1.50	0.59
3:M:76:ALA:HB1	6:M:702:BGL:H2	1.84	0.59
4:H:151:PRO:O	4:H:154:MET:HG3	2.03	0.59
4:H:204:LYS:C	4:H:206:ALA:H	2.10	0.59
1:C:230:ASN:OD1	1:C:232:ARG:HG2	2.02	0.59
1:C:280:PRO:O	1:C:282:ARG:HG2	2.02	0.58
4:H:215:LYS:H	4:H:218:HIS:CD2	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:VAL:HG12	1:C:294:LYS:H	1.69	0.58
1:C:156:LEU:HD12	1:C:157:LYS:H	1.67	0.58
2:L:169:GLY:HA2	2:L:175:PHE:CD1	2.39	0.58
2:L:169:GLY:HA3	7:L:602:BCL:HAC1	1.85	0.58
2:L:98:THR:HG21	9:L:707:LDA:H122	1.85	0.58
1:C:191:THR:HG21	1:C:235:ASN:ND2	2.19	0.58
2:L:265:ARG:HD2	2:L:269:GLU:OE2	2.04	0.58
7:L:602:BCL:HBB3	7:L:602:BCL:HMB1	1.85	0.58
2:L:221:ASN:O	2:L:225:ARG:HG3	2.04	0.57
2:L:88:LEU:HA	2:L:92:GLY:HA3	1.86	0.57
4:H:37:GLU:CD	4:H:80:ARG:HH22	2.12	0.57
1:C:37:VAL:HG23	1:C:301:MET:HE1	1.85	0.57
1:C:59:VAL:C	1:C:61:LYS:H	2.13	0.57
2:L:206:THR:OG1	2:L:207:ASN:ND2	2.38	0.57
3:M:134:LYS:O	3:M:137:GLU:HG2	2.05	0.56
7:M:603:BCL:CBB	7:M:603:BCL:HMB1	2.34	0.56
2:L:181:HIS:CE1	2:L:185:ILE:HD11	2.40	0.56
1:C:88:CYS:O	1:C:102:LYS:HB2	2.07	0.55
3:M:288:THR:CG2	3:M:289:VAL:HG23	2.36	0.55
4:H:105:ASP:H	4:H:108:LEU:HD23	1.70	0.55
2:L:18:GLY:H	4:H:259:LEU:CD1	2.20	0.55
3:M:34:ILE:HG22	3:M:47:ILE:HB	1.89	0.55
3:M:313:VAL:O	3:M:315:PRO:HD3	2.07	0.55
3:M:70:ILE:O	3:M:74:MET:HG3	2.07	0.55
4:H:31:ARG:NE	13:H:708:PEF:H112	2.22	0.55
2:L:44:LEU:O	2:L:48:LEU:HG	2.08	0.54
4:H:89:ALA:HB1	4:H:101:VAL:O	2.08	0.54
1:C:23:VAL:HG12	1:C:26:GLN:H	1.71	0.54
1:C:200:ASN:ND2	1:C:202:ALA:H	2.05	0.54
1:C:109:PHE:O	1:C:113:ARG:HG3	2.08	0.54
2:L:207:ASN:N	2:L:207:ASN:ND2	2.54	0.54
1:C:200:ASN:C	1:C:200:ASN:ND2	2.65	0.53
3:M:11:GLN:HE21	3:M:41:LYS:HE3	1.73	0.53
4:H:154:MET:HE1	4:H:202:PHE:HD2	1.73	0.53
3:M:148:ALA:O	3:M:151:ALA:HB3	2.09	0.53
4:H:137:ARG:HG3	4:H:137:ARG:O	2.09	0.53
1:C:32:GLN:HA	1:C:32:GLN:OE1	2.08	0.53
3:M:225:VAL:O	3:M:225:VAL:HG13	2.07	0.53
4:H:176:GLU:O	4:H:178:GLN:HG2	2.08	0.53
7:M:603:BCL:OBB	7:M:603:BCL:HHC	2.09	0.53
1:C:179:THR:O	1:C:183:ASP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD23	1:C:111:LEU:C	2.34	0.53
1:C:97:ASP:OD2	1:C:106:ARG:NH2	2.42	0.52
7:L:602:BCL:HMB1	7:L:602:BCL:CBB	2.39	0.52
3:M:22:LEU:HD11	3:M:29:ARG:HH11	1.74	0.52
1:C:106:ARG:HD3	5:C:609:HEM:O2D	2.09	0.52
3:M:300:HIS:CB	3:M:302:MET:HE3	2.40	0.52
3:M:22:LEU:HD21	3:M:29:ARG:NH1	2.24	0.52
1:C:97:ASP:CG	1:C:106:ARG:HH22	2.18	0.52
1:C:257:ILE:O	1:C:261:TYR:HB2	2.09	0.52
3:M:232:ARG:NH2	4:H:236:GLU:OE2	2.43	0.52
2:L:277:LEU:HB2	2:L:280:TRP:NE1	2.23	0.52
1:C:235:ASN:H	1:C:235:ASN:ND2	2.08	0.52
2:L:236:ALA:HA	2:L:239:ARG:HB2	1.91	0.52
1:C:282:ARG:HG2	1:C:282:ARG:HH11	1.75	0.52
4:H:145:ALA:O	4:H:146:GLU:C	2.53	0.52
1:C:100:TYR:O	1:C:104:VAL:HG23	2.09	0.52
2:L:193:LEU:HD23	2:L:197:MET:HG3	1.92	0.52
4:H:71:HIS:O	4:H:72:ASN:C	2.53	0.52
7:L:602:BCL:O1A	7:L:604:BCL:HBC1	2.09	0.51
3:M:198:ASN:HD22	3:M:199:PRO:N	2.07	0.51
4:H:157:VAL:HG23	4:H:210:LYS:HA	1.91	0.51
2:L:133:ILE:O	2:L:137:LEU:HG	2.09	0.51
1:C:11:ILE:HD13	1:C:226:THR:O	2.10	0.51
1:C:232:ARG:HH21	1:C:239:GLN:HE22	1.59	0.51
3:M:65:VAL:HG11	3:M:120:PHE:CD2	2.44	0.51
3:M:257:PHE:HB3	13:H:708:PEF:HN2	1.76	0.51
1:C:75:VAL:HG13	5:C:610:HEM:HMB2	1.92	0.51
4:H:134:VAL:CG2	4:H:174:ARG:HD2	2.40	0.51
2:L:69:LEU:HB2	6:L:703:BGL:C1'	2.40	0.51
3:M:131:ARG:HG3	3:M:131:ARG:NH1	2.25	0.51
4:H:7:HIS:HB3	4:H:9:ILE:CG1	2.27	0.51
3:M:22:LEU:CD2	3:M:29:ARG:HH12	2.23	0.51
4:H:171:TRP:NE1	4:H:183:GLU:HG3	2.23	0.51
1:C:77:THR:HA	1:C:81:PRO:HB3	1.93	0.51
2:L:182:MET:HB3	7:M:601:BCL:O1D	2.11	0.51
4:H:7:HIS:CG	4:H:8:TYR:N	2.65	0.51
2:L:115:ILE:O	2:L:119:LEU:HD12	2.11	0.50
3:M:128:TRP:HE1	8:M:605:BPH:HED1	1.76	0.50
3:M:234:ILE:HD12	3:M:234:ILE:H	1.76	0.50
4:H:248:LEU:O	4:H:255:ALA:HB2	2.10	0.50
1:C:200:ASN:HD22	1:C:201:PRO:N	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:216:THR:OG1	2:L:219:HIS:HD2	1.95	0.50
4:H:10:ASP:H	4:H:13:GLN:NE2	2.10	0.50
4:H:162:GLU:HB2	4:H:216:ALA:HB2	1.92	0.50
1:C:156:LEU:HD22	3:M:98:PRO:HB3	1.93	0.50
3:M:296:TRP:O	3:M:300:HIS:HD2	1.94	0.50
4:H:19:PHE:O	4:H:22:PHE:N	2.44	0.50
2:L:11:VAL:HG22	2:L:12:ARG:N	2.27	0.50
3:M:12:VAL:O	3:M:13:ARG:NH1	2.45	0.50
2:L:70:TRP:CZ2	6:L:703:BGL:H2'1	2.46	0.50
3:M:134:LYS:HB3	3:M:135:ARG:HH21	1.76	0.50
7:L:602:BCL:OBB	7:L:602:BCL:HHC	2.11	0.50
1:C:104:VAL:HG13	1:C:265:LEU:HD13	1.94	0.50
4:H:186:VAL:O	4:H:190:LYS:HA	2.12	0.50
3:M:22:LEU:HD11	3:M:29:ARG:NH1	2.27	0.50
4:H:31:ARG:NH1	4:H:34:ASP:OD2	2.44	0.50
4:H:126:THR:HG23	4:H:130:LEU:O	2.11	0.50
1:C:270:PRO:HG2	1:C:273:ARG:HG2	1.94	0.49
3:M:300:HIS:HB2	3:M:302:MET:HE3	1.94	0.49
4:H:130:LEU:O	4:H:131:PRO:C	2.53	0.49
2:L:143:ARG:CZ	2:L:147:MET:HE2	2.43	0.49
3:M:161:PHE:C	3:M:164:PRO:HD2	2.38	0.49
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.93	0.49
4:H:140:LYS:HD3	4:H:140:LYS:N	2.28	0.49
2:L:239:ARG:HD2	3:M:6:ILE:HA	1.94	0.49
2:L:278:PRO:C	2:L:280:TRP:N	2.66	0.49
2:L:205:VAL:CG1	3:M:141:MET:HE3	2.42	0.49
4:H:187:ALA:O	4:H:189:ASN:N	2.46	0.49
2:L:200:SER:HG	3:M:269:TRP:HD1	1.58	0.48
6:L:701:BGL:O3	6:L:701:BGL:H4'1	2.12	0.48
1:C:18:MET:HE3	1:C:229:HIS:O	2.13	0.48
3:M:252:ARG:HH22	13:H:708:PEF:H42	1.77	0.48
1:C:122:HIS:HD1	1:C:253:HIS:HD2	1.59	0.48
3:M:98:PRO:HB2	3:M:100:GLN:HG3	1.95	0.48
1:C:2:GLU:N	1:C:2:GLU:CD	2.72	0.48
3:M:128:TRP:CH2	7:M:601:BCL:H193	2.49	0.48
4:H:225:LEU:C	4:H:227:ASN:H	2.22	0.48
2:L:17:ILE:HD11	2:L:33:PHE:CD1	2.49	0.48
3:M:252:ARG:HH12	13:H:708:PEF:H51	1.78	0.48
4:H:189:ASN:HD22	4:H:191:LYS:CD	2.24	0.48
2:L:159:LEU:HD21	3:M:202:MET:HE2	1.96	0.48
3:M:113:TRP:HE3	3:M:116:ILE:HG21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:223:PHE:HE1	3:M:136:ALA:HB2	1.79	0.48
4:H:134:VAL:HB	4:H:135:PRO:HD2	1.96	0.47
1:C:63:LEU:HD21	1:C:307:GLY:HA3	1.96	0.47
8:L:606:BPH:HMB3	8:L:606:BPH:HBB3	1.97	0.47
3:M:82:VAL:O	3:M:82:VAL:HG12	2.14	0.47
4:H:134:VAL:HG11	4:H:174:ARG:NH1	2.29	0.47
2:L:193:LEU:O	2:L:197:MET:HG3	2.14	0.47
3:M:11:GLN:HE21	3:M:41:LYS:CE	2.27	0.47
3:M:198:ASN:ND2	3:M:200:PHE:H	2.12	0.47
3:M:231:ASP:C	3:M:233:GLU:H	2.22	0.47
3:M:128:TRP:O	3:M:132:THR:HG23	2.14	0.47
1:C:122:HIS:CE1	5:C:612:HEM:NC	2.82	0.47
2:L:31:VAL:HG12	2:L:32:GLY:N	2.27	0.47
2:L:239:ARG:NH1	3:M:6:ILE:O	2.47	0.47
3:M:149:PHE:O	3:M:153:ILE:HG13	2.14	0.47
3:M:288:THR:HG22	3:M:289:VAL:N	2.29	0.47
1:C:11:ILE:HG21	1:C:226:THR:O	2.15	0.47
6:L:704:BGL:C1	3:M:302:MET:HE2	2.35	0.47
1:C:37:VAL:CG2	1:C:301:MET:HE1	2.45	0.47
2:L:223:PHE:HD2	2:L:224:PHE:CD1	2.32	0.47
1:C:34:ASN:HB3	1:C:296:LEU:HA	1.97	0.47
2:L:225:ARG:O	2:L:229:GLY:HA2	2.15	0.47
3:M:4:GLN:HB3	3:M:6:ILE:HG12	1.96	0.47
4:H:151:PRO:HG2	4:H:170:VAL:HG21	1.97	0.47
1:C:158:PRO:O	1:C:160:GLY:N	2.48	0.47
2:L:223:PHE:HD2	2:L:224:PHE:HD1	1.63	0.47
3:M:63:GLY:O	3:M:67:ILE:HG13	2.14	0.47
3:M:196:TYR:CZ	7:M:603:BCL:HMC2	2.50	0.47
4:H:39:TYR:CE1	4:H:41:LEU:HD21	2.50	0.47
3:M:36:SER:HG	3:M:39:LEU:HB2	1.80	0.46
1:C:161:GLN:O	1:C:161:GLN:HG2	2.15	0.46
2:L:7:LYS:HD3	4:H:87:VAL:HG21	1.98	0.46
3:M:79:HIS:O	3:M:80:TRP:HB2	2.15	0.46
2:L:279:LEU:O	3:M:83:PHE:CZ	2.68	0.46
7:L:604:BCL:H172	7:L:604:BCL:H13	1.59	0.46
1:C:100:TYR:HB2	1:C:268:VAL:O	2.15	0.46
1:C:63:LEU:HD21	1:C:307:GLY:CA	2.46	0.46
2:L:202:ILE:O	2:L:205:VAL:HG22	2.15	0.46
3:M:134:LYS:HB3	3:M:135:ARG:NH2	2.31	0.46
3:M:178:ILE:HG23	7:M:601:BCL:HED1	1.98	0.46
4:H:14:ILE:HD12	4:H:14:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:TRP:O	1:C:123:VAL:HG22	2.16	0.46
1:C:128:VAL:HG11	5:C:612:HEM:CBC	2.45	0.46
3:M:128:TRP:HE1	8:M:605:BPH:CED	2.28	0.46
3:M:227:ARG:HG3	3:M:228:PHE:CD2	2.51	0.46
3:M:252:ARG:NH1	13:H:708:PEF:H51	2.30	0.46
1:C:151:LYS:HG2	1:C:152:TYR:N	2.31	0.46
3:M:36:SER:OG	3:M:39:LEU:HB2	2.16	0.46
7:M:601:BCL:H93	7:M:601:BCL:H62	1.78	0.46
1:C:281:LEU:HB2	5:C:610:HEM:HBD1	1.97	0.45
2:L:33:PHE:O	2:L:37:VAL:HG23	2.16	0.45
2:L:272:ASN:O	2:L:275:LEU:N	2.47	0.45
1:C:232:ARG:HE	1:C:239:GLN:HE22	1.64	0.45
3:M:137:GLU:HG3	3:M:138:ALA:N	2.30	0.45
4:H:244:ALA:O	4:H:247:LYS:HB2	2.17	0.45
4:H:122:HIS:C	4:H:122:HIS:CD2	2.94	0.45
1:C:122:HIS:HD1	1:C:253:HIS:CD2	2.34	0.45
2:L:241:GLY:HA3	3:M:215:PHE:CZ	2.52	0.45
3:M:5:ASN:HD22	3:M:226:SER:HB3	1.82	0.45
2:L:206:THR:C	2:L:207:ASN:ND2	2.74	0.45
4:H:144:ILE:HG22	4:H:145:ALA:N	2.31	0.45
4:H:104:GLY:O	4:H:106:PRO:HD3	2.16	0.45
3:M:174:VAL:HG21	12:M:613:CRT:H242	1.99	0.45
3:M:147:TRP:HA	3:M:147:TRP:CE3	2.52	0.44
2:L:215:LYS:CD	2:L:219:HIS:CE1	3.01	0.44
2:L:219:HIS:O	2:L:220:GLU:C	2.59	0.44
3:M:178:ILE:HG22	3:M:179:PHE:CD1	2.52	0.44
3:M:179:PHE:N	3:M:180:PRO:CD	2.79	0.44
4:H:248:LEU:HD12	4:H:255:ALA:HA	1.99	0.44
7:M:603:BCL:HMB1	7:M:603:BCL:HBB2	1.98	0.44
3:M:54:LEU:HG	3:M:58:LEU:HD22	1.99	0.44
2:L:11:VAL:HG22	2:L:12:ARG:H	1.82	0.44
2:L:76:PRO:HG3	2:L:153:GLY:O	2.17	0.44
2:L:206:THR:HG21	3:M:237:ILE:HD13	2.00	0.44
1:C:152:TYR:CZ	3:M:79:HIS:NE2	2.86	0.44
2:L:19:GLY:O	2:L:21:LEU:N	2.51	0.44
3:M:317:GLU:O	3:M:318:THR:C	2.60	0.44
12:M:613:CRT:H36	12:M:613:CRT:H341	1.86	0.44
4:H:204:LYS:O	4:H:206:ALA:N	2.51	0.44
2:L:251:TRP:HA	2:L:254:VAL:HG13	1.99	0.43
3:M:19:GLY:HA3	3:M:29:ARG:HH21	1.83	0.43
3:M:78:VAL:O	3:M:79:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LEU:O	1:C:208:GLU:HG3	2.17	0.43
3:M:142:SER:HB2	3:M:144:HIS:HD2	1.82	0.43
1:C:144:TRP:HE1	1:C:283:VAL:C	2.26	0.43
2:L:111:ARG:O	2:L:115:ILE:HG13	2.19	0.43
2:L:159:LEU:HD23	2:L:162:LEU:HD22	2.00	0.43
3:M:309:VAL:HG12	3:M:309:VAL:O	2.18	0.43
2:L:159:LEU:HD21	3:M:202:MET:CE	2.48	0.43
7:L:602:BCL:HBD	7:L:604:BCL:CBC	2.48	0.43
4:H:7:HIS:C	4:H:9:ILE:N	2.75	0.43
2:L:117:ARG:NH1	4:H:258:LEU:HD13	2.31	0.43
1:C:205:LYS:HD2	1:C:205:LYS:HA	1.84	0.43
8:L:606:BPH:H7C2	8:L:606:BPH:H112	1.74	0.43
3:M:75:LEU:HD13	3:M:80:TRP:HE3	1.79	0.43
3:M:214:LEU:HD23	3:M:214:LEU:HA	1.90	0.43
7:M:601:BCL:H62	7:M:601:BCL:H41	1.85	0.43
1:C:282:ARG:HH11	1:C:282:ARG:CG	2.31	0.43
2:L:249:ALA:CB	8:L:606:BPH:HBC3	2.40	0.43
3:M:90:PHE:HB2	3:M:91:TRP:CE3	2.53	0.43
1:C:59:VAL:C	1:C:61:LYS:N	2.77	0.43
1:C:144:TRP:CD1	1:C:284:SER:HB3	2.54	0.43
1:C:157:LYS:O	1:C:158:PRO:C	2.61	0.43
3:M:64:LEU:HD21	8:M:605:BPH:H8	2.01	0.43
3:M:137:GLU:C	3:M:139:LEU:N	2.77	0.43
2:L:223:PHE:CD2	2:L:224:PHE:CD1	3.07	0.42
7:L:604:BCL:H3A	7:L:604:BCL:H101	2.01	0.42
8:L:606:BPH:HHD	8:L:606:BPH:HAC2	1.71	0.42
3:M:67:ILE:HD11	8:M:605:BPH:H4C1	2.00	0.42
3:M:256:GLY:O	13:H:708:PEF:N	2.52	0.42
1:C:97:ASP:CG	1:C:106:ARG:NH2	2.77	0.42
1:C:290:GLN:O	1:C:291:ALA:HB3	2.19	0.42
7:M:601:BCL:HAC2	7:M:601:BCL:HHD	1.73	0.42
2:L:224:PHE:O	2:L:230:TYR:O	2.38	0.42
3:M:295:LEU:HD12	3:M:295:LEU:HA	1.90	0.42
7:M:601:BCL:HMB1	7:M:601:BCL:CBB	2.46	0.42
7:M:603:BCL:HBC2	7:M:603:BCL:H2C	1.86	0.42
3:M:227:ARG:HG3	3:M:228:PHE:CE2	2.55	0.42
4:H:133:ILE:HA	4:H:172:VAL:O	2.18	0.42
1:C:3:GLY:O	1:C:4:PRO:C	2.63	0.42
1:C:122:HIS:CD2	1:C:122:HIS:C	2.96	0.42
7:L:604:BCL:C1B	8:L:606:BPH:H202	2.48	0.42
4:H:192:LYS:NZ	4:H:228:PRO:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:258:LEU:O	4:H:259:LEU:C	2.62	0.42
4:H:135:PRO:HA	4:H:171:TRP:HA	2.01	0.42
4:H:183:GLU:CD	4:H:192:LYS:HD2	2.45	0.42
2:L:85:MET:HB3	9:L:707:LDA:O1	2.20	0.42
2:L:178:ASN:HB3	2:L:181:HIS:CB	2.50	0.42
1:C:4:PRO:HA	1:C:5:PRO:HA	1.68	0.42
1:C:11:ILE:HB	1:C:18:MET:O	2.20	0.42
1:C:245:THR:O	1:C:248:TRP:HB3	2.20	0.42
2:L:18:GLY:H	4:H:259:LEU:HD12	1.83	0.42
3:M:179:PHE:O	3:M:182:LEU:HB2	2.20	0.42
4:H:160:ASP:OD2	4:H:215:LYS:NZ	2.53	0.42
3:M:101:TYR:CD2	3:M:106:PRO:HB3	2.55	0.42
4:H:159:LEU:HD13	4:H:215:LYS:HG3	2.02	0.42
1:C:25:ARG:NH1	1:C:26:GLN:OE1	2.53	0.41
1:C:231:THR:HG22	1:C:234:PHE:CE2	2.54	0.41
2:L:278:PRO:O	2:L:279:LEU:C	2.61	0.41
4:H:69:LEU:N	4:H:69:LEU:HD23	2.35	0.41
4:H:140:LYS:HG2	4:H:141:GLU:OE1	2.20	0.41
7:L:604:BCL:HMD1	3:M:205:ILE:HD13	2.02	0.41
3:M:101:TYR:CE2	3:M:106:PRO:HB3	2.55	0.41
1:C:228:CYS:HA	1:C:241:THR:OG1	2.21	0.41
2:L:16:LEU:HD11	2:L:113:VAL:CG1	2.50	0.41
3:M:32:ARG:HD3	3:M:32:ARG:HA	1.41	0.41
3:M:128:TRP:CZ2	7:M:601:BCL:H193	2.55	0.41
2:L:17:ILE:HD11	2:L:33:PHE:CG	2.55	0.41
3:M:113:TRP:HA	3:M:113:TRP:CE3	2.56	0.41
4:H:204:LYS:C	4:H:206:ALA:N	2.76	0.41
2:L:232:ILE:HG12	2:L:236:ALA:HB3	2.03	0.41
2:L:279:LEU:O	3:M:83:PHE:HZ	2.03	0.41
4:H:105:ASP:CB	4:H:108:LEU:HD23	2.38	0.41
2:L:238:HIS:CD2	3:M:218:HIS:CD2	3.07	0.41
2:L:125:VAL:HG11	3:M:250:PHE:CE2	2.56	0.41
3:M:198:ASN:C	3:M:198:ASN:ND2	2.68	0.41
3:M:205:ILE:HG12	7:M:603:BCL:CHB	2.51	0.41
3:M:246:GLY:HA3	14:M:922:HOH:O	2.20	0.41
4:H:36:ARG:NH1	4:H:62:PRO:HG2	2.36	0.41
1:C:13:TYR:HB3	1:C:16:VAL:HG21	2.01	0.41
4:H:159:LEU:C	4:H:159:LEU:CD2	2.93	0.41
1:C:111:LEU:HD23	1:C:111:LEU:O	2.21	0.41
4:H:214:ILE:HB	4:H:218:HIS:HB2	2.02	0.41
1:C:252:ARG:N	1:C:252:ARG:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:241:GLY:HA3	3:M:215:PHE:CE1	2.56	0.41
2:L:265:ARG:HD2	2:L:269:GLU:CD	2.46	0.41
3:M:294:TYR:O	3:M:298:VAL:HG23	2.21	0.41
2:L:183:LEU:HD23	2:L:187:PHE:HE1	1.86	0.40
3:M:113:TRP:CE3	3:M:116:ILE:HG21	2.56	0.40
3:M:231:ASP:C	3:M:233:GLU:N	2.79	0.40
4:H:189:ASN:HD21	4:H:191:LYS:HB2	1.81	0.40
1:C:190:ILE:H	1:C:190:ILE:HD13	1.86	0.40
4:H:178:GLN:NE2	14:H:985:HOH:O	2.55	0.40
2:L:239:ARG:NH1	3:M:6:ILE:C	2.79	0.40
7:L:604:BCL:OBD	3:M:205:ILE:HD12	2.21	0.40
3:M:39:LEU:HD12	3:M:39:LEU:HA	1.95	0.40
2:L:253:ALA:O	2:L:257:LEU:HB2	2.21	0.40
3:M:259:ALA:HB1	3:M:263:SER:OG	2.21	0.40
2:L:215:LYS:HD2	2:L:219:HIS:CE1	2.56	0.40
2:L:234:ALA:O	2:L:237:ILE:HG22	2.22	0.40
3:M:122:THR:HG22	3:M:126:LEU:HD12	2.03	0.40
3:M:158:VAL:HA	3:M:162:ILE:HB	2.03	0.40
3:M:167:MET:HE2	3:M:167:MET:HB3	1.97	0.40
3:M:178:ILE:HG22	3:M:179:PHE:N	2.36	0.40
7:M:601:BCL:OBB	7:M:601:BCL:HHC	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	308/382 (81%)	268 (87%)	31 (10%)	9 (3%)	3 2
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	18 19
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	6 4
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	4 3

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	GLU
1	C	4	PRO
4	H	140	LYS
4	H	142	PHE
4	H	146	GLU
1	C	61	LYS
1	C	62	ASP
1	C	99	ILE
1	C	159	THR
2	L	20	ASP
3	M	28	PRO
4	H	188	ALA
4	H	205	LYS
3	M	2	GLU
3	M	23	PRO
3	M	30	ILE
3	M	37	TYR
4	H	177	PRO
3	M	33	PRO
4	H	206	ALA
4	H	213	ALA
4	H	257	PRO
1	C	162	ASN
1	C	165	SER
1	C	231	THR
2	L	31	VAL
4	H	227	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	259/300 (86%)	243 (94%)	16 (6%)	16	20
2	L	228/228 (100%)	211 (92%)	17 (8%)	12	14
3	M	254/258 (98%)	231 (91%)	23 (9%)	9	9
4	H	195/211 (92%)	159 (82%)	36 (18%)	1	1
All	All	936/997 (94%)	844 (90%)	92 (10%)	7	8

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	PRO
1	C	25	ARG
1	C	26	GLN
1	C	38	GLU
1	C	64	SER
1	C	108	MET
1	C	145	VAL
1	C	156	LEU
1	C	168	VAL
1	C	190	ILE
1	C	200	ASN
1	C	204	LEU
1	C	205	LYS
1	C	216	ASN
1	C	282	ARG
1	C	286	MET
2	L	8	LYS
2	L	10	ARG
2	L	17	ILE
2	L	61	THR
2	L	63	ASP
2	L	88	LEU
2	L	140	VAL
2	L	146	LEU
2	L	147	MET
2	L	183	LEU
2	L	207	ASN
2	L	209	GLN
2	L	239	ARG
2	L	247	SER
2	L	254	VAL
2	L	255	CYS
2	L	279	LEU

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Mol	Chain	Res	Type
3	M	2	GLU
3	M	4	GLN
3	M	24	LYS
3	M	30	ILE
3	M	32	ARG
3	M	34	ILE
3	M	36	SER
3	M	41	LYS
3	M	44	ASP
3	M	75	LEU
3	M	100	GLN
3	M	181	HIS
3	M	198	ASN
3	M	213	LEU
3	M	221	THR
3	M	223	LEU
3	M	225	VAL
3	M	231	ASP
3	M	234	ILE
3	M	255	MET
3	M	288	THR
3	M	295	LEU
3	M	310	VAL
4	H	13	GLN
4	H	14	ILE
4	H	16	ILE
4	H	21	LEU
4	H	61	LEU
4	H	72	ASN
4	H	75	THR
4	H	77	VAL
4	H	81	VAL
4	H	106	PRO
4	H	107	MET
4	H	108	LEU
4	H	116	SER
4	H	122	HIS
4	H	128	GLU
4	H	131	PRO
4	H	133	ILE
4	H	137	ARG
4	H	140	LYS

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Mol	Chain	Res	Type
4	H	141	GLU
4	H	143	SER
4	H	149	PRO
4	H	155	THR
4	H	157	VAL
4	H	159	LEU
4	H	160	ASP
4	H	177	PRO
4	H	183	GLU
4	H	186	VAL
4	H	193	VAL
4	H	200	SER
4	H	208	LYS
4	H	226	SER
4	H	230	GLN
4	H	258	LEU
4	H	259	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
1	C	55	GLN
1	C	93	ASN
1	C	200	ASN
1	C	206	GLN
1	C	235	ASN
1	C	239	GLN
1	C	253	HIS
1	C	260	ASN
1	C	290	GLN
2	L	95	GLN
2	L	171	GLN
2	L	174	HIS
2	L	207	ASN
2	L	219	HIS
3	M	5	ASN
3	M	100	GLN
3	M	143	GLN
3	M	144	HIS
3	M	198	ASN
3	M	258	ASN

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Mol	Chain	Res	Type
4	H	13	GLN
4	H	122	HIS
4	H	189	ASN
4	H	218	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	BPH	M	605	-	59,70,70	2.13	13 (22%)	59,101,101	2.43	19 (32%)
7	BCL	L	604	2	69,74,74	2.01	12 (17%)	79,115,115	2.20	22 (27%)
12	CRT	M	613	-	43,43,43	2.39	13 (30%)	48,54,54	2.61	5 (10%)
9	LDA	L	707	-	13,15,15	2.46	2 (15%)	14,17,17	0.64	0
6	BGL	L	703	-	20,20,20	0.93	1 (5%)	24,25,25	2.02	7 (29%)
6	BGL	M	702	-	20,20,20	1.09	1 (5%)	24,25,25	2.39	8 (33%)
13	PEF	H	708	-	46,46,46	2.19	7 (15%)	49,51,51	1.40	6 (12%)
11	MQ8	M	608	-	54,54,54	2.47	17 (31%)	67,69,69	2.79	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	C	611	1	50,50,50	1.49	10 (20%)	67,82,82	0.92	1 (1%)
6	BGL	M	705	-	20,20,20	1.30	2 (10%)	24,25,25	2.01	6 (25%)
6	BGL	M	706	-	20,20,20	0.98	1 (5%)	24,25,25	2.04	6 (25%)
7	BCL	M	603	3	69,74,74	1.85	8 (11%)	79,115,115	2.09	21 (26%)
6	BGL	L	704	-	20,20,20	1.25	2 (10%)	24,25,25	2.39	9 (37%)
5	HEM	C	612	1	50,50,50	1.38	6 (12%)	67,82,82	0.64	0
6	BGL	L	701	-	20,20,20	1.28	2 (10%)	24,25,25	1.95	8 (33%)
5	HEM	C	610	1	50,50,50	1.78	10 (20%)	67,82,82	1.01	4 (5%)
7	BCL	M	601	3	69,74,74	2.02	9 (13%)	79,115,115	2.20	21 (26%)
7	BCL	L	602	2	69,74,74	1.89	10 (14%)	79,115,115	2.10	19 (24%)
8	BPH	L	606	-	59,70,70	2.02	12 (20%)	59,101,101	2.54	20 (33%)
5	HEM	C	609	1	50,50,50	1.72	11 (22%)	67,82,82	0.96	2 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	M	605	-	-	11/37/105/105	0/5/6/6
7	BCL	L	604	2	-	8/41/137/137	-
12	CRT	M	613	-	-	5/51/51/51	-
9	LDA	L	707	-	-	4/13/13/13	-
6	BGL	L	703	-	-	6/11/31/31	0/1/1/1
6	BGL	M	702	-	-	7/11/31/31	0/1/1/1
13	PEF	H	708	-	-	34/50/50/50	-
11	MQ8	M	608	-	-	12/47/67/67	0/2/2/2
5	HEM	C	611	1	-	6/14/54/54	-
6	BGL	M	705	-	-	4/11/31/31	0/1/1/1
6	BGL	M	706	-	-	5/11/31/31	0/1/1/1
7	BCL	M	603	3	-	8/41/137/137	-
6	BGL	L	704	-	-	5/11/31/31	0/1/1/1
5	HEM	C	612	1	-	6/14/54/54	-
6	BGL	L	701	-	-	7/11/31/31	0/1/1/1
5	HEM	C	610	1	-	8/14/54/54	-
7	BCL	M	601	3	-	21/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	L	602	2	-	10/41/137/137	-
8	BPH	L	606	-	1/1/18/22	15/37/105/105	0/5/6/6
5	HEM	C	609	1	-	4/14/54/54	-

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	601	BCL	C3C-C4C	-12.13	1.36	1.51
7	L	604	BCL	C3C-C4C	-12.06	1.36	1.51
7	M	603	BCL	C3C-C4C	-10.55	1.38	1.51
7	L	602	BCL	C3C-C4C	-10.39	1.38	1.51
11	M	608	MQ8	C34-C33	8.93	1.72	1.50
13	H	708	PEF	O4-C10	8.28	1.47	1.22
12	M	613	CRT	C6-C5	7.94	1.54	1.32
12	M	613	CRT	C35-C36	7.53	1.52	1.32
8	M	605	BPH	C4C-C3C	-7.30	1.38	1.51
9	L	707	LDA	O1-N1	-7.04	1.24	1.42
8	L	606	BPH	C4C-C3C	-6.80	1.38	1.51
8	M	605	BPH	C2C-C3C	-6.28	1.49	1.54
5	C	609	HEM	FE-NA	6.19	2.15	1.95
8	M	605	BPH	C3A-C2A	-6.14	1.49	1.54
13	H	708	PEF	O5-C30	6.00	1.40	1.22
8	L	606	BPH	C2C-C3C	-5.92	1.49	1.54
5	C	610	HEM	FE-NC	5.91	2.14	1.95
8	L	606	BPH	C1D-C2D	5.80	1.45	1.39
11	M	608	MQ8	C30-C31	-5.63	1.35	1.53
13	H	708	PEF	P-O1P	5.59	1.70	1.50
9	L	707	LDA	C1-N1	-5.33	1.46	1.51
13	H	708	PEF	O2-C10	5.17	1.48	1.34
11	M	608	MQ8	C27-C28	5.14	1.44	1.33
8	M	605	BPH	C1D-C2D	5.12	1.45	1.39
11	M	608	MQ8	C42-C43	5.10	1.44	1.33
11	M	608	MQ8	C30-C28	4.92	1.61	1.51
7	L	602	BCL	O2D-CGD	4.83	1.45	1.33
11	M	608	MQ8	C12-C13	4.75	1.44	1.33
8	L	606	BPH	C3A-C2A	-4.58	1.50	1.54
7	M	603	BCL	MG-NA	4.41	2.16	2.06
8	M	605	BPH	O2D-CGD	4.39	1.44	1.33
13	H	708	PEF	O3-C30	4.30	1.45	1.33
7	M	603	BCL	O2D-CGD	4.23	1.43	1.33
11	M	608	MQ8	C32-C33	4.19	1.42	1.33
7	M	601	BCL	O2A-CGA	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	701	BGL	O2-C1'	4.03	1.54	1.43
6	M	702	BGL	O2-C1'	3.94	1.53	1.43
7	L	602	BCL	MG-NA	3.93	2.15	2.06
5	C	610	HEM	C1D-ND	-3.89	1.31	1.38
7	L	604	BCL	MG-NA	3.83	2.15	2.06
7	M	601	BCL	MG-NA	3.82	2.15	2.06
8	L	606	BPH	O2D-CGD	3.78	1.42	1.33
6	L	704	BGL	O2-C1'	3.77	1.53	1.43
7	M	601	BCL	O2D-CGD	3.73	1.42	1.33
6	M	705	BGL	O2-C1'	3.71	1.53	1.43
7	L	604	BCL	O2A-CGA	3.69	1.44	1.33
6	M	705	BGL	C1-C2	3.68	1.55	1.52
6	M	706	BGL	O2-C1'	3.67	1.53	1.43
12	M	613	CRT	C15-C16	3.62	1.44	1.34
12	M	613	CRT	C31-C30	3.57	1.44	1.34
6	L	704	BGL	C1-C2	3.56	1.55	1.52
7	L	602	BCL	C3B-C4B	3.55	1.48	1.41
5	C	612	HEM	CAB-C3B	-3.53	1.38	1.47
8	L	606	BPH	C1B-C2B	3.51	1.43	1.39
6	L	703	BGL	O2-C1'	3.49	1.52	1.43
5	C	611	HEM	CBC-CAC	3.33	1.46	1.30
5	C	610	HEM	CAB-C3B	-3.32	1.38	1.47
8	L	606	BPH	O2A-CGA	3.31	1.43	1.33
5	C	610	HEM	CBC-CAC	3.29	1.46	1.30
8	M	605	BPH	C1B-C2B	3.28	1.43	1.39
5	C	609	HEM	CBB-CAB	3.25	1.46	1.30
8	M	605	BPH	O2A-CGA	3.23	1.42	1.33
12	M	613	CRT	C10-C11	3.20	1.43	1.34
7	L	602	BCL	O2A-CGA	3.19	1.42	1.33
7	M	603	BCL	C3B-C4B	3.18	1.47	1.41
5	C	612	HEM	CBC-CAC	3.17	1.45	1.30
5	C	612	HEM	CBB-CAB	3.11	1.45	1.30
6	L	701	BGL	C1-C2	3.11	1.55	1.52
7	M	603	BCL	O2A-CGA	3.10	1.42	1.33
13	H	708	PEF	P-O2P	3.09	1.69	1.55
5	C	610	HEM	CBB-CAB	3.09	1.45	1.30
5	C	611	HEM	CAB-C3B	-3.08	1.39	1.47
7	M	601	BCL	C3B-C4B	3.07	1.47	1.41
12	M	613	CRT	C22-C23	3.05	1.42	1.35
12	M	613	CRT	C26-C25	2.97	1.42	1.34
5	C	611	HEM	CAC-C3C	-2.97	1.39	1.47
5	C	609	HEM	C4D-ND	-2.97	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	604	BCL	O2D-CGD	2.96	1.40	1.33
5	C	609	HEM	CAC-C3C	-2.95	1.39	1.47
5	C	609	HEM	CBC-CAC	2.95	1.44	1.30
7	L	604	BCL	C3B-C4B	2.93	1.46	1.41
8	L	606	BPH	C1A-C2A	-2.92	1.47	1.51
11	M	608	MQ8	C31-C32	-2.90	1.41	1.50
5	C	611	HEM	CBB-CAB	2.90	1.44	1.30
8	M	605	BPH	C3D-C2D	-2.89	1.34	1.39
5	C	612	HEM	CAC-C3C	-2.89	1.39	1.47
7	L	604	BCL	C2A-C1A	-2.84	1.45	1.52
12	M	613	CRT	C19-C17	2.84	1.42	1.35
5	C	609	HEM	C1B-NB	-2.83	1.35	1.40
5	C	612	HEM	FE-NC	2.82	2.04	1.95
5	C	609	HEM	CAB-C3B	-2.78	1.40	1.47
5	C	611	HEM	FE-NB	2.77	2.03	1.94
7	L	604	BCL	O2D-CED	-2.70	1.39	1.45
11	M	608	MQ8	C25-C23	2.66	1.56	1.51
7	M	601	BCL	O2D-CED	-2.63	1.39	1.45
7	L	602	BCL	O2D-CED	-2.63	1.39	1.45
12	M	613	CRT	C4-C1	2.62	1.57	1.52
8	L	606	BPH	O2D-CED	-2.62	1.39	1.45
11	M	608	MQ8	C22-C23	2.57	1.39	1.33
7	M	603	BCL	C2-C3	2.55	1.38	1.33
12	M	613	CRT	C4-C5	2.55	1.53	1.50
8	M	605	BPH	O2D-CED	-2.53	1.39	1.45
11	M	608	MQ8	C47-C48	2.53	1.40	1.32
7	M	601	BCL	C2C-C3C	-2.51	1.47	1.54
8	L	606	BPH	CHA-CBD	2.44	1.54	1.51
7	L	604	BCL	C1B-C2B	2.40	1.48	1.43
11	M	608	MQ8	C44-C43	2.39	1.56	1.51
5	C	610	HEM	CAC-C3C	-2.38	1.41	1.47
5	C	611	HEM	C1B-NB	-2.35	1.36	1.40
8	M	605	BPH	C3B-C2B	-2.35	1.35	1.39
12	M	613	CRT	C25-C23	-2.34	1.40	1.46
5	C	609	HEM	C2A-C3A	-2.33	1.32	1.38
11	M	608	MQ8	C17-C18	2.32	1.38	1.33
7	L	604	BCL	C1-C2	-2.29	1.42	1.49
7	L	602	BCL	O1D-CGD	2.29	1.27	1.21
12	M	613	CRT	C14-C12	2.27	1.41	1.35
11	M	608	MQ8	C39-C38	-2.27	1.45	1.50
5	C	610	HEM	CHC-C1C	-2.26	1.33	1.38
8	M	605	BPH	C4D-ND	-2.26	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	606	BPH	C1-C2	-2.25	1.42	1.49
5	C	610	HEM	FE-NB	2.23	2.01	1.94
5	C	609	HEM	O2D-CGD	-2.21	1.23	1.30
12	M	613	CRT	C16-C17	-2.17	1.41	1.46
5	C	609	HEM	C4C-NC	-2.16	1.35	1.39
11	M	608	MQ8	C35-C33	2.15	1.55	1.51
5	C	611	HEM	FE-NA	2.15	2.02	1.95
5	C	611	HEM	O2A-CGA	-2.14	1.23	1.30
5	C	610	HEM	C4D-C3D	-2.14	1.41	1.45
7	M	601	BCL	C2A-C1A	-2.14	1.47	1.52
11	M	608	MQ8	C16-C17	-2.14	1.44	1.50
7	M	601	BCL	C2-C3	2.13	1.38	1.33
5	C	610	HEM	C1C-NC	2.13	1.43	1.39
8	M	605	BPH	C1C-C2C	2.12	1.55	1.51
5	C	609	HEM	C4B-NB	2.11	1.43	1.38
13	H	708	PEF	P-O4P	2.09	1.67	1.59
7	L	602	BCL	MG-NB	-2.08	2.01	2.05
7	L	604	BCL	C3A-C2A	-2.08	1.48	1.54
7	M	603	BCL	O2D-CED	-2.08	1.40	1.45
7	L	604	BCL	MG-ND	-2.07	2.01	2.05
5	C	611	HEM	C4D-C3D	2.07	1.48	1.45
7	L	604	BCL	C2C-C3C	-2.07	1.48	1.54
7	L	602	BCL	C1-C2	-2.06	1.43	1.49
11	M	608	MQ8	C11-C12	-2.06	1.47	1.50
5	C	611	HEM	C1A-C2A	2.04	1.48	1.44
8	M	605	BPH	C1-C2	-2.04	1.43	1.49
5	C	612	HEM	O2D-CGD	-2.04	1.24	1.30
8	L	606	BPH	C2-C3	2.04	1.37	1.33
7	M	603	BCL	MG-ND	-2.03	2.01	2.05
7	L	602	BCL	C3A-C2A	-2.02	1.49	1.54

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	613	CRT	C37-C36-C35	-11.54	108.70	124.91
8	L	606	BPH	O2D-CGD-CBD	10.96	122.99	110.95
12	M	613	CRT	C4-C5-C6	-9.81	111.13	124.91
7	L	604	BCL	C4A-NA-C1A	8.88	110.73	106.68
7	M	601	BCL	C4A-NA-C1A	8.61	110.61	106.68
7	L	602	BCL	C4A-NA-C1A	8.38	110.50	106.68
11	M	608	MQ8	C11-C3-C4	-8.32	109.82	118.58
11	M	608	MQ8	C34-C33-C35	8.29	129.63	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	605	BPH	O2D-CGD-CBD	7.57	119.26	110.95
8	M	605	BPH	C4C-C3C-C2C	7.57	110.04	102.84
11	M	608	MQ8	C41-C40-C38	7.17	136.95	113.19
7	M	603	BCL	C4A-NA-C1A	7.10	109.92	106.68
11	M	608	MQ8	C35-C33-C32	-7.00	105.46	121.17
11	M	608	MQ8	C39-C38-C40	6.75	126.94	115.23
8	L	606	BPH	O1D-CGD-CBD	-6.37	115.06	124.72
6	M	706	BGL	C6-C5-C4	6.27	128.42	113.02
7	M	601	BCL	O2D-CGD-CBD	6.26	122.17	111.23
6	L	704	BGL	C6-C5-C4	6.16	128.13	113.02
7	L	602	BCL	C1D-ND-C4D	-6.15	101.99	106.31
7	M	603	BCL	O2D-CGD-CBD	6.08	121.87	111.23
6	M	702	BGL	C6-C5-C4	6.05	127.87	113.02
6	M	705	BGL	C6-C5-C4	6.01	127.78	113.02
7	L	604	BCL	O2D-CGD-CBD	5.99	121.70	111.23
11	M	608	MQ8	C31-C30-C28	5.88	132.68	113.19
7	M	603	BCL	C1C-NC-C4C	5.82	109.33	106.68
6	L	703	BGL	C6-C5-C4	5.59	126.75	113.02
7	M	601	BCL	C1C-NC-C4C	5.51	109.19	106.68
12	M	613	CRT	C36-C35-C33	-5.47	117.63	125.89
7	M	601	BCL	C1D-ND-C4D	-5.34	102.56	106.31
7	L	602	BCL	C1C-NC-C4C	5.34	109.11	106.68
12	M	613	CRT	C5-C6-C7	-5.32	117.85	125.89
8	L	606	BPH	C4C-C3C-C2C	5.24	107.83	102.84
8	M	605	BPH	C7-C6-C5	-5.24	99.30	113.26
6	L	701	BGL	C6-C5-C4	5.21	125.82	113.02
7	L	604	BCL	C1D-ND-C4D	-5.12	102.72	106.31
7	L	604	BCL	C1C-NC-C4C	4.89	108.91	106.68
8	M	605	BPH	O1D-CGD-CBD	-4.84	117.38	124.72
6	M	702	BGL	O5-C5-C4	-4.82	101.01	109.70
8	M	605	BPH	C4D-CHA-CBD	-4.66	106.22	108.45
7	M	603	BCL	C1D-ND-C4D	-4.63	103.07	106.31
6	L	704	BGL	O5-C5-C4	-4.62	101.37	109.70
7	M	601	BCL	O1D-CGD-CBD	-4.52	115.61	124.52
13	H	708	PEF	O3-C30-C31	4.45	125.39	111.83
11	M	608	MQ8	O1-C1-C10	-4.34	114.64	121.57
7	L	604	BCL	CAC-C3C-C4C	-4.29	103.07	112.58
7	M	603	BCL	O1D-CGD-CBD	-4.26	116.12	124.52
7	L	602	BCL	O2A-CGA-CBA	4.23	124.74	111.83
7	L	602	BCL	CED-O2D-CGD	4.13	125.28	115.92
8	M	605	BPH	OBD-CAD-CBD	-4.09	119.82	125.82
7	L	602	BCL	O2D-CGD-CBD	4.06	118.33	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	708	PEF	O3-C30-O5	-4.02	113.56	123.63
7	L	604	BCL	O1D-CGD-CBD	-4.01	116.61	124.52
13	H	708	PEF	O3-C3-C2	4.01	119.95	108.40
8	L	606	BPH	OBD-CAD-CBD	-3.99	119.96	125.82
7	M	601	BCL	O2A-CGA-CBA	3.93	123.82	111.83
11	M	608	MQ8	C11-C3-C2	3.93	131.63	124.89
7	M	603	BCL	O2A-CGA-CBA	3.70	123.12	111.83
8	L	606	BPH	C4D-CHA-CBD	-3.68	106.69	108.45
6	L	704	BGL	O6-C6-C5	3.68	123.85	111.33
7	M	603	BCL	C3C-C2C-C1C	3.67	107.79	101.87
7	L	604	BCL	CAB-C3B-C2B	3.66	135.35	127.74
6	L	703	BGL	O5-C5-C4	-3.64	103.14	109.70
8	L	606	BPH	OBb-CAB-C3B	3.64	126.07	119.99
6	M	702	BGL	O6-C6-C5	3.56	123.45	111.33
11	M	608	MQ8	C21-C22-C23	-3.55	119.49	127.62
6	M	702	BGL	C1-O5-C5	-3.51	106.86	113.65
7	M	603	BCL	OBb-CAB-C3B	3.44	126.51	120.43
6	M	706	BGL	O5-C5-C4	-3.44	103.50	109.70
13	H	708	PEF	C2-O2-C10	3.43	126.00	117.80
7	L	604	BCL	OBb-CAB-C3B	3.42	126.48	120.43
6	L	701	BGL	O6-C6-C5	3.41	122.96	111.33
11	M	608	MQ8	C31-C32-C33	-3.36	119.94	127.62
8	L	606	BPH	O2A-CGA-CBA	3.35	122.05	111.83
11	M	608	MQ8	C30-C31-C32	3.34	128.53	112.02
8	M	605	BPH	OBb-CAB-C3B	3.32	125.54	119.99
8	L	606	BPH	C9-C8-C7	3.31	123.08	111.27
8	M	605	BPH	CMA-C3A-C4A	-3.31	107.47	114.61
6	L	704	BGL	C4-C3-C2	-3.30	102.18	109.68
13	H	708	PEF	O2-C10-C11	3.29	118.59	111.48
11	M	608	MQ8	C2M-C2-C1	-3.28	110.63	116.68
11	M	608	MQ8	C36-C35-C33	3.27	124.03	113.19
7	L	604	BCL	C6-C5-C3	-3.26	105.52	113.47
7	L	602	BCL	CAB-C3B-C2B	3.26	134.51	127.74
6	L	704	BGL	O4-C4-C3	3.26	118.05	110.38
11	M	608	MQ8	C40-C38-C37	-3.25	113.87	121.17
7	L	604	BCL	C3C-C2C-C1C	3.24	107.11	101.87
6	L	703	BGL	O6-C6-C5	3.24	122.38	111.33
6	M	705	BGL	O5-C5-C4	-3.24	103.87	109.70
7	M	601	BCL	CAB-C3B-C2B	3.23	134.45	127.74
8	M	605	BPH	O2A-CGA-CBA	3.22	121.65	111.83
6	M	702	BGL	C3-C4-C5	-3.21	104.41	110.23
7	L	602	BCL	OBb-CAB-C3B	3.20	126.09	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	602	BCL	O1D-CGD-CBD	-3.20	118.21	124.52
7	M	603	BCL	CAB-C3B-C2B	3.19	134.38	127.74
7	M	601	BCL	OB B-CAB-C3B	3.19	126.07	120.43
7	M	601	BCL	C12-C11-C10	-3.19	98.99	113.28
6	M	702	BGL	O4-C4-C3	3.18	117.88	110.38
5	C	609	HEM	C4A-NA-C1A	-3.17	100.66	105.82
11	M	608	MQ8	C19-C18-C20	3.13	120.66	115.23
8	L	606	BPH	CMA-C3A-C4A	-3.13	107.87	114.61
11	M	608	MQ8	O1-C1-C2	3.12	124.56	120.45
6	M	705	BGL	O6-C6-C5	3.12	121.96	111.33
8	L	606	BPH	CMC-C2C-C1C	-3.10	107.92	114.61
7	M	601	BCL	C2C-C3C-C4C	3.08	105.95	101.34
7	L	602	BCL	O2A-CGA-O1A	-3.07	115.95	123.63
8	M	605	BPH	O2A-CGA-O1A	-3.04	116.02	123.63
6	L	704	BGL	C1-O5-C5	-3.04	107.77	113.65
6	M	706	BGL	C1-O5-C5	-3.04	107.78	113.65
7	M	603	BCL	CED-O2D-CGD	3.03	122.80	115.92
7	M	601	BCL	O2A-CGA-O1A	-3.03	116.06	123.63
8	M	605	BPH	C1-C2-C3	3.02	131.14	126.20
7	L	604	BCL	O2A-CGA-CBA	3.02	121.03	111.83
7	M	601	BCL	CED-O2D-CGD	3.00	122.72	115.92
6	M	705	BGL	C1-O5-C5	-2.97	107.90	113.65
6	L	704	BGL	C3-C4-C5	-2.97	104.85	110.23
6	L	703	BGL	C1-O5-C5	-2.97	107.91	113.65
7	L	602	BCL	C1-C2-C3	2.94	131.02	126.20
8	L	606	BPH	CED-O2D-CGD	2.89	122.48	115.92
8	M	605	BPH	CED-O2D-CGD	2.88	122.45	115.92
8	M	605	BPH	CBC-CAC-C3C	2.87	119.43	113.78
11	M	608	MQ8	C9-C10-C5	2.86	122.47	119.26
6	L	701	BGL	O5-C5-C4	-2.86	104.55	109.70
7	M	601	BCL	CAA-C2A-C1A	-2.85	102.64	111.97
5	C	609	HEM	C3B-C2B-C1B	2.85	108.55	106.41
8	L	606	BPH	CBC-CAC-C3C	2.83	119.35	113.78
8	L	606	BPH	O2A-CGA-O1A	-2.81	116.61	123.63
6	L	704	BGL	O3-C3-C2	2.79	117.10	109.94
8	M	605	BPH	CMC-C2C-C1C	-2.77	108.65	114.61
8	L	606	BPH	C3D-C4D-ND	2.76	111.24	107.71
6	M	706	BGL	O6-C6-C5	2.75	120.71	111.33
7	M	603	BCL	C1-C2-C3	2.75	130.71	126.20
7	L	604	BCL	C1-C2-C3	2.75	130.71	126.20
7	L	604	BCL	C2A-C1A-CHA	2.75	128.64	123.87
11	M	608	MQ8	C20-C18-C17	-2.75	114.99	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	604	BCL	CAA-C2A-C1A	-2.75	102.96	111.97
8	M	605	BPH	C3D-C4D-ND	2.73	111.21	107.71
7	M	603	BCL	O2A-CGA-O1A	-2.73	116.80	123.63
8	M	605	BPH	OBD-CAD-C3D	2.72	132.13	127.89
7	L	604	BCL	C3A-C2A-C1A	2.71	105.39	101.34
7	M	603	BCL	CHD-C1D-ND	-2.69	121.02	124.80
8	M	605	BPH	C4D-ND-C1D	-2.68	105.66	108.87
6	L	701	BGL	O4-C4-C3	2.67	116.67	110.38
7	L	604	BCL	CBB-CAB-C3B	-2.67	114.77	120.40
6	M	702	BGL	C4-C3-C2	-2.67	103.62	109.68
7	L	604	BCL	CED-O2D-CGD	2.64	121.91	115.92
7	M	603	BCL	C4D-CHA-C1A	2.63	124.38	121.24
6	M	706	BGL	C3-C4-C5	-2.62	105.49	110.23
7	M	601	BCL	CMC-C2C-C3C	-2.61	103.88	113.98
7	M	601	BCL	CBB-CAB-C3B	-2.61	114.90	120.40
7	L	604	BCL	O2A-CGA-O1A	-2.61	117.11	123.63
7	L	602	BCL	C3C-C2C-C1C	2.60	106.08	101.87
7	M	601	BCL	C1-C2-C3	2.58	130.43	126.20
6	M	702	BGL	O3-C3-C2	2.58	116.56	109.94
6	L	703	BGL	O4-C4-C3	2.57	116.44	110.38
11	M	608	MQ8	C5-C10-C1	-2.56	117.96	120.71
5	C	610	HEM	CAD-C3D-C2D	2.55	132.65	127.87
8	L	606	BPH	C11-C10-C8	-2.55	107.48	115.97
7	M	601	BCL	C3C-C2C-C1C	2.53	105.95	101.87
8	L	606	BPH	C17-C16-C15	-2.52	101.98	113.28
7	L	602	BCL	CHD-C1D-ND	-2.49	121.30	124.80
8	L	606	BPH	OBD-CAD-C3D	2.47	131.75	127.89
8	L	606	BPH	C1-C2-C3	2.47	130.24	126.20
12	M	613	CRT	C29-C28-C30	2.46	121.85	118.09
7	M	603	BCL	CGD-CBD-CAD	-2.44	102.95	110.85
7	M	603	BCL	CBB-CAB-C3B	-2.43	115.27	120.40
13	H	708	PEF	C3-C2-C1	-2.42	106.13	111.78
5	C	610	HEM	C4C-NC-C1C	-2.42	101.88	105.82
7	M	603	BCL	C2A-C3A-C4A	2.37	105.69	101.87
7	L	602	BCL	CBB-CAB-C3B	-2.34	115.46	120.40
8	M	605	BPH	C11-C12-C13	-2.33	108.21	115.97
6	L	701	BGL	O3-C3-C2	2.33	115.90	109.94
5	C	611	HEM	C3B-C2B-C1B	2.31	108.14	106.41
7	L	604	BCL	C11-C10-C8	-2.30	108.33	115.97
6	L	701	BGL	C1-O5-C5	-2.29	109.22	113.65
7	M	601	BCL	CHD-C1D-ND	-2.27	121.60	124.80
6	L	703	BGL	C3-C4-C5	-2.26	106.13	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	705	BGL	C3-C4-C5	-2.25	106.14	110.23
7	L	602	BCL	C4D-CHA-C1A	2.25	123.93	121.24
5	C	610	HEM	C4D-ND-C1D	2.25	107.87	105.21
7	M	603	BCL	C4-C3-C5	-2.25	111.33	115.23
7	M	601	BCL	CMC-C2C-C1C	-2.25	105.74	111.77
8	L	606	BPH	C4-C3-C5	-2.22	111.37	115.23
6	M	706	BGL	O4-C4-C3	2.21	115.58	110.38
7	M	601	BCL	C2A-C1A-CHA	2.18	127.65	123.87
7	L	604	BCL	C10-C8-C7	2.18	123.11	112.07
6	M	705	BGL	O3-C3-C2	2.18	115.52	109.94
7	M	603	BCL	CMC-C2C-C3C	-2.18	105.56	113.98
7	M	603	BCL	C9-C8-C10	-2.17	103.53	111.27
7	M	603	BCL	CMC-C2C-C1C	-2.16	105.96	111.77
7	L	602	BCL	C2A-C1A-CHA	2.15	127.61	123.87
7	L	602	BCL	C7-C6-C5	-2.15	107.54	113.26
8	L	606	BPH	C7-C6-C5	-2.14	107.55	113.26
8	M	605	BPH	C1C-C2C-C3C	-2.14	100.80	102.84
6	L	701	BGL	C3-C4-C5	-2.11	106.40	110.23
5	C	610	HEM	CHB-C1B-NB	2.11	126.98	124.37
11	M	608	MQ8	C44-C46-C47	2.09	122.37	112.02
7	L	604	BCL	CMC-C2C-C1C	-2.09	106.17	111.77
6	L	703	BGL	O3-C3-C2	2.08	115.26	109.94
7	M	601	BCL	CHB-C4A-NA	2.07	127.39	124.40
6	L	701	BGL	O2-C1'-C2'	2.06	116.36	109.37
7	L	602	BCL	C9-C8-C7	2.05	118.58	111.27
7	L	602	BCL	C3A-C2A-C1A	2.05	104.41	101.34
7	L	604	BCL	C17-C16-C15	-2.01	104.25	113.28
6	L	704	BGL	O2-C1'-C2'	2.01	116.17	109.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C8

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	610	HEM	C2C-C3C-CAC-CBC
5	C	611	HEM	C2B-C3B-CAB-CBB
5	C	611	HEM	C2C-C3C-CAC-CBC
5	C	611	HEM	C4C-C3C-CAC-CBC
5	C	612	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	C	612	HEM	C4C-C3C-CAC-CBC
6	L	703	BGL	C2'-C1'-O2-C2
6	M	705	BGL	C2'-C1'-O2-C2
7	L	602	BCL	C2C-C3C-CAC-CBC
7	L	602	BCL	C4C-C3C-CAC-CBC
7	L	604	BCL	C2C-C3C-CAC-CBC
7	L	604	BCL	C4C-C3C-CAC-CBC
7	M	601	BCL	C3A-C2A-CAA-CBA
7	M	601	BCL	C2C-C3C-CAC-CBC
7	M	601	BCL	C4C-C3C-CAC-CBC
7	M	603	BCL	C2C-C3C-CAC-CBC
7	M	603	BCL	C4C-C3C-CAC-CBC
7	M	603	BCL	CAD-CBD-CGD-O1D
7	M	603	BCL	CAD-CBD-CGD-O2D
8	L	606	BPH	C4C-C3C-CAC-CBC
8	L	606	BPH	C2C-C3C-CAC-CBC
11	M	608	MQ8	C28-C30-C31-C32
11	M	608	MQ8	C34-C33-C35-C36
12	M	613	CRT	C22-C23-C25-C26
12	M	613	CRT	C24-C23-C25-C26
13	H	708	PEF	O4P-C4-C5-N
13	H	708	PEF	C1-O3P-P-O1P
13	H	708	PEF	C1-O3P-P-O2P
13	H	708	PEF	C1-O3P-P-O4P
13	H	708	PEF	O5-C30-O3-C3
13	H	708	PEF	C31-C30-O3-C3
7	M	601	BCL	C4-C3-C5-C6
7	L	604	BCL	C3-C5-C6-C7
6	L	701	BGL	O5-C5-C6-O6
11	M	608	MQ8	C46-C47-C48-C49
8	M	605	BPH	CBA-CGA-O2A-C1
6	M	706	BGL	O5-C5-C6-O6
8	M	605	BPH	O1A-CGA-O2A-C1
11	M	608	MQ8	C33-C35-C36-C37
13	H	708	PEF	C32-C33-C34-C35
6	L	701	BGL	C4-C5-C6-O6
7	M	601	BCL	C2-C3-C5-C6
7	L	602	BCL	C6-C7-C8-C9
7	L	604	BCL	C6-C7-C8-C9
7	M	601	BCL	C6-C7-C8-C9
8	L	606	BPH	C6-C7-C8-C9
11	M	608	MQ8	C46-C47-C48-C50

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Mol	Chain	Res	Type	Atoms
6	M	706	BGL	C4-C5-C6-O6
6	L	704	BGL	O2-C1'-C2'-C3'
8	M	605	BPH	C10-C11-C12-C13
7	L	602	BCL	C2A-CAA-CBA-CGA
8	L	606	BPH	C15-C16-C17-C18
7	L	602	BCL	C15-C16-C17-C18
7	M	601	BCL	C8-C10-C11-C12
7	M	601	BCL	C10-C11-C12-C13
7	M	601	BCL	C15-C16-C17-C18
6	M	702	BGL	C4-C5-C6-O6
8	L	606	BPH	C8-C10-C11-C12
7	M	601	BCL	CBD-CGD-O2D-CED
11	M	608	MQ8	C43-C44-C46-C47
13	H	708	PEF	C19-C20-C21-C22
5	C	610	HEM	C3D-CAD-CBD-CGD
8	M	605	BPH	C5-C6-C7-C8
7	M	601	BCL	CBA-CGA-O2A-C1
7	M	601	BCL	O1A-CGA-O2A-C1
13	H	708	PEF	C14-C15-C16-C17
13	H	708	PEF	C31-C32-C33-C34
6	L	701	BGL	C3'-C4'-C5'-C6'
6	M	706	BGL	C1'-C2'-C3'-C4'
13	H	708	PEF	C34-C35-C36-C37
9	L	707	LDA	C11-C10-C9-C8
13	H	708	PEF	C1-C2-C3-O3
6	M	705	BGL	C4'-C5'-C6'-C7'
13	H	708	PEF	C20-C21-C22-C23
13	H	708	PEF	C17-C18-C19-C20
12	M	613	CRT	C5-C6-C7-C8
6	M	706	BGL	C3'-C4'-C5'-C6'
5	C	609	HEM	C2B-C3B-CAB-CBB
5	C	610	HEM	C2B-C3B-CAB-CBB
6	M	705	BGL	C3'-C4'-C5'-C6'
13	H	708	PEF	O3P-C1-C2-O2
5	C	610	HEM	C4C-C3C-CAC-CBC
5	C	611	HEM	C4B-C3B-CAB-CBB
6	M	702	BGL	C2'-C3'-C4'-C5'
8	M	605	BPH	C15-C16-C17-C18
13	H	708	PEF	C21-C22-C23-C24
6	L	703	BGL	C3'-C4'-C5'-C6'
7	M	601	BCL	C1A-C2A-CAA-CBA
6	L	704	BGL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	M	601	BCL	C6-C7-C8-C10
8	L	606	BPH	C11-C12-C13-C15
8	L	606	BPH	C12-C13-C15-C16
8	L	606	BPH	C13-C15-C16-C17
6	L	701	BGL	O2-C1'-C2'-C3'
8	L	606	BPH	C14-C13-C15-C16
6	M	705	BGL	O5-C5-C6-O6
7	M	603	BCL	C13-C15-C16-C17
7	L	604	BCL	C13-C15-C16-C17
11	M	608	MQ8	C32-C33-C35-C36
7	L	604	BCL	C15-C16-C17-C18
7	M	601	BCL	C13-C15-C16-C17
6	L	703	BGL	C4-C5-C6-O6
8	L	606	BPH	O2A-C1-C2-C3
6	M	702	BGL	O2-C1'-C2'-C3'
8	L	606	BPH	C2-C3-C5-C6
11	M	608	MQ8	C37-C38-C40-C41
6	M	702	BGL	C5'-C6'-C7'-C8'
9	L	707	LDA	C2-C3-C4-C5
7	L	602	BCL	C13-C15-C16-C17
8	L	606	BPH	C4-C3-C5-C6
7	L	602	BCL	C14-C13-C15-C16
7	M	601	BCL	C14-C13-C15-C16
8	L	606	BPH	C11-C12-C13-C14
6	M	702	BGL	C4'-C5'-C6'-C7'
13	H	708	PEF	O3P-C1-C2-C3
13	H	708	PEF	C39-C40-C41-C42
7	L	602	BCL	C12-C13-C15-C16
6	L	703	BGL	O2-C1'-C2'-C3'
6	M	702	BGL	C1'-C2'-C3'-C4'
6	M	706	BGL	C4'-C5'-C6'-C7'
7	M	601	BCL	O1D-CGD-O2D-CED
9	L	707	LDA	C9-C10-C11-C12
11	M	608	MQ8	C39-C38-C40-C41
6	M	702	BGL	O5-C5-C6-O6
7	M	601	BCL	C11-C10-C8-C9
13	H	708	PEF	C22-C23-C24-C25
7	M	601	BCL	C5-C6-C7-C8
7	L	604	BCL	C11-C10-C8-C7
11	M	608	MQ8	C24-C23-C25-C26
11	M	608	MQ8	C22-C23-C25-C26
6	L	704	BGL	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
13	H	708	PEF	C11-C12-C13-C14
6	L	703	BGL	C5'-C6'-C7'-C8'
13	H	708	PEF	C33-C34-C35-C36
7	L	604	BCL	C6-C7-C8-C10
8	M	605	BPH	C11-C12-C13-C15
6	L	701	BGL	C4'-C5'-C6'-C7'
13	H	708	PEF	O2-C2-C3-O3
8	M	605	BPH	C4C-C3C-CAC-CBC
6	L	704	BGL	C3'-C4'-C5'-C6'
13	H	708	PEF	C4-O4P-P-O1P
13	H	708	PEF	C15-C16-C17-C18
8	L	606	BPH	C11-C10-C8-C7
9	L	707	LDA	N1-C1-C2-C3
5	C	609	HEM	C4B-C3B-CAB-CBB
5	C	610	HEM	C4B-C3B-CAB-CBB
8	M	605	BPH	C11-C10-C8-C9
13	H	708	PEF	C40-C41-C42-C43
13	H	708	PEF	C3-C2-O2-C10
13	H	708	PEF	C12-C13-C14-C15
5	C	610	HEM	CAA-CBA-CGA-O1A
7	M	601	BCL	C12-C13-C15-C16
8	M	605	BPH	C11-C10-C8-C7
6	L	704	BGL	C2'-C3'-C4'-C5'
13	H	708	PEF	C13-C14-C15-C16
12	M	613	CRT	C5-C6-C7-C9
7	L	602	BCL	C11-C10-C8-C9
13	H	708	PEF	C35-C36-C37-C38
6	L	701	BGL	C2'-C1'-O2-C2
5	C	610	HEM	CAA-CBA-CGA-O2A
13	H	708	PEF	C16-C17-C18-C19
5	C	611	HEM	CAA-CBA-CGA-O2A
5	C	609	HEM	CAA-CBA-CGA-O2A
7	M	603	BCL	CAA-CBA-CGA-O2A
5	C	609	HEM	CAA-CBA-CGA-O1A
12	M	613	CRT	C35-C36-C37-C38
5	C	612	HEM	CAA-CBA-CGA-O2A
5	C	612	HEM	C2B-C3B-CAB-CBB
13	H	708	PEF	C1-C2-O2-C10
5	C	611	HEM	CAA-CBA-CGA-O1A
6	L	703	BGL	O5-C5-C6-O6
13	H	708	PEF	C38-C39-C40-C41
5	C	612	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	M	601	BCL	C2-C1-O2A-CGA
5	C	610	HEM	CAD-CBD-CGD-O2D
11	M	608	MQ8	C25-C26-C27-C28
6	L	701	BGL	C1-C2-O2-C1'
7	L	602	BCL	C2-C1-O2A-CGA
7	M	603	BCL	C11-C10-C8-C7
5	C	612	HEM	CAD-CBD-CGD-O1D
8	L	606	BPH	C3A-C2A-CAA-CBA
13	H	708	PEF	O2-C10-C11-C12
7	M	603	BCL	C11-C10-C8-C9
8	M	605	BPH	C11-C12-C13-C14
8	M	605	BPH	C13-C15-C16-C17
13	H	708	PEF	O4-C10-C11-C12

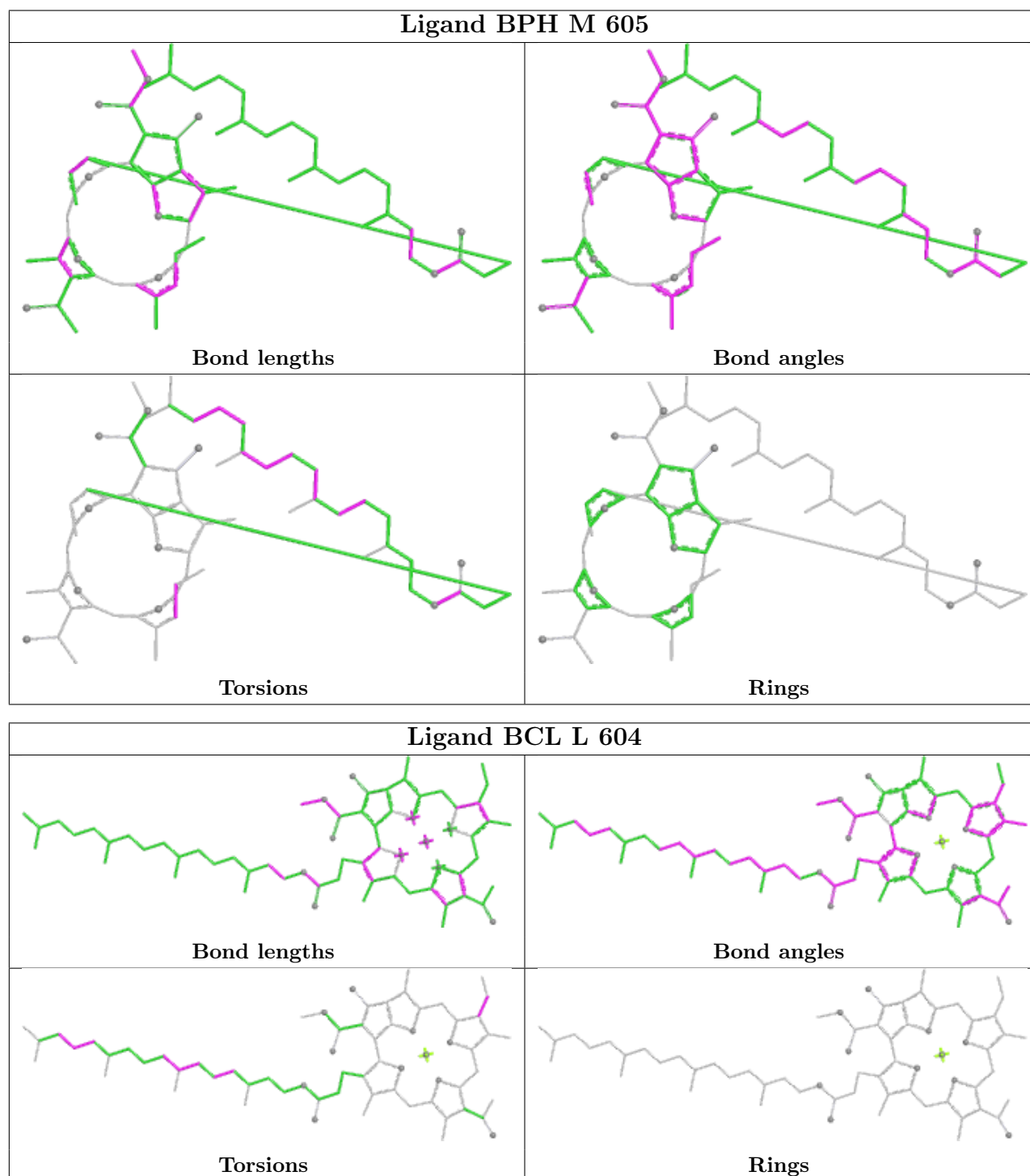
There are no ring outliers.

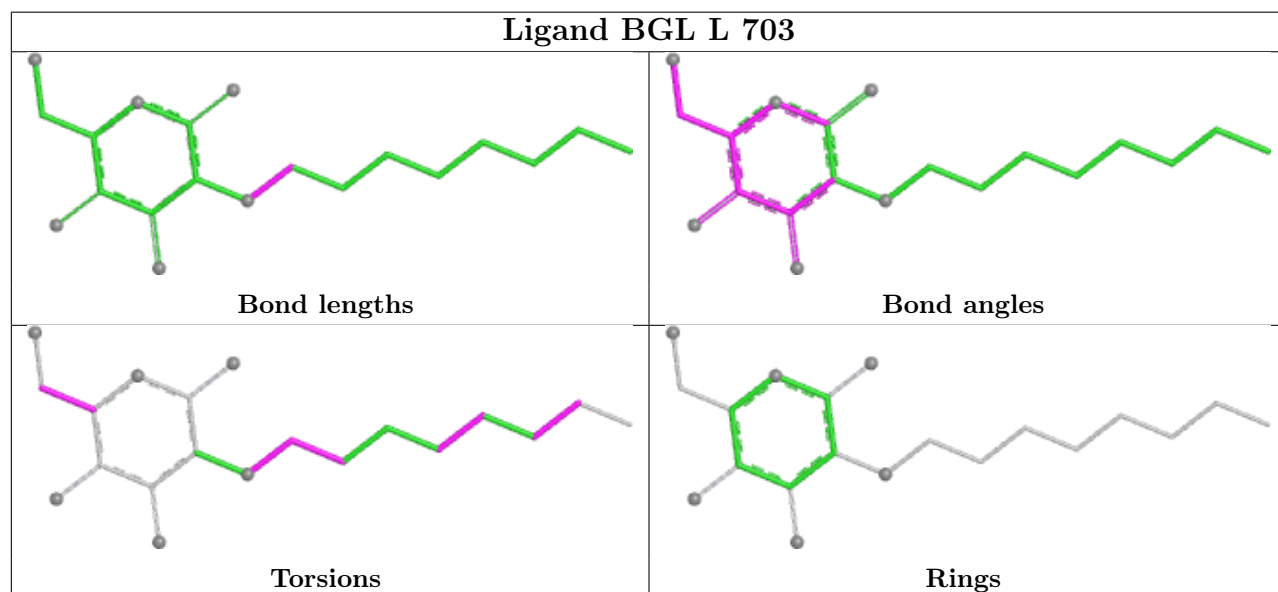
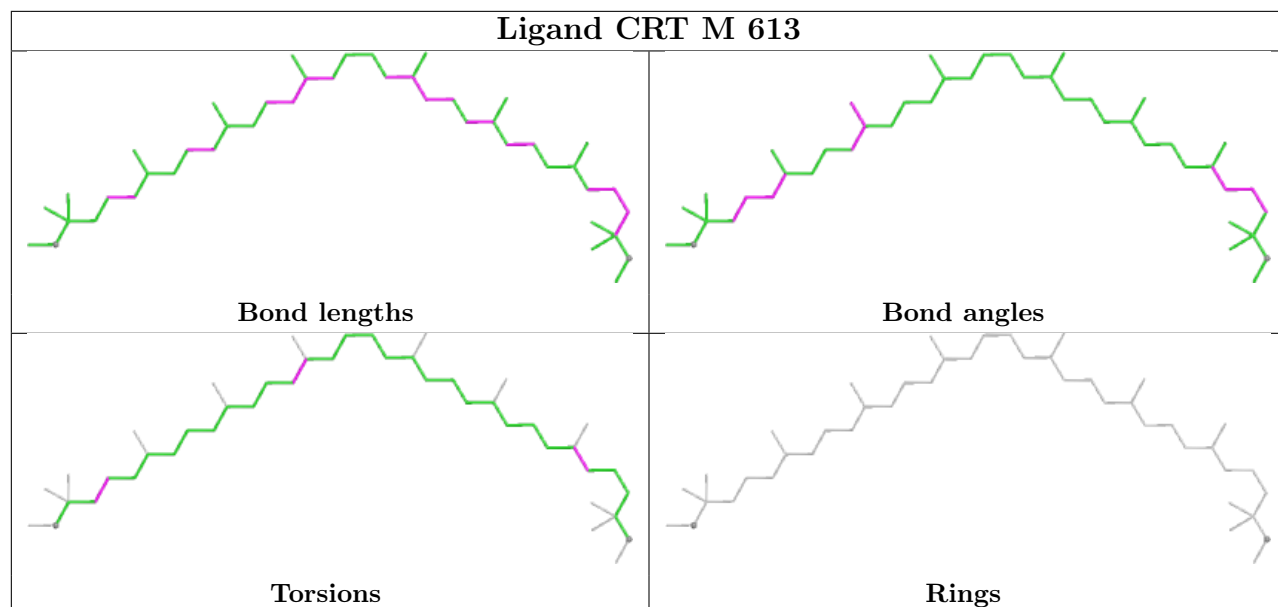
17 monomers are involved in 65 short contacts:

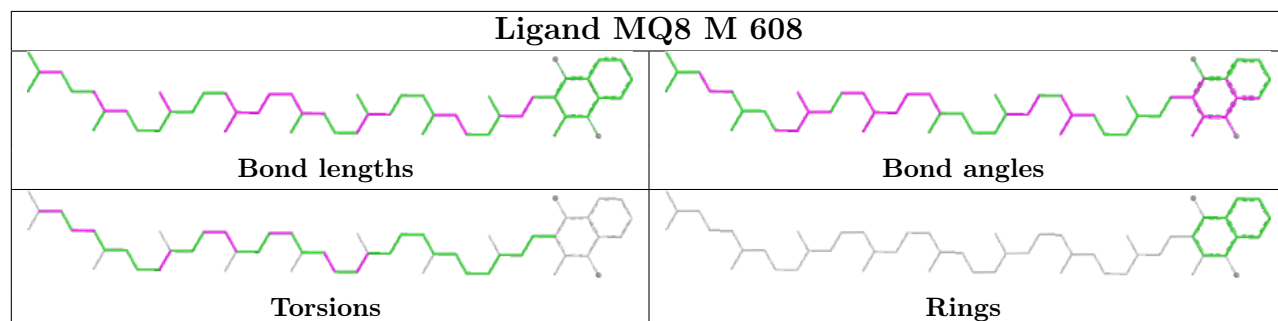
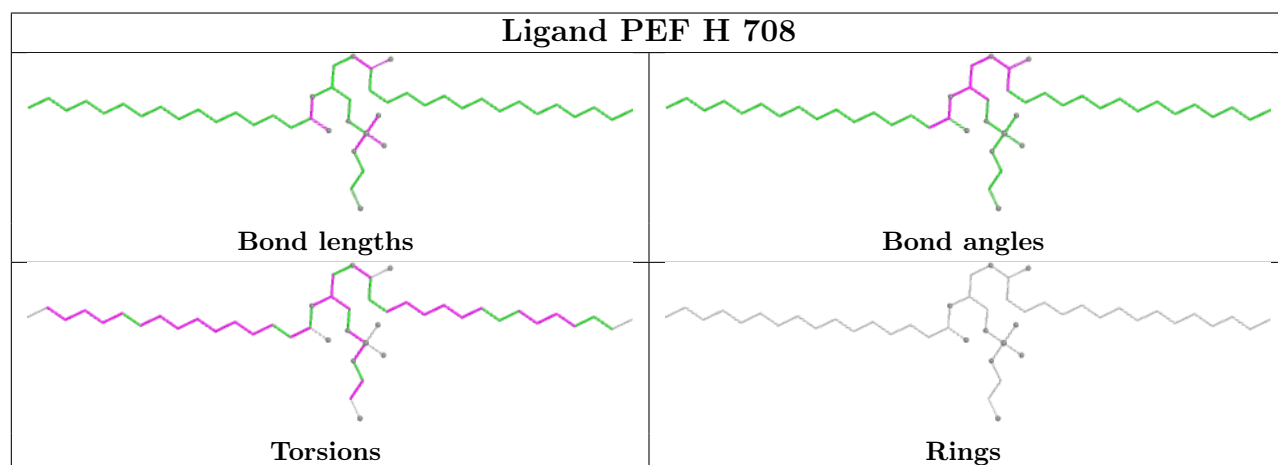
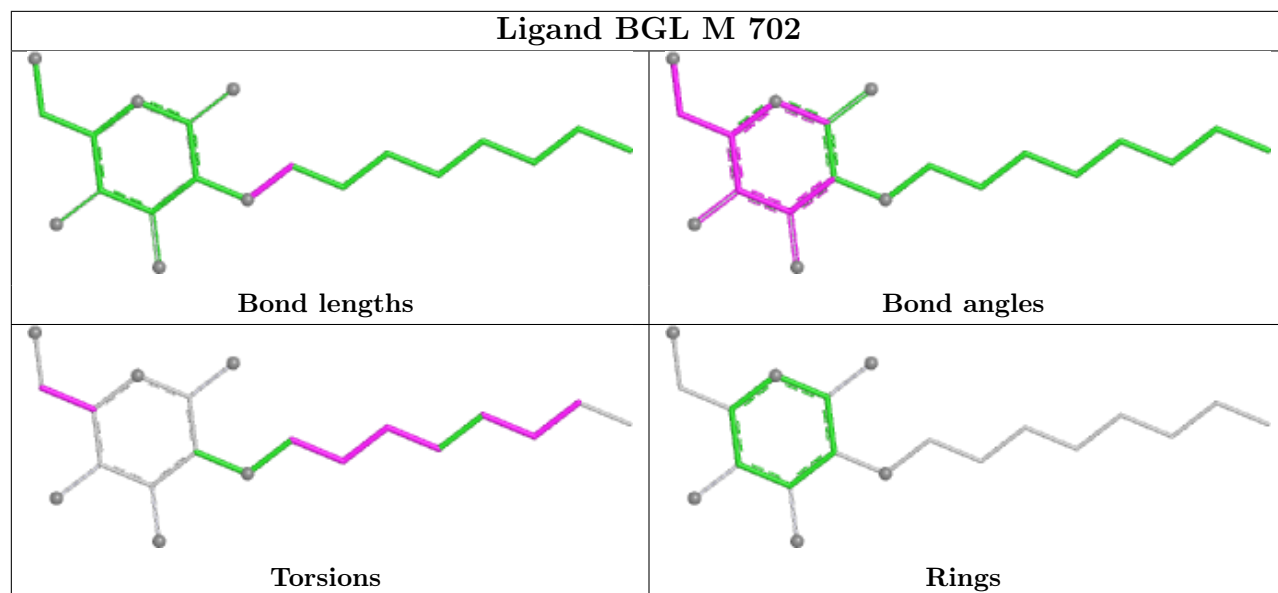
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	605	BPH	4	0
7	L	604	BCL	10	0
12	M	613	CRT	2	0
9	L	707	LDA	2	0
6	L	703	BGL	4	0
6	M	702	BGL	1	0
13	H	708	PEF	7	0
11	M	608	MQ8	1	0
7	M	603	BCL	6	0
6	L	704	BGL	2	0
5	C	612	HEM	2	0
6	L	701	BGL	3	0
5	C	610	HEM	2	0
7	M	601	BCL	10	0
7	L	602	BCL	7	0
8	L	606	BPH	7	0
5	C	609	HEM	1	0

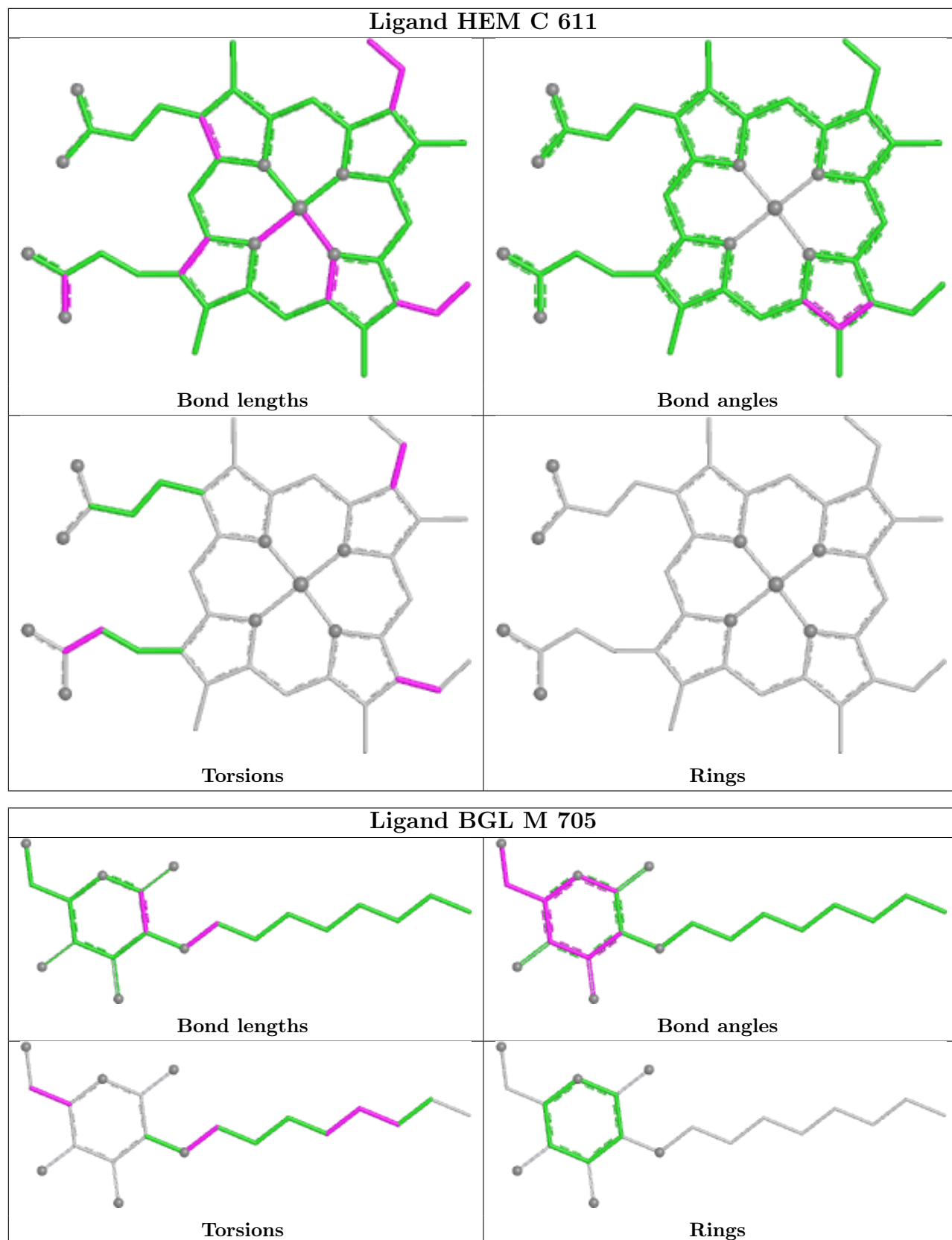
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

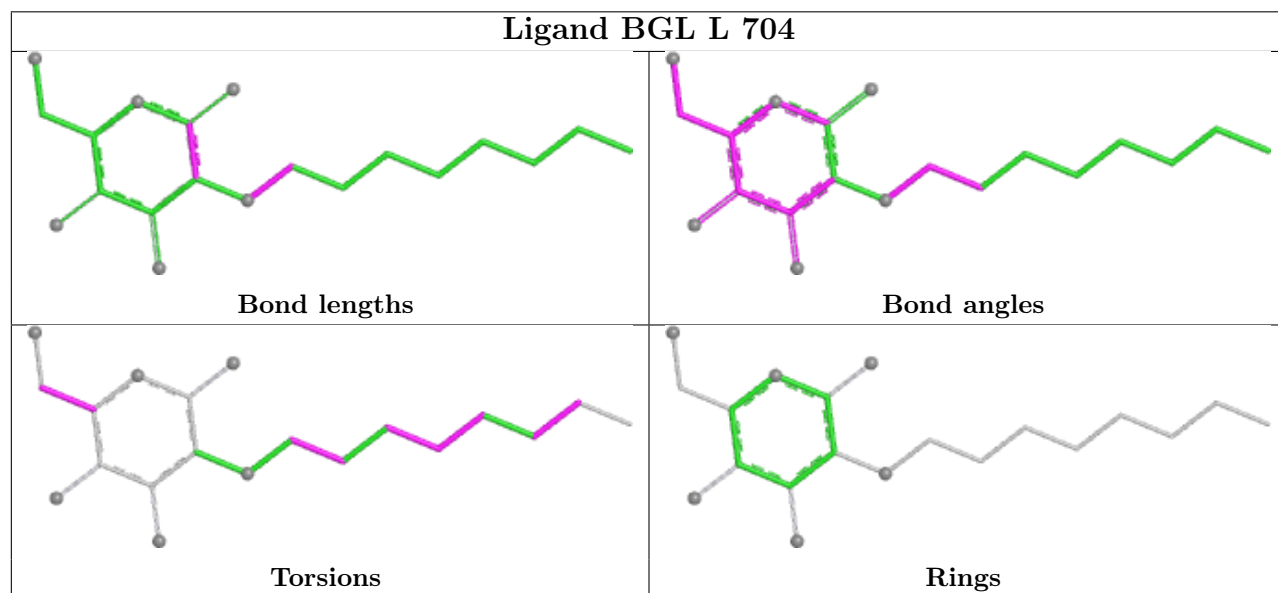
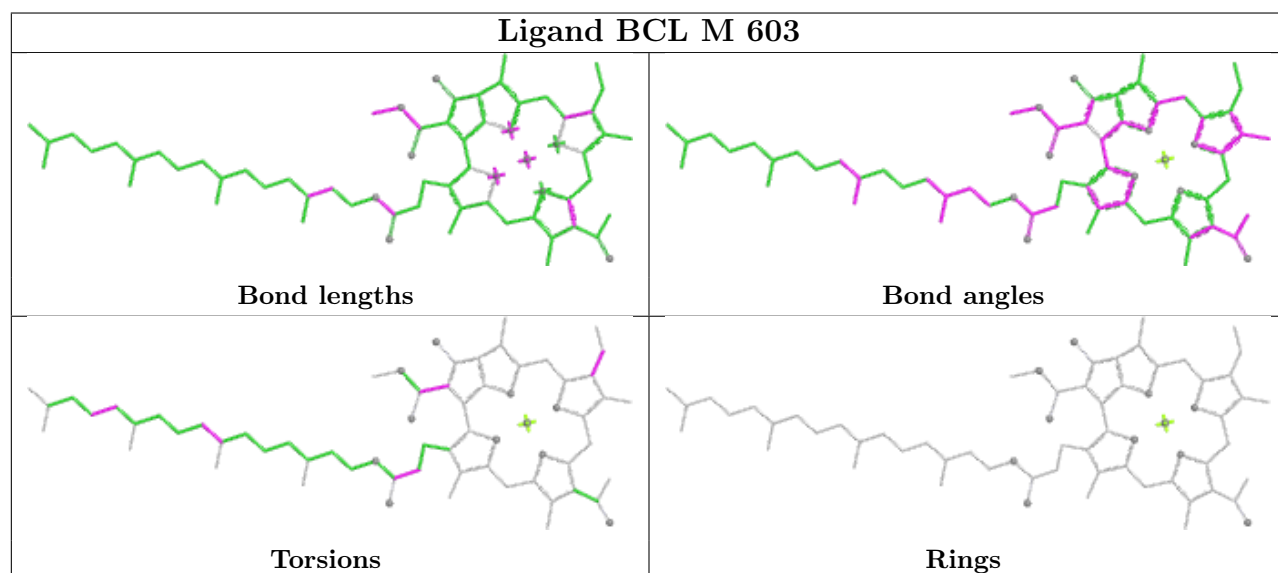
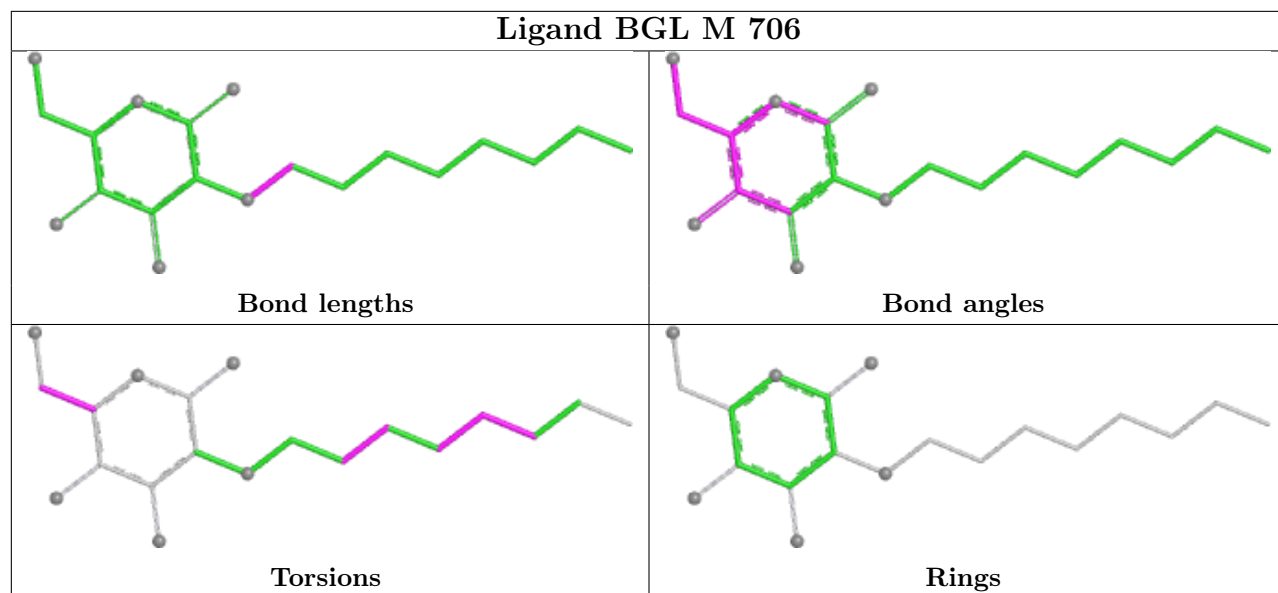
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

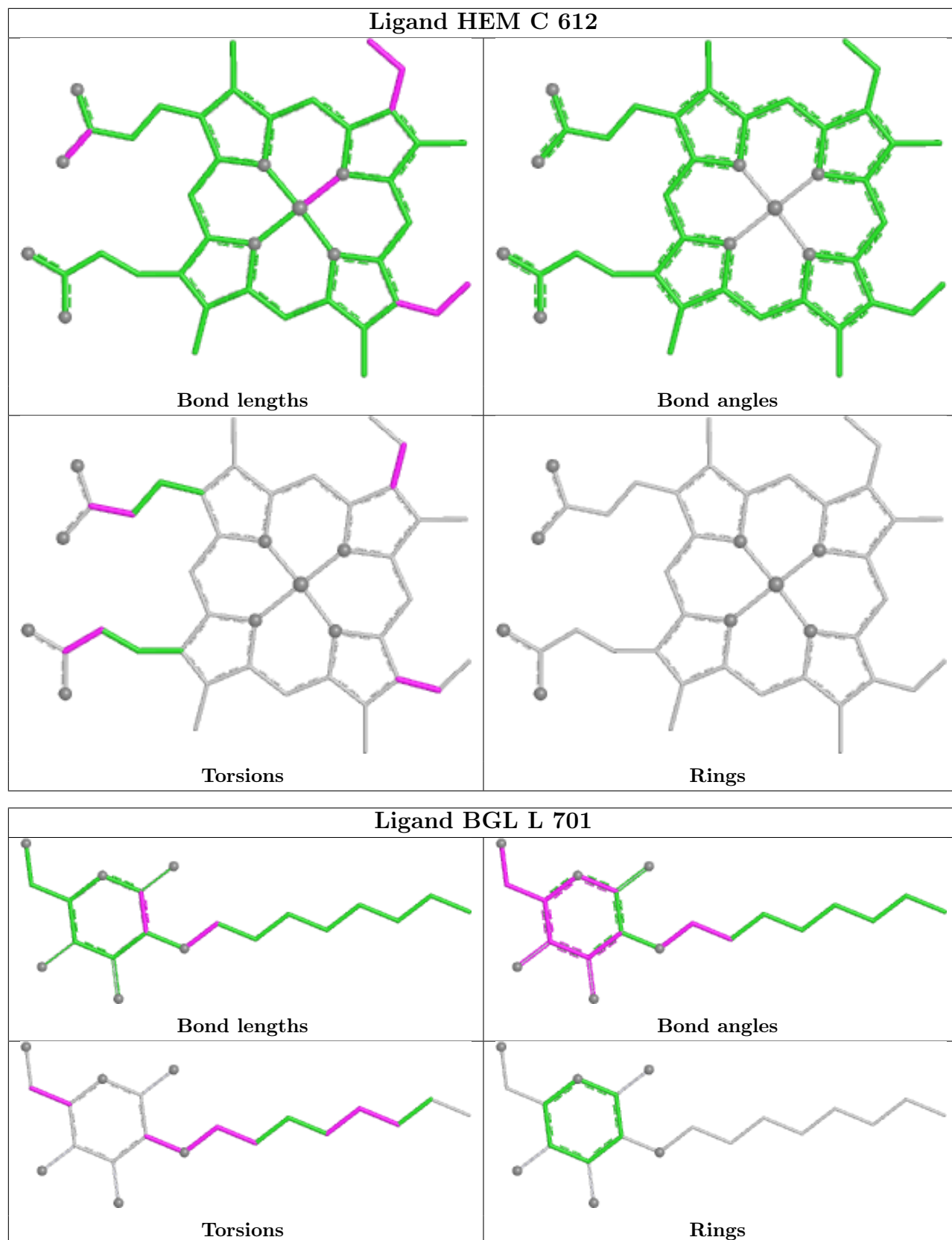


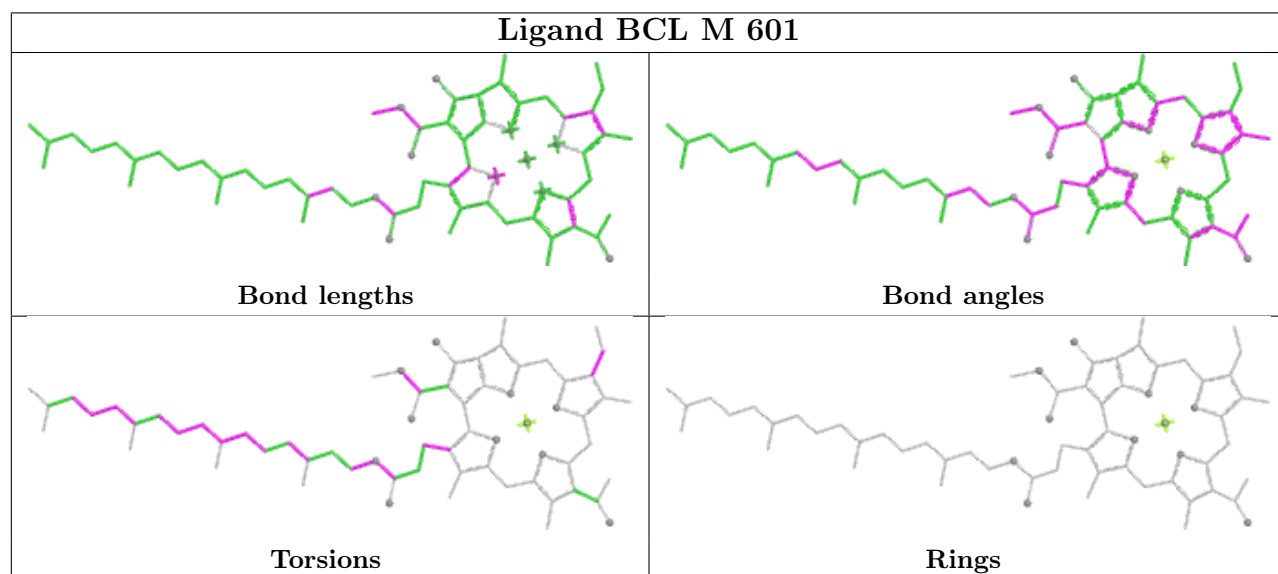
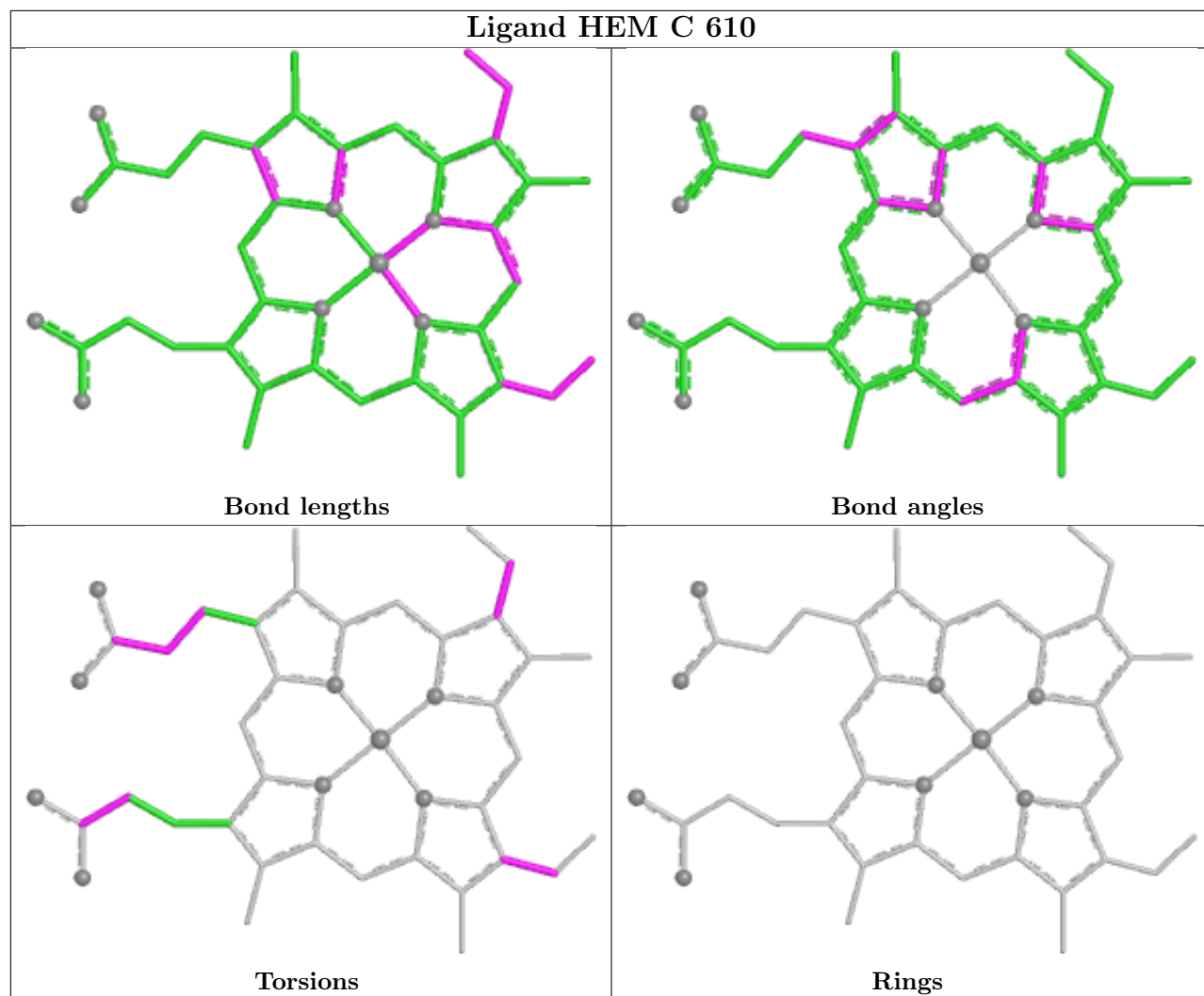


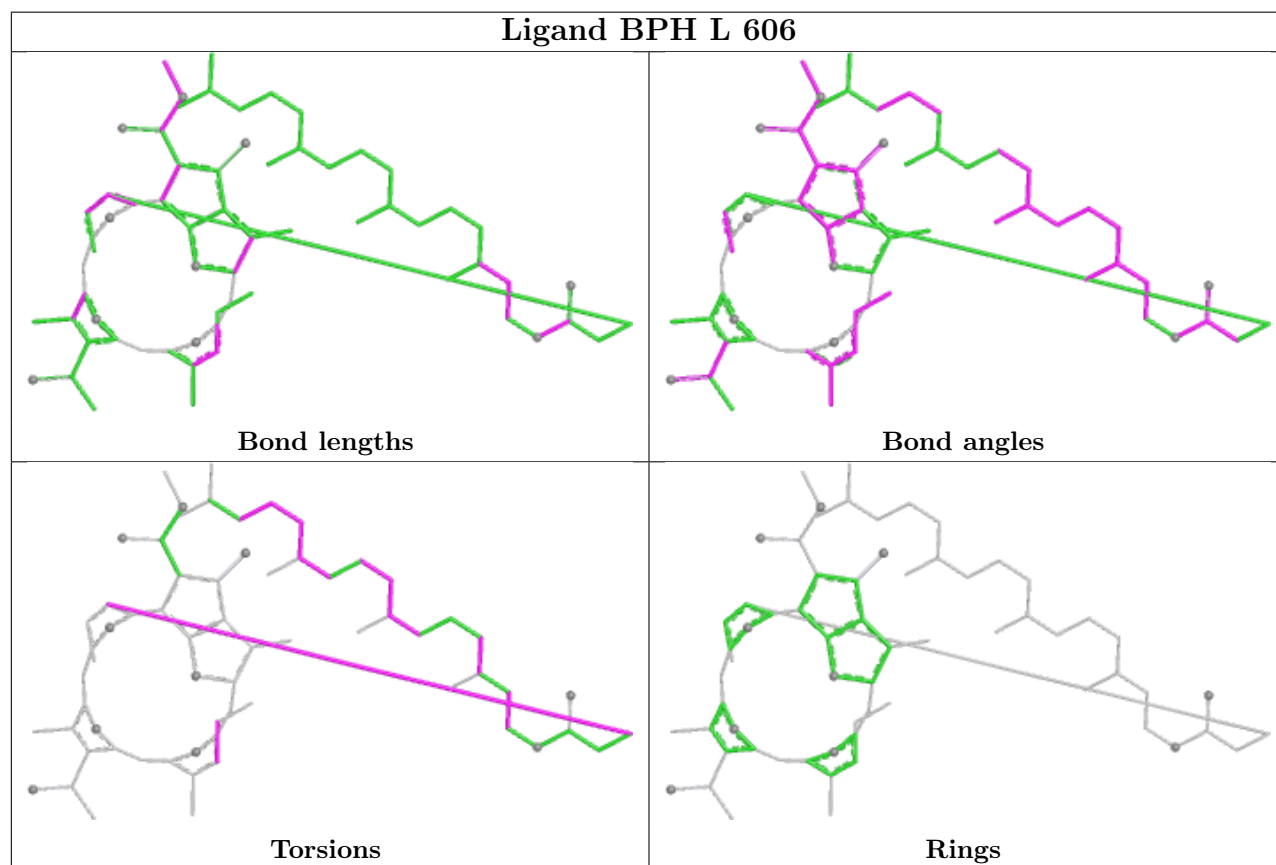
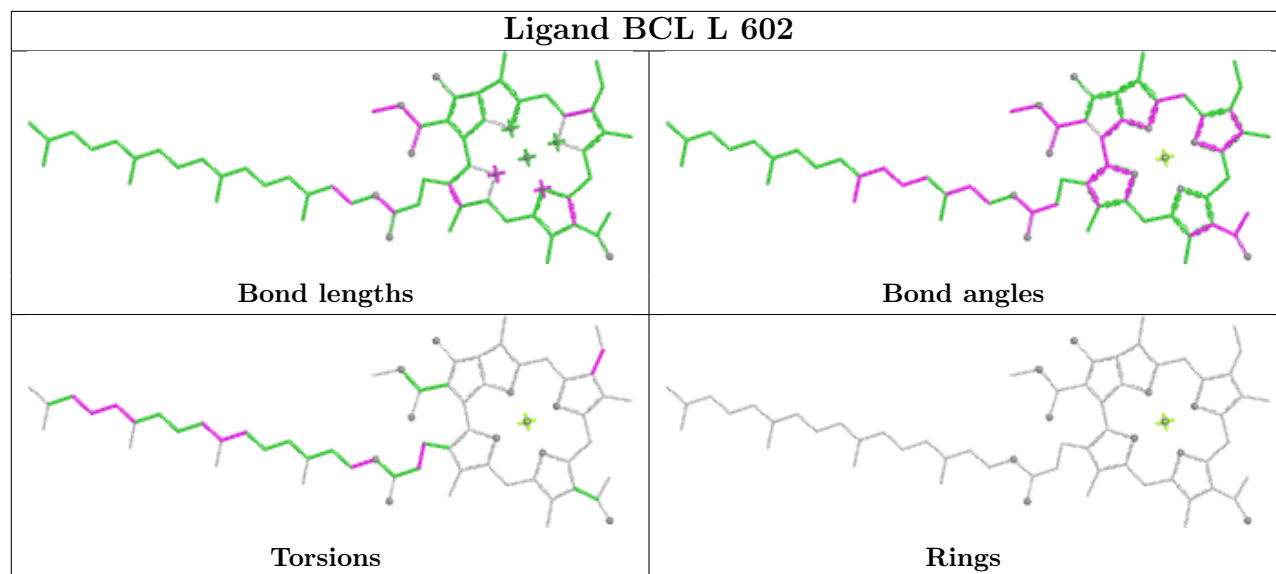


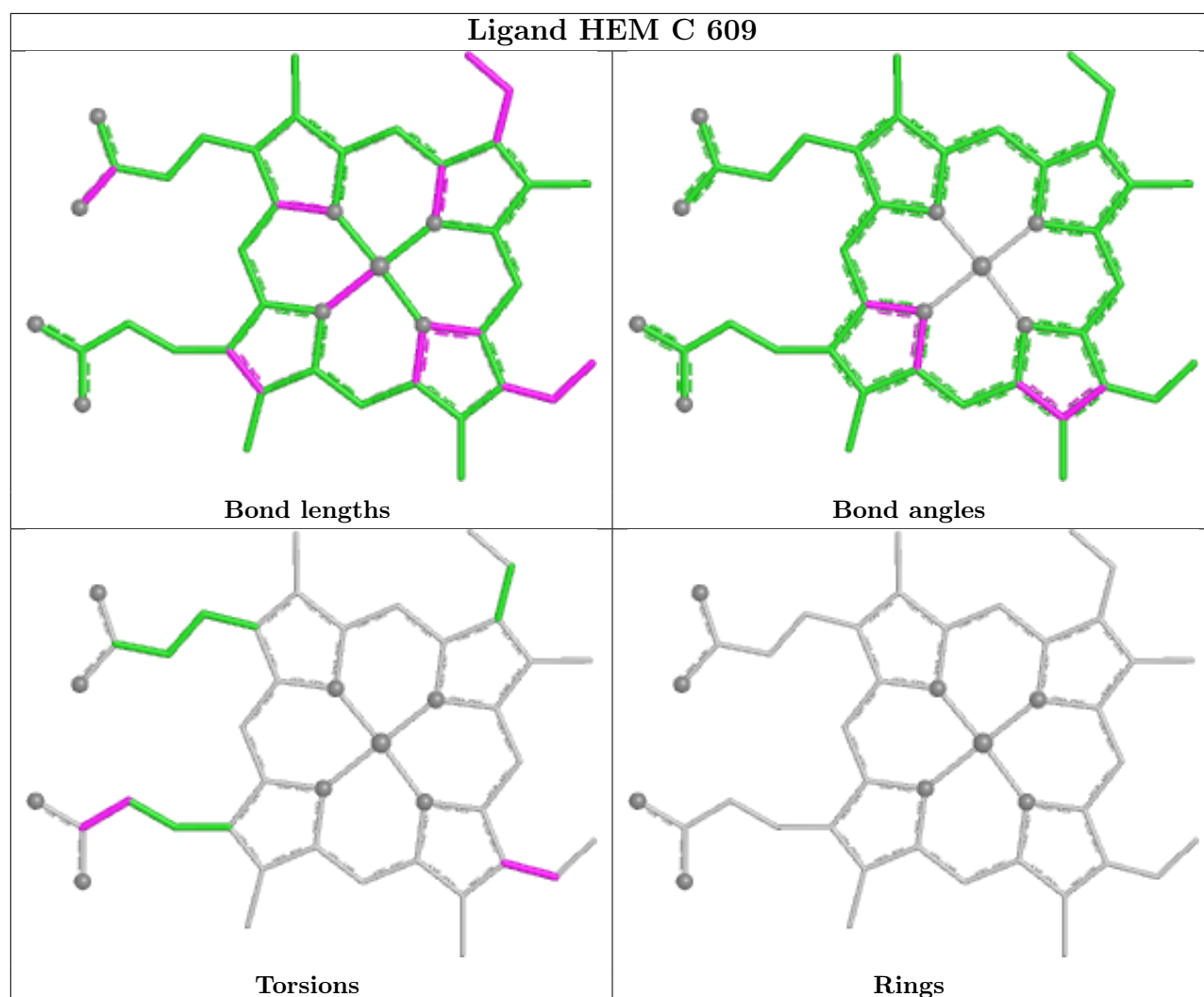












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.