Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:41 PM BST

PDB ID	:	1EYS
Title	:	CRYSTAL STRUCTURE OF PHOTOSYNTHETIC REACTION CENTER FROM A THERMOPHILIC BACTERIUM, THERMOCHROMATIUM TEPIDUM
Authors	:	Nogi, T.; Fathir, I.; Kobayashi, M.; Nozawa, T.; Miki, K.
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 following versions of software and data (see references ①) were used in the production of this report:

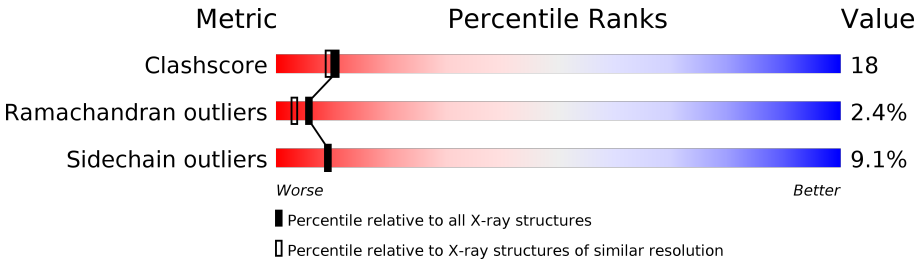
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	382	53% 24% • 19%
2	L	280	66% 31% •
3	M	324	60% 33% 5% • •
4	H	259	55% 29% 7% • 8%

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			

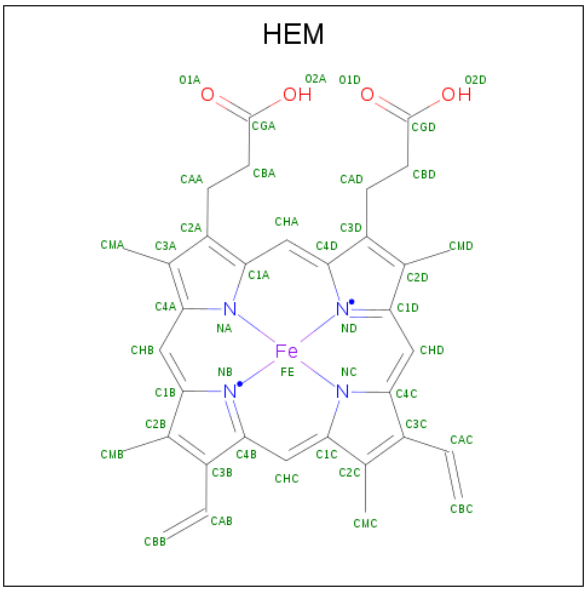
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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.

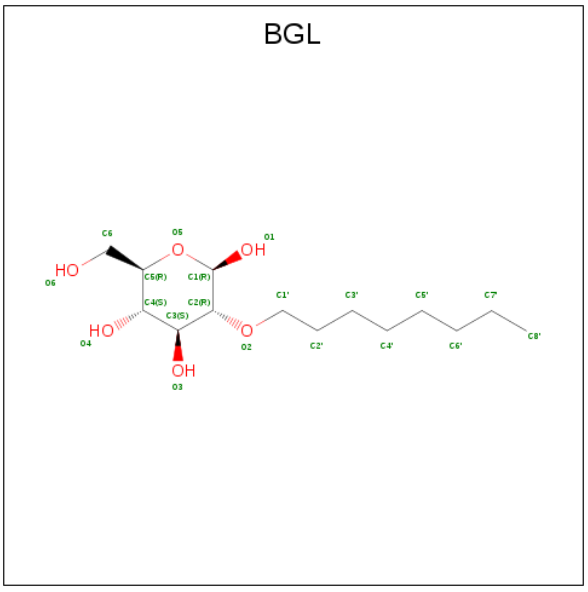
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	238	Total	C	N	O	S	0	0	0
			1837	1187	309	336	5			

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



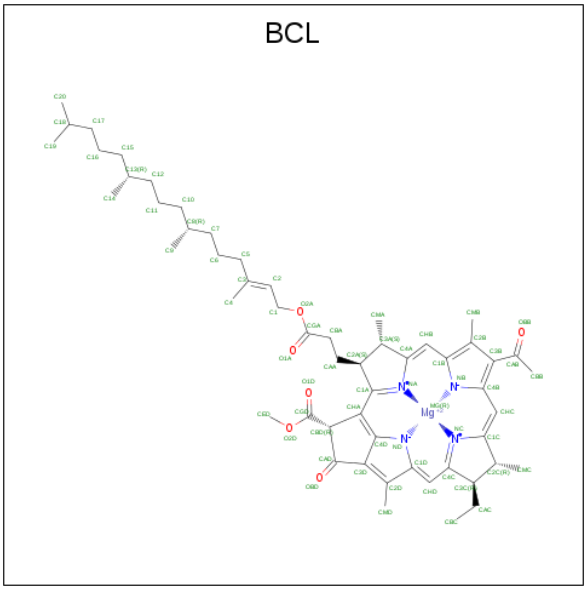
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



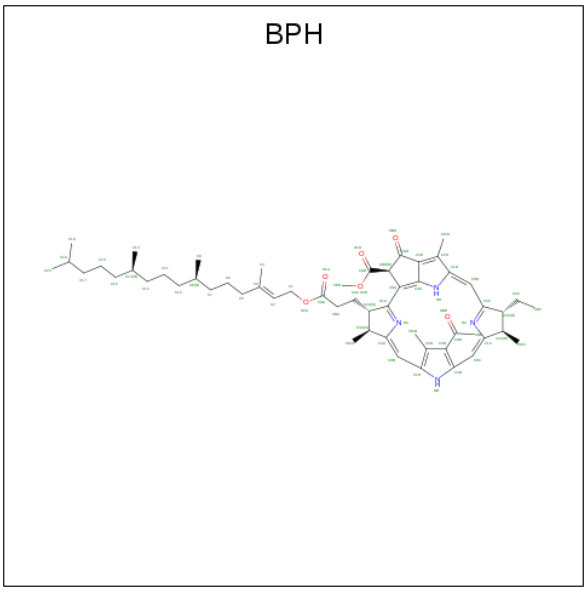
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 20 14 6	0	0
6	L	1	Total C O 20 14 6	0	0
6	L	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



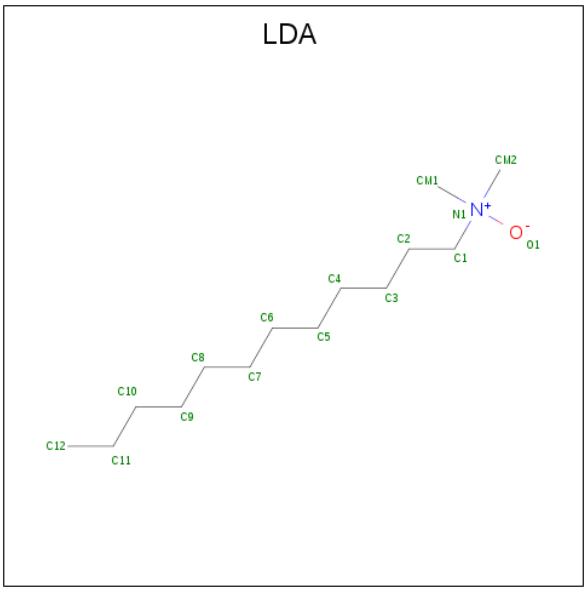
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C Mg N O 66 55 1 4 6	0	0
7	L	1	Total C Mg N O 66 55 1 4 6	0	0
7	M	1	Total C Mg N O 66 55 1 4 6	0	0
7	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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 (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

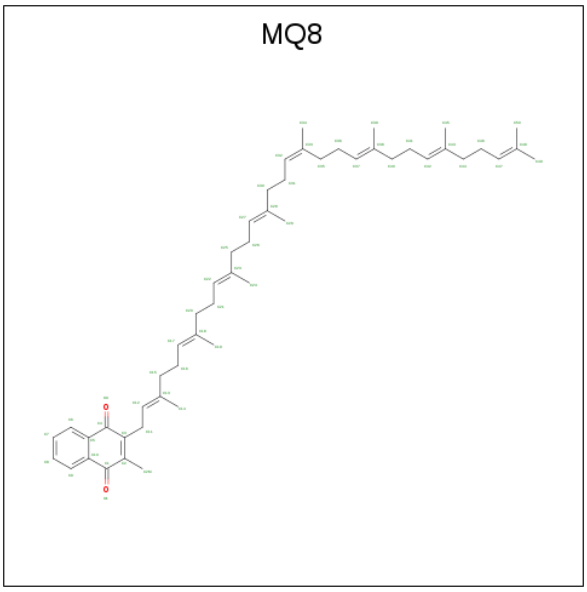


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

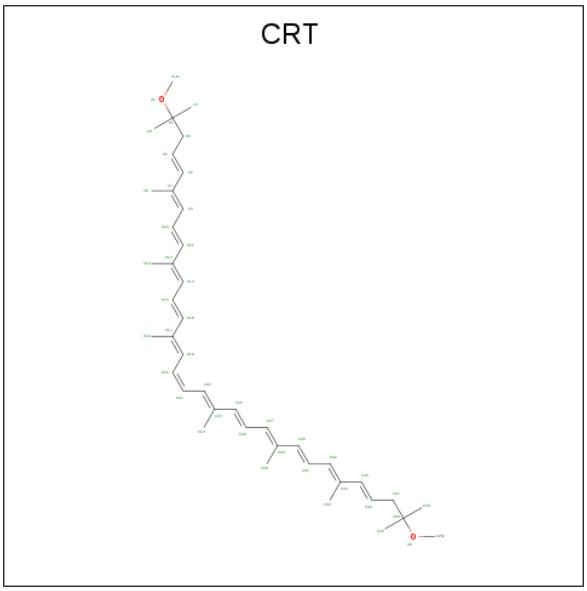
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

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



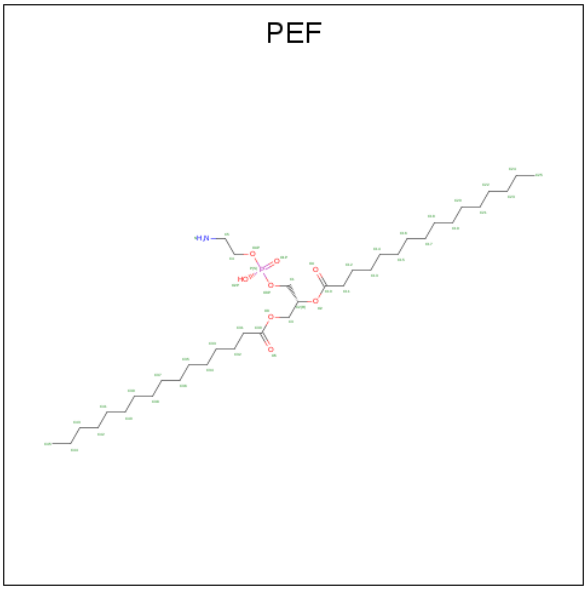
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 53 51 2	0	0

- Molecule 12 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



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

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



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

- Molecule 14 is water.

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

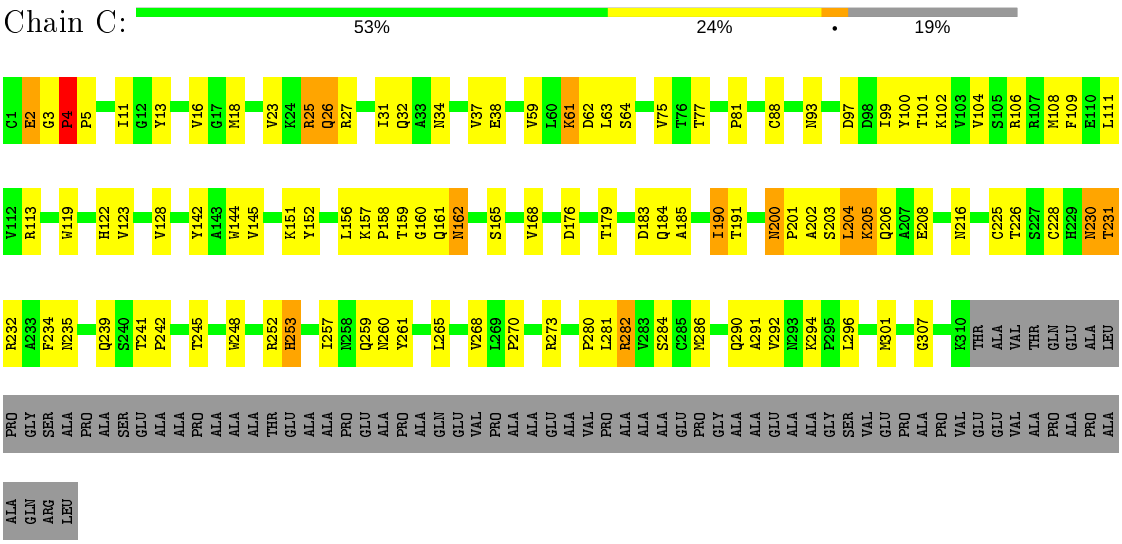
3 Residue-property plots (i)

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. 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.

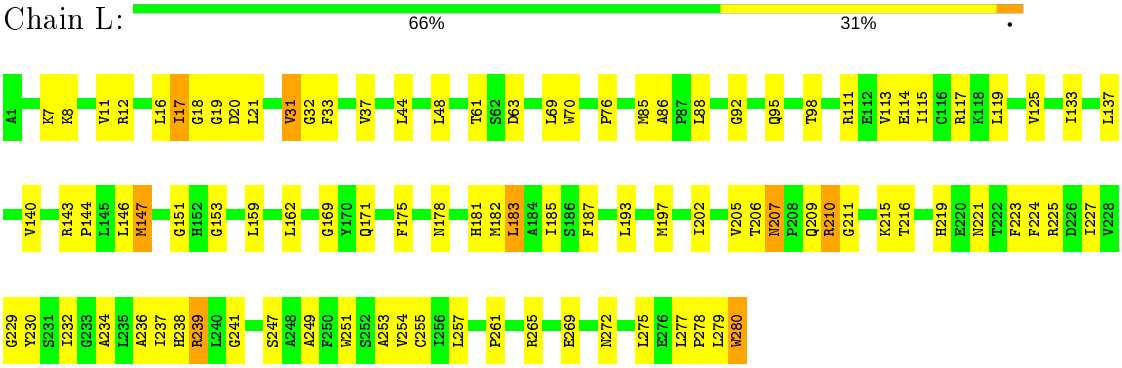
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



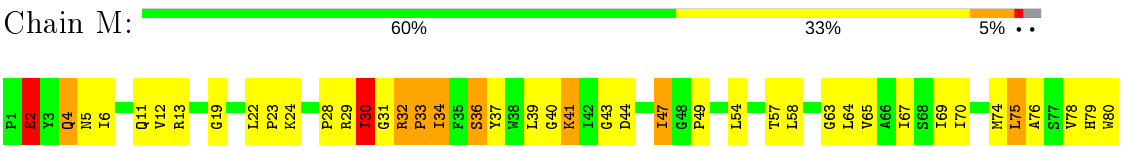
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

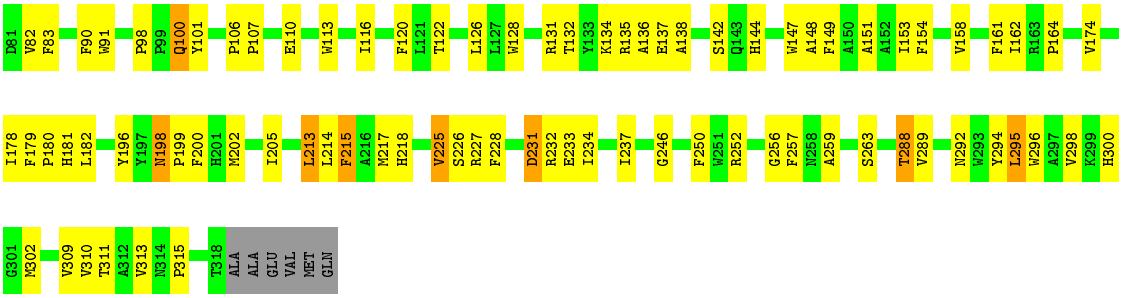
Chain L:



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

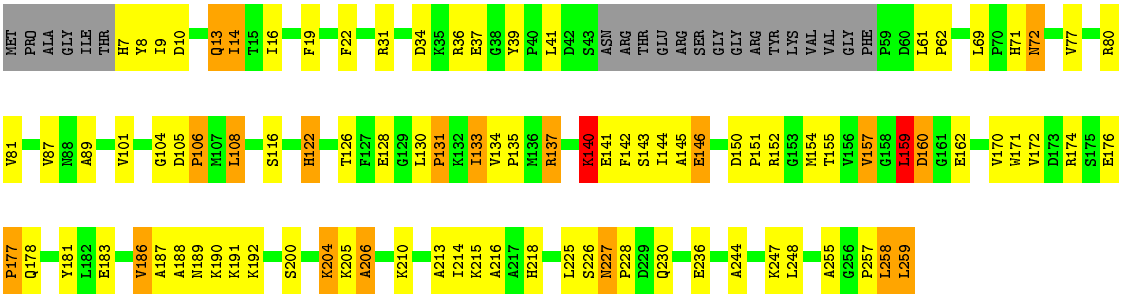
Chain M:





- Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:



4 Data and refinement statistics (i)

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: BCL, LDA, CRT, BPH, BGL, FE, MQ8, HEM, PEF

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	0.53	1/2471 (0.0%)	0.72	2/3374 (0.1%)
2	L	0.50	0/2320	0.65	0/3170
3	M	0.49	0/2637	0.67	1/3610 (0.0%)
4	H	0.47	0/1890	0.76	1/2576 (0.0%)
All	All	0.50	1/9318 (0.0%)	0.69	4/12730 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	CYS	CB-SG	-5.56	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	159	LEU	CA-CB-CG	7.48	132.51	115.30
1	C	230	ASN	N-CA-C	-6.83	92.55	111.00
3	M	47	ILE	N-CA-C	-5.57	95.95	111.00
1	C	3	GLY	N-CA-C	5.11	125.88	113.10

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	74	0
2	L	2233	0	2195	85	0
3	M	2537	0	2511	123	0
4	H	1837	0	1831	82	0
5	C	172	0	120	5	0
6	L	60	0	84	10	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	6	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	364	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 18.

All (364) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:H:171:TRP:HE1	4:H:183:GLU:HG3	1.57	0.69
2:L:117:ARG:HH12	4:H:258:LEU:CD1	2.04	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
3:M:198:ASN:HD22	3:M:198:ASN:C	1.96	0.67
7:M:601:BCL:HBB2	7:M:601:BCL:HMB1	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
6:L:704:BGL:H1	3:M:302:MET:HE2	1.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:70:TRP:CE2	6:L:703:BGL:H2'1	2.33	0.63
2:L:207:ASN:HD22	2:L:207:ASN:N	1.96	0.62
2:L:227:ILE:HD11	3:M:135:ARG:HB2	1.82	0.62
4:H:7:HIS:CG	4:H:8:TYR:N	2.65	0.62
2:L:143:ARG:HB3	2:L:144:PRO:HD3	1.82	0.61
1:C:200:ASN:HD22	1:C:200:ASN:C	2.03	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
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
3:M:288:THR:HG22	3:M:289:VAL:HG23	1.82	0.60
1:C:242:PRO:HD3	3:M:311:THR:O	2.01	0.60
4:H:7:HIS:CD2	4:H:8:TYR:H	2.18	0.60
3:M:128:TRP:O	3:M:131:ARG:HB3	2.02	0.59
3:M:11:GLN:NE2	3:M:41:LYS:HD2	2.17	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:HD22	1:C:235:ASN:H	1.50	0.59
4:H:151:PRO:O	4:H:154:MET:HG3	2.03	0.59
3:M:76:ALA:HB1	6:M:702:BGL:H2	1.84	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
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:HMB1	7:L:602:BCL:HBB3	1.85	0.58
4:H:7:HIS:C	4:H:9:ILE:H	2.07	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
2:L:143:ARG:CZ	2:L:147:MET:HE2	2.34	0.57
2:L:206:THR:OG1	2:L:207:ASN:ND2	2.38	0.57
3:M:232:ARG:HH22	4:H:236:GLU:CD	2.08	0.57
3:M:134:LYS:O	3:M:137:GLU:HG2	2.05	0.56
7:M:603:BCL:HMB1	7:M:603:BCL:CBB	2.34	0.56
2:L:181:HIS:CE1	2:L:185:ILE:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:207:ASN:ND2	2:L:207:ASN:N	2.54	0.55
1:C:88:CYS:O	1:C:102:LYS:HB2	2.07	0.55
4:H:105:ASP:H	4:H:108:LEU:HD23	1.70	0.55
3:M:288:THR:CG2	3:M:289:VAL:HG23	2.36	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
4:H:31:ARG:NE	13:H:708:PEF:H112	2.22	0.55
3:M:70:ILE:O	3:M:74:MET:HG3	2.07	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
4:H:204:LYS:C	4:H:206:ALA:H	2.10	0.54
1:C:200:ASN:ND2	1:C:202:ALA:H	2.05	0.54
1:C:23:VAL:HG12	1:C:26:GLN:H	1.71	0.54
1:C:109:PHE:O	1:C:113:ARG:HG3	2.08	0.54
3:M:225:VAL:HG13	3:M:225:VAL:O	2.07	0.53
3:M:11:GLN:HE21	3:M:41:LYS:HE3	1.73	0.53
3:M:148:ALA:O	3:M:151:ALA:HB3	2.09	0.53
4:H:137:ARG:O	4:H:137:ARG:HG3	2.09	0.53
1:C:32:GLN:OE1	1:C:32:GLN:HA	2.08	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
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
4:H:37:GLU:CD	4:H:80:ARG:HH22	2.12	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
1:C:59:VAL:C	1:C:61:LYS:H	2.13	0.52
3:M:22:LEU:HD21	3:M:29:ARG:NH1	2.24	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:ND2	1:C:235:ASN:H	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
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
2:L:70:TRP:HE1	6:L:704:BGL:HO1	1.57	0.52
4:H:157:VAL:HG23	4:H:210:LYS:HA	1.91	0.51
7:L:602:BCL:O1A	7:L:604:BCL:HBC1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:198:ASN:HD22	3:M:199:PRO:N	2.07	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:NH1	3:M:131:ARG:HG3	2.25	0.51
4:H:7:HIS:HB3	4:H:9:ILE:CG1	2.27	0.51
4:H:171:TRP:NE1	4:H:183:GLU:HG3	2.23	0.51
3:M:22:LEU:CD2	3:M:29:ARG:HH12	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:248:LEU:O	4:H:255:ALA:HB2	2.10	0.50
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:H	3:M:234:ILE:HD12	1.76	0.50
1:C:200:ASN:HD22	1:C:201:PRO:N	2.09	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
2:L:216:THR:OG1	2:L:219:HIS:HD2	1.95	0.50
3:M:296:TRP:O	3:M:300:HIS:HD2	1.94	0.50
1:C:156:LEU:HD22	3:M:98:PRO:HB3	1.93	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
4:H:126:THR:HG23	4:H:130:LEU:O	2.11	0.50
4:H:31:ARG:NH1	4:H:34:ASP:OD2	2.44	0.50
3:M:22:LEU:HD11	3:M:29:ARG:NH1	2.27	0.50
1:C:270:PRO:HG2	1:C:273:ARG:HG2	1.94	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
1:C:37:VAL:HG23	1:C:301:MET:HE3	1.94	0.49
2:L:239:ARG:HD2	3:M:6:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASN:ND2	1:C:200:ASN:C	2.65	0.49
4:H:187:ALA:O	4:H:189:ASN:N	2.46	0.49
6:L:701:BGL:O3	6:L:701:BGL:H4'1	2.12	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
3:M:128:TRP:CH2	7:M:601:BCL:H193	2.49	0.48
2:L:17:ILE:HD11	2:L:33:PHE:CD1	2.49	0.48
1:C:111:LEU:HD23	1:C:111:LEU:C	2.34	0.48
4:H:189:ASN:HD22	4:H:191:LYS:CD	2.24	0.48
3:M:252:ARG:HH12	13:H:708:PEF:H51	1.78	0.48
3:M:113:TRP:HE3	3:M:116:ILE:HG21	1.79	0.48
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
4:H:134:VAL:HG11	4:H:174:ARG:NH1	2.29	0.47
2:L:278:PRO:C	2:L:280:TRP:N	2.66	0.47
3:M:82:VAL:O	3:M:82:VAL:HG12	2.14	0.47
1:C:97:ASP:CG	1:C:106:ARG:HH22	2.18	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: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
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
2:L:239:ARG:NH1	3:M:6:ILE:O	2.47	0.47
1:C:11:ILE:HG21	1:C:226:THR:O	2.15	0.47
4:H:145:ALA:O	4:H:146:GLU:C	2.53	0.47
4:H:71:HIS:O	4:H:72:ASN:C	2.53	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
4:H:151:PRO:HG2	4:H:170:VAL:HG21	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
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
4:H:39:TYR:CE1	4:H:41:LEU:HD21	2.50	0.47
3:M:196:TYR:CZ	7:M:603:BCL:HMC2	2.50	0.47
3:M:63:GLY:O	3:M:67:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:36:SER:HG	3:M:39:LEU:HB2	1.80	0.46
1:C:161:GLN:HG2	1:C:161:GLN:O	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
4:H:130:LEU:O	4:H:131:PRO:C	2.53	0.46
7:L:604:BCL:H13	7:L:604:BCL:H172	1.59	0.46
2:L:279:LEU:O	3:M:83:PHE:CZ	2.68	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
4:H:14:ILE:O	4:H:14:ILE:HD12	2.16	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
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:252:ARG:NH1	13:H:708:PEF:H51	2.30	0.46
3:M:227:ARG:HG3	3:M:228:PHE:CD2	2.51	0.46
3:M:128:TRP:HE1	8:M:605:BPH:CED	2.28	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
3:M:198:ASN:ND2	3:M:198:ASN:C	2.68	0.45
1:C:232:ARG:HE	1:C:239:GLN:HE22	1.64	0.45
4:H:244:ALA:O	4:H:247:LYS:HB2	2.17	0.45
3:M:137:GLU:HG3	3:M:138:ALA:N	2.30	0.45
6:L:704:BGL:H1	3:M:302:MET:CE	2.45	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
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
3:M:161:PHE:C	3:M:164:PRO:HD2	2.38	0.44
2:L:215:LYS:CD	2:L:219:HIS:CE1	3.01	0.44
4:H:248:LEU:HD12	4:H:255:ALA:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:37:VAL:CG2	1:C:301:MET:HE3	2.48	0.44
2:L:206:THR:HG21	3:M:237:ILE:HD13	2.00	0.44
4:H:204:LYS:O	4:H:206:ALA:N	2.51	0.44
2:L:19:GLY:O	2:L:21:LEU:N	2.51	0.44
12:M:613:CRT:H36	12:M:613:CRT:H341	1.86	0.44
1:C:152:TYR:CZ	3:M:79:HIS:NE2	2.86	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
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:2:GLU:N	1:C:2:GLU:CD	2.72	0.43
4:H:225:LEU:C	4:H:227:ASN:H	2.22	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
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:H112	8:L:606:BPH:H7C2	1.74	0.43
3:M:214:LEU:HD23	3:M:214:LEU:HA	1.90	0.43
3:M:75:LEU:HD13	3:M:80:TRP:HE3	1.79	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:144:TRP:CD1	1:C:284:SER:HB3	2.54	0.43
3:M:231:ASP:C	3:M:233:GLU:H	2.22	0.43
3:M:64:LEU:HD21	8:M:605:BPH:H8	2.01	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:HAC2	8:L:606:BPH:HHD	1.71	0.42
3:M:256:GLY:O	13:H:708:PEF:N	2.52	0.42
3:M:67:ILE:HD11	8:M:605:BPH:H4C1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:133:ILE:HA	4:H:172:VAL:O	2.18	0.42
3:M:227:ARG:HG3	3:M:228:PHE:CE2	2.55	0.42
4:H:192:LYS:NZ	4:H:228:PRO:O	2.53	0.42
7:L:604:BCL:C1B	8:L:606:BPH:H202	2.48	0.42
4:H:135:PRO:HA	4:H:171:TRP:HA	2.01	0.42
3:M:2:GLU:HG2	4:H:247:LYS:HZ1	1.83	0.42
2:L:178:ASN:HB3	2:L:181:HIS:CB	2.50	0.42
2:L:85:MET:HB3	9:L:707:LDA:O1	2.20	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
1:C:4:PRO:HA	1:C:5:PRO:HA	1.68	0.42
4:H:160:ASP:OD2	4:H:215:LYS:NZ	2.53	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:159:LEU:HD13	4:H:215:LYS:HG3	2.02	0.42
3:M:101:TYR:CD2	3:M:106:PRO:HB3	2.55	0.42
1:C:231:THR:HG22	1:C:234:PHE:CE2	2.54	0.41
1:C:25:ARG:NH1	1:C:26:GLN:OE1	2.53	0.41
4:H:140:LYS:HG2	4:H:141:GLU:OE1	2.20	0.41
4:H:69:LEU:N	4:H:69:LEU:HD23	2.35	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:128:TRP:CZ2	7:M:601:BCL:H193	2.55	0.41
3:M:32:ARG:HA	3:M:32:ARG:HD3	1.41	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:105:ASP:CB	4:H:108:LEU:HD23	2.38	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
2:L:238:HIS:CD2	3:M:218:HIS:CD2	3.07	0.41
4:H:36:ARG:NH1	4:H:62:PRO:HG2	2.36	0.41
2:L:125:VAL:HG11	3:M:250:PHE:CE2	2.56	0.41
3:M:246:GLY:HA3	14:M:922:HOH:O	2.20	0.41
3:M:205:ILE:HG12	7:M:603:BCL:CHB	2.51	0.41
1:C:13:TYR:HB3	1:C:16:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:241:GLY:HA3	3:M:215:PHE:CE1	2.56	0.41
3:M:294:TYR:O	3:M:298:VAL:HG23	2.21	0.41
4:H:189:ASN:HD21	4:H:191:LYS:HB2	1.81	0.40
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
1:C:190:ILE:H	1:C:190:ILE:HD13	1.86	0.40
4:H:122:HIS:C	4:H:122:HIS:CD2	2.94	0.40
4:H:178:GLN:NE2	14:H:985:HOH:O	2.55	0.40
7:L:604:BCL:OBD	3:M:205:ILE:HD12	2.21	0.40
3:M:39:LEU:HA	3:M:39:LEU:HD12	1.95	0.40
2:L:206:THR:C	2:L:207:ASN:ND2	2.74	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:178:ILE:HG22	3:M:179:PHE:N	2.36	0.40
7:M:601:BCL:HHC	7:M:601:BCL:OBB	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%)	4 2
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	22 22
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	8 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	2 1
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	6 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 (i)

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%)	239 (92%)	20 (8%)	13 13
2	L	228/228 (100%)	212 (93%)	16 (7%)	15 16
3	M	254/258 (98%)	234 (92%)	20 (8%)	12 12
4	H	195/211 (92%)	166 (85%)	29 (15%)	3 2
All	All	936/997 (94%)	851 (91%)	85 (9%)	9 9

All (85) 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	93	ASN
1	C	108	MET
1	C	145	VAL
1	C	168	VAL
1	C	176	ASP
1	C	190	ILE
1	C	200	ASN
1	C	204	LEU
1	C	205	LYS
1	C	216	ASN
1	C	253	HIS
1	C	259	GLN
1	C	260	ASN
1	C	282	ARG
1	C	286	MET
2	L	8	LYS
2	L	17	ILE
2	L	61	THR
2	L	63	ASP
2	L	140	VAL
2	L	146	LEU
2	L	147	MET
2	L	171	GLN
2	L	183	LEU
2	L	207	ASN
2	L	209	GLN
2	L	210	ARG
2	L	239	ARG

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Mol	Chain	Res	Type
2	L	247	SER
2	L	255	CYS
2	L	280	TRP
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	215	PHE
3	M	225	VAL
3	M	231	ASP
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	61	LEU
4	H	72	ASN
4	H	77	VAL
4	H	81	VAL
4	H	106	PRO
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
4	H	143	SER
4	H	155	THR
4	H	157	VAL

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Mol	Chain	Res	Type
4	H	159	LEU
4	H	160	ASP
4	H	177	PRO
4	H	186	VAL
4	H	200	SER
4	H	204	LYS
4	H	226	SER
4	H	230	GLN
4	H	258	LEU
4	H	259	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
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	290	GLN
2	L	95	GLN
2	L	174	HIS
2	L	207	ASN
2	L	219	HIS
3	M	100	GLN
3	M	144	HIS
3	M	198	ASN
3	M	300	HIS
4	H	13	GLN
4	H	122	HIS
4	H	189	ASN
4	H	218	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	L	606	-	64,70,70	1.57	8 (12%)	76,101,101	2.03	25 (32%)
7	BCL	L	604	2	58,74,74	2.17	10 (17%)	69,115,115	2.41	26 (37%)
6	BGL	M	705	-	20,20,20	1.28	2 (10%)	24,25,25	2.04	6 (25%)
9	LDA	L	707	-	12,15,15	2.14	1 (8%)	14,17,17	0.64	0
6	BGL	M	702	-	20,20,20	1.07	1 (5%)	24,25,25	2.42	8 (33%)
5	HEM	C	609	1	27,50,50	2.20	10 (37%)	17,82,82	0.95	0
12	CRT	M	613	-	41,43,43	2.75	14 (34%)	50,54,54	1.44	4 (8%)
11	MQ8	M	608	-	54,54,54	2.41	16 (29%)	66,69,69	2.90	21 (31%)
6	BGL	L	704	-	20,20,20	1.23	2 (10%)	24,25,25	2.42	8 (33%)
5	HEM	C	612	1	27,50,50	1.91	6 (22%)	17,82,82	0.88	0
6	BGL	L	703	-	20,20,20	0.92	1 (5%)	24,25,25	2.04	7 (29%)
6	BGL	M	706	-	20,20,20	0.97	1 (5%)	24,25,25	2.07	6 (25%)
5	HEM	C	611	1	27,50,50	2.08	9 (33%)	17,82,82	1.16	0
5	HEM	C	610	1	27,50,50	2.00	7 (25%)	17,82,82	1.18	1 (5%)
7	BCL	L	602	2	58,74,74	2.07	8 (13%)	69,115,115	2.23	21 (30%)
6	BGL	L	701	-	20,20,20	1.25	2 (10%)	24,25,25	1.96	7 (29%)
8	BPH	M	605	-	64,70,70	1.67	8 (12%)	76,101,101	2.01	18 (23%)
7	BCL	M	603	3	58,74,74	2.03	6 (10%)	69,115,115	2.28	23 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	M	601	3	58,74,74	2.23	10 (17%)	69,115,115	2.47	25 (36%)
13	PEF	H	708	-	46,46,46	2.17	7 (15%)	49,51,51	1.38	6 (12%)

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	L	606	-	1/1/18/22	21/54/105/105	0/5/6/6
7	BCL	L	604	2	-	8/37/137/137	-
6	BGL	M	705	-	-	4/11/31/31	0/1/1/1
9	LDA	L	707	-	-	4/13/13/13	-
6	BGL	M	702	-	-	8/11/31/31	0/1/1/1
5	HEM	C	609	1	-	0/6/54/54	-
12	CRT	M	613	-	-	5/51/51/51	-
11	MQ8	M	608	-	-	12/47/67/67	0/2/2/2
6	BGL	L	704	-	-	5/11/31/31	0/1/1/1
5	HEM	C	612	1	-	0/6/54/54	-
6	BGL	L	703	-	-	6/11/31/31	0/1/1/1
6	BGL	M	706	-	-	5/11/31/31	0/1/1/1
5	HEM	C	611	1	-	0/6/54/54	-
5	HEM	C	610	1	-	1/6/54/54	-
7	BCL	L	602	2	-	10/37/137/137	-
6	BGL	L	701	-	-	7/11/31/31	0/1/1/1
8	BPH	M	605	-	-	14/54/105/105	0/5/6/6
7	BCL	M	603	3	-	10/37/137/137	-
7	BCL	M	601	3	-	23/37/137/137	-
13	PEF	H	708	-	-	35/50/50/50	-

All (129) 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
8	M	605	BPH	C3C-C4C	-8.84	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	608	MQ8	C34-C33	8.50	1.72	1.50
12	M	613	CRT	C6-C5	8.45	1.54	1.32
13	H	708	PEF	O4-C10	8.31	1.47	1.22
8	L	606	BPH	C3C-C4C	-8.19	1.38	1.50
12	M	613	CRT	C35-C36	8.01	1.52	1.32
9	L	707	LDA	O1-N1	-7.38	1.24	1.42
13	H	708	PEF	O5-C30	6.02	1.40	1.22
7	L	602	BCL	C4B-NB	5.76	1.40	1.35
7	M	601	BCL	C4B-NB	5.59	1.40	1.35
11	M	608	MQ8	C30-C31	-5.52	1.35	1.53
13	H	708	PEF	P-O1P	5.44	1.70	1.50
7	M	603	BCL	C4B-NB	5.40	1.40	1.35
12	M	613	CRT	C22-C23	5.32	1.42	1.35
7	L	604	BCL	C4B-NB	5.31	1.39	1.35
13	H	708	PEF	O2-C10	5.18	1.48	1.34
5	C	610	HEM	C3B-C2B	-5.07	1.33	1.40
11	M	608	MQ8	C27-C28	4.96	1.44	1.33
12	M	613	CRT	C19-C17	4.96	1.42	1.35
11	M	608	MQ8	C42-C43	4.93	1.44	1.33
5	C	612	HEM	C3B-CAB	-4.89	1.38	1.47
11	M	608	MQ8	C30-C28	4.88	1.61	1.51
7	L	602	BCL	O2D-CGD	4.88	1.45	1.33
5	C	609	HEM	C3B-C2B	-4.87	1.33	1.40
5	C	611	HEM	C3C-C2C	-4.79	1.33	1.40
5	C	610	HEM	C3B-CAB	-4.61	1.38	1.47
11	M	608	MQ8	C12-C13	4.59	1.44	1.33
8	M	605	BPH	O2D-CGD	4.43	1.44	1.33
7	M	603	BCL	MG-NA	4.41	2.16	2.06
5	C	612	HEM	C3C-C2C	-4.37	1.34	1.40
5	C	611	HEM	C3B-CAB	-4.31	1.39	1.47
13	H	708	PEF	O3-C30	4.29	1.45	1.33
7	M	603	BCL	O2D-CGD	4.28	1.43	1.33
5	C	610	HEM	C3C-C2C	-4.14	1.34	1.40
7	M	601	BCL	O2A-CGA	4.09	1.45	1.33
5	C	611	HEM	C3C-CAC	-4.07	1.39	1.47
11	M	608	MQ8	C32-C33	4.05	1.42	1.33
5	C	609	HEM	C3C-CAC	-4.04	1.39	1.47
5	C	609	HEM	C3C-C2C	-4.01	1.34	1.40
5	C	612	HEM	C3B-C2B	-3.99	1.34	1.40
12	M	613	CRT	C14-C12	3.97	1.41	1.35
5	C	612	HEM	C3C-CAC	-3.96	1.39	1.47
6	L	701	BGL	O2-C1'	3.95	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	602	BCL	MG-NA	3.93	2.15	2.06
5	C	609	HEM	C3B-CAB	-3.90	1.40	1.47
6	M	702	BGL	O2-C1'	3.86	1.53	1.43
7	L	604	BCL	MG-NA	3.83	2.15	2.06
8	L	606	BPH	O2D-CGD	3.82	1.42	1.33
7	M	601	BCL	MG-NA	3.82	2.15	2.06
7	M	601	BCL	O2D-CGD	3.77	1.42	1.33
12	M	613	CRT	C15-C16	3.71	1.44	1.34
6	L	704	BGL	O2-C1'	3.69	1.53	1.43
7	L	604	BCL	O2A-CGA	3.69	1.44	1.33
12	M	613	CRT	C31-C30	3.66	1.44	1.34
6	M	705	BGL	O2-C1'	3.64	1.53	1.43
6	M	705	BGL	C1-C2	3.60	1.55	1.52
6	M	706	BGL	O2-C1'	3.60	1.53	1.43
5	C	611	HEM	C3B-C2B	-3.59	1.35	1.40
6	L	704	BGL	C1-C2	3.49	1.55	1.52
6	L	703	BGL	O2-C1'	3.42	1.52	1.43
5	C	609	HEM	C4A-NA	3.41	1.43	1.36
5	C	609	HEM	C4B-NB	3.32	1.43	1.36
5	C	610	HEM	C3C-CAC	-3.30	1.41	1.47
8	L	606	BPH	O2A-CGA	3.30	1.43	1.33
12	M	613	CRT	C10-C11	3.28	1.43	1.34
12	M	613	CRT	C27-C28	3.27	1.40	1.35
8	M	605	BPH	O2A-CGA	3.23	1.42	1.33
7	L	602	BCL	O2A-CGA	3.19	1.42	1.33
7	M	603	BCL	O2A-CGA	3.09	1.42	1.33
13	H	708	PEF	P-O2P	3.06	1.69	1.55
12	M	613	CRT	C26-C25	3.05	1.42	1.34
6	L	701	BGL	C1-C2	3.05	1.55	1.52
7	L	604	BCL	O2D-CGD	2.99	1.40	1.33
7	L	604	BCL	C2A-C1A	-2.84	1.45	1.52
7	L	602	BCL	C3D-C2D	-2.78	1.34	1.39
8	L	606	BPH	C2A-C1A	-2.69	1.47	1.51
11	M	608	MQ8	C31-C32	-2.68	1.41	1.50
11	M	608	MQ8	C47-C48	2.67	1.40	1.32
5	C	611	HEM	C4D-C3D	2.64	1.48	1.42
5	C	609	HEM	C1A-NA	2.64	1.41	1.36
11	M	608	MQ8	C25-C23	2.64	1.56	1.51
8	M	605	BPH	C3D-C2D	-2.64	1.34	1.39
5	C	611	HEM	CBC-CAC	2.58	1.46	1.29
7	L	604	BCL	O2D-CED	-2.57	1.39	1.45
5	C	610	HEM	CBC-CAC	2.56	1.46	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	609	HEM	CBB-CAB	2.53	1.46	1.29
7	M	601	BCL	O2D-CED	-2.50	1.39	1.45
7	L	602	BCL	O2D-CED	-2.50	1.39	1.45
11	M	608	MQ8	C22-C23	2.50	1.39	1.33
8	L	606	BPH	O2D-CED	-2.49	1.39	1.45
7	M	603	BCL	C2-C3	2.48	1.38	1.33
5	C	612	HEM	CBC-CAC	2.47	1.45	1.29
7	M	601	BCL	C2C-C3C	-2.43	1.47	1.54
5	C	612	HEM	CBB-CAB	2.42	1.45	1.29
8	M	605	BPH	O2D-CED	-2.41	1.39	1.45
5	C	610	HEM	CBB-CAB	2.41	1.45	1.29
5	C	610	HEM	C1D-ND	-2.41	1.31	1.36
11	M	608	MQ8	C44-C43	2.38	1.56	1.51
5	C	611	HEM	C1D-ND	2.37	1.41	1.36
12	M	613	CRT	C4-C5	2.36	1.53	1.50
12	M	613	CRT	C25-C23	-2.33	1.40	1.45
7	L	602	BCL	O1D-CGD	2.31	1.27	1.21
8	L	606	BPH	CHC-C1C	2.31	1.41	1.36
5	C	609	HEM	CBC-CAC	2.31	1.44	1.29
11	M	608	MQ8	C11-C12	-2.30	1.47	1.50
7	M	601	BCL	C1B-NB	2.30	1.37	1.35
12	M	613	CRT	C32-C33	2.29	1.38	1.35
5	C	611	HEM	CBB-CAB	2.27	1.44	1.29
8	L	606	BPH	C4C-NC	2.26	1.42	1.37
11	M	608	MQ8	C17-C18	2.26	1.38	1.33
8	M	605	BPH	CHC-C1C	2.25	1.41	1.36
7	L	604	BCL	C3D-C2D	-2.17	1.35	1.39
12	M	613	CRT	C16-C17	-2.16	1.41	1.45
11	M	608	MQ8	C39-C38	-2.15	1.45	1.50
7	L	604	BCL	C1-C2	-2.14	1.42	1.49
7	M	601	BCL	C2A-C1A	-2.14	1.47	1.52
11	M	608	MQ8	C35-C33	2.14	1.55	1.51
8	L	606	BPH	C1-C2	-2.10	1.42	1.49
5	C	609	HEM	C1D-ND	2.10	1.40	1.36
7	M	601	BCL	C2-C3	2.08	1.38	1.33
5	C	611	HEM	C4A-NA	2.07	1.40	1.36
8	M	605	BPH	C4C-NC	2.05	1.41	1.37
13	H	708	PEF	P-O4P	2.05	1.67	1.59
8	M	605	BPH	C1C-NC	2.02	1.41	1.37
7	L	604	BCL	C3A-C2A	-2.01	1.48	1.54

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	604	BCL	C4A-NA-C1A	8.95	110.73	106.71
7	M	601	BCL	C4A-NA-C1A	8.67	110.61	106.71
11	M	608	MQ8	C34-C33-C35	8.53	129.63	115.27
7	L	602	BCL	C4A-NA-C1A	8.45	110.50	106.71
11	M	608	MQ8	C11-C3-C4	-8.11	109.82	118.50
11	M	608	MQ8	C35-C33-C32	-7.74	105.46	121.12
11	M	608	MQ8	C41-C40-C38	7.29	136.95	112.98
7	M	603	BCL	C4A-NA-C1A	7.14	109.92	106.71
11	M	608	MQ8	C39-C38-C40	6.94	126.94	115.27
8	M	605	BPH	CAC-C3C-C2C	6.81	131.28	114.26
8	L	606	BPH	O2D-CGD-CBD	6.60	122.99	111.27
6	M	706	BGL	C6-C5-C4	6.58	128.42	113.00
6	L	704	BGL	C6-C5-C4	6.46	128.13	113.00
6	M	702	BGL	C6-C5-C4	6.35	127.87	113.00
6	M	705	BGL	C6-C5-C4	6.31	127.78	113.00
7	M	601	BCL	O2D-CGD-CBD	6.13	122.17	111.27
11	M	608	MQ8	C31-C30-C28	5.99	132.68	112.98
7	M	603	BCL	O2D-CGD-CBD	5.96	121.87	111.27
7	L	604	BCL	O2D-CGD-CBD	5.87	121.70	111.27
6	L	703	BGL	C6-C5-C4	5.87	126.75	113.00
7	M	603	BCL	C1C-NC-C4C	5.84	109.33	106.71
8	M	605	BPH	C2C-C3C-C4C	5.81	110.04	101.34
7	M	601	BCL	C1C-NC-C4C	5.54	109.19	106.71
6	L	701	BGL	C6-C5-C4	5.47	125.82	113.00
12	M	613	CRT	C36-C35-C33	-5.47	117.63	125.89
7	L	602	BCL	C1C-NC-C4C	5.35	109.11	106.71
8	L	606	BPH	CAC-C3C-C2C	5.34	127.60	114.26
12	M	613	CRT	C5-C6-C7	-5.32	117.85	125.89
8	M	605	BPH	C7-C6-C5	-5.18	99.30	113.36
11	M	608	MQ8	C30-C31-C32	5.07	128.53	111.88
7	L	604	BCL	C1C-NC-C4C	4.90	108.91	106.71
6	M	702	BGL	O5-C5-C4	-4.78	101.01	109.69
8	L	606	BPH	O1D-CGD-CBD	-4.60	115.06	124.48
6	L	704	BGL	O5-C5-C4	-4.58	101.37	109.69
8	M	605	BPH	O2D-CGD-CBD	4.50	119.26	111.27
7	L	604	BCL	C4B-C3B-CAB	-4.48	118.48	127.13
7	M	601	BCL	C4B-C3B-CAB	-4.44	118.56	127.13
7	M	601	BCL	O1D-CGD-CBD	-4.34	115.61	124.48
8	L	606	BPH	C2C-C3C-C4C	4.33	107.83	101.34
7	M	601	BCL	CAC-C3C-C2C	4.32	125.05	114.26
13	H	708	PEF	O3-C30-C31	4.30	125.39	111.91
7	L	604	BCL	CAC-C3C-C4C	-4.29	103.07	112.58
11	M	608	MQ8	O1-C1-C10	-4.28	114.64	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	602	BCL	C4B-C3B-CAB	-4.26	118.91	127.13
8	M	605	BPH	OBD-CAD-CBD	-4.25	119.82	125.89
7	M	601	BCL	OBD-CAD-CBD	-4.21	119.88	125.89
8	L	606	BPH	OBD-CAD-CBD	-4.15	119.96	125.89
7	L	602	BCL	CED-O2D-CGD	4.13	125.28	115.94
7	L	604	BCL	CHD-C4C-NC	-4.13	120.49	125.08
7	M	603	BCL	O1D-CGD-CBD	-4.09	116.12	124.48
7	L	602	BCL	O2A-CGA-CBA	4.09	124.74	111.91
7	M	603	BCL	C4B-C3B-CAB	-4.05	119.31	127.13
7	M	603	BCL	CHD-C4C-NC	-4.03	120.60	125.08
7	M	603	BCL	OBD-CAD-CBD	-3.98	120.21	125.89
7	L	602	BCL	O2D-CGD-CBD	3.98	118.33	111.27
13	H	708	PEF	O3-C30-O5	-3.97	113.56	123.59
13	H	708	PEF	O3-C3-C2	3.96	119.95	108.43
7	L	604	BCL	O1D-CGD-CBD	-3.85	116.61	124.48
7	M	601	BCL	O2A-CGA-CBA	3.79	123.82	111.91
7	M	603	BCL	OBB-CAB-C3B	3.67	126.51	119.99
7	M	603	BCL	C3C-C2C-C1C	3.67	107.79	101.87
6	L	704	BGL	O6-C6-C5	3.66	123.85	111.29
7	L	604	BCL	OBB-CAB-C3B	3.65	126.48	119.99
6	L	703	BGL	O5-C5-C4	-3.61	103.14	109.69
6	M	702	BGL	C1-O5-C5	-3.61	106.86	113.66
11	M	608	MQ8	C40-C38-C37	-3.58	113.87	121.12
7	M	603	BCL	O2A-CGA-CBA	3.57	123.12	111.91
6	M	702	BGL	O6-C6-C5	3.54	123.45	111.29
7	L	602	BCL	OBD-CAD-CBD	-3.51	120.88	125.89
8	M	605	BPH	O1D-CGD-CBD	-3.47	117.38	124.48
7	L	602	BCL	OBB-CAB-C3B	3.44	126.09	119.99
7	M	601	BCL	OBB-CAB-C3B	3.43	126.07	119.99
6	M	706	BGL	O5-C5-C4	-3.41	103.50	109.69
11	M	608	MQ8	C2M-C2-C1	-3.40	110.63	116.27
6	L	701	BGL	O6-C6-C5	3.40	122.96	111.29
11	M	608	MQ8	C21-C22-C23	-3.39	119.49	127.66
11	M	608	MQ8	C36-C35-C33	3.36	124.03	112.98
7	L	602	BCL	CHD-C4C-NC	-3.35	121.35	125.08
13	H	708	PEF	C2-O2-C10	3.34	126.00	117.79
6	L	704	BGL	O4-C4-C3	3.33	118.05	110.35
11	M	608	MQ8	O1-C1-C2	3.32	124.56	120.25
13	H	708	PEF	O2-C10-C11	3.29	118.59	111.50
6	L	704	BGL	C4-C3-C2	-3.28	102.18	109.68
6	M	702	BGL	C3-C4-C5	-3.27	104.41	110.24
8	L	606	BPH	C9-C8-C7	3.26	123.08	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	702	BGL	O4-C4-C3	3.26	117.88	110.35
7	L	604	BCL	C3C-C2C-C1C	3.24	107.11	101.87
7	M	601	BCL	CHD-C4C-NC	-3.23	121.48	125.08
8	L	606	BPH	O2A-CGA-CBA	3.23	122.05	111.91
6	L	703	BGL	O6-C6-C5	3.23	122.38	111.29
6	M	705	BGL	O5-C5-C4	-3.21	103.87	109.69
11	M	608	MQ8	C31-C32-C33	-3.21	119.94	127.66
11	M	608	MQ8	C19-C18-C20	3.20	120.66	115.27
11	M	608	MQ8	C44-C46-C47	3.19	122.37	111.88
7	M	601	BCL	C4D-C3D-CAD	-3.18	106.70	108.47
7	L	604	BCL	OBD-CAD-CBD	-3.14	121.42	125.89
6	L	704	BGL	C1-O5-C5	-3.12	107.77	113.66
6	M	706	BGL	C1-O5-C5	-3.12	107.78	113.66
8	L	606	BPH	C4D-CHA-C1A	-3.11	122.83	130.51
6	M	705	BGL	O6-C6-C5	3.11	121.96	111.29
8	M	605	BPH	O2A-CGA-CBA	3.10	121.65	111.91
7	M	601	BCL	C12-C11-C10	-3.10	98.99	113.24
7	M	601	BCL	C2C-C3C-C4C	3.08	105.95	101.34
7	L	602	BCL	O1D-CGD-CBD	-3.07	118.21	124.48
8	L	606	BPH	OBB-CAB-C3B	3.06	126.07	120.41
6	M	705	BGL	C1-O5-C5	-3.05	107.90	113.66
6	L	703	BGL	C1-O5-C5	-3.05	107.91	113.66
7	M	603	BCL	CED-O2D-CGD	3.03	122.80	115.94
7	L	602	BCL	O2A-CGA-O1A	-3.03	115.95	123.59
7	L	604	BCL	C6-C5-C3	-3.03	105.52	113.45
11	M	608	MQ8	C20-C18-C17	-3.03	114.99	121.12
6	L	704	BGL	C3-C4-C5	-3.02	104.85	110.24
8	M	605	BPH	O2A-CGA-O1A	-3.00	116.02	123.59
7	M	601	BCL	CED-O2D-CGD	3.00	122.72	115.94
7	M	601	BCL	O2A-CGA-O1A	-2.99	116.06	123.59
8	M	605	BPH	C1-C2-C3	2.95	131.14	126.04
7	M	603	BCL	C4D-C3D-CAD	-2.94	106.83	108.47
7	L	604	BCL	O2A-CGA-CBA	2.91	121.03	111.91
8	L	606	BPH	CED-O2D-CGD	2.89	122.48	115.94
11	M	608	MQ8	C9-C10-C5	2.88	122.47	119.26
8	M	605	BPH	CED-O2D-CGD	2.88	122.45	115.94
7	L	602	BCL	C1-C2-C3	2.88	131.02	126.04
7	M	601	BCL	CAA-C2A-C1A	-2.85	102.64	111.97
6	L	701	BGL	O5-C5-C4	-2.83	104.55	109.69
8	M	605	BPH	OBB-CAB-C3B	2.77	125.54	120.41
8	L	606	BPH	O2A-CGA-O1A	-2.77	116.61	123.59
7	L	604	BCL	C4D-C3D-CAD	-2.76	106.93	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	604	BCL	CAA-C2A-C1A	-2.75	102.96	111.97
6	M	706	BGL	O6-C6-C5	2.75	120.71	111.29
11	M	608	MQ8	C40-C41-C42	-2.74	102.86	111.88
6	L	701	BGL	O4-C4-C3	2.74	116.67	110.35
7	L	604	BCL	C2A-C1A-CHA	2.74	128.64	123.86
7	L	604	BCL	C3A-C2A-C1A	2.71	105.39	101.34
6	L	704	BGL	O3-C3-C2	2.70	117.10	109.94
7	M	603	BCL	C1-C2-C3	2.70	130.71	126.04
7	L	604	BCL	C1-C2-C3	2.70	130.71	126.04
7	M	603	BCL	CMB-C2B-C1B	-2.69	124.33	128.46
7	M	603	BCL	O2A-CGA-O1A	-2.69	116.80	123.59
8	M	605	BPH	CBC-CAC-C3C	2.68	119.43	113.47
7	M	601	BCL	OBD-CAD-C3D	2.67	132.42	127.98
6	M	706	BGL	C3-C4-C5	-2.66	105.49	110.24
6	M	702	BGL	C4-C3-C2	-2.66	103.62	109.68
8	L	606	BPH	CBC-CAC-C3C	2.64	119.35	113.47
7	L	604	BCL	CED-O2D-CGD	2.64	121.91	115.94
6	L	703	BGL	O4-C4-C3	2.63	116.44	110.35
7	L	604	BCL	CMB-C2B-C1B	-2.61	124.45	128.46
8	L	606	BPH	C11-C10-C8	-2.61	107.48	115.92
7	L	602	BCL	C3C-C2C-C1C	2.60	106.08	101.87
8	M	605	BPH	C4D-CHA-C1A	-2.58	124.15	130.51
7	L	604	BCL	O2A-CGA-O1A	-2.57	117.11	123.59
7	M	603	BCL	OBD-CAD-C3D	2.57	132.24	127.98
7	M	601	BCL	C1-C2-C3	2.54	130.43	126.04
7	M	601	BCL	C3C-C2C-C1C	2.53	105.95	101.87
11	M	608	MQ8	C5-C10-C1	-2.51	117.96	120.68
8	M	605	BPH	OBD-CAD-C3D	2.50	132.13	127.98
6	M	702	BGL	O3-C3-C2	2.50	116.56	109.94
7	M	601	BCL	CMC-C2C-C3C	-2.47	103.88	113.83
8	M	605	BPH	C4D-C3D-CAD	-2.45	106.32	107.87
7	L	602	BCL	OBD-CAD-C3D	2.45	132.05	127.98
8	L	606	BPH	C17-C16-C15	-2.45	101.98	113.24
8	L	606	BPH	C4D-C3D-CAD	-2.44	106.32	107.87
8	L	606	BPH	C4A-NA-C1A	2.44	110.11	108.14
8	L	606	BPH	C1-C2-C3	2.42	130.24	126.04
8	L	606	BPH	CBB-CAB-C3B	-2.42	115.25	120.43
7	M	603	BCL	CGD-CBD-CAD	-2.40	102.95	110.73
12	M	613	CRT	C29-C28-C30	2.39	121.85	118.08
13	H	708	PEF	C3-C2-C1	-2.39	106.13	111.79
8	L	606	BPH	C3A-C4A-NA	-2.39	108.97	113.05
8	M	605	BPH	C4A-NA-C1A	2.39	110.07	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	605	BPH	C11-C12-C13	-2.38	108.21	115.92
7	M	601	BCL	CMB-C2B-C1B	-2.38	124.80	128.46
7	M	603	BCL	C2A-C3A-C4A	2.37	105.69	101.87
8	M	605	BPH	CBB-CAB-C3B	-2.36	115.40	120.43
6	L	701	BGL	C1-O5-C5	-2.36	109.22	113.66
7	L	604	BCL	C11-C10-C8	-2.35	108.33	115.92
7	M	603	BCL	C4-C3-C5	-2.34	111.33	115.27
5	C	610	HEM	CMD-C2D-C1D	-2.33	124.88	128.46
8	L	606	BPH	C4-C3-C5	-2.32	111.37	115.27
7	L	602	BCL	C4B-CHC-C1C	-2.31	125.54	130.12
6	L	703	BGL	C3-C4-C5	-2.30	106.13	110.24
6	M	705	BGL	C3-C4-C5	-2.30	106.14	110.24
7	M	603	BCL	C4B-CHC-C1C	-2.28	125.61	130.12
8	L	606	BPH	OBD-CAD-C3D	2.27	131.75	127.98
6	M	706	BGL	O4-C4-C3	2.26	115.58	110.35
6	L	701	BGL	O3-C3-C2	2.25	115.90	109.94
7	M	601	BCL	CMC-C2C-C1C	-2.25	105.74	111.77
12	M	613	CRT	C29-C28-C27	-2.22	119.81	122.92
7	M	601	BCL	C4B-CHC-C1C	-2.21	125.75	130.12
8	L	606	BPH	C3A-C2A-C1A	2.21	104.28	101.64
7	L	602	BCL	C1D-CHD-C4C	2.20	129.13	125.88
7	L	602	BCL	CMB-C2B-C1B	-2.20	125.08	128.46
8	L	606	BPH	CAB-C3B-C2B	2.19	134.82	127.18
7	M	601	BCL	C2A-C1A-CHA	2.17	127.65	123.86
7	M	603	BCL	CMC-C2C-C1C	-2.16	105.96	111.77
6	L	701	BGL	C3-C4-C5	-2.15	106.40	110.24
7	M	603	BCL	C9-C8-C10	-2.14	103.53	111.29
7	L	602	BCL	C7-C6-C5	-2.14	107.54	113.36
7	L	602	BCL	C2A-C1A-CHA	2.14	127.61	123.86
8	L	606	BPH	C7-C6-C5	-2.14	107.55	113.36
7	L	604	BCL	C4B-CHC-C1C	-2.11	125.95	130.12
6	M	705	BGL	O3-C3-C2	2.11	115.52	109.94
7	L	604	BCL	C1D-CHD-C4C	2.10	128.98	125.88
8	L	606	BPH	CHD-C4C-NC	-2.09	122.72	125.20
7	L	604	BCL	C10-C8-C7	2.09	123.11	112.13
7	L	604	BCL	CMC-C2C-C1C	-2.09	106.17	111.77
7	M	601	BCL	CHB-C4A-NA	2.08	127.39	124.51
7	L	602	BCL	C3A-C2A-C1A	2.05	104.41	101.34
7	M	603	BCL	CMC-C2C-C3C	-2.05	105.56	113.83
7	L	604	BCL	CMB-C2B-C3B	2.04	128.50	124.68
11	M	608	MQ8	C2M-C2-C3	2.04	127.72	124.40
7	L	602	BCL	C9-C8-C7	2.01	118.58	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	703	BGL	O3-C3-C2	2.01	115.26	109.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C8

All (178) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	604	BCL	C2C-C3C-CAC-CBC
7	L	604	BCL	C4C-C3C-CAC-CBC
6	M	705	BGL	C2'-C1'-O2-C2
8	L	606	BPH	C4C-C3C-CAC-CBC
8	L	606	BPH	C2C-C3C-CAC-CBC
8	L	606	BPH	C4B-C3B-CAB-CBB
8	L	606	BPH	O2A-C1-C2-C3
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
5	C	610	HEM	C3D-CAD-CBD-CGD
6	L	703	BGL	C2'-C1'-O2-C2
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
7	L	602	BCL	C2C-C3C-CAC-CBC
7	L	602	BCL	C4C-C3C-CAC-CBC
8	M	605	BPH	C4C-C3C-CAC-CBC
8	M	605	BPH	C4B-C3B-CAB-CBB
8	M	605	BPH	C4B-C3B-CAB-OBB
8	M	605	BPH	C2B-C3B-CAB-CBB
8	M	605	BPH	C2B-C3B-CAB-OBB
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	601	BCL	C3A-C2A-CAA-CBA
7	M	601	BCL	C2C-C3C-CAC-CBC
7	M	601	BCL	C4C-C3C-CAC-CBC
7	M	601	BCL	C4-C3-C5-C6
13	H	708	PEF	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
13	H	708	PEF	C31-C30-O3-C3
11	M	608	MQ8	C46-C47-C48-C49
7	L	602	BCL	C2A-CAA-CBA-CGA
7	L	604	BCL	C3-C5-C6-C7
6	L	701	BGL	O5-C5-C6-O6
8	M	605	BPH	CBA-CGA-O2A-C1
13	H	708	PEF	C32-C33-C34-C35
6	M	706	BGL	O5-C5-C6-O6
8	M	605	BPH	O1A-CGA-O2A-C1
11	M	608	MQ8	C46-C47-C48-C50
7	M	601	BCL	C2-C3-C5-C6
11	M	608	MQ8	C33-C35-C36-C37
6	L	701	BGL	C4-C5-C6-O6
6	M	706	BGL	C4-C5-C6-O6
7	L	604	BCL	C6-C7-C8-C9
8	L	606	BPH	C6-C7-C8-C9
7	L	602	BCL	C6-C7-C8-C9
7	M	601	BCL	C6-C7-C8-C9
12	M	613	CRT	C5-C6-C7-C8
8	M	605	BPH	C10-C11-C12-C13
8	L	606	BPH	C15-C16-C17-C18
7	M	601	BCL	C8-C10-C11-C12
7	M	601	BCL	C10-C11-C12-C13
7	L	602	BCL	C15-C16-C17-C18
6	L	704	BGL	O2-C1'-C2'-C3'
7	M	601	BCL	C15-C16-C17-C18
6	M	702	BGL	C4-C5-C6-O6
11	M	608	MQ8	C43-C44-C46-C47
13	H	708	PEF	C19-C20-C21-C22
7	M	601	BCL	CBD-CGD-O2D-CED
8	L	606	BPH	C8-C10-C11-C12
8	M	605	BPH	C5-C6-C7-C8
13	H	708	PEF	C14-C15-C16-C17
13	H	708	PEF	C31-C32-C33-C34
6	L	701	BGL	C3'-C4'-C5'-C6'
11	M	608	MQ8	C39-C38-C40-C41
9	L	707	LDA	C11-C10-C9-C8
13	H	708	PEF	C20-C21-C22-C23
13	H	708	PEF	C34-C35-C36-C37
13	H	708	PEF	C17-C18-C19-C20
6	M	705	BGL	C4'-C5'-C6'-C7'
6	M	706	BGL	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
6	M	705	BGL	C3'-C4'-C5'-C6'
7	M	601	BCL	CBA-CGA-O2A-C1
6	M	702	BGL	C2'-C3'-C4'-C5'
7	M	601	BCL	O1A-CGA-O2A-C1
13	H	708	PEF	C1-C2-C3-O3
6	L	703	BGL	C3'-C4'-C5'-C6'
6	M	706	BGL	C1'-C2'-C3'-C4'
11	M	608	MQ8	C37-C38-C40-C41
8	M	605	BPH	C11-C10-C8-C7
7	M	601	BCL	C12-C13-C15-C16
8	M	605	BPH	C15-C16-C17-C18
13	H	708	PEF	C21-C22-C23-C24
13	H	708	PEF	O3P-C1-C2-O2
8	L	606	BPH	C2-C3-C5-C6
8	L	606	BPH	C14-C13-C15-C16
7	L	602	BCL	C11-C10-C8-C9
8	M	605	BPH	C11-C10-C8-C9
7	M	601	BCL	C1A-C2A-CAA-CBA
8	L	606	BPH	C13-C15-C16-C17
8	L	606	BPH	C4-C3-C5-C6
6	L	701	BGL	O2-C1'-C2'-C3'
6	L	704	BGL	O5-C5-C6-O6
6	M	705	BGL	O5-C5-C6-O6
7	M	603	BCL	C13-C15-C16-C17
9	L	707	LDA	C2-C3-C4-C5
6	M	702	BGL	C5'-C6'-C7'-C8'
7	L	604	BCL	C13-C15-C16-C17
8	L	606	BPH	C2B-C3B-CAB-CBB
7	L	604	BCL	C15-C16-C17-C18
7	L	602	BCL	C13-C15-C16-C17
7	M	601	BCL	C13-C15-C16-C17
6	M	702	BGL	C4'-C5'-C6'-C7'
6	L	703	BGL	C4-C5-C6-O6
6	M	702	BGL	O2-C1'-C2'-C3'
13	H	708	PEF	C39-C40-C41-C42
8	L	606	BPH	C11-C12-C13-C15
8	L	606	BPH	C12-C13-C15-C16
7	M	601	BCL	C6-C7-C8-C10
8	L	606	BPH	C11-C12-C13-C14
7	M	601	BCL	C14-C13-C15-C16
9	L	707	LDA	N1-C1-C2-C3
13	H	708	PEF	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	M	608	MQ8	C32-C33-C35-C36
6	M	706	BGL	C4'-C5'-C6'-C7'
7	M	601	BCL	O1D-CGD-O2D-CED
6	L	703	BGL	O2-C1'-C2'-C3'
9	L	707	LDA	C9-C10-C11-C12
6	M	702	BGL	C1'-C2'-C3'-C4'
13	H	708	PEF	C22-C23-C24-C25
7	M	601	BCL	C2-C1-O2A-CGA
8	L	606	BPH	C11-C10-C8-C9
7	L	602	BCL	C14-C13-C15-C16
7	M	601	BCL	C11-C10-C8-C9
7	M	601	BCL	C5-C6-C7-C8
6	M	702	BGL	O5-C5-C6-O6
6	L	704	BGL	C5'-C6'-C7'-C8'
7	L	604	BCL	C11-C10-C8-C7
11	M	608	MQ8	C22-C23-C25-C26
7	L	602	BCL	C12-C13-C15-C16
7	M	601	BCL	C11-C10-C8-C7
8	L	606	BPH	C4B-C3B-CAB-OBB
7	M	603	BCL	CHA-CBD-CGD-O1D
7	M	603	BCL	CHA-CBD-CGD-O2D
13	H	708	PEF	C11-C12-C13-C14
6	L	703	BGL	C5'-C6'-C7'-C8'
11	M	608	MQ8	C24-C23-C25-C26
13	H	708	PEF	C33-C34-C35-C36
6	L	701	BGL	C4'-C5'-C6'-C7'
7	L	604	BCL	C6-C7-C8-C10
8	M	605	BPH	C11-C12-C13-C15
6	L	704	BGL	C3'-C4'-C5'-C6'
13	H	708	PEF	O2-C2-C3-O3
13	H	708	PEF	C15-C16-C17-C18
8	L	606	BPH	C2B-C3B-CAB-OBB
7	L	602	BCL	C2-C1-O2A-CGA
8	L	606	BPH	C11-C10-C8-C7
6	L	701	BGL	C2'-C1'-O2-C2
13	H	708	PEF	C40-C41-C42-C43
13	H	708	PEF	C12-C13-C14-C15
6	L	704	BGL	C2'-C3'-C4'-C5'
13	H	708	PEF	C13-C14-C15-C16
12	M	613	CRT	C5-C6-C7-C9
13	H	708	PEF	C3-C2-O2-C10
13	H	708	PEF	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
13	H	708	PEF	C16-C17-C18-C19
7	M	603	BCL	CAA-CBA-CGA-O2A
8	L	606	BPH	CAD-CBD-CGD-O2D
13	H	708	PEF	C1-C2-O2-C10
7	M	603	BCL	CAD-CBD-CGD-O2D
7	M	601	BCL	CAD-CBD-CGD-O2D
13	H	708	PEF	C38-C39-C40-C41
6	L	703	BGL	O5-C5-C6-O6
6	L	701	BGL	C1-C2-O2-C1'
8	M	605	BPH	C11-C12-C13-C14
7	M	603	BCL	C11-C10-C8-C9
11	M	608	MQ8	C25-C26-C27-C28
13	H	708	PEF	O2-C10-C11-C12
8	L	606	BPH	C1A-C2A-CAA-CBA
6	M	702	BGL	C2'-C1'-O2-C2
13	H	708	PEF	C4-O4P-P-O1P
13	H	708	PEF	C5-C4-O4P-P
12	M	613	CRT	C35-C36-C37-C38
7	M	603	BCL	C11-C10-C8-C7
13	H	708	PEF	O4-C10-C11-C12

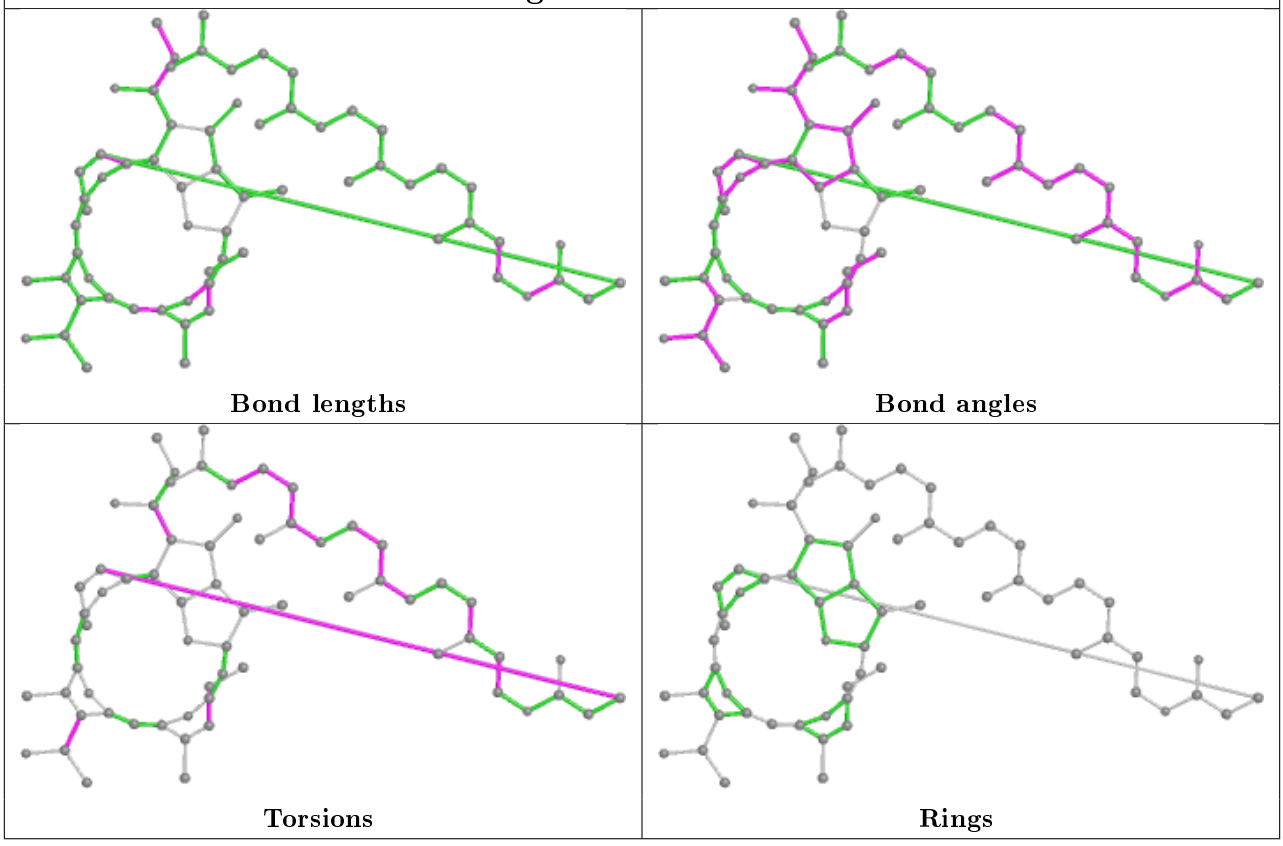
There are no ring outliers.

17 monomers are involved in 65 short contacts:

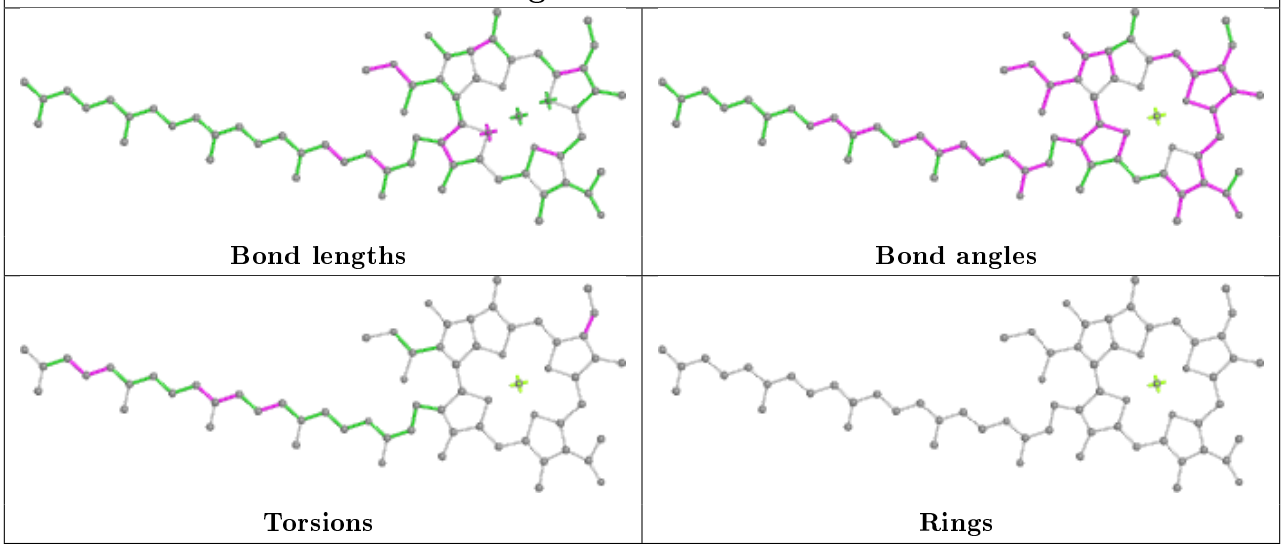
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	606	BPH	6	0
7	L	604	BCL	10	0
9	L	707	LDA	2	0
6	M	702	BGL	1	0
5	C	609	HEM	1	0
12	M	613	CRT	2	0
11	M	608	MQ8	1	0
6	L	704	BGL	3	0
5	C	612	HEM	2	0
6	L	703	BGL	4	0
5	C	610	HEM	2	0
7	L	602	BCL	7	0
6	L	701	BGL	3	0
8	M	605	BPH	4	0
7	M	603	BCL	6	0
7	M	601	BCL	10	0
13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

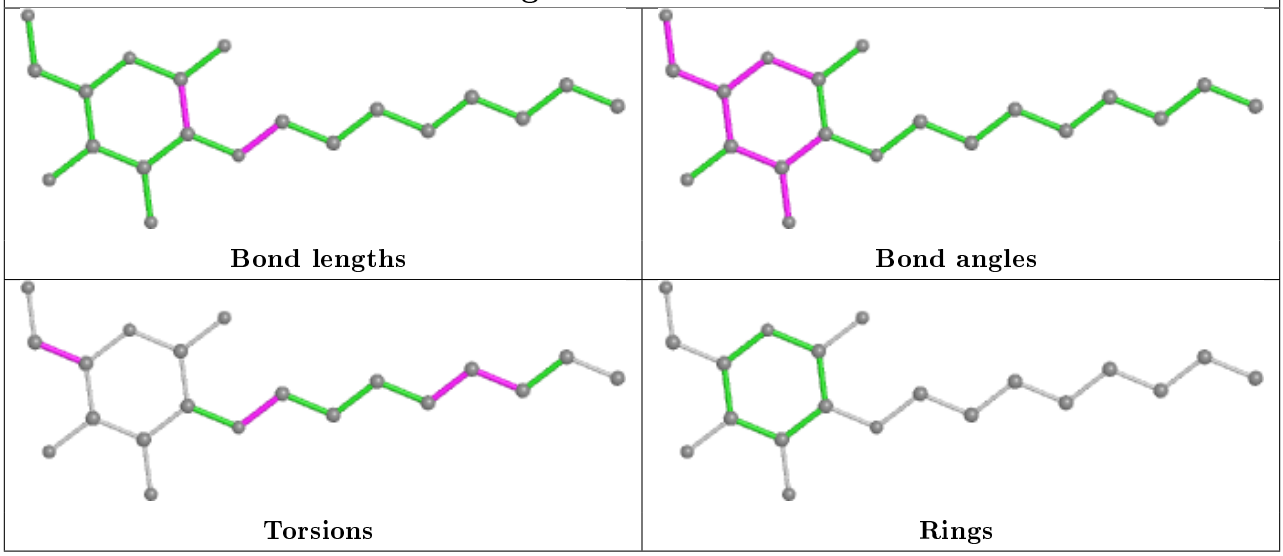
Ligand BPH L 606



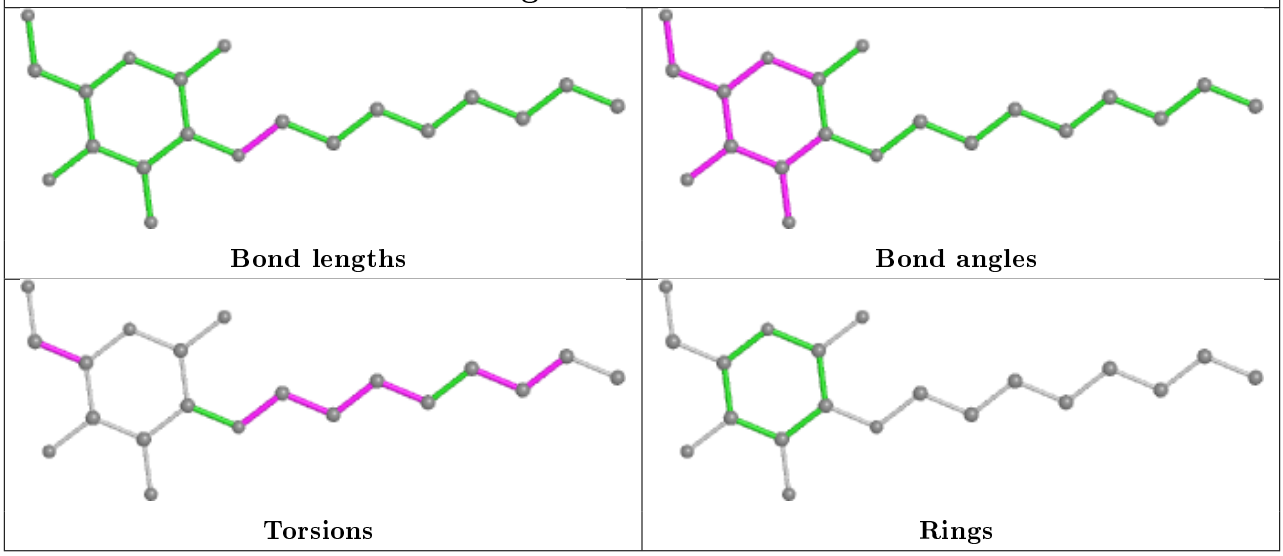
Ligand BCL L 604



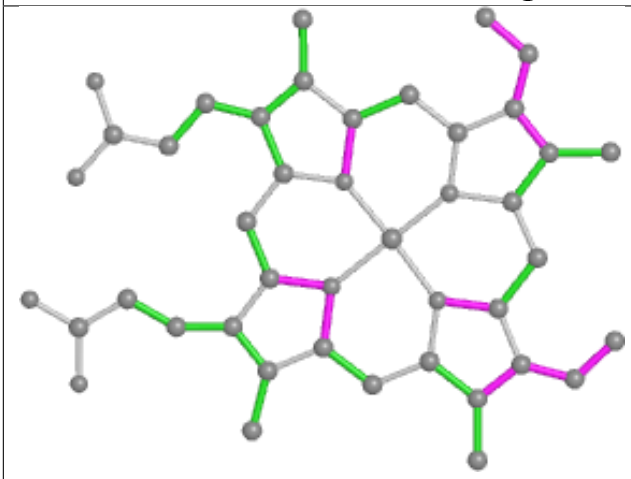
Ligand BGL M 705



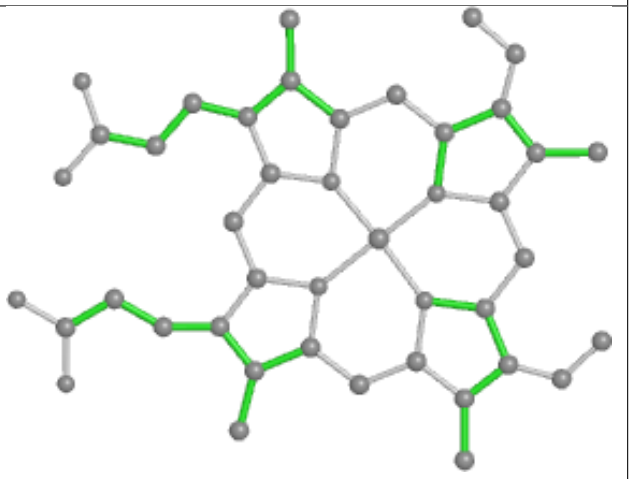
Ligand BGL M 702



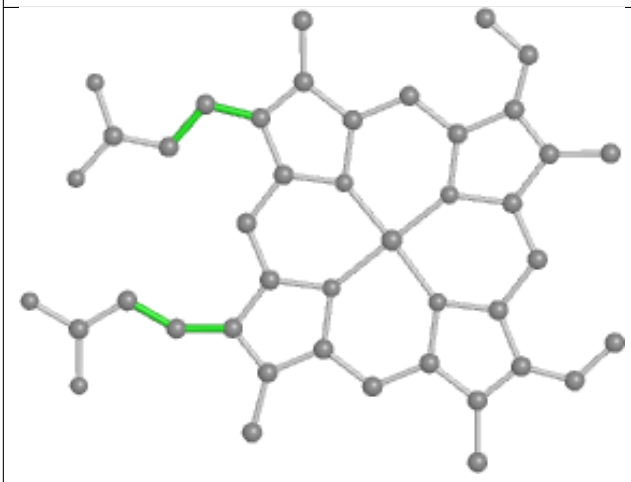
Ligand HEM C 609



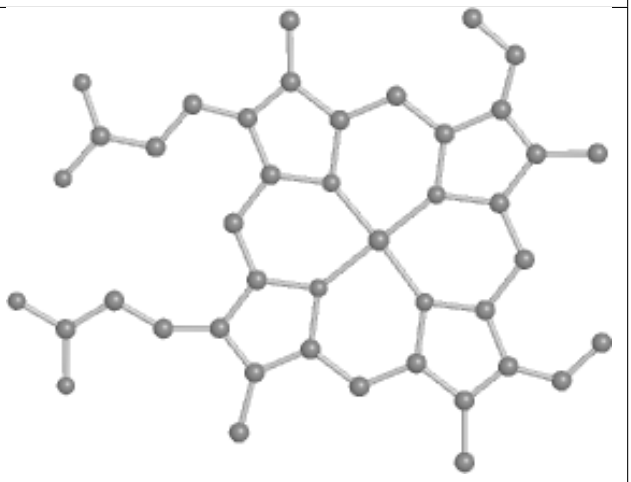
Bond lengths



Bond angles

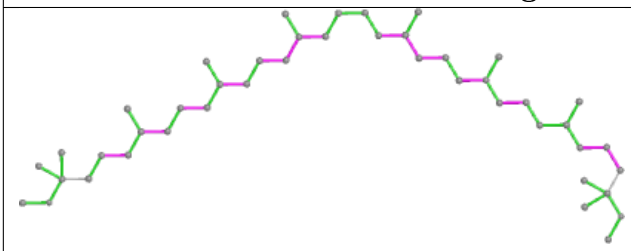


Torsions

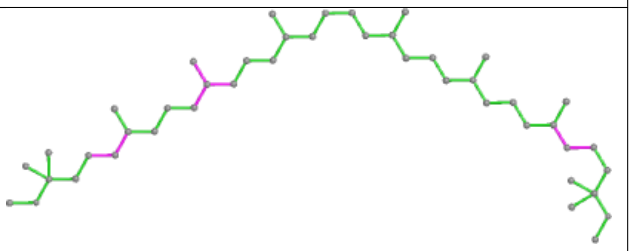


Rings

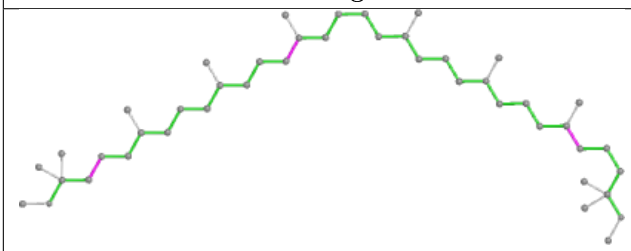
Ligand CRT M 613



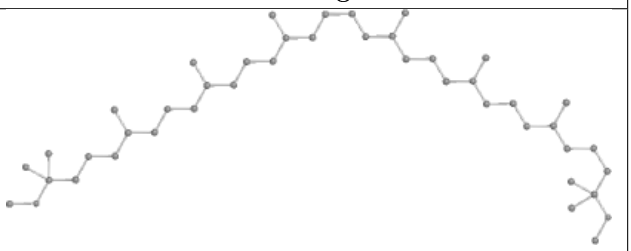
Bond lengths



Bond angles

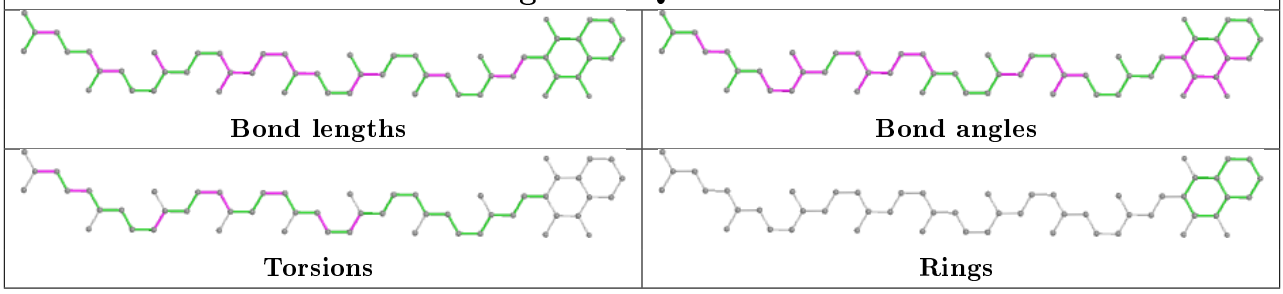


Torsions

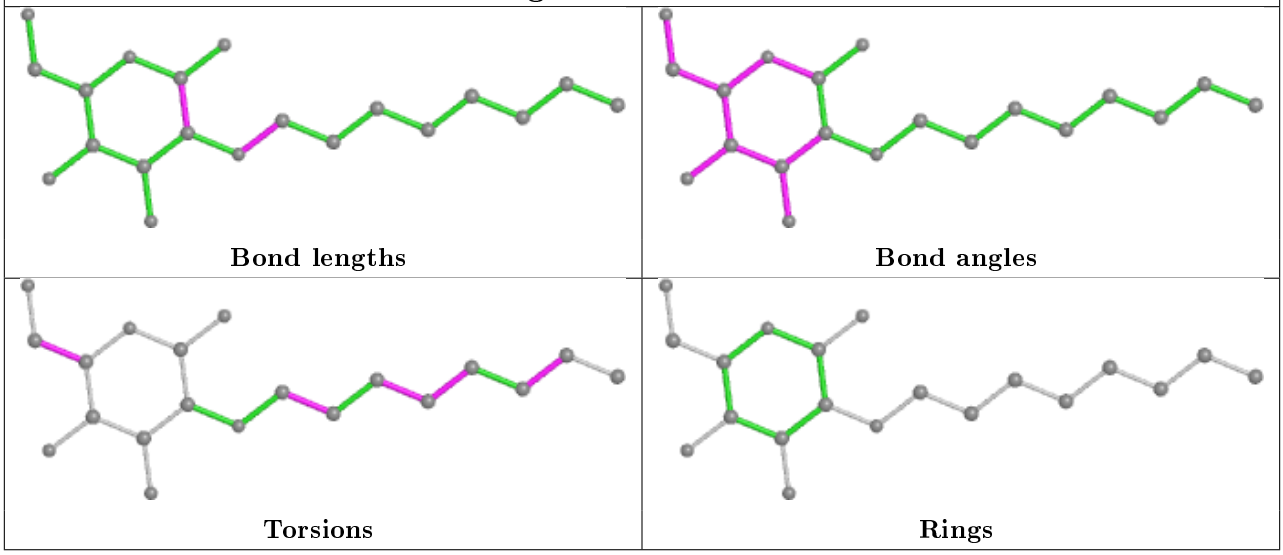


Rings

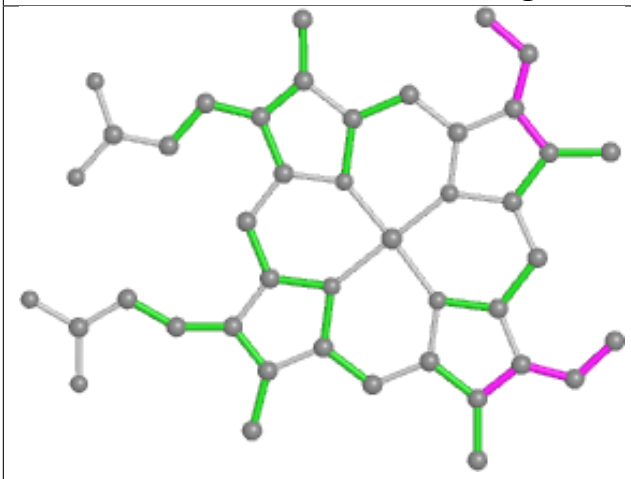
Ligand MQ8 M 608



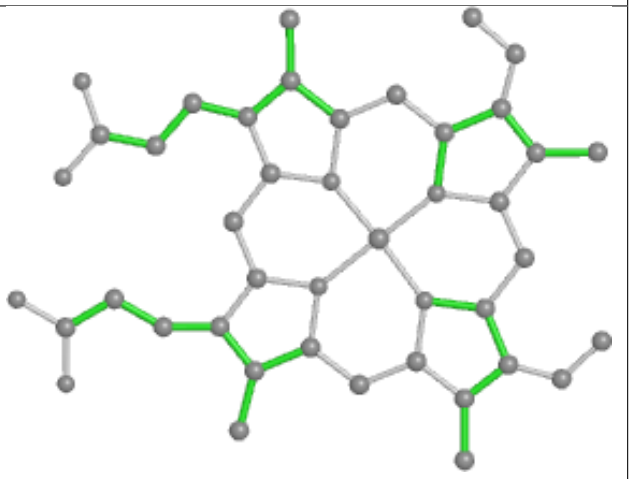
Ligand BGL L 704



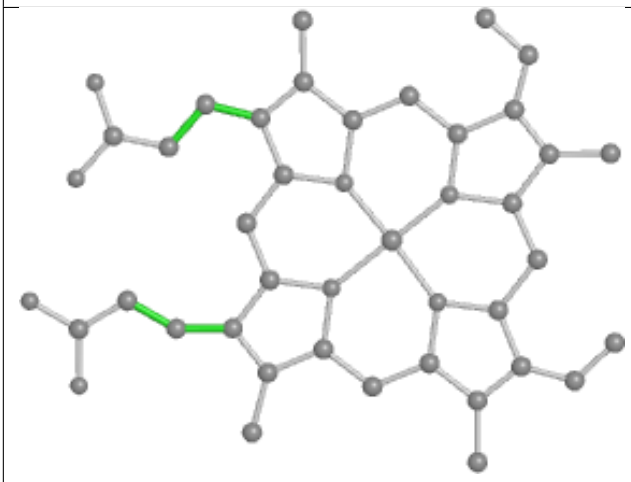
Ligand HEM C 612



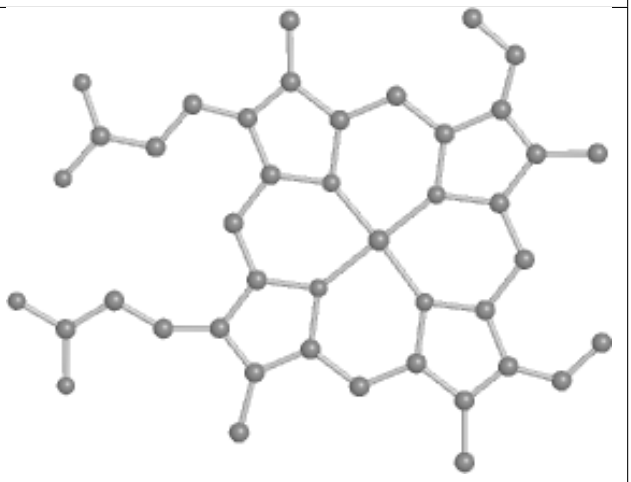
Bond lengths



Bond angles

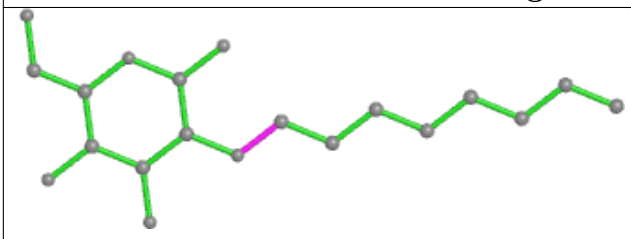


Torsions

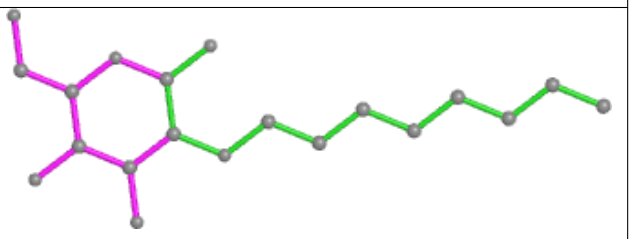


Rings

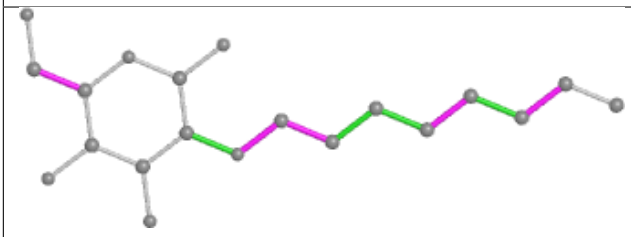
Ligand BGL L 703



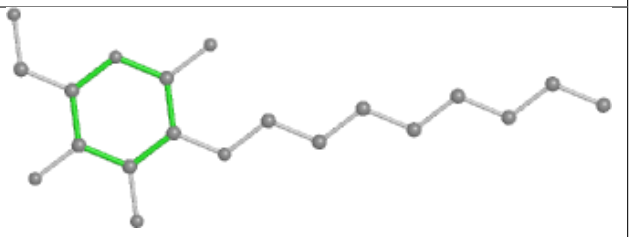
Bond lengths



Bond angles

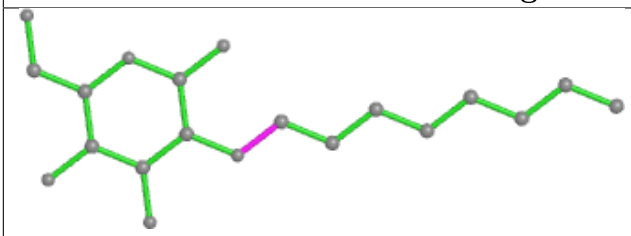


Torsions

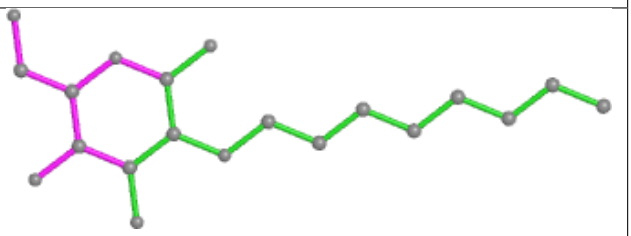


Rings

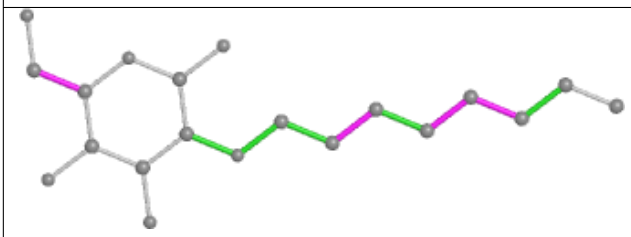
Ligand BGL M 706



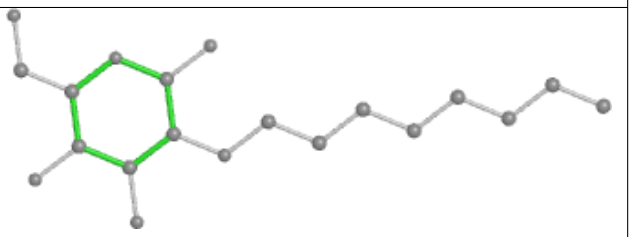
Bond lengths



Bond angles

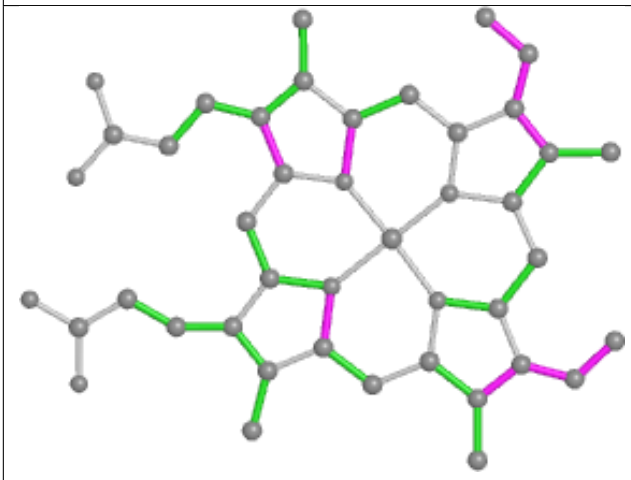


Torsions

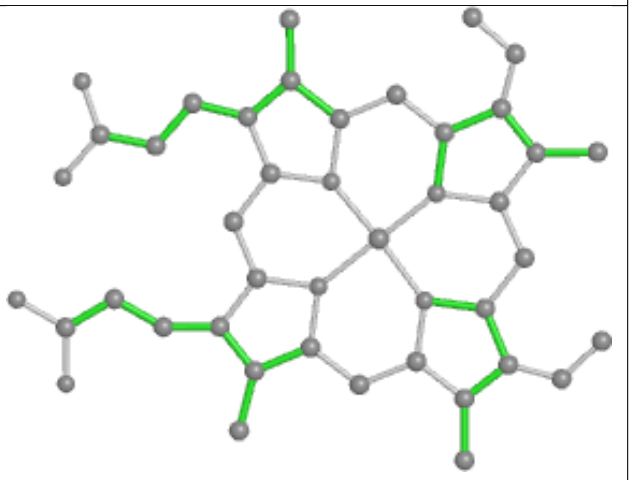


Rings

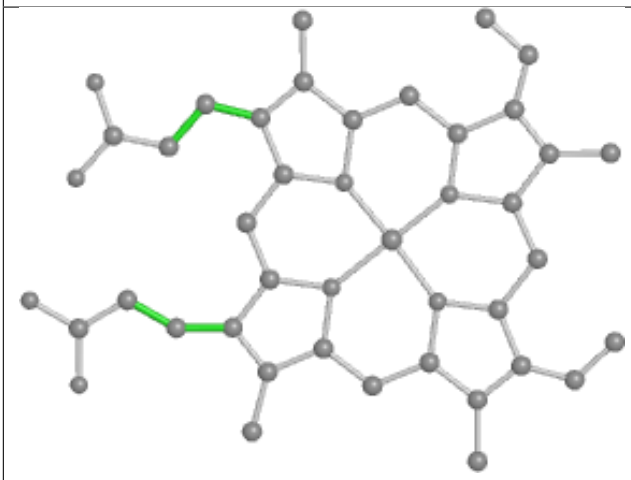
Ligand HEM C 611



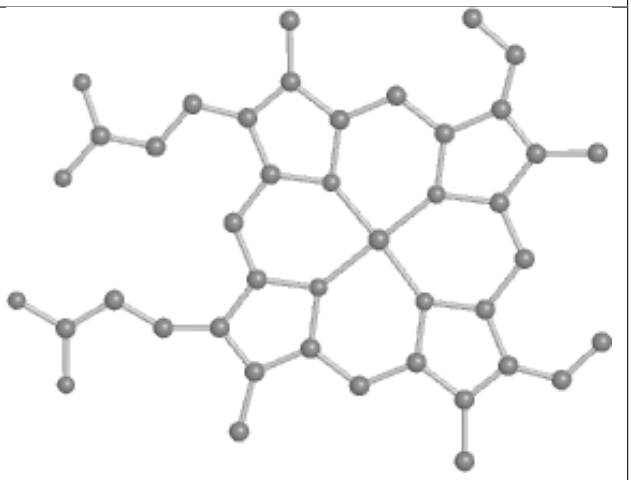
Bond lengths



Bond angles

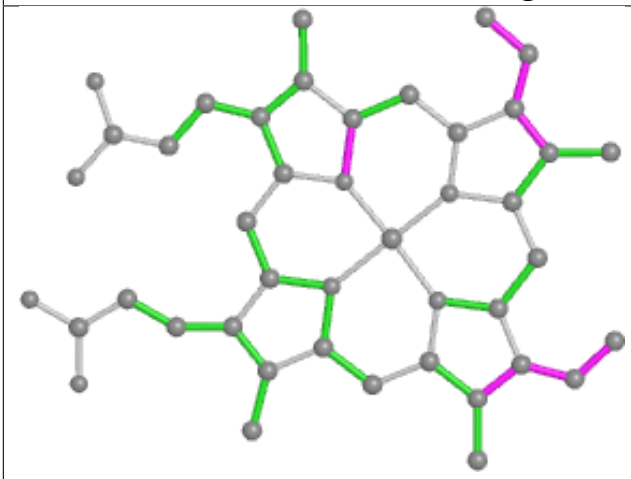


Torsions

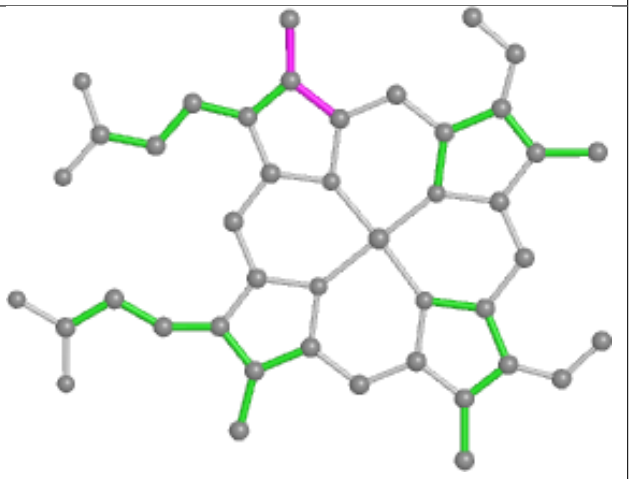


Rings

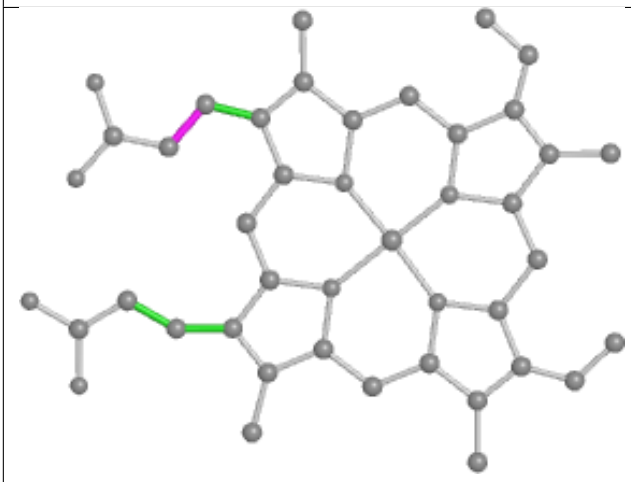
Ligand HEM C 610



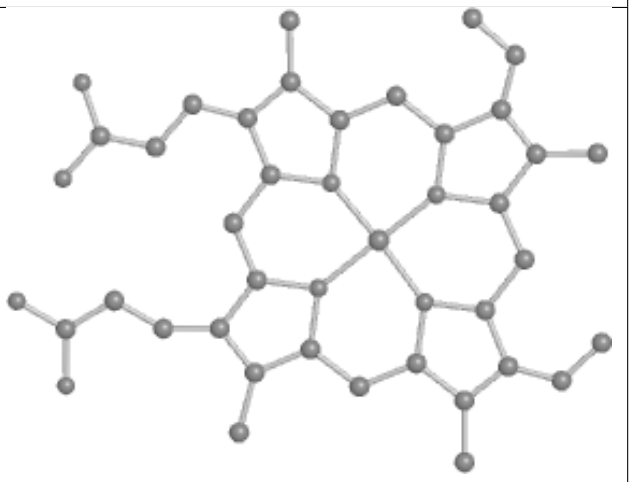
Bond lengths



Bond angles

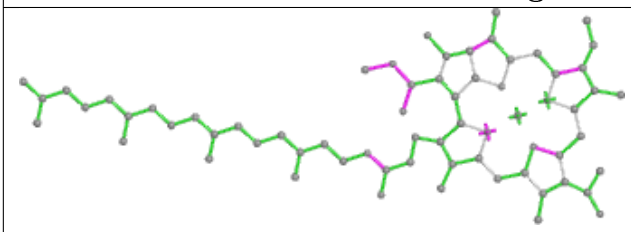


Torsions

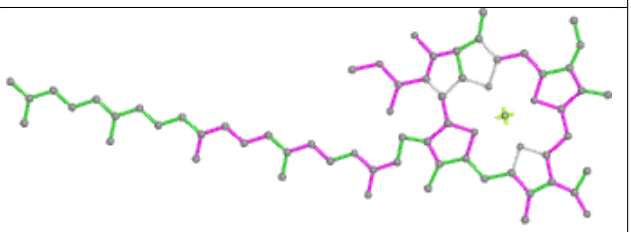


Rings

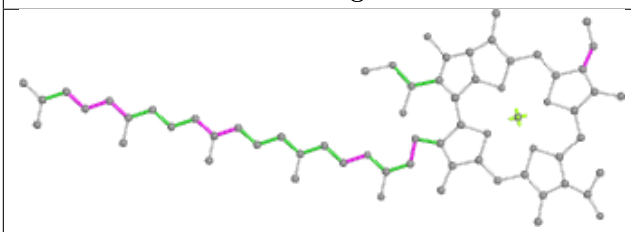
Ligand BCL L 602



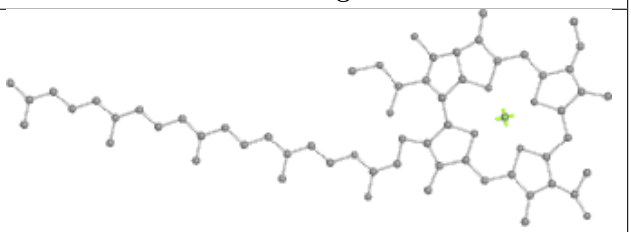
Bond lengths



Bond angles

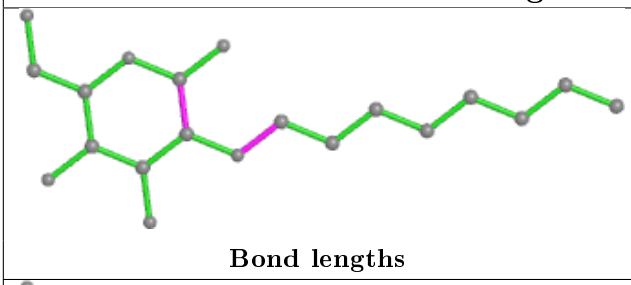


Torsions

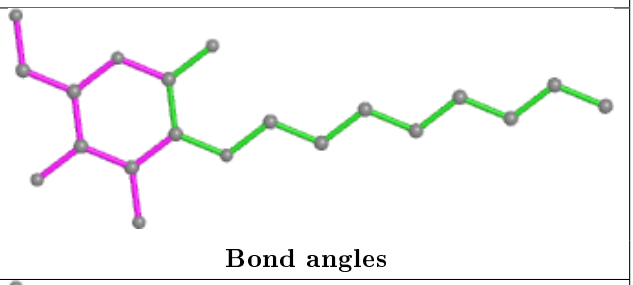


Rings

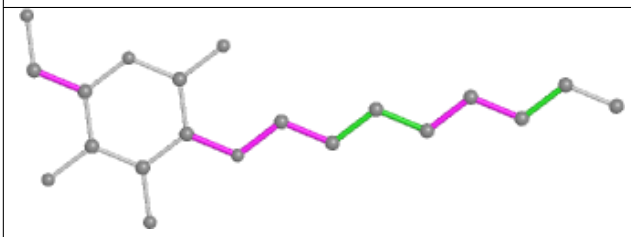
Ligand BGL L 701



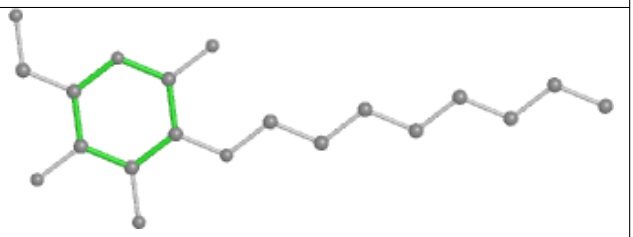
Bond lengths



Bond angles

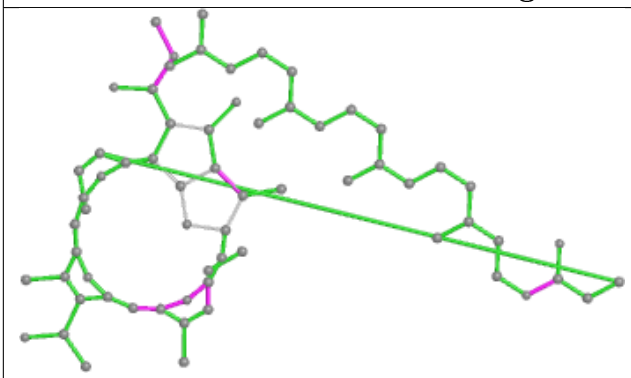


Torsions

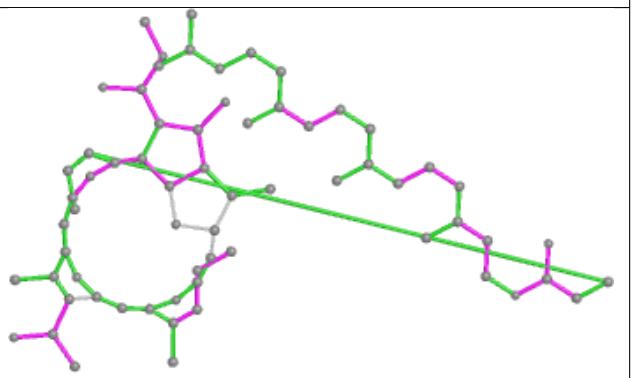


Rings

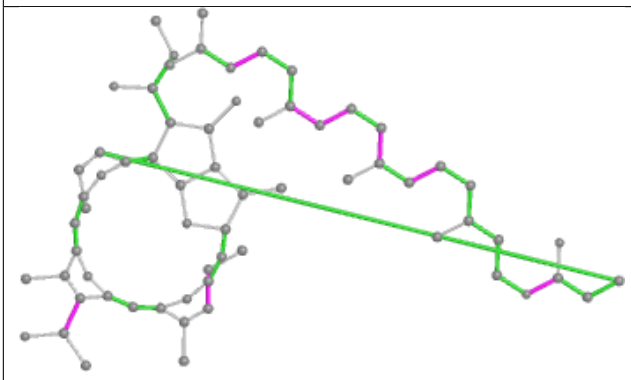
Ligand BPH M 605



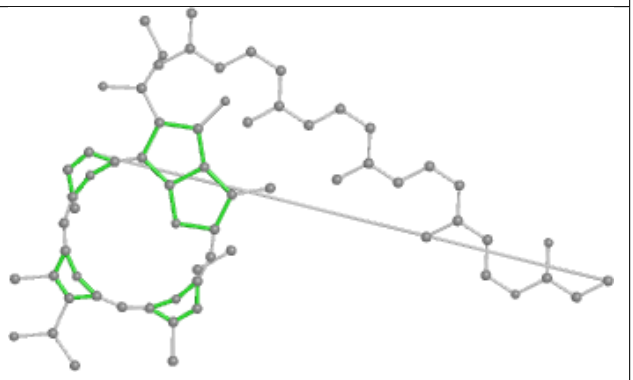
Bond lengths



Bond angles

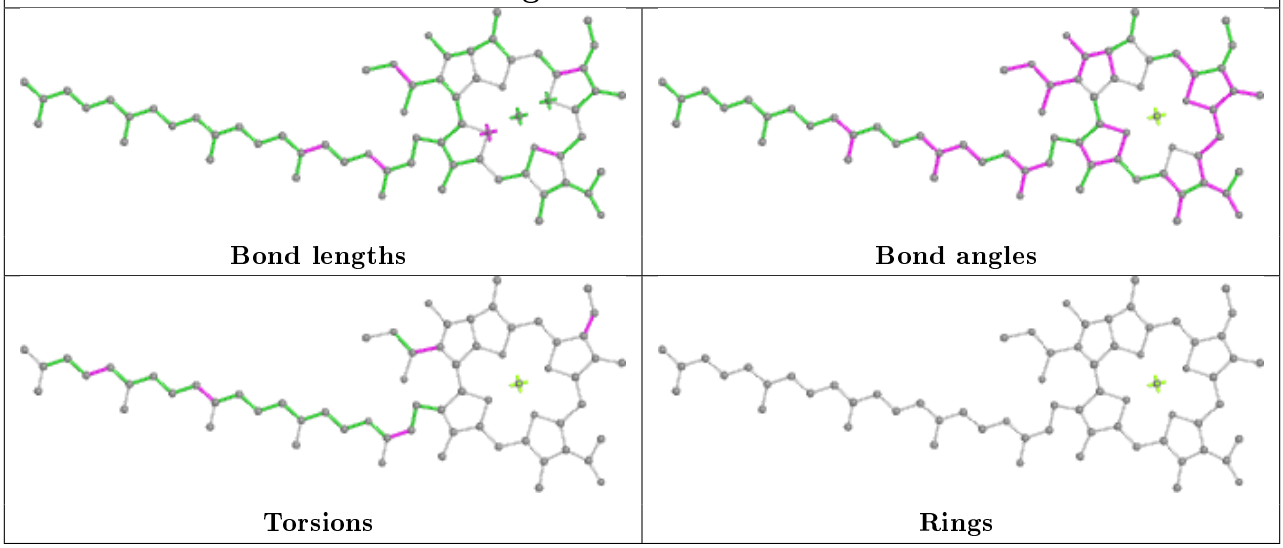


Torsions

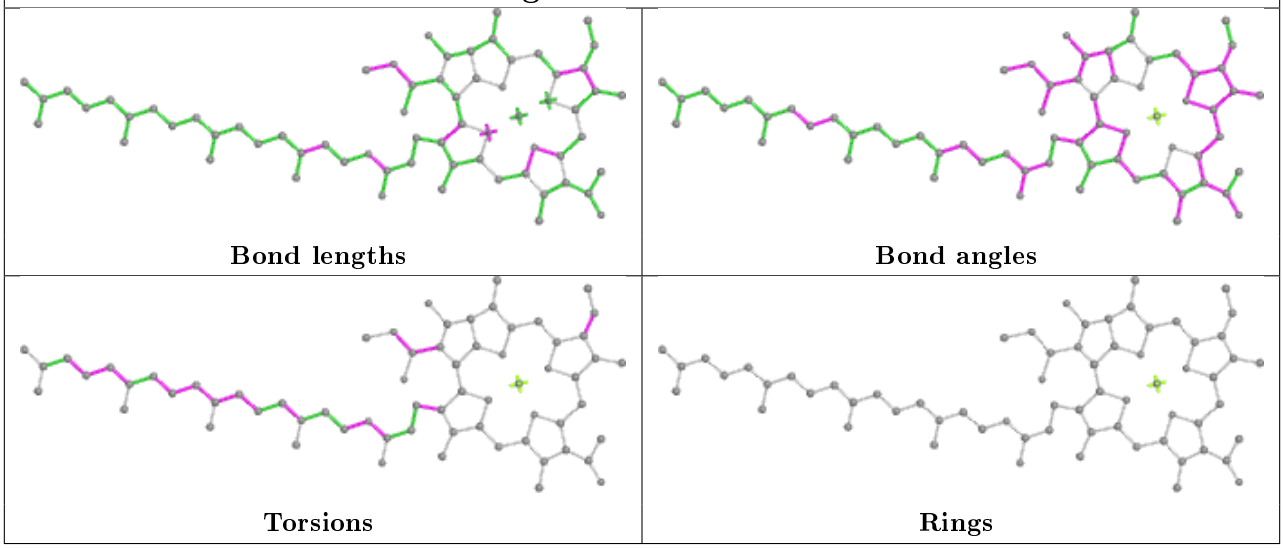


Rings

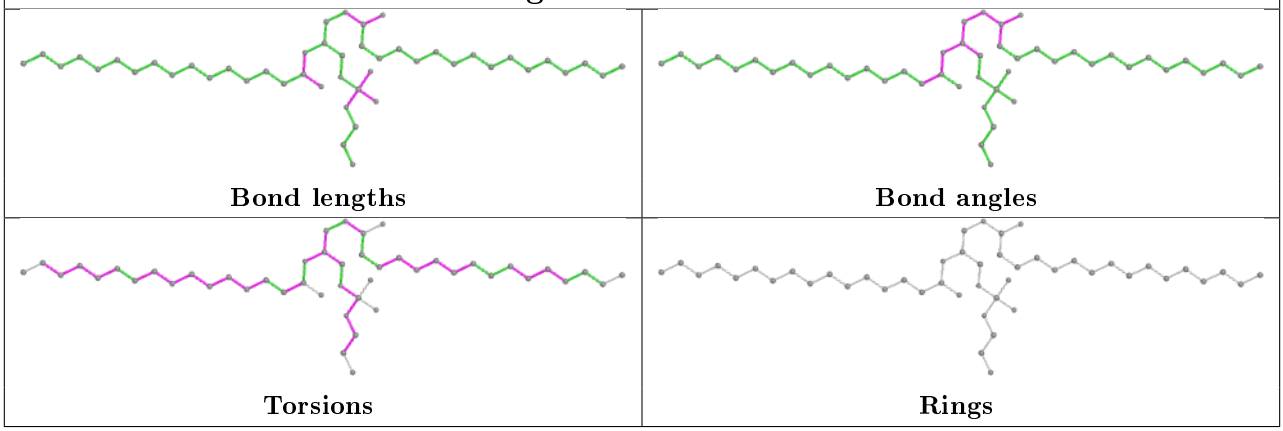
Ligand BCL M 603



Ligand BCL M 601



Ligand PEF H 708



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.