Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:18 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

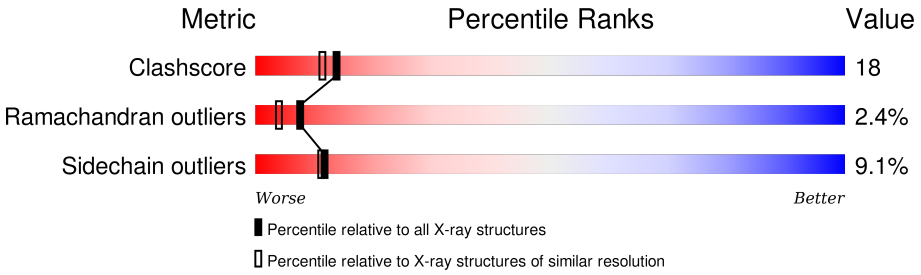
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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			

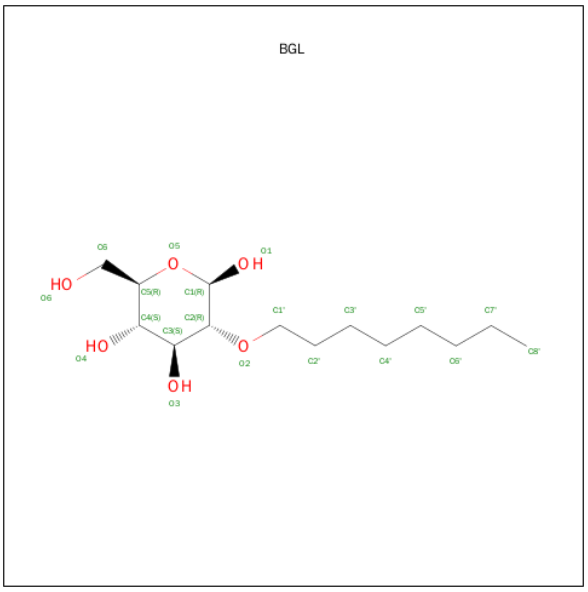
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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 SUGAR (B-2-OCTYLGLUCOSIDE) (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).

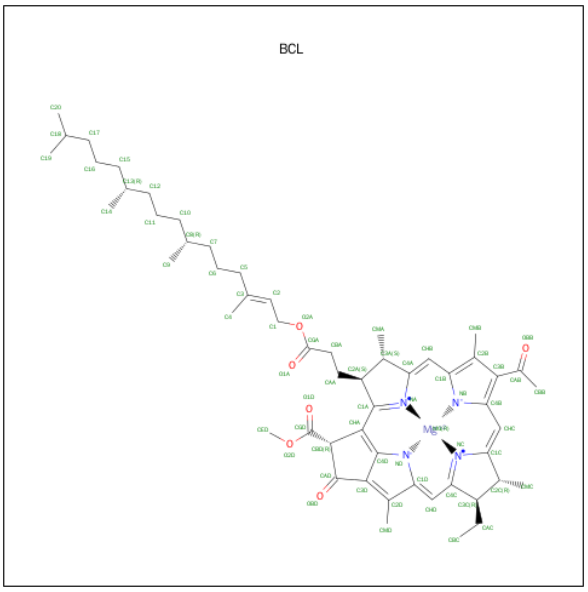


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0
5	L	1	Total C O 20 14 6	0	0
5	L	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

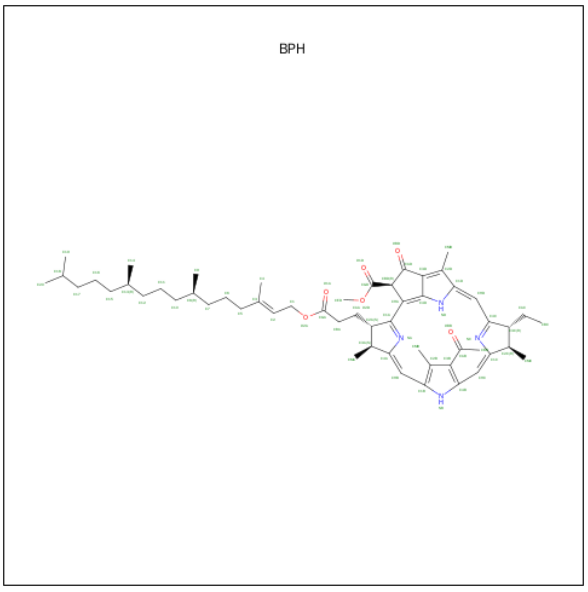
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0

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



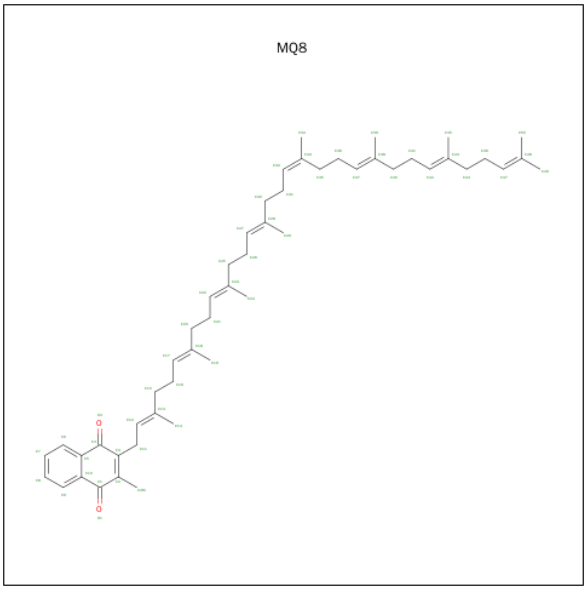
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



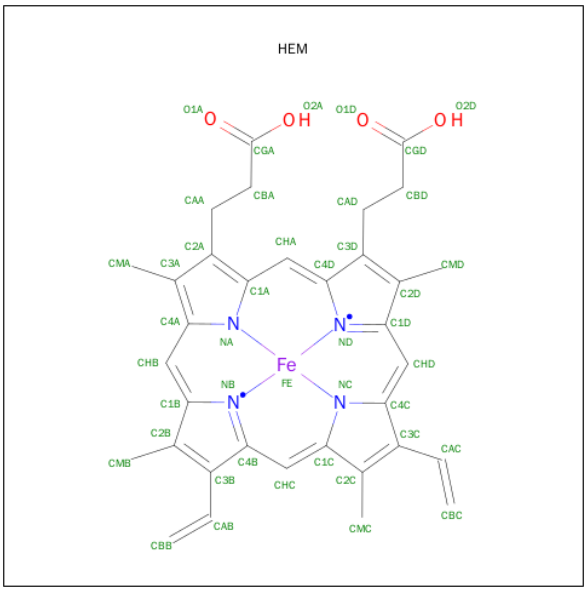
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



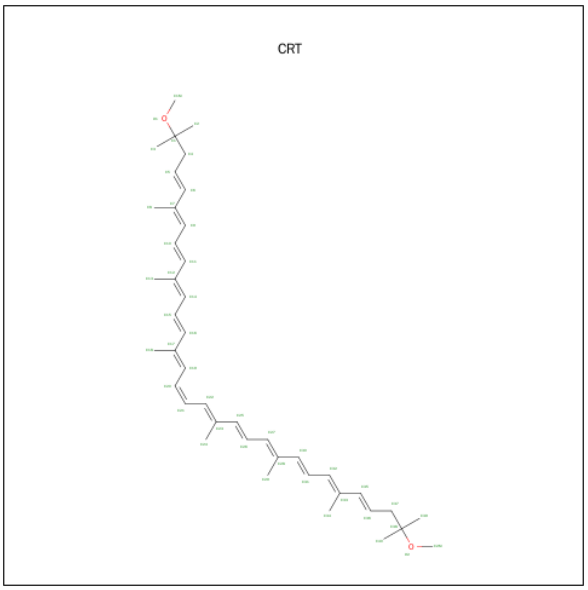
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



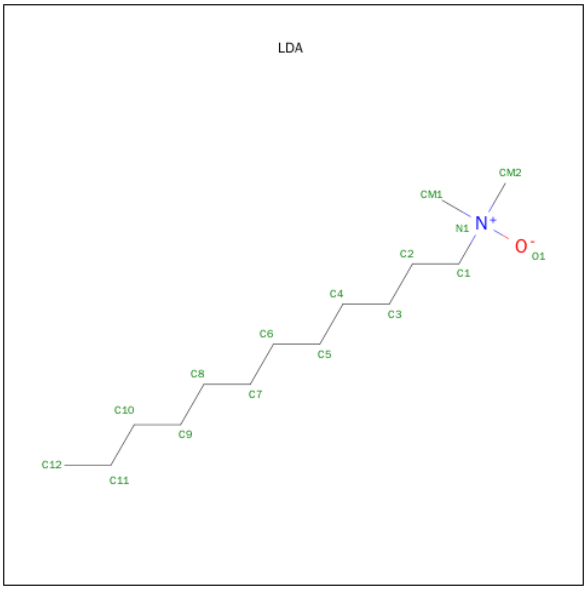
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



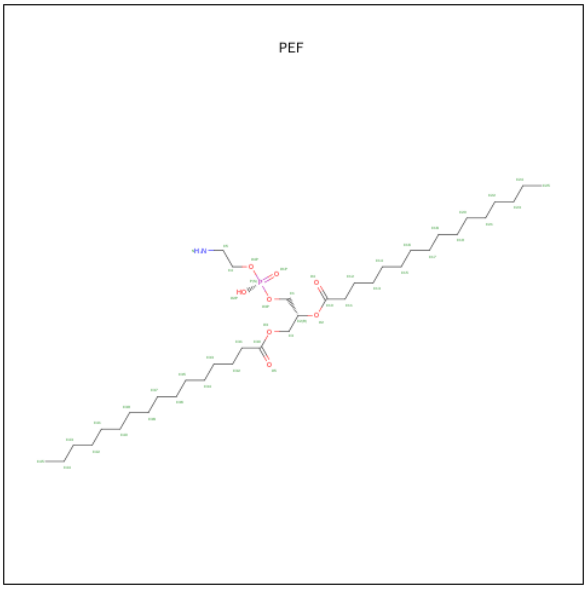
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 44 42 2	0	0

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C N O 16 14 1 1	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	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	H	22	Total	O	0	0
			22	22		
14	L	37	Total	O	0	0
			37	37		
14	M	35	Total	O	0	0
			35	35		

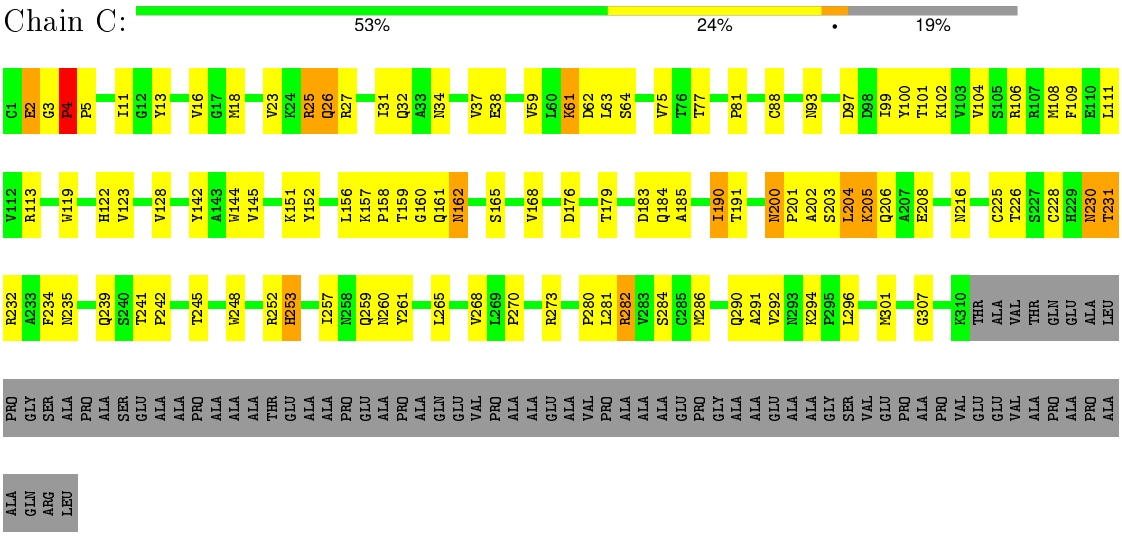
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

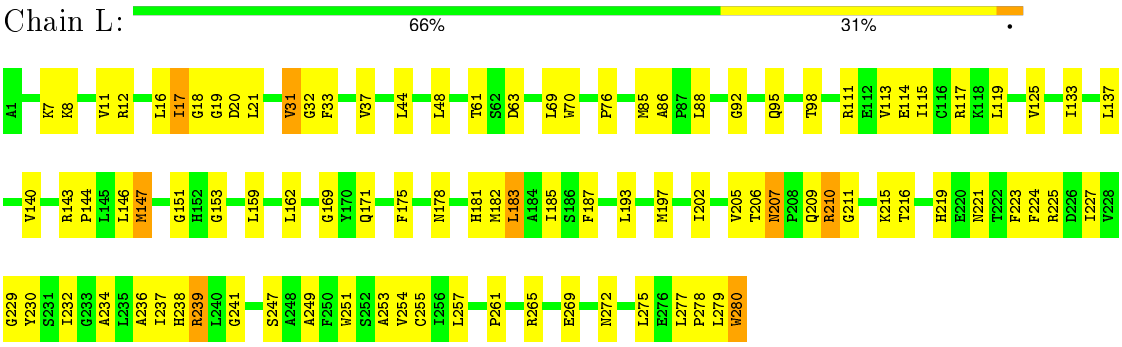
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



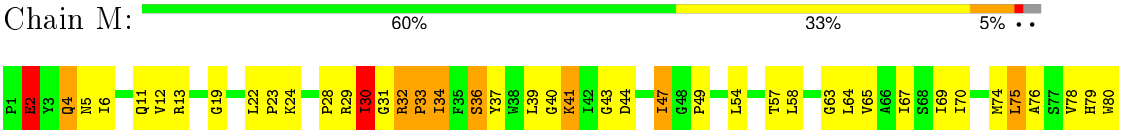
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

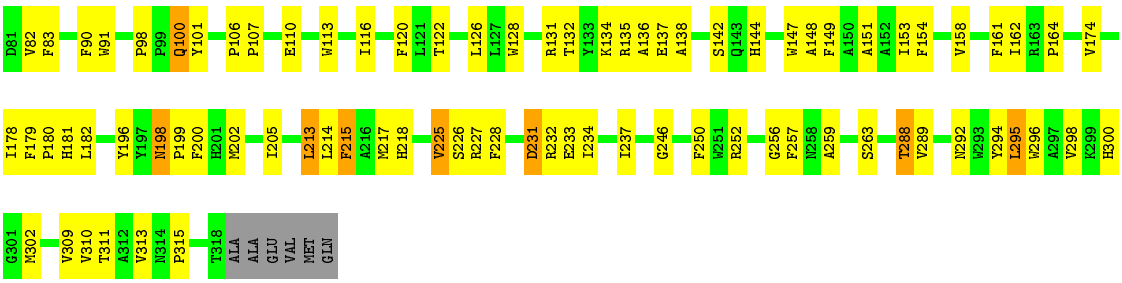
Chain L:



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

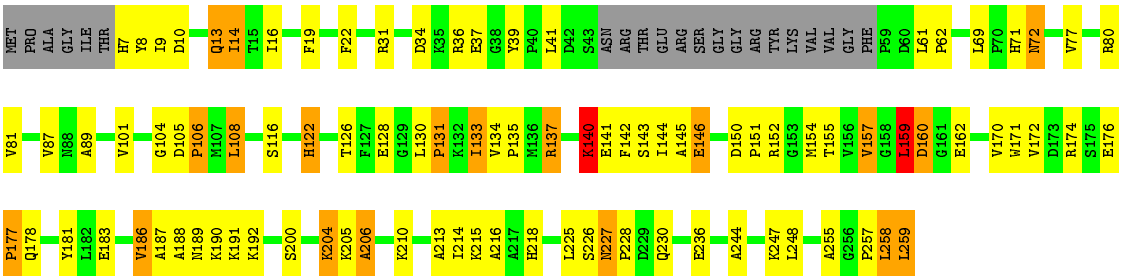
Chain M:





• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	L	60	0	84	10	0
5	M	60	0	84	1	0
6	M	1	0	0	0	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	M	53	0	72	1	0
10	C	172	0	120	5	0
11	M	44	0	60	2	0
12	L	16	0	31	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
9: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)
4:H:189:ASN:ND2	4:H:191:LYS:HB2	2.03	0.74
1:C:27:ARG:O	1:C:31:ILE:HG13	1.87	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	5: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:69:ILE:HD13	3:M:116:ILE:CG2	2.18	0.70
3:M:30:ILE:HG13	3:M:31:GLY:N	2.07	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
3:M:113:TRP:O	3:M:116:ILE:HG22	1.94	0.67
1:C:4:PRO:HD3	2:L:261:PRO:O	1.93	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
5: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	5: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	5:L:703:BGL:H2'1	2.33	0.63
2:L:227:ILE:HD11	3:M:135:ARG:HB2	1.82	0.62
2:L:207:ASN:HD22	2:L:207:ASN:N	1.96	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
7:L:604:BCL:HMB1	7:L:604:BCL:HBB2	1.83	0.60
2:L:16:LEU:HG	2:L:114:GLU:HG2	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: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	5:L:703:BGL:H1'1	1.84	0.59
4:H:151:PRO:O	4:H:154:MET:HG3	2.03	0.59
3:M:76:ALA:HB1	5:M:702:BGL:H2	1.84	0.59
1:C:235:ASN:HD22	1:C:235:ASN:H	1.50	0.59
1:C:230:ASN:OD1	1:C:232:ARG:HG2	2.02	0.59
4:H:215:LYS:H	4:H:218:HIS:CD2	2.13	0.58
1:C:280:PRO:O	1:C:282:ARG:HG2	2.02	0.58
1:C:292:VAL:HG12	1:C:294:LYS:H	1.69	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
1:C:156:LEU:HD12	1:C:157:LYS:H	1.67	0.58
2:L:98:THR:HG21	12:L:707:LDA:H122	1.85	0.58
1:C:191:THR:HG21	1:C:235:ASN:ND2	2.19	0.58
7:L:602:BCL:HMB1	7:L:602:BCL:HBB3	1.85	0.58
2:L:265:ARG:HD2	2:L:269:GLU:OE2	2.04	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
4:H:105:ASP:H	4:H:108:LEU:HD23	1.70	0.55
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
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
7:L:602:BCL:HMB1	7:L:602:BCL:CBB	2.39	0.52
1:C:97:ASP:OD2	1:C:106:ARG:NH2	2.42	0.52
3:M:22:LEU:HD11	3:M:29:ARG:HH11	1.74	0.52
4:H:37:GLU:CD	4:H:80:ARG:HH22	2.12	0.52
1:C:106:ARG:HD3	10: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
3:M:232:ARG:NH2	4:H:236:GLU:OE2	2.43	0.52
1:C:257:ILE:O	1:C:261:TYR:HB2	2.09	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
2:L:70:TRP:HE1	5:L:704:BGL:HO1	1.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:257:PHE:HB3	13:H:708:PEF:HN2	1.76	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
1:C:11:ILE:HD13	1:C:226:THR:O	2.10	0.51
4:H:134:VAL:CG2	4:H:174:ARG:HD2	2.40	0.51
1:C:75:VAL:HG13	10:C:610:HEM:HMB2	1.92	0.51
3:M:131:ARG:NH1	3:M:131:ARG:HG3	2.25	0.51
2:L:69:LEU:HB2	5:L:703:BGL:C1'	2.40	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
2:L:182:MET:HB3	7:M:601:BCL:O1D	2.11	0.51
1:C:77:THR:HA	1:C:81:PRO:HB3	1.93	0.51
3:M:128:TRP:HE1	8:M:605:BPH:HED1	1.76	0.50
2:L:115:ILE:O	2:L:119:LEU:HD12	2.11	0.50
3:M:234:ILE:H	3:M:234:ILE:HD12	1.76	0.50
4:H:248:LEU:O	4:H:255:ALA:HB2	2.10	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
1:C:200:ASN:HD22	1:C:201:PRO:N	2.09	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
3:M:12:VAL:O	3:M:13:ARG:NH1	2.45	0.50
2:L:11:VAL:HG22	2:L:12:ARG:N	2.27	0.50
2:L:70:TRP:CZ2	5: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
4:H:186:VAL:O	4:H:190:LYS:HA	2.12	0.50
1:C:104:VAL:HG13	1:C:265:LEU:HD13	1.94	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
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
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.93	0.49
4:H:140:LYS:N	4:H:140:LYS:HD3	2.28	0.49
2:L:239:ARG:HD2	3:M:6:ILE:HA	1.94	0.49
1:C:37:VAL:HG23	1:C:301:MET:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:187:ALA:O	4:H:189:ASN:N	2.46	0.49
1:C:200:ASN:ND2	1:C:200:ASN:C	2.65	0.49
5:L:701:BGL:O3	5: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
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
1:C:111:LEU:HD23	1:C:111:LEU:C	2.34	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
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:63:LEU:HD21	1:C:307:GLY:HA3	1.96	0.47
3:M:198:ASN:ND2	3:M:200:PHE:H	2.12	0.47
3:M:11:GLN:HE21	3:M:41:LYS:CE	2.27	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:128:TRP:O	3:M:132:THR:HG23	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:122:HIS:CE1	10:C:612:HEM:NC	2.82	0.47
3:M:149:PHE:O	3:M:153:ILE:HG13	2.14	0.47
2:L:31:VAL:HG12	2:L:32:GLY:N	2.27	0.47
1:C:11:ILE:HG21	1:C:226:THR:O	2.15	0.47
2:L:223:PHE:HD2	2:L:224:PHE:CD1	2.32	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
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:34:ASN:HB3	1:C:296:LEU:HA	1.97	0.47
2:L:223:PHE:HD2	2:L:224:PHE:HD1	1.63	0.47
1:C:158:PRO:O	1:C:160:GLY:N	2.48	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
4:H:39:TYR:CE1	4:H:41:LEU:HD21	2.50	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:O	1:C:161:GLN:HG2	2.15	0.46
3:M:79:HIS:O	3:M:80:TRP:HB2	2.15	0.46
2:L:7:LYS:HD3	4:H:87:VAL:HG21	1.98	0.46
7:L:604:BCL:H13	7:L:604:BCL:H172	1.59	0.46
4:H:130:LEU:O	4:H:131:PRO:C	2.53	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
3:M:178:ILE:HG23	7:M:601:BCL:HED1	1.98	0.46
3:M:134:LYS:HB3	3:M:135:ARG:NH2	2.31	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
4:H:14:ILE:HD12	4:H:14:ILE:O	2.16	0.46
1:C:119:TRP:O	1:C:123:VAL:HG22	2.16	0.46
3:M:252:ARG:NH1	13:H:708:PEF:H51	2.30	0.46
3:M:128:TRP:HE1	8:M:605:BPH:CED	2.28	0.46
1:C:128:VAL:HG11	10:C:612:HEM:CBC	2.45	0.46
3:M:227:ARG:HG3	3:M:228:PHE:CD2	2.51	0.46
1:C:151:LYS:HG2	1:C:152:TYR:N	2.31	0.46
7:M:601:BCL:H93	7:M:601:BCL:H62	1.78	0.46
3:M:36:SER:OG	3:M:39:LEU:HB2	2.16	0.46
2:L:33:PHE:O	2:L:37:VAL:HG23	2.16	0.45
1:C:281:LEU:HB2	10:C:610:HEM:HBD1	1.97	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
3:M:137:GLU:HG3	3:M:138:ALA:N	2.30	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
5: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
3:M:5:ASN:HD22	3:M:226:SER:HB3	1.82	0.45
2:L:241:GLY:HA3	3:M:215:PHE:CZ	2.52	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	11: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
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

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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:76:PRO:HG3	2:L:153:GLY:O	2.17	0.44
2:L:11:VAL:HG22	2:L:12:ARG:H	1.82	0.44
2:L:206:THR:HG21	3:M:237:ILE:HD13	2.00	0.44
1:C:37:VAL:CG2	1:C:301:MET:HE3	2.48	0.44
1:C:152:TYR:CZ	3:M:79:HIS:NE2	2.86	0.44
4:H:204:LYS:O	4:H:206:ALA:N	2.51	0.44
11:M:613:CRT:H36	11:M:613:CRT:H341	1.86	0.44
2:L:19:GLY:O	2:L:21:LEU:N	2.51	0.44
3:M:78:VAL:O	3:M:79:HIS:HB2	2.18	0.43
3:M:19:GLY:HA3	3:M:29:ARG:HH21	1.83	0.43
2:L:251:TRP:HA	2:L:254:VAL:HG13	1.99	0.43
3:M:142:SER:HB2	3:M:144:HIS:HD2	1.82	0.43
1:C:204:LEU:O	1:C:208:GLU:HG3	2.17	0.43
1:C:2:GLU:N	1:C:2:GLU:CD	2.72	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
4:H:225:LEU:C	4:H:227:ASN:H	2.22	0.43
7:L:602:BCL:HBD	7:L:604:BCL:CBC	2.48	0.43
2:L:159:LEU:HD21	3:M:202:MET:CE	2.48	0.43
2:L:117:ARG:NH1	4:H:258:LEU:HD13	2.31	0.43
3:M:75:LEU:HD13	3:M:80:TRP:HE3	1.79	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
1:C:205:LYS:HD2	1:C:205:LYS:HA	1.84	0.43
7:M:601:BCL:H62	7:M:601:BCL:H41	1.85	0.43
2:L:249:ALA:CB	8:L:606:BPH:HBC3	2.40	0.43
1:C:282:ARG:HH11	1:C:282:ARG:CG	2.31	0.43
3:M:90:PHE:HB2	3:M:91:TRP:CE3	2.53	0.43
3:M:64:LEU:HD21	8:M:605:BPH:H8	2.01	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
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
2:L:223:PHE:CD2	2:L:224:PHE:CD1	3.07	0.42
7:M:601:BCL:HAC2	7:M:601:BCL:HHD	1.73	0.42
1:C:290:GLN:O	1:C:291:ALA:HB3	2.19	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
7:M:603:BCL:HBC2	7:M:603:BCL:H2C	1.86	0.42
7:M:601:BCL:CBB	7:M:601:BCL:HMB1	2.46	0.42
3:M:295:LEU:HD12	3:M:295:LEU:HA	1.90	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
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
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	12:L:707:LDA:O1	2.20	0.42
4:H:160:ASP:OD2	4:H:215:LYS:NZ	2.53	0.42
3:M:179:PHE:O	3:M:182:LEU:HB2	2.20	0.42
1:C:4:PRO:HA	1:C:5:PRO:HA	1.68	0.42
2:L:18:GLY:H	4:H:259:LEU:HD12	1.83	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
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: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
1:C:231:THR:HG22	1:C:234:PHE:CE2	2.54	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
3:M:128:TRP:CZ2	7:M:601:BCL:H193	2.55	0.41
2:L:16:LEU:HD11	2:L:113:VAL:CG1	2.50	0.41
3:M:32:ARG:HA	3:M:32:ARG:HD3	1.41	0.41
1:C:228:CYS:HA	1:C:241:THR:OG1	2.21	0.41
3:M:113:TRP:HA	3:M:113:TRP:CE3	2.56	0.41
2:L:17:ILE:HD11	2:L:33:PHE:CG	2.55	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
3:M:205:ILE:HG12	7:M:603:BCL:CHB	2.51	0.41
4:H:36:ARG:NH1	4:H:62:PRO:HG2	2.36	0.41
3:M:246:GLY:HA3	14:M:922:HOH:O	2.20	0.41
2:L:125:VAL:HG11	3:M:250:PHE:CE2	2.56	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)
4:H:214:ILE:HB	4:H:218:HIS:HB2	2.02	0.41
1:C:111:LEU:HD23	1:C:111:LEU:O	2.21	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
1:C:252:ARG:N	1:C:252:ARG:HD2	2.35	0.41
3:M:113:TRP:CE3	3:M:116:ILE:HG21	2.56	0.40
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
4:H:178:GLN:NE2	14:H:985:HOH:O	2.55	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
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
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
3:M:158:VAL:HA	3:M:162:ILE:HB	2.03	0.40
2:L:215:LYS:HD2	2:L:219:HIS:CE1	2.56	0.40
3:M:122:THR:HG22	3:M:126:LEU:HD12	2.03	0.40
2:L:234:ALA:O	2:L:237:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	6 2
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	26 25
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	10 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	3 1
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	7 4

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%)	16 16
2	L	228/228 (100%)	212 (93%)	16 (7%)	19 19
3	M	254/258 (98%)	234 (92%)	20 (8%)	15 15
4	H	195/211 (92%)	166 (85%)	29 (15%)	4 3
All	All	936/997 (94%)	851 (91%)	85 (9%)	12 11

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 carbohydrates 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	$\#\|Z\| > 2$
10	HEM	C	609	1	30,50,50	3.11	12 (40%)	24,82,82	2.10	6 (25%)
10	HEM	C	610	1	30,50,50	3.38	13 (43%)	24,82,82	2.20	7 (29%)
10	HEM	C	611	1	30,50,50	3.18	11 (36%)	24,82,82	2.13	6 (25%)
10	HEM	C	612	1	30,50,50	3.19	11 (36%)	24,82,82	2.09	6 (25%)
13	PEF	H	708	-	45,46,46	2.15	6 (13%)	46,51,51	1.43	6 (13%)
7	BCL	L	602	2	53,74,74	1.87	7 (13%)	57,115,115	1.93	12 (21%)
7	BCL	L	604	2	53,74,74	2.02	5 (9%)	57,115,115	2.18	16 (28%)
8	BPH	L	606	-	64,70,70	1.18	7 (10%)	73,101,101	2.13	19 (26%)
5	BGL	L	701	-	19,20,20	1.06	1 (5%)	23,25,25	2.06	8 (34%)
5	BGL	L	703	-	19,20,20	0.92	1 (5%)	23,25,25	2.10	8 (34%)
5	BGL	L	704	-	19,20,20	0.96	1 (5%)	23,25,25	2.50	9 (39%)
12	LDA	L	707	-	15,15,15	4.08	2 (13%)	16,17,17	0.97	1 (6%)
7	BCL	M	601	3	53,74,74	2.07	7 (13%)	57,115,115	2.28	17 (29%)
7	BCL	M	603	3	53,74,74	1.84	4 (7%)	57,115,115	2.09	12 (21%)
8	BPH	M	605	-	64,70,70	1.22	6 (9%)	73,101,101	1.98	16 (21%)
9	MQ8	M	608	-	54,54,54	2.62	17 (31%)	68,69,69	3.05	24 (35%)
11	CRT	M	613	-	41,43,43	2.74	15 (36%)	46,54,54	2.58	6 (13%)
5	BGL	M	702	-	19,20,20	1.03	1 (5%)	23,25,25	2.49	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BGL	M	705	-	19,20,20	1.00	1 (5%)	23,25,25	2.09	7 (30%)
5	BGL	M	706	-	19,20,20	0.98	1 (5%)	23,25,25	2.11	8 (34%)

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

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	707	LDA	O1-N1	-15.39	1.24	1.39
7	M	601	BCL	C3C-C4C	-11.88	1.36	1.51
7	L	604	BCL	C3C-C4C	-11.81	1.36	1.51
7	M	603	BCL	C3C-C4C	-10.33	1.38	1.51
7	L	602	BCL	C3C-C4C	-10.18	1.38	1.51
10	C	611	HEM	C3B-C4B	-9.42	1.43	1.51
10	C	609	HEM	C3B-C4B	-8.53	1.44	1.51
10	C	612	HEM	C3B-C4B	-8.11	1.44	1.51
10	C	610	HEM	C3D-C4D	-7.92	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	612	HEM	C3B-CAB	-7.11	1.38	1.51
10	C	610	HEM	C3B-CAB	-6.82	1.38	1.51
10	C	612	HEM	C2D-C3D	-6.76	1.34	1.54
10	C	611	HEM	C2D-C3D	-6.72	1.34	1.54
10	C	609	HEM	C2D-C3D	-6.52	1.34	1.54
10	C	611	HEM	C3B-CAB	-6.48	1.39	1.51
10	C	611	HEM	C3C-CAC	-6.33	1.39	1.51
10	C	609	HEM	C3C-CAC	-6.29	1.39	1.51
10	C	610	HEM	C2D-C3D	-6.23	1.35	1.54
10	C	612	HEM	C3C-CAC	-6.21	1.39	1.51
10	C	609	HEM	C3B-CAB	-6.05	1.40	1.51
10	C	612	HEM	C3D-C4D	-5.67	1.44	1.51
10	C	610	HEM	C3B-C4B	-5.57	1.46	1.51
10	C	610	HEM	C3C-CAC	-5.49	1.41	1.51
9	M	608	MQ8	C30-C31	-5.40	1.35	1.53
10	C	611	HEM	C2C-C1C	-5.35	1.42	1.52
10	C	612	HEM	C2C-C1C	-5.03	1.43	1.52
10	C	609	HEM	C2C-C1C	-4.26	1.44	1.52
10	C	610	HEM	C2C-C1C	-4.16	1.44	1.52
10	C	609	HEM	C3D-C4D	-3.93	1.46	1.51
7	L	604	BCL	C2A-C1A	-3.15	1.45	1.52
9	M	608	MQ8	C31-C32	-3.15	1.41	1.50
10	C	612	HEM	C2B-C1B	-3.11	1.41	1.51
10	C	611	HEM	C2B-C1B	-2.98	1.42	1.51
12	L	707	LDA	C1-N1	-2.97	1.46	1.51
10	C	609	HEM	C2B-C1B	-2.90	1.42	1.51
10	C	610	HEM	C2B-C1B	-2.87	1.42	1.51
10	C	609	HEM	C2D-C1D	-2.63	1.43	1.51
8	L	606	BPH	C2A-C1A	-2.63	1.47	1.51
7	L	604	BCL	O2D-CED	-2.48	1.39	1.45
7	M	601	BCL	O2D-CED	-2.42	1.39	1.45
7	L	602	BCL	O2D-CED	-2.41	1.39	1.45
7	M	601	BCL	C2A-C1A	-2.41	1.47	1.52
8	L	606	BPH	O2D-CED	-2.41	1.39	1.45
10	C	611	HEM	C3D-C4D	-2.37	1.48	1.51
10	C	611	HEM	C2D-C1D	-2.35	1.44	1.51
7	L	602	BCL	C3D-C2D	-2.35	1.34	1.40
10	C	612	HEM	C2D-C1D	-2.33	1.44	1.51
8	M	605	BPH	O2D-CED	-2.33	1.39	1.45
9	M	608	MQ8	C39-C38	-2.33	1.45	1.50
9	M	608	MQ8	C16-C17	-2.32	1.44	1.50
7	M	601	BCL	C2C-C3C	-2.30	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	613	CRT	C25-C23	-2.24	1.40	1.45
8	M	605	BPH	C3D-C2D	-2.24	1.34	1.40
9	M	608	MQ8	C11-C12	-2.22	1.47	1.50
9	M	608	MQ8	C46-C47	-2.16	1.44	1.50
11	M	613	CRT	C16-C17	-2.07	1.41	1.45
7	L	602	BCL	C2-C3	2.06	1.37	1.33
8	L	606	BPH	C4C-NC	2.11	1.42	1.37
10	C	609	HEM	CHD-C4C	2.18	1.41	1.36
9	M	608	MQ8	C44-C43	2.18	1.56	1.51
10	C	612	HEM	FE-NC	2.20	2.04	1.95
8	M	605	BPH	C2-C3	2.27	1.37	1.33
7	L	602	BCL	O1D-CGD	2.31	1.27	1.21
11	M	613	CRT	C32-C33	2.32	1.38	1.35
10	C	610	HEM	CHD-C4C	2.40	1.42	1.36
8	M	605	BPH	CHC-C1C	2.41	1.41	1.36
9	M	608	MQ8	C25-C23	2.43	1.56	1.51
8	L	606	BPH	C2-C3	2.45	1.37	1.33
8	L	606	BPH	CHC-C1C	2.47	1.41	1.36
9	M	608	MQ8	C47-C48	2.54	1.40	1.32
7	M	601	BCL	C2-C3	2.56	1.38	1.33
10	C	611	HEM	CBB-CAB	2.60	1.44	1.29
10	C	609	HEM	CBC-CAC	2.64	1.44	1.29
11	M	613	CRT	C4-C5	2.68	1.53	1.50
10	C	610	HEM	CBB-CAB	2.76	1.45	1.29
10	C	612	HEM	CBB-CAB	2.77	1.45	1.29
9	M	608	MQ8	C17-C18	2.77	1.38	1.33
10	C	612	HEM	CBC-CAC	2.82	1.45	1.29
7	L	604	BCL	O2D-CGD	2.87	1.40	1.33
10	C	609	HEM	CBB-CAB	2.89	1.46	1.29
11	M	613	CRT	C4-C1	2.92	1.57	1.53
10	C	610	HEM	CBC-CAC	2.93	1.46	1.29
10	C	611	HEM	CBC-CAC	2.96	1.46	1.29
7	M	603	BCL	O2A-CGA	3.01	1.42	1.33
11	M	613	CRT	C26-C25	3.04	1.42	1.34
7	M	603	BCL	C2-C3	3.05	1.38	1.33
9	M	608	MQ8	C22-C23	3.06	1.39	1.33
7	L	602	BCL	O2A-CGA	3.10	1.42	1.33
8	M	605	BPH	O2A-CGA	3.14	1.42	1.33
10	C	610	HEM	C4C-NC	3.20	1.40	1.36
8	L	606	BPH	O2A-CGA	3.21	1.43	1.33
11	M	613	CRT	C10-C11	3.27	1.43	1.34
11	M	613	CRT	C27-C28	3.30	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	703	BGL	O2-C1'	3.41	1.52	1.42
13	H	708	PEF	P-O2P	3.45	1.69	1.54
7	L	604	BCL	O2A-CGA	3.58	1.44	1.33
5	M	706	BGL	O2-C1'	3.59	1.53	1.42
7	M	601	BCL	O2D-CGD	3.61	1.42	1.33
5	M	705	BGL	O2-C1'	3.62	1.53	1.42
11	M	613	CRT	C31-C30	3.64	1.44	1.34
10	C	611	HEM	C1C-NC	3.64	1.40	1.36
8	L	606	BPH	O2D-CGD	3.66	1.42	1.33
5	L	704	BGL	O2-C1'	3.68	1.53	1.42
11	M	613	CRT	C15-C16	3.69	1.44	1.34
5	M	702	BGL	O2-C1'	3.84	1.53	1.42
10	C	609	HEM	C1C-NC	3.87	1.40	1.36
5	L	701	BGL	O2-C1'	3.94	1.54	1.42
7	M	601	BCL	O2A-CGA	3.97	1.45	1.33
11	M	613	CRT	C14-C12	4.01	1.41	1.35
7	M	603	BCL	O2D-CGD	4.09	1.43	1.33
13	H	708	PEF	O3-C30	4.17	1.45	1.33
8	M	605	BPH	O2D-CGD	4.24	1.44	1.33
9	M	608	MQ8	C30-C28	4.51	1.61	1.51
7	L	602	BCL	O2D-CGD	4.67	1.45	1.33
10	C	610	HEM	FE-NC	4.79	2.14	1.95
13	H	708	PEF	O2-C10	4.87	1.48	1.34
9	M	608	MQ8	C32-C33	4.96	1.42	1.33
11	M	613	CRT	C19-C17	5.00	1.42	1.35
13	H	708	PEF	P-O1P	5.20	1.70	1.51
11	M	613	CRT	C22-C23	5.36	1.42	1.35
9	M	608	MQ8	C12-C13	5.62	1.44	1.33
13	H	708	PEF	O5-C30	5.94	1.40	1.22
9	M	608	MQ8	C42-C43	6.04	1.44	1.33
9	M	608	MQ8	C27-C28	6.08	1.44	1.33
10	C	610	HEM	C1C-NC	6.14	1.43	1.36
11	M	613	CRT	C35-C36	7.55	1.52	1.31
11	M	613	CRT	C6-C5	7.96	1.54	1.31
13	H	708	PEF	O4-C10	8.23	1.47	1.22
9	M	608	MQ8	C34-C33	9.04	1.72	1.50

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	613	CRT	C37-C36-C35	-11.22	108.70	124.67
11	M	613	CRT	C4-C5-C6	-9.51	111.13	124.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	608	MQ8	C35-C33-C32	-8.22	105.46	121.05
9	M	608	MQ8	C11-C3-C4	-7.58	109.82	118.47
8	L	606	BPH	O1D-CGD-CBD	-6.67	115.06	124.62
7	M	601	BCL	O1D-CGD-CBD	-6.29	115.61	124.62
7	M	603	BCL	O1D-CGD-CBD	-5.93	116.12	124.62
7	L	604	BCL	O1D-CGD-CBD	-5.59	116.61	124.62
11	M	613	CRT	C36-C35-C33	-5.32	117.63	125.75
11	M	613	CRT	C5-C6-C7	-5.18	117.85	125.75
8	M	605	BPH	O1D-CGD-CBD	-5.05	117.38	124.62
8	M	605	BPH	C7-C6-C5	-4.66	99.30	113.06
5	M	702	BGL	O5-C5-C4	-4.62	101.01	109.68
7	L	602	BCL	O1D-CGD-CBD	-4.48	118.21	124.62
5	L	704	BGL	O5-C5-C4	-4.43	101.37	109.68
7	L	604	BCL	CAC-C3C-C4C	-4.29	103.07	112.58
9	M	608	MQ8	O1-C1-C10	-4.11	114.64	121.55
8	M	605	BPH	OBD-CAD-CBD	-4.05	119.82	125.94
7	M	601	BCL	OBD-CAD-CBD	-4.01	119.88	125.94
8	L	606	BPH	OBD-CAD-CBD	-3.96	119.96	125.94
7	L	604	BCL	CHD-C4C-NC	-3.94	120.49	125.06
13	H	708	PEF	O3-C30-O5	-3.85	113.56	123.49
7	M	603	BCL	CHD-C4C-NC	-3.84	120.60	125.06
9	M	608	MQ8	C21-C22-C23	-3.81	119.49	127.76
7	M	603	BCL	OBD-CAD-CBD	-3.79	120.21	125.94
9	M	608	MQ8	C40-C38-C37	-3.78	113.87	121.05
9	M	608	MQ8	C31-C32-C33	-3.60	119.94	127.76
5	M	702	BGL	C1-O5-C5	-3.58	106.86	113.47
5	L	703	BGL	O5-C5-C4	-3.49	103.14	109.68
9	M	608	MQ8	C2M-C2-C1	-3.48	110.63	116.27
5	L	704	BGL	C4-C3-C2	-3.38	102.18	109.60
9	M	608	MQ8	C40-C41-C42	-3.37	102.86	111.69
7	L	602	BCL	OBD-CAD-CBD	-3.35	120.88	125.94
5	M	702	BGL	C3-C4-C5	-3.32	104.41	110.20
5	M	706	BGL	O5-C5-C4	-3.29	103.50	109.68
7	L	602	BCL	CHD-C4C-NC	-3.20	121.35	125.06
9	M	608	MQ8	C20-C18-C17	-3.19	114.99	121.05
7	L	604	BCL	C6-C5-C3	-3.17	105.52	112.48
5	M	705	BGL	O5-C5-C4	-3.10	103.87	109.68
7	M	601	BCL	CHD-C4C-NC	-3.08	121.48	125.06
5	L	704	BGL	C1-O5-C5	-3.08	107.77	113.47
5	M	706	BGL	C1-O5-C5	-3.08	107.78	113.47
5	L	704	BGL	C3-C4-C5	-3.06	104.85	110.20
5	M	705	BGL	C1-O5-C5	-3.01	107.90	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	703	BGL	C1-O5-C5	-3.00	107.91	113.47
7	L	604	BCL	OBD-CAD-CBD	-3.00	121.42	125.94
7	L	602	BCL	O2A-CGA-O1A	-2.92	115.95	123.49
8	M	605	BPH	O2A-CGA-O1A	-2.90	116.02	123.49
7	M	601	BCL	O2A-CGA-O1A	-2.88	116.06	123.49
5	L	701	BGL	C1-C2-C3	-2.86	105.40	110.45
7	M	601	BCL	C12-C11-C10	-2.82	98.99	112.99
7	M	601	BCL	CAA-C2A-C1A	-2.79	102.64	112.47
5	L	701	BGL	O5-C5-C4	-2.73	104.55	109.68
5	M	702	BGL	C4-C3-C2	-2.72	103.62	109.60
5	M	706	BGL	C3-C4-C5	-2.70	105.49	110.20
7	L	604	BCL	CAA-C2A-C1A	-2.70	102.96	112.47
7	M	603	BCL	C4-C3-C5	-2.67	111.33	115.41
8	L	606	BPH	O2A-CGA-O1A	-2.67	116.61	123.49
8	L	606	BPH	C4-C3-C5	-2.65	111.37	115.41
8	L	606	BPH	C3A-C4A-NA	-2.63	108.97	113.57
7	M	603	BCL	O2A-CGA-O1A	-2.59	116.80	123.49
5	L	704	BGL	C1-C2-C3	-2.56	105.93	110.45
13	H	708	PEF	C3-C2-C1	-2.54	106.13	112.07
7	L	604	BCL	O2A-CGA-O1A	-2.47	117.11	123.49
9	M	608	MQ8	C5-C10-C1	-2.46	117.96	120.66
5	M	702	BGL	C1-C2-C3	-2.45	106.11	110.45
7	M	603	BCL	CMB-C2B-C1B	-2.44	124.33	128.36
8	L	606	BPH	C11-C10-C8	-2.41	107.48	115.49
12	L	707	LDA	O1-N1-C1	-2.37	107.60	110.27
8	L	606	BPH	CBB-CAB-C3B	-2.37	115.25	120.52
7	L	604	BCL	CMB-C2B-C1B	-2.37	124.45	128.36
7	M	601	BCL	CMC-C2C-C3C	-2.37	103.88	114.35
5	L	703	BGL	C3-C4-C5	-2.33	106.13	110.20
5	M	705	BGL	C3-C4-C5	-2.32	106.14	110.20
8	M	605	BPH	CBB-CAB-C3B	-2.31	115.40	120.52
5	L	701	BGL	C1-O5-C5	-2.30	109.22	113.47
9	M	608	MQ8	C39-C38-C37	-2.29	119.00	123.50
7	M	603	BCL	CGD-CBD-CAD	-2.27	102.95	110.62
5	M	705	BGL	C1-C2-C3	-2.25	106.48	110.45
8	L	606	BPH	C17-C16-C15	-2.22	101.98	112.99
8	M	605	BPH	C3A-C4A-NA	-2.20	109.72	113.57
8	M	605	BPH	C11-C12-C13	-2.19	108.21	115.49
8	M	605	BPH	C4-C3-C5	-2.19	112.06	115.41
9	M	608	MQ8	C24-C23-C22	-2.19	119.21	123.50
5	L	701	BGL	C3-C4-C5	-2.18	106.40	110.20
5	L	703	BGL	C1-C2-C3	-2.17	106.61	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	604	BCL	C11-C10-C8	-2.16	108.33	115.49
7	M	601	BCL	CMB-C2B-C1B	-2.15	124.80	128.36
10	C	610	HEM	C4B-CHC-C1C	-2.15	122.23	125.82
9	M	608	MQ8	C29-C28-C27	-2.10	119.39	123.50
11	M	613	CRT	C29-C28-C27	-2.09	119.81	122.90
5	M	706	BGL	C1-C2-C3	-2.05	106.83	110.45
7	L	602	BCL	C1D-CHD-C4C	2.01	129.13	126.07
8	L	606	BPH	CAB-C3B-C2B	2.02	134.82	127.14
7	L	602	BCL	C2A-C1A-CHA	2.02	127.61	123.89
7	M	601	BCL	C2A-C1A-CHA	2.05	127.65	123.89
8	M	605	BPH	C4A-NA-C1A	2.08	110.07	108.21
7	M	601	BCL	CHB-C4A-NA	2.08	127.39	124.51
9	M	608	MQ8	C35-C36-C37	2.11	117.21	111.69
5	M	706	BGL	O3-C3-C2	2.11	114.87	109.87
8	L	606	BPH	C4A-NA-C1A	2.12	110.11	108.21
7	L	602	BCL	C6-C5-C3	2.23	117.39	112.48
11	M	613	CRT	C29-C28-C30	2.25	121.85	118.10
5	L	703	BGL	O3-C3-C2	2.28	115.26	109.87
7	L	604	BCL	C3A-C2A-C1A	2.30	105.39	101.50
5	M	706	BGL	O4-C4-C3	2.33	115.58	110.34
8	L	606	BPH	CBC-CAC-C3C	2.36	119.35	113.57
5	M	705	BGL	O3-C3-C2	2.39	115.52	109.87
8	M	605	BPH	CBC-CAC-C3C	2.40	119.43	113.57
10	C	610	HEM	C2D-C3D-C4D	2.43	105.62	101.50
7	L	604	BCL	CED-O2D-CGD	2.52	121.91	115.99
5	L	701	BGL	O3-C3-C2	2.55	115.90	109.87
7	L	604	BCL	C2A-C1A-CHA	2.58	128.64	123.89
7	M	601	BCL	C2C-C3C-C4C	2.62	105.95	101.50
10	C	610	HEM	CAD-C3D-C4D	2.63	121.73	112.47
8	M	605	BPH	OBB-CAB-C3B	2.71	125.54	120.31
5	L	703	BGL	O4-C4-C3	2.71	116.44	110.34
7	M	603	BCL	C4A-NA-C1A	2.75	109.92	106.36
8	M	605	BPH	CED-O2D-CGD	2.76	122.45	115.99
8	L	606	BPH	CED-O2D-CGD	2.77	122.48	115.99
5	L	701	BGL	O4-C4-C3	2.81	116.67	110.34
5	M	702	BGL	O3-C3-C2	2.82	116.56	109.87
9	M	608	MQ8	C9-C10-C5	2.83	122.47	119.26
10	C	612	HEM	CMD-C2D-C3D	2.83	126.87	114.35
5	M	706	BGL	O6-C6-C5	2.84	120.71	111.33
7	M	601	BCL	CED-O2D-CGD	2.87	122.72	115.99
7	M	603	BCL	CED-O2D-CGD	2.90	122.80	115.99
10	C	609	HEM	CMD-C2D-C3D	2.98	127.53	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	606	BPH	OBB-CAB-C3B	2.99	126.07	120.31
8	L	606	BPH	C3C-C4C-NC	2.99	110.92	107.93
7	L	604	BCL	O2A-CGA-CBA	3.00	121.03	111.90
10	C	611	HEM	CMD-C2D-C3D	3.01	127.67	114.35
10	C	610	HEM	CMD-C2D-C3D	3.03	127.77	114.35
5	L	704	BGL	O3-C3-C2	3.05	117.10	109.87
8	L	606	BPH	C9-C8-C7	3.12	123.08	111.08
8	M	605	BPH	O2A-CGA-CBA	3.20	121.65	111.90
7	L	602	BCL	C4A-NA-C1A	3.21	110.50	106.36
5	M	705	BGL	O6-C6-C5	3.22	121.96	111.33
10	C	612	HEM	C2D-C3D-C4D	3.22	106.96	101.50
13	H	708	PEF	O2-C10-C11	3.25	118.59	111.53
7	M	601	BCL	C4A-NA-C1A	3.28	110.61	106.36
8	L	606	BPH	O2A-CGA-CBA	3.33	122.05	111.90
5	L	703	BGL	O6-C6-C5	3.34	122.38	111.33
5	M	702	BGL	O4-C4-C3	3.35	117.88	110.34
10	C	609	HEM	C2D-C3D-C4D	3.36	107.19	101.50
7	L	604	BCL	C4A-NA-C1A	3.38	110.73	106.36
13	H	708	PEF	C2-O2-C10	3.38	126.00	117.89
10	C	611	HEM	CAD-C3D-C4D	3.39	124.43	112.47
5	L	704	BGL	O4-C4-C3	3.43	118.05	110.34
9	M	608	MQ8	O1-C1-C2	3.43	124.56	120.27
9	M	608	MQ8	C19-C18-C20	3.44	120.66	115.41
9	M	608	MQ8	C36-C35-C33	3.47	124.03	112.71
5	L	701	BGL	O6-C6-C5	3.52	122.96	111.33
10	C	612	HEM	CAD-C3D-C4D	3.53	124.92	112.47
5	M	702	BGL	O6-C6-C5	3.67	123.45	111.33
10	C	611	HEM	C2D-C3D-C4D	3.67	107.72	101.50
7	M	603	BCL	O2A-CGA-CBA	3.68	123.12	111.90
8	L	606	BPH	C2C-C3C-C4C	3.73	107.83	101.50
5	L	704	BGL	O6-C6-C5	3.79	123.85	111.33
10	C	609	HEM	CAD-C3D-C4D	3.80	125.89	112.47
7	M	601	BCL	OBB-CAB-C3B	3.83	126.07	120.00
7	L	602	BCL	OBB-CAB-C3B	3.85	126.09	120.00
7	M	601	BCL	O2A-CGA-CBA	3.91	123.82	111.90
10	C	611	HEM	CMC-C2C-C3C	3.93	126.34	116.53
10	C	610	HEM	CMC-C2C-C3C	3.96	126.41	116.53
7	L	602	BCL	CED-O2D-CGD	3.96	125.28	115.99
10	C	612	HEM	CMC-C2C-C3C	3.97	126.45	116.53
10	C	609	HEM	CMC-C2C-C3C	4.05	126.63	116.53
9	M	608	MQ8	C44-C46-C47	4.08	122.37	111.69
7	L	604	BCL	OBB-CAB-C3B	4.09	126.48	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	603	BCL	OBB-CAB-C3B	4.11	126.51	120.00
13	H	708	PEF	O3-C3-C2	4.18	119.95	108.69
10	C	609	HEM	CMB-C2B-C3B	4.20	127.01	116.53
7	L	602	BCL	O2A-CGA-CBA	4.21	124.74	111.90
10	C	610	HEM	CMB-C2B-C3B	4.32	127.31	116.53
7	M	601	BCL	CAC-C3C-C2C	4.34	125.05	114.13
10	C	611	HEM	CMB-C2B-C3B	4.38	127.46	116.53
13	H	708	PEF	O3-C30-C31	4.43	125.39	111.90
10	C	612	HEM	CMB-C2B-C3B	4.66	128.16	116.53
10	C	609	HEM	CAD-C3D-C2D	4.75	126.88	113.22
8	M	605	BPH	C2C-C3C-C4C	5.04	110.04	101.50
10	C	611	HEM	CAD-C3D-C2D	5.09	127.85	113.22
7	L	602	BCL	O2D-CGD-CBD	5.13	118.33	111.30
10	C	612	HEM	CAD-C3D-C2D	5.16	128.07	113.22
5	L	701	BGL	C6-C5-C4	5.19	125.82	113.02
8	L	606	BPH	CAC-C3C-C2C	5.36	127.60	114.13
5	L	703	BGL	C6-C5-C4	5.57	126.75	113.02
8	M	605	BPH	O2D-CGD-CBD	5.80	119.26	111.30
5	M	705	BGL	C6-C5-C4	5.99	127.78	113.02
5	M	702	BGL	C6-C5-C4	6.02	127.87	113.02
5	L	704	BGL	C6-C5-C4	6.13	128.13	113.02
9	M	608	MQ8	C31-C30-C28	6.13	132.68	112.71
5	M	706	BGL	C6-C5-C4	6.25	128.42	113.02
9	M	608	MQ8	C30-C31-C32	6.43	128.53	111.69
10	C	610	HEM	CAD-C3D-C2D	6.76	132.65	113.22
8	M	605	BPH	CAC-C3C-C2C	6.82	131.28	114.13
9	M	608	MQ8	C41-C40-C38	7.44	136.95	112.71
9	M	608	MQ8	C39-C38-C40	7.55	126.94	115.41
7	L	604	BCL	O2D-CGD-CBD	7.58	121.70	111.30
7	M	603	BCL	O2D-CGD-CBD	7.70	121.87	111.30
7	M	601	BCL	O2D-CGD-CBD	7.92	122.17	111.30
8	L	606	BPH	O2D-CGD-CBD	8.52	122.99	111.30
9	M	608	MQ8	C34-C33-C35	9.31	129.63	115.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C8

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 65 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.