WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2014 – 03:59 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 wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
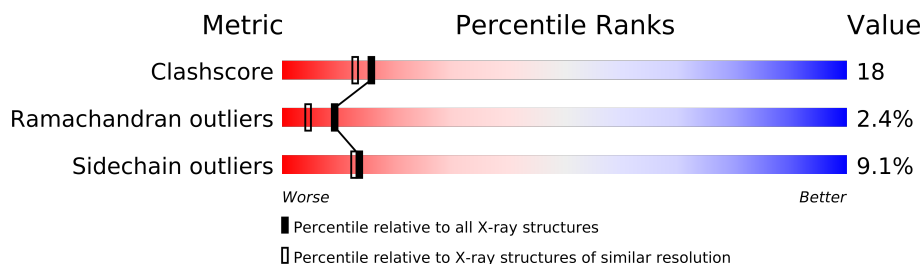A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		2.4%
Sidechain outliers		9.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2　Entry composition　ⓘ

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

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: $C_{14}H_{28}O_6$).
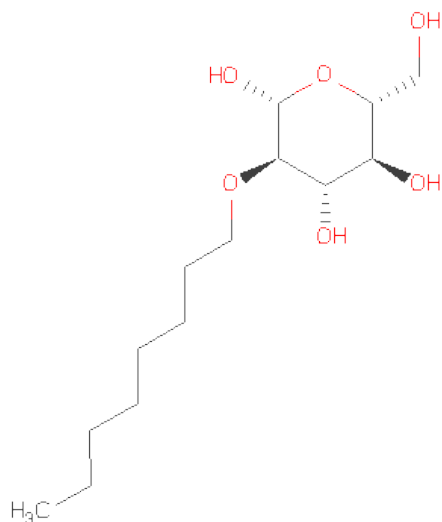
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total 20	C 14	O 6	0	0
5	M	1	Total 20	C 14	O 6	0	0
5	L	1	Total 20	C 14	O 6	0	0
5	L	1	Total 20	C 14	O 6	0	0
5	M	1	Total 20	C 14	O 6	0	0
5	M	1	Total 20	C 14	O 6	0	0

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

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

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).
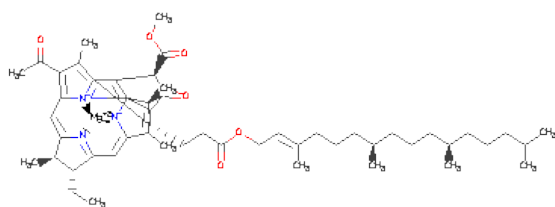
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).
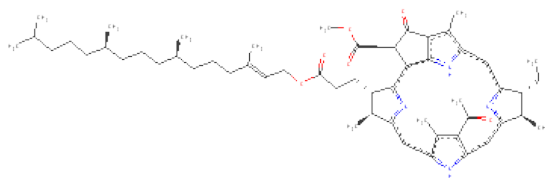
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total 65	C 55	N 4	O 6	0	0
8	L	1	Total 65	C 55	N 4	O 6	0	0

- Molecule 9 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).
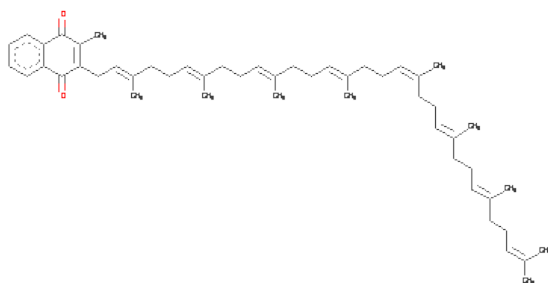
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total 53	C 51	O 2	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
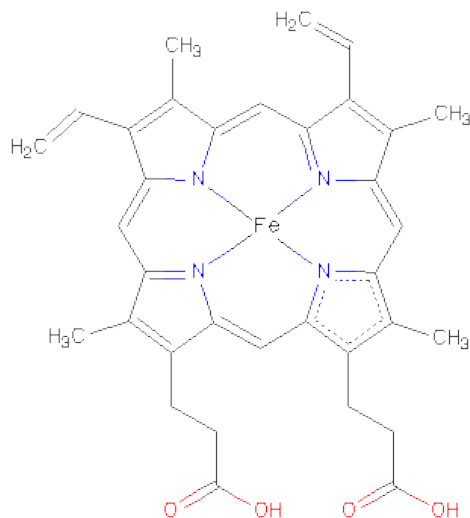
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).
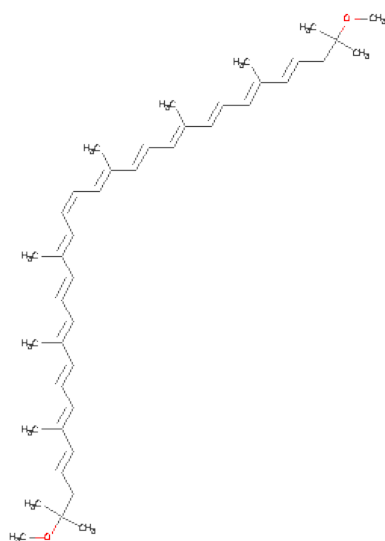
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total 44	C 42	O 2	0	0

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).
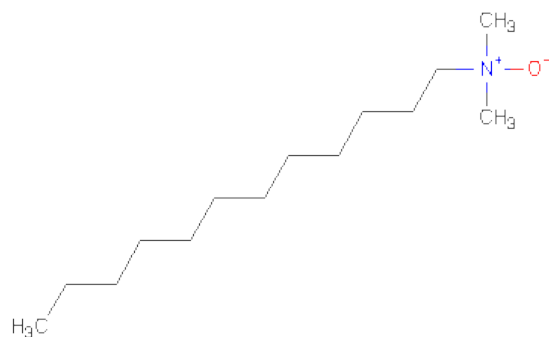
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 13 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).
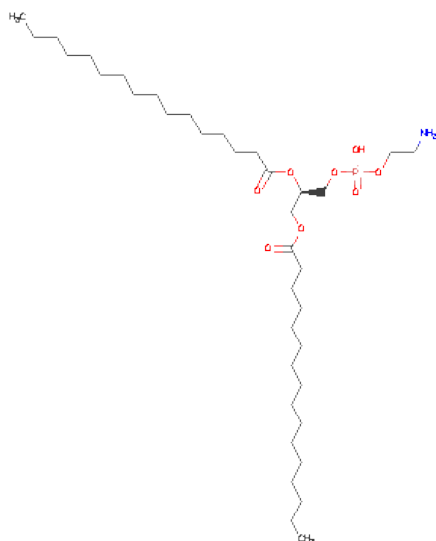
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	H	1	Total 47	C 37	N 1	O 8	P 1	0	0

• Molecule 14 is water.

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

3 Residue-property plots ⓘ

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.
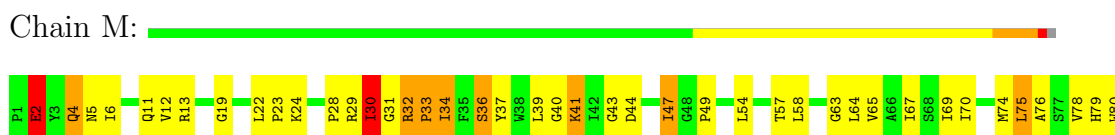
Note EDS was not executed.

• Molecule 1: PHOTOSYNTHETIC REACTION CENTER
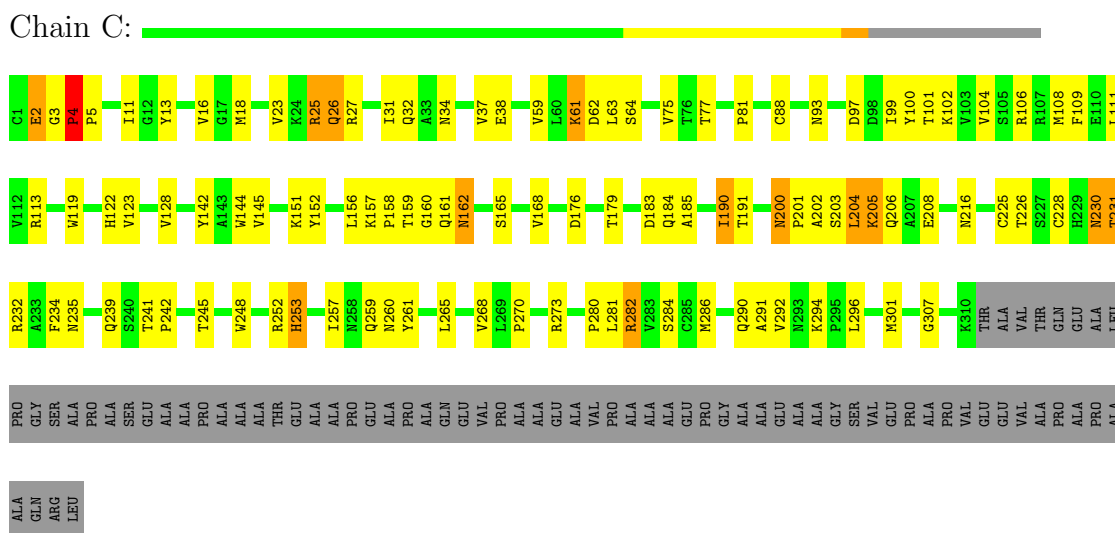
Chain C:

• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:

• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M:

D81 V82 F83 F90 W91 P98 P99 Q100 Y101 P106 P107 E110 W113 I116 F120 L121 T122 L126 L127 W128 R131 T132 Y133 K134 R135 A136 E137 A138 S142 Q143 H144 W147 A148 F149 A150 A151 A152 I153 F154 V158 F161 I162 R163 P164 V174

I178 F179 P180 H181 L182 Y196 Y197 N198 P199 F200 H201 M202 I205 L213 L214 F215 A216 M217 H218 V225 S226 R227 F228 D231 R232 E233 I234 I237 G246 F250 W251 R252 G256 F257 N258 A259 S263 T288 V289 N292 W293 Y294 L295 W296 A297 V298 K299 H300

G301 M302 V309 V310 T311 A312 V313 N314 P315 T318 ALA ALA GLU VAL MET GLN

● Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:

MET PRO ALA GLY ILE THR H7 Y8 I9 D10 Q13 I14 T15 I16 F19 F22 R31 D34 K35 R36 E37 G38 Y39 P40 L41 D42 S43 ASN ARG THR GLU ARG SER GLY GLY ARG TYR LYS VAL VAL GLY PHE P59 D60 L61 P62 L69 P70 H71 N72 V77 R80

V81 V87 N88 A89 V101 G104 D105 P106 M107 L108 S116 H122 T126 F127 E128 G129 L130 P131 K132 I133 V134 P135 M136 R137 K140 E141 F142 S143 I144 A145 E146 D150 P151 R152 G153 M154 T155 V156 V157 G158 L159 D160 G161 E162 V170 W171 V172 D173 R174 S175 E176

P177 Q178 Y181 L182 E183 V186 A187 A188 N189 K190 K191 K192 S200 K204 K205 A206 K210 A213 I214 K215 A216 A217 H218 L225 S226 N227 P228 D229 Q230 E236 A244 K247 L248 A255 G256 P257 L258 L259

4 Data and refinement statistics ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

The worst 5 of 364 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	7	3
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	30	28
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	12	7
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	4	1
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	9	4

5 of 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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	259/300 (86%)	239 (92%)	20 (8%)	18	18
2	L	228/228 (100%)	212 (93%)	16 (7%)	21	22
3	M	254/258 (98%)	234 (92%)	20 (8%)	18	17
4	H	195/211 (92%)	166 (85%)	29 (15%)	4	3
All	All	936/997 (94%)	851 (91%)	85 (9%)	14	13

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	24	LYS
3	M	181	HIS
4	H	186	VAL
3	M	30	ILE
3	M	41	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	174	HIS
2	L	207	ASN
4	H	13	GLN
1	C	290	GLN
2	L	95	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	49,50,50	2.83	16 (32%)	46,82,82	1.69	7 (15%)
10	HEM	C	610	1	49,50,50	3.17	17 (34%)	46,82,82	1.45	6 (13%)
10	HEM	C	611	1	49,50,50	3.29	12 (24%)	46,82,82	1.48	5 (10%)
10	HEM	C	612	1	49,50,50	2.46	7 (14%)	46,82,82	1.15	3 (6%)
13	PEF	H	708	-	46,46,46	2.10	6 (13%)	51,51,51	1.36	6 (11%)
7	BCL	L	602	2	74,74,74	2.07	13 (17%)	97,115,115	1.79	26 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	BCL	L	604	2	74,74,74	2.19	12 (16%)	97,115,115	1.94	26 (26%)
8	BPH	L	606	-	70,70,70	1.56	10 (14%)	94,101,101	1.90	23 (24%)
5	BGL	L	701	-	20,20,20	1.28	2 (10%)	25,25,25	1.98	8 (32%)
5	BGL	L	703	-	20,20,20	0.88	1 (5%)	25,25,25	2.02	8 (32%)
5	BGL	L	704	-	20,20,20	1.29	2 (10%)	25,25,25	2.41	9 (36%)
12	LDA	L	707	-	15,15,15	4.07	2 (13%)	17,17,17	1.70	1 (5%)
7	BCL	M	601	3	74,74,74	2.18	15 (20%)	97,115,115	1.98	29 (29%)
7	BCL	M	603	3	74,74,74	2.05	12 (16%)	97,115,115	1.87	25 (25%)
8	BPH	M	605	-	70,70,70	1.57	9 (12%)	94,101,101	1.90	22 (23%)
9	MQ8	M	608	-	54,54,54	2.52	17 (31%)	69,69,69	3.04	24 (34%)
11	CRT	M	613	-	43,43,43	2.60	15 (34%)	54,54,54	2.06	6 (11%)
5	BGL	M	702	-	20,20,20	1.05	1 (5%)	25,25,25	2.40	10 (40%)
5	BGL	M	705	-	20,20,20	1.34	2 (10%)	25,25,25	2.02	7 (28%)
5	BGL	M	706	-	20,20,20	0.96	1 (5%)	25,25,25	2.04	7 (28%)

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	-	0/14/114/114	0/0/8/8
10	HEM	C	610	1	-	0/14/114/114	0/0/8/8
10	HEM	C	611	1	-	0/14/114/114	0/0/8/8
10	HEM	C	612	1	-	0/14/114/114	0/0/8/8
13	PEF	H	708	-	-	0/50/50/50	0/0/0/0
7	BCL	L	602	2	-	0/41/137/137	0/0/9/9
7	BCL	L	604	2	-	0/41/137/137	0/0/9/9
8	BPH	L	606	-	2/2/18/22	0/49/105/105	0/0/6/6
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	-	0/41/137/137	0/0/9/9
7	BCL	M	603	3	-	0/41/137/137	0/0/9/9
8	BPH	M	605	-	2/2/18/22	0/49/105/105	0/0/6/6
9	MQ8	M	608	-	-	0/47/67/67	0/0/2/2
11	CRT	M	613	-	-	0/51/51/51	0/0/0/0
5	BGL	M	702	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BGL	M	705	-	-	0/11/31/31	0/1/1/1
5	BGL	M	706	-	-	0/11/31/31	0/1/1/1

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	611	HEM	C3D-C4D	15.99	1.48	1.44
12	L	707	LDA	O1-N1	-15.38	1.24	1.39
10	C	610	HEM	C3D-C4D	-12.62	1.41	1.44
7	M	601	BCL	C3C-C4C	-11.88	1.36	1.51
7	L	604	BCL	C3C-C4C	-11.81	1.36	1.51

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	613	CRT	C37-C36-C35	-9.82	108.70	124.95
9	M	608	MQ8	C34-C33-C35	9.36	129.63	115.39
9	M	608	MQ8	C11-C3-C4	-8.48	109.82	118.67
11	M	613	CRT	C4-C5-C6	-8.36	111.13	124.95
9	M	608	MQ8	C35-C33-C32	-8.12	105.46	121.08

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C13
8	L	606	BPH	C8
8	M	605	BPH	C8
8	M	605	BPH	C13

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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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.