wwPDB X-ray Structure Validation Summary Report (i)

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 wwPDB X-ray Structure 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/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:

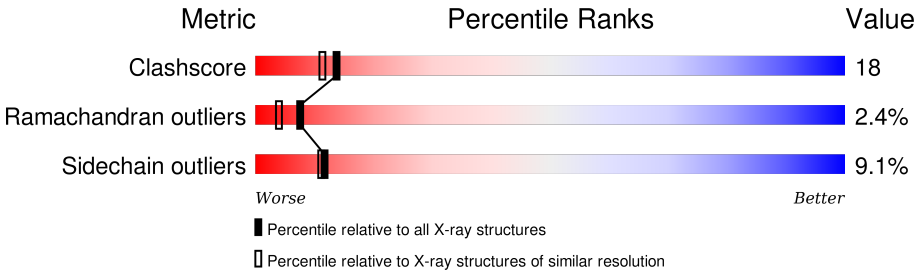
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (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	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 (i)

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			

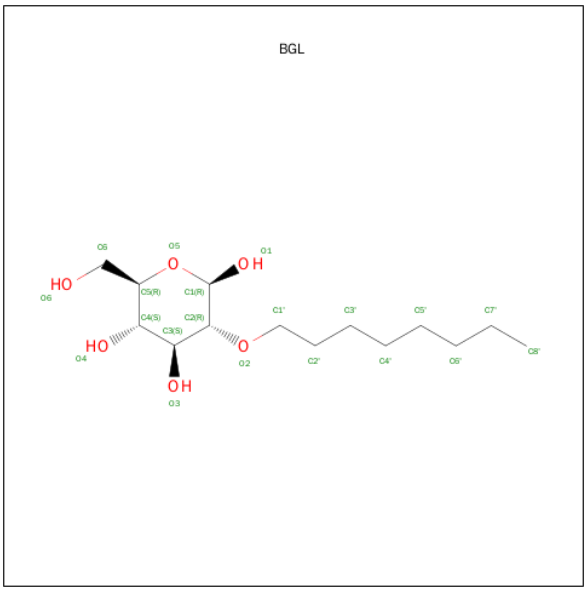
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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: $C_{14}H_{28}O_6$).

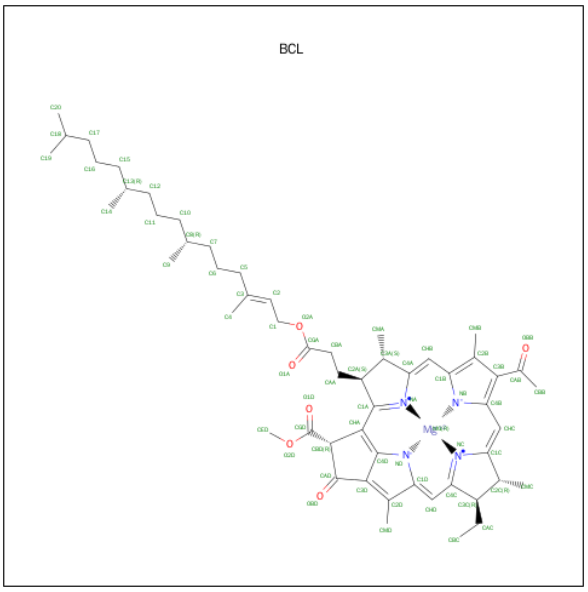


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0
5	L	1	Total C O 20 14 6	0	0
5	L	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0
5	M	1	Total C O 20 14 6	0	0

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

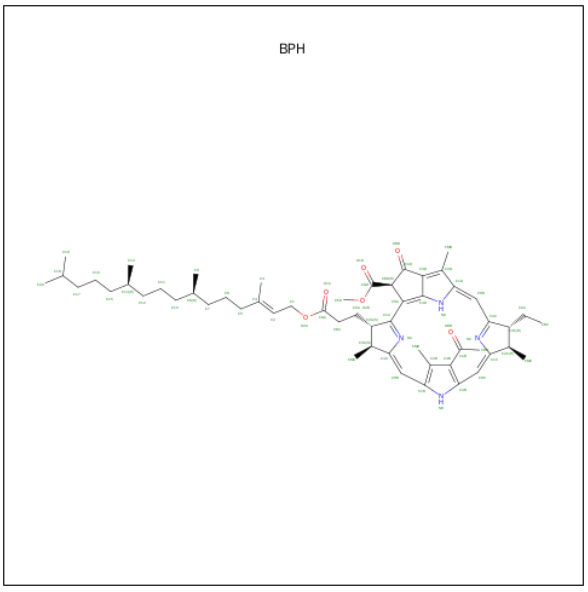
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0

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



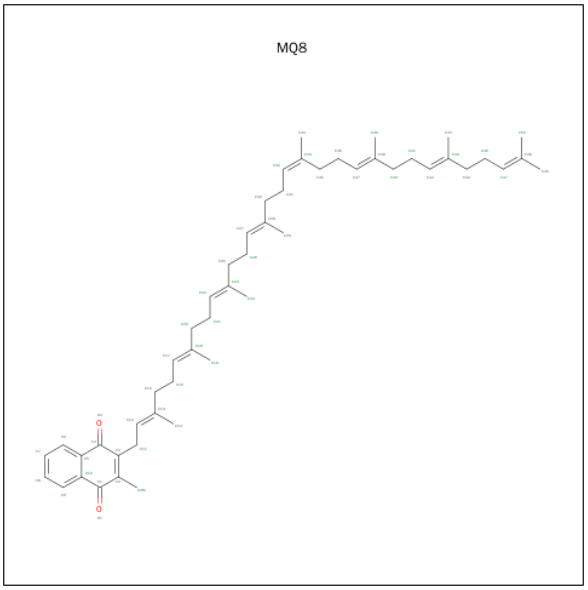
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



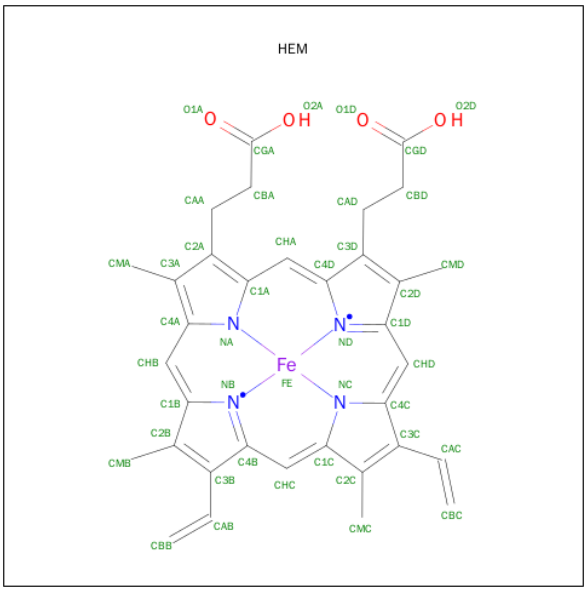
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



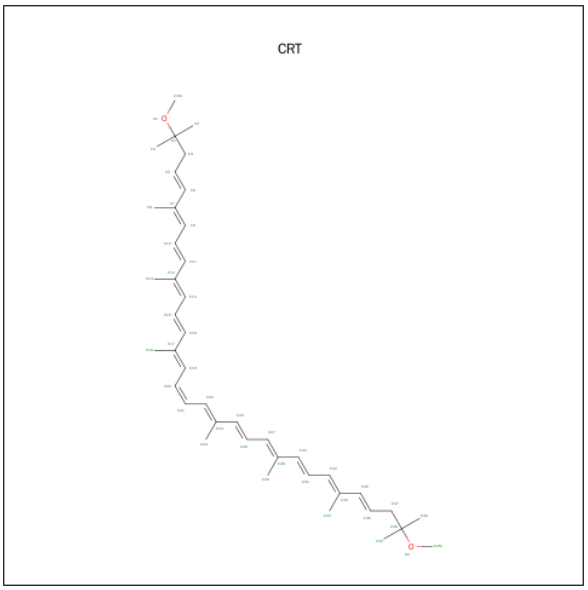
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			53	51	2		

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



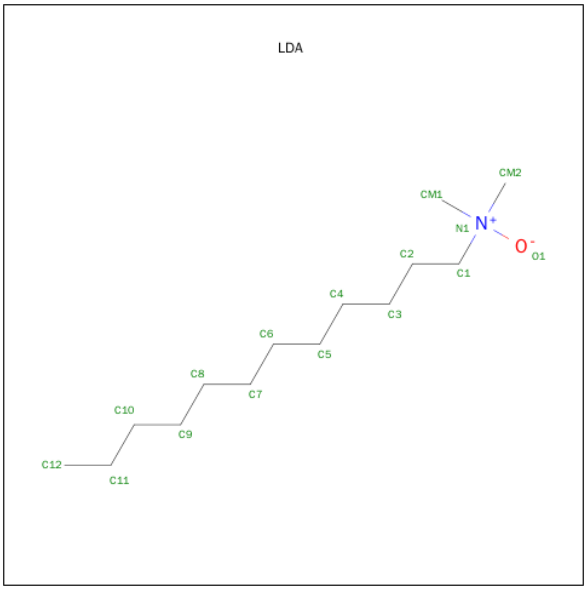
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



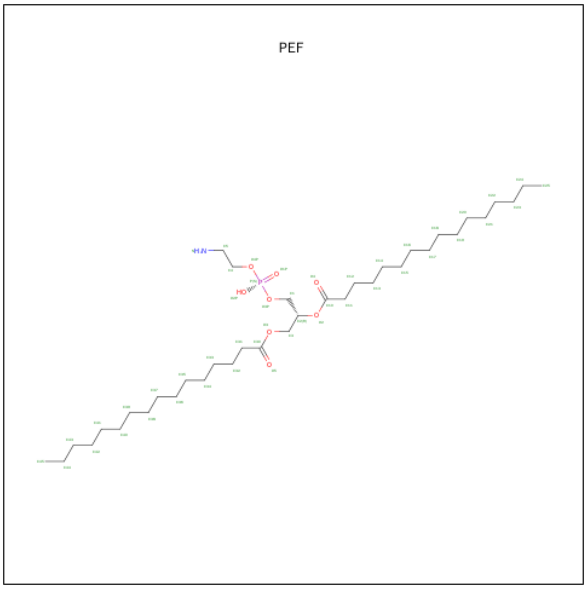
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 44 42 2	0	0

- 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		

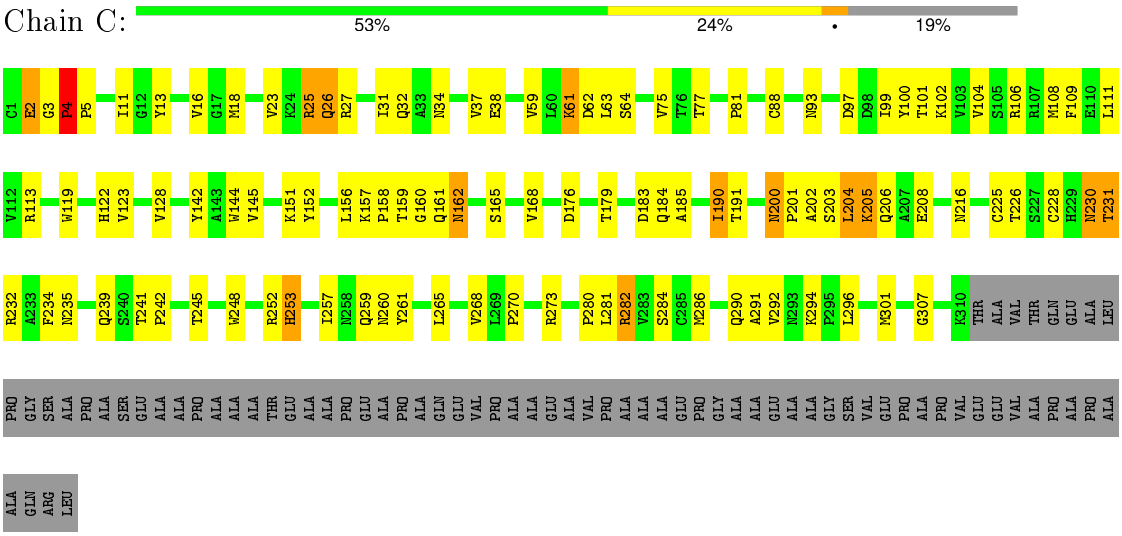
3 Residue-property plots (i)

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.

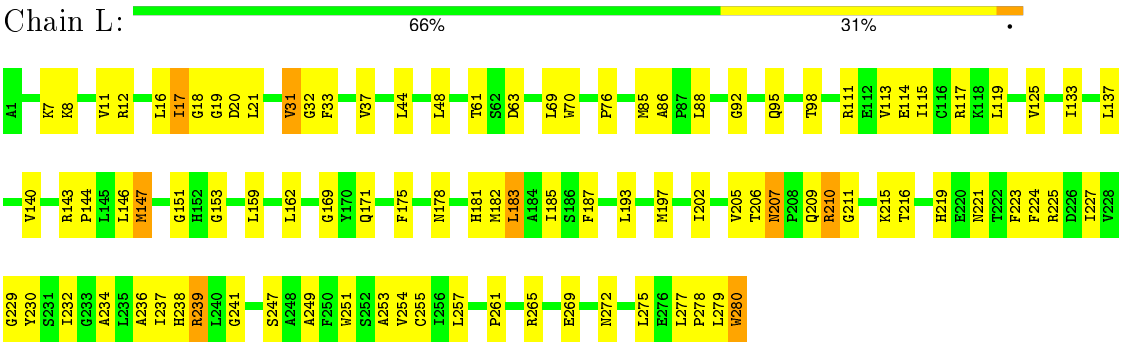
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



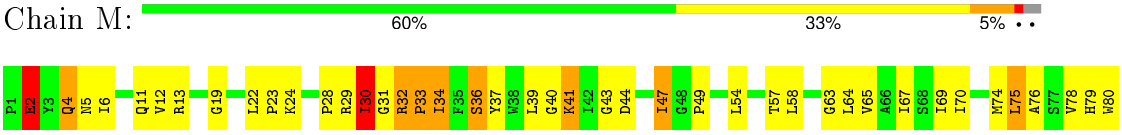
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

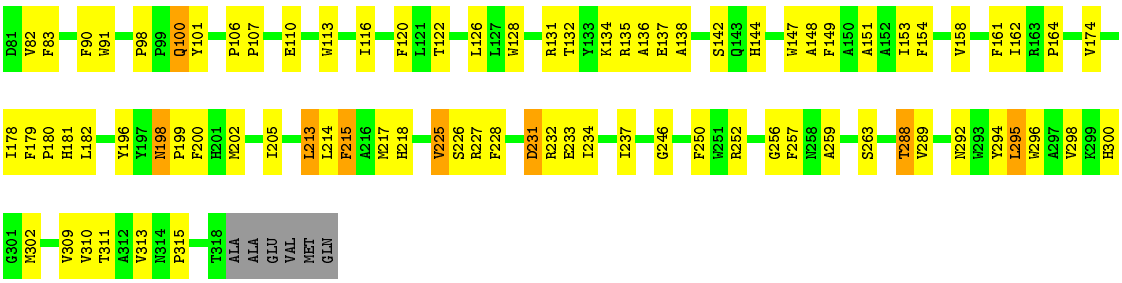
Chain L:



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

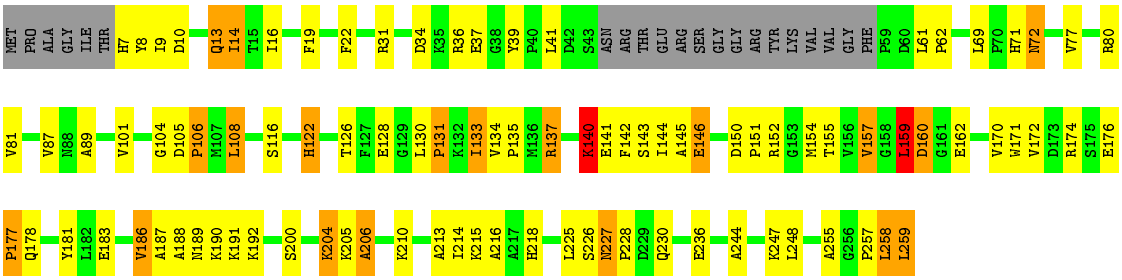
Chain M:





• 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.

The worst 5 of 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

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
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

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 (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

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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 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
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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.