WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 01:11 am GMT

PDB ID	:	2VEE
Title	:	Structure of protoglobin from Methanosarcina acetivorans C2A
Authors	:	Nardini, M.; Pesce, A.; Thijs, L.; Saito, J.A.; Dewilde, S.; Alam, M.; Ascenzi, P.; Coletta, M.; Ciaccio, C.; Moens, L.; Bolognesi, M.
Deposited on	:	2007-10-22
Resolution	:	2.60 Å(reported)

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

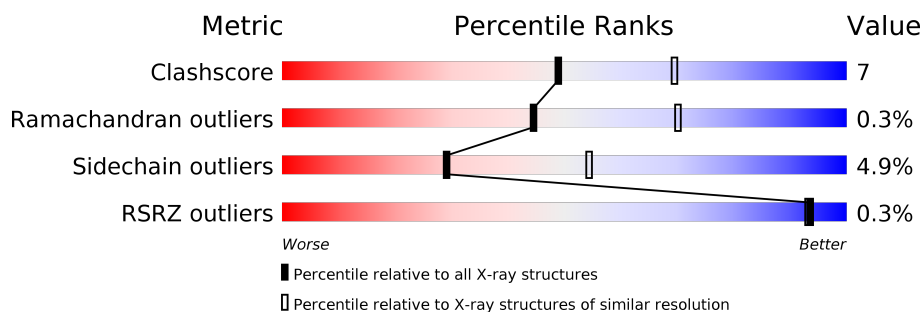|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.60 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		7
Ramachandran outliers		0.3%
Sidechain outliers		4.9%
RSRZ outliers		0.3%

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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	195	78% 18% • •
1	B	195	% 85% 10% • •
1	C	195	80% 16% • •
1	D	195	81% 15% • •
1	E	195	% 74% 21% • •
1	F	195	% 81% 14% • •
1	G	195	80% 17% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	195	

82%   13%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13310 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 PROTOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	B	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	C	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	D	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	E	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	F	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	G	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			
1	H	190	Total	C	N	O	S	0	0	0
			1591	1033	258	297	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
B	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
C	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
D	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
E	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
F	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
G	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9
H	101	SER	CYS	ENGINEERED MUTATION	UNP Q8TLY9

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	29	Total	O	0	0
			29	29		
3	C	26	Total	O	0	0
			26	26		
3	D	29	Total	O	0	0
			29	29		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	25	Total 25	O 25	0	0
3	F	32	Total 32	O 32	0	0
3	G	24	Total 24	O 24	0	0
3	H	34	Total 34	O 34	0	0

3   Residue-property plots ⓘ

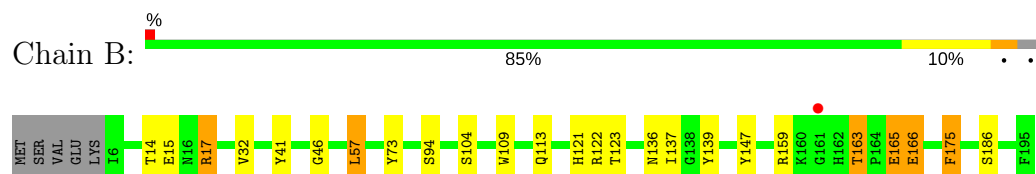These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.
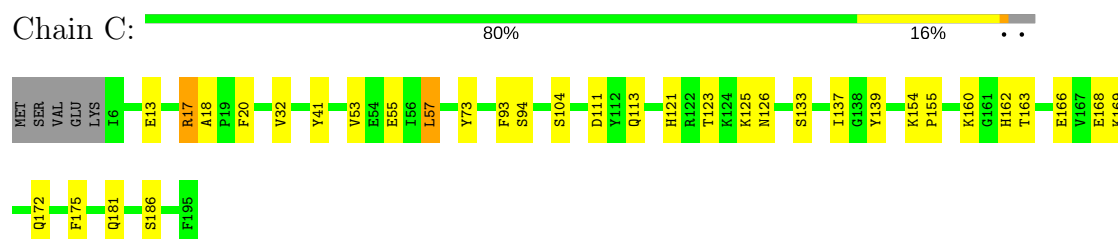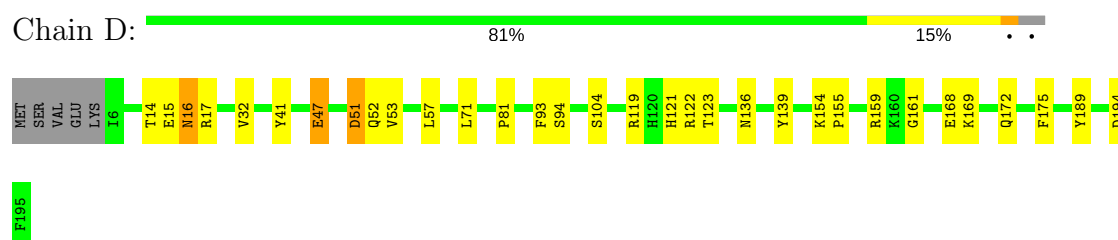
- Molecule 1: PROTOGLOBIN

Chain A:

- Molecule 1: PROTOGLOBIN

Chain B:

- Molecule 1: PROTOGLOBIN

Chain C:

- Molecule 1: PROTOGLOBIN

Chain D:

- Molecule 1: PROTOGLOBIN

Chain E:

MET SER VAL GLU LYS I6 R17 F20 K26 V32 Y41 I42 Q43 E47 V48 Q52 E55 I56 L57 D58 L71 Y72 Y73 P81 R90 F93 L98 N102 Q113 L118 H121 R122 T123 K124 K125 N126 S133 N136 I137 G138 Y139

A144 P148 K154 P155 R159 K160 G161 H162 E166 Q172 F175 K176 W185 S186 Y189 V190 F195

• Molecule 1: PROTOGLOBIN

Chain F:

%

81%   14%

MET SER VAL GLU LYS I6 E15 E39 Q43 Q52 V53 L57 W60 F93 S94 S101 Q113 R119 H120 H121 R122 T123 K124 K125 N126 S133 V134 P135 N136 Y139 V143 K154 P155 R159 K160 G161 H162 Q172 F175 K176 W185 S186

Y189 F195

• Molecule 1: PROTOGLOBIN

Chain G:

80%   17%

MET SER VAL GLU LYS I6 K29 V32 Q43 K44 V48 V53 L57 Y72 F93 S94 S101 W109 Q113 H121 R122 T123 V134 P135 N136 Y139 F145 P148 K154 P155 R159 K160 T163 E166 V167 E168 K169 M170 Y171 Q172

F175 S186 Y189 D194 F195

• Molecule 1: PROTOGLOBIN

Chain H:

82%   13%

MET SER VAL GLU LYS I6 T14 E15 V32 E37 Y41 Q52 V53 E54 L57 Y72 Y73 F93 L98 N102 Q113 R119 H120 H121 R122 T123 K124 K125 N126 I137 G138 Y139 I149 R159 K160 T163 E166 Q181 W185 S186

Y189 F195

4 Data and refinement statistics (i)

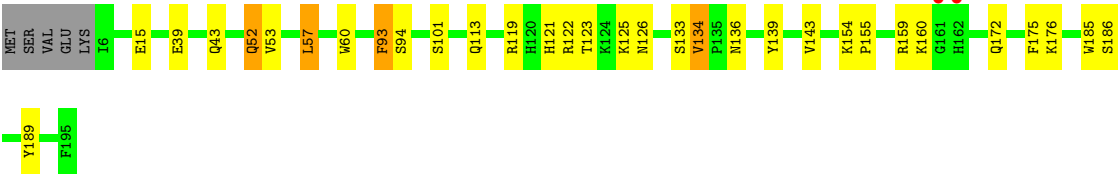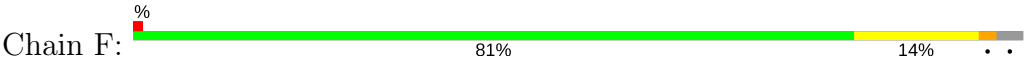| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.93Å 48.53Å 161.07Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	160.13 – 2.60 50.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (160.13-2.60) 51.0 (50.12-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.263 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.0	EDS
L-test for twinning[2]	$< |L| > = 0.53, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13310	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6228e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.38	0/1641	0.53	0/2231
1	B	0.38	0/1641	0.52	0/2231
1	C	0.39	0/1641	0.55	0/2231
1	D	0.38	0/1641	0.54	0/2231
1	E	0.38	0/1641	0.54	0/2231
1	F	0.39	0/1641	0.54	0/2231
1	G	0.37	0/1641	0.53	0/2231
1	H	0.38	0/1641	0.54	0/2231
All	All	0.38	0/13128	0.54	0/17848

There are no bond length outliers.

There are no bond angle outliers.

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	A	1591	0	1519	28	0
1	B	1591	0	1519	15	0
1	C	1591	0	1519	18	0
1	D	1591	0	1519	16	0
1	E	1591	0	1519	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1591	0	1519	21	0
1	G	1591	0	1519	20	0
1	H	1591	0	1519	19	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	4	0
2	H	43	0	30	2	0
3	A	39	0	0	0	0
3	B	29	0	0	0	0
3	C	26	0	0	1	0
3	D	29	0	0	1	0
3	E	25	0	0	1	0
3	F	32	0	0	0	0
3	G	24	0	0	0	0
3	H	34	0	0	0	0
All	All	13310	0	12392	174	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 7.

All (174) 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)
1:A:14:THR:O	1:A:15:GLU:HG3	1.24	1.25
1:A:14:THR:O	1:A:15:GLU:CG	1.95	1.14
1:E:17:ARG:HH11	1:E:17:ARG:HG3	1.05	1.08
1:C:57:LEU:HD21	1:C:94:SER:HB2	1.55	0.89
1:B:57:LEU:HD21	1:B:94:SER:HB2	1.54	0.88
1:F:57:LEU:HD21	1:F:94:SER:HB3	1.57	0.86
1:B:163:THR:HG23	1:B:166:GLU:HB2	1.61	0.82
1:E:17:ARG:NH1	1:E:17:ARG:HG3	1.84	0.79
1:D:14:THR:HG22	1:D:16:ASN:H	1.49	0.78
1:G:57:LEU:HD21	1:G:94:SER:HB2	1.66	0.77
1:C:17:ARG:HA	3:C:2002:HOH:O	1.87	0.73
1:B:121:HIS:HD2	1:B:123:THR:OG1	1.70	0.73
2:E:1196:HEM:HMB1	2:E:1196:HEM:HBB2	1.70	0.73
1:E:17:ARG:CG	1:E:17:ARG:HH11	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD11	1:D:94:SER:HB2	1.77	0.67
1:D:121:HIS:HD2	1:D:123:THR:OG1	1.78	0.67
1:F:53:VAL:CG1	1:F:94:SER:HB2	2.26	0.66
2:G:1196:HEM:HBB2	2:G:1196:HEM:HMB2	1.77	0.65
1:B:14:THR:O	1:B:15:GLU:HB2	1.99	0.62
1:H:52:GLN:NE2	1:H:159:ARG:HD2	2.15	0.62
1:C:154:LYS:HB3	1:C:155:PRO:HD3	1.81	0.61
1:A:57:LEU:HD11	1:A:94:SER:HB2	1.84	0.60
2:C:1196:HEM:HMB1	2:C:1196:HEM:HBB2	1.84	0.60
1:F:53:VAL:HG13	1:F:94:SER:HB2	1.84	0.59
1:G:53:VAL:HG11	1:G:94:SER:OG	2.03	0.59
1:H:57:LEU:HD21	1:H:93:PHE:HB3	1.83	0.58
1:F:57:LEU:CD2	1:F:94:SER:HB3	2.31	0.58
1:C:41:TYR:HE2	1:C:166:GLU:HG3	1.69	0.58
1:A:14:THR:O	1:A:15:GLU:HG2	2.01	0.57
1:C:41:TYR:CZ	1:C:169:LYS:HE2	2.40	0.56
1:E:17:ARG:NH1	1:E:17:ARG:CG	2.58	0.56
1:E:57:LEU:HD21	1:E:93:PHE:HB3	1.88	0.56
1:F:125:LYS:HE2	1:F:134:VAL:O	2.06	0.56
2:E:1196:HEM:CMB	2:E:1196:HEM:HBB2	2.34	0.55
1:F:39:GLU:O	1:F:43:GLN:HG3	2.06	0.55
1:D:53:VAL:HG11	1:D:94:SER:OG	2.05	0.55
1:G:154:LYS:HB3	1:G:155:PRO:HD3	1.87	0.55
1:G:139:TYR:HB2	1:G:189:TYR:CD2	2.42	0.55
1:E:58:ASP:OD1	1:E:90:ARG:NH2	2.39	0.55
1:B:41:TYR:HE2	1:B:166:GLU:HG2	1.72	0.54
1:B:165:GLU:HG2	1:B:166:GLU:N	2.22	0.54
1:A:14:THR:C	1:A:15:GLU:CG	2.76	0.54
2:F:1196:HEM:HBB2	2:F:1196:HEM:HMB1	1.90	0.53
1:F:121:HIS:HD2	1:F:123:THR:OG1	1.91	0.53
1:H:52:GLN:HE22	1:H:159:ARG:HD2	1.72	0.53
1:A:122:ARG:N	1:A:136:ASN:HD22	2.06	0.53
2:D:1196:HEM:HBB2	2:D:1196:HEM:HMB1	1.90	0.53
1:A:122:ARG:H	1:A:136:ASN:HD22	1.58	0.52
1:E:43:GLN:NE2	3:E:2009:HOH:O	2.41	0.52
1:G:145:PHE:HB3	2:G:1196:HEM:HAB	1.91	0.52
1:E:122:ARG:N	1:E:136:ASN:HD22	2.08	0.52
1:A:154:LYS:HB3	1:A:155:PRO:HD3	1.92	0.52
1:E:139:TYR:OH	1:E:186:SER:HB3	2.09	0.52
1:C:53:VAL:HG11	1:C:94:SER:OG	2.10	0.52
1:E:121:HIS:HD2	1:E:123:THR:OG1	1.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LYS:O	1:A:126:ASN:HB2	2.10	0.51
1:B:122:ARG:N	1:B:136:ASN:HD22	2.08	0.51
1:A:54:GLU:HA	1:A:54:GLU:OE2	2.10	0.51
2:G:1196:HEM:HBB2	2:G:1196:HEM:CMB	2.40	0.51
2:D:1196:HEM:CMB	2:D:1196:HEM:HBB2	2.41	0.51
1:E:126:ASN:OD1	1:E:133:SER:HB3	2.12	0.50
1:A:194:ASP:OD2	1:C:121:HIS:HE1	1.94	0.50
1:E:113:GLN:NE2	1:E:185:TRP:HE1	2.10	0.50
1:H:14:THR:O	1:H:15:GLU:HB2	2.12	0.50
1:H:121:HIS:O	1:H:125:LYS:HB2	2.12	0.50
1:G:121:HIS:HD2	1:G:123:THR:OG1	1.94	0.49
2:C:1196:HEM:HBB2	2:C:1196:HEM:CMB	2.42	0.49
1:C:121:HIS:HD2	1:C:123:THR:OG1	1.96	0.49
1:H:163:THR:HB	1:H:166:GLU:HB2	1.94	0.49
2:A:1196:HEM:HBB2	2:A:1196:HEM:HMB1	1.95	0.49
1:D:139:TYR:HB2	1:D:189:TYR:CD2	2.49	0.48
1:F:53:VAL:HG11	1:F:94:SER:HB2	1.96	0.48
1:B:175:PHE:O	1:B:175:PHE:HD1	1.97	0.48
1:F:60:TRP:CZ3	1:F:93:PHE:CE1	3.01	0.48
1:A:14:THR:C	1:A:15:GLU:HG3	2.17	0.48
1:A:51:ASP:HB2	1:A:160:LYS:NZ	2.29	0.48
1:G:72:TYR:CZ	1:G:134:VAL:HG11	2.49	0.48
1:E:118:LEU:HD22	1:E:123:THR:HG21	1.96	0.47
1:E:186:SER:O	1:E:190:VAL:HG23	2.13	0.47
1:E:52:GLN:O	1:E:55:GLU:HB2	2.14	0.47
1:G:145:PHE:HA	1:G:148:PRO:HD2	1.95	0.47
2:A:1196:HEM:HBB2	2:A:1196:HEM:CMB	2.44	0.47
1:G:145:PHE:CB	2:G:1196:HEM:HAB	2.45	0.47
1:F:125:LYS:O	1:F:126:ASN:HB2	2.13	0.47
1:H:98:LEU:O	1:H:102:ASN:HB2	2.14	0.47
1:B:73:TYR:CE1	1:B:137:ILE:HA	2.50	0.47
1:F:139:TYR:CZ	1:F:186:SER:HB3	2.50	0.47
1:A:139:TYR:HB2	1:A:189:TYR:CD2	2.50	0.47
1:G:122:ARG:HB3	1:G:136:ASN:HB2	1.97	0.47
1:H:113:GLN:NE2	1:H:181:GLN:HG2	2.29	0.47
1:C:125:LYS:O	1:C:126:ASN:HB2	2.14	0.47
1:C:160:LYS:HB3	1:C:162:HIS:HD2	1.80	0.46
1:D:121:HIS:CD2	1:D:123:THR:OG1	2.65	0.46
1:H:125:LYS:O	1:H:126:ASN:HB2	2.15	0.46
1:G:122:ARG:N	1:G:136:ASN:HD22	2.13	0.46
1:D:168:GLU:O	1:D:172:GLN:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:TYR:HE2	1:E:166:GLU:HG3	1.81	0.46
1:A:53:VAL:HG11	1:A:94:SER:OG	2.16	0.46
1:G:139:TYR:OH	1:G:186:SER:HB3	2.16	0.45
1:A:47:GLU:H	1:A:47:GLU:HG2	1.42	0.45
1:C:126:ASN:OD1	1:C:133:SER:HB3	2.16	0.45
1:F:113:GLN:NE2	1:F:185:TRP:HE1	2.14	0.45
1:G:109:TRP:O	1:G:113:GLN:HG2	2.17	0.45
1:D:47:GLU:HG2	1:D:47:GLU:H	1.52	0.45
1:B:17:ARG:NH2	1:C:13:GLU:HA	2.31	0.45
1:A:139:TYR:OH	1:A:186:SER:HB3	2.17	0.45
1:H:54:GLU:OE2	1:H:54:GLU:HA	2.17	0.45
1:B:109:TRP:O	1:B:113:GLN:HG2	2.17	0.45
1:G:44:LYS:O	1:G:48:VAL:HG23	2.17	0.45
1:F:52:GLN:HE21	1:F:159:ARG:HH11	1.63	0.45
1:H:139:TYR:OH	1:H:186:SER:HB3	2.18	0.44
2:B:1196:HEM:HBB2	2:B:1196:HEM:CMB	2.46	0.44
1:G:29:LYS:HA	1:G:32:VAL:HG12	1.98	0.44
1:H:121:HIS:HD2	1:H:123:THR:OG1	2.01	0.44
1:A:51:ASP:HB2	1:A:160:LYS:HZ1	1.82	0.44
1:D:122:ARG:HB3	1:D:136:ASN:HB2	1.99	0.44
1:F:122:ARG:N	1:F:136:ASN:HD22	2.15	0.44
1:F:119:ARG:NH1	2:F:1196:HEM:O2A	2.50	0.44
1:E:139:TYR:HB2	1:E:189:TYR:CD2	2.53	0.43
1:E:172:GLN:O	1:E:176:LYS:HG3	2.18	0.43
1:E:73:TYR:CE1	1:E:137:ILE:HA	2.53	0.43
1:A:139:TYR:CZ	1:A:186:SER:HB3	2.53	0.43
1:F:126:ASN:OD1	1:F:133:SER:HB3	2.18	0.43
1:A:72:TYR:CZ	1:A:134:VAL:HG11	2.53	0.43
1:C:73:TYR:CE1	1:C:137:ILE:HA	2.54	0.43
1:D:71:LEU:HD21	1:D:81:PRO:HG3	1.99	0.43
1:C:18:ALA:HB2	1:C:111:ASP:HA	2.01	0.43
1:D:119:ARG:NH1	2:D:1196:HEM:O2A	2.51	0.43
1:F:139:TYR:OH	1:F:186:SER:HB3	2.19	0.43
1:A:168:GLU:O	1:A:172:GLN:HG2	2.18	0.43
1:E:154:LYS:HB3	1:E:155:PRO:HD3	2.00	0.43
1:A:109:TRP:O	1:A:113:GLN:HG2	2.18	0.43
1:C:139:TYR:OH	1:C:186:SER:HB3	2.19	0.43
2:B:1196:HEM:HMB1	2:B:1196:HEM:HBB2	2.01	0.42
1:B:147:TYR:CD2	1:B:147:TYR:C	2.92	0.42
1:E:47:GLU:H	1:E:47:GLU:HG2	1.56	0.42
1:A:121:HIS:CD2	1:A:123:THR:H	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LEU:O	1:E:102:ASN:ND2	2.51	0.42
1:A:121:HIS:HD2	1:A:123:THR:OG1	2.02	0.42
1:D:41:TYR:CZ	1:D:169:LYS:HD3	2.55	0.42
1:G:122:ARG:H	1:G:136:ASN:HD22	1.67	0.42
1:B:175:PHE:CD1	1:B:175:PHE:C	2.92	0.42
1:E:48:VAL:HG13	1:E:160:LYS:HB2	2.01	0.42
2:F:1196:HEM:HBB2	2:F:1196:HEM:CMB	2.50	0.42
1:C:113:GLN:NE2	1:C:181:GLN:HG2	2.34	0.42
1:D:154:LYS:HB3	1:D:155:PRO:HD3	2.02	0.42
1:F:154:LYS:HB3	1:F:155:PRO:HD3	2.02	0.42
1:H:139:TYR:HB2	1:H:189:TYR:CD2	2.55	0.42
1:A:186:SER:O	1:A:190:VAL:HG23	2.20	0.41
1:G:166:GLU:O	1:G:170:MET:HG3	2.19	0.41
1:H:149:ILE:HG13	2:H:1196:HEM:HBB2	2.01	0.41
1:F:172:GLN:O	1:F:176:LYS:HG3	2.20	0.41
1:H:73:TYR:CE1	1:H:137:ILE:HA	2.55	0.41
1:A:57:LEU:HD21	1:A:93:PHE:HB3	2.02	0.41
1:G:168:GLU:O	1:G:172:GLN:HG2	2.20	0.41
1:G:43:GLN:HG3	1:G:101:SER:O	2.20	0.41
1:C:160:LYS:HB3	1:C:162:HIS:CD2	2.56	0.41
1:F:139:TYR:HB2	1:F:189:TYR:CD2	2.55	0.41
1:G:194:ASP:OD2	1:H:121:HIS:HE1	2.04	0.41
1:H:119:ARG:NH1	2:H:1196:HEM:O2A	2.48	0.41
1:B:139:TYR:CZ	1:B:186:SER:HB3	2.56	0.41
1:H:113:GLN:NE2	1:H:185:TRP:HE1	2.17	0.41
1:A:73:TYR:CE1	1:A:137:ILE:HA	2.55	0.41
1:F:139:TYR:CE2	1:F:143:VAL:CG2	3.04	0.41
1:E:144:ALA:O	1:E:148:PRO:HD2	2.21	0.41
1:H:37:GLU:O	1:H:41:TYR:HD1	2.04	0.41
1:D:52:GLN:HA	3:D:2012:HOH:O	2.20	0.40
1:E:139:TYR:CZ	1:E:186:SER:HB3	2.56	0.40
1:B:121:HIS:HE1	1:D:194:ASP:OD2	2.03	0.40
1:D:51:ASP:HB3	1:D:52:GLN:HG3	2.03	0.40
1:E:125:LYS:O	1:E:126:ASN:HB2	2.21	0.40
1:E:71:LEU:HD21	1:E:81:PRO:HG3	2.04	0.40
1:A:126:ASN:OD1	1:A:133:SER:HB3	2.21	0.40
1:C:168:GLU:O	1:C:172:GLN:HG2	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	A	188/195 (96%)	178 (95%)	10 (5%)	0	100	100
1	B	188/195 (96%)	178 (95%)	9 (5%)	1 (0%)	32	58
1	C	188/195 (96%)	179 (95%)	9 (5%)	0	100	100
1	D	188/195 (96%)	181 (96%)	6 (3%)	1 (0%)	32	58
1	E	188/195 (96%)	179 (95%)	8 (4%)	1 (0%)	32	58
1	F	188/195 (96%)	179 (95%)	8 (4%)	1 (0%)	32	58
1	G	188/195 (96%)	181 (96%)	7 (4%)	0	100	100
1	H	188/195 (96%)	178 (95%)	9 (5%)	1 (0%)	32	58
All	All	1504/1560 (96%)	1433 (95%)	66 (4%)	5 (0%)	44	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	160	LYS
1	E	72	TYR
1	H	72	TYR
1	B	46	GLY
1	D	161	GLY

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	A	167/172 (97%)	158 (95%)	9 (5%)	26	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	167/172 (97%)	158 (95%)	9 (5%)	26	49
1	C	167/172 (97%)	158 (95%)	9 (5%)	26	49
1	D	167/172 (97%)	157 (94%)	10 (6%)	22	44
1	E	167/172 (97%)	157 (94%)	10 (6%)	22	44
1	F	167/172 (97%)	160 (96%)	7 (4%)	34	62
1	G	167/172 (97%)	161 (96%)	6 (4%)	40	68
1	H	167/172 (97%)	161 (96%)	6 (4%)	40	68
All	All	1336/1376 (97%)	1270 (95%)	66 (5%)	29	54

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	16	ASN
1	A	17	ARG
1	A	20	PHE
1	A	32	VAL
1	A	47	GLU
1	A	93	PHE
1	A	101	SER
1	A	159	ARG
1	B	17	ARG
1	B	32	VAL
1	B	57	LEU
1	B	104	SER
1	B	159	ARG
1	B	163	THR
1	B	165	GLU
1	B	166	GLU
1	B	175	PHE
1	C	17	ARG
1	C	20	PHE
1	C	32	VAL
1	C	55	GLU
1	C	57	LEU
1	C	93	PHE
1	C	104	SER
1	C	163	THR
1	C	175	PHE
1	D	15	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	16	ASN
1	D	17	ARG
1	D	32	VAL
1	D	47	GLU
1	D	51	ASP
1	D	93	PHE
1	D	104	SER
1	D	159	ARG
1	D	175	PHE
1	E	17	ARG
1	E	20	PHE
1	E	26	LYS
1	E	32	VAL
1	E	43	GLN
1	E	47	GLU
1	E	57	LEU
1	E	93	PHE
1	E	159	ARG
1	E	175	PHE
1	F	15	GLU
1	F	52	GLN
1	F	57	LEU
1	F	93	PHE
1	F	101	SER
1	F	134	VAL
1	F	175	PHE
1	G	57	LEU
1	G	93	PHE
1	G	159	ARG
1	G	160	LYS
1	G	163	THR
1	G	175	PHE
1	H	14	THR
1	H	32	VAL
1	H	57	LEU
1	H	93	PHE
1	H	160	LYS
1	H	166	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	136	ASN
1	B	52	GLN
1	B	121	HIS
1	B	136	ASN
1	C	52	GLN
1	C	113	GLN
1	C	121	HIS
1	C	162	HIS
1	D	16	ASN
1	D	113	GLN
1	D	121	HIS
1	D	136	ASN
1	D	162	HIS
1	E	43	GLN
1	E	52	GLN
1	E	113	GLN
1	E	121	HIS
1	E	136	ASN
1	F	52	GLN
1	F	113	GLN
1	F	121	HIS
1	F	136	ASN
1	G	16	ASN
1	G	52	GLN
1	G	69	HIS
1	G	113	GLN
1	G	121	HIS
1	G	136	ASN
1	H	52	GLN
1	H	113	GLN
1	H	121	HIS
1	H	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

8 ligands are modelled in this entry.

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	$\#|Z| > 2$
2	HEM	A	1196	1	28,50,50	2.21	7 (25%)	17,82,82	1.64	4 (23%)
2	HEM	B	1196	1	28,50,50	2.22	7 (25%)	17,82,82	1.64	4 (23%)
2	HEM	C	1196	1	28,50,50	2.20	7 (25%)	17,82,82	1.59	3 (17%)
2	HEM	D	1196	1	28,50,50	2.24	7 (25%)	17,82,82	1.52	3 (17%)
2	HEM	E	1196	1	28,50,50	2.18	7 (25%)	17,82,82	1.70	5 (29%)
2	HEM	F	1196	1	28,50,50	2.15	7 (25%)	17,82,82	1.66	5 (29%)
2	HEM	G	1196	1	28,50,50	2.19	7 (25%)	17,82,82	1.69	6 (35%)
2	HEM	H	1196	1	28,50,50	2.18	6 (21%)	17,82,82	1.95	6 (35%)

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
2	HEM	A	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	B	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	C	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	D	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	E	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	F	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	G	1196	1	-	0/6/54/54	0/0/8/8
2	HEM	H	1196	1	-	0/6/54/54	0/0/8/8

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1196	HEM	C3C-C2C	-4.91	1.33	1.40
2	E	1196	HEM	C3C-C2C	-4.84	1.34	1.40
2	D	1196	HEM	C3C-C2C	-4.72	1.34	1.40
2	B	1196	HEM	C3C-C2C	-4.61	1.34	1.40
2	A	1196	HEM	C3C-C2C	-4.59	1.34	1.40
2	C	1196	HEM	C3C-C2C	-4.58	1.34	1.40
2	G	1196	HEM	C3C-C2C	-4.49	1.34	1.40
2	F	1196	HEM	C3C-C2C	-4.46	1.34	1.40
2	D	1196	HEM	C3B-C2B	-4.42	1.34	1.40
2	A	1196	HEM	C3B-C2B	-4.42	1.34	1.40
2	E	1196	HEM	C3B-C2B	-4.31	1.34	1.40
2	B	1196	HEM	C3B-C2B	-4.28	1.34	1.40
2	H	1196	HEM	C3B-C2B	-4.08	1.35	1.40
2	G	1196	HEM	C3B-C2B	-3.97	1.35	1.40
2	F	1196	HEM	C3B-C2B	-3.85	1.35	1.40
2	C	1196	HEM	C3B-C2B	-3.85	1.35	1.40
2	E	1196	HEM	C4D-ND	2.02	1.39	1.36
2	D	1196	HEM	CAA-C2A	2.07	1.55	1.52
2	E	1196	HEM	CAA-C2A	2.07	1.55	1.52
2	A	1196	HEM	CAA-C2A	2.17	1.55	1.52
2	C	1196	HEM	CAA-C2A	2.23	1.55	1.52
2	B	1196	HEM	CAA-C2A	2.26	1.55	1.52
2	A	1196	HEM	C4D-ND	2.26	1.39	1.36
2	H	1196	HEM	C4D-ND	2.36	1.39	1.36
2	G	1196	HEM	CAA-C2A	2.36	1.56	1.52
2	F	1196	HEM	CAA-C2A	2.38	1.56	1.52
2	G	1196	HEM	C4D-ND	2.42	1.39	1.36
2	F	1196	HEM	C4D-ND	2.44	1.39	1.36
2	C	1196	HEM	C4D-ND	2.44	1.39	1.36
2	D	1196	HEM	C4D-ND	2.51	1.39	1.36
2	B	1196	HEM	C4D-ND	2.77	1.40	1.36
2	F	1196	HEM	C3C-CAC	3.51	1.54	1.47
2	G	1196	HEM	C3C-CAC	3.53	1.54	1.47
2	H	1196	HEM	C3C-CAC	3.57	1.54	1.47
2	E	1196	HEM	C3C-CAC	3.59	1.54	1.47
2	E	1196	HEM	C3B-CAB	3.59	1.55	1.47
2	C	1196	HEM	C3C-CAC	3.62	1.54	1.47
2	D	1196	HEM	C3C-CAC	3.68	1.55	1.47
2	A	1196	HEM	C3C-CAC	3.75	1.55	1.47
2	G	1196	HEM	C3B-CAB	3.84	1.55	1.47
2	B	1196	HEM	C3B-CAB	3.85	1.55	1.47
2	D	1196	HEM	C3B-CAB	3.85	1.55	1.47
2	H	1196	HEM	C3B-CAB	3.86	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1196	HEM	C3C-CAC	3.88	1.55	1.47
2	A	1196	HEM	C3B-CAB	3.89	1.55	1.47
2	F	1196	HEM	C3B-CAB	3.91	1.55	1.47
2	C	1196	HEM	C3B-CAB	3.93	1.55	1.47
2	H	1196	HEM	C3D-C2D	5.44	1.53	1.37
2	E	1196	HEM	C3D-C2D	5.44	1.53	1.37
2	G	1196	HEM	C3D-C2D	5.55	1.54	1.37
2	B	1196	HEM	C3D-C2D	5.55	1.54	1.37
2	A	1196	HEM	C3D-C2D	5.56	1.54	1.37
2	F	1196	HEM	C3D-C2D	5.57	1.54	1.37
2	C	1196	HEM	C3D-C2D	5.58	1.54	1.37
2	D	1196	HEM	C3D-C2D	5.65	1.54	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1196	HEM	CBD-CAD-C3D	-4.88	103.15	112.47
2	B	1196	HEM	CBD-CAD-C3D	-3.43	105.92	112.47
2	E	1196	HEM	C1D-C2D-C3D	-3.30	104.70	107.00
2	A	1196	HEM	CBD-CAD-C3D	-2.99	106.77	112.47
2	A	1196	HEM	CAA-CBA-CGA	-2.89	107.73	112.66
2	H	1196	HEM	CAA-CBA-CGA	-2.87	107.76	112.66
2	G	1196	HEM	CMA-C3A-C4A	-2.84	124.09	128.46
2	D	1196	HEM	CAA-CBA-CGA	-2.81	107.86	112.66
2	G	1196	HEM	C1D-C2D-C3D	-2.73	105.09	107.00
2	E	1196	HEM	CAA-CBA-CGA	-2.72	108.00	112.66
2	H	1196	HEM	C1D-C2D-C3D	-2.69	105.12	107.00
2	A	1196	HEM	C1D-C2D-C3D	-2.68	105.13	107.00
2	C	1196	HEM	CBD-CAD-C3D	-2.67	107.36	112.47
2	F	1196	HEM	C1D-C2D-C3D	-2.64	105.16	107.00
2	E	1196	HEM	CBD-CAD-C3D	-2.59	107.52	112.47
2	G	1196	HEM	CBD-CAD-C3D	-2.58	107.54	112.47
2	E	1196	HEM	CMA-C3A-C4A	-2.43	124.74	128.46
2	B	1196	HEM	CMA-C3A-C4A	-2.40	124.78	128.46
2	B	1196	HEM	C1D-C2D-C3D	-2.35	105.36	107.00
2	F	1196	HEM	CAA-CBA-CGA	-2.31	108.72	112.66
2	C	1196	HEM	C1D-C2D-C3D	-2.28	105.41	107.00
2	F	1196	HEM	CMA-C3A-C4A	-2.22	125.06	128.46
2	D	1196	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
2	H	1196	HEM	CMA-C3A-C4A	-2.20	125.09	128.46
2	F	1196	HEM	CAD-CBD-CGD	-2.18	108.93	112.66
2	G	1196	HEM	C3C-C4C-NC	-2.04	107.08	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1196	HEM	C4C-C3C-C2C	2.17	108.42	106.90
2	G	1196	HEM	C4C-C3C-C2C	2.23	108.45	106.90
2	E	1196	HEM	C4A-C3A-C2A	2.43	108.69	107.00
2	H	1196	HEM	C4A-C3A-C2A	2.58	108.79	107.00
2	A	1196	HEM	C4A-C3A-C2A	2.68	108.86	107.00
2	D	1196	HEM	C4A-C3A-C2A	2.79	108.93	107.00
2	G	1196	HEM	C4A-C3A-C2A	2.80	108.94	107.00
2	F	1196	HEM	C4A-C3A-C2A	2.86	108.99	107.00
2	B	1196	HEM	C4A-C3A-C2A	2.91	109.02	107.00
2	C	1196	HEM	C4A-C3A-C2A	3.11	109.16	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1196	HEM	2	0
2	B	1196	HEM	2	0
2	C	1196	HEM	2	0
2	D	1196	HEM	3	0
2	E	1196	HEM	2	0
2	F	1196	HEM	3	0
2	G	1196	HEM	4	0
2	H	1196	HEM	2	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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	190/195 (97%)	-0.63	0	100	100	22, 29, 43, 51	0
1	B	190/195 (97%)	-0.59	1 (0%)	90	89	22, 29, 43, 50	0
1	C	190/195 (97%)	-0.63	0	100	100	22, 29, 43, 51	0
1	D	190/195 (97%)	-0.65	0	100	100	22, 29, 43, 51	0
1	E	190/195 (97%)	-0.59	2 (1%)	80	77	22, 29, 43, 51	0
1	F	190/195 (97%)	-0.63	2 (1%)	80	77	21, 29, 43, 51	0
1	G	190/195 (97%)	-0.58	0	100	100	21, 29, 43, 51	0
1	H	190/195 (97%)	-0.61	0	100	100	22, 29, 43, 50	0
All	All	1520/1560 (97%)	-0.61	5 (0%)	93	93	21, 29, 43, 51	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	161	GLY	3.9
1	B	161	GLY	3.1
1	E	161	GLY	2.3
1	F	162	HIS	2.1
1	E	162	HIS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	HEM	H	1196	43/43	0.97	0.13	-0.03	7,20,22,24	0
2	HEM	F	1196	43/43	0.97	0.12	-0.19	7,20,22,24	0
2	HEM	D	1196	43/43	0.98	0.12	-0.33	7,20,22,24	0
2	HEM	A	1196	43/43	0.98	0.12	-0.47	7,20,22,24	0
2	HEM	E	1196	43/43	0.98	0.12	-0.68	7,20,22,24	0
2	HEM	C	1196	43/43	0.98	0.12	-0.80	7,20,22,24	0
2	HEM	B	1196	43/43	0.98	0.11	-0.88	7,20,22,24	0
2	HEM	G	1196	43/43	0.97	0.11	-1.26	7,20,22,24	0

6.5 Other polymers (i)

There are no such residues in this entry.