Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:33 AM GMT

PDB ID	:	2R7A
Title	:	Crystal Structure of a Periplasmic Heme Binding Protein from Shigella dysenteriae
Authors	:	Ho, W.W.; Li, H.; Poulos, T.L.
Deposited on	:	2007-09-07
Resolution	:	2.05 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 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	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 2.05 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
Rfree		0.250
Clashscore		16
Ramachandran outliers		0.3%
Sidechain outliers		2.1%
RSRZ outliers		5.8%

Worse ————————————————————————— *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
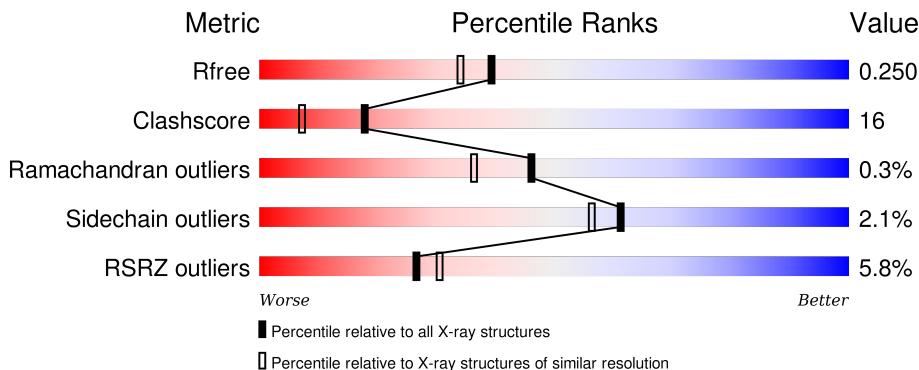
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	256	3% · 73% green, 27% yellow
1	B	256	2% · 72% green, 27% yellow ·
1	C	256	4% · 71% green, 27% yellow ·
1	D	256	14% · 64% green, 34% yellow ·
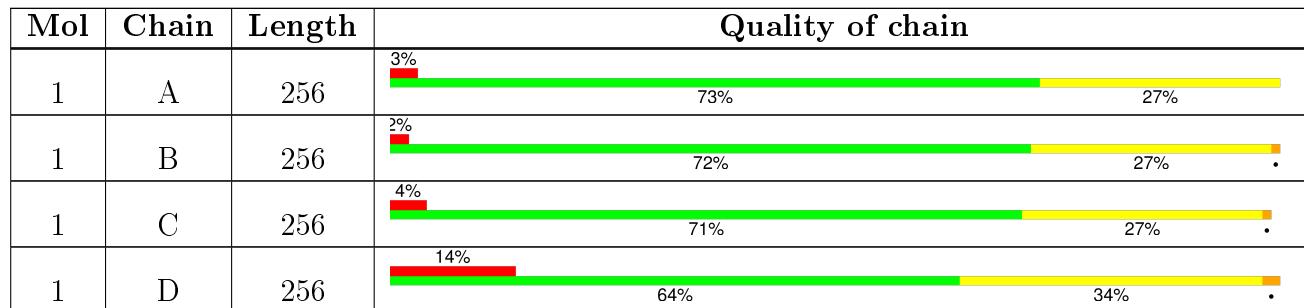
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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
2	HEM	A	600	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8283 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 Bacterial heme binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1934	1216	344	369	5			
1	B	256	Total	C	N	O	S	0	0	0
			1939	1219	345	370	5			
1	C	255	Total	C	N	O	S	0	0	0
			1934	1216	344	369	5			
1	D	255	Total	C	N	O	S	0	0	0
			1934	1216	344	369	5			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
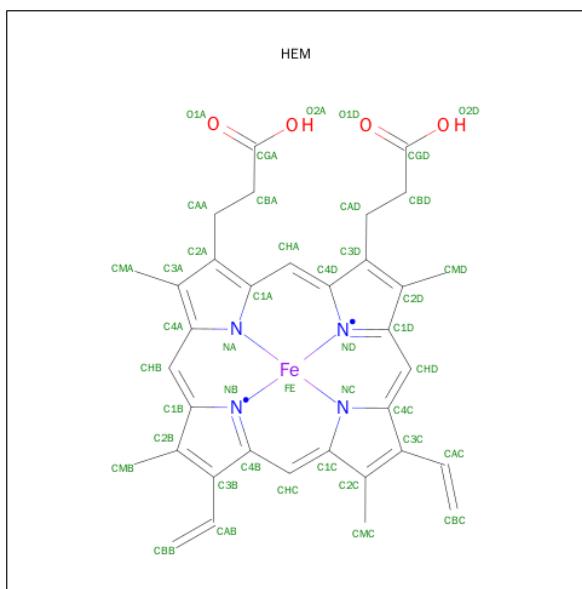
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	144	Total　O 144　　144	0	0
3	B	144	Total　O 144　　144	0	0
3	C	106	Total　O 106　　106	0	0
3	D	105	Total　O 105　　105	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.

- Molecule 1: Bacterial heme binding protein

- Molecule 1: Bacterial heme binding protein

- Molecule 1: Bacterial heme binding protein

S269 L270 H271 Q272 Q273 P276 Q277

• Molecule 1: Bacterial heme binding protein

14%

Chain D:

64%

34%

ALA A23 E24 R25 I26 V27 V28 A29 S32 L36 I37 M40 G41 A42 G43 E44 R45 V49 D50 L62 P63 H64 I65 G66 Y67 W68 K69 Q70 L71 S72 S73 E74 G75 I76 L77 R80 P81 D82 S83 T86 W87 Q88 D89 A90 G91 P92 Q93 I94 V95 L96 D97 Q98 L99

R100 A101 Q102 K103 V104 M105 V106 V107 T108 L109 V112 P113 K128 T129 L130 Q135 G136 D137 A138 Q142 R149 V150 V154 K158 A159 P160 V161 M164 F165 G170 G171 N194 E207 S208 L209 V216 T220 S221 Q222 M223 V224 D225 G226 D227 I228 N229

T238 W243 R247 I248 I249 T250 V251 D252 L255 I256 L257 G258 P261 A264 D265 V266 V267 E268 H271 Q272 Q273 L274 W275 P276 Q277

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.70Å 73.31Å 73.32Å 70.25° 79.02° 90.22°	Depositor
Resolution (Å)	43.86 – 2.05 43.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.86-2.05) 85.9 (43.86-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	2.28 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.255 0.207 , 0.250	Depositor DCC
R_{free} test set	6417 reflections (11.22%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Outliers	0 of 67701 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8283	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.31	0/1965	0.56	0/2676
1	B	0.32	0/1970	0.57	0/2683
1	C	0.31	0/1965	0.56	0/2676
1	D	0.29	0/1965	0.55	0/2676
All	All	0.31	0/7865	0.56	0/10711

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 (i)

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	1934	0	1977	55	0
1	B	1939	0	1983	59	0
1	C	1934	0	1978	62	0
1	D	1934	0	1978	84	0
2	A	43	0	30	3	0
3	A	144	0	0	8	0
3	B	144	0	0	5	0
3	C	106	0	0	5	0
3	D	105	0	0	9	0
All	All	8283	0	7946	248	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 16.

All (248) 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:220:THR:H	1:A:223:MET:HE3	1.21	1.06
1:D:44:GLU:HG3	1:D:45:ARG:HG3	1.49	0.94
1:A:240:THR:HG22	1:A:242:ALA:H	1.37	0.90
1:B:98:GLN:NE2	1:C:207:GLU:HG2	1.88	0.88
1:D:135:GLN:H	1:D:135:GLN:NE2	1.75	0.84
1:B:160:PRO:HB2	1:B:193:GLU:HG3	1.60	0.80
1:B:94:ILE:HD13	1:C:207:GLU:HA	1.62	0.80
1:A:65:ILE:HG22	1:A:66:GLY:H	1.48	0.79
1:D:86:THR:HG22	1:D:87:TRP:H	1.50	0.77
1:A:162:LYS:HB2	1:A:215:GLU:HG3	1.68	0.75
1:B:36:LEU:HD23	1:B:261:PRO:HG3	1.66	0.75
1:D:165:PHE:CZ	1:D:256:ILE:HD12	2.22	0.75
1:D:135:GLN:HE21	1:D:135:GLN:H	1.35	0.74
1:C:92:PRO:HG2	1:C:95:VAL:HG23	1.67	0.74
1:B:98:GLN:HE22	1:C:207:GLU:HG2	1.48	0.74
1:D:65:ILE:HD12	1:D:76:ILE:HG12	1.69	0.73
1:C:249:ILE:HG23	1:C:273:GLN:OE1	1.89	0.73
1:A:240:THR:HG22	1:A:242:ALA:N	2.04	0.72
1:C:165:PHE:CZ	1:C:256:ILE:HD12	2.25	0.71
1:D:207:GLU:CD	1:D:207:GLU:H	1.91	0.71
1:B:92:PRO:HG2	1:B:95:VAL:HG23	1.73	0.70
1:D:249:ILE:HG23	1:D:273:GLN:OE1	1.93	0.69
1:D:86:THR:HG22	1:D:87:TRP:N	2.06	0.69
1:A:171:GLY:HA2	1:C:168:SER:O	1.94	0.68
1:A:68:TRP:HA	1:A:71:LEU:HD13	1.73	0.68
1:A:168:SER:O	1:C:171:GLY:HA2	1.92	0.68
1:A:166:ILE:O	1:A:223:MET:HE1	1.94	0.67
1:B:141:THR:O	1:B:145:GLN:HG3	1.95	0.67
1:C:141:THR:O	1:C:145:GLN:HG2	1.93	0.67
1:A:223:MET:HE2	3:A:663:HOH:O	1.93	0.66
1:C:87:TRP:CE3	1:C:111:ARG:HB3	2.30	0.66
1:D:24:GLU:HG2	1:D:25:ARG:HG3	1.79	0.65
1:D:252:ASP:HB3	1:D:255:LEU:HD23	1.79	0.65
1:C:117:GLU:HG3	3:D:286:HOH:O	1.97	0.65
1:A:187:LEU:HD23	1:A:270:LEU:HD21	1.79	0.64
1:D:25:ARG:HE	1:D:80:ARG:HG3	1.62	0.64
1:A:220:THR:N	1:A:223:MET:HE3	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG22	1:A:66:GLY:N	2.13	0.63
1:D:29:ALA:HA	1:D:50:ASP:HB3	1.81	0.63
1:C:100:ARG:NH1	1:C:106:VAL:HB	2.14	0.63
1:A:252:ASP:HB3	1:A:255:LEU:HD23	1.80	0.63
1:C:238:THR:HG22	1:C:239:HIS:ND1	2.13	0.63
1:D:108:THR:HG22	3:D:302:HOH:O	1.98	0.62
1:D:62:LEU:O	1:D:64:HIS:HD2	1.83	0.62
1:D:68:TRP:O	1:D:71:LEU:HG	2.00	0.62
1:A:150:VAL:O	1:A:154:VAL:HG23	1.99	0.61
1:A:257:LEU:HD22	2:A:600:HEM:HBA1	1.82	0.61
1:D:150:VAL:O	1:D:154:VAL:HG23	2.00	0.61
1:B:74:GLU:H	1:B:74:GLU:CD	2.04	0.60
1:A:134:GLU:HG2	3:A:614:HOH:O	2.01	0.60
1:B:61:LYS:HE3	1:D:74:GLU:OE1	2.01	0.60
1:A:68:TRP:HA	1:A:71:LEU:CD1	2.30	0.60
1:D:25:ARG:NE	1:D:80:ARG:HG3	2.16	0.60
1:D:255:LEU:HB3	1:D:266:VAL:HG21	1.84	0.60
1:D:100:ARG:NH1	1:D:106:VAL:HB	2.16	0.60
1:C:96:LEU:HD13	3:C:381:HOH:O	2.00	0.60
1:D:32:SER:OG	1:D:258:GLY:HA3	2.01	0.60
1:B:94:ILE:CD1	1:C:207:GLU:HA	2.31	0.59
1:D:36:LEU:HD23	1:D:261:PRO:HD3	1.83	0.59
1:B:179:LYS:HE3	1:B:197:THR:HA	1.84	0.58
1:B:168:SER:O	1:D:171:GLY:HA2	2.03	0.58
1:A:72:SER:HA	3:A:655:HOH:O	2.04	0.58
1:D:220:THR:HG22	1:D:256:ILE:HD11	1.86	0.57
1:B:148:GLU:O	1:B:152:GLN:HG3	2.03	0.57
1:D:63:PRO:HD3	3:D:280:HOH:O	2.03	0.57
1:D:100:ARG:HH11	1:D:106:VAL:HB	1.69	0.57
1:C:264:ALA:O	1:C:268:GLU:HG3	2.05	0.57
1:B:165:PHE:CZ	1:B:256:ILE:HD12	2.40	0.57
1:D:164:MET:SD	1:D:209:LEU:HD11	2.44	0.56
1:A:249:ILE:HG23	1:A:273:GLN:OE1	2.04	0.56
1:B:164:MET:SD	1:B:209:LEU:HD11	2.46	0.56
1:B:63:PRO:HA	3:D:339:HOH:O	2.06	0.56
1:B:268:GLU:O	1:B:272:GLN:HG3	2.06	0.56
1:A:62:LEU:O	1:A:64:HIS:HD2	1.89	0.56
1:D:68:TRP:HA	1:D:71:LEU:HD21	1.86	0.55
1:D:227:ASP:OD2	1:D:229:ASN:HB2	2.06	0.55
1:C:187:LEU:HD23	1:C:270:LEU:HD21	1.87	0.55
1:B:124:ARG:NH1	3:B:355:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:256:ILE:HG13	2.06	0.55
1:B:251:VAL:HG13	1:B:256:ILE:HD13	1.88	0.55
1:A:255:LEU:HD12	1:A:266:VAL:CG2	2.38	0.54
1:A:149:ARG:NH1	3:A:683:HOH:O	2.40	0.54
1:B:178:GLY:N	1:B:200:GLN:O	2.42	0.53
1:C:220:THR:HG22	1:C:256:ILE:HD11	1.90	0.53
1:C:93:GLN:NE2	1:C:96:LEU:HD12	2.24	0.53
1:A:221:SER:HA	1:A:250:THR:OG1	2.10	0.52
1:D:228:ILE:HD11	1:D:248:ILE:HD12	1.92	0.52
1:A:167:LEU:HD21	1:A:169:ALA:HB2	1.92	0.52
1:C:164:MET:SD	1:C:209:LEU:HD11	2.50	0.52
1:C:232:ARG:HG2	1:C:232:ARG:HH11	1.74	0.52
1:B:264:ALA:O	1:B:268:GLU:HG3	2.10	0.52
1:D:88:GLN:HG2	1:D:108:THR:OG1	2.11	0.51
1:A:55:TYR:CG	1:A:56:PRO:HA	2.45	0.51
1:A:220:THR:HA	1:A:251:VAL:O	2.09	0.51
1:C:251:VAL:HG13	1:C:256:ILE:HD13	1.92	0.51
1:C:165:PHE:CE2	1:C:167:LEU:HB2	2.46	0.51
1:D:112:VAL:HA	1:D:113:PRO:C	2.30	0.51
1:A:24:GLU:HB3	1:A:82:ASP:OD2	2.09	0.51
1:A:29:ALA:HB3	1:A:86:THR:HB	1.93	0.51
1:D:29:ALA:O	1:D:86:THR:HG23	2.10	0.51
1:D:220:THR:HA	1:D:251:VAL:O	2.09	0.51
1:C:179:LYS:HE2	1:C:197:THR:HA	1.92	0.51
1:B:94:ILE:HD12	1:C:210:ILE:HB	1.92	0.51
1:A:227:ASP:HB3	1:A:230:ARG:HH11	1.76	0.51
1:B:223:MET:HE2	3:D:308:HOH:O	2.09	0.51
1:D:23:ALA:HB3	1:D:26:ILE:HD11	1.93	0.51
2:A:600:HEM:HAD2	3:A:722:HOH:O	2.09	0.51
1:C:65:ILE:HG21	1:C:75:GLY:HA3	1.92	0.50
1:B:100:ARG:NH1	1:B:106:VAL:HB	2.25	0.50
1:C:144:ASN:O	1:C:148:GLU:HG3	2.12	0.50
1:A:134:GLU:HG2	1:A:135:GLN:OE1	2.10	0.50
1:A:255:LEU:HB3	1:A:266:VAL:HG21	1.93	0.50
1:A:84:VAL:HG21	1:A:99:LEU:HD13	1.94	0.50
1:A:109:LEU:HD12	1:A:109:LEU:N	2.27	0.50
1:B:249:ILE:HG22	1:B:250:THR:N	2.26	0.50
1:B:270:LEU:HA	1:B:273:GLN:NE2	2.26	0.50
1:D:88:GLN:HA	1:D:108:THR:OG1	2.12	0.49
1:C:220:THR:HA	1:C:251:VAL:O	2.12	0.49
1:C:253:GLN:HA	1:C:256:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:O	1:A:108:THR:HA	2.11	0.49
1:D:255:LEU:HB3	1:D:266:VAL:CG2	2.42	0.49
1:D:159:ALA:HB3	1:D:275:TRP:HE1	1.77	0.49
1:D:135:GLN:N	1:D:135:GLN:NE2	2.54	0.49
1:D:86:THR:CG2	1:D:87:TRP:N	2.75	0.49
1:D:112:VAL:HB	1:D:113:PRO:HA	1.95	0.49
1:D:86:THR:CG2	1:D:87:TRP:H	2.21	0.49
1:C:179:LYS:HE2	1:C:196:ALA:O	2.12	0.48
1:D:65:ILE:CD1	1:D:76:ILE:HG12	2.41	0.48
1:D:68:TRP:HA	1:D:71:LEU:CD2	2.43	0.48
1:A:93:GLN:NE2	1:A:97:ASP:OD2	2.46	0.48
1:B:165:PHE:CE2	1:B:167:LEU:HB2	2.49	0.48
1:D:221:SER:HA	1:D:250:THR:CG2	2.44	0.48
1:A:171:GLY:H	2:A:600:HEM:CBB	2.26	0.48
1:B:164:MET:HG2	1:B:214:PRO:HG3	1.96	0.48
1:C:153:ASN:O	1:C:156:ALA:HB3	2.14	0.48
1:D:276:PRO:O	1:D:277:GLN:HB2	2.12	0.48
1:B:109:LEU:N	1:B:109:LEU:HD12	2.29	0.48
1:D:62:LEU:HA	3:D:280:HOH:O	2.14	0.47
1:B:157:LYS:HD3	1:B:275:TRP:CE2	2.48	0.47
1:B:94:ILE:HD12	1:C:210:ILE:HD12	1.97	0.47
1:A:112:VAL:HA	1:A:113:PRO:C	2.35	0.47
1:C:55:TYR:CG	1:C:56:PRO:HA	2.49	0.47
1:D:83:SER:HA	1:D:105:ASN:O	2.15	0.47
1:B:65:ILE:HG21	1:B:75:GLY:HA3	1.95	0.47
1:B:194:ASN:HD22	1:B:195:VAL:N	2.12	0.47
1:A:44:GLU:HG3	1:A:45:ARG:HG3	1.97	0.47
1:D:165:PHE:CE1	1:D:256:ILE:HD12	2.49	0.47
1:C:92:PRO:HG2	1:C:95:VAL:CG2	2.42	0.47
1:C:227:ASP:HB3	1:C:230:ARG:HH11	1.79	0.47
1:C:88:GLN:HE22	1:D:149:ARG:HH22	1.63	0.46
1:A:112:VAL:HB	1:A:113:PRO:HA	1.97	0.46
1:C:87:TRP:CD2	1:C:111:ARG:HB3	2.50	0.46
1:B:227:ASP:HB3	1:B:230:ARG:NH1	2.30	0.46
1:C:62:LEU:O	1:C:64:HIS:HD2	1.98	0.46
1:C:178:GLY:N	1:C:200:GLN:O	2.47	0.46
1:D:62:LEU:O	1:D:64:HIS:CD2	2.66	0.46
1:D:36:LEU:O	1:D:40:MET:HB2	2.15	0.46
1:A:29:ALA:HA	1:A:50:ASP:HB3	1.98	0.46
1:B:124:ARG:NH2	3:B:363:HOH:O	2.49	0.46
1:C:232:ARG:HG2	1:C:232:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:O	1:B:108:THR:HA	2.16	0.46
1:B:94:ILE:CD1	1:C:210:ILE:HD12	2.46	0.46
1:D:49:VAL:O	1:D:64:HIS:HA	2.16	0.46
1:B:134:GLU:HB2	3:B:373:HOH:O	2.16	0.46
1:B:220:THR:HA	1:B:251:VAL:O	2.15	0.46
1:B:132:VAL:N	1:B:133:PRO:CD	2.78	0.46
1:D:138:ALA:O	1:D:142:GLN:HG2	2.16	0.46
1:D:77:LEU:HD21	1:D:99:LEU:HD23	1.98	0.46
1:A:102:GLN:HB3	3:A:675:HOH:O	2.15	0.45
1:C:36:LEU:O	1:C:40:MET:HB2	2.16	0.45
1:C:44:GLU:HG3	3:C:362:HOH:O	2.17	0.45
1:D:44:GLU:HG3	1:D:45:ARG:N	2.32	0.45
1:A:134:GLU:CG	1:A:135:GLN:OE1	2.64	0.45
1:D:86:THR:O	1:D:108:THR:HA	2.16	0.45
1:D:264:ALA:O	1:D:268:GLU:HG3	2.16	0.45
1:B:55:TYR:CG	1:B:56:PRO:HA	2.52	0.45
1:B:162:LYS:HB2	1:B:215:GLU:HG3	1.99	0.45
1:C:36:LEU:HD23	1:C:261:PRO:HG3	1.99	0.44
1:C:94:ILE:O	1:C:94:ILE:HG12	2.16	0.44
1:D:104:VAL:O	1:D:106:VAL:HG23	2.16	0.44
1:C:268:GLU:O	1:C:272:GLN:HG3	2.17	0.44
1:C:227:ASP:HB3	1:C:230:ARG:NH1	2.33	0.44
1:D:62:LEU:HD23	3:D:280:HOH:O	2.16	0.44
1:D:67:TYR:CD2	1:D:69:LYS:HB2	2.53	0.44
1:D:106:VAL:HG12	1:D:107:VAL:N	2.33	0.43
1:A:167:LEU:HA	1:A:223:MET:HE1	2.00	0.43
1:A:272:GLN:HG2	3:A:737:HOH:O	2.18	0.43
3:C:374:HOH:O	1:D:271:HIS:HE1	1.99	0.43
1:B:94:ILE:HD12	1:C:210:ILE:CD1	2.49	0.43
1:C:86:THR:O	1:C:108:THR:HA	2.19	0.43
1:A:264:ALA:O	1:A:268:GLU:HG3	2.18	0.43
1:C:151:GLN:HG2	3:C:337:HOH:O	2.18	0.43
1:D:88:GLN:HE21	1:D:108:THR:HG23	1.83	0.43
1:B:263:ILE:O	1:B:266:VAL:HG12	2.19	0.43
1:B:276:PRO:O	1:B:277:GLN:NE2	2.52	0.43
1:B:161:VAL:HG23	1:B:275:TRP:CZ2	2.54	0.43
1:B:194:ASN:ND2	1:B:196:ALA:H	2.17	0.43
1:D:28:VAL:HG21	1:D:37:ILE:HD12	2.01	0.43
1:C:132:VAL:N	1:C:133:PRO:CD	2.82	0.43
1:C:88:GLN:HA	1:C:108:THR:HB	2.01	0.43
1:B:270:LEU:HA	1:B:273:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:N	1:A:200:GLN:O	2.46	0.42
1:A:23:ALA:N	1:A:82:ASP:HB2	2.34	0.42
1:D:272:GLN:NE2	3:D:374:HOH:O	2.51	0.42
1:D:29:ALA:HB3	1:D:86:THR:CG2	2.49	0.42
1:C:100:ARG:NH2	3:C:376:HOH:O	2.53	0.42
1:B:222:GLN:CD	1:B:222:GLN:H	2.23	0.42
1:D:108:THR:C	1:D:109:LEU:HD12	2.40	0.42
1:C:167:LEU:HG	1:C:168:SER:N	2.34	0.42
1:D:224:VAL:O	1:D:225:ASP:C	2.58	0.42
1:D:98:GLN:O	1:D:101:ALA:HB3	2.20	0.42
1:C:150:VAL:O	1:C:154:VAL:HG23	2.20	0.42
1:D:29:ALA:HB3	1:D:86:THR:HG23	2.01	0.42
1:C:95:VAL:HA	1:C:98:GLN:HE21	1.85	0.42
1:B:167:LEU:HD11	1:B:253:GLN:OE1	2.20	0.42
1:C:243:TRP:CE3	1:C:248:ILE:CD1	3.03	0.42
1:D:26:ILE:N	1:D:45:ARG:O	2.53	0.42
1:B:187:LEU:HD23	1:B:270:LEU:HD21	2.01	0.42
1:D:216:VAL:HG22	1:D:247:ARG:HB3	2.01	0.42
1:C:216:VAL:HG11	1:C:249:ILE:HD12	2.01	0.42
1:B:124:ARG:NE	3:B:363:HOH:O	2.53	0.41
1:D:222:GLN:CD	1:D:222:GLN:H	2.23	0.41
1:B:36:LEU:HD23	1:B:261:PRO:CG	2.43	0.41
1:A:49:VAL:O	1:A:64:HIS:HA	2.20	0.41
1:C:153:ASN:OD1	1:C:271:HIS:HE1	2.03	0.41
1:A:255:LEU:HD22	1:A:255:LEU:N	2.35	0.41
1:C:84:VAL:HG23	1:C:104:VAL:HG11	2.02	0.41
1:A:164:MET:SD	1:A:209:LEU:CD1	3.08	0.41
1:C:153:ASN:HD22	1:C:153:ASN:C	2.23	0.41
1:B:251:VAL:CG1	1:B:256:ILE:HD13	2.49	0.41
1:D:221:SER:HA	1:D:250:THR:HG21	2.02	0.41
1:A:37:ILE:HG12	1:A:130:LEU:HD11	2.02	0.41
1:D:220:THR:H	1:D:223:MET:HE3	1.86	0.41
1:B:247:ARG:HA	1:B:247:ARG:HD2	1.94	0.41
1:D:23:ALA:O	1:D:45:ARG:HD3	2.20	0.41
1:C:216:VAL:HG12	1:C:217:ILE:N	2.36	0.41
1:B:202:LYS:HE2	3:B:369:HOH:O	2.20	0.41
1:A:103:LYS:HE2	3:A:679:HOH:O	2.20	0.41
1:D:164:MET:SD	1:D:209:LEU:CD1	3.09	0.41
1:A:88:GLN:HG3	1:A:109:LEU:C	2.40	0.41
1:D:98:GLN:O	1:D:102:GLN:HG2	2.20	0.41
1:B:195:VAL:HG11	1:B:212:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ALA:HB3	1:D:86:THR:OG1	2.21	0.40
1:D:42:ALA:C	1:D:44:GLU:H	2.23	0.40
1:B:220:THR:HG22	1:B:256:ILE:HD11	2.04	0.40
1:B:273:GLN:HB2	1:B:273:GLN:HE21	1.66	0.40
1:D:264:ALA:HB3	3:D:331:HOH:O	2.21	0.40
1:D:238:THR:HA	1:D:243:TRP:CG	2.57	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	253/256 (99%)	246 (97%)	7 (3%)	0	100	100
1	B	254/256 (99%)	241 (95%)	12 (5%)	1 (0%)	39	28
1	C	253/256 (99%)	246 (97%)	7 (3%)	0	100	100
1	D	253/256 (99%)	243 (96%)	8 (3%)	2 (1%)	24	12
All	All	1013/1024 (99%)	976 (96%)	34 (3%)	3 (0%)	46	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	VAL
1	D	225	ASP
1	B	159	ALA

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	207/207 (100%)	205 (99%)	2 (1%)	82	81
1	B	207/207 (100%)	203 (98%)	4 (2%)	65	60
1	C	207/207 (100%)	203 (98%)	4 (2%)	65	60
1	D	207/207 (100%)	200 (97%)	7 (3%)	44	36
All	All	828/828 (100%)	811 (98%)	17 (2%)	61	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	194	ASN
1	B	74	GLU
1	B	194	ASN
1	B	207	GLU
1	B	223	MET
1	C	153	ASN
1	C	194	ASN
1	C	232	ARG
1	C	238	THR
1	D	105	ASN
1	D	135	GLN
1	D	137	ASP
1	D	158	LYS
1	D	194	ASN
1	D	207	GLU
1	D	227	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	105	ASN
1	A	131	GLN
1	A	194	ASN
1	A	198	HIS
1	A	229	ASN
1	A	254	ASN
1	A	271	HIS

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Mol	Chain	Res	Type
1	B	64	HIS
1	B	98	GLN
1	B	105	ASN
1	B	135	GLN
1	B	194	ASN
1	B	198	HIS
1	B	253	GLN
1	B	271	HIS
1	B	272	GLN
1	B	273	GLN
1	C	64	HIS
1	C	93	GLN
1	C	98	GLN
1	C	105	ASN
1	C	131	GLN
1	C	194	ASN
1	C	198	HIS
1	C	200	GLN
1	C	245	ASN
1	C	254	ASN
1	C	271	HIS
1	C	277	GLN
1	D	64	HIS
1	D	88	GLN
1	D	105	ASN
1	D	131	GLN
1	D	135	GLN
1	D	145	GLN
1	D	153	ASN
1	D	194	ASN
1	D	198	HIS
1	D	254	ASN
1	D	271	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	600	1	30,50,50	2.72	9 (30%)	24,82,82	2.09	9 (37%)

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	600	1	-	0/10/54/54	0/0/8/8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-CAB	-6.13	1.39	1.51
2	A	600	HEM	C3B-C4B	-6.09	1.46	1.51
2	A	600	HEM	C2D-C3D	-6.00	1.36	1.54
2	A	600	HEM	C3C-CAC	-5.92	1.40	1.51
2	A	600	HEM	C2C-C1C	-3.31	1.46	1.52
2	A	600	HEM	C3D-C4D	-3.24	1.47	1.51
2	A	600	HEM	CHC-C1C	2.07	1.41	1.36
2	A	600	HEM	C1C-NC	3.53	1.40	1.36
2	A	600	HEM	C4C-NC	4.49	1.41	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	CAA-C2A-C3A	-2.33	122.34	129.00
2	A	600	HEM	CBA-CAA-C2A	2.22	116.50	112.53
2	A	600	HEM	CAA-C2A-C1A	2.27	129.47	127.01
2	A	600	HEM	CMD-C2D-C3D	2.33	124.64	114.35
2	A	600	HEM	C2D-C3D-C4D	2.80	106.25	101.50
2	A	600	HEM	CAD-C3D-C2D	3.08	122.08	113.22
2	A	600	HEM	CMC-C2C-C3C	3.46	125.16	116.53
2	A	600	HEM	CMB-C2B-C3B	4.10	126.76	116.53
2	A	600	HEM	CAD-C3D-C4D	5.44	131.65	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	255/256 (99%)	-0.02	7 (2%)	58	64	22, 34, 51, 67	0
1	B	256/256 (100%)	0.04	6 (2%)	64	70	21, 34, 49, 69	0
1	C	255/256 (99%)	0.05	9 (3%)	48	54	23, 35, 56, 76	0
1	D	255/256 (99%)	0.59	37 (14%)	3	3	20, 42, 80, 89	0
All	All	1021/1024 (99%)	0.17	59 (5%)	26	30	20, 35, 62, 89	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	VAL	8.4
1	C	23	ALA	7.5
1	D	23	ALA	6.6
1	D	159	ALA	6.3
1	B	22	ALA	5.9
1	D	99	LEU	5.5
1	C	156	ALA	4.9
1	D	82	ASP	4.2
1	D	129	THR	4.1
1	C	277	GLN	4.0
1	D	101	ALA	4.0
1	A	23	ALA	3.9
1	D	90	ALA	3.8
1	C	158	LYS	3.7
1	D	92	PRO	3.7
1	D	26	ILE	3.7
1	B	159	ALA	3.7
1	D	100	ARG	3.6
1	D	158	LYS	3.6
1	A	155	ALA	3.6
1	B	156	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	158	LYS	3.5
1	C	276	PRO	3.4
1	D	91	GLY	3.4
1	B	155	ALA	3.4
1	D	106	VAL	3.4
1	D	103	LYS	3.4
1	D	93	GLN	3.3
1	D	94	ILE	3.3
1	D	105	ASN	3.2
1	D	95	VAL	3.2
1	D	96	LEU	3.2
1	D	112	VAL	3.1
1	D	130	LEU	3.1
1	B	158	LYS	3.1
1	D	68	TRP	3.1
1	D	73	SER	2.9
1	B	277	GLN	2.8
1	C	152	GLN	2.8
1	D	170	GLY	2.8
1	D	66	GLY	2.7
1	D	107	VAL	2.7
1	C	155	ALA	2.6
1	D	70	GLN	2.6
1	A	159	ALA	2.5
1	D	83	SER	2.5
1	D	67	TYR	2.5
1	D	108	THR	2.2
1	A	67	TYR	2.2
1	D	24	GLU	2.2
1	C	154	VAL	2.2
1	D	89	ASP	2.2
1	D	41	GLY	2.1
1	A	169	ALA	2.1
1	D	72	SER	2.1
1	C	272	GLN	2.1
1	A	154	VAL	2.1
1	D	80	ARG	2.0
1	D	128	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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(Å²)	Q<0.9
2	HEM	A	600	43/43	0.83	0.23	2.76	31,52,55,56	10

6.5 Other polymers (i)

There are no such residues in this entry.