Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:36 AM GMT

PDB ID	:	2RFB
Title	:	Crystal Structure of a Cytochrome P450 from the Thermoacidophilic Archaeon Picrophilus Torridus
Authors	:	Ho, W.W.; Li, H.; Poulos, T.L.; Nishida, C.R.; Ortiz de Montellano, P.R.
Deposited on	:	2007-09-28
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

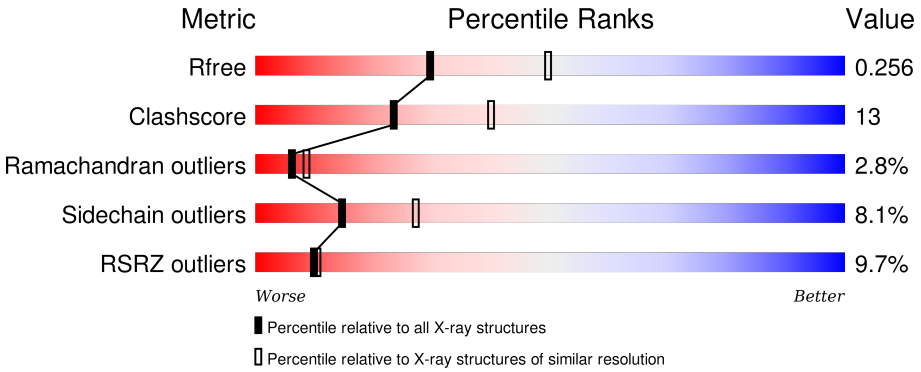
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	343	4% 70% 24%
1	B	343	12% 69% 22% 6%
1	C	343	13% 63% 31%

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	SO4	A	920	-	-	-	X
2	SO4	C	910	-	-	X	X

2 Entry composition

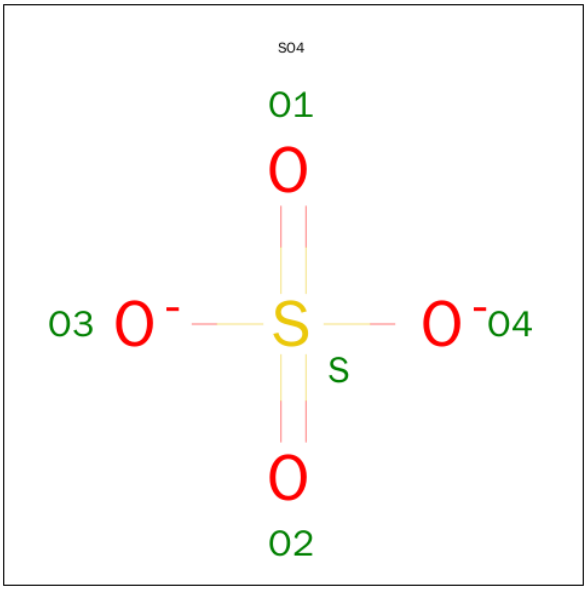
There are 4 unique types of molecules in this entry. The entry contains 8465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2752	1763	467	511	11			
1	B	335	Total	C	N	O	S	0	0	0
			2721	1744	460	505	12			
1	C	333	Total	C	N	O	S	0	0	0
			2708	1736	458	503	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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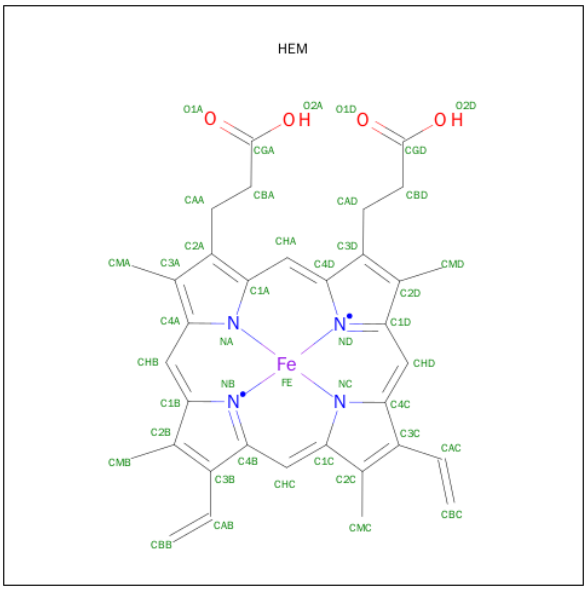
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

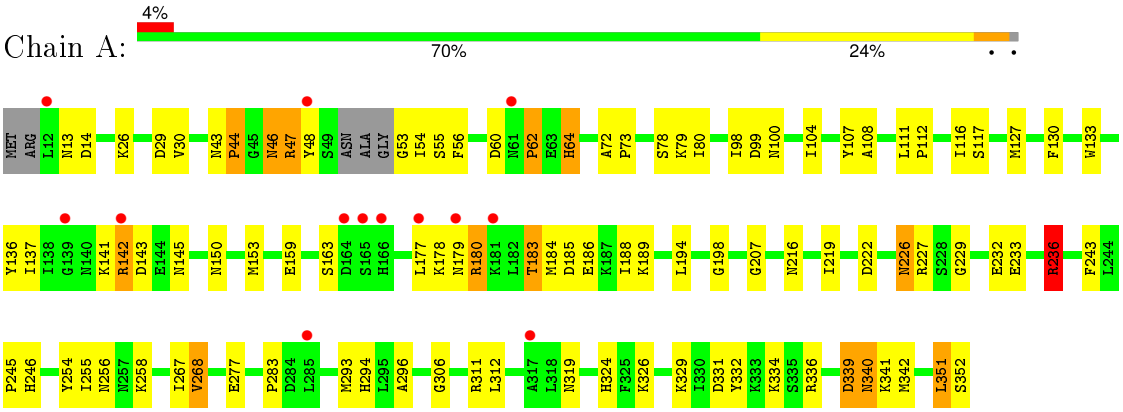
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	33	Total O 33 33	0	0
4	C	26	Total O 26 26	0	0

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.

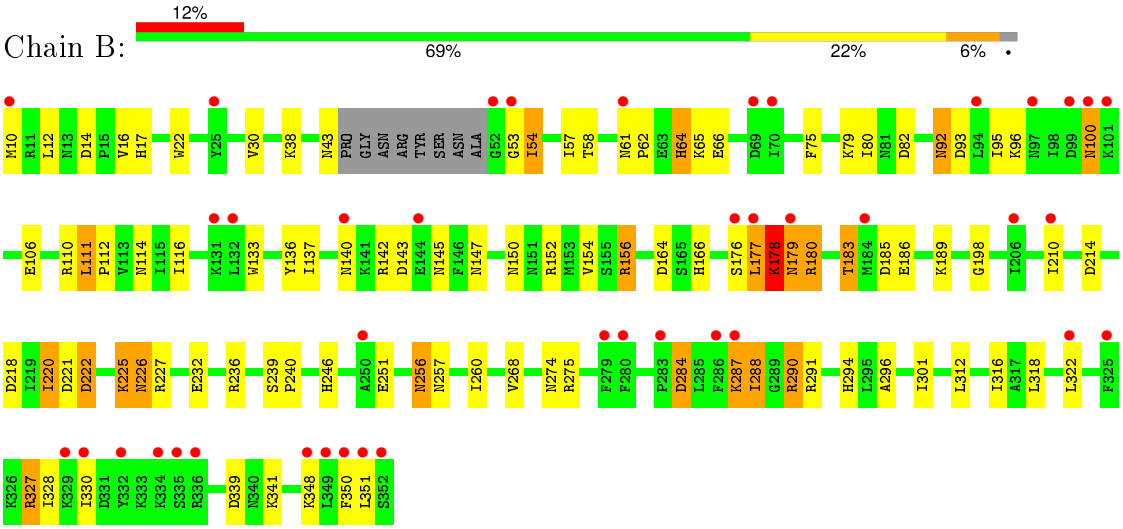
- Molecule 1: Cytochrome P450

Chain A:



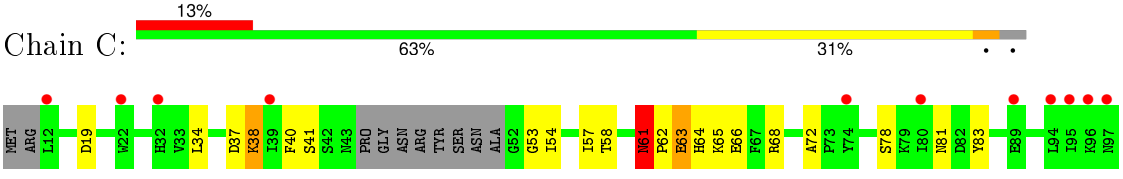
- Molecule 1: Cytochrome P450

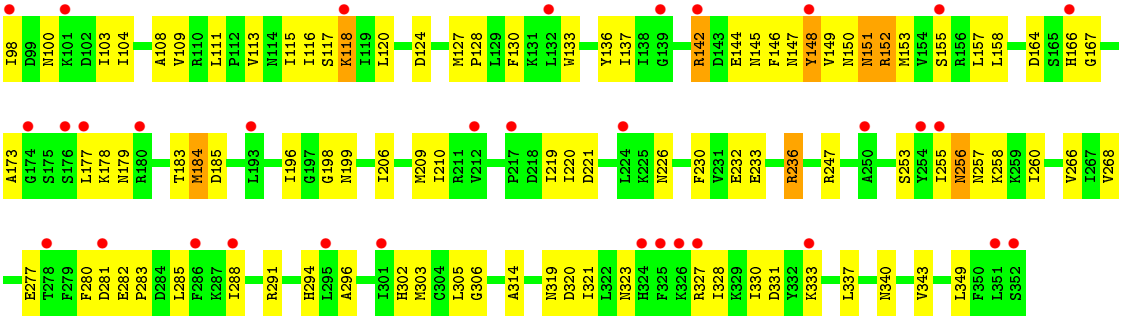
Chain B:



- Molecule 1: Cytochrome P450

Chain C:




I98 D99 N100 K101 D102 I103 I104
A108 V109 R110 L111 P112 V113 N114 I115 I116 S117 K118 I119 L120
D124
M127 P128 L129 F130 K131 L132 W133
Y136 I137 I138 G139
R142 D143 E144 N145 F146 N147 Y148 V149 N150 N151 R152 M153 V154 S155 R156 L157 L158
D164 S165 H166 G167
A173 G174 S175 S176 L177 K178 N179 R180
T183 M184 D185
L193
I196 G197 G198 N199
I206
M209 I210 R211 V212
P217 D218 I219 I220 D221
L224 K225 N226
F230 V231 E232 E233
R236
R247
A250
S253 Y254 I255 N256 N257 K258 K259 I260
V266 I267 V268
E277 T278 F279 F280 D281 E282 P283 D284 L285 F286 K287 I288
R291
H294 L295 A296
I301 H302 M303 C304 L305 G306
A314
N319 D320 I321 L322 N323 H324 F325 K326 R327 I328 K329 I330 D331 Y332 K333
L337
N340
V343
L349 F350 L351 S352

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.79Å 168.46Å 88.23Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	48.51 – 2.50 48.50 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.51-2.50) 98.1 (48.50-2.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.268 0.205 , 0.256	Depositor DCC
R_{free} test set	2414 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 79.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 48274 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8465	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4

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	0.82	0/2809	0.88	4/3785 (0.1%)
1	B	0.89	11/2776 (0.4%)	0.74	6/3739 (0.2%)
1	C	0.56	1/2763 (0.0%)	0.66	1/3722 (0.0%)
All	All	0.77	12/8348 (0.1%)	0.77	11/11246 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	LYS	CD-CE	19.91	2.01	1.51
1	B	221	ASP	CG-OD1	13.05	1.55	1.25
1	B	225	LYS	CD-CE	11.32	1.79	1.51
1	B	287	LYS	CE-NZ	11.23	1.77	1.49
1	B	221	ASP	CG-OD2	8.83	1.45	1.25
1	B	222	ASP	CG-OD1	7.56	1.42	1.25
1	B	290	ARG	NE-CZ	7.01	1.42	1.33
1	B	226	ASN	CB-CG	5.53	1.63	1.51
1	B	218	ASP	CG-OD2	5.47	1.38	1.25
1	B	220	ILE	CB-CG2	5.18	1.68	1.52
1	B	218	ASP	CG-OD1	5.01	1.36	1.25
1	C	280	PHE	CE1-CZ	5.00	1.46	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	ARG	NE-CZ-NH2	-9.67	115.46	120.30
1	B	221	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	B	287	LYS	CD-CE-NZ	-6.36	97.08	111.70
1	B	287	LYS	CG-CD-CE	-6.17	93.40	111.90
1	B	222	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	236	ARG	CG-CD-NE	-5.66	99.91	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	222	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	C	61	ASN	C-N-CD	5.51	139.98	128.40
1	A	236	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	221	ASP	OD1-CG-OD2	5.12	133.02	123.30
1	B	290	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	2752	0	2756	76	0
1	B	2721	0	2727	69	0
1	C	2708	0	2716	72	0
2	A	15	0	0	1	0
2	C	5	0	0	4	0
3	A	43	0	30	5	0
3	B	43	0	30	3	0
3	C	43	0	30	6	0
4	A	76	0	0	7	0
4	B	33	0	0	3	0
4	C	26	0	0	1	0
All	All	8465	0	8289	221	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 13.

All (221) 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:B:225:LYS:CD	1:B:225:LYS:CE	1.79	1.55
1:B:287:LYS:CE	1:B:287:LYS:NZ	1.77	1.47
1:B:287:LYS:CE	1:B:287:LYS:CD	2.01	1.37
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:HH11	1:B:156:ARG:HG3	1.23	1.01
1:A:133:TRP:HE1	1:A:150:ASN:HD22	1.18	0.90
1:A:294:HIS:HD2	1:A:296:ALA:H	1.19	0.88
1:C:61:ASN:HD21	1:C:65:LYS:HG2	1.40	0.87
1:C:133:TRP:HE1	1:C:150:ASN:HD22	1.24	0.85
1:A:133:TRP:HE1	1:A:150:ASN:ND2	1.75	0.84
1:C:232:GLU:OE1	1:C:294:HIS:HE1	1.59	0.83
3:C:410:HEM:HBC2	3:C:410:HEM:HHD	1.62	0.82
1:B:143:ASP:HB3	1:B:145:ASN:H	1.45	0.81
1:B:288:ILE:HD12	1:B:288:ILE:H	1.46	0.80
1:C:166:HIS:CD2	1:C:167:GLY:H	1.98	0.79
1:C:166:HIS:HD2	1:C:167:GLY:H	1.32	0.77
1:B:177:LEU:O	1:B:179:ASN:N	2.17	0.76
1:C:61:ASN:ND2	1:C:65:LYS:HG2	2.01	0.75
1:A:26:LYS:HE3	1:A:29:ASP:OD2	1.88	0.74
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.00	0.73
1:B:287:LYS:CE	1:B:287:LYS:CG	2.69	0.71
1:A:142:ARG:NH1	1:A:142:ARG:HG3	2.01	0.70
1:A:183:THR:HG22	1:A:186:GLU:H	1.55	0.70
1:B:30:VAL:HG13	1:B:268:VAL:CG1	2.23	0.69
1:B:225:LYS:CG	1:B:225:LYS:CE	2.70	0.69
1:A:48:TYR:CE2	1:A:246:HIS:HE1	2.11	0.68
1:C:232:GLU:OE1	1:C:294:HIS:CE1	2.46	0.68
1:B:136:TYR:HE2	1:B:143:ASP:HB2	1.57	0.68
1:B:53:GLY:HA2	1:B:189:LYS:HD3	1.74	0.68
1:B:178:LYS:O	1:B:179:ASN:HB2	1.94	0.68
1:B:246:HIS:NE2	4:B:419:HOH:O	2.22	0.68
1:A:339:ASP:N	1:A:339:ASP:OD1	2.25	0.67
1:B:294:HIS:HD2	1:B:296:ALA:H	1.42	0.67
1:B:54:ILE:O	1:B:57:ILE:HG22	1.94	0.67
1:A:226:ASN:ND2	1:A:229:GLY:H	1.93	0.67
1:B:328:ILE:HG23	1:B:351:LEU:HD11	1.77	0.67
1:A:331:ASP:OD2	1:A:334:LYS:NZ	2.18	0.67
1:C:198:GLY:HA2	3:C:410:HEM:C2C	2.30	0.66
1:B:180:ARG:NH2	1:B:186:GLU:OE1	2.29	0.66
1:A:277:GLU:CG	1:A:283:PRO:HG3	2.26	0.66
1:C:210:ILE:HD11	1:C:321:ILE:HD13	1.78	0.66
1:C:236:ARG:NH2	1:C:283:PRO:O	2.27	0.66
1:A:294:HIS:HD2	1:A:296:ALA:N	1.91	0.65
1:C:83:TYR:HD2	1:C:118:LYS:HZ1	1.45	0.65
1:B:92:ASN:O	1:B:95:ILE:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:HG2	1:A:283:PRO:HG3	1.79	0.64
1:B:176:SER:O	1:B:177:LEU:HB2	1.97	0.64
1:C:220:ILE:HD11	1:C:328:ILE:HD11	1.81	0.62
1:B:64:HIS:CD2	1:B:65:LYS:HG2	2.35	0.62
1:C:103:ILE:HD12	1:C:349:LEU:HD22	1.80	0.62
1:C:282:GLU:HB3	1:C:285:LEU:HG	1.82	0.62
1:A:340:ASN:HD22	1:A:341:LYS:N	1.98	0.62
1:B:133:TRP:HE1	1:B:150:ASN:HD22	1.48	0.61
1:A:48:TYR:HE2	1:A:246:HIS:HE1	1.48	0.61
1:B:30:VAL:HG13	1:B:268:VAL:HG13	1.82	0.61
1:C:117:SER:HA	1:C:120:LEU:HD12	1.82	0.60
1:C:294:HIS:HD2	1:C:296:ALA:H	1.50	0.60
1:B:183:THR:HG22	1:B:186:GLU:H	1.67	0.60
1:B:232:GLU:OE2	1:B:294:HIS:HE1	1.85	0.60
1:A:47:ARG:HA	1:A:47:ARG:HH11	1.67	0.59
1:C:104:ILE:HA	1:C:108:ALA:HB3	1.83	0.59
1:A:30:VAL:HG13	1:A:268:VAL:HG13	1.84	0.59
1:C:184:MET:N	1:C:184:MET:SD	2.64	0.59
1:C:233:GLU:OE2	1:C:236:ARG:NH1	2.35	0.58
1:A:232:GLU:OE2	1:A:294:HIS:HE1	1.87	0.58
1:A:55:SER:OG	1:A:56:PHE:N	2.36	0.58
1:C:340:ASN:HB3	1:C:343:VAL:HG22	1.86	0.58
1:C:281:ASP:CB	2:C:910:SO4:O1	2.52	0.58
1:A:64:HIS:HE1	3:A:410:HEM:O2D	1.87	0.58
1:B:275:ARG:HH11	1:B:284:ASP:HB3	1.70	0.57
1:B:53:GLY:HA2	1:B:189:LYS:CD	2.35	0.57
1:A:53:GLY:HA2	4:A:980:HOH:O	2.04	0.57
1:A:142:ARG:NH1	1:A:142:ARG:CG	2.63	0.57
1:A:78:SER:HA	4:A:955:HOH:O	2.03	0.57
1:B:198:GLY:HA2	3:B:410:HEM:C2C	2.40	0.57
1:A:44:PRO:HB2	1:A:46:ASN:H	1.69	0.56
1:A:294:HIS:CD2	1:A:296:ALA:H	2.11	0.56
1:C:83:TYR:HD2	1:C:118:LYS:NZ	2.01	0.56
1:B:256:ASN:O	1:B:257:ASN:HB2	2.05	0.56
1:C:206:ILE:O	1:C:210:ILE:HD12	2.05	0.56
1:C:288:ILE:H	1:C:288:ILE:HD12	1.69	0.56
1:C:277:GLU:HG3	1:C:283:PRO:HG3	1.87	0.56
1:B:136:TYR:CE2	1:B:143:ASP:HB2	2.41	0.55
1:C:61:ASN:ND2	1:C:64:HIS:HD2	2.04	0.55
1:B:348:LYS:HD2	1:B:350:PHE:HE1	1.71	0.55
1:C:37:ASP:OD2	1:C:38:LYS:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:HE2	1:A:246:HIS:CE1	2.24	0.55
1:A:185:ASP:O	1:A:189:LYS:HG2	2.06	0.54
1:C:111:LEU:O	1:C:115:ILE:HD12	2.08	0.54
1:C:281:ASP:HB3	2:C:910:SO4:O1	2.07	0.54
1:C:209:MET:CE	1:C:314:ALA:HB1	2.38	0.54
1:B:348:LYS:HD2	1:B:350:PHE:CE1	2.43	0.54
1:C:155:SER:HA	1:C:158:LEU:HD12	1.89	0.54
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.02	0.53
3:C:410:HEM:HHD	3:C:410:HEM:CBC	2.35	0.53
1:A:98:ILE:CD1	1:A:107:TYR:HB2	2.39	0.52
1:C:117:SER:HB3	1:C:130:PHE:CE2	2.43	0.52
1:A:184:MET:O	1:A:188:ILE:HG12	2.10	0.52
1:A:329:LYS:O	1:A:352:SER:N	2.30	0.52
1:B:220:ILE:HG12	1:B:322:LEU:HD22	1.92	0.52
1:A:311:ARG:HD2	4:A:938:HOH:O	2.08	0.52
1:A:332:TYR:O	1:A:336:ARG:NH2	2.43	0.52
1:C:78:SER:O	1:C:81:ASN:HB3	2.10	0.52
1:B:177:LEU:HG	1:B:178:LYS:H	1.75	0.52
1:C:109:VAL:O	1:C:113:VAL:HG23	2.10	0.52
1:A:99:ASP:O	1:A:100:ASN:HB2	2.09	0.51
1:B:246:HIS:O	1:B:246:HIS:CG	2.63	0.51
1:C:40:PHE:CZ	1:C:255:ILE:HD11	2.46	0.51
1:A:14:ASP:OD1	1:A:26:LYS:NZ	2.42	0.51
1:A:311:ARG:NH1	4:A:938:HOH:O	2.41	0.51
1:A:255:ILE:O	1:A:256:ASN:C	2.48	0.51
1:A:277:GLU:HG3	1:A:283:PRO:HG3	1.93	0.51
1:A:306:GLY:HA3	3:A:410:HEM:C3C	2.46	0.51
1:B:30:VAL:HG13	1:B:268:VAL:HG11	1.92	0.51
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.09	0.51
1:B:64:HIS:HE1	3:B:410:HEM:O2D	1.94	0.51
1:C:72:ALA:HA	1:C:305:LEU:HD11	1.93	0.50
1:B:110:ARG:O	1:B:114:ASN:ND2	2.41	0.50
1:C:281:ASP:HB2	2:C:910:SO4:O1	2.11	0.50
1:C:302:HIS:O	1:C:303:MET:C	2.50	0.50
1:A:183:THR:HB	1:A:186:GLU:OE1	2.12	0.50
1:A:48:TYR:CE2	1:A:246:HIS:CE1	2.95	0.50
1:C:137:ILE:HG23	1:C:196:ILE:HD11	1.93	0.50
1:A:340:ASN:ND2	1:A:342:MET:H	2.10	0.50
1:B:75:PHE:HA	1:B:80:ILE:CD1	2.42	0.50
1:A:326:LYS:N	2:A:900:SO4:O3	2.44	0.49
1:A:294:HIS:CD2	1:A:296:ALA:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:MET:HE1	1:C:314:ALA:HB1	1.95	0.49
1:A:351:LEU:O	1:A:352:SER:HB3	2.13	0.49
1:A:73:PRO:O	1:A:79:LYS:HG3	2.13	0.49
1:B:178:LYS:O	1:B:179:ASN:CB	2.61	0.49
1:A:216:ASN:O	1:A:219:ILE:HG22	2.13	0.48
1:C:306:GLY:HA3	3:C:410:HEM:C3C	2.48	0.48
1:A:183:THR:HG22	1:A:186:GLU:N	2.25	0.48
1:C:127:MET:N	1:C:128:PRO:HD2	2.29	0.48
1:A:47:ARG:HA	1:A:47:ARG:NH1	2.27	0.48
1:A:233:GLU:OE1	1:A:236:ARG:HD3	2.13	0.48
1:A:254:TYR:HA	1:A:258:LYS:O	2.14	0.48
1:C:209:MET:HB3	1:C:230:PHE:HE2	1.78	0.48
1:A:98:ILE:HD12	1:A:107:TYR:HB2	1.96	0.48
1:B:43:ASN:OD1	1:B:43:ASN:C	2.52	0.47
1:A:183:THR:HG23	1:A:185:ASP:H	1.79	0.47
1:A:277:GLU:HG2	1:A:283:PRO:CG	2.44	0.47
1:A:13:ASN:ND2	4:A:977:HOH:O	2.47	0.47
1:A:245:PRO:HA	1:A:267:ILE:HG23	1.96	0.47
1:C:327:ARG:HB3	4:C:924:HOH:O	2.13	0.47
1:C:34:LEU:HD21	1:C:268:VAL:HG21	1.97	0.47
1:C:136:TYR:HB3	1:C:146:PHE:CD1	2.50	0.47
1:B:111:LEU:N	1:B:112:PRO:HD2	2.29	0.46
1:B:142:ARG:HG2	1:B:142:ARG:O	2.16	0.46
1:C:151:ASN:O	1:C:152:ARG:C	2.54	0.46
1:B:156:ARG:NH1	1:B:156:ARG:CG	2.75	0.46
1:C:142:ARG:O	1:C:142:ARG:HD2	2.15	0.46
1:B:150:ASN:O	1:B:154:VAL:HG23	2.15	0.46
1:A:198:GLY:HA2	3:A:410:HEM:C2C	2.50	0.46
1:A:293:MET:HG2	1:A:294:HIS:O	2.16	0.46
1:A:194:LEU:O	3:A:410:HEM:HBC2	2.15	0.45
1:C:63:GLU:HG2	1:C:64:HIS:N	2.31	0.45
1:A:99:ASP:OD2	1:A:324:HIS:HE1	1.97	0.45
1:A:136:TYR:HE2	1:A:143:ASP:HB2	1.80	0.45
1:B:227:ARG:HG2	1:B:318:LEU:HD23	1.99	0.45
1:C:116:ILE:HG22	1:C:120:LEU:HD11	1.98	0.45
1:C:281:ASP:HB2	2:C:910:SO4:S	2.57	0.45
1:B:17:HIS:HB2	1:B:22:TRP:CZ3	2.52	0.44
1:A:179:ASN:O	1:A:180:ARG:HB2	2.17	0.44
1:C:68:ARG:NH1	3:C:410:HEM:O2D	2.45	0.44
1:B:185:ASP:OD2	1:B:189:LYS:HD2	2.18	0.44
1:B:54:ILE:HG13	1:B:58:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ILE:O	1:C:256:ASN:C	2.56	0.44
1:C:136:TYR:OH	1:C:145:ASN:HB2	2.18	0.44
1:B:316:ILE:HG23	4:B:421:HOH:O	2.17	0.44
1:C:210:ILE:HG22	1:C:330:ILE:HD11	2.00	0.44
1:A:207:GLY:HA3	4:A:936:HOH:O	2.17	0.43
1:C:149:VAL:O	1:C:152:ARG:HB3	2.17	0.43
1:A:341:LYS:NZ	4:A:997:HOH:O	2.44	0.43
1:A:133:TRP:CD2	1:A:153:MET:HG2	2.54	0.43
1:A:111:LEU:N	1:A:112:PRO:HD2	2.34	0.43
1:B:328:ILE:HA	1:B:351:LEU:HD21	1.99	0.43
1:C:57:ILE:HG23	1:C:58:THR:HG23	2.00	0.43
1:B:54:ILE:H	1:B:54:ILE:HG12	1.19	0.43
1:C:147:ASN:O	1:C:148:TYR:C	2.56	0.43
1:B:93:ASP:HA	1:B:96:LYS:HE3	2.01	0.43
1:B:176:SER:HB3	1:B:177:LEU:H	1.61	0.42
1:B:14:ASP:OD1	1:B:256:ASN:O	2.36	0.42
1:B:236:ARG:NH1	1:B:274:ASN:O	2.52	0.42
1:A:72:ALA:HB3	1:A:73:PRO:HD3	2.02	0.42
1:A:43:ASN:OD1	1:A:43:ASN:N	2.52	0.42
1:A:60:ASP:C	1:A:62:PRO:HD2	2.40	0.42
1:B:287:LYS:NZ	1:B:287:LYS:CD	2.83	0.42
1:B:246:HIS:CD2	4:B:419:HOH:O	2.67	0.42
3:A:410:HEM:HAB	3:A:410:HEM:HHC	1.66	0.42
1:C:331:ASP:OD1	1:C:333:LYS:HB2	2.19	0.42
1:C:83:TYR:CD2	1:C:118:LYS:NZ	2.82	0.41
1:A:232:GLU:OE1	1:A:311:ARG:NE	2.39	0.41
1:C:117:SER:CB	1:C:130:PHE:CE2	3.03	0.41
1:C:157:LEU:HA	1:C:157:LEU:HD23	1.94	0.41
3:B:410:HEM:HBC2	3:B:410:HEM:CMC	2.50	0.41
1:C:258:LYS:O	1:C:260:ILE:HD12	2.21	0.41
1:C:66:GLU:HG2	1:C:177:LEU:HD23	2.01	0.41
1:C:66:GLU:HA	1:C:177:LEU:HD23	2.02	0.41
1:B:100:ASN:HD22	1:B:100:ASN:C	2.23	0.41
1:A:104:ILE:HA	1:A:108:ALA:HB3	2.03	0.41
1:B:177:LEU:HD12	1:B:177:LEU:HA	1.95	0.41
1:C:152:ARG:HB3	1:C:153:MET:H	1.72	0.41
1:B:210:ILE:HG22	1:B:330:ILE:HD11	2.02	0.41
1:C:61:ASN:HA	1:C:64:HIS:HB3	2.02	0.41
1:C:61:ASN:ND2	1:C:64:HIS:CD2	2.86	0.41
1:B:64:HIS:CD2	1:B:301:ILE:HD12	2.56	0.41
1:A:227:ARG:CD	1:A:319:ASN:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:HA	1:A:26:LYS:HE2	2.02	0.41
1:B:232:GLU:OE2	1:B:294:HIS:CE1	2.68	0.41
1:C:256:ASN:O	1:C:257:ASN:HB2	2.20	0.41
1:B:239:SER:HA	1:B:240:PRO:HD3	1.95	0.41
1:A:243:PHE:CE2	1:A:342:MET:HA	2.55	0.41
1:B:79:LYS:O	1:B:82:ASP:HB2	2.21	0.40
1:C:198:GLY:HA2	3:C:410:HEM:CMC	2.51	0.40
1:B:179:ASN:O	1:B:180:ARG:HB2	2.21	0.40
1:C:319:ASN:O	1:C:323:ASN:HB2	2.20	0.40
1:A:117:SER:HB3	1:A:130:PHE:CE2	2.57	0.40
1:C:41:SER:O	1:C:247:ARG:HA	2.21	0.40
1:B:287:LYS:HB2	1:B:290:ARG:NE	2.37	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	334/343 (97%)	308 (92%)	20 (6%)	6 (2%)	11 18
1	B	331/343 (96%)	286 (86%)	35 (11%)	10 (3%)	5 7
1	C	329/343 (96%)	289 (88%)	28 (8%)	12 (4%)	4 5
All	All	994/1029 (97%)	883 (89%)	83 (8%)	28 (3%)	6 9

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	B	12	LEU
1	B	177	LEU
1	B	178	LYS
1	B	179	ASN

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Mol	Chain	Res	Type
1	C	19	ASP
1	B	66	GLU
1	C	53	GLY
1	C	62	PRO
1	C	152	ARG
1	C	256	ASN
1	A	46	ASN
1	A	62	PRO
1	B	62	PRO
1	B	256	ASN
1	C	173	ALA
1	A	163	SER
1	A	178	LYS
1	A	180	ARG
1	C	61	ASN
1	C	151	ASN
1	C	178	LYS
1	C	179	ASN
1	C	199	ASN
1	B	61	ASN
1	B	180	ARG
1	C	148	TYR
1	B	327	ARG

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	307/310 (99%)	287 (94%)	20 (6%)	21 39
1	B	303/310 (98%)	272 (90%)	31 (10%)	9 17
1	C	302/310 (97%)	279 (92%)	23 (8%)	16 30
All	All	912/930 (98%)	838 (92%)	74 (8%)	15 27

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	54	ILE
1	A	64	HIS
1	A	80	ILE
1	A	116	ILE
1	A	127	MET
1	A	137	ILE
1	A	141	LYS
1	A	142	ARG
1	A	145	ASN
1	A	159	GLU
1	A	177	LEU
1	A	183	THR
1	A	226	ASN
1	A	236	ARG
1	A	268	VAL
1	A	312	LEU
1	A	339	ASP
1	A	340	ASN
1	A	351	LEU
1	B	10	MET
1	B	16	VAL
1	B	38	LYS
1	B	54	ILE
1	B	64	HIS
1	B	92	ASN
1	B	100	ASN
1	B	106	GLU
1	B	111	LEU
1	B	116	ILE
1	B	137	ILE
1	B	140	ASN
1	B	147	ASN
1	B	152	ARG
1	B	156	ARG
1	B	164	ASP
1	B	166	HIS
1	B	178	LYS
1	B	183	THR
1	B	214	ASP
1	B	222	ASP
1	B	226	ASN
1	B	251	GLU

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Mol	Chain	Res	Type
1	B	260	ILE
1	B	284	ASP
1	B	288	ILE
1	B	291	ARG
1	B	312	LEU
1	B	327	ARG
1	B	339	ASP
1	B	341	LYS
1	C	38	LYS
1	C	54	ILE
1	C	61	ASN
1	C	63	GLU
1	C	98	ILE
1	C	100	ASN
1	C	118	LYS
1	C	124	ASP
1	C	142	ARG
1	C	144	GLU
1	C	164	ASP
1	C	183	THR
1	C	184	MET
1	C	185	ASP
1	C	219	ILE
1	C	221	ASP
1	C	226	ASN
1	C	236	ARG
1	C	253	SER
1	C	266	VAL
1	C	291	ARG
1	C	320	ASP
1	C	337	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	64	HIS
1	A	150	ASN
1	A	151	ASN
1	A	199	ASN
1	A	226	ASN
1	A	246	HIS

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Mol	Chain	Res	Type
1	A	294	HIS
1	A	319	ASN
1	A	324	HIS
1	A	340	ASN
1	B	64	HIS
1	B	92	ASN
1	B	100	ASN
1	B	150	ASN
1	B	166	HIS
1	B	199	ASN
1	B	208	ASN
1	B	226	ASN
1	B	256	ASN
1	B	294	HIS
1	C	61	ASN
1	C	64	HIS
1	C	100	ASN
1	C	150	ASN
1	C	166	HIS
1	C	226	ASN
1	C	246	HIS
1	C	294	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
3	HEM	A	410	1	30,50,50	3.54	16 (53%)	24,82,82	3.21	14 (58%)
2	SO4	A	900	-	4,4,4	0.11	0	6,6,6	0.26	0
2	SO4	A	910	-	4,4,4	0.18	0	6,6,6	0.62	0
2	SO4	A	920	-	4,4,4	0.15	0	6,6,6	0.40	0
3	HEM	B	410	1	30,50,50	2.35	6 (20%)	24,82,82	2.40	9 (37%)
3	HEM	C	410	1	30,50,50	2.31	6 (20%)	24,82,82	2.35	10 (41%)
2	SO4	C	910	-	4,4,4	1.24	0	6,6,6	0.38	0

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
3	HEM	A	410	1	-	0/10/54/54	0/0/8/8
2	SO4	A	900	-	-	0/0/0/0	0/0/0/0
2	SO4	A	910	-	-	0/0/0/0	0/0/0/0
2	SO4	A	920	-	-	0/0/0/0	0/0/0/0
3	HEM	B	410	1	-	0/10/54/54	0/0/8/8
3	HEM	C	410	1	-	0/10/54/54	0/0/8/8
2	SO4	C	910	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	HEM	C3B-C4B	-11.30	1.41	1.51
3	B	410	HEM	C3B-C4B	-9.01	1.43	1.51
3	C	410	HEM	C3B-C4B	-8.31	1.44	1.51
3	A	410	HEM	C3D-C4D	-8.09	1.41	1.51
3	C	410	HEM	C3D-C4D	-6.19	1.43	1.51
3	B	410	HEM	C3D-C4D	-4.77	1.45	1.51
3	C	410	HEM	C2C-C1C	-3.29	1.46	1.52
3	B	410	HEM	C2C-C1C	-3.22	1.46	1.52
3	C	410	HEM	C2D-C1D	-2.22	1.44	1.51
3	C	410	HEM	C2B-C1B	-2.22	1.44	1.51
3	A	410	HEM	C2B-C1B	-2.17	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	HEM	C2C-C1C	-2.12	1.48	1.52
3	A	410	HEM	C2D-C1D	-2.11	1.44	1.51
3	B	410	HEM	C2D-C1D	-2.06	1.45	1.51
3	B	410	HEM	CAA-C2A	2.20	1.55	1.52
3	A	410	HEM	CBB-CAB	2.38	1.43	1.29
3	A	410	HEM	FE-NB	2.47	2.10	1.97
3	C	410	HEM	C3B-CAB	2.60	1.56	1.51
3	A	410	HEM	CMB-C2B	2.86	1.59	1.53
3	A	410	HEM	CMC-C2C	2.98	1.60	1.53
3	A	410	HEM	CAA-C2A	3.08	1.57	1.52
3	A	410	HEM	C1C-NC	3.23	1.40	1.36
3	B	410	HEM	FE-NC	3.30	2.08	1.95
3	A	410	HEM	CHC-C1C	3.42	1.44	1.36
3	A	410	HEM	C3C-CAC	3.83	1.58	1.51
3	A	410	HEM	FE-NC	4.89	2.15	1.95
3	A	410	HEM	CMA-C3A	4.90	1.61	1.51
3	A	410	HEM	C3B-CAB	5.29	1.61	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	410	HEM	CMA-C3A-C4A	-4.91	120.24	128.36
3	B	410	HEM	C3C-CAC-CBC	-4.56	117.46	124.46
3	A	410	HEM	CAA-CBA-CGA	-4.47	104.55	112.75
3	C	410	HEM	C3C-CAC-CBC	-3.93	118.42	124.46
3	A	410	HEM	C3B-C4B-CHC	-3.05	118.87	123.16
3	C	410	HEM	CBD-CAD-C3D	-2.72	105.64	113.55
3	A	410	HEM	C2C-C1C-NC	-2.65	105.74	110.21
3	B	410	HEM	CBD-CAD-C3D	-2.34	106.75	113.55
3	A	410	HEM	CAA-C2A-C1A	-2.28	124.53	127.01
3	C	410	HEM	CAA-C2A-C1A	-2.13	124.70	127.01
3	A	410	HEM	CBD-CAD-C3D	-2.07	107.52	113.55
3	C	410	HEM	C2C-C1C-CHC	2.24	127.09	123.68
3	C	410	HEM	C2D-C3D-C4D	2.30	105.40	101.50
3	B	410	HEM	C2D-C3D-C4D	2.31	105.41	101.50
3	A	410	HEM	C2D-C3D-C4D	2.31	105.42	101.50
3	A	410	HEM	CMD-C2D-C3D	2.54	125.60	114.35
3	A	410	HEM	CHC-C4B-NB	2.61	130.80	124.52
3	B	410	HEM	CMD-C2D-C3D	2.63	125.98	114.35
3	B	410	HEM	C2C-C1C-CHC	2.65	127.72	123.68
3	A	410	HEM	CAD-C3D-C4D	2.70	121.99	112.47
3	C	410	HEM	CMD-C2D-C3D	2.82	126.84	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	410	HEM	CMC-C2C-C3C	3.44	125.13	116.53
3	A	410	HEM	CMA-C3A-C2A	3.62	132.81	125.24
3	C	410	HEM	CAD-C3D-C4D	3.78	125.80	112.47
3	B	410	HEM	CMC-C2C-C3C	3.93	126.35	116.53
3	B	410	HEM	CMB-C2B-C3B	4.38	127.45	116.53
3	B	410	HEM	CAD-C3D-C2D	4.47	126.06	113.22
3	B	410	HEM	CAD-C3D-C4D	4.55	128.51	112.47
3	C	410	HEM	CMB-C2B-C3B	4.63	128.08	116.53
3	C	410	HEM	CAD-C3D-C2D	5.42	128.80	113.22
3	A	410	HEM	CMB-C2B-C3B	6.47	132.67	116.53
3	A	410	HEM	C2C-C1C-CHC	6.51	133.59	123.68
3	A	410	HEM	CAD-C3D-C2D	6.74	132.58	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	HEM	5	0
2	A	900	SO4	1	0
3	B	410	HEM	3	0
3	C	410	HEM	6	0
2	C	910	SO4	4	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

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, 95^{th} 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	338/343 (98%)	0.70	13 (3%) 44 49	59, 68, 85, 114	0
1	B	335/343 (97%)	0.79	41 (12%) 5 5	58, 69, 82, 86	0
1	C	333/343 (97%)	0.92	44 (13%) 4 4	57, 70, 80, 88	0
All	All	1006/1029 (97%)	0.80	98 (9%) 10 10	57, 69, 82, 114	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	SER	7.9
1	A	177	LEU	6.3
1	B	177	LEU	5.7
1	A	166	HIS	5.7
1	B	351	LEU	5.6
1	C	177	LEU	5.4
1	B	350	PHE	5.3
1	C	98	ILE	5.1
1	C	351	LEU	5.0
1	C	12	LEU	4.9
1	A	142	ARG	4.8
1	B	61	ASN	4.7
1	C	96	LYS	4.3
1	B	100	ASN	4.2
1	C	95	ILE	4.2
1	C	250	ALA	4.0
1	C	325	PHE	3.9
1	B	325	PHE	3.8
1	B	99	ASP	3.6
1	B	334	LYS	3.6
1	B	140	ASN	3.6
1	A	165	SER	3.5
1	B	332	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	280	PHE	3.5
1	B	335	SER	3.4
1	B	330	ILE	3.3
1	C	89	GLU	3.3
1	C	288	ILE	3.3
1	C	327	ARG	3.2
1	B	70	ILE	3.2
1	B	322	LEU	3.2
1	C	295	LEU	3.2
1	C	352	SER	3.2
1	C	94	LEU	3.1
1	B	287	LYS	3.1
1	A	48	TYR	3.1
1	B	250	ALA	3.1
1	C	97	ASN	3.0
1	C	166	HIS	3.0
1	B	144	GLU	3.0
1	A	181	LYS	2.9
1	A	179	ASN	2.8
1	A	164	ASP	2.8
1	C	39	ILE	2.8
1	B	348	LYS	2.8
1	B	283	PRO	2.7
1	C	326	LYS	2.7
1	B	206	ILE	2.6
1	C	254	TYR	2.6
1	C	255	ILE	2.6
1	B	179	ASN	2.6
1	C	281	ASP	2.6
1	C	278	THR	2.5
1	B	279	PHE	2.5
1	B	52	GLY	2.5
1	C	32	HIS	2.5
1	C	212	VAL	2.5
1	C	148	TYR	2.5
1	B	97	ASN	2.5
1	C	174	GLY	2.5
1	C	139	GLY	2.5
1	C	155	SER	2.5
1	C	22	TRP	2.5
1	C	74	TYR	2.4
1	B	101	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	193	LEU	2.4
1	C	224	LEU	2.4
1	C	333	LYS	2.4
1	A	12	LEU	2.4
1	B	94	LEU	2.4
1	B	184	MET	2.4
1	C	286	PHE	2.3
1	B	349	LEU	2.3
1	C	301	ILE	2.3
1	B	176	SER	2.3
1	C	142	ARG	2.2
1	C	176	SER	2.2
1	C	217	PRO	2.2
1	A	317	ALA	2.2
1	B	210	ILE	2.2
1	B	25	TYR	2.2
1	A	139	GLY	2.2
1	C	101	LYS	2.2
1	B	286	PHE	2.1
1	A	61	ASN	2.1
1	C	324	HIS	2.1
1	B	69	ASP	2.1
1	C	118	LYS	2.1
1	B	336	ARG	2.1
1	B	329	LYS	2.1
1	B	10	MET	2.1
1	B	131	LYS	2.1
1	C	80	ILE	2.0
1	B	132	LEU	2.0
1	C	132	LEU	2.0
1	C	180	ARG	2.0
1	B	53	GLY	2.0
1	A	285	LEU	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

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, 95^{th} 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	SO4	C	910	5/5	0.91	0.41	4.61	89,89,91,92	0
2	SO4	A	920	5/5	0.94	0.25	3.64	90,90,91,92	0
3	HEM	C	410	43/43	0.94	0.19	-0.01	62,64,67,70	0
2	SO4	A	910	5/5	0.94	0.20	-0.25	76,78,78,79	0
3	HEM	B	410	43/43	0.96	0.16	-0.85	61,65,67,67	0
3	HEM	A	410	43/43	0.98	0.18	-0.98	60,67,71,75	0
2	SO4	A	900	5/5	0.95	0.16	-0.98	86,87,88,89	0

6.5 Other polymers

There are no such residues in this entry.