Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:11 PM GMT

PDB ID : 4HGJ
Title : Crystal structure of P450 BM3 5F5 heme domain variant
Authors : Shehzad, A.; Panneerselvam, S.; Bocola, M.; Mueller-Dieckmann, J.; Wilmanns, M.; Schwaneberg, U.
Deposited on : 2012-10-08
Resolution : 1.90 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 (i) symbol.

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

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 1.90 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.

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
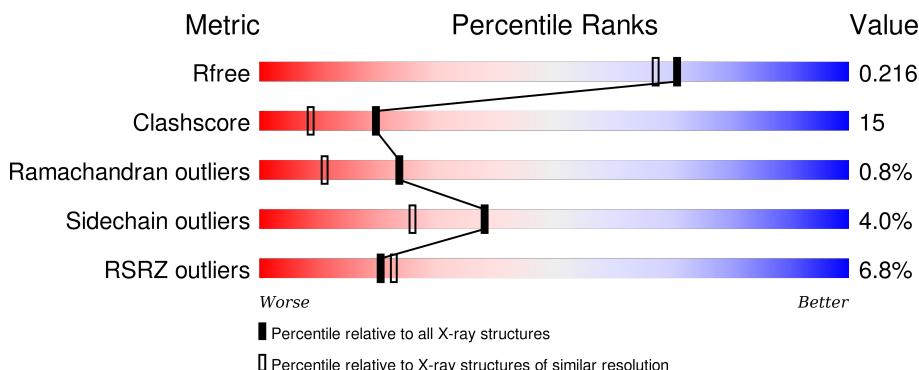
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	455	
1	B	455	
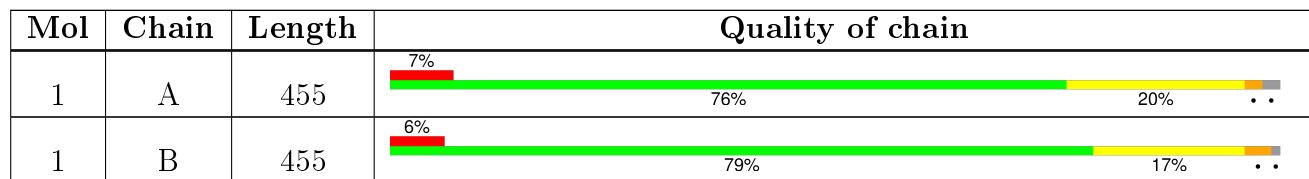
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	502	-	-	-	X
3	GOL	A	503	-	-	-	X
3	GOL	A	505	-	-	-	X
3	GOL	B	501	-	-	-	X
3	GOL	B	503	-	-	-	X
4	MES	A	504	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8336 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 Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total 3708	C 2375	N 627	O 688	S 18	0	15	0
1	B	451	Total 3697	C 2366	N 628	O 686	S 17	0	11	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
A	235	ALA	THR	ENGINEERED MUTATION	UNP P14779
B	87	ALA	PHE	ENGINEERED MUTATION	UNP P14779
B	235	ALA	THR	ENGINEERED MUTATION	UNP P14779

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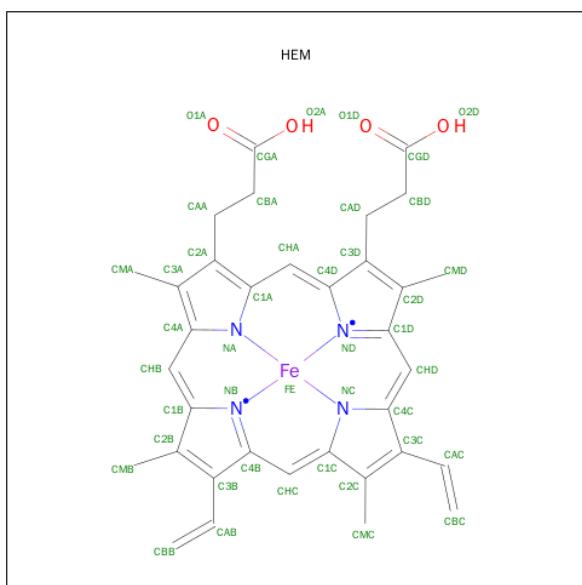
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
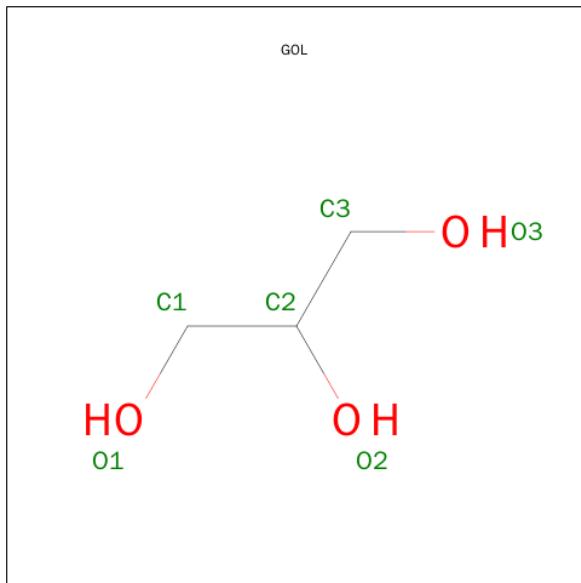
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

O1
C2   C6
C3   C5
H
N$^+$
N4

C8   C7

S
O2S   O   O1S

O$^-$
O3S
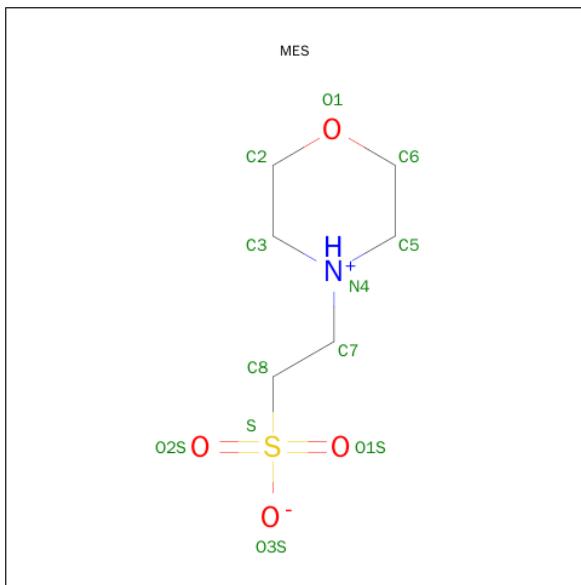
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O	0	0
			391	391		
5	B	412	Total	O	0	0
			412	412		

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: Bifunctional P-450/NADPH-P450 reductase
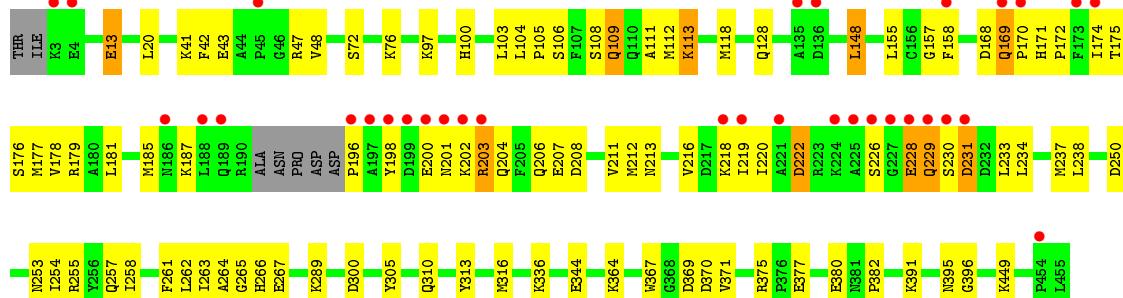
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase
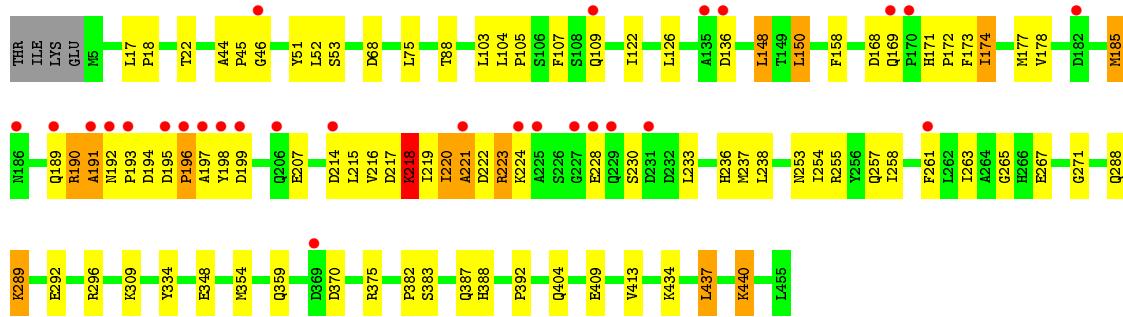
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.01Å 148.37Å 64.15Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	19.93 – 1.90 19.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.93-1.90) 97.5 (19.93-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.69 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.182 , 0.217 0.182 , 0.216	Depositor DCC
R_{free} test set	4174 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 83473 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8336	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: GOL, MES, 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	0.49	0/3820	0.57	0/5155
1	B	0.46	1/3815 (0.0%)	0.56	1/5156 (0.0%)
All	All	0.47	1/7635 (0.0%)	0.57	1/10311 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	GLU	CB-CG	-5.35	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	LEU	CA-CB-CG	5.13	127.09	115.30

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	3708	0	3700	106	0
1	B	3697	0	3697	108	0
2	A	43	0	30	4	0
2	B	43	0	30	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	18	0	24	5	0
3	B	12	0	16	0	0
4	A	12	0	12	0	0
5	A	391	0	0	12	0
5	B	412	0	0	21	0
All	All	8336	0	7509	224	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 15.

All (224) 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:177:MET:HG3	1:A:212:MET:CE	1.82	1.09
1:B:437:LEU:H	1:B:437:LEU:HD12	1.17	1.08
1:B:171:HIS:HB3	1:B:174:ILE:CG1	1.90	1.02
1:B:185:MET:HE1	1:B:437:LEU:HB3	1.43	0.99
1:B:440[A]:LYS:HD2	5:B:999:HOH:O	1.63	0.97
1:B:171:HIS:CG	1:B:172:PRO:HD2	2.00	0.96
1:A:179:ARG:NE	1:A:204:GLN:OE1	1.99	0.96
2:B:502:HEM:HBC2	2:B:502:HEM:HHD	1.48	0.95
1:B:171:HIS:HB3	1:B:174:ILE:HG12	1.49	0.95
1:B:214:ASP:O	1:B:218:LYS:HD3	1.68	0.93
1:A:370:ASP:OD2	1:A:375:ARG:NH1	2.03	0.92
1:B:437:LEU:H	1:B:437:LEU:CD1	1.82	0.91
1:A:234:LEU:HA	1:A:237:MET:HE2	1.52	0.89
1:A:234:LEU:HA	1:A:237:MET:CE	2.02	0.89
1:A:200:GLU:O	1:A:203:ARG:HG3	1.72	0.89
1:A:181:LEU:O	1:A:185:MET:HG3	1.72	0.88
1:B:292:GLU:OE2	1:B:296[A]:ARG:NH1	2.07	0.88
1:B:189:GLN:O	1:B:191:ALA:N	2.08	0.87
1:A:202:LYS:O	1:A:206:GLN:HG2	1.73	0.86
1:B:177:MET:SD	1:B:263:ILE:HG12	2.16	0.86
1:B:185:MET:CE	1:B:437:LEU:HB3	2.07	0.85
1:A:41:LYS:NZ	1:A:43:GLU:OE2	2.11	0.83
1:A:177:MET:HG3	1:A:212:MET:HE2	1.58	0.83
1:A:395:ASN:HA	3:A:502:GOL:H11	1.61	0.81
1:B:158:PHE:HZ	1:B:261[B]:PHE:HD2	1.28	0.81
1:A:128[B]:GLN:NE2	5:A:855:HOH:O	2.05	0.80
1:A:174:ILE:O	1:A:178:VAL:HG23	1.82	0.78
1:B:217:ASP:OD1	5:B:896:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG11	1:B:255:ARG:HB2	1.66	0.77
1:B:440[A]:LYS:CD	5:B:999:HOH:O	2.23	0.77
1:A:177:MET:SD	1:A:263:ILE:HG12	2.26	0.76
1:B:267:GLU:OE1	1:B:437:LEU:HD21	1.84	0.76
1:A:177:MET:CG	1:A:212:MET:CE	2.64	0.76
1:A:226:SER:OG	1:A:228:GLU:HG2	1.87	0.74
1:B:189:GLN:O	1:B:190:ARG:C	2.24	0.72
1:B:288:GLN:OE1	5:B:909:HOH:O	2.07	0.72
1:A:177:MET:CB	1:A:212:MET:HE3	2.20	0.71
2:B:502:HEM:HBB2	2:B:502:HEM:HMB2	1.71	0.71
2:B:502:HEM:HBC1	5:B:994:HOH:O	1.90	0.71
2:B:502:HEM:HBB2	2:B:502:HEM:CMB	2.21	0.70
1:A:103:LEU:HD13	1:A:261[B]:PHE:HZ	1.55	0.70
1:B:237:MET:HE3	1:B:258:ILE:HG13	1.74	0.69
1:B:437:LEU:N	1:B:437:LEU:HD12	2.00	0.69
1:A:109[B]:GLN:O	1:A:112:MET:HB2	1.93	0.69
1:A:174:ILE:HG22	1:A:178:VAL:CG2	2.23	0.68
1:A:267[B]:GLU:OE1	1:A:267[B]:GLU:HA	1.93	0.68
1:B:309:LYS:NZ	5:B:667:HOH:O	2.22	0.68
1:B:158:PHE:CZ	1:B:261[B]:PHE:HD2	2.12	0.67
2:B:502:HEM:CBC	5:B:994:HOH:O	2.43	0.67
1:A:229:GLN:OE1	1:A:229:GLN:HA	1.93	0.67
1:A:177:MET:HG3	1:A:212:MET:HE1	1.77	0.66
1:B:193:PRO:O	1:B:194:ASP:OD1	2.14	0.65
1:A:168:ASP:N	1:B:168:ASP:OD1	2.24	0.65
1:B:107:PHE:CZ	1:B:261[A]:PHE:CE1	2.84	0.65
1:B:171:HIS:ND1	1:B:172:PRO:HD2	2.11	0.64
1:A:106[B]:SER:HB3	1:A:233:LEU:HD23	1.78	0.64
1:B:222:ASP:OD2	5:B:809:HOH:O	2.15	0.64
1:B:171:HIS:HB3	1:B:174:ILE:CD1	2.27	0.64
1:B:109:GLN:CD	1:B:309:LYS:HZ3	2.00	0.64
1:A:220:ILE:HD11	1:A:258:ILE:CD1	2.27	0.64
1:A:207:GLU:O	1:A:211:VAL:HG23	1.97	0.63
1:A:13:GLU:CD	1:A:13:GLU:H	2.02	0.63
1:A:336:LYS:NZ	3:A:503:GOL:O2	2.31	0.63
1:B:171:HIS:CD2	1:B:172:PRO:HD2	2.33	0.62
1:A:187:LYS:NZ	5:A:820:HOH:O	2.32	0.62
1:A:203:ARG:O	1:A:207:GLU:HG2	2.01	0.61
1:A:204:GLN:O	1:A:207:GLU:HG3	1.99	0.61
1:B:237:MET:CE	1:B:258:ILE:HG13	2.31	0.61
1:A:108[B]:SER:O	1:A:112:MET:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106[A]:SER:HB3	1:A:233:LEU:HD23	1.82	0.60
1:B:289:LYS:HD2	5:B:745:HOH:O	2.00	0.60
1:A:218:LYS:O	1:A:222:ASP:HB2	2.00	0.60
1:B:292:GLU:CD	1:B:296[A]:ARG:NH1	2.56	0.59
1:A:174:ILE:HG22	1:A:178:VAL:HG23	1.83	0.59
1:B:440[A]:LYS:HE3	5:B:999:HOH:O	2.03	0.59
1:B:194:ASP:O	1:B:195:ASP:C	2.42	0.58
1:B:292:GLU:CD	1:B:296[A]:ARG:HH12	2.07	0.58
1:A:47:ARG:NH2	5:A:940:HOH:O	2.34	0.58
1:A:169:GLN:HB2	1:A:170:PRO:HD2	1.85	0.57
1:B:171:HIS:CB	1:B:174:ILE:HG12	2.29	0.57
1:A:310:GLN:HG3	5:A:977:HOH:O	2.03	0.57
1:A:395:ASN:HA	3:A:502:GOL:C1	2.31	0.57
1:A:204:GLN:O	1:A:207:GLU:CG	2.53	0.56
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.88	0.56
1:B:440[B]:LYS:CE	5:B:1012:HOH:O	2.53	0.56
1:B:122:ILE:HG22	1:B:148:LEU:HD22	1.88	0.55
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.41	0.55
1:A:177:MET:HB2	1:A:212:MET:HE3	1.87	0.55
1:B:370:ASP:OD2	1:B:375[B]:ARG:NH1	2.37	0.55
1:A:177:MET:HA	1:A:212:MET:CE	2.36	0.55
1:B:267:GLU:OE1	1:B:437:LEU:CD2	2.54	0.55
1:A:316:MET:CE	1:A:377:GLU:HA	2.37	0.55
1:A:174:ILE:CG2	1:A:178:VAL:CG2	2.85	0.54
1:B:437:LEU:N	1:B:437:LEU:CD1	2.54	0.54
1:B:192:ASN:O	1:B:198:TYR:CE2	2.60	0.54
1:B:215:LEU:O	1:B:219:ILE:HG13	2.08	0.54
1:A:382:PRO:HG3	5:A:809:HOH:O	2.07	0.54
1:B:196:PRO:O	1:B:199:ASP:HB2	2.08	0.54
1:A:264:ALA:HA	5:A:770:HOH:O	2.07	0.54
1:B:158:PHE:CE1	1:B:258:ILE:HG12	2.43	0.54
1:A:158[B]:PHE:HZ	1:A:262:LEU:HD21	1.73	0.54
1:B:171:HIS:HB3	1:B:174:ILE:HD11	1.90	0.54
1:B:107:PHE:CZ	1:B:261[A]:PHE:HE1	2.25	0.53
2:B:502:HEM:HMB2	2:B:502:HEM:CBB	2.37	0.53
1:B:265:GLY:HA2	2:B:502:HEM:HBB2	1.88	0.53
1:A:108[A]:SER:O	1:A:111[A]:ALA:HB3	2.09	0.53
1:A:198:TYR:HD1	1:A:201:ASN:OD1	1.92	0.53
1:B:292:GLU:OE1	1:B:296[A]:ARG:NH1	2.42	0.53
1:B:228:GLU:HA	1:B:228:GLU:OE2	2.08	0.53
1:B:150:LEU:HD11	1:B:174:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:TYR:CD1	1:A:201:ASN:OD1	2.62	0.53
1:A:169:GLN:CB	1:A:170:PRO:HD2	2.39	0.53
1:B:150:LEU:HD11	1:B:174:ILE:CD1	2.37	0.53
1:A:106[A]:SER:HB3	1:A:233:LEU:CD2	2.38	0.53
1:A:250:ASP:O	1:A:254:ILE:HG13	2.09	0.53
1:A:267[A]:GLU:HB3	5:A:761:HOH:O	2.09	0.52
1:B:238:LEU:HD23	1:B:254:ILE:HD13	1.92	0.52
1:A:264:ALA:O	5:A:770:HOH:O	2.18	0.52
1:A:289:LYS:HD3	1:A:313:TYR:CZ	2.44	0.52
1:B:265:GLY:HA2	2:B:502:HEM:CBB	2.40	0.52
1:B:288:GLN:CD	5:B:909:HOH:O	2.47	0.52
1:B:193:PRO:C	1:B:194:ASP:OD1	2.48	0.52
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.92	0.52
1:B:223:ARG:HD2	5:B:1007:HOH:O	2.10	0.51
1:B:195:ASP:O	1:B:197:ALA:N	2.43	0.51
1:B:237:MET:CE	1:B:254:ILE:HG23	2.39	0.51
1:B:109:GLN:CD	1:B:309:LYS:NZ	2.63	0.51
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.41	0.51
1:A:177:MET:HA	1:A:212:MET:HE1	1.93	0.50
1:A:106[B]:SER:HB3	1:A:233:LEU:CD2	2.40	0.50
1:A:41:LYS:NZ	1:A:43:GLU:CD	2.64	0.50
1:A:253:ASN:O	1:A:257:GLN:HG2	2.12	0.50
1:A:174:ILE:HG22	1:A:178:VAL:HG21	1.93	0.50
1:B:219:ILE:O	1:B:222:ASP:HB2	2.11	0.50
1:B:174:ILE:O	1:B:178:VAL:HG23	2.11	0.50
1:B:440[A]:LYS:CE	5:B:999:HOH:O	2.53	0.50
1:B:171:HIS:CE1	1:B:172:PRO:HD2	2.47	0.49
1:B:253:ASN:O	1:B:257:GLN:HG2	2.12	0.49
1:B:440[B]:LYS:HE2	5:B:1012:HOH:O	2.10	0.49
1:B:392:PRO:O	2:B:502:HEM:CBC	2.60	0.49
1:B:51:TYR:CE2	1:B:354:MET:HG2	2.46	0.49
1:A:257:GLN:O	1:A:261[A]:PHE:HD1	1.96	0.49
1:A:174:ILE:CG2	1:A:178:VAL:HG23	2.42	0.49
1:A:177:MET:CB	1:A:212:MET:CE	2.88	0.49
1:B:104:LEU:N	1:B:105:PRO:HD2	2.28	0.49
1:A:266:HIS:C	1:A:266:HIS:CD2	2.87	0.49
1:A:204:GLN:HA	1:A:207:GLU:HG2	1.96	0.48
1:A:148:LEU:HD13	1:A:148:LEU:C	2.33	0.48
1:A:177:MET:CA	1:A:212:MET:HE3	2.43	0.48
1:B:434:LYS:HB3	1:B:440[A]:LYS:HD3	1.95	0.48
1:A:158[B]:PHE:CD1	1:A:219:ILE:HD13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:O	1:B:254:ILE:HD11	2.14	0.48
1:B:216:VAL:CG1	1:B:255:ARG:HB2	2.42	0.48
1:B:440[B]:LYS:NZ	5:B:851:HOH:O	2.45	0.47
1:B:404[B]:GLN:OE1	5:B:657:HOH:O	2.20	0.47
1:A:364:LYS:HD3	1:A:369:ASP:HA	1.95	0.47
1:B:44:ALA:HB1	1:B:45:PRO:HD2	1.95	0.47
1:A:118[A]:MET:SD	1:A:155:LEU:HD21	2.54	0.47
1:B:237:MET:HE2	1:B:254:ILE:HG23	1.94	0.47
1:A:158[B]:PHE:CE1	1:A:219:ILE:HD13	2.50	0.47
1:A:158[B]:PHE:HB3	1:A:234:LEU:HB2	1.97	0.47
1:A:234:LEU:CA	1:A:237:MET:HE2	2.35	0.47
1:B:17:LEU:HB3	1:B:18:PRO:HD3	1.95	0.47
1:B:68:ASP:HB3	1:B:334:TYR:CE1	2.50	0.47
1:B:103:LEU:HD21	1:B:237:MET:HG3	1.97	0.47
1:B:148:LEU:HD11	1:B:413:VAL:HG21	1.97	0.47
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.45	0.46
1:B:107:PHE:HZ	1:B:261[A]:PHE:CE1	2.33	0.46
1:B:257:GLN:O	1:B:261[A]:PHE:HD2	1.98	0.46
1:B:173:PHE:HD2	1:B:174:ILE:HD13	1.80	0.45
1:A:113:LYS:HD2	1:A:305:TYR:CE2	2.51	0.45
1:A:179:ARG:CZ	1:A:204:GLN:OE1	2.64	0.45
1:A:204:GLN:CA	1:A:207:GLU:HG2	2.47	0.45
1:B:220:ILE:HG23	1:B:238:LEU:HD21	1.99	0.45
1:A:396:GLY:H	3:A:502:GOL:C1	2.30	0.45
1:A:300:ASP:OD2	5:A:926:HOH:O	2.21	0.45
1:A:230[B]:SER:OG	1:A:231:ASP:N	2.48	0.45
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.99	0.44
1:B:237:MET:CE	1:B:258:ILE:CG1	2.94	0.44
1:A:213:ASN:OD1	1:A:255:ARG:HD3	2.17	0.44
1:A:175:THR:CG2	1:A:179:ARG:HH12	2.31	0.44
1:B:236:HIS:CE1	5:B:1010:HOH:O	2.70	0.44
1:A:157:GLY:C	1:A:158[A]:PHE:CG	2.91	0.44
1:A:171:HIS:CG	1:A:172:PRO:HD2	2.52	0.44
1:B:223:ARG:HG3	1:B:223:ARG:O	2.18	0.43
1:A:100:HIS:HE1	3:A:505:GOL:O2	2.01	0.43
1:B:288:GLN:NE2	5:B:909:HOH:O	2.51	0.43
1:B:382:PRO:HD2	5:B:953:HOH:O	2.18	0.43
1:A:43:GLU:HG2	1:A:48:VAL:HG22	2.00	0.43
1:B:171:HIS:CG	1:B:172:PRO:CD	2.87	0.43
1:B:171:HIS:HB3	1:B:174:ILE:HG13	1.92	0.43
1:B:107:PHE:CE2	1:B:261[A]:PHE:CE1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:HD22	1:B:88:THR:HG22	2.01	0.43
1:A:200:GLU:O	1:A:203:ARG:CG	2.55	0.43
1:B:46:GLY:N	5:B:913:HOH:O	2.27	0.43
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.79	0.42
1:A:196:PRO:C	1:A:198:TYR:N	2.72	0.42
1:B:220:ILE:O	1:B:221:ALA:C	2.58	0.42
1:A:266:HIS:N	5:A:759:HOH:O	2.52	0.42
1:A:104:LEU:HB3	1:A:105:PRO:HD3	2.02	0.42
1:A:104:LEU:N	1:A:105:PRO:CD	2.83	0.42
1:B:271:GLY:HA2	1:B:440[B]:LYS:HG3	2.00	0.42
2:B:502:HEM:HHD	2:B:502:HEM:CBC	2.35	0.42
1:A:169:GLN:HG2	1:A:169:GLN:H	1.38	0.41
1:B:53:SER:HB3	1:B:359:GLN:HB3	2.01	0.41
1:A:47:ARG:HD2	5:A:942:HOH:O	2.19	0.41
1:B:107:PHE:CE2	1:B:233:LEU:HD21	2.56	0.41
1:A:72:SER:O	1:A:76:LYS:HG3	2.21	0.41
1:A:216:VAL:HG13	1:A:258:ILE:HD13	2.02	0.41
1:A:255:ARG:HA	1:A:258:ILE:HD12	2.03	0.41
1:B:173:PHE:CD2	1:B:173:PHE:C	2.95	0.41
1:B:195:ASP:C	1:B:197:ALA:H	2.24	0.41
1:A:220:ILE:HG23	1:A:238:LEU:HD21	2.03	0.41
1:B:171:HIS:O	1:B:174:ILE:HG12	2.21	0.41
1:B:216:VAL:O	1:B:220:ILE:HG13	2.21	0.41
1:A:169:GLN:CB	1:A:170:PRO:CD	2.99	0.41
1:A:97:LYS:HB2	5:A:740:HOH:O	2.21	0.40
1:A:176:SER:O	1:A:208:ASP:HB3	2.21	0.40
1:B:158:PHE:HZ	1:B:261[B]:PHE:CD2	2.20	0.40
1:A:177:MET:HA	1:A:212:MET:HE3	2.03	0.40
1:A:20:LEU:HG	1:A:42:PHE:CZ	2.56	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	459/455 (101%)	438 (95%)	20 (4%)	1 (0%)	52	42
1	B	460/455 (101%)	436 (95%)	18 (4%)	6 (1%)	15	4
All	All	919/910 (101%)	874 (95%)	38 (4%)	7 (1%)	24	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	ARG
1	B	191	ALA
1	B	220	ILE
1	B	221	ALA
1	B	218	LYS
1	A	228	GLU
1	B	196	PRO

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	405/397 (102%)	391 (96%)	14 (4%)	43	31
1	B	404/397 (102%)	384 (95%)	20 (5%)	30	18
All	All	809/794 (102%)	775 (96%)	34 (4%)	38	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	109[A]	GLN
1	A	109[B]	GLN
1	A	113	LYS
1	A	148	LEU
1	A	169	GLN
1	A	203	ARG
1	A	222	ASP
1	A	229	GLN

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Mol	Chain	Res	Type
1	A	231	ASP
1	A	344	GLU
1	A	380	GLU
1	A	391	LYS
1	A	449	LYS
1	B	22	THR
1	B	52	LEU
1	B	126	LEU
1	B	136	ASP
1	B	150	LEU
1	B	169	GLN
1	B	174	ILE
1	B	185	MET
1	B	207	GLU
1	B	218	LYS
1	B	223	ARG
1	B	224	LYS
1	B	230	SER
1	B	289	LYS
1	B	383	SER
1	B	409[A]	GLU
1	B	409[B]	GLU
1	B	437	LEU
1	B	440[A]	LYS
1	B	440[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	501	1,5	30,50,50	2.20	8 (26%)	24,82,82	2.42	10 (41%)
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.25	0
3	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.57	0
4	MES	A	504	-	11,12,12	0.90	0	14,16,16	3.15	6 (42%)
3	GOL	A	505	-	5,5,5	0.31	0	5,5,5	0.38	0
3	GOL	B	501	-	5,5,5	0.29	0	5,5,5	0.46	0
2	HEM	B	502	1,5	30,50,50	2.27	7 (23%)	24,82,82	2.37	11 (45%)
3	GOL	B	503	-	5,5,5	0.32	0	5,5,5	0.29	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
2	HEM	A	501	1,5	-	0/10/54/54	0/0/8/8
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
3	GOL	A	503	-	-	0/4/4/4	0/0/0/0
4	MES	A	504	-	-	0/6/14/14	0/1/1/1
3	GOL	A	505	-	-	0/4/4/4	0/0/0/0
3	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	HEM	B	502	1,5	-	0/10/54/54	0/0/8/8
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	C3B-C4B	-7.33	1.45	1.51
2	A	501	HEM	C3B-C4B	-7.27	1.45	1.51
2	B	502	HEM	C3D-C4D	-4.99	1.45	1.51
2	A	501	HEM	C3D-C4D	-4.98	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	C2C-C1C	-4.42	1.44	1.52
2	A	501	HEM	C2C-C1C	-3.40	1.46	1.52
2	B	502	HEM	C2D-C1D	-2.17	1.44	1.51
2	A	501	HEM	C2D-C1D	-2.08	1.45	1.51
2	A	501	HEM	CAA-C2A	2.18	1.55	1.52
2	A	501	HEM	C3C-CAC	2.32	1.55	1.51
2	B	502	HEM	C4C-NC	2.34	1.38	1.36
2	A	501	HEM	C4C-NC	2.74	1.39	1.36
2	A	501	HEM	FE-ND	2.86	2.12	1.97
2	B	502	HEM	C1C-NC	2.98	1.39	1.36
2	B	502	HEM	FE-ND	3.02	2.13	1.97

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	MES	O3S-S-O2S	-4.15	101.95	111.61
2	B	502	HEM	CBA-CAA-C2A	-3.92	105.51	112.53
2	A	501	HEM	CBA-CAA-C2A	-3.42	106.39	112.53
2	A	501	HEM	CBD-CAD-C3D	-2.96	104.93	113.55
4	A	504	MES	O3S-S-O1S	-2.85	104.97	111.61
2	B	502	HEM	C3B-CAB-CBB	-2.84	120.10	124.46
2	B	502	HEM	CMA-C3A-C4A	-2.39	124.40	128.36
2	B	502	HEM	CBD-CAD-C3D	-2.38	106.63	113.55
2	B	502	HEM	C3C-CAC-CBC	-2.34	120.87	124.46
2	A	501	HEM	C3B-CAB-CBB	-2.33	120.88	124.46
2	A	501	HEM	C2C-C1C-CHC	2.12	126.90	123.68
2	B	502	HEM	CMD-C2D-C3D	2.70	126.30	114.35
2	B	502	HEM	C2D-C3D-C4D	2.88	106.38	101.50
2	A	501	HEM	C2D-C3D-C4D	2.89	106.39	101.50
2	A	501	HEM	CMD-C2D-C3D	3.00	127.63	114.35
4	A	504	MES	O1S-S-C8	3.04	109.50	106.91
2	B	502	HEM	CMB-C2B-C3B	3.33	124.84	116.53
2	B	502	HEM	CMC-C2C-C3C	3.38	124.98	116.53
2	A	501	HEM	CAD-C3D-C4D	3.89	126.18	112.47
2	A	501	HEM	CMC-C2C-C3C	3.92	126.31	116.53
2	B	502	HEM	CAD-C3D-C4D	4.33	127.75	112.47
2	B	502	HEM	CAD-C3D-C2D	4.40	125.87	113.22
2	A	501	HEM	CMB-C2B-C3B	4.46	127.67	116.53
2	A	501	HEM	CAD-C3D-C2D	4.94	127.41	113.22
4	A	504	MES	C7-N4-C3	5.00	124.09	111.27
4	A	504	MES	C5-N4-C3	5.18	120.13	108.90
4	A	504	MES	O2S-S-C8	6.20	112.19	106.91

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
2	A	501	HEM	4	0
3	A	502	GOL	3	0
3	A	503	GOL	1	0
3	A	505	GOL	1	0
2	B	502	HEM	10	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	448/455 (98%)	0.10	33 (7%)	17	19	12, 23, 59, 82	0
1	B	451/455 (99%)	0.17	28 (6%)	24	27	12, 23, 57, 95	0
All	All	899/910 (98%)	0.13	61 (6%)	20	23	12, 23, 58, 95	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	11.5
1	B	192	ASN	8.1
1	B	196	PRO	7.5
1	A	198	TYR	6.5
1	B	225	ALA	6.3
1	B	193	PRO	5.9
1	B	195	ASP	5.5
1	A	196	PRO	5.3
1	B	221	ALA	5.3
1	A	227	GLY	5.1
1	A	225	ALA	5.1
1	A	229	GLN	4.9
1	B	228	GLU	4.6
1	B	229	GLN	4.6
1	B	227	GLY	4.5
1	A	197	ALA	4.3
1	A	169	GLN	4.2
1	A	173	PHE	3.9
1	A	170	PRO	3.8
1	B	197	ALA	3.8
1	B	261[A]	PHE	3.7
1	B	224	LYS	3.7
1	B	198	TYR	3.5
1	A	228	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASP	3.4
1	B	46	GLY	3.2
1	A	199	ASP	3.2
1	A	221	ALA	3.1
1	B	136	ASP	3.1
1	B	231	ASP	3.0
1	A	201	ASN	3.0
1	A	218	LYS	3.0
1	A	200	GLU	2.9
1	A	202	LYS	2.9
1	B	109	GLN	2.7
1	A	188	LEU	2.7
1	B	214	ASP	2.6
1	A	203	ARG	2.6
1	A	226	SER	2.6
1	A	230[A]	SER	2.6
1	A	219	ILE	2.5
1	A	158[A]	PHE	2.5
1	B	186	ASN	2.5
1	A	45	PRO	2.5
1	B	135	ALA	2.4
1	A	136	ASP	2.4
1	B	182	ASP	2.4
1	A	186	ASN	2.3
1	B	170	PRO	2.3
1	A	174	ILE	2.3
1	A	189	GLN	2.3
1	B	189	GLN	2.2
1	A	224	LYS	2.2
1	A	4	GLU	2.2
1	A	454	PRO	2.2
1	B	206	GLN	2.1
1	A	231	ASP	2.1
1	A	3	LYS	2.1
1	A	135	ALA	2.1
1	B	169	GLN	2.1
1	B	369	ASP	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($Å^2$)	Q<0.9
3	GOL	A	503	6/6	0.92	0.23	29.71	24,40,43,50	0
4	MES	A	504	12/12	0.76	0.25	13.40	34,52,89,93	0
3	GOL	B	501	6/6	0.88	0.19	5.79	24,37,45,54	0
3	GOL	A	502	6/6	0.80	0.17	4.52	30,40,41,51	0
3	GOL	A	505	6/6	0.91	0.17	3.46	27,31,39,43	0
3	GOL	B	503	6/6	0.88	0.24	2.58	39,47,51,51	0
2	HEM	B	502	43/43	0.98	0.09	-0.35	9,15,21,31	0
2	HEM	A	501	43/43	0.98	0.07	-0.72	10,16,22,26	0

6.5 Other polymers (i)

There are no such residues in this entry.