Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:32 AM GMT

PDB ID	:	2R50
Title	:	The crystal structure of nonsymbiotic corn hemoglobin 1
Authors	:	Smagghe, B.J.; Hoy, J.A.; Hargrove, M.S.
Deposited on	:	2007-09-02
Resolution	:	2.20 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 (1)) were used in the production of this report:

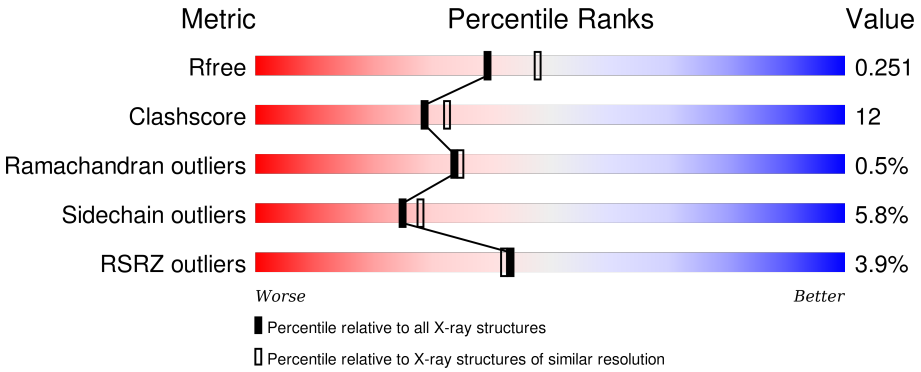
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	5% 68% 17% • 12%
1	B	165	% 68% 19% • 12%
1	C	165	4% 65% 21% •• 11%
1	D	165	4% 62% 23% • 12%

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	D	166	-	-	X	-
4	ACY	B	168	-	-	X	-

2 Entry composition

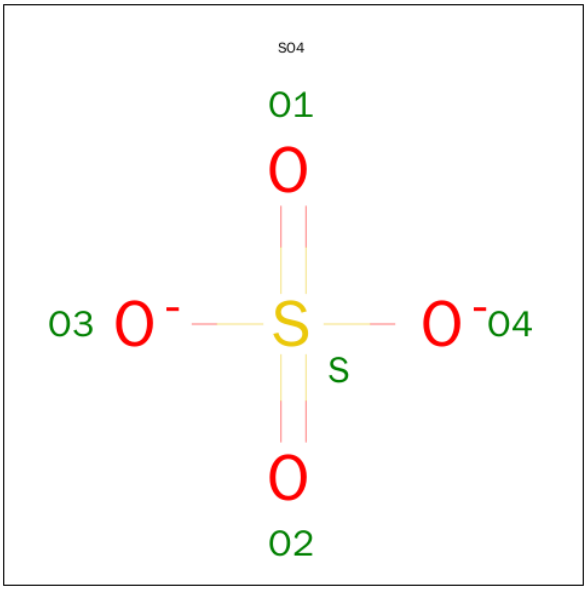
There are 5 unique types of molecules in this entry. The entry contains 5368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Non-symbiotic hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1145	741	195	201	8			
1	B	146	Total	C	N	O	S	0	0	0
			1143	738	195	202	8			
1	C	147	Total	C	N	O	S	0	0	0
			1155	748	196	203	8			
1	D	145	Total	C	N	O	S	0	0	0
			1136	733	194	201	8			

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



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

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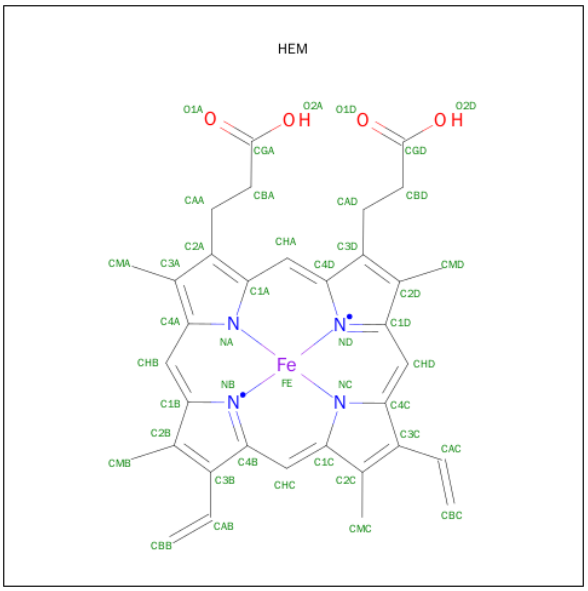
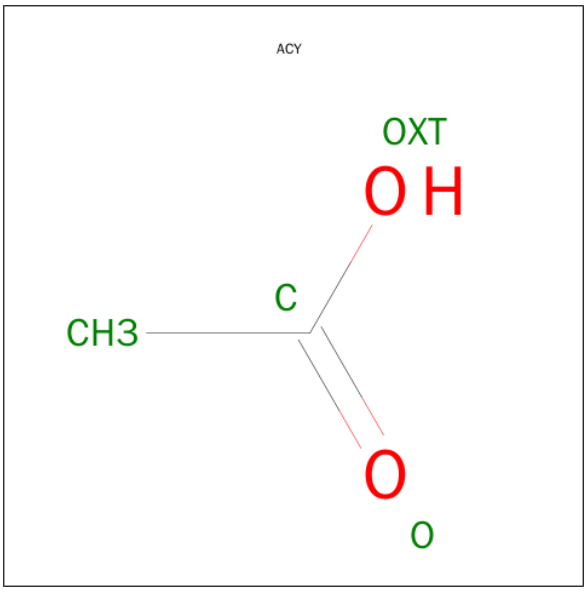
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- 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
3	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

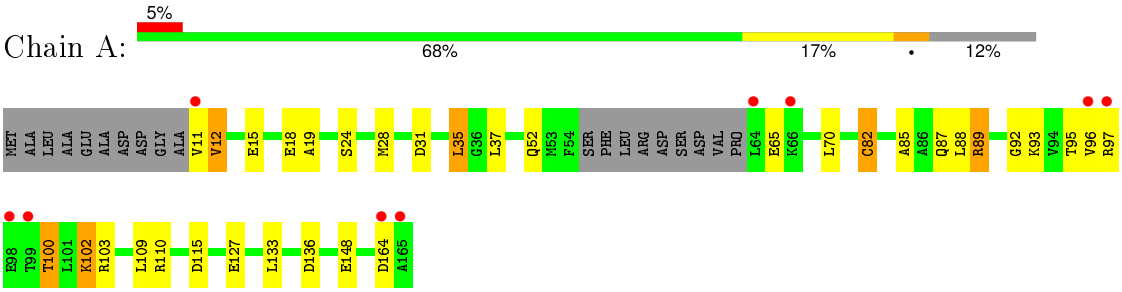
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	161	Total O 161 161	0	0
5	B	172	Total O 172 172	0	0
5	C	142	Total O 142 142	0	0
5	D	109	Total O 109 109	0	0

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.

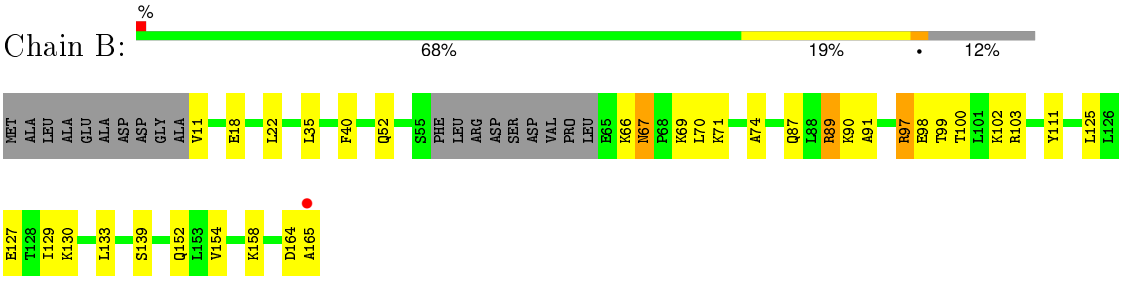
- Molecule 1: Non-symbiotic hemoglobin

Chain A:



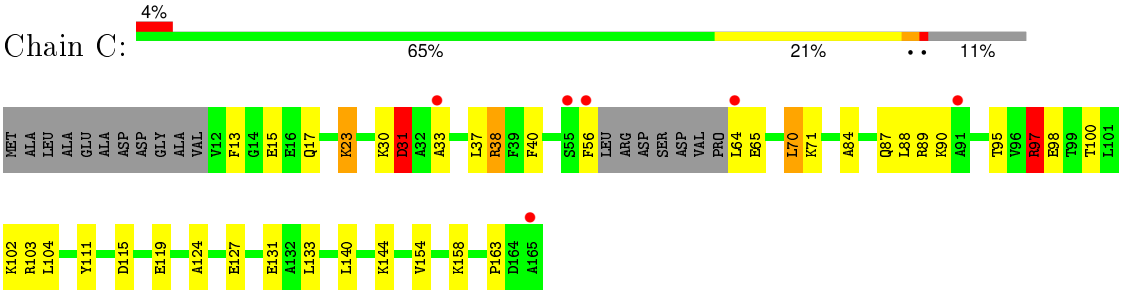
- Molecule 1: Non-symbiotic hemoglobin

Chain B:



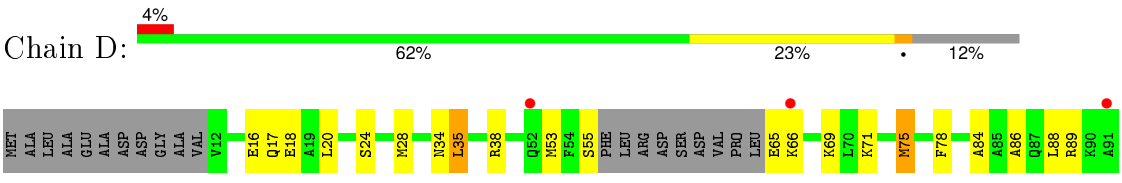
- Molecule 1: Non-symbiotic hemoglobin

Chain C:



- Molecule 1: Non-symbiotic hemoglobin

Chain D:




G92
K93
V94
T95
V96
R97
E98
T99
A106
L109
R110
V113
A114
D115
E119
L125
I129
K130
L133
L140
E141
M142
K143
K144
Q152
K158
D164
A165

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.75Å 89.73Å 157.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.06 – 2.20 26.24 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.06-2.20) 80.0 (26.24-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.201 , 0.253 0.204 , 0.251	Depositor DCC
R_{free} test set	1873 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	1 of 50255 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5368	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 25.50 % 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 3.1319e-03.*

[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, ACY, 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	1.17	1/1166 (0.1%)	0.96	4/1565 (0.3%)
1	B	1.20	2/1164 (0.2%)	0.92	1/1562 (0.1%)
1	C	1.19	2/1177 (0.2%)	0.94	3/1579 (0.2%)
1	D	1.13	1/1157 (0.1%)	0.93	2/1552 (0.1%)
All	All	1.17	6/4664 (0.1%)	0.94	10/6258 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	MET	CG-SD	-9.82	1.55	1.81
1	C	131	GLU	CD-OE1	-5.67	1.19	1.25
1	B	130	LYS	CE-NZ	5.23	1.62	1.49
1	A	82	CYS	CB-SG	-5.22	1.73	1.81
1	B	71	LYS	CE-NZ	5.08	1.61	1.49
1	C	124	ALA	CA-CB	-5.01	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	164	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	115	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	31	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	136	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	142	MET	CA-CB-CG	-5.46	104.01	113.30
1	C	38	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	31	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	55	SER	CA-C-O	-5.11	109.36	120.10
1	C	97	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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	1145	0	1188	26	0
1	B	1143	0	1182	21	0
1	C	1155	0	1193	32	0
1	D	1136	0	1173	34	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	2	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	B	4	0	3	2	0
4	D	4	0	3	0	0
5	A	161	0	0	6	0
5	B	172	0	0	5	1
5	C	142	0	0	11	1
5	D	109	0	0	6	0
All	All	5368	0	4862	111	1

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 12.

All (111) 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:C:65:GLU:O	5:C:303:HOH:O	1.82	0.97
1:C:23:LYS:NZ	1:C:23:LYS:HB2	1.82	0.94
1:A:15:GLU:HG2	5:A:243:HOH:O	1.72	0.88
1:C:23:LYS:HB2	1:C:23:LYS:HZ3	1.42	0.82
1:C:154:VAL:HG12	1:C:158:LYS:HE2	1.63	0.80
1:A:35:LEU:HG	5:A:251:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG13	5:A:236:HOH:O	1.81	0.79
1:B:97:ARG:HH21	1:B:99:THR:HG23	1.46	0.79
1:D:75:MET:HE1	5:D:257:HOH:O	1.82	0.78
1:D:34:ASN:O	1:D:38:ARG:HG3	1.86	0.74
1:B:139:SER:OG	5:B:300:HOH:O	2.06	0.73
1:C:98:GLU:HG2	1:C:102:LYS:HE2	1.72	0.71
1:C:37:LEU:HB2	5:C:305:HOH:O	1.90	0.71
1:A:87:GLN:HG3	1:A:95:THR:HG22	1.75	0.67
1:D:16:GLU:HG3	1:D:17:GLN:NE2	2.10	0.67
1:C:37:LEU:HG	5:C:258:HOH:O	1.94	0.66
1:A:102:LYS:HD3	1:A:102:LYS:H	1.61	0.66
1:D:125:LEU:O	1:D:129:ILE:HG12	1.95	0.65
1:B:125:LEU:O	1:B:129:ILE:HG13	1.96	0.65
1:B:127:GLU:OE2	5:B:237:HOH:O	2.14	0.65
1:C:64:LEU:HG	1:C:65:GLU:H	1.62	0.64
1:C:38:ARG:NH2	5:C:302:HOH:O	2.25	0.64
1:D:16:GLU:HG3	1:D:17:GLN:HE22	1.65	0.61
1:D:16:GLU:O	1:D:20:LEU:HG	2.01	0.60
1:C:111:TYR:OH	2:C:166:SO4:O2	2.15	0.60
1:A:89:ARG:HB3	1:A:89:ARG:HH11	1.67	0.59
1:A:93:LYS:HB2	5:A:297:HOH:O	2.01	0.59
1:B:52:GLN:HB2	5:B:317:HOH:O	2.03	0.59
1:A:88:LEU:HD23	1:A:93:LYS:HA	1.87	0.57
1:D:66:LYS:HA	1:D:71:LYS:NZ	2.20	0.56
1:C:90:LYS:HG2	5:C:267:HOH:O	2.05	0.56
1:A:37:LEU:HD11	1:A:65:GLU:HG3	1.87	0.56
1:A:100:THR:HG21	1:A:102:LYS:CE	2.36	0.55
1:C:40:PHE:HB3	1:C:70:LEU:HD11	1.89	0.55
1:A:87:GLN:HG3	1:A:95:THR:CG2	2.37	0.53
1:A:100:THR:HG21	1:A:102:LYS:HE2	1.88	0.53
1:A:19:ALA:HA	5:A:240:HOH:O	2.08	0.53
1:A:92:GLY:O	1:A:93:LYS:HB3	2.09	0.53
1:A:18:GLU:OE1	1:A:89:ARG:HD3	2.09	0.52
1:C:127:GLU:CD	5:C:275:HOH:O	2.47	0.52
1:B:89:ARG:HG3	1:B:90:LYS:N	2.24	0.52
1:B:40:PHE:HE1	1:B:70:LEU:O	1.91	0.52
1:D:129:ILE:O	1:D:133:LEU:HB2	2.09	0.52
1:C:31:ASP:HB3	5:C:253:HOH:O	2.08	0.52
1:D:18:GLU:OE2	1:D:86:ALA:HA	2.10	0.51
1:C:33:ALA:HB2	5:C:300:HOH:O	2.10	0.51
1:A:109:LEU:HD21	1:D:110:ARG:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:78:PHE:CE2	2.47	0.50
1:D:164:ASP:HB2	2:D:166:SO4:S	2.51	0.50
1:D:164:ASP:HB2	2:D:166:SO4:O2	2.13	0.49
1:D:110:ARG:HH11	1:D:110:ARG:HG3	1.76	0.49
1:C:115:ASP:O	1:C:119:GLU:HG3	2.13	0.49
1:B:69:LYS:HD3	3:B:167:HEM:O2D	2.13	0.48
1:C:64:LEU:HD23	1:C:64:LEU:N	2.28	0.48
1:B:165:ALA:HB2	5:C:240:HOH:O	2.14	0.48
1:D:99:THR:HG22	5:D:275:HOH:O	2.13	0.48
1:D:20:LEU:HB3	1:D:142:MET:HG3	1.94	0.48
1:B:11:VAL:HG21	1:B:152:GLN:NE2	2.29	0.48
1:B:40:PHE:CE1	1:B:74:ALA:HB2	2.49	0.47
1:C:30:LYS:O	1:C:31:ASP:HB2	2.14	0.47
1:D:78:PHE:HE1	1:D:129:ILE:HD11	1.78	0.47
1:B:40:PHE:CG	4:B:168:ACY:H3	2.50	0.47
1:B:154:VAL:HG12	1:B:158:LYS:HE2	1.98	0.46
1:A:24:SER:O	1:A:28:MET:HG3	2.15	0.46
1:A:110:ARG:HA	1:D:109:LEU:HD21	1.97	0.46
1:D:84:ALA:O	1:D:88:LEU:HG	2.16	0.46
1:D:66:LYS:HA	1:D:71:LYS:HZ1	1.80	0.46
1:A:11:VAL:O	1:A:12:VAL:HB	2.16	0.46
1:D:38:ARG:NH1	1:D:38:ARG:HB3	2.31	0.45
1:C:37:LEU:HD13	5:C:257:HOH:O	2.17	0.45
1:A:96:VAL:O	1:A:96:VAL:HG23	2.17	0.45
1:A:82:CYS:O	1:A:85:ALA:HB3	2.17	0.45
1:D:96:VAL:O	1:D:97:ARG:C	2.55	0.44
1:C:100:THR:HG23	1:C:103:ARG:HH22	1.81	0.44
1:C:100:THR:O	1:C:104:LEU:HG	2.17	0.44
1:D:130:LYS:HE3	5:D:239:HOH:O	2.18	0.44
1:B:87:GLN:O	1:B:91:ALA:HB3	2.18	0.44
1:C:140:LEU:HG	1:C:144:LYS:HZ3	1.83	0.44
1:D:152:GLN:NE2	5:D:259:HOH:O	2.49	0.44
1:C:71:LYS:HB2	1:C:71:LYS:NZ	2.33	0.43
1:C:13:PHE:CZ	1:C:17:GLN:HB3	2.53	0.43
1:C:127:GLU:OE2	5:C:173:HOH:O	2.21	0.43
1:B:40:PHE:CE1	1:B:70:LEU:O	2.70	0.43
1:C:23:LYS:CB	1:C:23:LYS:HZ2	2.30	0.43
1:C:84:ALA:O	1:C:88:LEU:HG	2.18	0.43
1:A:96:VAL:HB	1:A:100:THR:HG23	2.01	0.43
1:D:106:ALA:O	1:D:110:ARG:HB2	2.19	0.43
1:D:140:LEU:HG	1:D:144:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	5:A:324:HOH:O	2.19	0.43
1:C:40:PHE:CB	1:C:70:LEU:HD11	2.49	0.42
1:B:97:ARG:NH1	5:B:208:HOH:O	2.50	0.42
3:B:167:HEM:HBC2	5:B:176:HOH:O	2.18	0.42
1:D:115:ASP:OD2	1:D:158:LYS:HE3	2.20	0.42
1:A:89:ARG:HB3	1:A:89:ARG:NH1	2.34	0.42
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.84	0.42
1:D:53:MET:CE	1:D:113:VAL:HG22	2.50	0.41
1:B:74:ALA:HA	4:B:168:ACY:O	2.20	0.41
1:C:56:PHE:N	1:C:56:PHE:CD2	2.87	0.41
1:C:97:ARG:HE	1:C:97:ARG:HA	1.85	0.41
1:B:98:GLU:O	1:B:102:LYS:HG3	2.20	0.41
1:D:93:LYS:O	1:D:95:THR:HG23	2.21	0.41
1:A:15:GLU:HA	1:A:89:ARG:HD2	2.03	0.41
1:D:34:ASN:CB	5:D:263:HOH:O	2.68	0.41
1:D:78:PHE:HE1	1:D:129:ILE:CD1	2.33	0.41
1:D:115:ASP:O	1:D:119:GLU:HG3	2.21	0.41
1:B:100:THR:HG23	1:B:103:ARG:HH21	1.86	0.41
1:D:24:SER:HB2	1:D:28:MET:HE1	2.03	0.41
1:B:111:TYR:CZ	1:C:163:PRO:HB3	2.56	0.40
1:C:87:GLN:OE1	1:C:95:THR:N	2.51	0.40
1:B:18:GLU:HG2	1:B:22:LEU:HD12	2.03	0.40
1:D:158:LYS:HD3	5:D:176:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:322:HOH:O	5:C:285:HOH:O[3_645]	2.19	0.01

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	142/165 (86%)	135 (95%)	6 (4%)	1 (1%)	26	25
1	B	142/165 (86%)	139 (98%)	2 (1%)	1 (1%)	26	25
1	C	143/165 (87%)	136 (95%)	6 (4%)	1 (1%)	26	25
1	D	141/165 (86%)	137 (97%)	4 (3%)	0	100	100
All	All	568/660 (86%)	547 (96%)	18 (3%)	3 (0%)	34	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	ASP
1	B	67	ASN
1	A	12	VAL

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	117/131 (89%)	108 (92%)	9 (8%)	16	16
1	B	117/131 (89%)	111 (95%)	6 (5%)	29	34
1	C	118/131 (90%)	112 (95%)	6 (5%)	29	34
1	D	116/131 (88%)	110 (95%)	6 (5%)	29	33
All	All	468/524 (89%)	441 (94%)	27 (6%)	25	28

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	52	GLN
1	A	70	LEU
1	A	89	ARG
1	A	100	THR
1	A	102	LYS
1	A	127	GLU
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	148	GLU
1	B	35	LEU
1	B	66	LYS
1	B	67	ASN
1	B	89	ARG
1	B	97	ARG
1	B	133	LEU
1	C	15	GLU
1	C	23	LYS
1	C	70	LEU
1	C	89	ARG
1	C	97	ARG
1	C	133	LEU
1	D	35	LEU
1	D	65	GLU
1	D	69	LYS
1	D	75	MET
1	D	89	ARG
1	D	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	C	52	GLN
1	D	52	GLN
1	D	152	GLN

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 (i)

11 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	166	1	30,50,50	2.75	10 (33%)	24,82,82	2.21	7 (29%)
2	SO4	B	166	-	4,4,4	0.34	0	6,6,6	0.55	0
3	HEM	B	167	1	30,50,50	3.12	12 (40%)	24,82,82	2.48	8 (33%)
4	ACY	B	168	-	1,3,3	1.44	0	0,3,3	0.00	-
2	SO4	C	166	-	4,4,4	0.21	0	6,6,6	0.35	0
2	SO4	C	167	-	4,4,4	0.34	0	6,6,6	1.20	1 (16%)
3	HEM	C	168	1	30,50,50	2.57	9 (30%)	24,82,82	2.13	7 (29%)
2	SO4	D	166	-	4,4,4	0.27	0	6,6,6	0.42	0
2	SO4	D	167	-	4,4,4	0.42	0	6,6,6	0.53	0
3	HEM	D	168	1	30,50,50	2.92	11 (36%)	24,82,82	2.46	9 (37%)
4	ACY	D	169	-	1,3,3	1.06	0	0,3,3	0.00	-

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	166	1	-	0/10/54/54	0/0/8/8
2	SO4	B	166	-	-	0/0/0/0	0/0/0/0
3	HEM	B	167	1	-	0/10/54/54	0/0/8/8
4	ACY	B	168	-	-	0/0/0/0	0/0/0/0
2	SO4	C	166	-	-	0/0/0/0	0/0/0/0
2	SO4	C	167	-	-	0/0/0/0	0/0/0/0
3	HEM	C	168	1	-	0/10/54/54	0/0/8/8
2	SO4	D	166	-	-	0/0/0/0	0/0/0/0
2	SO4	D	167	-	-	0/0/0/0	0/0/0/0
3	HEM	D	168	1	-	0/10/54/54	0/0/8/8
4	ACY	D	169	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	167	HEM	C3B-C4B	-8.37	1.44	1.51
3	C	168	HEM	C2D-C3D	-7.26	1.32	1.54
3	A	166	HEM	C2D-C3D	-7.16	1.33	1.54
3	B	167	HEM	C3B-CAB	-7.00	1.38	1.51
3	C	168	HEM	C3B-CAB	-6.85	1.38	1.51
3	D	168	HEM	C2D-C3D	-6.57	1.34	1.54
3	A	166	HEM	C3B-C4B	-6.50	1.46	1.51
3	D	168	HEM	C3B-C4B	-6.42	1.46	1.51
3	B	167	HEM	C3D-C4D	-6.40	1.43	1.51
3	B	167	HEM	C2D-C3D	-6.35	1.35	1.54
3	D	168	HEM	C3D-C4D	-6.25	1.43	1.51
3	A	166	HEM	C3D-C4D	-5.63	1.44	1.51
3	D	168	HEM	C3B-CAB	-5.45	1.41	1.51
3	C	168	HEM	C3D-C4D	-5.34	1.44	1.51
3	D	168	HEM	C3C-CAC	-5.18	1.41	1.51
3	A	166	HEM	C3B-CAB	-5.18	1.41	1.51
3	B	167	HEM	C3C-CAC	-5.14	1.41	1.51
3	A	166	HEM	C2C-C1C	-4.31	1.44	1.52
3	A	166	HEM	C3C-CAC	-4.14	1.43	1.51
3	C	168	HEM	C2C-C1C	-4.05	1.44	1.52
3	D	168	HEM	C2C-C1C	-3.92	1.45	1.52
3	C	168	HEM	C3C-CAC	-3.77	1.44	1.51
3	B	167	HEM	C2C-C1C	-3.19	1.46	1.52
3	B	167	HEM	C2B-C1B	-2.82	1.42	1.51
3	D	168	HEM	C2D-C1D	-2.71	1.43	1.51
3	B	167	HEM	C2D-C1D	-2.66	1.43	1.51
3	A	166	HEM	C2D-C1D	-2.42	1.43	1.51
3	A	166	HEM	C2B-C1B	-2.03	1.45	1.51
3	D	168	HEM	CBB-CAB	2.01	1.40	1.29
3	B	167	HEM	CBC-CAC	2.02	1.41	1.29
3	C	168	HEM	C4C-NC	2.20	1.38	1.36
3	C	168	HEM	CBC-CAC	2.37	1.43	1.29
3	A	166	HEM	CBC-CAC	2.38	1.43	1.29
3	C	168	HEM	CBB-CAB	2.40	1.43	1.29
3	A	166	HEM	CBB-CAB	2.48	1.43	1.29
3	D	168	HEM	CBC-CAC	2.60	1.44	1.29
3	C	168	HEM	C1C-NC	2.60	1.39	1.36
3	B	167	HEM	C1C-NC	2.68	1.39	1.36
3	B	167	HEM	C4C-NC	2.69	1.39	1.36
3	B	167	HEM	CBB-CAB	2.80	1.45	1.29
3	D	168	HEM	C4C-NC	3.08	1.39	1.36
3	D	168	HEM	C1C-NC	4.22	1.41	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	168	HEM	C3C-CAC-CBC	-3.09	119.71	124.46
2	C	167	SO4	O2-S-O1	-2.72	100.89	109.50
3	B	167	HEM	C3B-CAB-CBB	-2.49	120.63	124.46
3	A	166	HEM	C3C-CAC-CBC	-2.10	121.24	124.46
3	C	168	HEM	CMD-C2D-C3D	2.35	124.74	114.35
3	D	168	HEM	C2D-C3D-C4D	2.37	105.51	101.50
3	A	166	HEM	CMD-C2D-C3D	2.63	125.99	114.35
3	D	168	HEM	CMD-C2D-C3D	2.86	126.98	114.35
3	B	167	HEM	CMD-C2D-C3D	2.87	127.06	114.35
3	C	168	HEM	C2D-C3D-C4D	2.90	106.42	101.50
3	D	168	HEM	CAA-CBA-CGA	2.94	118.14	112.75
3	C	168	HEM	CBA-CAA-C2A	3.21	118.28	112.53
3	A	166	HEM	CBA-CAA-C2A	3.34	118.52	112.53
3	B	167	HEM	C2D-C3D-C4D	3.60	107.61	101.50
3	D	168	HEM	CMC-C2C-C3C	3.65	125.64	116.53
3	D	168	HEM	CAD-C3D-C4D	3.78	125.80	112.47
3	B	167	HEM	CAD-C3D-C2D	3.98	124.65	113.22
3	C	168	HEM	CAD-C3D-C4D	3.99	126.56	112.47
3	A	166	HEM	CMB-C2B-C3B	4.00	126.52	116.53
3	C	168	HEM	CMB-C2B-C3B	4.03	126.59	116.53
3	A	166	HEM	CAD-C3D-C2D	4.29	125.56	113.22
3	B	167	HEM	CAD-C3D-C4D	4.31	127.67	112.47
3	A	166	HEM	CMC-C2C-C3C	4.34	127.35	116.53
3	C	168	HEM	CMC-C2C-C3C	4.34	127.36	116.53
3	D	168	HEM	CBA-CAA-C2A	4.49	120.57	112.53
3	B	167	HEM	CBA-CAA-C2A	4.60	120.77	112.53
3	C	168	HEM	CAD-C3D-C2D	4.75	126.86	113.22
3	D	168	HEM	CMB-C2B-C3B	4.75	128.40	116.53
3	B	167	HEM	CMC-C2C-C3C	4.76	128.40	116.53
3	A	166	HEM	CAD-C3D-C4D	4.92	129.82	112.47
3	B	167	HEM	CMB-C2B-C3B	5.05	129.15	116.53
3	D	168	HEM	CAD-C3D-C2D	5.37	128.66	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	167	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	168	ACY	2	0
2	C	166	SO4	1	0
2	D	166	SO4	2	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	146/165 (88%)	-0.07	9 (6%)	24	23	24, 39, 72, 91	0
1	B	146/165 (88%)	-0.29	1 (0%)	89	88	22, 39, 61, 82	1 (0%)
1	C	147/165 (89%)	0.02	6 (4%)	41	39	26, 40, 69, 93	0
1	D	145/165 (87%)	0.04	7 (4%)	34	34	26, 42, 73, 93	0
All	All	584/660 (88%)	-0.08	23 (3%)	43	42	22, 40, 72, 93	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	ALA	7.9
1	A	165	ALA	7.9
1	C	165	ALA	7.2
1	B	165	ALA	7.1
1	A	97	ARG	5.3
1	C	33	ALA	4.4
1	A	96	VAL	4.3
1	D	66	LYS	3.3
1	D	97	ARG	3.1
1	D	52	GLN	3.0
1	A	99	THR	2.8
1	C	55	SER	2.8
1	C	56	PHE	2.6
1	A	66	LYS	2.6
1	D	91	ALA	2.6
1	C	91	ALA	2.5
1	D	95	THR	2.4
1	A	98	GLU	2.3
1	C	64	LEU	2.3
1	A	11	VAL	2.2
1	A	164	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	2.0
1	D	164	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, 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
4	ACY	D	169	4/4	0.92	0.15	1.19	37,38,38,38	0
4	ACY	B	168	4/4	0.88	0.17	0.67	40,42,42,42	0
3	HEM	C	168	43/43	0.94	0.16	0.59	28,35,54,58	0
3	HEM	D	168	43/43	0.94	0.15	0.53	33,38,61,63	0
3	HEM	A	166	43/43	0.95	0.16	0.44	26,33,57,67	0
3	HEM	B	167	43/43	0.96	0.14	0.04	29,34,60,66	0
2	SO4	D	167	5/5	0.92	0.13	-0.53	73,73,76,77	0
2	SO4	D	166	5/5	0.94	0.12	-0.72	80,81,81,82	0
2	SO4	B	166	5/5	0.99	0.07	-0.93	54,57,59,61	0
2	SO4	C	166	5/5	0.97	0.08	-0.98	68,68,72,75	0
2	SO4	C	167	5/5	0.90	0.19	-	62,64,65,67	5

6.5 Other polymers (i)

There are no such residues in this entry.