



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 24, 2017 – 09:21 PM EST

PDB ID : 5OHF
Title : Globin sensor domain of AfGcHK (FeIII form) in complex with cyanide, partially reduced
Authors : Skalova, T.; Kolenko, P.; Dohnalek, J.; Stranava, M.; Martinkova, M.
Deposited on : 2017-07-16
Resolution : 1.80 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

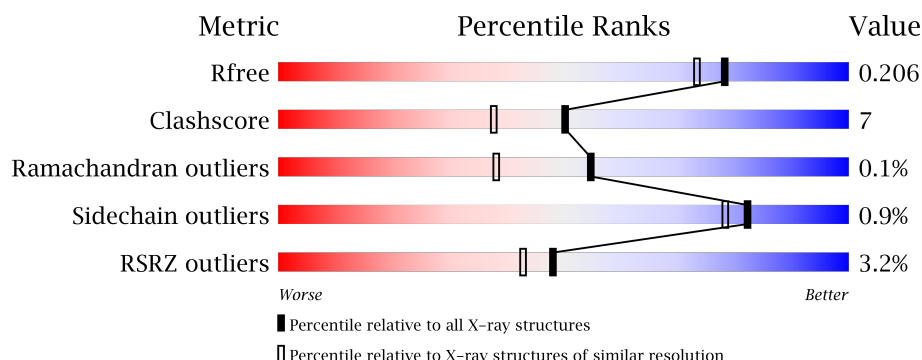
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 $\leq 5\%$. 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	161	<div> <div>2%</div> <div>89% 5% 6%</div> </div>
1	B	161	<div> <div>%</div> <div>91% 6%</div> </div>
1	C	161	<div> <div>3%</div> <div>88% 9%</div> </div>
1	D	161	<div> <div>%</div> <div>92% 6%</div> </div>
1	E	161	<div> <div>%</div> <div>91% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	161	 .% 94% 5%
1	G	161	 12% 58% 32% 9%
1	H	161	 3% 84% 9% 6%

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	CYN	G	201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12325 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.

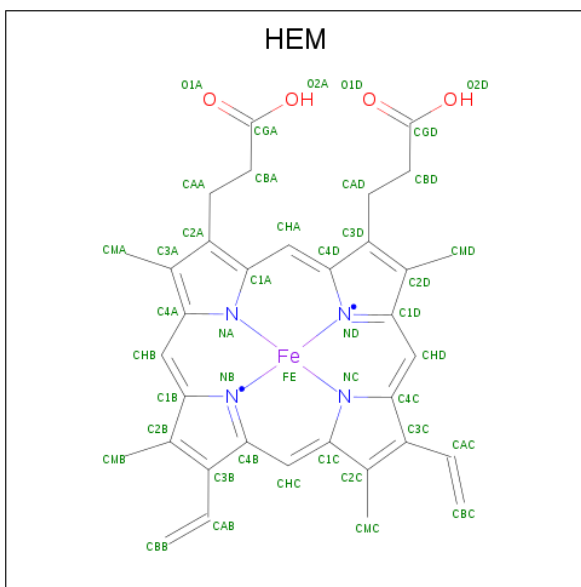
- Molecule 1 is a protein called Globin-coupled histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	4	0
			1259	807	232	215	5			
1	B	152	Total	C	N	O	S	0	6	0
			1276	814	240	217	5			
1	C	147	Total	C	N	O	S	0	4	0
			1232	793	232	203	4			
1	D	152	Total	C	N	O	S	0	3	0
			1259	804	238	213	4			
1	E	152	Total	C	N	O	S	0	1	0
			1240	790	232	214	4			
1	F	153	Total	C	N	O	S	0	0	0
			1243	791	233	215	4			
1	G	147	Total	C	N	O	S	0	94	0
			1968	1261	369	330	8			
1	H	152	Total	C	N	O	S	0	23	0
			1422	907	265	246	4			

There are 8 discrepancies between the modelled and reference sequences:

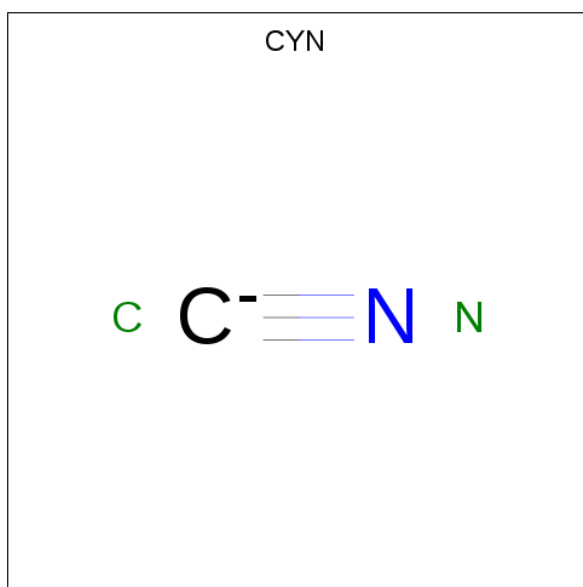
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A7HD43
B	1	GLY	-	expression tag	UNP A7HD43
C	1	GLY	-	expression tag	UNP A7HD43
D	1	GLY	-	expression tag	UNP A7HD43
E	1	GLY	-	expression tag	UNP A7HD43
F	1	GLY	-	expression tag	UNP A7HD43
G	1	GLY	-	expression tag	UNP A7HD43
H	1	GLY	-	expression tag	UNP A7HD43

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 86	C 68	Fe 2	N 8	O 8	0	1
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			2	1	1		
3	B	1	Total	C	N	0	0
			2	1	1		
3	C	1	Total	C	N	0	0
			2	1	1		
3	D	1	Total	C	N	0	0
			2	1	1		
3	E	1	Total	C	N	0	0
			2	1	1		
3	F	1	Total	C	N	0	0
			2	1	1		
3	G	1	Total	C	N	0	0
			2	1	1		
3	H	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	131	Total O 131 131	0	0
6	B	157	Total O 157 157	0	0
6	C	113	Total O 113 113	0	0
6	D	130	Total O 130 130	0	0
6	E	139	Total O 139 139	0	0
6	F	151	Total O 151 151	0	0
6	G	58	Total O 59 59	0	1
6	H	137	Total O 137 137	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

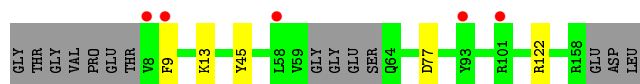
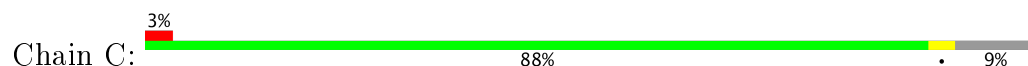
- Molecule 1: Globin-coupled histidine kinase



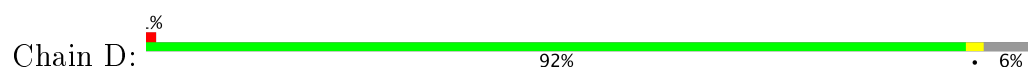
- Molecule 1: Globin-coupled histidine kinase



- Molecule 1: Globin-coupled histidine kinase



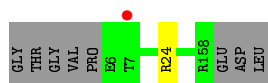
- Molecule 1: Globin-coupled histidine kinase



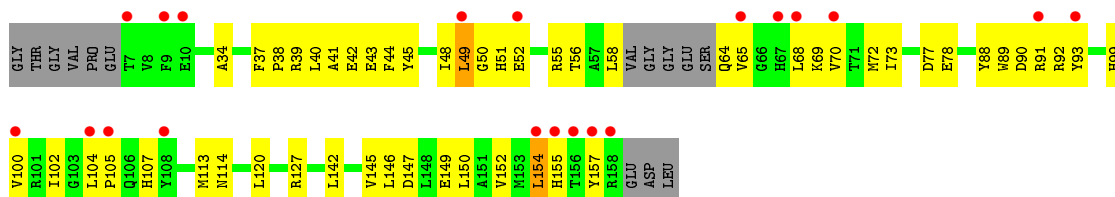
- Molecule 1: Globin-coupled histidine kinase



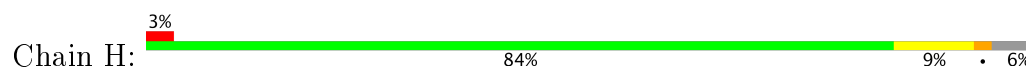
- Molecule 1: Globin-coupled histidine kinase



- Molecule 1: Globin-coupled histidine kinase



- Molecule 1: Globin-coupled histidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.69 Å 77.69 Å 441.24 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 1.80 49.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.17-1.80) 100.0 (49.17-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.190 , 0.239 0.200 , 0.206	Depositor DCC
R_{free} test set	6224 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, CL, CYN, NA

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	0.51	0/1306	0.74	0/1766
1	B	0.49	0/1323	0.72	1/1787 (0.1%)
1	C	0.47	0/1279	0.71	0/1728
1	D	0.49	0/1303	0.73	2/1761 (0.1%)
1	E	0.49	0/1277	0.74	0/1727
1	F	0.50	0/1277	0.71	1/1727 (0.1%)
1	G	0.37	0/2021	0.56	0/2730
1	H	0.45	0/1473	0.68	1/1990 (0.1%)
All	All	0.47	0/11259	0.69	5/15216 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	158	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	122	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	24	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	H	139	ARG	NE-CZ-NH1	5.00	122.80	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	1259	0	1239	6	0
1	B	1276	0	1256	2	0
1	C	1232	0	1219	5	0
1	D	1259	0	1239	2	0
1	E	1240	0	1210	7	0
1	F	1243	0	1210	0	0
1	G	1968	0	1935	78	0
1	H	1422	0	1386	23	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
2	E	43	0	30	3	0
2	F	43	0	30	2	0
2	G	86	0	60	24	0
2	H	43	0	30	1	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	1	0
3	F	2	0	0	0	0
3	G	2	0	0	5	0
3	H	2	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	E	1	0	0	0	0
6	A	131	0	0	0	0
6	B	157	0	0	0	0
6	C	113	0	0	1	0
6	D	130	0	0	1	0
6	E	139	0	0	3	0
6	F	151	0	0	0	0
6	G	59	0	0	4	0
6	H	137	0	0	1	0
All	All	12325	0	10964	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (146) 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:E:122:ARG:NH2	1:E:126:GLU:OE2	1.67	1.26
1:E:43[B]:GLU:OE2	6:E:301:HOH:O	1.66	1.10
2:G:200[A]:HEM:HHA	2:G:200[A]:HEM:HBA1	1.40	1.04
1:G:69[B]:LYS:O	1:G:73[B]:ILE:HG13	1.59	1.03
1:G:39[B]:ARG:HH12	1:G:40[B]:LEU:CD2	1.71	1.03
1:H:22[B]:ASP:OD1	6:H:301:HOH:O	1.77	1.02
1:H:8[B]:VAL:O	1:H:12[B]:LEU:HD13	1.59	1.01
2:G:200[A]:HEM:HBC2	2:G:200[A]:HEM:HMC1	1.39	1.00
2:G:200[A]:HEM:HMB1	2:G:200[A]:HEM:HBB2	1.46	0.97
2:G:200[B]:HEM:HBC2	2:G:200[B]:HEM:HMC1	1.44	0.96
1:G:39[B]:ARG:HH12	1:G:40[B]:LEU:HD21	1.29	0.96
2:G:200[B]:HEM:HMB1	2:G:200[B]:HEM:HBB2	1.49	0.93
1:G:39[B]:ARG:NH1	1:G:40[B]:LEU:CD2	2.34	0.89
1:G:89[B]:TRP:O	1:G:93[B]:TYR:CD2	2.26	0.87
1:G:107[B]:HIS:CD2	1:H:12[B]:LEU:HD11	2.10	0.87
2:G:200[B]:HEM:HBC2	2:G:200[B]:HEM:CMC	2.08	0.84
1:C:9[B]:PHE:CE1	1:C:13:LYS:HG3	2.11	0.83
2:G:200[A]:HEM:CMB	2:G:200[A]:HEM:HBB2	2.10	0.81
2:G:200[A]:HEM:HBC2	2:G:200[A]:HEM:CMC	2.07	0.80
1:G:107[B]:HIS:HB2	1:H:12[B]:LEU:HD21	1.65	0.78
1:G:39[B]:ARG:NH1	1:G:40[B]:LEU:HD21	1.98	0.77
1:G:107[B]:HIS:HD2	1:H:12[B]:LEU:HD11	1.50	0.77
1:E:43[B]:GLU:CD	6:E:301:HOH:O	2.14	0.77
1:C:9[B]:PHE:CE1	1:C:13:LYS:CG	2.64	0.76
1:G:93[B]:TYR:CE1	1:G:152[B]:VAL:HG13	2.21	0.76
1:G:68[A]:LEU:HD21	2:G:200[A]:HEM:HBD1	1.68	0.76
1:G:39[B]:ARG:HH12	1:G:40[B]:LEU:HD23	1.52	0.75
1:G:58[A]:LEU:HB3	1:G:64[A]:GLN:OE1	1.86	0.75
1:G:92[A]:ARG:HD2	1:G:149[A]:GLU:OE1	1.87	0.74
1:H:104:LEU:HD23	1:H:109:MET:HE3	1.70	0.74
1:G:39[B]:ARG:NH1	1:G:40[B]:LEU:HD23	2.03	0.73
1:H:45:TYR:OH	3:H:201:CYN:N	2.21	0.72
2:G:200[B]:HEM:HBB2	2:G:200[B]:HEM:CMB	2.16	0.71
2:G:200[A]:HEM:CBA	2:G:200[A]:HEM:HHA	2.18	0.71
1:G:45[A]:TYR:OH	3:G:201:CYN:N	2.21	0.68
1:G:100[B]:VAL:HG22	1:G:157[B]:TYR:CZ	2.29	0.67
2:G:200[A]:HEM:CBC	2:G:200[A]:HEM:HMC1	2.23	0.66
1:G:70[B]:VAL:HG23	6:G:302:HOH:O	1.97	0.65
1:G:45[B]:TYR:OH	1:G:68[B]:LEU:HB3	1.96	0.64
1:H:7[B]:THR:O	1:H:11[B]:GLU:HB2	1.99	0.63
2:G:200[B]:HEM:C1B	3:G:201:CYN:N	2.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93[B]:TYR:CD1	1:G:152[B]:VAL:HG13	2.34	0.61
1:G:70[B]:VAL:HG22	6:G:354:HOH:O	1.99	0.61
2:G:200[B]:HEM:CBC	2:G:200[B]:HEM:HMC1	2.26	0.60
1:G:37:PHE:CE2	1:G:77[B]:ASP:HA	2.37	0.59
1:G:155[B]:HIS:O	1:G:155[B]:HIS:CD2	2.56	0.58
1:G:42[B]:GLU:OE1	1:G:69[B]:LYS:HE2	2.03	0.58
1:G:92[A]:ARG:HD3	1:G:149[A]:GLU:OE2	2.04	0.58
1:G:39[B]:ARG:NH2	1:G:43[B]:GLU:OE1	2.37	0.58
1:G:78[A]:GLU:OE1	1:G:91[A]:ARG:NH2	2.37	0.58
2:E:201:HEM:HMC1	2:E:201:HEM:HBC2	1.86	0.57
1:G:72[B]:MET:HE1	2:G:200[B]:HEM:CHB	2.35	0.57
1:H:22[B]:ASP:O	1:H:25[B]:ALA:HB3	2.06	0.56
1:G:48[B]:ILE:C	1:G:50[B]:GLY:H	2.09	0.56
1:C:45:TYR:OH	3:C:201:CYN:N	2.24	0.55
1:A:93[A]:TYR:CE1	1:A:156:THR:HG22	2.42	0.55
2:D:200:HEM:HBC2	2:D:200:HEM:HMC1	1.88	0.55
1:G:88[B]:TYR:CZ	1:G:92[B]:ARG:NH1	2.73	0.54
1:G:42[B]:GLU:OE1	1:G:69[B]:LYS:CE	2.55	0.54
1:G:92[B]:ARG:HG2	1:G:149[B]:GLU:OE2	2.08	0.54
1:H:12[B]:LEU:O	1:H:16[B]:VAL:HG22	2.06	0.54
1:G:68[A]:LEU:CD2	2:G:200[A]:HEM:HBD1	2.37	0.54
2:G:200[A]:HEM:CHA	2:G:200[A]:HEM:CBA	2.81	0.54
1:G:72[B]:MET:HE1	2:G:200[B]:HEM:HHB	1.89	0.53
2:G:200[A]:HEM:HMB1	2:G:200[A]:HEM:CBB	2.30	0.53
1:G:99[B]:HIS:HA	1:G:102[B]:ILE:HG12	1.91	0.53
1:G:72[B]:MET:CE	2:G:200[B]:HEM:CHB	2.87	0.53
2:C:200:HEM:HMB1	2:C:200:HEM:HBB2	1.91	0.52
1:G:48[B]:ILE:HG22	1:G:49[B]:LEU:N	2.25	0.52
1:E:122:ARG:CZ	1:E:126:GLU:OE2	2.52	0.51
2:B:200:HEM:HBC2	2:B:200:HEM:HMC1	1.92	0.51
1:G:41[A]:ALA:O	1:G:45[A]:TYR:HD2	1.94	0.51
2:G:200[B]:HEM:HMB1	2:G:200[B]:HEM:CBB	2.33	0.50
2:G:200[B]:HEM:CMD	2:G:200[B]:HEM:HBD2	2.42	0.49
1:G:107[B]:HIS:HD2	1:H:12[B]:LEU:CD1	2.21	0.49
2:C:200:HEM:HMC1	2:C:200:HEM:HBC2	1.94	0.49
1:A:93[A]:TYR:CD1	1:A:156:THR:HG22	2.49	0.48
1:G:107[B]:HIS:HB2	1:H:12[B]:LEU:HD11	1.95	0.48
1:C:122:ARG:NH2	6:C:301:HOH:O	2.37	0.48
1:G:88[B]:TYR:OH	1:G:149[B]:GLU:OE1	2.22	0.47
2:H:200:HEM:HMB1	2:H:200:HEM:HBB2	1.95	0.47
1:G:72[A]:MET:HE3	3:G:201:CYN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7[B]:THR:O	1:H:11[B]:GLU:CB	2.62	0.47
1:G:89[B]:TRP:CE3	1:G:152[B]:VAL:HG21	2.49	0.47
1:A:45:TYR:OH	3:A:201:CYN:N	2.34	0.47
1:G:147[B]:ASP:OD2	1:H:117:ARG:NE	2.47	0.47
2:D:200:HEM:HBB2	2:D:200:HEM:HMB1	1.96	0.47
1:H:104:LEU:HD23	1:H:109:MET:CE	2.42	0.47
1:A:149:GLU:O	1:A:153[B]:MET:HG2	2.15	0.46
1:G:68[A]:LEU:HD21	2:G:200[A]:HEM:CBD	2.42	0.46
1:G:51[B]:HIS:O	1:G:52[B]:GLU:C	2.54	0.46
1:B:93[A]:TYR:CE2	1:B:156:THR:HG22	2.50	0.46
1:E:122:ARG:NH2	1:E:126:GLU:CD	2.61	0.46
1:E:91:ARG:NH2	6:E:304:HOH:O	2.47	0.46
1:G:113[B]:MET:SD	1:G:146[B]:LEU:HD22	2.55	0.46
1:G:40[B]:LEU:CD1	1:G:120[B]:LEU:HD21	2.45	0.46
1:G:45[B]:TYR:O	1:G:49[B]:LEU:HB2	2.16	0.45
1:G:65[A]:VAL:HG12	1:G:69[A]:LYS:HE3	1.98	0.45
1:A:8:VAL:HG22	1:A:93[B]:TYR:OH	2.17	0.45
2:F:200:HEM:HMC1	2:F:200:HEM:HBC2	1.97	0.45
1:G:107[B]:HIS:CD2	1:H:12[B]:LEU:CD1	2.91	0.45
1:G:92[B]:ARG:HG3	6:G:317[B]:HOH:O	2.16	0.45
1:H:8[B]:VAL:O	1:H:12[B]:LEU:CD1	2.49	0.45
1:D:93[B]:TYR:CE2	1:D:97[B]:ARG:HD3	2.52	0.45
1:E:45:TYR:OH	3:E:202:CYN:N	2.40	0.44
1:G:34:ALA:HA	1:G:37:PHE:CE2	2.52	0.44
1:H:12[B]:LEU:N	1:H:12[B]:LEU:HD12	2.32	0.44
1:G:114[A]:ASN:ND2	1:H:147:ASP:OD2	2.36	0.44
1:H:7[A]:THR:N	1:H:9[A]:PHE:CE1	2.86	0.44
1:B:45:TYR:OH	3:B:201:CYN:N	2.36	0.44
1:G:52[A]:GLU:HG2	1:G:55[A]:ARG:HH21	1.83	0.44
1:G:107[B]:HIS:CG	1:H:12[B]:LEU:HD11	2.52	0.44
1:D:153:MET:HG3	6:D:322:HOH:O	2.18	0.43
2:B:200:HEM:HBC2	2:B:200:HEM:CMC	2.49	0.43
1:G:90[B]:ASP:HA	1:G:93[B]:TYR:HD2	1.83	0.43
1:G:52[B]:GLU:O	1:G:56[B]:THR:HG23	2.19	0.43
1:H:134:GLU:OE1	1:H:137:ARG:NH1	2.51	0.43
1:C:9[B]:PHE:CD1	1:C:13:LYS:HG3	2.52	0.43
2:A:200:HEM:HBB2	2:A:200:HEM:HMB1	2.01	0.43
1:G:99[B]:HIS:NE2	3:G:201:CYN:C	2.65	0.43
2:F:200:HEM:HBB2	2:F:200:HEM:HMB1	2.01	0.42
1:G:89[B]:TRP:O	1:G:93[B]:TYR:CE2	2.72	0.42
1:A:8:VAL:O	1:A:12:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:HEM:HBB2	2:E:201:HEM:HMB1	2.02	0.42
1:G:92[B]:ARG:CG	1:G:149[B]:GLU:OE2	2.68	0.42
2:C:200:HEM:CMB	2:C:200:HEM:HBB2	2.50	0.41
1:G:38[B]:PRO:HG3	1:G:73[B]:ILE:HD13	2.02	0.41
1:G:88[B]:TYR:CE2	1:G:92[B]:ARG:NH1	2.88	0.41
1:G:127:ARG:NH2	6:G:310:HOH:O	2.53	0.41
2:E:201:HEM:CMC	2:E:201:HEM:HBC2	2.48	0.41
1:G:100[B]:VAL:HG22	1:G:157[B]:TYR:CE2	2.54	0.41
1:G:88[B]:TYR:CE1	1:G:92[B]:ARG:HD3	2.56	0.41
1:G:155[B]:HIS:C	1:G:155[B]:HIS:CD2	2.93	0.41
1:G:150[A]:LEU:O	1:G:154[A]:LEU:HD23	2.21	0.41
1:G:150[B]:LEU:O	1:G:154[B]:LEU:HD23	2.20	0.41
1:G:48[B]:ILE:C	1:G:50[B]:GLY:N	2.74	0.41
1:H:7[B]:THR:O	1:H:11[B]:GLU:CG	2.68	0.41
1:G:41[B]:ALA:O	1:G:44[B]:PHE:HB3	2.20	0.41
1:G:92[B]:ARG:HD3	1:G:149[B]:GLU:OE1	2.20	0.41
1:G:72[B]:MET:HE3	2:G:200[B]:HEM:C1B	2.56	0.41
1:G:41[A]:ALA:O	1:G:45[A]:TYR:CD2	2.75	0.40
1:G:49[B]:LEU:HD11	1:G:65[B]:VAL:HG11	2.03	0.40
2:D:200:HEM:HBB2	2:D:200:HEM:CMB	2.51	0.40
1:G:104[B]:LEU:HD12	1:G:105[B]:PRO:HD2	2.03	0.40
1:G:142:LEU:O	1:G:145[B]:VAL:HG12	2.22	0.40
1:G:99[B]:HIS:CE1	3:G:201:CYN:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	154/161 (96%)	152 (99%)	2 (1%)	0	100	100
1	B	156/161 (97%)	154 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	147/161 (91%)	145 (99%)	2 (1%)	0	100	100
1	D	153/161 (95%)	151 (99%)	2 (1%)	0	100	100
1	E	151/161 (94%)	150 (99%)	1 (1%)	0	100	100
1	F	151/161 (94%)	149 (99%)	2 (1%)	0	100	100
1	G	234/161 (145%)	215 (92%)	17 (7%)	2 (1%)	20	6
1	H	172/161 (107%)	171 (99%)	1 (1%)	0	100	100
All	All	1318/1288 (102%)	1287 (98%)	29 (2%)	2 (0%)	55	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	49[A]	LEU
1	G	49[B]	LEU

5.3.2 Protein sidechains ⓘ

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	125/128 (98%)	124 (99%)	1 (1%)	85	81
1	B	127/128 (99%)	126 (99%)	1 (1%)	85	81
1	C	122/128 (95%)	121 (99%)	1 (1%)	85	81
1	D	124/128 (97%)	124 (100%)	0	100	100
1	E	122/128 (95%)	121 (99%)	1 (1%)	85	81
1	F	122/128 (95%)	122 (100%)	0	100	100
1	G	194/128 (152%)	192 (99%)	2 (1%)	80	75
1	H	140/128 (109%)	132 (94%)	8 (6%)	24	9
All	All	1076/1024 (105%)	1062 (99%)	14 (1%)	82	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	B	126	GLU
1	C	77	ASP
1	E	7	THR
1	G	154[A]	LEU
1	G	154[B]	LEU
1	H	9[A]	PHE
1	H	9[B]	PHE
1	H	10[A]	GLU
1	H	10[B]	GLU
1	H	11[A]	GLU
1	H	11[B]	GLU
1	H	12[A]	LEU
1	H	12[B]	LEU

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](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

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	200	1,3	28,50,50	0.68	0	17,82,82	1.23	2 (11%)
3	CYN	A	201	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	B	200	1,3	28,50,50	0.84	1 (3%)	17,82,82	1.40	2 (11%)
3	CYN	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	C	200	1,3	28,50,50	0.97	2 (7%)	17,82,82	1.15	1 (5%)
3	CYN	C	201	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	D	200	1	28,50,50	0.87	2 (7%)	17,82,82	1.64	5 (29%)
3	CYN	D	201	-	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	E	201	-	28,50,50	0.89	1 (3%)	17,82,82	1.23	1 (5%)
3	CYN	E	202	-	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	F	200	1	28,50,50	0.82	1 (3%)	17,82,82	1.42	1 (5%)
3	CYN	F	201	-	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	G	200[A]	1,3	28,50,50	0.89	2 (7%)	17,82,82	1.38	2 (11%)
2	HEM	G	200[B]	1	28,50,50	0.91	2 (7%)	17,82,82	1.38	3 (17%)
3	CYN	G	201	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	H	200	1,3	28,50,50	0.75	1 (3%)	17,82,82	1.36	3 (17%)
3	CYN	H	201	2	0,1,1	0.00	-	0,0,0	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
2	HEM	A	200	1,3	-	0/6/54/54	0/0/8/8
3	CYN	A	201	2	-	0/0/0/0	0/0/0/0
2	HEM	B	200	1,3	-	0/6/54/54	0/0/8/8
3	CYN	B	201	2	-	0/0/0/0	0/0/0/0
2	HEM	C	200	1,3	-	0/6/54/54	0/0/8/8
3	CYN	C	201	2	-	0/0/0/0	0/0/0/0
2	HEM	D	200	1	-	0/6/54/54	0/0/8/8
3	CYN	D	201	-	-	0/0/0/0	0/0/0/0
2	HEM	E	201	-	-	0/6/54/54	0/0/8/8
3	CYN	E	202	-	-	0/0/0/0	0/0/0/0
2	HEM	F	200	1	-	0/6/54/54	0/0/8/8
3	CYN	F	201	-	-	0/0/0/0	0/0/0/0
2	HEM	G	200[A]	1,3	-	0/6/54/54	0/0/8/8
2	HEM	G	200[B]	1	-	0/6/54/54	0/0/8/8
3	CYN	G	201	2	-	0/0/0/0	0/0/0/0
2	HEM	H	200	1,3	-	0/6/54/54	0/0/8/8
3	CYN	H	201	2	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200	HEM	C1B-NB	-3.08	1.33	1.36
2	D	200	HEM	C1B-NB	-2.66	1.33	1.36
2	G	200[A]	HEM	C3B-C2B	-2.66	1.36	1.40
2	E	201	HEM	C1B-NB	-2.65	1.33	1.36
2	G	200[B]	HEM	C3B-C2B	-2.64	1.36	1.40
2	F	200	HEM	C1B-NB	-2.57	1.33	1.36
2	H	200	HEM	C1B-NB	-2.43	1.33	1.36
2	G	200[A]	HEM	C1B-NB	-2.32	1.34	1.36
2	C	200	HEM	C3B-C2B	-2.23	1.37	1.40
2	B	200	HEM	C4D-ND	-2.14	1.34	1.36
2	G	200[B]	HEM	C1B-NB	-2.12	1.34	1.36
2	D	200	HEM	C3B-C2B	-2.03	1.37	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	200	HEM	CMA-C3A-C4A	-2.90	124.01	128.46
2	G	200[B]	HEM	CAA-CBA-CGA	-2.72	108.01	112.66
2	F	200	HEM	CAA-CBA-CGA	-2.68	108.08	112.66
2	D	200	HEM	CAA-CBA-CGA	-2.68	108.09	112.66
2	B	200	HEM	CAA-CBA-CGA	-2.62	108.18	112.66
2	G	200[A]	HEM	CAD-CBD-CGD	-2.46	108.46	112.66
2	D	200	HEM	C1D-C2D-C3D	-2.41	105.32	107.00
2	G	200[B]	HEM	C3B-C4B-NB	-2.36	106.16	109.21
2	A	200	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
2	E	201	HEM	CAA-CBA-CGA	-2.35	108.64	112.66
2	D	200	HEM	CAD-CBD-CGD	-2.35	108.65	112.66
2	D	200	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
2	D	200	HEM	CBA-CAA-C2A	-2.08	108.50	112.48
2	B	200	HEM	CBA-CAA-C2A	-2.04	108.59	112.48
2	A	200	HEM	CAD-CBD-CGD	-2.02	109.20	112.66
2	G	200[B]	HEM	CAD-CBD-CGD	-2.02	109.21	112.66
2	G	200[A]	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
2	C	200	HEM	CMB-C2B-C3B	2.05	128.70	124.89
2	H	200	HEM	CMB-C2B-C3B	2.05	128.70	124.89
2	H	200	HEM	CMA-C3A-C2A	2.12	128.94	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	HEM	1	0
3	A	201	CYN	1	0
2	B	200	HEM	2	0
3	B	201	CYN	1	0
2	C	200	HEM	3	0
3	C	201	CYN	1	0
2	D	200	HEM	3	0
2	E	201	HEM	3	0
3	E	202	CYN	1	0
2	F	200	HEM	2	0
2	G	200[A]	HEM	12	0
2	G	200[B]	HEM	12	0
3	G	201	CYN	5	0
2	H	200	HEM	1	0
3	H	201	CYN	1	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, 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	152/161 (94%)	-0.08	3 (1%) 65 61	16, 25, 42, 69	3 (1%)
1	B	152/161 (94%)	-0.26	2 (1%) 77 74	16, 26, 38, 52	5 (3%)
1	C	147/161 (91%)	0.06	5 (3%) 46 41	19, 29, 48, 60	3 (2%)
1	D	152/161 (94%)	-0.01	1 (0%) 87 86	17, 28, 44, 62	1 (0%)
1	E	152/161 (94%)	-0.09	2 (1%) 77 74	17, 26, 38, 50	4 (2%)
1	F	153/161 (95%)	-0.12	1 (0%) 87 86	16, 25, 44, 56	3 (1%)
1	G	147/161 (91%)	0.97	20 (13%) 3 2	17, 30, 50, 62	1 (0%)
1	H	152/161 (94%)	0.17	5 (3%) 47 41	16, 27, 41, 50	2 (1%)
All	All	1207/1288 (93%)	0.08	39 (3%) 48 43	16, 27, 44, 69	22 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	VAL	6.3
1	G	65[A]	VAL	5.3
1	C	9[A]	PHE	4.9
1	C	8	VAL	3.8
1	G	156[A]	THR	3.6
1	A	9	PHE	3.5
1	G	67[A]	HIS	3.5
1	H	9[A]	PHE	3.3
1	G	49[A]	LEU	3.3
1	G	70[A]	VAL	3.2
1	G	10	GLU	3.2
1	C	58	LEU	3.1
1	G	7	THR	3.1
1	G	93[A]	TYR	3.0
1	G	104[A]	LEU	2.9
1	H	14[A]	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	93	TYR	2.8
1	H	12[A]	LEU	2.7
1	G	91[A]	ARG	2.7
1	G	157[A]	TYR	2.6
1	G	108[A]	TYR	2.5
1	G	52[A]	GLU	2.5
1	G	9	PHE	2.5
1	B	9	PHE	2.4
1	A	7	THR	2.4
1	G	68[A]	LEU	2.3
1	H	155	HIS	2.2
1	D	158	ARG	2.2
1	F	7	THR	2.1
1	G	100[A]	VAL	2.1
1	G	155[A]	HIS	2.1
1	E	7	THR	2.1
1	H	7[A]	THR	2.1
1	C	101	ARG	2.1
1	B	8	VAL	2.1
1	G	105[A]	PRO	2.1
1	E	9	PHE	2.1
1	G	158[A]	ARG	2.0
1	G	154[A]	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 [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(\AA^2)	Q<0.9
2	HEM	G	200[B]	43/43	0.92	0.24	1.44	26,30,34,36	43
2	HEM	G	200[A]	43/43	0.92	0.24	1.22	18,21,31,33	43
2	HEM	B	200	43/43	0.97	0.11	1.07	18,20,40,43	0
2	HEM	A	200	43/43	0.97	0.12	0.61	19,21,39,41	0
2	HEM	E	201	43/43	0.97	0.10	0.48	19,21,34,36	0
2	HEM	C	200	43/43	0.95	0.15	0.41	25,29,38,45	4
2	HEM	D	200	43/43	0.97	0.11	0.24	21,24,36,44	4
2	HEM	F	200	43/43	0.97	0.11	0.24	19,22,39,42	0
2	HEM	H	200	43/43	0.98	0.10	-0.38	19,21,35,39	0
3	CYN	G	201	2/2	0.97	0.14	-0.51	21,21,21,25	2
4	CL	E	203	1/1	0.99	0.09	-0.56	23,23,23,23	0
4	CL	A	202	1/1	0.99	0.08	-0.68	27,27,27,27	0
4	CL	G	202	1/1	0.99	0.07	-1.50	33,33,33,33	0
4	CL	C	202	1/1	0.99	0.04	-6.01	32,32,32,32	0
4	CL	D	202	1/1	0.97	0.05	-	47,47,47,47	0
3	CYN	A	201	2/2	0.96	0.15	-	16,16,16,20	0
3	CYN	F	201	2/2	0.92	0.23	-	22,22,22,27	0
5	NA	E	204	1/1	0.98	0.09	-	47,47,47,47	0
3	CYN	D	201	2/2	0.95	0.21	-	22,22,22,25	0
3	CYN	E	202	2/2	0.99	0.13	-	16,16,16,18	0
3	CYN	H	201	2/2	0.95	0.15	-	19,19,19,24	0
3	CYN	B	201	2/2	0.97	0.14	-	17,17,17,22	0
3	CYN	C	201	2/2	0.98	0.14	-	22,22,22,28	0

6.5 Other polymers

There are no such residues in this entry.