Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:07 AM GMT

PDB ID	:	2VXH
Title	:	THE CRYSTAL STRUCTURE OF CHLORITE DISMUTASE: A DETOX ENZYME PRODUCING MOLECULAR OXYGEN
Authors	:	De Geus, D.C.; Thomassen, E.A.J.; Hagedoorn, P.L.; Pannu, N.S.; Abrahams, J.P.
Deposited on	:	2008-07-04
Resolution	:	2.10 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:

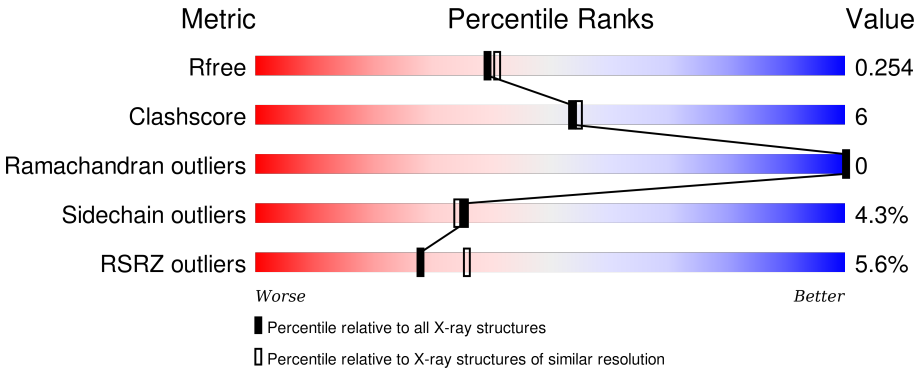
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	251	3% 78% 11% • 9%
1	B	251	2% 78% 12% • 8%
1	C	251	4% 80% 8% • 9%
1	D	251	9% 79% 10% • 8%
1	E	251	3% 80% 11% 8%

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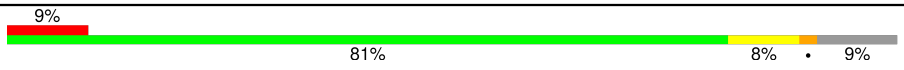
Mol	Chain	Length	Quality of chain
1	F	251	

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
4	CO3	A	1003	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11790 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 CHLORITE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1818	1167	303	342	6			
1	B	230	Total	C	N	O	S	0	0	0
			1826	1171	304	345	6			
1	C	228	Total	C	N	O	S	0	0	0
			1814	1163	302	343	6			
1	D	230	Total	C	N	O	S	0	0	0
			1830	1175	305	344	6			
1	E	230	Total	C	N	O	S	0	0	0
			1830	1175	305	344	6			
1	F	229	Total	C	N	O	S	0	0	0
			1821	1169	303	343	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q673K5
A	-1	SER	-	EXPRESSION TAG	UNP Q673K5
A	0	HIS	-	EXPRESSION TAG	UNP Q673K5
A	6	ALA	PRO	CONFLICT	UNP Q673K5
B	-2	GLY	-	EXPRESSION TAG	UNP Q673K5
B	-1	SER	-	EXPRESSION TAG	UNP Q673K5
B	0	HIS	-	EXPRESSION TAG	UNP Q673K5
B	6	ALA	PRO	CONFLICT	UNP Q673K5
C	-2	GLY	-	EXPRESSION TAG	UNP Q673K5
C	-1	SER	-	EXPRESSION TAG	UNP Q673K5
C	0	HIS	-	EXPRESSION TAG	UNP Q673K5
C	6	ALA	PRO	CONFLICT	UNP Q673K5
D	-2	GLY	-	EXPRESSION TAG	UNP Q673K5
D	-1	SER	-	EXPRESSION TAG	UNP Q673K5
D	0	HIS	-	EXPRESSION TAG	UNP Q673K5
D	6	ALA	PRO	CONFLICT	UNP Q673K5
E	-2	GLY	-	EXPRESSION TAG	UNP Q673K5

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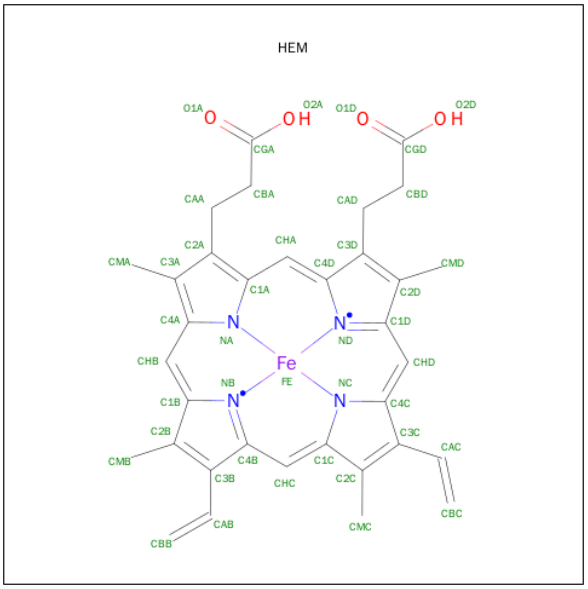
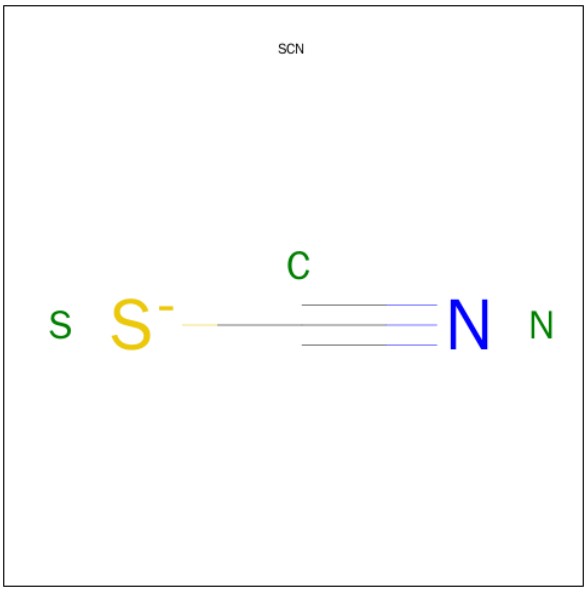
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	EXPRESSION TAG	UNP Q673K5
E	0	HIS	-	EXPRESSION TAG	UNP Q673K5
E	6	ALA	PRO	CONFLICT	UNP Q673K5
F	-2	GLY	-	EXPRESSION TAG	UNP Q673K5
F	-1	SER	-	EXPRESSION TAG	UNP Q673K5
F	0	HIS	-	EXPRESSION TAG	UNP Q673K5
F	6	ALA	PRO	CONFLICT	UNP Q673K5

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



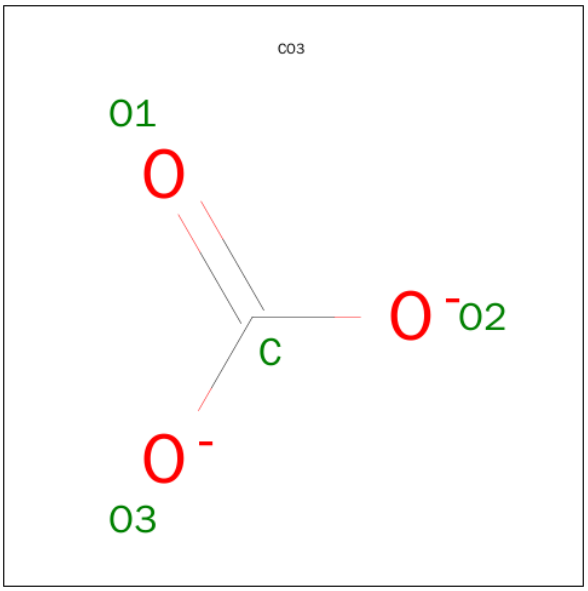
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0

- Molecule 5 is water.

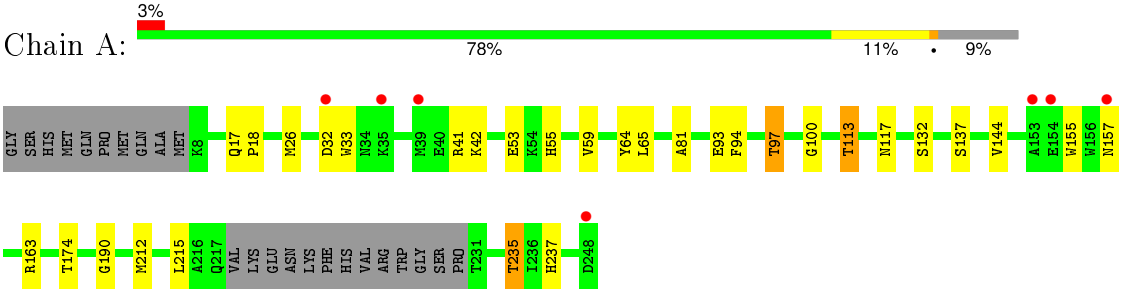
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	110	Total O 110 110	0	0
5	B	98	Total O 98 98	0	0
5	C	93	Total O 93 93	0	0
5	D	66	Total O 66 66	0	0
5	E	114	Total O 114 114	0	0
5	F	74	Total O 74 74	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

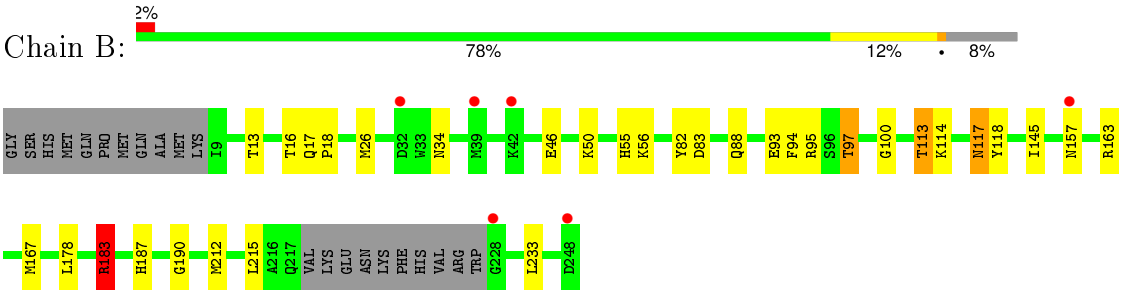
- Molecule 1: CHLORITE DISMUTASE

Chain A:



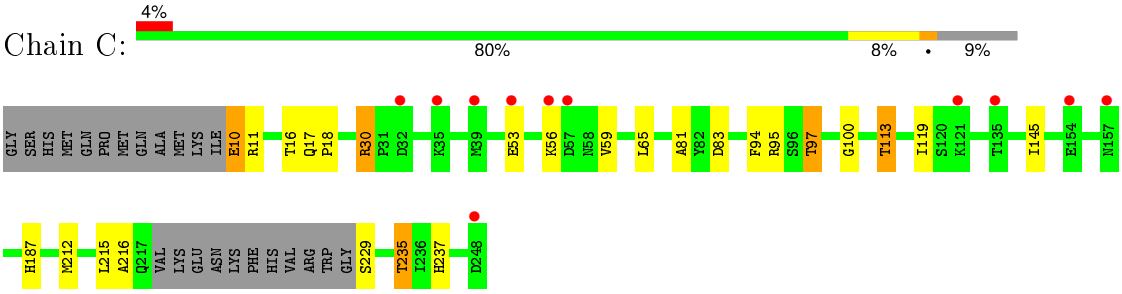
- Molecule 1: CHLORITE DISMUTASE

Chain B:



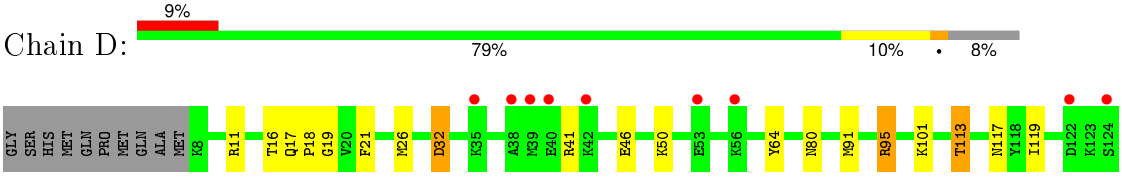
- Molecule 1: CHLORITE DISMUTASE

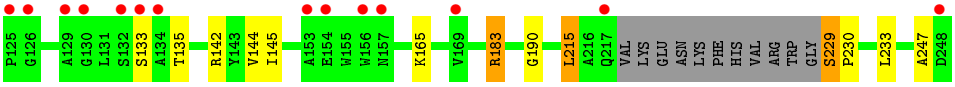
Chain C:



- Molecule 1: CHLORITE DISMUTASE

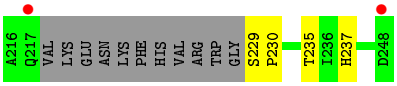
Chain D:





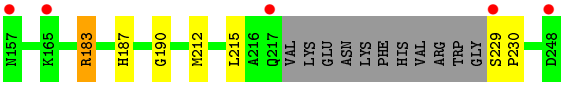
• Molecule 1: CHLORITE DISMUTASE

Chain E:



• Molecule 1: CHLORITE DISMUTASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.46Å 169.34Å 60.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.68 – 2.10 37.64 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.68-2.10) 100.0 (37.64-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.255 0.218 , 0.254	Depositor DCC
R_{free} test set	4994 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.4	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 99931 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11790	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, CO3, SCN

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	0.64	1/1857 (0.1%)	0.66	0/2516
1	B	0.58	1/1866 (0.1%)	0.64	2/2530 (0.1%)
1	C	0.57	0/1854	0.62	0/2514
1	D	0.58	0/1870	0.63	2/2535 (0.1%)
1	E	0.60	0/1870	0.65	1/2535 (0.0%)
1	F	0.61	0/1861	0.67	0/2524
All	All	0.60	2/11178 (0.0%)	0.65	5/15154 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	TYR	C-N	-5.42	1.21	1.34
1	A	137	SER	CB-OG	-5.17	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	183	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	11	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	E	11	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	183	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	183	ARG	NE-CZ-NH1	5.04	122.82	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	1818	0	1828	24	0
1	B	1826	0	1831	26	0
1	C	1814	0	1817	33	0
1	D	1830	0	1841	24	0
1	E	1830	0	1841	28	0
1	F	1821	0	1828	22	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
2	E	43	0	30	0	0
2	F	43	0	30	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	A	110	0	0	2	0
5	B	98	0	0	8	0
5	C	93	0	0	5	0
5	D	66	0	0	1	0
5	E	114	0	0	2	0
5	F	74	0	0	4	0
All	All	11790	0	11166	145	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 6.

All (145) 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:138:GLY:HA3	5:E:2066:HOH:O	1.42	1.19
1:E:229:SER:HB3	1:E:230:PRO:CD	1.75	1.17
1:C:10:GLU:HA	1:C:10:GLU:OE2	1.43	1.09
1:E:229:SER:HB3	1:E:230:PRO:HD2	1.42	0.97
1:A:235:THR:HG23	1:A:237:HIS:NE2	1.82	0.94
1:D:229:SER:HB2	1:D:230:PRO:HD3	1.50	0.94
1:D:229:SER:HB2	1:D:230:PRO:CD	2.00	0.92
1:A:97:THR:HG22	1:A:100:GLY:H	1.34	0.92
1:B:17:GLN:O	1:B:113:THR:HG21	1.71	0.91
1:A:17:GLN:O	1:A:113:THR:HG21	1.71	0.91
1:D:17:GLN:O	1:D:113:THR:HG21	1.71	0.90
1:E:17:GLN:O	1:E:113:THR:HG21	1.72	0.89
1:E:18:PRO:HA	1:E:113:THR:HG22	1.55	0.89
1:C:97:THR:HG22	1:C:100:GLY:H	1.38	0.89
1:C:18:PRO:HA	1:C:113:THR:HG22	1.54	0.88
1:F:18:PRO:HA	1:F:113:THR:HG22	1.59	0.85
1:E:229:SER:HB3	1:E:230:PRO:HD3	1.59	0.84
1:F:17:GLN:O	1:F:113:THR:HG21	1.77	0.84
1:E:229:SER:CB	1:E:230:PRO:CD	2.56	0.83
1:E:235:THR:HG23	1:E:237:HIS:CE1	2.13	0.83
1:C:17:GLN:O	1:C:113:THR:HG21	1.78	0.83
1:B:97:THR:HG22	1:B:100:GLY:H	1.41	0.82
1:E:229:SER:CB	1:E:230:PRO:HD2	2.11	0.81
1:D:145:ILE:HD11	1:D:233:LEU:HD13	1.64	0.79
1:C:235:THR:HG23	1:C:237:HIS:NE2	1.96	0.79
1:E:235:THR:CG2	1:E:237:HIS:HE1	1.99	0.76
1:F:18:PRO:HA	1:F:113:THR:CG2	2.17	0.75
1:A:18:PRO:HA	1:A:113:THR:HG22	1.68	0.75
1:F:97:THR:HG22	1:F:100:GLY:H	1.50	0.75
1:D:18:PRO:HA	1:D:113:THR:CG2	2.17	0.73
1:C:18:PRO:HA	1:C:113:THR:CG2	2.19	0.72
1:E:235:THR:HG23	1:E:237:HIS:HE1	1.55	0.71
1:A:235:THR:CG2	1:A:237:HIS:NE2	2.54	0.71
1:C:235:THR:HG23	1:C:237:HIS:CD2	2.27	0.70
1:A:163:ARG:NH2	5:A:2073:HOH:O	2.25	0.69
1:C:83:ASP:OD1	1:D:142:ARG:NH1	2.26	0.68
1:C:187:HIS:HD2	5:C:2071:HOH:O	1.77	0.68
1:A:235:THR:HG23	1:A:237:HIS:CD2	2.31	0.66
1:B:18:PRO:HA	1:B:113:THR:HG22	1.77	0.64
1:D:46:GLU:HG3	1:D:50:LYS:HE2	1.78	0.64
1:B:18:PRO:HA	1:B:113:THR:CG2	2.26	0.64
1:E:55:HIS:HE1	1:E:93:GLU:OE1	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ARG:NH1	5:D:2035:HOH:O	2.24	0.63
1:C:30:ARG:CG	1:C:30:ARG:HH11	2.11	0.62
1:B:187:HIS:HD2	5:B:2033:HOH:O	1.82	0.62
1:B:55:HIS:HE1	1:B:93:GLU:OE1	1.82	0.62
1:C:94:PHE:O	1:C:97:THR:HB	2.00	0.61
1:B:46:GLU:HG3	1:B:50:LYS:HE2	1.80	0.61
1:A:18:PRO:HA	1:A:113:THR:CG2	2.31	0.61
1:B:94:PHE:O	1:B:97:THR:HB	2.01	0.60
1:F:229:SER:CB	1:F:230:PRO:HD2	2.31	0.60
1:A:94:PHE:O	1:A:97:THR:HB	2.01	0.59
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.67	0.59
1:B:117:ASN:ND2	5:B:2047:HOH:O	2.36	0.58
1:C:83:ASP:HB2	5:C:2034:HOH:O	2.02	0.58
1:C:65:LEU:HB3	1:C:235:THR:HG22	1.85	0.57
1:D:229:SER:CB	1:D:230:PRO:CD	2.78	0.57
1:A:65:LEU:HB3	1:A:235:THR:HG22	1.85	0.57
1:E:18:PRO:HA	1:E:113:THR:CG2	2.33	0.56
1:D:17:GLN:O	1:D:113:THR:CG2	2.51	0.56
1:B:13:THR:O	1:B:17:GLN:HG3	2.05	0.56
1:E:17:GLN:O	1:E:113:THR:CG2	2.50	0.56
1:A:212:MET:HG3	1:E:190:GLY:HA3	1.87	0.56
1:A:17:GLN:O	1:A:113:THR:CG2	2.51	0.56
1:F:229:SER:CB	1:F:230:PRO:CD	2.84	0.56
1:C:95:ARG:HD2	5:C:2037:HOH:O	2.05	0.55
1:D:18:PRO:HA	1:D:113:THR:HG22	1.88	0.55
1:D:19:GLY:N	1:D:113:THR:HG22	2.23	0.54
1:F:229:SER:HB2	1:F:230:PRO:HD2	1.89	0.54
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.24	0.53
1:B:17:GLN:O	1:B:113:THR:CG2	2.51	0.53
1:C:10:GLU:OE2	1:C:10:GLU:CA	2.28	0.53
1:A:64:TYR:CD1	1:A:144:VAL:HG11	2.44	0.53
1:C:229:SER:N	5:C:2084:HOH:O	2.41	0.53
1:F:152:ASN:OD1	1:F:154:GLU:HB2	2.07	0.53
1:B:163:ARG:NH2	5:B:2065:HOH:O	2.42	0.53
1:E:235:THR:CG2	1:E:237:HIS:CE1	2.80	0.52
1:A:97:THR:HG22	1:A:100:GLY:N	2.16	0.52
1:A:212:MET:HG3	1:E:190:GLY:CA	2.40	0.52
1:C:235:THR:HG21	5:F:2030:HOH:O	2.09	0.52
1:D:145:ILE:CD1	1:D:233:LEU:HD13	2.36	0.52
1:F:97:THR:CG2	1:F:100:GLY:H	2.19	0.52
1:F:119:ILE:HG13	2:F:1001:HEM:HMA3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:HIS:CE1	1:B:93:GLU:OE1	2.62	0.51
1:F:187:HIS:HE1	5:F:2054:HOH:O	1.91	0.51
1:B:178:LEU:HD21	2:B:1001:HEM:HMB3	1.93	0.51
1:C:30:ARG:HH11	1:C:30:ARG:HB3	1.76	0.50
1:A:55:HIS:HE1	1:A:93:GLU:OE1	1.93	0.50
1:D:18:PRO:HA	1:D:113:THR:HG23	1.92	0.50
1:A:59:VAL:HG12	1:A:81:ALA:HB2	1.94	0.49
1:D:32:ASP:OD1	1:D:32:ASP:N	2.41	0.48
1:C:97:THR:HG22	1:C:100:GLY:N	2.18	0.48
1:C:59:VAL:HG12	1:C:81:ALA:HB2	1.96	0.48
1:A:157:ASN:HB3	5:A:2071:HOH:O	2.14	0.47
1:B:17:GLN:HG2	5:B:2004:HOH:O	2.14	0.47
1:C:235:THR:CG2	1:C:237:HIS:NE2	2.72	0.47
1:C:212:MET:HG3	1:F:190:GLY:HA3	1.95	0.47
1:E:53:GLU:O	1:E:56:LYS:HB2	2.15	0.47
1:A:190:GLY:HA3	1:F:212:MET:HG3	1.97	0.47
1:C:119:ILE:HG13	2:C:1001:HEM:HMA3	1.95	0.47
1:B:34:ASN:HD21	1:D:101:LYS:HG2	1.78	0.47
1:B:183:ARG:NH2	5:B:2076:HOH:O	2.47	0.46
1:B:95:ARG:HD2	5:B:2042:HOH:O	2.15	0.46
1:E:8:LYS:HD3	1:E:9:ILE:H	1.81	0.46
1:F:32:ASP:HB3	1:F:35:LYS:HE3	1.98	0.45
1:C:53:GLU:O	1:C:56:LYS:HB2	2.17	0.45
1:D:91:MET:O	1:D:95:ARG:HG2	2.17	0.44
1:C:30:ARG:CG	1:C:30:ARG:NH1	2.77	0.44
1:F:95:ARG:HG3	5:F:2034:HOH:O	2.17	0.44
1:C:17:GLN:O	1:C:113:THR:CG2	2.59	0.44
1:D:119:ILE:HG13	2:D:1001:HEM:HMA3	1.99	0.44
1:A:235:THR:HG21	5:E:2045:HOH:O	2.17	0.44
1:C:30:ARG:CB	1:C:30:ARG:HH11	2.29	0.44
1:E:27:PHE:HE1	1:E:95:ARG:HD3	1.83	0.44
1:F:183:ARG:HD3	2:F:1001:HEM:C2B	2.53	0.44
1:B:95:ARG:CD	5:B:2042:HOH:O	2.66	0.44
1:C:212:MET:HG3	1:F:190:GLY:CA	2.48	0.44
1:B:88:GLN:OE1	1:E:235:THR:HG21	2.18	0.43
1:B:114:LYS:NZ	1:E:210:ASN:ND2	2.66	0.43
1:C:216:ALA:O	1:F:156:TRP:HB3	2.18	0.43
1:F:97:THR:HG22	1:F:100:GLY:N	2.25	0.43
1:B:212:MET:HG3	1:D:190:GLY:HA3	1.99	0.43
1:D:41:ARG:NH2	1:D:247:ALA:O	2.52	0.43
1:E:235:THR:HG21	1:E:237:HIS:HE1	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:TYR:CD1	1:D:144:VAL:HG11	2.54	0.43
1:A:174:THR:HB	2:A:1001:HEM:C3B	2.54	0.43
1:D:215:LEU:HA	1:D:215:LEU:HD12	1.86	0.43
1:B:83:ASP:OD2	5:B:2036:HOH:O	2.21	0.42
1:B:118:TYR:CD2	1:B:167:MET:HG3	2.54	0.42
1:C:10:GLU:HB3	1:C:11:ARG:H	1.69	0.42
1:E:59:VAL:HG12	1:E:81:ALA:HB2	2.01	0.42
1:E:55:HIS:CE1	1:E:93:GLU:OE1	2.67	0.41
1:F:187:HIS:CE1	5:F:2054:HOH:O	2.70	0.41
1:B:145:ILE:HD11	1:B:233:LEU:HD13	2.02	0.41
1:B:190:GLY:HA3	1:E:212:MET:HG3	2.01	0.41
1:A:155:TRP:CE2	1:A:163:ARG:HD2	2.55	0.41
1:E:118:TYR:CD2	1:E:167:MET:HG3	2.56	0.41
1:F:94:PHE:O	1:F:97:THR:HB	2.21	0.41
1:E:8:LYS:CD	1:E:9:ILE:H	2.34	0.41
1:A:33:TRP:CH2	1:A:41:ARG:HG2	2.56	0.41
1:D:21:PHE:O	1:D:80:ASN:HA	2.21	0.41
1:C:187:HIS:CD2	5:C:2071:HOH:O	2.61	0.40
1:F:36:VAL:O	1:F:41:ARG:HD2	2.22	0.40
1:A:97:THR:CG2	1:A:100:GLY:H	2.19	0.40
1:D:145:ILE:HD11	1:D:233:LEU:CD1	2.43	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	224/251 (89%)	221 (99%)	3 (1%)	0	100	100
1	B	226/251 (90%)	223 (99%)	3 (1%)	0	100	100
1	C	224/251 (89%)	221 (99%)	3 (1%)	0	100	100
1	D	226/251 (90%)	223 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	226/251 (90%)	223 (99%)	3 (1%)	0	100	100
1	F	225/251 (90%)	221 (98%)	4 (2%)	0	100	100
All	All	1351/1506 (90%)	1332 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	200/220 (91%)	190 (95%)	10 (5%)	30	27
1	B	201/220 (91%)	192 (96%)	9 (4%)	34	32
1	C	200/220 (91%)	192 (96%)	8 (4%)	38	38
1	D	202/220 (92%)	190 (94%)	12 (6%)	24	20
1	E	202/220 (92%)	198 (98%)	4 (2%)	63	68
1	F	201/220 (91%)	192 (96%)	9 (4%)	34	32
All	All	1206/1320 (91%)	1154 (96%)	52 (4%)	35	34

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	32	ASP
1	A	42	LYS
1	A	53	GLU
1	A	97	THR
1	A	113	THR
1	A	117	ASN
1	A	132	SER
1	A	215	LEU
1	A	235	THR
1	B	16	THR
1	B	26	MET

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Mol	Chain	Res	Type
1	B	56	LYS
1	B	97	THR
1	B	113	THR
1	B	117	ASN
1	B	157	ASN
1	B	183	ARG
1	B	215	LEU
1	C	10	GLU
1	C	16	THR
1	C	30	ARG
1	C	97	THR
1	C	113	THR
1	C	145	ILE
1	C	215	LEU
1	C	235	THR
1	D	16	THR
1	D	26	MET
1	D	32	ASP
1	D	95	ARG
1	D	113	THR
1	D	117	ASN
1	D	133	SER
1	D	135	THR
1	D	165	LYS
1	D	183	ARG
1	D	215	LEU
1	D	229	SER
1	E	16	THR
1	E	112	VAL
1	E	145	ILE
1	E	215	LEU
1	F	16	THR
1	F	32	ASP
1	F	39	MET
1	F	95	ARG
1	F	97	THR
1	F	113	THR
1	F	117	ASN
1	F	183	ARG
1	F	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	117	ASN
1	A	217	GLN
1	B	34	ASN
1	B	55	HIS
1	B	102	ASN
1	B	117	ASN
1	B	157	ASN
1	B	187	HIS
1	B	237	HIS
1	C	102	ASN
1	C	157	ASN
1	C	187	HIS
1	D	157	ASN
1	D	209	ASN
1	E	55	HIS
1	E	72	ASN
1	E	157	ASN
1	E	210	ASN
1	E	217	GLN
1	E	237	HIS
1	F	80	ASN
1	F	102	ASN
1	F	157	ASN
1	F	187	HIS
1	F	209	ASN
1	F	210	ASN

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)

17 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	1001	1,3	30,50,50	2.34	10 (33%)	24,82,82	2.78	15 (62%)
3	SCN	A	1002	2	2,2,2	1.23	0	1,1,1	1.18	0
4	CO3	A	1003	-	0,3,3	0.00	-	0,3,3	0.00	-
2	HEM	B	1001	1,3	30,50,50	2.40	10 (33%)	24,82,82	2.57	14 (58%)
3	SCN	B	1002	2	2,2,2	1.37	0	1,1,1	0.96	0
4	CO3	B	1003	-	0,3,3	0.00	-	0,3,3	0.00	-
2	HEM	C	1001	1,3	30,50,50	2.27	12 (40%)	24,82,82	2.68	15 (62%)
3	SCN	C	1002	2	2,2,2	1.26	0	1,1,1	0.64	0
4	CO3	C	1003	-	0,3,3	0.00	-	0,3,3	0.00	-
2	HEM	D	1001	1,3	30,50,50	2.10	9 (30%)	24,82,82	2.67	16 (66%)
3	SCN	D	1002	2	2,2,2	1.16	0	1,1,1	0.49	0
2	HEM	E	1001	1,3	30,50,50	2.24	9 (30%)	24,82,82	2.76	14 (58%)
3	SCN	E	1002	2	2,2,2	1.21	0	1,1,1	0.20	0
4	CO3	E	1003	-	0,3,3	0.00	-	0,3,3	0.00	-
2	HEM	F	1001	1,3	30,50,50	2.31	8 (26%)	24,82,82	2.62	13 (54%)
3	SCN	F	1002	2	2,2,2	1.20	0	1,1,1	0.10	0
4	CO3	F	1003	-	0,3,3	0.00	-	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
2	HEM	A	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	A	1002	2	-	0/0/0/0	0/0/0/0
4	CO3	A	1003	-	-	0/0/0/0	0/0/0/0
2	HEM	B	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	B	1002	2	-	0/0/0/0	0/0/0/0
4	CO3	B	1003	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	C	1002	2	-	0/0/0/0	0/0/0/0
4	CO3	C	1003	-	-	0/0/0/0	0/0/0/0
2	HEM	D	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	D	1002	2	-	0/0/0/0	0/0/0/0
2	HEM	E	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	E	1002	2	-	0/0/0/0	0/0/0/0
4	CO3	E	1003	-	-	0/0/0/0	0/0/0/0
2	HEM	F	1001	1,3	-	0/10/54/54	0/0/8/8
3	SCN	F	1002	2	-	0/0/0/0	0/0/0/0
4	CO3	F	1003	-	-	0/0/0/0	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	HEM	C3B-C4B	-7.85	1.44	1.51
2	A	1001	HEM	C3B-C4B	-7.47	1.45	1.51
2	E	1001	HEM	C3B-C4B	-6.96	1.45	1.51
2	F	1001	HEM	C3B-C4B	-6.88	1.45	1.51
2	D	1001	HEM	C3B-C4B	-6.42	1.46	1.51
2	C	1001	HEM	C3B-C4B	-6.19	1.46	1.51
2	F	1001	HEM	C3D-C4D	-5.88	1.44	1.51
2	E	1001	HEM	C3D-C4D	-5.80	1.44	1.51
2	C	1001	HEM	C3D-C4D	-5.54	1.44	1.51
2	B	1001	HEM	C3D-C4D	-4.89	1.45	1.51
2	D	1001	HEM	C3D-C4D	-4.59	1.45	1.51
2	A	1001	HEM	C3D-C4D	-4.45	1.45	1.51
2	A	1001	HEM	C2C-C1C	-4.13	1.44	1.52
2	D	1001	HEM	C2C-C1C	-3.84	1.45	1.52
2	C	1001	HEM	C2C-C1C	-3.80	1.45	1.52
2	F	1001	HEM	C2C-C1C	-3.70	1.45	1.52
2	B	1001	HEM	C2C-C1C	-3.44	1.46	1.52
2	E	1001	HEM	C2C-C1C	-2.92	1.47	1.52
2	C	1001	HEM	C2B-C1B	-2.36	1.44	1.51
2	D	1001	HEM	C2D-C1D	-2.33	1.44	1.51
2	E	1001	HEM	C2D-C1D	-2.26	1.44	1.51
2	A	1001	HEM	C2B-C1B	-2.21	1.44	1.51
2	E	1001	HEM	C2B-C1B	-2.20	1.44	1.51
2	F	1001	HEM	C2B-C1B	-2.17	1.44	1.51
2	F	1001	HEM	C2D-C1D	-2.13	1.44	1.51
2	D	1001	HEM	C2B-C1B	-2.08	1.45	1.51
2	C	1001	HEM	CAA-C2A	2.02	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	HEM	FE-ND	2.09	2.08	1.97
2	D	1001	HEM	CAA-C2A	2.12	1.55	1.52
2	A	1001	HEM	C3B-CAB	2.13	1.55	1.51
2	A	1001	HEM	C1C-NC	2.13	1.38	1.36
2	D	1001	HEM	C3B-CAB	2.13	1.55	1.51
2	C	1001	HEM	C4C-NC	2.18	1.38	1.36
2	B	1001	HEM	C3B-CAB	2.18	1.55	1.51
2	F	1001	HEM	C3B-CAB	2.20	1.55	1.51
2	C	1001	HEM	C1C-NC	2.20	1.38	1.36
2	E	1001	HEM	C4C-NC	2.22	1.38	1.36
2	C	1001	HEM	C3B-CAB	2.24	1.55	1.51
2	D	1001	HEM	FE-ND	2.27	2.09	1.97
2	C	1001	HEM	FE-NB	2.30	2.09	1.97
2	C	1001	HEM	C3C-CAC	2.34	1.55	1.51
2	B	1001	HEM	C3C-CAC	2.35	1.55	1.51
2	A	1001	HEM	C4C-NC	2.36	1.38	1.36
2	B	1001	HEM	C1C-NC	2.41	1.39	1.36
2	E	1001	HEM	C3C-CAC	2.56	1.56	1.51
2	F	1001	HEM	FE-ND	2.63	2.11	1.97
2	B	1001	HEM	FE-ND	2.69	2.11	1.97
2	B	1001	HEM	FE-NB	2.79	2.12	1.97
2	A	1001	HEM	FE-ND	2.81	2.12	1.97
2	A	1001	HEM	FE-NB	2.84	2.12	1.97
2	C	1001	HEM	FE-ND	2.84	2.12	1.97
2	D	1001	HEM	FE-NC	3.18	2.08	1.95
2	B	1001	HEM	C4C-NC	3.26	1.40	1.36
2	C	1001	HEM	FE-NC	3.58	2.09	1.95
2	B	1001	HEM	FE-NC	3.59	2.09	1.95
2	E	1001	HEM	FE-NC	3.73	2.10	1.95
2	A	1001	HEM	FE-NC	3.80	2.10	1.95
2	F	1001	HEM	FE-NC	4.59	2.13	1.95

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1001	HEM	C3B-CAB-CBB	-5.15	116.56	124.46
2	A	1001	HEM	C3B-CAB-CBB	-5.12	116.61	124.46
2	B	1001	HEM	C3B-CAB-CBB	-3.94	118.42	124.46
2	D	1001	HEM	CAA-C2A-C1A	-3.40	123.32	127.01
2	F	1001	HEM	C3C-CAC-CBC	-3.39	119.26	124.46
2	A	1001	HEM	CAA-CBA-CGA	-3.34	106.63	112.75
2	C	1001	HEM	C3B-CAB-CBB	-3.32	119.36	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	HEM	CBD-CAD-C3D	-3.27	104.04	113.55
2	A	1001	HEM	CBD-CAD-C3D	-3.21	104.20	113.55
2	D	1001	HEM	C3B-CAB-CBB	-3.18	119.57	124.46
2	A	1001	HEM	CMA-C3A-C4A	-3.16	123.14	128.36
2	C	1001	HEM	C3C-CAC-CBC	-3.11	119.69	124.46
2	F	1001	HEM	CAA-CBA-CGA	-3.03	107.20	112.75
2	F	1001	HEM	CBD-CAD-C3D	-3.02	104.77	113.55
2	E	1001	HEM	CBD-CAD-C3D	-3.01	104.78	113.55
2	D	1001	HEM	CMA-C3A-C4A	-2.99	123.42	128.36
2	B	1001	HEM	CMA-C3A-C4A	-2.97	123.46	128.36
2	B	1001	HEM	CBD-CAD-C3D	-2.88	105.17	113.55
2	F	1001	HEM	C3B-CAB-CBB	-2.83	120.11	124.46
2	C	1001	HEM	C3B-C4B-NB	-2.78	106.31	111.63
2	C	1001	HEM	CMA-C3A-C4A	-2.76	123.79	128.36
2	E	1001	HEM	C3B-C4B-NB	-2.66	106.53	111.63
2	D	1001	HEM	CBD-CAD-C3D	-2.55	106.14	113.55
2	B	1001	HEM	C3B-C4B-NB	-2.50	106.85	111.63
2	A	1001	HEM	C3B-C4B-NB	-2.49	106.87	111.63
2	B	1001	HEM	CAA-C2A-C1A	-2.47	124.32	127.01
2	E	1001	HEM	CMA-C3A-C4A	-2.38	124.43	128.36
2	A	1001	HEM	C2C-C1C-NC	-2.37	106.21	110.21
2	A	1001	HEM	CAA-C2A-C1A	-2.35	124.46	127.01
2	C	1001	HEM	CAA-C2A-C1A	-2.33	124.48	127.01
2	D	1001	HEM	CAA-CBA-CGA	-2.31	108.51	112.75
2	E	1001	HEM	CAA-CBA-CGA	-2.29	108.56	112.75
2	F	1001	HEM	C3B-C4B-NB	-2.28	107.28	111.63
2	E	1001	HEM	C2C-C1C-NC	-2.25	106.41	110.21
2	B	1001	HEM	C2C-C1C-NC	-2.22	106.47	110.21
2	C	1001	HEM	CAA-CBA-CGA	-2.13	108.85	112.75
2	D	1001	HEM	C2C-C1C-NC	-2.09	106.69	110.21
2	D	1001	HEM	C3B-C4B-NB	-2.02	107.76	111.63
2	D	1001	HEM	CBA-CAA-C2A	2.07	116.25	112.53
2	D	1001	HEM	C2C-C1C-CHC	2.09	126.87	123.68
2	A	1001	HEM	C2C-C1C-CHC	2.38	127.30	123.68
2	A	1001	HEM	C2D-C3D-C4D	2.41	105.59	101.50
2	B	1001	HEM	C2D-C3D-C4D	2.42	105.60	101.50
2	C	1001	HEM	C2C-C1C-CHC	2.46	127.42	123.68
2	A	1001	HEM	CMD-C2D-C3D	2.47	125.29	114.35
2	F	1001	HEM	C3B-C4B-CHC	2.52	126.72	123.16
2	C	1001	HEM	CMD-C2D-C3D	2.54	125.57	114.35
2	D	1001	HEM	C3B-C4B-CHC	2.58	126.80	123.16
2	C	1001	HEM	C2D-C3D-C4D	2.62	105.94	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	HEM	C3B-C4B-CHC	2.63	126.87	123.16
2	D	1001	HEM	C2D-C3D-C4D	2.72	106.11	101.50
2	F	1001	HEM	C2C-C1C-CHC	2.73	127.83	123.68
2	B	1001	HEM	CMD-C2D-C3D	2.81	126.77	114.35
2	F	1001	HEM	C2D-C3D-C4D	2.84	106.32	101.50
2	B	1001	HEM	C3B-C4B-CHC	2.86	127.20	123.16
2	B	1001	HEM	C2C-C1C-CHC	2.89	128.07	123.68
2	E	1001	HEM	C2D-C3D-C4D	2.91	106.44	101.50
2	E	1001	HEM	CMD-C2D-C3D	2.92	127.28	114.35
2	D	1001	HEM	CMD-C2D-C3D	2.96	127.45	114.35
2	F	1001	HEM	CMD-C2D-C3D	2.98	127.52	114.35
2	E	1001	HEM	C2C-C1C-CHC	3.00	128.25	123.68
2	A	1001	HEM	C3B-C4B-CHC	3.06	127.47	123.16
2	E	1001	HEM	C3B-C4B-CHC	3.30	127.81	123.16
2	F	1001	HEM	CAD-C3D-C4D	3.57	125.06	112.47
2	B	1001	HEM	CMC-C2C-C3C	3.73	125.85	116.53
2	B	1001	HEM	CMB-C2B-C3B	3.78	125.98	116.53
2	C	1001	HEM	CMC-C2C-C3C	3.84	126.12	116.53
2	B	1001	HEM	CAD-C3D-C4D	3.92	126.30	112.47
2	C	1001	HEM	CAD-C3D-C4D	3.93	126.33	112.47
2	E	1001	HEM	CAD-C3D-C4D	3.94	126.36	112.47
2	A	1001	HEM	CMB-C2B-C3B	3.95	126.39	116.53
2	F	1001	HEM	CMC-C2C-C3C	4.06	126.66	116.53
2	E	1001	HEM	CMC-C2C-C3C	4.26	127.18	116.53
2	A	1001	HEM	CMC-C2C-C3C	4.30	127.26	116.53
2	D	1001	HEM	CAD-C3D-C4D	4.31	127.66	112.47
2	E	1001	HEM	CMB-C2B-C3B	4.43	127.59	116.53
2	A	1001	HEM	CAD-C3D-C2D	4.45	126.00	113.22
2	A	1001	HEM	CAD-C3D-C4D	4.51	128.36	112.47
2	D	1001	HEM	CAD-C3D-C2D	4.52	126.21	113.22
2	F	1001	HEM	CMB-C2B-C3B	4.56	127.90	116.53
2	D	1001	HEM	CMC-C2C-C3C	4.60	128.02	116.53
2	C	1001	HEM	CMB-C2B-C3B	4.67	128.19	116.53
2	D	1001	HEM	CMB-C2B-C3B	4.80	128.52	116.53
2	E	1001	HEM	CAD-C3D-C2D	4.86	127.18	113.22
2	C	1001	HEM	CAD-C3D-C2D	5.04	127.72	113.22
2	B	1001	HEM	CAD-C3D-C2D	5.18	128.10	113.22
2	F	1001	HEM	CAD-C3D-C2D	5.35	128.60	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	HEM	1	0
2	B	1001	HEM	1	0
2	C	1001	HEM	1	0
2	D	1001	HEM	1	0
2	F	1001	HEM	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	228/251 (90%)	0.02	7 (3%) 52 61	15, 24, 44, 53	0
1	B	230/251 (91%)	0.09	6 (2%) 59 66	15, 24, 44, 53	0
1	C	228/251 (90%)	0.16	11 (4%) 34 43	15, 25, 44, 53	0
1	D	230/251 (91%)	0.24	23 (10%) 9 13	15, 25, 44, 53	0
1	E	230/251 (91%)	0.17	8 (3%) 48 57	15, 24, 44, 52	0
1	F	229/251 (91%)	0.43	22 (9%) 10 14	15, 24, 44, 53	0
All	All	1375/1506 (91%)	0.19	77 (5%) 28 36	15, 24, 45, 53	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	153	ALA	6.2
1	F	133	SER	6.1
1	D	39	MET	5.9
1	C	39	MET	5.1
1	F	157	ASN	5.1
1	A	157	ASN	4.9
1	D	133	SER	4.7
1	F	248	ASP	4.5
1	D	153	ALA	4.4
1	D	38	ALA	4.3
1	D	248	ASP	4.2
1	E	134	ALA	4.2
1	F	134	ALA	4.0
1	F	129	ALA	4.0
1	D	156	TRP	3.9
1	F	126	GLY	3.9
1	B	39	MET	3.9
1	C	32	ASP	3.9
1	F	122	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	248	ASP	3.7
1	C	35	LYS	3.7
1	F	127	LEU	3.7
1	F	130	GLY	3.6
1	D	157	ASN	3.6
1	D	217	GLN	3.6
1	F	217	GLN	3.5
1	F	38	ALA	3.5
1	F	125	PRO	3.4
1	D	125	PRO	3.4
1	E	154	GLU	3.4
1	F	154	GLU	3.4
1	E	248	ASP	3.3
1	B	248	ASP	3.3
1	C	57	ASP	3.1
1	D	169	VAL	3.1
1	D	129	ALA	3.1
1	D	132	SER	3.0
1	D	126	GLY	3.0
1	D	130	GLY	3.0
1	A	154	GLU	3.0
1	D	124	SER	2.9
1	C	53	GLU	2.8
1	E	138	GLY	2.8
1	D	42	LYS	2.8
1	F	39	MET	2.8
1	E	157	ASN	2.8
1	C	157	ASN	2.7
1	E	217	GLN	2.7
1	F	229	SER	2.7
1	C	154	GLU	2.7
1	C	56	LYS	2.6
1	D	35	LYS	2.6
1	A	35	LYS	2.6
1	C	121	LYS	2.6
1	F	152	ASN	2.5
1	D	122	ASP	2.5
1	A	248	ASP	2.5
1	A	39	MET	2.5
1	E	53	GLU	2.4
1	B	157	ASN	2.4
1	F	121	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	56	LYS	2.3
1	B	32	ASP	2.3
1	F	32	ASP	2.3
1	A	32	ASP	2.3
1	C	135	THR	2.2
1	B	228	GLY	2.2
1	D	134	ALA	2.1
1	F	42	LYS	2.1
1	E	42	LYS	2.1
1	A	153	ALA	2.1
1	F	165	LYS	2.1
1	D	53	GLU	2.1
1	B	42	LYS	2.0
1	F	124	SER	2.0
1	D	154	GLU	2.0
1	D	40	GLU	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	CO3	A	1003	4/4	0.78	0.17	2.77	38,38,39,40	0
4	CO3	F	1003	4/4	0.85	0.14	1.34	48,49,49,49	0
4	CO3	C	1003	4/4	0.81	0.17	1.05	40,41,41,42	0
4	CO3	E	1003	4/4	0.88	0.15	0.76	33,35,35,35	0
4	CO3	B	1003	4/4	0.86	0.12	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SCN	C	1002	3/3	0.96	0.10	-0.06	20,20,20,22	0
2	HEM	D	1001	43/43	0.97	0.10	-0.30	20,24,26,28	0
2	HEM	F	1001	43/43	0.97	0.10	-0.56	23,25,28,30	0
2	HEM	C	1001	43/43	0.97	0.10	-0.74	17,19,21,23	0
2	HEM	A	1001	43/43	0.97	0.09	-0.75	14,17,20,22	0
2	HEM	E	1001	43/43	0.98	0.10	-1.01	14,17,20,22	0
3	SCN	D	1002	3/3	0.96	0.08	-1.18	18,18,18,20	0
3	SCN	F	1002	3/3	0.98	0.09	-1.29	21,21,22,22	0
2	HEM	B	1001	43/43	0.99	0.09	-1.66	15,18,24,25	0
3	SCN	B	1002	3/3	0.98	0.09	-1.86	18,18,19,20	0
3	SCN	A	1002	3/3	0.96	0.07	-3.04	19,19,20,22	0
3	SCN	E	1002	3/3	0.99	0.09	-3.30	16,16,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.