Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:42 PM GMT

PDB ID	:	5A13
Title	:	Crystal structure of Chlorite Dismutase from Magnetospirillum sp. in complex with thiocyanate
Authors	:	Correia, H.D.; Santos-Silva, T.
Deposited on	:	2015-04-27
Resolution	:	1.75 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:

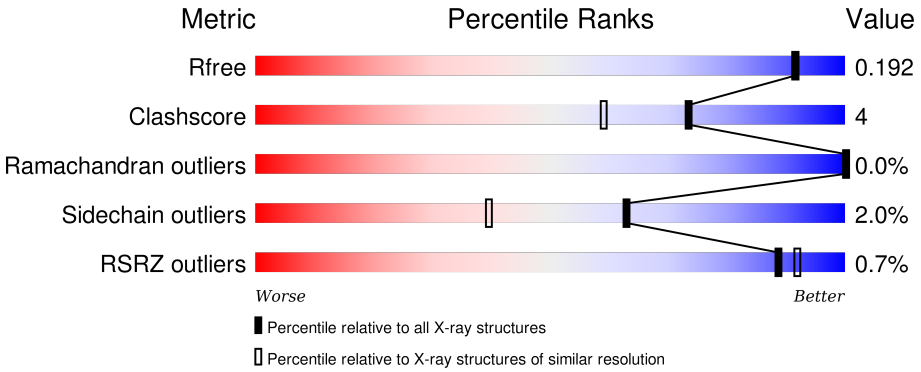
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	245	89% 9%
1	B	245	92% 7%
1	C	245	91% 7%
1	D	245	92% 5%
1	E	245	90% 8%

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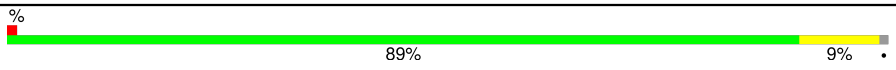
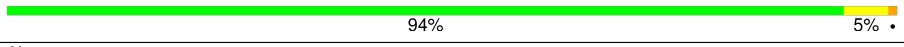
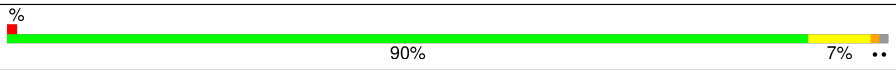
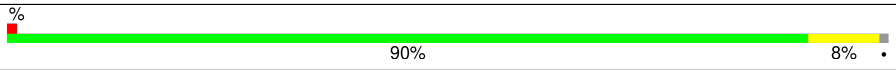
Mol	Chain	Length	Quality of chain
1	F	245	
1	G	245	
1	H	245	
1	I	245	
1	J	245	

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	SCN	C	251	-	-	X	-
4	GOL	A	252	-	-	-	X
4	GOL	B	252	-	-	-	X
4	GOL	C	252	-	-	-	X
4	GOL	C	253	-	-	-	X
4	GOL	D	253	-	-	-	X
4	GOL	E	252	-	-	-	X
4	GOL	F	252	-	-	-	X

2 Entry composition (i)

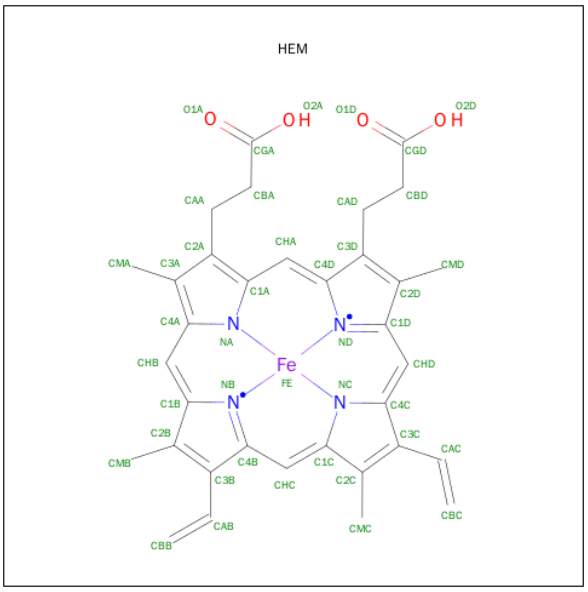
There are 5 unique types of molecules in this entry. The entry contains 21916 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

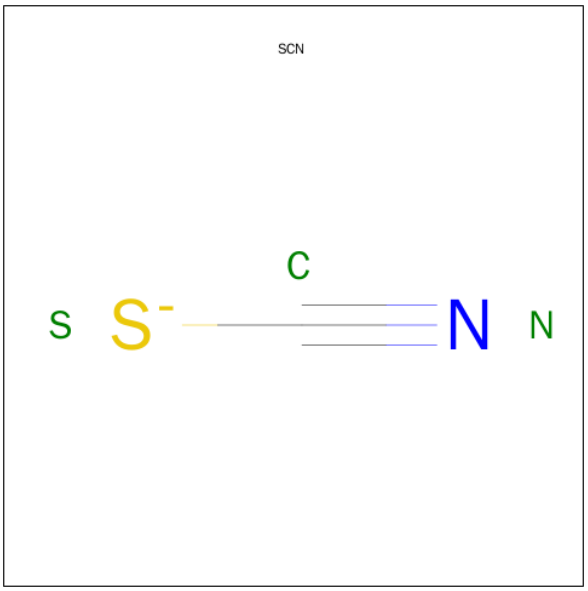
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	7	0
			1926	1231	329	357	9			
1	B	245	Total	C	N	O	S	0	9	0
			1961	1252	336	364	9			
1	C	242	Total	C	N	O	S	0	8	0
			1935	1235	333	359	8			
1	D	242	Total	C	N	O	S	0	4	0
			1910	1216	326	361	7			
1	E	242	Total	C	N	O	S	0	11	0
			1949	1244	335	362	8			
1	F	242	Total	C	N	O	S	0	6	0
			1918	1224	326	360	8			
1	G	245	Total	C	N	O	S	0	9	0
			1959	1249	335	366	9			
1	H	242	Total	C	N	O	S	0	3	0
			1905	1214	327	357	7			
1	I	242	Total	C	N	O	S	0	5	0
			1917	1222	329	359	7			
1	J	242	Total	C	N	O	S	0	3	0
			1909	1215	329	358	7			

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



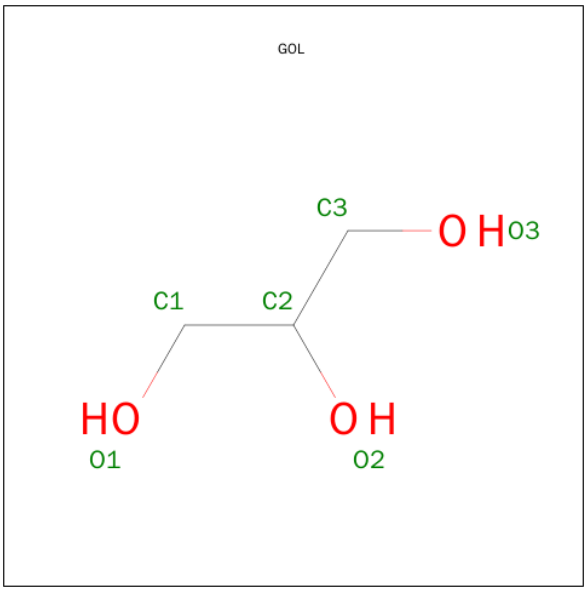
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	J	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
3	G	1	Total C N S 3 1 1 1	0	0
3	H	1	Total C N S 3 1 1 1	0	0
3	I	1	Total C N S 3 1 1 1	0	0
3	J	1	Total C N S 3 1 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

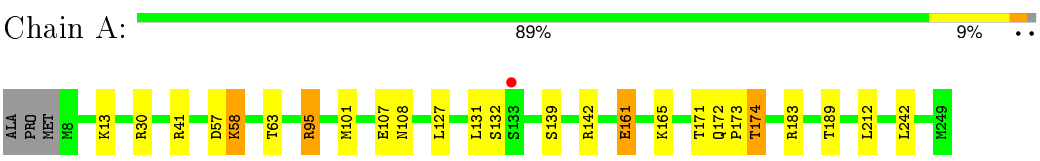
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	230	Total O 230 230	0	0
5	B	233	Total O 233 233	0	0
5	C	239	Total O 239 239	0	0
5	D	156	Total O 156 156	0	0
5	E	199	Total O 199 199	0	0
5	F	246	Total O 246 246	0	0
5	G	229	Total O 229 229	0	0
5	H	202	Total O 202 202	0	0
5	I	174	Total O 174 174	0	0
5	J	175	Total O 175 175	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.

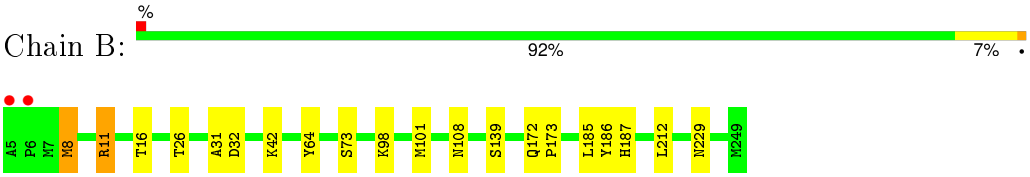
- Molecule 1: CHLORITE DISMUTASE

Chain A:



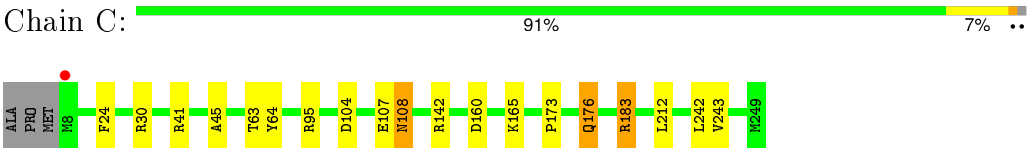
- Molecule 1: CHLORITE DISMUTASE

Chain B:



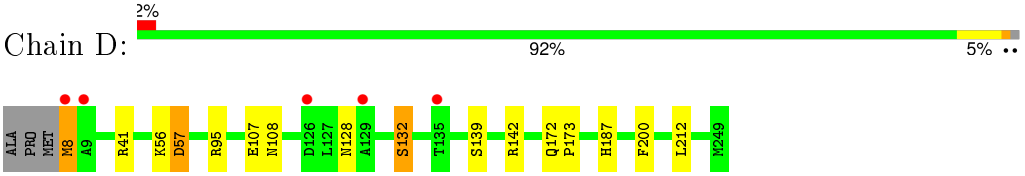
- Molecule 1: CHLORITE DISMUTASE

Chain C:



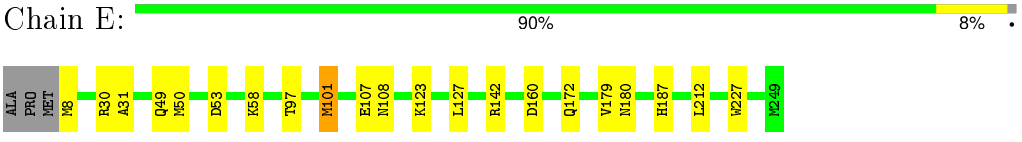
- Molecule 1: CHLORITE DISMUTASE

Chain D:



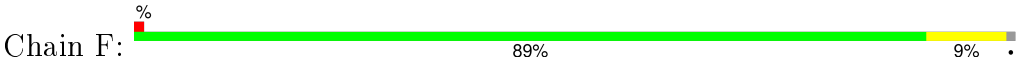
- Molecule 1: CHLORITE DISMUTASE

Chain E:



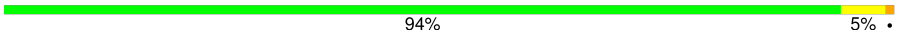
- Molecule 1: CHLORITE DISMUTASE

Chain F:



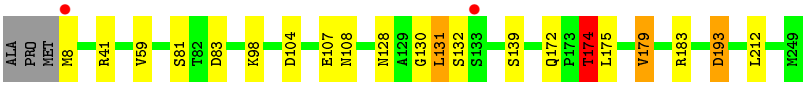
• Molecule 1: CHLORITE DISMUTASE

Chain G:



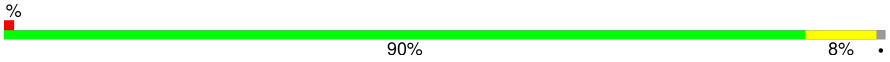
• Molecule 1: CHLORITE DISMUTASE

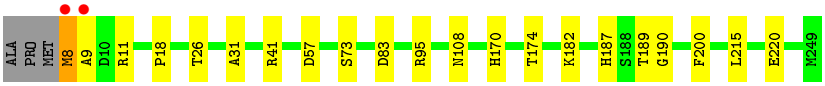
Chain H:



• Molecule 1: CHLORITE DISMUTASE

Chain I:





• Molecule 1: CHLORITE DISMUTASE

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.03Å 124.48Å 133.38Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	49.11 – 1.75 48.37 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.11-1.75) 99.7 (48.37-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.151 , 0.183 0.164 , 0.192	Depositor DCC
R_{free} test set	12628 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.8	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 261115 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21916	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 62.38 % 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 1.1362e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, SCN, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.89	2/1985 (0.1%)	0.94	6/2694 (0.2%)
1	B	0.82	0/2027	0.90	6/2753 (0.2%)
1	C	0.83	1/1997 (0.1%)	0.89	5/2709 (0.2%)
1	D	0.86	1/1960 (0.1%)	0.91	3/2662 (0.1%)
1	E	0.85	1/2020 (0.0%)	0.91	3/2742 (0.1%)
1	F	0.82	1/1974 (0.1%)	0.90	5/2680 (0.2%)
1	G	0.80	0/2025	0.89	2/2750 (0.1%)
1	H	0.90	1/1952 (0.1%)	0.96	7/2650 (0.3%)
1	I	0.82	0/1970	0.90	2/2675 (0.1%)
1	J	0.85	1/1953 (0.1%)	0.91	5/2651 (0.2%)
All	All	0.84	8/19863 (0.0%)	0.91	44/26966 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	F	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	107	GLU	CD-OE1	8.25	1.34	1.25
1	C	107	GLU	CD-OE1	7.12	1.33	1.25
1	A	107	GLU	CD-OE1	6.86	1.33	1.25
1	A	161	GLU	CD-OE2	6.16	1.32	1.25
1	F	107	GLU	CD-OE1	6.05	1.32	1.25
1	D	107	GLU	CD-OE1	6.00	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	107	GLU	CD-OE1	5.44	1.31	1.25
1	E	107	GLU	CD-OE1	5.04	1.31	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	142	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	D	142	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	H	41	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	41	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	F	10	ASP	CB-CG-OD1	6.95	124.56	118.30
1	J	78	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	142	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	H	41	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	G	41	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	I	83	ASP	CB-CG-OD1	6.55	124.20	118.30
1	J	78	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	41	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	E	160	ASP	CB-CG-OD1	5.85	123.56	118.30
1	H	174	THR	N-CA-CB	-5.83	99.22	110.30
1	F	10	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	I	41	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	8	MET	CA-CB-CG	5.68	122.95	113.30
1	H	104	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	142	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	41	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	160	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	101	MET	CG-SD-CE	5.57	109.10	100.20
1	F	152	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	41	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	32	ASP	CB-CG-OD1	5.47	123.22	118.30
1	H	193	ASP	CB-CG-OD1	5.47	123.22	118.30
1	G	10	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	J	164	LEU	CB-CG-CD1	5.37	120.13	111.00
1	B	11[A]	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	11[B]	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	160	ASP	CB-CG-OD1	5.30	123.07	118.30
1	F	83	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	95[A]	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	95[B]	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	131	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	32	ASP	CB-CG-OD2	-5.19	113.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	101[A]	MET	CG-SD-CE	-5.18	91.91	100.20
1	E	101[B]	MET	CG-SD-CE	-5.18	91.91	100.20
1	D	41	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	F	163	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	H	179	VAL	CB-CA-C	-5.11	101.69	111.40
1	J	10	ASP	CB-CG-OD1	5.10	122.89	118.30
1	J	41	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	H	83	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	8	MET	Peptide
1	F	133	SER	Peptide

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	1926	0	1971	24	0
1	B	1961	0	2008	16	0
1	C	1935	0	1981	21	0
1	D	1910	0	1930	9	0
1	E	1949	0	2000	30	0
1	F	1918	0	1951	14	0
1	G	1959	0	2000	10	0
1	H	1905	0	1933	17	0
1	I	1917	0	1948	16	0
1	J	1909	0	1933	12	0
2	A	43	0	30	12	0
2	B	43	0	30	2	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
2	E	43	0	30	4	0
2	F	43	0	30	1	0
2	G	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	43	0	30	10	0
2	I	43	0	30	1	0
2	J	43	0	30	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	2	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	2	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	12	0	16	0	0
4	I	12	0	16	0	0
4	J	6	0	8	0	0
5	A	230	0	0	3	0
5	B	233	0	0	4	0
5	C	239	0	0	8	0
5	D	156	0	0	3	0
5	E	199	0	0	6	0
5	F	246	0	0	3	0
5	G	229	0	0	3	0
5	H	202	0	0	3	0
5	I	174	0	0	3	0
5	J	175	0	0	4	0
All	All	21916	0	20067	164	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 4.

All (164) 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:50:MET:HG3	5:E:2033:HOH:O	1.47	1.12
1:C:45:ALA:HA	1:C:243[B]:VAL:HG21	1.43	0.99
1:I:8:MET:HB2	1:I:9:ALA:HA	1.43	0.98
1:J:49:GLN:NE2	1:J:53:ASP:OD2	1.98	0.97
1:E:212[B]:LEU:HD11	1:E:227:TRP:CH2	2.02	0.94
1:A:174:THR:HG23	2:A:250:HEM:CMB	1.97	0.93
1:E:212[B]:LEU:CD1	1:E:227:TRP:CH2	2.52	0.92
1:H:174:THR:HG23	2:H:250:HEM:HMB1	1.53	0.88
1:A:189:THR:HG22	1:E:212[B]:LEU:HD12	1.59	0.84
1:A:174:THR:CG2	2:A:250:HEM:CMB	2.55	0.84
1:A:174:THR:HG23	2:A:250:HEM:C2B	2.13	0.84
1:H:174:THR:HG23	2:H:250:HEM:CMB	2.08	0.84
5:F:2089:HOH:O	1:I:95[B]:ARG:NH2	2.06	0.83
1:C:183[B]:ARG:NH1	3:C:251:SCN:N	2.26	0.83
1:A:174:THR:HG23	2:A:250:HEM:HMB1	1.61	0.82
1:B:229[B]:ASN:OD1	5:B:2217:HOH:O	1.98	0.81
1:H:174:THR:CG2	2:H:250:HEM:CMB	2.62	0.78
1:A:174:THR:CG2	2:A:250:HEM:C2B	2.68	0.76
1:D:212:LEU:HD11	2:D:250:HEM:HBC2	1.67	0.74
1:E:212[B]:LEU:HD21	2:E:250:HEM:HBC2	1.68	0.73
1:D:56:LYS:HE2	5:D:2044:HOH:O	1.89	0.72
1:A:127:LEU:HD21	1:A:172:GLN:NE2	2.04	0.72
1:B:16:THR:O	4:B:252:GOL:H31	1.90	0.70
1:G:212:LEU:HD11	2:G:250:HEM:HBC2	1.76	0.67
1:J:229:ASN:HB3	5:J:2167:HOH:O	1.95	0.66
1:J:95[A]:ARG:NH2	5:J:2064:HOH:O	2.29	0.63
1:E:97:THR:O	1:E:101[A]:MET:HG3	1.98	0.63
1:I:170:HIS:HD2	1:I:220:GLU:OE1	1.81	0.63
1:A:95[B]:ARG:NH2	5:A:2102:HOH:O	2.31	0.62
1:C:165[B]:LYS:HG3	5:C:2171:HOH:O	2.00	0.61
1:B:11[B]:ARG:NH2	5:B:2009:HOH:O	2.27	0.61
1:G:187:HIS:HD2	5:G:2178:HOH:O	1.83	0.61
5:C:2030:HOH:O	1:E:30[B]:ARG:NH1	2.22	0.60
1:E:49[B]:GLN:NE2	1:E:53:ASP:OD2	2.34	0.60
1:A:161:GLU:O	1:A:165:LYS:HD3	2.01	0.60
1:E:212[B]:LEU:HD13	1:E:227:TRP:CH2	2.36	0.60
1:B:212:LEU:HD11	2:B:250:HEM:HBC2	1.83	0.60
5:G:2216:HOH:O	1:H:193:ASP:OD2	2.15	0.60
5:H:2084:HOH:O	1:J:187:HIS:HD2	1.83	0.59
1:A:189:THR:CG2	1:E:212[B]:LEU:HD12	2.30	0.59
1:D:95[A]:ARG:NH2	5:D:2075:HOH:O	2.15	0.59
1:C:45:ALA:CA	1:C:243[B]:VAL:HG21	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:CD1	2:B:250:HEM:HBC2	2.33	0.59
1:A:212:LEU:HD11	2:A:250:HEM:HBC2	1.83	0.59
1:E:179:VAL:HG23	1:E:180[B]:ASN:ND2	2.18	0.59
1:C:176:GLN:HG2	5:C:2178:HOH:O	2.02	0.58
1:E:212[B]:LEU:HD11	1:E:227:TRP:CZ2	2.38	0.57
1:C:183[B]:ARG:NH1	2:C:250:HEM:C1B	2.72	0.57
1:B:185[B]:LEU:HD22	1:B:187:HIS:NE2	2.18	0.57
1:I:8:MET:SD	1:I:8:MET:N	2.77	0.57
1:H:174:THR:CG2	2:H:250:HEM:C2B	2.87	0.57
1:F:212[B]:LEU:HG	1:I:190:GLY:HA2	1.87	0.57
1:A:174:THR:CG2	2:A:250:HEM:HMB2	2.34	0.56
1:E:212[A]:LEU:HD11	2:E:250:HEM:HBC2	1.86	0.56
1:F:212[B]:LEU:HD12	1:F:227:TRP:CH2	2.39	0.56
1:C:95[A]:ARG:NH2	5:C:2025:HOH:O	2.35	0.56
1:E:142[A]:ARG:HD2	5:E:2103:HOH:O	2.06	0.55
1:H:212:LEU:HD11	2:H:250:HEM:HBC2	1.88	0.55
1:F:212[B]:LEU:HG	1:I:190:GLY:CA	2.36	0.55
5:F:2103:HOH:O	1:I:187:HIS:HD2	1.89	0.55
5:C:2100:HOH:O	1:E:187:HIS:HD2	1.90	0.54
1:I:57:ASP:HB3	5:I:2001:HOH:O	2.07	0.54
1:D:187:HIS:HD2	5:D:2131:HOH:O	1.90	0.53
1:F:212[B]:LEU:CD1	1:F:227:TRP:CH2	2.91	0.53
1:A:174:THR:HG21	2:A:250:HEM:C2B	2.41	0.52
1:J:229:ASN:CB	5:J:2167:HOH:O	2.55	0.52
1:G:46:ALA:O	1:G:50:MET:HG3	2.08	0.52
2:J:250:HEM:HBC2	2:J:250:HEM:HHD	1.92	0.52
1:H:183:ARG:HD3	5:H:2157:HOH:O	2.09	0.52
1:C:45:ALA:HB2	1:C:243[B]:VAL:HG23	1.91	0.52
1:I:8:MET:HB2	1:I:9:ALA:CA	2.28	0.52
1:C:183[B]:ARG:NH2	5:C:2188:HOH:O	2.20	0.52
1:D:212:LEU:CD1	2:D:250:HEM:HBC2	2.40	0.51
1:H:128:ASN:HA	1:H:131:LEU:HD13	1.93	0.51
1:H:174:THR:HG23	2:H:250:HEM:C2B	2.45	0.51
1:G:212:LEU:CD1	2:G:250:HEM:HBC2	2.41	0.51
1:D:128:ASN:O	1:D:132:SER:OG	2.29	0.51
1:C:173:PRO:O	1:C:176:GLN:HG3	2.11	0.51
1:B:185[B]:LEU:HD23	1:B:186:TYR:N	2.25	0.51
1:A:101[B]:MET:HG2	5:A:2100:HOH:O	2.10	0.50
1:B:31:ALA:HB1	1:C:30[B]:ARG:NH2	2.27	0.50
1:H:174:THR:HG21	2:H:250:HEM:C2B	2.47	0.50
1:G:63:THR:HB	1:G:242:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD11	2:A:250:HEM:CBC	2.41	0.49
1:C:45:ALA:HA	1:C:243[B]:VAL:CG2	2.29	0.49
1:D:8:MET:N	1:D:57[B]:ASP:OD1	2.46	0.49
1:B:11[B]:ARG:NE	5:B:2009:HOH:O	2.17	0.49
1:B:172[B]:GLN:HB3	1:B:173:PRO:HD3	1.94	0.49
1:C:212:LEU:HD11	2:C:250:HEM:HBC2	1.95	0.49
1:A:63:THR:HB	1:A:242:LEU:HD22	1.94	0.48
1:H:174:THR:HG21	2:H:250:HEM:CMB	2.41	0.48
1:D:172:GLN:HB3	1:D:173:PRO:HD3	1.95	0.48
1:B:172[A]:GLN:HB2	1:B:173:PRO:HD3	1.96	0.48
1:H:172:GLN:HG2	5:H:2150:HOH:O	2.12	0.48
1:E:123:LYS:HE3	5:E:2085:HOH:O	2.12	0.48
1:C:63:THR:HB	1:C:242:LEU:HD22	1.95	0.48
1:E:212[B]:LEU:CD2	2:E:250:HEM:HBC2	2.43	0.47
1:C:212:LEU:CD1	2:C:250:HEM:HBC2	2.45	0.47
1:G:212:LEU:HD11	2:G:250:HEM:CBC	2.44	0.47
1:J:59:VAL:HG12	1:J:81:SER:HB2	1.97	0.47
1:E:58:LYS:NZ	5:E:2040:HOH:O	2.48	0.47
1:G:30[B]:ARG:CZ	1:I:31:ALA:HB1	2.45	0.47
1:F:119:ILE:O	1:F:119:ILE:HG22	2.15	0.47
1:E:30[B]:ARG:CG	5:E:2021:HOH:O	2.62	0.46
1:E:30[B]:ARG:HG2	5:E:2021:HOH:O	2.15	0.46
1:H:59:VAL:HG12	1:H:81:SER:HB2	1.98	0.46
1:G:24:PHE:O	1:G:108:ASN:HA	2.15	0.46
1:H:212:LEU:CD1	2:H:250:HEM:HBC2	2.45	0.45
1:F:11:ARG:HD3	5:F:2009:HOH:O	2.16	0.45
1:J:98:LYS:HD3	1:J:98:LYS:HA	1.79	0.45
1:E:49[A]:GLN:NE2	1:E:53:ASP:OD1	2.48	0.45
1:J:8:MET:HA	1:J:57:ASP:HA	1.99	0.45
1:H:130:GLY:C	1:H:132:SER:H	2.20	0.45
1:H:174:THR:HG22	1:H:175:LEU:N	2.32	0.44
1:B:16:THR:O	4:B:252:GOL:C3	2.63	0.44
1:C:183[B]:ARG:NH1	2:C:250:HEM:CHB	2.81	0.44
1:F:26:THR:HB	1:F:73:SER:CB	2.47	0.44
1:C:45:ALA:CB	1:C:243[B]:VAL:CG2	2.96	0.44
1:H:174:THR:CG2	2:H:250:HEM:HMB2	2.44	0.44
2:I:250:HEM:HBC2	2:I:250:HEM:HHD	2.00	0.44
1:F:212[B]:LEU:HD13	1:F:212[B]:LEU:HA	1.70	0.43
1:A:183:ARG:HD2	2:A:250:HEM:C3B	2.52	0.43
1:C:104:ASP:OD1	5:C:2029:HOH:O	2.21	0.43
1:E:127:LEU:HD21	1:E:172[A]:GLN:NE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95[A]:ARG:NH2	5:A:2023:HOH:O	2.46	0.43
1:F:189:THR:HG22	1:J:212:LEU:HB3	2.00	0.43
1:F:63:THR:HB	1:F:242:LEU:HD22	2.01	0.43
1:A:171:THR:O	1:A:174:THR:HB	2.18	0.43
1:C:183[B]:ARG:NH1	2:C:250:HEM:C4A	2.87	0.43
1:F:46:ALA:O	1:F:50:MET:HG3	2.19	0.43
1:B:185[B]:LEU:CD2	1:B:187:HIS:NE2	2.81	0.43
1:A:13:LYS:HA	1:A:13:LYS:HE2	2.01	0.43
1:I:11:ARG:HD3	5:I:2006:HOH:O	2.18	0.43
5:C:2033:HOH:O	1:E:30[B]:ARG:NH1	2.37	0.43
1:E:127:LEU:HD21	1:E:172[A]:GLN:HE21	1.83	0.43
1:F:212[B]:LEU:HB3	1:I:189:THR:HG22	2.00	0.42
1:I:95[A]:ARG:NH2	5:I:2073:HOH:O	2.50	0.42
1:I:26:THR:HB	1:I:73:SER:CB	2.49	0.42
2:F:250:HEM:HHD	2:F:250:HEM:HBC2	2.02	0.42
1:J:16[B]:THR:O	1:J:16[B]:THR:HG22	2.19	0.42
2:A:250:HEM:CMC	2:A:250:HEM:HBC2	2.50	0.42
1:A:30[A]:ARG:NH2	1:E:31:ALA:HB1	2.34	0.42
1:C:24:PHE:O	1:C:108:ASN:HA	2.20	0.42
1:G:139:SER:HB2	5:G:2136:HOH:O	2.19	0.42
1:A:57:ASP:CG	1:A:58:LYS:HD2	2.40	0.42
2:A:250:HEM:HBB2	2:A:250:HEM:HHC	2.02	0.42
1:E:212[B]:LEU:HD22	1:E:212[B]:LEU:HA	1.46	0.41
1:F:130:GLY:O	1:F:133:SER:HB3	2.20	0.41
1:A:30[A]:ARG:CZ	1:E:31:ALA:HB1	2.50	0.41
1:J:229:ASN:ND2	5:J:2163:HOH:O	2.48	0.41
1:G:200:PHE:CZ	2:G:250:HEM:C2C	3.09	0.41
1:B:11[B]:ARG:CZ	5:B:2009:HOH:O	2.57	0.41
1:B:26:THR:HB	1:B:73:SER:CB	2.50	0.41
1:I:182:LYS:O	1:I:200:PHE:HA	2.20	0.41
1:E:212[B]:LEU:HD13	1:E:227:TRP:HH2	1.84	0.41
1:E:212[B]:LEU:HD21	2:E:250:HEM:CBC	2.45	0.41
1:C:183[B]:ARG:NH1	3:C:251:SCN:C	2.82	0.41
1:J:200:PHE:CZ	2:J:250:HEM:C2C	3.09	0.41
1:I:174:THR:HG21	1:I:215:LEU:HD21	2.03	0.41
1:D:200:PHE:CZ	2:D:250:HEM:C2C	3.09	0.40
1:A:172:GLN:CB	1:A:173:PRO:CD	2.99	0.40
1:F:134:ALA:O	1:F:135:THR:HG22	2.21	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	247/245 (101%)	244 (99%)	3 (1%)	0	100	100
1	B	252/245 (103%)	247 (98%)	5 (2%)	0	100	100
1	C	248/245 (101%)	243 (98%)	5 (2%)	0	100	100
1	D	244/245 (100%)	240 (98%)	4 (2%)	0	100	100
1	E	251/245 (102%)	248 (99%)	3 (1%)	0	100	100
1	F	246/245 (100%)	241 (98%)	5 (2%)	0	100	100
1	G	252/245 (103%)	249 (99%)	3 (1%)	0	100	100
1	H	243/245 (99%)	237 (98%)	5 (2%)	1 (0%)	39	19
1	I	245/245 (100%)	239 (98%)	6 (2%)	0	100	100
1	J	243/245 (99%)	239 (98%)	4 (2%)	0	100	100
All	All	2471/2450 (101%)	2427 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	131	LEU

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	208/203 (102%)	203 (98%)	5 (2%)	57	31
1	B	212/203 (104%)	206 (97%)	6 (3%)	51	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	209/203 (103%)	204 (98%)	5 (2%)	57 31
1	D	205/203 (101%)	200 (98%)	5 (2%)	57 31
1	E	212/203 (104%)	210 (99%)	2 (1%)	84 72
1	F	207/203 (102%)	202 (98%)	5 (2%)	57 31
1	G	212/203 (104%)	209 (99%)	3 (1%)	74 58
1	H	204/203 (100%)	198 (97%)	6 (3%)	50 24
1	I	206/203 (102%)	203 (98%)	3 (2%)	72 55
1	J	204/203 (100%)	201 (98%)	3 (2%)	72 55
All	All	2079/2030 (102%)	2036 (98%)	43 (2%)	63 37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	108	ASN
1	A	132	SER
1	A	139	SER
1	A	174	THR
1	B	8	MET
1	B	42	LYS
1	B	64	TYR
1	B	98	LYS
1	B	108	ASN
1	B	139	SER
1	C	64	TYR
1	C	108	ASN
1	C	176	GLN
1	C	183[A]	ARG
1	C	183[B]	ARG
1	D	57[A]	ASP
1	D	57[B]	ASP
1	D	108	ASN
1	D	132	SER
1	D	139	SER
1	E	8	MET
1	E	108	ASN
1	F	108	ASN
1	F	132	SER
1	F	133	SER

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Mol	Chain	Res	Type
1	F	135	THR
1	F	139	SER
1	G	56	LYS
1	G	108	ASN
1	G	139	SER
1	H	8	MET
1	H	98	LYS
1	H	108	ASN
1	H	139	SER
1	H	174	THR
1	H	179	VAL
1	I	8	MET
1	I	18	PRO
1	I	108	ASN
1	J	8	MET
1	J	98	LYS
1	J	108	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	C	176	GLN
1	D	49	GLN
1	D	187	HIS
1	E	187	HIS
1	G	49	GLN
1	G	187	HIS
1	I	170	HIS
1	I	187	HIS
1	J	117	ASN
1	J	187	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

34 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	250	1,3	24,50,50	1.24	3 (12%)	16,82,82	2.20	5 (31%)
3	SCN	A	251	2	2,2,2	1.24	0	1,1,1	0.06	0
4	GOL	A	252	-	5,5,5	0.33	0	5,5,5	0.33	0
2	HEM	B	250	1,3	24,50,50	0.92	1 (4%)	16,82,82	1.77	3 (18%)
3	SCN	B	251	2	2,2,2	1.34	0	1,1,1	0.02	0
4	GOL	B	252	-	5,5,5	0.59	0	5,5,5	1.29	1 (20%)
2	HEM	C	250	1,3	24,50,50	0.85	1 (4%)	16,82,82	1.03	2 (12%)
3	SCN	C	251	2	2,2,2	1.66	1 (50%)	1,1,1	0.17	0
4	GOL	C	252	-	5,5,5	0.40	0	5,5,5	0.49	0
4	GOL	C	253	-	5,5,5	0.25	0	5,5,5	0.50	0
2	HEM	D	250	1,3	24,50,50	0.91	1 (4%)	16,82,82	2.17	5 (31%)
3	SCN	D	251	2	2,2,2	1.22	0	1,1,1	0.36	0
4	GOL	D	252	-	5,5,5	0.30	0	5,5,5	0.74	0
4	GOL	D	253	-	5,5,5	0.32	0	5,5,5	0.82	0
2	HEM	E	250	1,3	24,50,50	1.01	2 (8%)	16,82,82	1.96	5 (31%)
3	SCN	E	251	2	2,2,2	1.25	0	1,1,1	0.10	0
4	GOL	E	252	-	5,5,5	0.35	0	5,5,5	0.27	0
2	HEM	F	250	1,3	24,50,50	1.08	2 (8%)	16,82,82	1.66	5 (31%)
3	SCN	F	251	2	2,2,2	1.80	1 (50%)	1,1,1	0.19	0
4	GOL	F	252	-	5,5,5	0.29	0	5,5,5	0.66	0
2	HEM	G	250	1,3	24,50,50	0.89	1 (4%)	16,82,82	1.77	4 (25%)
3	SCN	G	251	2	2,2,2	1.64	1 (50%)	1,1,1	0.42	0
4	GOL	G	252	-	5,5,5	0.24	0	5,5,5	0.37	0
2	HEM	H	250	1,3	24,50,50	1.51	2 (8%)	16,82,82	1.35	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SCN	H	251	2	2,2,2	1.57	1 (50%)	1,1,1	0.11	0
4	GOL	H	252	-	5,5,5	0.27	0	5,5,5	0.49	0
4	GOL	H	253	-	5,5,5	0.31	0	5,5,5	0.54	0
2	HEM	I	250	1,3	24,50,50	1.04	2 (8%)	16,82,82	1.76	4 (25%)
3	SCN	I	251	2	2,2,2	1.43	0	1,1,1	0.16	0
4	GOL	I	252	-	5,5,5	0.57	0	5,5,5	0.49	0
4	GOL	I	253	-	5,5,5	0.39	0	5,5,5	0.85	0
2	HEM	J	250	1,3	24,50,50	1.21	2 (8%)	16,82,82	2.03	7 (43%)
3	SCN	J	251	2	2,2,2	1.44	0	1,1,1	0.01	0
4	GOL	J	252	-	5,5,5	0.73	0	5,5,5	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	A	251	2	-	0/0/0/0	0/0/0/0
4	GOL	A	252	-	-	0/4/4/4	0/0/0/0
2	HEM	B	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	B	251	2	-	0/0/0/0	0/0/0/0
4	GOL	B	252	-	-	0/4/4/4	0/0/0/0
2	HEM	C	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	C	251	2	-	0/0/0/0	0/0/0/0
4	GOL	C	252	-	-	0/4/4/4	0/0/0/0
4	GOL	C	253	-	-	0/4/4/4	0/0/0/0
2	HEM	D	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	D	251	2	-	0/0/0/0	0/0/0/0
4	GOL	D	252	-	-	0/4/4/4	0/0/0/0
4	GOL	D	253	-	-	0/4/4/4	0/0/0/0
2	HEM	E	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	E	251	2	-	0/0/0/0	0/0/0/0
4	GOL	E	252	-	-	0/4/4/4	0/0/0/0
2	HEM	F	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	F	251	2	-	0/0/0/0	0/0/0/0
4	GOL	F	252	-	-	0/4/4/4	0/0/0/0
2	HEM	G	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	G	251	2	-	0/0/0/0	0/0/0/0
4	GOL	G	252	-	-	0/4/4/4	0/0/0/0
2	HEM	H	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	H	251	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	252	-	-	0/4/4/4	0/0/0/0
4	GOL	H	253	-	-	0/4/4/4	0/0/0/0
2	HEM	I	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	I	251	2	-	0/0/0/0	0/0/0/0
4	GOL	I	252	-	-	0/4/4/4	0/0/0/0
4	GOL	I	253	-	-	0/4/4/4	0/0/0/0
2	HEM	J	250	1,3	-	0/6/54/54	0/0/8/8
3	SCN	J	251	2	-	0/0/0/0	0/0/0/0
4	GOL	J	252	-	-	0/4/4/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	250	HEM	C3B-C2B	-4.99	1.34	1.40
2	A	250	HEM	C3B-C2B	-3.77	1.35	1.40
2	F	250	HEM	C3B-C2B	-3.42	1.36	1.40
2	I	250	HEM	C3B-C2B	-3.35	1.36	1.40
2	J	250	HEM	C3B-C2B	-3.13	1.36	1.40
2	E	250	HEM	C3B-C2B	-3.12	1.36	1.40
2	J	250	HEM	C3C-C2C	-3.07	1.36	1.40
2	D	250	HEM	C3B-C2B	-2.90	1.36	1.40
2	B	250	HEM	C3B-C2B	-2.62	1.37	1.40
2	H	250	HEM	C1B-NB	-2.62	1.33	1.36
3	F	251	SCN	C-S	-2.54	1.48	1.63
2	I	250	HEM	C4D-ND	-2.42	1.33	1.36
3	C	251	SCN	C-S	-2.35	1.49	1.63
2	C	250	HEM	C4C-NC	-2.35	1.33	1.36
3	G	251	SCN	C-S	-2.32	1.49	1.63
2	A	250	HEM	C4D-ND	-2.24	1.33	1.36
3	H	251	SCN	C-S	-2.22	1.50	1.63
2	G	250	HEM	C3B-C2B	-2.16	1.37	1.40
2	F	250	HEM	C4D-ND	-2.15	1.33	1.36
2	A	250	HEM	C3C-CAC	2.16	1.52	1.47
2	E	250	HEM	C4C-NC	2.58	1.40	1.36

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	250	HEM	C3C-CAC-CBC	-5.72	114.90	126.40
2	D	250	HEM	C3B-CAB-CBB	-4.80	116.74	126.40
2	I	250	HEM	C3B-CAB-CBB	-4.43	117.49	126.40
2	D	250	HEM	CBD-CAD-C3D	-3.76	105.87	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	250	HEM	C3B-CAB-CBB	-3.67	119.02	126.40
2	F	250	HEM	C3B-C4B-NB	-3.64	104.50	109.21
2	D	250	HEM	C3B-C4B-NB	-3.63	104.52	109.21
2	H	250	HEM	C3B-C4B-NB	-3.46	104.73	109.21
2	G	250	HEM	CBD-CAD-C3D	-3.46	106.40	112.47
2	E	250	HEM	C3B-CAB-CBB	-3.41	119.54	126.40
2	B	250	HEM	C3B-CAB-CBB	-3.41	119.55	126.40
2	B	250	HEM	CBD-CAD-C3D	-3.34	106.60	112.47
2	I	250	HEM	CBD-CAD-C3D	-3.25	106.78	112.47
2	E	250	HEM	CBD-CAD-C3D	-3.18	106.89	112.47
2	J	250	HEM	C3B-CAB-CBB	-3.15	120.07	126.40
2	A	250	HEM	C3B-CAB-CBB	-3.00	120.36	126.40
2	E	250	HEM	C3B-C4B-NB	-2.96	105.39	109.21
2	A	250	HEM	C3B-C4B-NB	-2.96	105.39	109.21
2	J	250	HEM	C3C-CAC-CBC	-2.91	120.55	126.40
2	A	250	HEM	CBD-CAD-C3D	-2.87	107.43	112.47
2	H	250	HEM	CBD-CAD-C3D	-2.78	107.60	112.47
2	J	250	HEM	C3C-C4C-NC	-2.76	105.73	110.94
2	J	250	HEM	C3B-C4B-NB	-2.65	105.79	109.21
2	F	250	HEM	CBD-CAD-C3D	-2.51	108.06	112.47
2	B	250	HEM	CMA-C3A-C4A	-2.50	124.06	128.31
2	F	250	HEM	C3B-CAB-CBB	-2.46	121.45	126.40
2	J	250	HEM	CAA-CBA-CGA	-2.44	108.04	112.78
2	F	250	HEM	C3C-C4C-NC	-2.33	106.55	110.94
4	B	252	GOL	C3-C2-C1	-2.27	101.50	111.06
2	C	250	HEM	CBD-CAD-C3D	-2.16	108.67	112.47
2	C	250	HEM	C3C-C4C-NC	-2.15	106.88	110.94
2	F	250	HEM	CMA-C3A-C4A	-2.14	124.67	128.31
2	E	250	HEM	CMA-C3A-C4A	-2.13	124.69	128.31
2	J	250	HEM	CBD-CAD-C3D	-2.11	108.77	112.47
2	D	250	HEM	CAA-CBA-CGA	-2.10	108.69	112.78
2	I	250	HEM	C3B-C4B-NB	-2.10	106.49	109.21
2	G	250	HEM	C3C-C4C-NC	-2.04	107.09	110.94
2	I	250	HEM	CMA-C3A-C4A	-2.03	124.86	128.31
2	D	250	HEM	CMC-C2C-C3C	2.19	129.37	125.09
2	G	250	HEM	CMC-C2C-C3C	2.93	130.81	125.09
2	J	250	HEM	CAD-CBD-CGD	3.28	119.16	112.78
2	A	250	HEM	CMC-C2C-C3C	3.40	131.74	125.09
2	E	250	HEM	CBA-CAA-C2A	3.45	118.56	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	250	HEM	12	0
2	B	250	HEM	2	0
4	B	252	GOL	2	0
2	C	250	HEM	5	0
3	C	251	SCN	2	0
2	D	250	HEM	3	0
2	E	250	HEM	4	0
2	F	250	HEM	1	0
2	G	250	HEM	4	0
2	H	250	HEM	10	0
2	I	250	HEM	1	0
2	J	250	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	242/245 (98%)	-0.41	1 (0%) 93 94	9, 16, 32, 62	0
1	B	245/245 (100%)	-0.39	2 (0%) 87 91	10, 16, 32, 68	0
1	C	242/245 (98%)	-0.44	1 (0%) 93 94	9, 15, 29, 61	0
1	D	242/245 (98%)	-0.17	5 (2%) 67 73	10, 18, 36, 126	0
1	E	242/245 (98%)	-0.44	0 100 100	9, 16, 33, 55	0
1	F	242/245 (98%)	-0.44	2 (0%) 87 91	10, 15, 32, 58	0
1	G	245/245 (100%)	-0.43	1 (0%) 93 94	10, 16, 31, 51	0
1	H	242/245 (98%)	-0.35	2 (0%) 87 91	10, 16, 34, 78	0
1	I	242/245 (98%)	-0.31	2 (0%) 87 91	10, 16, 31, 96	0
1	J	242/245 (98%)	-0.38	1 (0%) 93 94	10, 17, 36, 64	0
All	All	2426/2450 (99%)	-0.38	17 (0%) 89 92	9, 16, 33, 126	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	MET	10.2
1	H	8	MET	6.8
1	B	5	ALA	6.2
1	I	8	MET	5.6
1	F	134	ALA	4.8
1	J	8	MET	4.0
1	G	5	ALA	4.0
1	I	9	ALA	3.5
1	C	8	MET	3.4
1	A	133	SER	3.2
1	F	8	MET	3.1
1	B	6	PRO	2.6
1	D	126	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	129	ALA	2.3
1	H	133	SER	2.3
1	D	135	THR	2.2
1	D	9	ALA	2.2

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	GOL	F	252	6/6	0.94	0.12	7.35	18,24,41,42	0
4	GOL	A	252	6/6	0.96	0.11	6.14	24,26,35,47	0
4	GOL	E	252	6/6	0.97	0.12	5.96	20,25,35,41	0
4	GOL	B	252	6/6	0.89	0.14	4.24	25,30,46,52	0
4	GOL	C	252	6/6	0.95	0.10	3.64	20,27,32,38	0
4	GOL	C	253	6/6	0.97	0.13	3.37	16,24,29,37	0
4	GOL	D	253	6/6	0.96	0.13	2.77	16,25,28,36	0
4	GOL	H	253	6/6	0.95	0.12	1.73	19,30,34,38	0
4	GOL	H	252	6/6	0.95	0.08	1.63	21,29,34,40	0
2	HEM	B	250	43/43	0.97	0.09	1.37	11,15,21,27	0
4	GOL	I	253	6/6	0.95	0.10	1.15	17,30,30,34	0
3	SCN	J	251	3/3	0.99	0.07	1.03	17,17,19,22	0
4	GOL	J	252	6/6	0.95	0.10	0.84	22,24,36,41	0
2	HEM	D	250	43/43	0.96	0.10	0.81	14,20,28,41	0
4	GOL	G	252	6/6	0.96	0.08	0.66	21,27,32,35	0
2	HEM	J	250	43/43	0.98	0.07	0.45	10,14,16,24	0
2	HEM	G	250	43/43	0.98	0.08	0.41	8,14,20,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	I	250	43/43	0.97	0.09	0.37	12,15,20,30	0
4	GOL	I	252	6/6	0.97	0.07	0.20	19,26,30,33	0
2	HEM	A	250	43/43	0.98	0.08	0.02	11,15,23,26	0
3	SCN	D	251	3/3	0.98	0.08	-0.03	23,23,25,25	0
2	HEM	E	250	43/43	0.98	0.07	-0.03	9,13,18,21	0
2	HEM	H	250	43/43	0.98	0.08	-0.04	11,14,20,29	0
2	HEM	C	250	43/43	0.98	0.07	-0.30	9,13,17,23	0
2	HEM	F	250	43/43	0.98	0.07	-0.33	9,12,15,29	0
4	GOL	D	252	6/6	0.97	0.07	-0.54	22,33,37,43	0
3	SCN	F	251	3/3	0.99	0.06	-0.65	15,15,18,18	0
3	SCN	C	251	3/3	0.99	0.07	-0.98	16,16,18,19	0
3	SCN	E	251	3/3	0.99	0.06	-1.35	11,11,13,16	0
3	SCN	G	251	3/3	1.00	0.05	-1.57	15,15,19,20	0
3	SCN	B	251	3/3	0.99	0.06	-1.67	14,14,15,17	0
3	SCN	I	251	3/3	0.99	0.06	-1.94	15,15,17,18	0
3	SCN	H	251	3/3	0.99	0.05	-2.21	19,19,20,26	0
3	SCN	A	251	3/3	0.99	0.05	-2.41	15,15,18,21	0

6.5 Other polymers

There are no such residues in this entry.