Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GG9
Title	:	CRYSTAL STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI, HIS128ASN VARIANT.
Authors	:	Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on	:	2000-08-11
Resolution	:	1.89 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:

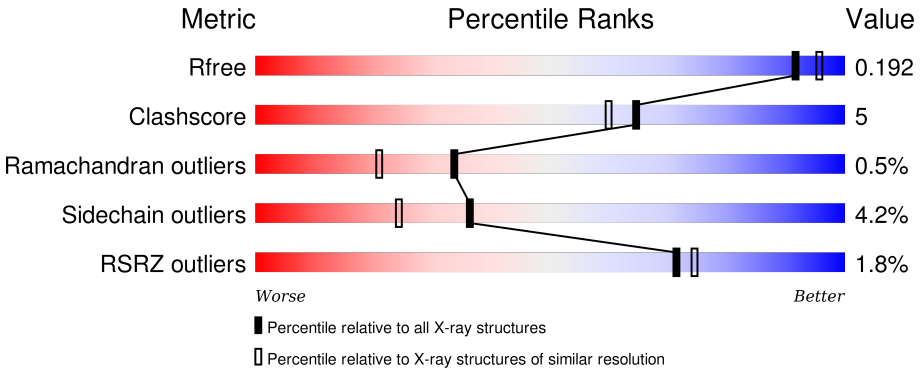
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	753	2% 83% 12%
1	B	753	2% 82% 12%
1	C	753	2% 83% 11%
1	D	753	% 83% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26587 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.

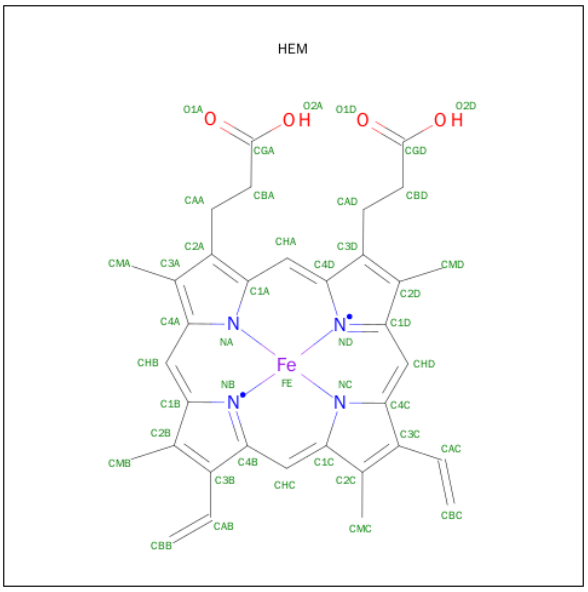
- Molecule 1 is a protein called CATALASE HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	B	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	C	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	D	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ASN	HIS	ENGINEERED	UNP P21179
B	128	ASN	HIS	ENGINEERED	UNP P21179
C	128	ASN	HIS	ENGINEERED	UNP P21179
D	128	ASN	HIS	ENGINEERED	UNP P21179

- 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		

- Molecule 3 is water.

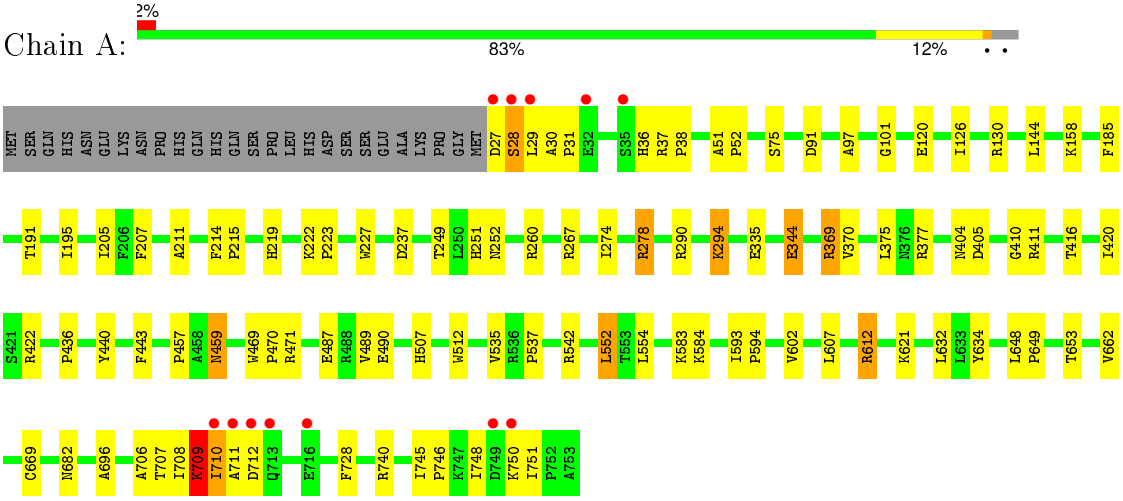
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	916	Total	O	0	0
			916	916		
3	B	807	Total	O	0	0
			807	807		
3	C	818	Total	O	0	0
			818	818		
3	D	898	Total	O	0	0
			898	898		

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.

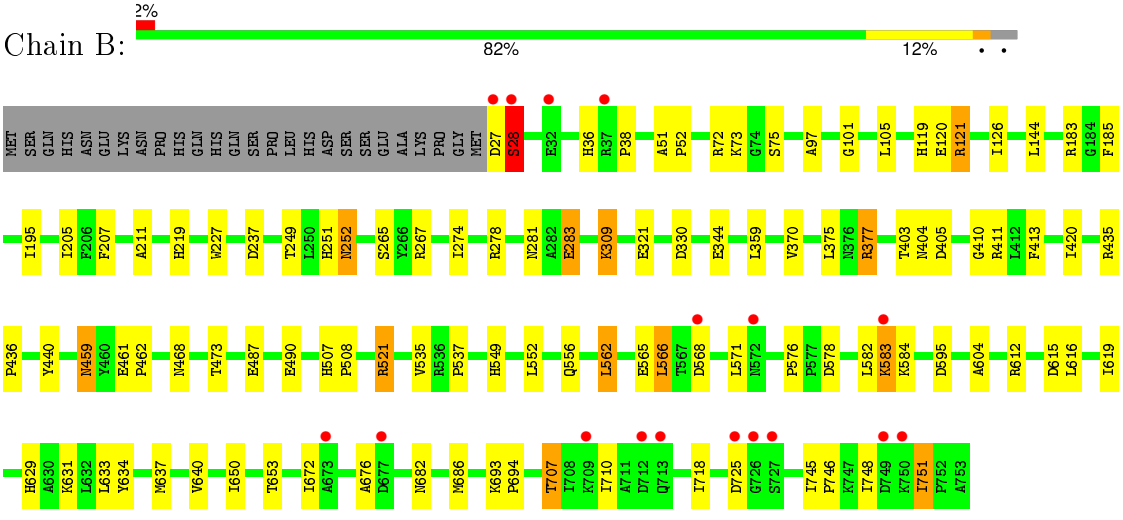
- Molecule 1: CATALASE HPII

Chain A:



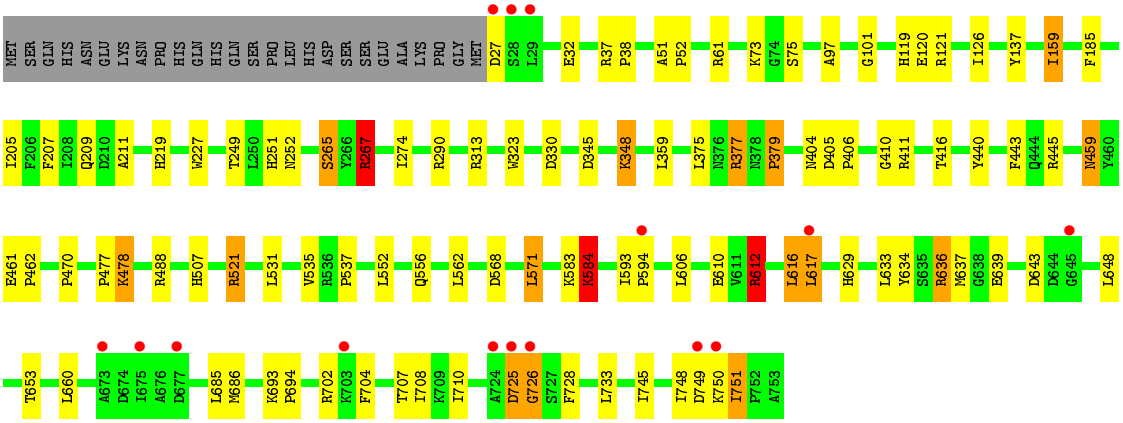
- Molecule 1: CATALASE HPII

Chain B:



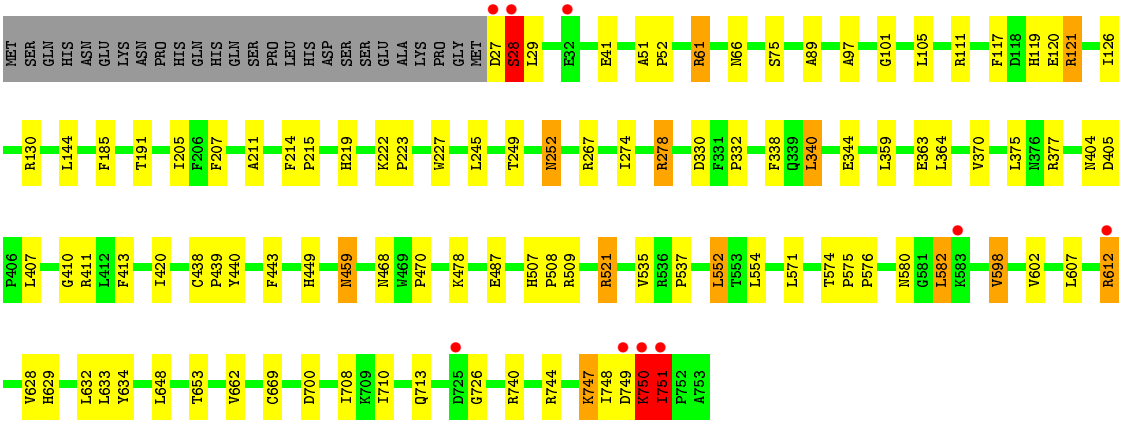
- Molecule 1: CATALASE HPII

Chain C:



- Molecule 1: CATALASE HPII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.04Å 132.34Å 121.20Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.63 – 1.89 14.93 – 1.89	Depositor EDS
% Data completeness (in resolution range)	89.0 (87.63-1.89) 89.5 (14.93-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.188 0.147 , 0.192	Depositor DCC
R_{free} test set	9905 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	8.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.1	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 196723 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26587	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

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	0.40	0/5899	0.97	12/8020 (0.1%)
1	B	0.40	0/5899	0.94	6/8020 (0.1%)
1	C	0.40	0/5899	0.95	7/8020 (0.1%)
1	D	0.40	0/5899	0.98	12/8020 (0.1%)
All	All	0.40	0/23596	0.96	37/32080 (0.1%)

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	C	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	377	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	D	377	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	D	740	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	344	GLU	CA-CB-CG	8.18	131.40	113.40
1	B	121	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	D	278	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	D	61	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	B	521	ARG	CD-NE-CZ	7.58	134.22	123.60
1	C	726	GLY	N-CA-C	-7.29	94.88	113.10
1	D	61	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	278	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	D	130	ARG	NE-CZ-NH2	-6.91	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	369	ARG	CD-NE-CZ	6.79	133.10	123.60
1	C	445	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	260	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	422	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	D	612	ARG	CD-NE-CZ	6.30	132.43	123.60
1	D	449	HIS	CA-CB-CG	6.02	123.83	113.60
1	A	740	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	369	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	D	61	ARG	CD-NE-CZ	5.77	131.68	123.60
1	D	111	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	B	28	SER	N-CA-CB	5.72	119.08	110.50
1	C	267	ARG	CD-NE-CZ	5.71	131.59	123.60
1	D	521	ARG	CG-CD-NE	5.64	123.64	111.80
1	C	377	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	130	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	121	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	612	ARG	CD-NE-CZ	5.36	131.10	123.60
1	C	702	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	542	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	278	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	C	290	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	290	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	72	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	403	THR	N-CA-CB	5.01	119.81	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	Mainchain

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	5744	0	5577	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5744	0	5577	73	0
1	C	5744	0	5577	62	0
1	D	5744	0	5577	61	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	916	0	0	10	1
3	B	807	0	0	6	1
3	C	818	0	0	9	0
3	D	898	0	0	5	0
All	All	26587	0	22428	232	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.58	0.84
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.50	0.77
1:D:27:ASP:O	1:D:28:SER:HB2	1.86	0.76
1:A:708:ILE:O	1:A:710:ILE:HB	1.89	0.72
1:D:700:ASP:HB2	3:D:1657:HOH:O	1.89	0.71
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.71	0.70
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.74	0.69
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.77	0.67
1:B:267:ARG:HG3	3:B:1245:HOH:O	1.95	0.66
1:D:267:ARG:HG3	3:D:864:HOH:O	1.96	0.65
1:B:281:ASN:OD1	1:B:283:GLU:HG3	1.96	0.64
1:B:583:LYS:O	1:B:584:LYS:HB3	1.96	0.64
1:C:725:ASP:CA	1:C:728:PHE:HB3	2.29	0.63
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.79	0.63
1:B:748:ILE:O	1:B:751:ILE:HG22	1.98	0.63
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.80	0.61
1:D:612:ARG:HD2	1:D:669:CYS:HB3	1.83	0.61
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.83	0.61
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.82	0.61
1:C:583:LYS:O	1:C:584:LYS:HB3	2.01	0.60
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.31	0.59
1:B:309:LYS:HD3	1:C:313:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.84	0.59
1:B:583:LYS:HE2	1:B:583:LYS:H	1.68	0.59
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.86	0.59
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.19	0.58
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.33	0.58
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.86	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.51	0.57
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.86	0.57
1:C:748:ILE:O	1:C:751:ILE:HG22	2.05	0.57
1:B:121:ARG:HG2	1:C:126:ILE:HD12	1.86	0.57
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.87	0.56
1:B:413:PHE:HB2	1:D:105:LEU:HD11	1.87	0.56
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.86	0.56
1:C:751:ILE:HB	3:C:1496:HOH:O	2.05	0.56
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.70	0.56
1:B:583:LYS:CE	1:B:583:LYS:H	2.20	0.55
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.88	0.55
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.87	0.55
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.20	0.55
1:D:750:LYS:HD3	1:D:751:ILE:H	1.71	0.55
1:D:748:ILE:O	1:D:751:ILE:HG22	2.05	0.55
1:B:745:ILE:O	1:B:748:ILE:HG12	2.07	0.54
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.38	0.54
1:C:686:MET:HG2	1:C:751:ILE:HD11	1.89	0.54
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.90	0.54
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.89	0.53
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.43	0.53
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.38	0.53
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.44	0.53
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.91	0.53
1:A:748:ILE:O	1:A:751:ILE:HG13	2.09	0.53
1:C:704:PHE:O	1:C:707:THR:HG22	2.08	0.53
1:D:629:HIS:HD2	3:D:1183:HOH:O	1.92	0.52
1:A:751:ILE:O	1:A:751:ILE:HD12	2.08	0.52
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.91	0.52
1:D:602:VAL:HG13	1:D:662:VAL:HA	1.91	0.52
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.45	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.58	0.52
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.92	0.52
1:D:97:ALA:O	1:D:101:GLY:HA3	2.10	0.52
1:B:634:TYR:O	1:B:653:THR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ILE:HB	3:B:1540:HOH:O	2.11	0.51
1:A:267:ARG:HG3	3:A:1183:HOH:O	2.09	0.51
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.25	0.51
1:C:616:LEU:HD12	1:C:648:LEU:HD21	1.92	0.51
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.92	0.51
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.40	0.51
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.46	0.51
1:D:535:VAL:O	1:D:537:PRO:HD3	2.11	0.51
1:B:207:PHE:O	1:B:249:THR:HA	2.11	0.50
1:B:468:ASN:HD22	1:D:27:ASP:N	2.09	0.50
1:A:207:PHE:O	1:A:249:THR:HA	2.12	0.50
1:C:137:TYR:HB2	1:C:159:ILE:HD13	1.93	0.50
1:B:36:HIS:HD1	1:B:36:HIS:H	1.59	0.50
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.27	0.50
1:A:416:THR:HA	3:A:1670:HOH:O	2.12	0.50
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.42	0.49
1:A:158:LYS:HE2	3:A:1641:HOH:O	2.12	0.49
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.48	0.49
1:A:750:LYS:O	1:A:750:LYS:HE3	2.12	0.49
1:B:640:VAL:HG13	1:B:650:ILE:HD11	1.95	0.48
1:B:359:LEU:H	1:B:507:HIS:CD2	2.30	0.48
1:B:629:HIS:HD2	3:B:1055:HOH:O	1.96	0.48
1:C:535:VAL:O	1:C:537:PRO:HD3	2.12	0.48
1:C:610:GLU:O	1:C:610:GLU:HG3	2.13	0.48
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.95	0.48
1:A:120:GLU:HB2	1:D:126:ILE:HD11	1.94	0.48
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.97	0.48
1:A:30:ALA:HB1	1:A:36:HIS:CD2	2.49	0.48
1:D:222:LYS:HB3	1:D:223:PRO:HD2	1.95	0.47
1:C:583:LYS:HG2	3:C:1524:HOH:O	2.14	0.47
1:D:607:LEU:HD11	1:D:632:LEU:HB3	1.96	0.47
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.95	0.47
1:B:97:ALA:O	1:B:101:GLY:HA3	2.14	0.47
1:A:708:ILE:O	1:A:709:LYS:C	2.53	0.47
1:B:126:ILE:HD11	1:C:120:GLU:HB2	1.95	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.44	0.47
1:A:52:PRO:HG3	3:C:1017:HOH:O	2.15	0.47
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.30	0.47
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.97	0.47
1:A:602:VAL:HG13	1:A:662:VAL:HA	1.97	0.47
1:C:359:LEU:H	1:C:507:HIS:CD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD11	1:D:413:PHE:HB2	1.96	0.47
2:A:760:HEM:HBC2	2:A:760:HEM:CMC	2.45	0.46
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.97	0.46
1:B:27:ASP:HB3	3:B:1503:HOH:O	2.15	0.46
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.97	0.46
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.98	0.46
1:B:578:ASP:HB3	1:B:582:LEU:O	2.15	0.46
1:D:521:ARG:HD3	3:D:1651:HOH:O	2.15	0.46
1:A:535:VAL:O	1:A:537:PRO:HD3	2.16	0.46
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.98	0.46
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.98	0.46
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.97	0.46
1:B:211:ALA:HB3	1:B:410:GLY:HA3	1.97	0.45
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.81	0.45
1:C:612:ARG:HD3	1:C:643:ASP:OD2	2.15	0.45
1:B:411:ARG:HG2	2:B:760:HEM:C2C	2.51	0.45
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.52	0.45
1:B:461:GLU:HA	1:B:462:PRO:C	2.36	0.45
1:A:707:THR:HG23	3:A:1538:HOH:O	2.16	0.45
1:C:636:ARG:NH2	1:C:639:GLU:O	2.49	0.45
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.51	0.45
1:A:294:LYS:NZ	3:A:1022:HOH:O	2.48	0.45
1:C:207:PHE:O	1:C:249:THR:HA	2.17	0.45
1:D:27:ASP:HB2	1:D:29:LEU:HD21	1.97	0.45
1:B:120:GLU:HB2	1:C:126:ILE:HD11	1.97	0.45
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.51	0.45
1:A:709:LYS:O	1:A:710:ILE:HD12	2.17	0.45
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.99	0.45
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.45
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.46	0.44
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.98	0.44
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.52	0.44
1:D:574:THR:HG22	3:D:1241:HOH:O	2.18	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.21	0.44
1:B:126:ILE:CD1	1:C:120:GLU:HB2	2.46	0.44
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.33	0.44
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.17	0.44
1:A:195:ILE:HD11	1:A:436:PRO:HA	1.99	0.44
1:B:507:HIS:N	1:B:508:PRO:CD	2.80	0.44
1:B:195:ILE:HD11	1:B:436:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:O	1:A:405:ASP:C	2.56	0.44
1:C:404:ASN:O	1:C:405:ASP:C	2.54	0.44
1:C:416:THR:HA	3:C:810:HOH:O	2.18	0.44
1:D:207:PHE:O	1:D:249:THR:HA	2.18	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.17	0.43
1:A:31:PRO:HD2	1:A:36:HIS:HB3	2.00	0.43
1:A:222:LYS:HB3	1:A:223:PRO:CD	2.48	0.43
1:C:745:ILE:HD13	3:C:1533:HOH:O	2.17	0.43
3:A:909:HOH:O	1:C:52:PRO:HG3	2.19	0.43
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.43
1:B:672:ILE:HG22	1:B:676:ALA:HB2	2.01	0.43
1:A:745:ILE:N	1:A:746:PRO:HD2	2.33	0.43
1:B:183:ARG:HG2	3:B:1128:HOH:O	2.19	0.43
1:C:556:GLN:NE2	3:C:1371:HOH:O	2.52	0.43
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	2.00	0.43
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.43
1:C:617:LEU:HD13	3:C:1537:HOH:O	2.18	0.43
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.67	0.43
1:B:507:HIS:N	1:B:508:PRO:HD2	2.33	0.43
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.53	0.43
1:A:612:ARG:HG3	3:A:1597:HOH:O	2.19	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.42
1:D:214:PHE:HB3	1:D:215:PRO:HD3	2.00	0.42
1:B:549:HIS:O	1:B:576:PRO:HD3	2.18	0.42
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.54	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.40	0.42
1:D:411:ARG:HG2	2:D:760:HEM:C2C	2.54	0.42
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.84	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.55	0.42
1:A:158:LYS:HB3	3:A:1641:HOH:O	2.19	0.42
1:B:604:ALA:HA	1:B:631:LYS:HG3	2.02	0.42
1:B:252:ASN:HA	1:B:252:ASN:HD22	1.64	0.42
1:B:27:ASP:O	1:B:28:SER:HB2	2.20	0.42
1:B:435:ARG:HA	1:B:436:PRO:HD3	1.93	0.42
1:D:438:CYS:HB2	1:D:439:PRO:CD	2.49	0.42
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.01	0.42
1:A:126:ILE:HD12	1:D:121:ARG:CZ	2.49	0.42
1:B:637:MET:HB2	1:C:562:LEU:HA	2.02	0.42
1:B:344:GLU:H	1:B:344:GLU:CD	2.22	0.42
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.23	0.42
1:C:97:ALA:O	1:C:101:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:LYS:HA	1:B:694:PRO:HD3	1.88	0.42
1:C:552:LEU:HD22	1:C:556:GLN:HG3	2.02	0.41
1:D:407:LEU:HD11	2:D:760:HEM:HMC2	2.02	0.41
1:A:512:TRP:CZ3	1:A:554:LEU:HD13	2.54	0.41
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.20	0.41
1:C:411:ARG:HG2	2:C:760:HEM:C2C	2.55	0.41
1:D:363:GLU:HB2	1:D:582:LEU:HD21	2.02	0.41
1:B:404:ASN:O	1:B:405:ASP:C	2.59	0.41
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.90	0.41
1:B:126:ILE:HD12	1:C:121:ARG:HG2	2.02	0.41
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.35	0.41
1:B:73:LYS:HD3	3:B:1563:HOH:O	2.21	0.41
1:C:209:GLN:O	1:C:406:PRO:HG2	2.20	0.41
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.55	0.41
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.50	0.41
1:C:521:ARG:HG2	3:C:1533:HOH:O	2.19	0.41
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.37	0.41
1:D:574:THR:HA	1:D:575:PRO:HD3	1.91	0.41
1:C:265:SER:OG	1:C:267:ARG:HB2	2.21	0.41
1:A:489:VAL:HG22	3:A:1673:HOH:O	2.20	0.41
1:A:583:LYS:O	1:A:584:LYS:HB3	2.20	0.41
1:A:27:ASP:O	1:A:28:SER:C	2.59	0.41
1:B:552:LEU:HD22	1:B:556:GLN:HG3	2.03	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.20	0.41
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.97	0.41
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.91	0.41
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.96	0.41
1:D:267:ARG:HG2	1:D:332:PRO:HB3	2.02	0.41
1:A:648:LEU:HA	1:A:649:PRO:HD3	1.95	0.41
1:A:97:ALA:O	1:A:101:GLY:HA3	2.21	0.41
1:A:126:ILE:HD13	1:D:117:PHE:O	2.21	0.41
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.85	0.41
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.02	0.41
1:A:552:LEU:HB3	3:A:1668:HOH:O	2.20	0.40
1:B:562:LEU:HA	1:C:637:MET:HB2	2.03	0.40
1:B:535:VAL:O	1:B:537:PRO:HD3	2.21	0.40
1:A:706:ALA:O	1:A:709:LYS:HD2	2.21	0.40
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.40
1:D:507:HIS:N	1:D:508:PRO:CD	2.84	0.40
1:C:267:ARG:HD3	3:C:797:HOH:O	2.21	0.40
1:B:473:THR:O	1:D:89:ALA:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ASN:O	1:D:405:ASP:C	2.58	0.40
1:C:686:MET:CG	1:C:751:ILE:HD11	2.51	0.40
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.55	0.40
1:D:507:HIS:N	1:D:508:PRO:HD2	2.36	0.40
1:B:615:ASP:O	1:B:619:ILE:HG13	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1269:HOH:O	3:B:1515:HOH:O[2_545]	1.51	0.69

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	725/753 (96%)	702 (97%)	19 (3%)	4 (1%)	30	17
1	B	725/753 (96%)	703 (97%)	19 (3%)	3 (0%)	39	27
1	C	725/753 (96%)	707 (98%)	15 (2%)	3 (0%)	39	27
1	D	725/753 (96%)	702 (97%)	18 (2%)	5 (1%)	26	14
All	All	2900/3012 (96%)	2814 (97%)	71 (2%)	15 (0%)	34	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	711	ALA
1	B	28	SER
1	C	725	ASP
1	D	28	SER

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Mol	Chain	Res	Type
1	A	709	LYS
1	C	584	LYS
1	D	726	GLY
1	D	750	LYS
1	D	751	ILE
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER
1	D	75	SER

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	612/636 (96%)	594 (97%)	18 (3%)	50	40
1	B	612/636 (96%)	588 (96%)	24 (4%)	39	27
1	C	612/636 (96%)	576 (94%)	36 (6%)	24	12
1	D	612/636 (96%)	588 (96%)	24 (4%)	39	27
All	All	2448/2544 (96%)	2346 (96%)	102 (4%)	36	24

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	294	LYS
1	A	344	GLU
1	A	375	LEU
1	A	440	TYR

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Mol	Chain	Res	Type
1	A	459	ASN
1	A	552	LEU
1	A	612	ARG
1	A	621	LYS
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	265	SER
1	B	283	GLU
1	B	309	LYS
1	B	321	GLU
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	633	LEU
1	B	707	THR
1	B	751	ILE
1	C	27	ASP
1	C	32	GLU
1	C	61	ARG
1	C	73	LYS
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	252	ASN
1	C	265	SER
1	C	267	ARG

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Mol	Chain	Res	Type
1	C	348	LYS
1	C	375	LEU
1	C	377	ARG
1	C	379	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	660	LEU
1	C	685	LEU
1	C	733	LEU
1	C	749	ASP
1	C	750	LYS
1	C	751	ILE
1	D	28	SER
1	D	41	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	598	VAL

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Mol	Chain	Res	Type
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA

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)

4 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	760	1	30,50,50	2.42	8 (26%)	24,82,82	2.49	9 (37%)
2	HEM	B	760	1	30,50,50	2.38	5 (16%)	24,82,82	2.52	8 (33%)
2	HEM	C	760	1	30,50,50	2.47	7 (23%)	24,82,82	2.45	8 (33%)
2	HEM	D	760	1	30,50,50	2.43	7 (23%)	24,82,82	2.62	8 (33%)

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	760	1	-	0/10/54/54	0/0/8/8
2	HEM	B	760	1	-	0/10/54/54	0/0/8/8
2	HEM	C	760	1	-	0/10/54/54	0/0/8/8
2	HEM	D	760	1	-	0/10/54/54	0/0/8/8

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	C2D-C3D	-7.28	1.32	1.54
2	B	760	HEM	C2D-C3D	-7.14	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C2D-C3D	-7.05	1.33	1.54
2	C	760	HEM	C2D-C3D	-6.98	1.33	1.54
2	C	760	HEM	C3B-C4B	-6.96	1.45	1.51
2	D	760	HEM	C3B-C4B	-6.63	1.45	1.51
2	B	760	HEM	C3B-C4B	-6.48	1.46	1.51
2	A	760	HEM	C3B-C4B	-6.27	1.46	1.51
2	A	760	HEM	C3D-C4D	-5.15	1.45	1.51
2	D	760	HEM	C3D-C4D	-5.06	1.45	1.51
2	B	760	HEM	C3D-C4D	-4.70	1.45	1.51
2	C	760	HEM	C3D-C4D	-4.64	1.45	1.51
2	C	760	HEM	C2C-C1C	-4.17	1.44	1.52
2	B	760	HEM	C2C-C1C	-4.01	1.45	1.52
2	A	760	HEM	C2C-C1C	-4.01	1.45	1.52
2	D	760	HEM	C2C-C1C	-3.84	1.45	1.52
2	A	760	HEM	C2D-C1D	-2.11	1.45	1.51
2	D	760	HEM	C2B-C1B	-2.08	1.45	1.51
2	D	760	HEM	C2D-C1D	-2.06	1.45	1.51
2	C	760	HEM	C2D-C1D	-2.04	1.45	1.51
2	A	760	HEM	C3C-CAC	2.11	1.55	1.51
2	A	760	HEM	C4C-NC	2.22	1.38	1.36
2	D	760	HEM	C1C-NC	2.28	1.38	1.36
2	B	760	HEM	C1C-NC	2.56	1.39	1.36
2	C	760	HEM	C1C-NC	2.73	1.39	1.36
2	C	760	HEM	C4C-NC	2.98	1.39	1.36
2	A	760	HEM	C1C-NC	2.98	1.39	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	760	HEM	CAA-C2A-C1A	-5.12	121.45	127.01
2	B	760	HEM	CAA-C2A-C1A	-4.18	122.47	127.01
2	A	760	HEM	C3C-CAC-CBC	-3.75	118.70	124.46
2	D	760	HEM	C3C-CAC-CBC	-3.15	119.62	124.46
2	A	760	HEM	CMA-C3A-C4A	-2.75	123.81	128.36
2	C	760	HEM	CMA-C3A-C4A	-2.65	123.98	128.36
2	C	760	HEM	CAA-C2A-C1A	-2.34	124.47	127.01
2	B	760	HEM	CMA-C3A-C4A	-2.29	124.57	128.36
2	A	760	HEM	CAA-C2A-C1A	-2.07	124.76	127.01
2	D	760	HEM	CAD-C3D-C4D	2.86	122.56	112.47
2	C	760	HEM	CAD-C3D-C4D	2.98	122.97	112.47
2	B	760	HEM	CAD-C3D-C4D	3.16	123.61	112.47
2	A	760	HEM	CAD-C3D-C4D	3.30	124.10	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760	HEM	CMD-C2D-C3D	3.39	129.34	114.35
2	D	760	HEM	CMD-C2D-C3D	3.41	129.43	114.35
2	C	760	HEM	CMD-C2D-C3D	3.45	129.59	114.35
2	B	760	HEM	CMD-C2D-C3D	3.58	130.17	114.35
2	A	760	HEM	C2D-C3D-C4D	3.95	108.20	101.50
2	B	760	HEM	C2D-C3D-C4D	3.96	108.21	101.50
2	C	760	HEM	C2D-C3D-C4D	3.96	108.21	101.50
2	D	760	HEM	C2D-C3D-C4D	4.15	108.53	101.50
2	A	760	HEM	CMC-C2C-C3C	4.37	127.45	116.53
2	D	760	HEM	CMC-C2C-C3C	4.38	127.47	116.53
2	D	760	HEM	CMB-C2B-C3B	4.53	127.83	116.53
2	C	760	HEM	CMC-C2C-C3C	4.55	127.90	116.53
2	B	760	HEM	CMC-C2C-C3C	4.61	128.04	116.53
2	B	760	HEM	CMB-C2B-C3B	4.83	128.59	116.53
2	C	760	HEM	CMB-C2B-C3B	5.00	129.02	116.53
2	A	760	HEM	CAD-C3D-C2D	5.04	127.69	113.22
2	A	760	HEM	CMB-C2B-C3B	5.04	129.12	116.53
2	B	760	HEM	CAD-C3D-C2D	5.14	128.00	113.22
2	C	760	HEM	CAD-C3D-C2D	5.40	128.74	113.22
2	D	760	HEM	CAD-C3D-C2D	5.45	128.88	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	3	0
2	B	760	HEM	2	0
2	C	760	HEM	2	0
2	D	760	HEM	3	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	727/753 (96%)	-0.51	12 (1%)	73	76	3, 8, 25, 47	1 (0%)
1	B	727/753 (96%)	-0.43	17 (2%)	64	67	3, 9, 28, 46	1 (0%)
1	C	727/753 (96%)	-0.47	15 (2%)	67	70	3, 9, 27, 45	1 (0%)
1	D	727/753 (96%)	-0.56	9 (1%)	81	83	3, 8, 26, 46	1 (0%)
All	All	2908/3012 (96%)	-0.49	53 (1%)	71	74	3, 8, 27, 47	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	10.3
1	A	27	ASP	8.0
1	B	726	GLY	6.8
1	A	28	SER	6.0
1	C	28	SER	5.7
1	D	27	ASP	5.7
1	A	712	ASP	5.7
1	B	27	ASP	5.2
1	A	710	ILE	5.0
1	A	32	GLU	4.7
1	A	713	GLN	4.6
1	D	28	SER	3.9
1	C	27	ASP	3.9
1	D	749	ASP	3.6
1	C	726	GLY	3.6
1	B	750	LYS	3.2
1	D	32	GLU	3.2
1	C	594	PRO	3.0
1	B	28	SER	3.0
1	B	713	GLN	3.0
1	B	677	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	32	GLU	2.8
1	A	29	LEU	2.8
1	C	749	ASP	2.8
1	B	749	ASP	2.8
1	D	725	ASP	2.7
1	C	675	ILE	2.6
1	B	712	ASP	2.6
1	D	751	ILE	2.5
1	B	583	LYS	2.5
1	C	29	LEU	2.5
1	C	645	GLY	2.4
1	D	750	LYS	2.4
1	B	673	ALA	2.4
1	C	750	LYS	2.4
1	C	677	ASP	2.4
1	B	572	ASN	2.3
1	B	725	ASP	2.3
1	C	724	ALA	2.3
1	C	725	ASP	2.3
1	C	673	ALA	2.3
1	A	750	LYS	2.2
1	B	727	SER	2.2
1	C	703	LYS	2.2
1	C	617	LEU	2.2
1	B	37	ARG	2.1
1	A	716	GLU	2.1
1	A	749	ASP	2.1
1	B	709	LYS	2.0
1	D	612	ARG	2.0
1	B	568	ASP	2.0
1	A	35	SER	2.0
1	D	583	LYS	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
2	HEM	B	760	43/43	0.99	0.06	-0.27	3,5,6,6	0
2	HEM	D	760	43/43	0.99	0.06	-0.41	2,4,5,6	0
2	HEM	C	760	43/43	0.99	0.06	-0.47	4,6,7,7	0
2	HEM	A	760	43/43	0.99	0.06	-0.55	3,4,6,6	0

6.5 Other polymers (i)

There are no such residues in this entry.