



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:09 AM GMT

PDB ID : 1A00
Title : HEMOGLOBIN (VAL BETA1 MET, TRP BETA37 TYR) MUTANT
Authors : Kavanaugh, J.S.; Arnone, A.
Deposited on : 1997-12-08
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

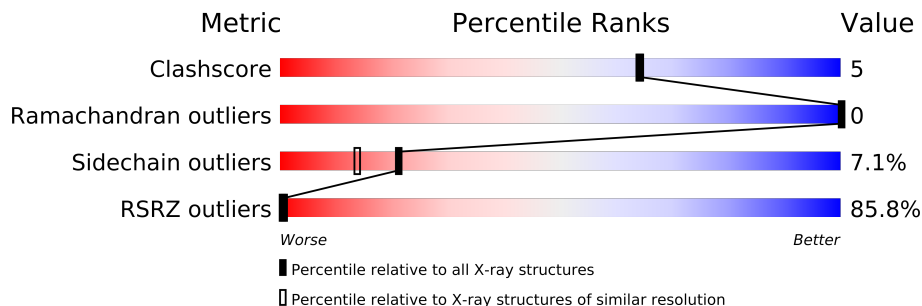
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HEM	C	142	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4770 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HEMOGLOBIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

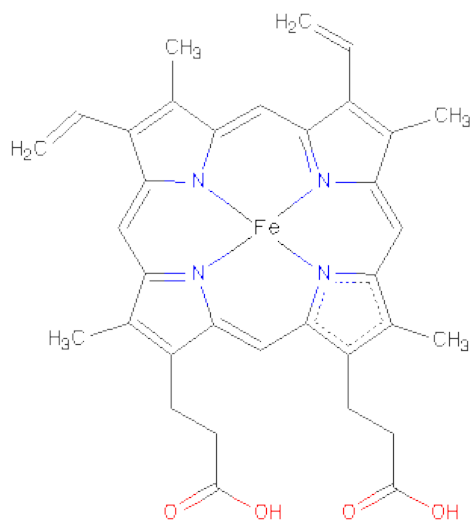
- Molecule 2 is a protein called HEMOGLOBIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1122	722	194	202	4			
2	D	146	Total	C	N	O	S	0	0	0
			1122	722	194	202	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	TYR	TRP	ENGINEERED	UNP P68871
D	37	TYR	TRP	ENGINEERED	UNP P68871

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

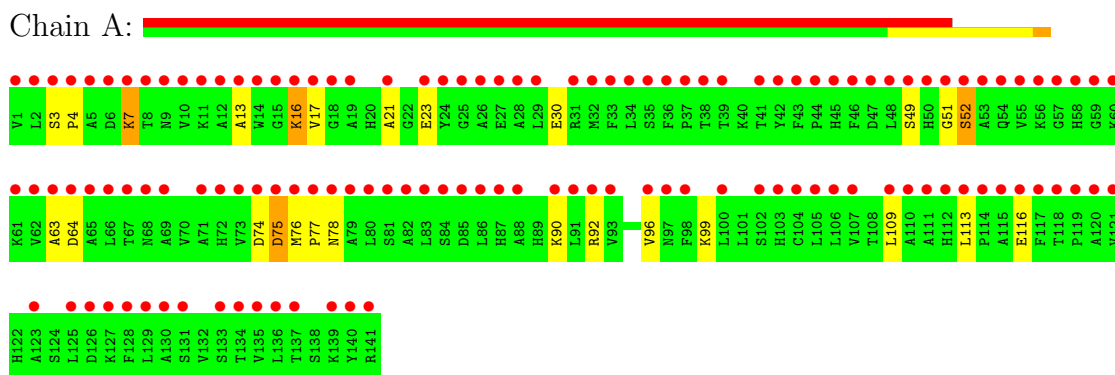
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	52	Total	O	0	0
			52	52		
4	C	66	Total	O	0	0
			66	66		
4	D	46	Total	O	0	0
			46	46		

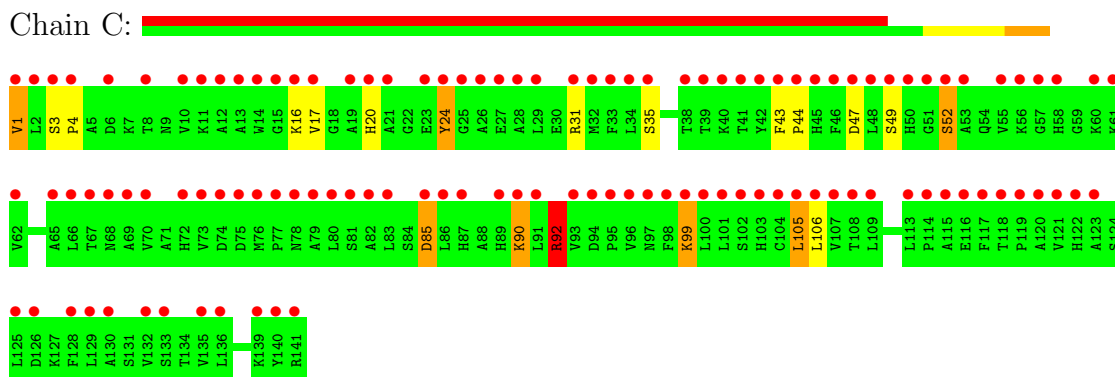
3 Residue-property plots

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.

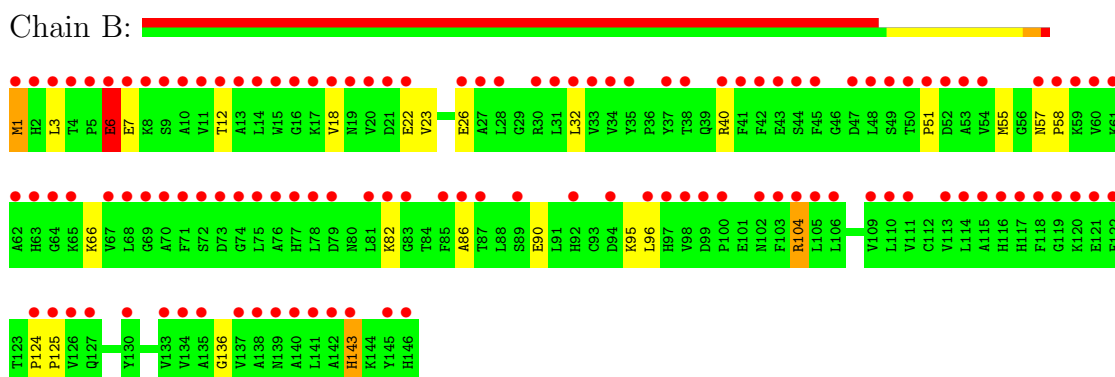
• Molecule 1: HEMOGLOBIN (ALPHA CHAIN)



• Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

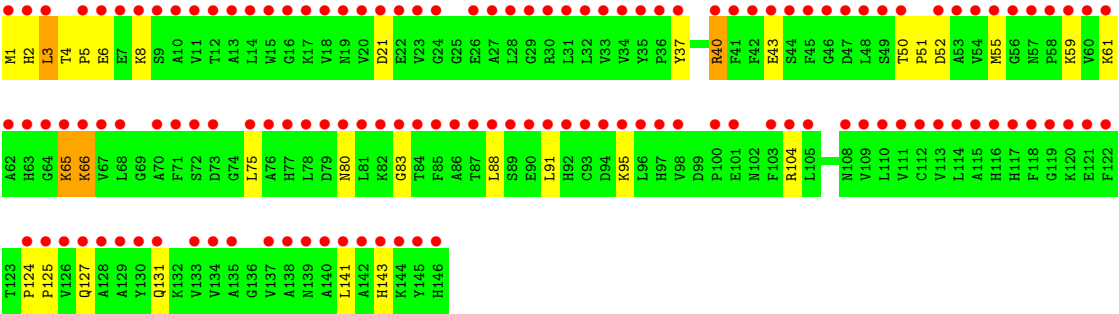


• Molecule 2: HEMOGLOBIN (BETA CHAIN)



● Molecule 2: HEMOGLOBIN (BETA CHAIN)

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.10Å 112.00Å 63.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 46.61 – 1.73	Depositor EDS
% Data completeness (in resolution range)	97.1 (8.00-2.00) 67.5 (46.61-1.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.73Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , 0.223 0.527 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 485.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42867 reflections	Xtriage
F_o, F_c correlation	0.40	EDS
Total number of atoms	4770	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.81	0/1097	1.33	7/1491 (0.5%)
1	C	0.83	0/1097	1.50	12/1491 (0.8%)
2	B	0.84	0/1151	1.33	3/1561 (0.2%)
2	D	0.82	0/1151	1.39	8/1561 (0.5%)
All	All	0.82	0/4496	1.39	30/6104 (0.5%)

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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	NE-CZ-NH2	-20.75	109.92	120.30
2	D	40	ARG	NE-CZ-NH1	12.78	126.69	120.30
1	C	85	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	C	85	ASP	CB-CG-OD1	7.70	125.23	118.30
2	D	66	LYS	CA-CB-CG	7.68	130.29	113.40
1	C	99	LYS	CB-CA-C	7.13	124.67	110.40
1	A	75	ASP	CB-CG-OD2	-7.09	111.92	118.30
2	D	40	ARG	CD-NE-CZ	7.08	133.51	123.60
1	C	1	VAL	CG1-CB-CG2	7.00	122.10	110.90
1	C	105	LEU	CA-CB-CG	6.76	130.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	92	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	D	52	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	92	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	A	92	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	24	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	D	2	HIS	CA-CB-CG	-6.08	103.25	113.60
1	C	99	LYS	CA-CB-CG	6.02	126.64	113.40
2	B	6	GLU	CA-CB-CG	6.00	126.59	113.40
2	B	40	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	106	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	30	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	23	GLU	CA-CB-CG	5.51	125.52	113.40
1	A	64	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	74	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	D	52	ASP	CB-CG-OD1	5.17	122.95	118.30
2	D	2	HIS	N-CA-CB	5.16	119.88	110.60
1	C	47	ASP	O-C-N	5.15	130.94	122.70
2	D	141	LEU	CA-CB-CG	5.09	127.00	115.30
2	B	143	HIS	CA-CB-CG	-5.02	105.07	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	104	ARG	Sidechain
2	D	40	ARG	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	14	0
1	C	1069	0	1073	10	0
2	B	1122	0	1117	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1122	0	1117	12	0
3	A	43	0	30	0	0
3	B	43	0	30	4	0
3	C	43	0	30	0	0
3	D	43	0	30	1	0
4	A	52	0	0	1	0
4	B	52	0	0	0	0
4	C	66	0	0	0	0
4	D	46	0	0	1	0
All	All	4770	0	4500	49	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:147:HEM:HBC2	3:B:147:HEM:HMC1	1.71	0.72
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	2.20	0.71
1:A:96:VAL:O	1:A:99:LYS:HG2	1.96	0.66
2:D:124:PRO:HB2	2:D:125:PRO:HD3	1.80	0.63
1:C:49:SER:O	1:C:52:SER:HB3	2.03	0.58
1:A:96:VAL:HB	1:A:99:LYS:NZ	2.18	0.57
2:B:51:PRO:O	2:B:55:MET:HG2	2.07	0.55
2:B:1:MET:HG3	2:B:136:GLY:HA3	1.88	0.55
1:A:75:ASP:OD2	1:A:78:ASN:HB2	2.07	0.54
2:D:80:ASN:ND2	2:D:83:GLY:HA3	2.22	0.54
1:C:35:SER:HB3	2:D:131:GLN:HG3	1.89	0.54
2:D:143:HIS:HB3	4:D:414:HOH:O	2.07	0.53
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.89	0.53
1:A:13:ALA:O	1:A:17:VAL:HG23	2.10	0.51
1:C:90:LYS:HB3	1:C:90:LYS:NZ	2.26	0.50
2:B:6:GLU:CD	2:B:6:GLU:H	2.15	0.50
1:A:76:MET:N	1:A:77:PRO:CD	2.75	0.50
2:D:91:LEU:HD12	2:D:95:LYS:HB2	1.94	0.49
1:C:3:SER:HB2	1:C:4:PRO:HD2	1.94	0.49
1:C:90:LYS:O	1:C:92:ARG:HD3	2.13	0.49
1:A:3:SER:O	1:A:7:LYS:HG3	2.13	0.48
1:C:3:SER:HB2	1:C:4:PRO:CD	2.44	0.47
2:B:86:ALA:O	2:B:90:GLU:HG3	2.14	0.47
1:A:51:GLY:O	1:A:52:SER:C	2.51	0.47
2:B:82:LYS:HE3	2:B:143:HIS:CD2	2.50	0.46
2:D:50:THR:HB	2:D:51:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:HG3	1:A:116:GLU:HG2	1.97	0.45
3:B:147:HEM:CBC	3:B:147:HEM:HMC1	2.44	0.45
2:D:51:PRO:O	2:D:55:MET:HG2	2.18	0.44
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.99	0.44
2:B:3:LEU:HA	2:B:7:GLU:OE1	2.18	0.44
2:D:88:LEU:HD23	2:D:91:LEU:HD23	2.00	0.43
2:D:3:LEU:HD23	2:D:3:LEU:N	2.33	0.43
2:B:18:VAL:HG13	2:B:23:VAL:HG21	2.00	0.43
2:B:95:LYS:HD3	2:B:95:LYS:HA	1.72	0.43
1:A:21:ALA:HB1	1:A:63:ALA:HB1	2.01	0.43
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.19	0.43
3:D:147:HEM:HBC2	3:D:147:HEM:CMC	2.49	0.42
2:D:21:ASP:HA	2:D:65:LYS:HG3	2.00	0.42
1:C:20:HIS:HB3	1:C:24:TYR:CE1	2.55	0.42
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.55	0.42
2:D:4:THR:HB	2:D:5:PRO:HD2	2.02	0.41
1:C:43:PHE:N	1:C:44:PRO:CD	2.84	0.41
1:A:49:SER:O	1:A:52:SER:HB3	2.21	0.41
1:A:96:VAL:HB	1:A:99:LYS:HZ3	1.85	0.41
1:A:76:MET:HB2	1:A:77:PRO:HD3	2.03	0.41
2:B:96:LEU:HD13	3:B:147:HEM:C3D	2.57	0.40
1:A:4:PRO:HD2	4:A:308:HOH:O	2.21	0.40
2:B:57:ASN:HA	2:B:58:PRO:HD3	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	566/574 (99%)	554 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	108 (96%)	5 (4%)	39	32
1	C	113/113 (100%)	105 (93%)	8 (7%)	21	14
2	B	118/118 (100%)	110 (93%)	8 (7%)	22	15
2	D	118/118 (100%)	106 (90%)	12 (10%)	11	5
All	All	462/462 (100%)	429 (93%)	33 (7%)	21	14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	LYS
1	A	52	SER
1	A	90	LYS
1	A	109	LEU
2	B	1	MET
2	B	6	GLU
2	B	12	THR
2	B	22	GLU
2	B	26	GLU
2	B	32	LEU
2	B	66	LYS
2	B	104	ARG
1	C	1	VAL
1	C	16	LYS
1	C	52	SER
1	C	85	ASP
1	C	90	LYS

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Mol	Chain	Res	Type
1	C	92	ARG
1	C	99	LYS
1	C	105	LEU
2	D	1	MET
2	D	3	LEU
2	D	6	GLU
2	D	8	LYS
2	D	37	TYR
2	D	43	GLU
2	D	59	LYS
2	D	61	LYS
2	D	65	LYS
2	D	66	LYS
2	D	75	LEU
2	D	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
2	B	63	HIS
2	B	139	ASN
2	D	80	ASN
2	D	117	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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$
3	HEM	A	142	1	49,50,50	2.22	14 (28%)	46,82,82	2.03	10 (21%)
3	HEM	B	147	2	49,50,50	2.24	14 (28%)	46,82,82	1.81	13 (28%)
3	HEM	C	142	1	49,50,50	2.24	12 (24%)	46,82,82	1.83	13 (28%)
3	HEM	D	147	2	49,50,50	2.46	14 (28%)	46,82,82	1.60	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	142	1	-	0/14/114/114	0/0/8/8
3	HEM	B	147	2	-	0/14/114/114	0/0/8/8
3	HEM	C	142	1	-	0/14/114/114	0/0/8/8
3	HEM	D	147	2	-	0/14/114/114	0/0/8/8

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	C2D-C1D	7.16	1.46	1.44
3	D	147	HEM	C3D-C2D	-6.55	1.32	1.43
3	C	142	HEM	C3D-C2D	-6.07	1.33	1.43
3	B	147	HEM	C3C-C2C	-6.02	1.33	1.43
3	D	147	HEM	C3C-C2C	-6.02	1.33	1.43
3	B	147	HEM	C3D-C2D	-5.97	1.33	1.43
3	C	142	HEM	C3C-C2C	-5.82	1.33	1.43
3	A	142	HEM	C3D-C2D	-5.58	1.34	1.43
3	A	142	HEM	C3C-C2C	-5.41	1.34	1.43
3	C	142	HEM	C3B-C2B	-5.17	1.34	1.43
3	D	147	HEM	C3B-C2B	-5.11	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C4A-C3A	5.07	1.46	1.40
3	A	142	HEM	C4A-C3A	4.98	1.46	1.40
3	B	147	HEM	C3B-C2B	-4.97	1.35	1.43
3	C	142	HEM	C3D-C4D	-4.91	1.43	1.44
3	B	147	HEM	C3C-CAC	4.85	1.55	1.40
3	D	147	HEM	C3B-CAB	4.84	1.55	1.40
3	C	142	HEM	C3C-CAC	4.76	1.55	1.40
3	A	142	HEM	C3B-C2B	-4.73	1.35	1.43
3	D	147	HEM	C3C-CAC	4.57	1.54	1.40
3	C	142	HEM	C3B-CAB	4.47	1.54	1.40
3	A	142	HEM	C3B-CAB	4.31	1.54	1.40
3	A	142	HEM	C3D-C4D	-4.29	1.43	1.44
3	A	142	HEM	C3C-CAC	4.26	1.53	1.40
3	D	147	HEM	C4A-C3A	4.24	1.45	1.40
3	B	147	HEM	C3B-CAB	4.10	1.53	1.40
3	C	142	HEM	C4A-C3A	3.92	1.45	1.40
3	A	142	HEM	FE-NA	3.55	2.07	1.92
3	C	142	HEM	FE-NA	3.13	2.05	1.92
3	A	142	HEM	CHA-C4D	3.02	1.40	1.35
3	B	147	HEM	CMC-C2C	2.93	1.56	1.47
3	D	147	HEM	CMB-C2B	2.90	1.56	1.47
3	B	147	HEM	CAA-C2A	2.75	1.56	1.52
3	B	147	HEM	FE-NA	2.55	2.03	1.92
3	A	142	HEM	CMB-C2B	2.54	1.55	1.47
3	B	147	HEM	CMB-C2B	2.53	1.55	1.47
3	D	147	HEM	CMD-C2D	2.49	1.55	1.47
3	C	142	HEM	CHA-C4D	2.47	1.39	1.35
3	B	147	HEM	FE-NB	2.41	2.06	1.97
3	A	142	HEM	FE-NC	2.41	2.06	1.97
3	B	147	HEM	CMD-C2D	2.41	1.54	1.47
3	D	147	HEM	CMA-C3A	2.38	1.56	1.51
3	A	142	HEM	CMD-C2D	2.35	1.54	1.47
3	D	147	HEM	FE-NC	2.32	2.06	1.97
3	D	147	HEM	CMC-C2C	2.31	1.54	1.47
3	C	142	HEM	CMB-C2B	2.31	1.54	1.47
3	A	142	HEM	CMC-C2C	2.31	1.54	1.47
3	A	142	HEM	C2D-C1D	2.27	1.45	1.44
3	C	142	HEM	CMD-C2D	2.23	1.54	1.47
3	D	147	HEM	FE-NA	2.20	2.01	1.92
3	C	142	HEM	CMC-C2C	2.15	1.54	1.47
3	B	147	HEM	FE-NC	2.08	2.05	1.97
3	D	147	HEM	CAA-C2A	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CMA-C3A	2.01	1.55	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	C3B-C4B-NB	-6.73	109.19	114.00
3	A	142	HEM	C3B-C4B-NB	-6.42	109.41	114.00
3	C	142	HEM	C3B-C4B-NB	-6.33	109.47	114.00
3	B	147	HEM	C3B-C4B-NB	-6.00	109.71	114.00
3	A	142	HEM	C4A-CHB-C1B	-5.31	120.48	127.47
3	A	142	HEM	CBA-CAA-C2A	4.47	120.56	112.69
3	C	142	HEM	CMA-C3A-C4A	-4.18	122.20	128.62
3	A	142	HEM	CHD-C1D-ND	3.60	127.57	124.58
3	B	147	HEM	C2D-C1D-ND	-3.34	108.98	112.93
3	A	142	HEM	CMA-C3A-C4A	-3.33	123.50	128.62
3	D	147	HEM	C2D-C1D-ND	-3.32	109.01	112.93
3	A	142	HEM	C1A-CHA-C4D	-3.20	123.26	127.47
3	B	147	HEM	C4A-CHB-C1B	-3.15	123.33	127.47
3	C	142	HEM	CMA-C3A-C2A	3.10	130.78	124.94
3	A	142	HEM	CHB-C1B-NB	3.05	128.49	124.31
3	C	142	HEM	CHD-C4C-NC	3.04	127.38	124.73
3	B	147	HEM	CMA-C3A-C4A	-2.98	124.03	128.62
3	C	142	HEM	CBD-CAD-C3D	-2.87	108.11	114.37
3	A	142	HEM	C2D-C1D-ND	-2.80	109.62	112.93
3	B	147	HEM	CHD-C1D-ND	2.78	126.90	124.58
3	B	147	HEM	C1A-CHA-C4D	-2.76	123.84	127.47
3	C	142	HEM	C1A-CHA-C4D	-2.63	124.01	127.47
3	D	147	HEM	C1A-CHA-C4D	-2.60	124.05	127.47
3	B	147	HEM	C1A-C2A-C3A	2.57	109.58	106.92
3	C	142	HEM	CHD-C1D-ND	2.56	126.71	124.58
3	C	142	HEM	C2D-C1D-ND	-2.55	109.92	112.93
3	B	147	HEM	O1D-CGD-CBD	-2.54	114.30	123.03
3	D	147	HEM	O2D-CGD-O1D	2.47	129.59	123.30
3	C	142	HEM	C4A-CHB-C1B	-2.43	124.28	127.47
3	C	142	HEM	CBA-CAA-C2A	2.39	116.91	112.69
3	B	147	HEM	CMA-C3A-C2A	2.39	129.44	124.94
3	C	142	HEM	O2A-CGA-O1A	2.27	129.06	123.30
3	A	142	HEM	CMA-C3A-C2A	2.24	129.17	124.94
3	D	147	HEM	CMA-C3A-C4A	-2.18	125.28	128.62
3	B	147	HEM	CBA-CAA-C2A	-2.16	108.89	112.69
3	D	147	HEM	O1D-CGD-CBD	-2.15	115.62	123.03
3	C	142	HEM	O1A-CGA-CBA	-2.15	115.64	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CMD-C2D-C3D	2.08	130.31	125.60
3	C	142	HEM	O1D-CGD-CBD	-2.07	115.89	123.03
3	B	147	HEM	O1A-CGA-CBA	-2.05	115.97	123.03
3	A	142	HEM	CHB-C4A-NA	2.03	127.97	124.58
3	B	147	HEM	CHB-C4A-NA	2.02	127.96	124.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/141 (100%)	5.15	126 (89%) 0 1	8, 18, 45, 58	0
1	C	141/141 (100%)	4.42	116 (82%) 0 1	6, 13, 33, 47	0
2	B	146/146 (100%)	4.87	118 (80%) 0 1	7, 16, 49, 64	0
2	D	146/146 (100%)	5.50	132 (90%) 0 1	8, 19, 48, 103	0
All	All	574/574 (100%)	4.99	492 (85%) 0 1	6, 17, 45, 103	0

All (492) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	44	SER	24.5
2	D	33	VAL	23.5
2	B	33	VAL	23.5
1	A	34	LEU	22.7
2	D	77	HIS	22.5
2	D	44	SER	20.0
1	C	1	VAL	19.2
1	A	111	ALA	18.7
1	A	79	ALA	17.1
2	B	34	VAL	16.9
1	A	42	TYR	16.7
1	C	24	TYR	16.4
2	D	71	PHE	15.7
1	A	135	VAL	15.4
1	A	12	ALA	15.2
2	D	42	PHE	15.1
2	B	141	LEU	13.8
2	D	140	ALA	13.6
2	D	3	LEU	13.6
2	B	31	LEU	13.5
2	B	26	GLU	13.3

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Mol	Chain	Res	Type	RSRZ
2	B	1	MET	13.3
1	C	34	LEU	13.3
1	C	119	PRO	13.0
2	B	52	ASP	12.9
2	B	109	VAL	12.7
1	A	58	HIS	12.4
2	B	16	GLY	12.4
2	D	27	ALA	12.3
2	D	45	PHE	12.1
2	B	53	ALA	12.1
2	D	36	PRO	11.9
2	B	87	THR	11.8
2	B	63	HIS	11.8
1	A	76	MET	11.7
2	D	85	PHE	11.6
2	B	38	THR	11.5
2	D	16	GLY	11.5
1	A	43	PHE	11.4
1	A	98	PHE	11.3
2	D	88	LEU	11.2
2	D	91	LEU	11.1
1	A	97	ASN	10.8
1	C	55	VAL	10.7
1	C	25	GLY	10.6
1	A	140	TYR	10.5
1	A	14	TRP	10.5
2	D	110	LEU	10.4
1	C	15	GLY	10.2
1	C	80	LEU	10.2
2	D	105	LEU	10.2
1	C	81	SER	10.2
1	A	86	LEU	10.2
1	C	73	VAL	10.1
1	A	15	GLY	10.0
1	C	20	HIS	10.0
2	D	142	ALA	9.9
2	D	2	HIS	9.9
2	B	83	GLY	9.8
2	B	122	PHE	9.7
2	D	1	MET	9.7
1	A	52	SER	9.7
2	D	82	LYS	9.6

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Mol	Chain	Res	Type	RSRZ
2	B	137	VAL	9.5
1	A	107	VAL	9.4
2	D	31	LEU	9.4
1	C	113	LEU	9.3
2	D	66	LYS	9.1
2	D	15	TRP	9.1
2	B	100	PRO	9.0
2	D	76	ALA	9.0
1	C	48	LEU	8.9
2	D	122	PHE	8.9
2	B	121	GLU	8.8
2	D	7	GLU	8.8
2	D	13	ALA	8.7
2	D	46	GLY	8.7
1	A	17	VAL	8.6
1	A	93	VAL	8.6
2	D	34	VAL	8.6
1	C	133	SER	8.5
2	B	62	ALA	8.5
2	D	103	PHE	8.5
1	C	47	ASP	8.4
2	B	64	GLY	8.4
1	C	10	VAL	8.3
1	A	115	ALA	8.3
2	D	118	PHE	8.2
1	A	16	LYS	8.1
2	B	27	ALA	8.1
1	C	125	LEU	8.1
1	C	140	TYR	8.1
2	B	54	VAL	8.0
1	C	26	ALA	7.9
2	D	109	VAL	7.9
1	C	2	LEU	7.8
1	A	67	THR	7.8
1	A	80	LEU	7.8
1	C	58	HIS	7.7
1	A	126	ASP	7.7
1	C	82	ALA	7.7
2	D	32	LEU	7.7
1	A	27	GLU	7.6
1	A	24	TYR	7.6
2	D	54	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLY	7.5
1	A	128	PHE	7.5
1	C	116	GLU	7.5
2	B	70	ALA	7.4
1	C	33	PHE	7.3
2	D	28	LEU	7.3
2	B	3	LEU	7.3
1	A	26	ALA	7.2
1	C	129	LEU	7.2
2	B	17	LYS	7.2
2	B	140	ALA	7.2
2	B	127	GLN	7.2
1	C	141	ARG	7.2
2	D	37	TYR	7.1
2	B	68	LEU	7.1
1	A	25	GLY	7.1
2	B	50	THR	7.0
2	B	75	LEU	7.0
1	C	41	THR	7.0
2	B	125	PRO	6.9
1	C	132	VAL	6.8
2	D	113	VAL	6.8
1	A	33	PHE	6.8
2	D	22	GLU	6.8
1	A	114	PRO	6.8
2	B	113	VAL	6.6
2	D	124	PRO	6.6
2	D	53	ALA	6.5
2	B	115	ALA	6.5
1	C	101	LEU	6.5
2	B	11	VAL	6.5
2	D	98	VAL	6.4
1	A	100	LEU	6.4
1	C	91	LEU	6.4
2	D	23	VAL	6.4
2	B	32	LEU	6.4
2	D	134	VAL	6.4
2	D	68	LEU	6.4
1	A	28	ALA	6.4
2	D	48	LEU	6.3
2	D	114	LEU	6.3
1	C	38	THR	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	61	LYS	6.2
2	B	51	PRO	6.2
2	D	90	GLU	6.1
1	A	123	ALA	6.1
1	A	136	LEU	6.1
1	A	137	THR	6.1
1	A	59	GLY	6.1
1	A	87	HIS	6.0
1	A	2	LEU	5.9
2	D	121	GLU	5.9
1	A	117	PHE	5.9
1	A	119	PRO	5.8
2	D	93	CYS	5.8
2	B	48	LEU	5.8
1	A	109	LEU	5.7
2	B	49	SER	5.7
1	C	17	VAL	5.7
2	D	63	HIS	5.7
1	A	1	VAL	5.7
1	C	61	LYS	5.7
1	A	6	ASP	5.6
2	D	78	LEU	5.6
2	D	145	TYR	5.6
2	D	119	GLY	5.6
1	A	57	GLY	5.5
2	D	141	LEU	5.5
2	B	118	PHE	5.5
1	A	38	THR	5.5
1	A	73	VAL	5.4
2	B	133	VAL	5.4
1	C	29	LEU	5.4
2	D	75	LEU	5.4
1	C	28	ALA	5.4
2	B	103	PHE	5.4
1	A	120	ALA	5.4
2	D	137	VAL	5.2
1	C	103	HIS	5.2
1	C	52	SER	5.2
1	A	83	LEU	5.2
2	D	11	VAL	5.1
2	B	45	PHE	5.1
1	A	55	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	93	VAL	5.1
1	A	19	ALA	5.1
1	C	14	TRP	5.1
1	A	61	LYS	5.1
2	B	5	PRO	5.0
1	A	60	LYS	5.0
1	A	105	LEU	5.0
1	C	100	LEU	5.0
2	D	96	LEU	5.0
2	B	19	ASN	5.0
2	B	98	VAL	4.9
2	B	85	PHE	4.9
2	B	94	ASP	4.9
1	A	50	HIS	4.9
2	B	110	LEU	4.9
1	C	6	ASP	4.9
2	D	92	HIS	4.9
2	D	41	PHE	4.9
1	C	115	ALA	4.8
1	A	78	ASN	4.8
1	C	87	HIS	4.8
1	A	110	ALA	4.8
1	A	44	PRO	4.8
1	A	92	ARG	4.8
2	B	142	ALA	4.8
1	A	129	LEU	4.8
1	C	128	PHE	4.8
2	D	100	PRO	4.7
1	C	78	ASN	4.7
2	B	61	LYS	4.7
2	D	79	ASP	4.7
2	D	52	ASP	4.7
1	C	39	THR	4.7
2	B	15	TRP	4.7
1	C	105	LEU	4.6
1	C	104	CYS	4.6
2	B	130	TYR	4.6
2	D	35	TYR	4.6
1	A	62	VAL	4.6
2	B	60	VAL	4.6
2	B	119	GLY	4.6
2	B	9	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	106	LEU	4.5
2	D	120	LYS	4.5
2	D	87	THR	4.4
2	D	49	SER	4.4
2	B	146	HIS	4.4
2	B	76	ALA	4.4
2	D	108	ASN	4.4
1	A	139	LYS	4.3
2	B	8	LYS	4.3
1	C	106	LEU	4.3
2	D	29	GLY	4.3
1	A	125	LEU	4.3
2	D	30	ARG	4.3
1	A	84	SER	4.3
2	B	22	GLU	4.3
2	B	42	PHE	4.3
2	D	70	ALA	4.3
2	D	81	LEU	4.3
2	D	133	VAL	4.3
1	C	77	PRO	4.3
1	C	74	ASP	4.3
1	A	104	CYS	4.2
2	B	77	HIS	4.2
2	B	14	LEU	4.2
2	D	139	ASN	4.2
2	B	92	HIS	4.2
1	C	83	LEU	4.2
2	B	35	TYR	4.1
1	C	67	THR	4.1
2	B	96	LEU	4.1
2	B	41	PHE	4.1
2	D	40	ARG	4.1
1	C	11	LYS	4.1
1	A	13	ALA	4.1
1	C	19	ALA	4.0
2	D	97	HIS	4.0
1	A	63	ALA	4.0
1	C	76	MET	4.0
2	B	120	LYS	4.0
1	A	91	LEU	4.0
2	B	78	LEU	4.0
1	C	117	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	35	SER	3.9
2	D	128	ALA	3.9
2	D	94	ASP	3.9
1	C	16	LYS	3.9
1	C	79	ALA	3.9
2	B	86	ALA	3.9
1	C	96	VAL	3.8
1	A	133	SER	3.8
2	D	129	ALA	3.8
1	C	89	HIS	3.8
1	C	35	SER	3.8
1	C	70	VAL	3.8
2	D	111	VAL	3.8
2	D	56	GLY	3.7
2	B	102	ASN	3.7
1	A	130	ALA	3.7
1	C	85	ASP	3.7
2	D	57	ASN	3.7
1	A	8	THR	3.7
2	D	83	GLY	3.7
1	C	32	MET	3.7
1	A	18	GLY	3.7
2	D	60	VAL	3.7
1	C	108	THR	3.6
1	A	113	LEU	3.6
2	B	10	ALA	3.6
1	A	72	HIS	3.6
2	D	143	HIS	3.6
1	A	53	ALA	3.6
2	D	55	MET	3.6
1	A	46	PHE	3.6
2	B	81	LEU	3.6
1	C	94	ASP	3.6
1	C	46	PHE	3.6
2	B	58	PRO	3.6
2	B	138	ALA	3.6
2	B	2	HIS	3.6
1	A	82	ALA	3.5
2	D	115	ALA	3.5
1	C	122	HIS	3.5
2	D	67	VAL	3.5
1	A	49	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	134	VAL	3.5
1	A	69	ALA	3.5
2	B	6	GLU	3.5
1	A	29	LEU	3.5
1	C	65	ALA	3.5
2	B	7	GLU	3.4
1	C	139	LYS	3.4
1	C	51	GLY	3.4
2	D	24	GLY	3.4
2	D	9	SER	3.4
2	B	69	GLY	3.4
1	A	31	ARG	3.4
2	D	19	ASN	3.4
1	A	75	ASP	3.4
1	C	62	VAL	3.4
1	C	95	PRO	3.4
2	B	47	ASP	3.4
1	A	3	SER	3.4
1	C	72	HIS	3.4
2	D	125	PRO	3.4
1	A	74	ASP	3.4
1	C	136	LEU	3.3
2	B	114	LEU	3.3
1	A	9	ASN	3.3
2	B	104	ARG	3.3
1	C	98	PHE	3.3
1	C	66	LEU	3.3
1	A	96	VAL	3.3
2	B	18	VAL	3.3
1	C	126	ASP	3.3
1	C	45	HIS	3.3
1	A	103	HIS	3.2
2	B	20	VAL	3.2
2	D	21	ASP	3.2
1	A	5	ALA	3.2
1	C	21	ALA	3.2
2	B	145	TYR	3.2
1	C	90	LYS	3.2
1	C	130	ALA	3.2
1	A	37	PRO	3.2
1	C	102	SER	3.2
2	D	17	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	3.2
2	B	4	THR	3.1
2	D	50	THR	3.1
2	D	59	LYS	3.1
2	D	10	ALA	3.1
1	A	11	LYS	3.1
2	D	20	VAL	3.1
1	A	48	LEU	3.1
1	C	109	LEU	3.1
1	C	50	HIS	3.1
2	D	84	THR	3.1
1	A	10	VAL	3.1
2	D	12	THR	3.0
1	A	102	SER	3.0
2	D	104	ARG	3.0
1	C	49	SER	3.0
2	B	143	HIS	3.0
2	D	65	LYS	3.0
1	A	121	VAL	3.0
1	C	31	ARG	3.0
1	C	107	VAL	3.0
2	B	30	ARG	3.0
2	D	101	GLU	2.9
1	A	71	ALA	2.9
2	B	71	PHE	2.9
2	D	135	ALA	2.9
2	B	139	ASN	2.9
2	B	89	SER	2.9
2	D	47	ASP	2.9
1	A	88	ALA	2.9
1	A	68	ASN	2.9
1	C	60	LYS	2.9
2	B	57	ASN	2.9
2	B	105	LEU	2.9
1	C	121	VAL	2.9
2	B	43	GLU	2.9
2	D	18	VAL	2.9
1	A	131	SER	2.9
1	A	77	PRO	2.9
2	B	99	ASP	2.8
1	C	40	LYS	2.8
1	A	39	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	80	ASN	2.8
2	D	62	ALA	2.8
1	A	141	ARG	2.8
1	A	47	ASP	2.8
2	D	43	GLU	2.8
1	C	135	VAL	2.8
2	B	65	LYS	2.8
1	C	56	LYS	2.8
2	D	126	VAL	2.8
2	D	112	CYS	2.8
1	C	12	ALA	2.8
1	C	123	ALA	2.8
2	D	26	GLU	2.8
2	D	14	LEU	2.7
1	C	69	ALA	2.7
2	D	116	HIS	2.7
1	C	114	PRO	2.7
1	C	53	ALA	2.7
1	C	42	TYR	2.7
2	B	37	TYR	2.7
2	D	72	SER	2.7
1	A	45	HIS	2.7
1	A	134	THR	2.7
2	D	64	GLY	2.7
2	D	6	GLU	2.6
1	A	66	LEU	2.6
1	C	97	ASN	2.6
1	A	64	ASP	2.6
2	B	79	ASP	2.6
1	A	4	PRO	2.6
1	A	116	GLU	2.6
1	A	56	LYS	2.6
1	A	32	MET	2.6
2	D	86	ALA	2.6
1	A	23	GLU	2.6
2	D	127	GLN	2.5
1	C	43	PHE	2.5
1	A	127	LYS	2.5
1	A	90	LYS	2.5
2	D	146	HIS	2.5
1	A	36	PHE	2.5
2	B	12	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	112	HIS	2.5
2	B	82	LYS	2.5
2	B	40	ARG	2.5
2	D	73	ASP	2.5
1	C	8	THR	2.4
2	B	74	GLY	2.4
1	A	7	LYS	2.4
1	A	81	SER	2.4
2	B	67	VAL	2.4
1	C	23	GLU	2.4
1	C	99	LYS	2.4
1	C	44	PRO	2.4
2	D	95	LYS	2.4
1	A	118	THR	2.4
1	A	21	ALA	2.4
1	C	75	ASP	2.4
2	D	8	LYS	2.4
2	D	117	HIS	2.4
2	B	28	LEU	2.3
1	C	13	ALA	2.3
1	C	118	THR	2.3
2	B	97	HIS	2.3
1	C	3	SER	2.3
2	B	111	VAL	2.2
1	C	27	GLU	2.2
2	D	131	GLN	2.2
2	B	124	PRO	2.2
2	D	5	PRO	2.2
2	D	138	ALA	2.2
1	A	54	GLN	2.2
2	B	13	ALA	2.2
2	D	58	PRO	2.2
1	C	120	ALA	2.2
2	B	126	VAL	2.2
1	C	4	PRO	2.2
1	C	68	ASN	2.2
2	B	116	HIS	2.2
1	A	41	THR	2.1
2	B	59	LYS	2.1
2	B	21	ASP	2.1
2	B	73	ASP	2.1
2	D	89	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	86	LEU	2.1
1	A	85	ASP	2.1
2	B	117	HIS	2.1
2	B	72	SER	2.1
2	D	130	TYR	2.1
2	D	144	LYS	2.1
2	B	135	ALA	2.0
1	C	57	GLY	2.0
1	A	65	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	C	142	43/43	0.53	1.40	6,9,24,42	0
3	HEM	A	142	43/43	0.34	-0.59	9,14,30,49	0
3	HEM	B	147	43/43	0.31	-0.62	2,10,37,46	0
3	HEM	D	147	43/43	0.36	-0.73	10,18,51,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.