



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:16 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

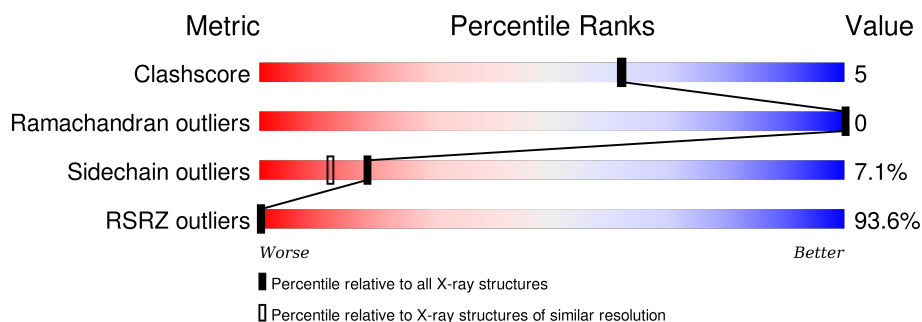
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>96%</div> <div>82%16%.</div> </div>
1	C	141	<div> <div>91%</div> <div>86%9%5%.</div> </div>
2	B	146	<div> <div>90%</div> <div>82%15%..</div> </div>
2	D	146	<div> <div>97%</div> <div>78%19%. .</div> </div>

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	HEM	A	142	-	-	-	X
3	HEM	C	142	-	-	-	X
3	HEM	D	147	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4770 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 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

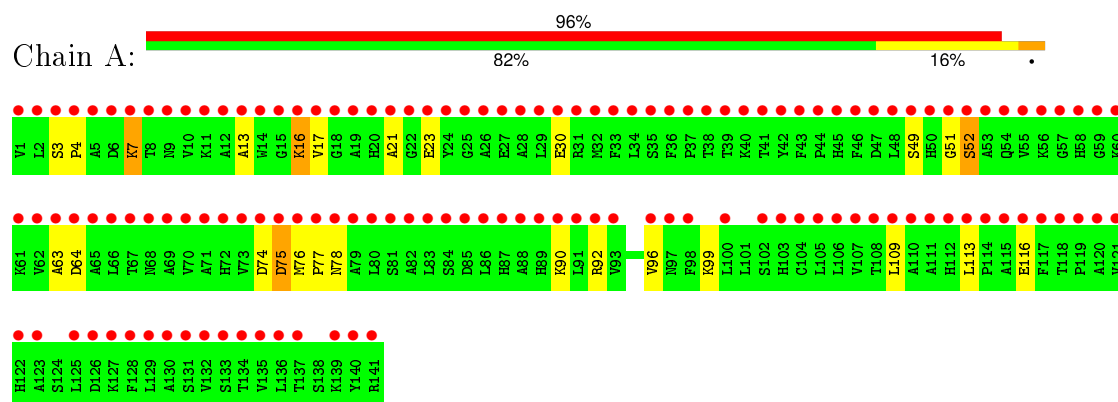
- Molecule 4 is water.

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		

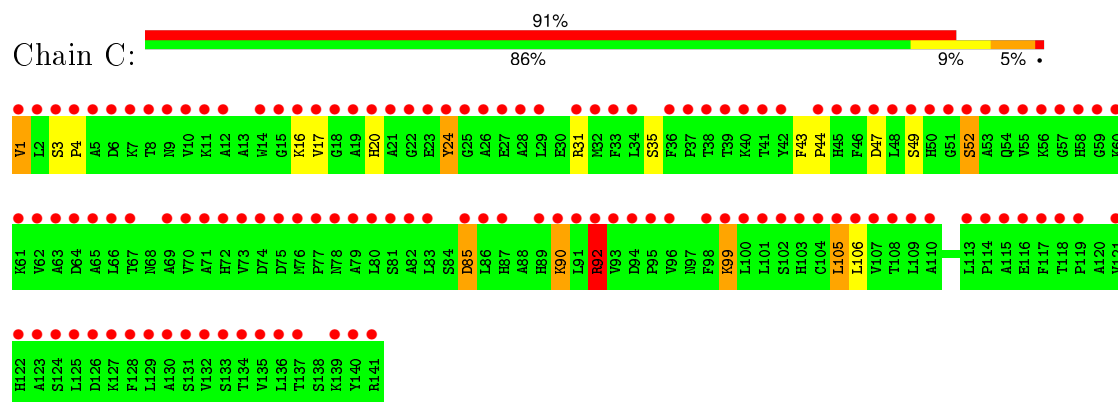
3 Residue-property plots

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.

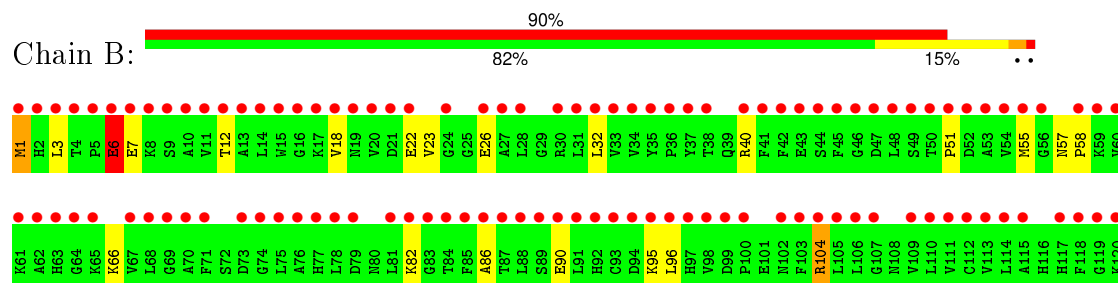
• Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

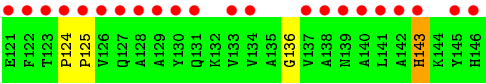


• Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

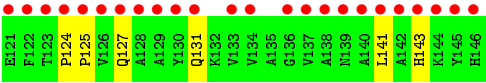
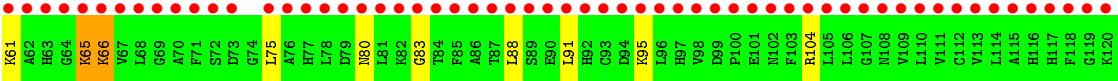
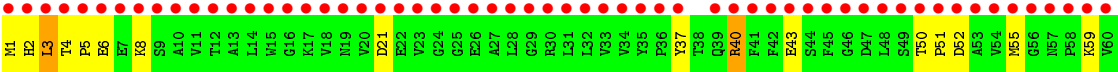
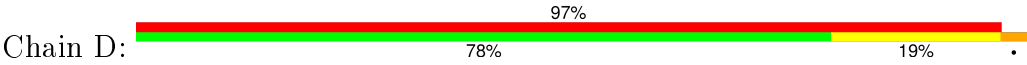


• Molecule 2: HEMOGLOBIN (BETA CHAIN)





● Molecule 2: HEMOGLOBIN (BETA CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.10 Å 112.00 Å 63.80 Å 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 1.73 Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , 0.223 0.493 , (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)	0.41 , 1498.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.81	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 Too-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 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	1069	0	1073	14	0
1	C	1069	0	1073	10	0
2	B	1122	0	1117	11	0
2	D	1122	0	1117	12	0
3	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (49) 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)
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	Interatomic distance (Å)	Clash overlap (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 [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	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
All	All	566/574 (99%)	554 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	108 (96%)	5 (4%)	35	30
1	C	113/113 (100%)	105 (93%)	8 (7%)	18	12
2	B	118/118 (100%)	110 (93%)	8 (7%)	20	13
2	D	118/118 (100%)	106 (90%)	12 (10%)	9	5
All	All	462/462 (100%)	429 (93%)	33 (7%)	18	12

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

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Mol	Chain	Res	Type
1	C	16	LYS
1	C	52	SER
1	C	85	ASP
1	C	90	LYS
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	30,50,50	2.65	9 (30%)	24,82,82	2.82	11 (45%)
3	HEM	B	147	2	30,50,50	2.57	12 (40%)	24,82,82	2.82	12 (50%)
3	HEM	C	142	1	30,50,50	2.64	8 (26%)	24,82,82	2.79	12 (50%)
3	HEM	D	147	2	30,50,50	2.87	10 (33%)	24,82,82	2.83	10 (41%)

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	-	0/10/54/54	0/0/8/8
3	HEM	B	147	2	-	0/10/54/54	0/0/8/8
3	HEM	C	142	1	-	0/10/54/54	0/0/8/8
3	HEM	D	147	2	-	0/10/54/54	0/0/8/8

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	C3B-C4B	-9.25	1.43	1.51
3	A	142	HEM	C3B-C4B	-8.38	1.44	1.51
3	C	142	HEM	C3B-C4B	-7.67	1.45	1.51
3	D	147	HEM	C2D-C3D	-7.40	1.32	1.54
3	C	142	HEM	C2D-C3D	-7.12	1.33	1.54
3	B	147	HEM	C2D-C3D	-7.06	1.33	1.54
3	A	142	HEM	C2D-C3D	-6.83	1.34	1.54
3	B	147	HEM	C3B-C4B	-6.50	1.46	1.51
3	C	142	HEM	C3D-C4D	-6.42	1.43	1.51
3	A	142	HEM	C3D-C4D	-6.30	1.43	1.51
3	D	147	HEM	C3D-C4D	-5.21	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3D-C4D	-5.13	1.45	1.51
3	C	142	HEM	C2C-C1C	-4.17	1.44	1.52
3	D	147	HEM	C2C-C1C	-4.05	1.44	1.52
3	B	147	HEM	C2C-C1C	-3.97	1.45	1.52
3	A	142	HEM	C2C-C1C	-3.28	1.46	1.52
3	C	142	HEM	C2B-C1B	-2.28	1.44	1.51
3	B	147	HEM	C2D-C1D	-2.15	1.44	1.51
3	A	142	HEM	C2B-C1B	-2.14	1.44	1.51
3	B	147	HEM	C2B-C1B	-2.13	1.44	1.51
3	D	147	HEM	C2B-C1B	-2.13	1.44	1.51
3	C	142	HEM	C2D-C1D	-2.12	1.44	1.51
3	A	142	HEM	C2D-C1D	-2.06	1.45	1.51
3	A	142	HEM	C1C-NC	2.05	1.38	1.36
3	B	147	HEM	CMA-C3A	2.05	1.55	1.51
3	D	147	HEM	CAA-C2A	2.11	1.55	1.52
3	C	142	HEM	C3C-CAC	2.17	1.55	1.51
3	A	142	HEM	C4C-NC	2.20	1.38	1.36
3	D	147	HEM	C3B-CAB	2.31	1.55	1.51
3	B	147	HEM	C3C-CAC	2.32	1.55	1.51
3	D	147	HEM	CMA-C3A	2.42	1.56	1.51
3	B	147	HEM	C1C-NC	2.43	1.39	1.36
3	B	147	HEM	FE-NC	2.48	2.05	1.95
3	C	142	HEM	C1C-NC	2.49	1.39	1.36
3	D	147	HEM	FE-NC	2.71	2.06	1.95
3	A	142	HEM	FE-NC	2.81	2.06	1.95
3	B	147	HEM	CAA-C2A	2.83	1.56	1.52
3	B	147	HEM	C4C-NC	2.96	1.39	1.36
3	D	147	HEM	C1C-NC	3.66	1.40	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C3C-CAC-CBC	-5.40	116.17	124.46
3	A	142	HEM	CAA-C2A-C1A	-5.04	121.54	127.01
3	D	147	HEM	C3B-CAB-CBB	-4.84	117.03	124.46
3	D	147	HEM	CAA-C2A-C1A	-4.74	121.86	127.01
3	C	142	HEM	C3B-CAB-CBB	-4.38	117.74	124.46
3	B	147	HEM	CAA-C2A-C1A	-4.24	122.40	127.01
3	C	142	HEM	CMA-C3A-C4A	-3.73	122.20	128.36
3	D	147	HEM	C3C-CAC-CBC	-3.49	119.11	124.46
3	C	142	HEM	CAA-C2A-C1A	-3.02	123.73	127.01
3	A	142	HEM	CMA-C3A-C4A	-2.94	123.50	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CMA-C3A-C4A	-2.62	124.03	128.36
3	C	142	HEM	C3C-CAC-CBC	-2.48	120.66	124.46
3	A	142	HEM	C1D-CHD-C4C	-2.11	122.30	125.82
3	B	147	HEM	CBA-CAA-C2A	-2.03	108.89	112.53
3	B	147	HEM	C1D-CHD-C4C	-2.01	122.47	125.82
3	B	147	HEM	CMA-C3A-C2A	2.01	129.44	125.24
3	D	147	HEM	CAA-CBA-CGA	2.10	116.59	112.75
3	A	142	HEM	C2C-C1C-CHC	2.25	127.11	123.68
3	C	142	HEM	CBA-CAA-C2A	2.44	116.91	112.53
3	B	147	HEM	CAD-C3D-C4D	2.58	121.58	112.47
3	D	147	HEM	CAD-C3D-C4D	2.60	121.64	112.47
3	C	142	HEM	CMA-C3A-C2A	2.65	130.78	125.24
3	A	142	HEM	CAD-C3D-C4D	2.97	122.94	112.47
3	D	147	HEM	CMD-C2D-C3D	3.25	128.75	114.35
3	C	142	HEM	CMD-C2D-C3D	3.33	129.10	114.35
3	A	142	HEM	CMD-C2D-C3D	3.50	129.82	114.35
3	B	147	HEM	CMD-C2D-C3D	3.61	130.31	114.35
3	C	142	HEM	CAD-C3D-C4D	3.74	125.66	112.47
3	C	142	HEM	CAD-C3D-C2D	3.94	124.56	113.22
3	D	147	HEM	C2D-C3D-C4D	4.09	108.43	101.50
3	A	142	HEM	C2D-C3D-C4D	4.27	108.74	101.50
3	A	142	HEM	CBA-CAA-C2A	4.48	120.56	112.53
3	C	142	HEM	CMB-C2B-C3B	4.56	127.91	116.53
3	B	147	HEM	C2D-C3D-C4D	4.63	109.36	101.50
3	A	142	HEM	CMC-C2C-C3C	4.68	128.20	116.53
3	B	147	HEM	CMC-C2C-C3C	4.72	128.31	116.53
3	D	147	HEM	CMC-C2C-C3C	4.78	128.45	116.53
3	C	142	HEM	C2D-C3D-C4D	4.81	109.65	101.50
3	B	147	HEM	CMB-C2B-C3B	4.82	128.56	116.53
3	C	142	HEM	CMC-C2C-C3C	4.91	128.79	116.53
3	D	147	HEM	CMB-C2B-C3B	4.91	128.80	116.53
3	A	142	HEM	CAD-C3D-C2D	5.17	128.07	113.22
3	A	142	HEM	CMB-C2B-C3B	5.22	129.56	116.53
3	B	147	HEM	CAD-C3D-C2D	5.47	128.95	113.22
3	D	147	HEM	CAD-C3D-C2D	5.81	129.91	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	4	0
3	D	147	HEM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/141 (100%)	6.18	135 (95%) 0 0	8, 18, 45, 58	0
1	C	141/141 (100%)	5.33	129 (91%) 0 0	6, 13, 33, 47	0
2	B	146/146 (100%)	5.61	131 (89%) 0 0	7, 16, 49, 64	0
2	D	146/146 (100%)	6.60	142 (97%) 0 0	8, 19, 48, 103	0
All	All	574/574 (100%)	5.93	537 (93%) 0 0	6, 17, 45, 103	0

All (537) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	77	HIS	28.1
2	D	44	SER	27.9
1	A	34	LEU	26.5
1	A	79	ALA	24.5
2	D	33	VAL	22.8
2	B	33	VAL	22.6
2	B	44	SER	22.2
1	A	111	ALA	22.0
2	B	1	MET	21.3
1	A	52	SER	20.2
1	C	1	VAL	18.6
2	D	16	GLY	16.9
2	B	31	LEU	16.7
1	C	119	PRO	16.6
1	A	135	VAL	16.3
1	C	15	GLY	16.1
2	B	70	ALA	16.0
2	D	27	ALA	15.8
2	B	83	GLY	15.7
2	D	140	ALA	15.7
1	C	20	HIS	15.5

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Mol	Chain	Res	Type	RSRZ
2	D	42	PHE	15.4
1	C	24	TYR	15.4
1	C	133	SER	15.3
1	A	12	ALA	15.2
2	D	13	ALA	15.0
2	B	38	THR	15.0
2	D	142	ALA	14.8
1	C	132	VAL	14.7
2	D	3	LEU	14.4
2	B	87	THR	14.2
1	A	97	ASN	14.1
1	C	82	ALA	13.9
2	B	137	VAL	13.8
1	C	55	VAL	13.8
2	B	26	GLU	13.7
2	B	53	ALA	13.6
2	B	141	LEU	13.6
2	D	36	PRO	13.2
2	B	64	GLY	13.2
1	A	115	ALA	12.8
1	A	42	TYR	12.7
1	A	26	ALA	12.6
2	D	31	LEU	12.5
1	C	73	VAL	12.4
1	A	107	VAL	12.2
1	A	140	TYR	12.1
1	A	28	ALA	12.0
2	D	71	PHE	12.0
2	D	37	TYR	11.9
2	D	88	LEU	11.7
2	B	34	VAL	11.6
2	D	40	ARG	11.5
1	A	59	GLY	11.5
1	C	113	LEU	11.5
2	D	66	LYS	11.3
2	D	2	HIS	11.3
2	D	15	TRP	11.2
1	A	67	THR	11.1
1	C	52	SER	11.0
2	D	61	LYS	11.0
1	A	123	ALA	11.0
1	C	25	GLY	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	10.8
1	A	17	VAL	10.8
2	D	93	CYS	10.7
2	D	53	ALA	10.5
2	D	82	LYS	10.5
1	A	58	HIS	10.5
2	B	63	HIS	10.4
1	A	86	LEU	10.4
1	C	34	LEU	10.4
2	B	109	VAL	10.2
2	D	96	LEU	10.2
2	B	142	ALA	10.2
2	D	85	PHE	10.2
2	D	76	ALA	10.2
2	B	122	PHE	10.1
2	D	122	PHE	10.0
1	A	129	LEU	10.0
1	C	81	SER	10.0
2	D	54	VAL	10.0
1	A	98	PHE	9.9
1	C	33	PHE	9.8
2	B	16	GLY	9.7
1	C	26	ALA	9.5
2	D	22	GLU	9.4
2	D	141	LEU	9.4
2	D	105	LEU	9.4
1	C	47	ASP	9.2
2	D	103	PHE	9.2
2	B	2	HIS	9.1
2	B	54	VAL	9.1
2	D	34	VAL	9.0
1	C	38	THR	8.9
2	D	46	GLY	8.9
1	C	136	LEU	8.8
1	C	48	LEU	8.7
2	B	62	ALA	8.7
1	A	128	PHE	8.6
2	D	7	GLU	8.6
2	B	100	PRO	8.5
1	A	24	TYR	8.5
2	B	52	ASP	8.5
1	A	43	PHE	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	27	GLU	8.5
1	A	25	GLY	8.5
1	C	93	VAL	8.4
2	D	124	PRO	8.4
1	A	126	ASP	8.4
1	A	51	GLY	8.4
2	B	49	SER	8.3
2	D	121	GLU	8.3
1	C	10	VAL	8.2
2	D	92	HIS	8.1
1	A	63	ALA	8.1
2	D	113	VAL	8.0
1	A	119	PRO	8.0
1	C	28	ALA	8.0
1	A	105	LEU	8.0
2	B	121	GLU	7.9
2	B	127	GLN	7.9
2	D	45	PHE	7.8
2	D	110	LEU	7.8
2	B	58	PRO	7.8
2	D	98	VAL	7.8
2	D	80	ASN	7.7
1	A	47	ASP	7.7
2	B	76	ALA	7.7
2	D	90	GLU	7.7
2	D	78	LEU	7.6
1	C	67	THR	7.6
1	A	10	VAL	7.6
1	C	125	LEU	7.5
1	A	93	VAL	7.5
2	D	100	PRO	7.5
1	A	88	ALA	7.5
2	D	41	PHE	7.5
1	A	18	GLY	7.5
2	B	68	LEU	7.5
1	A	104	CYS	7.4
2	B	98	VAL	7.4
1	C	6	ASP	7.4
1	A	137	THR	7.3
1	A	75	ASP	7.3
1	C	45	HIS	7.2
1	C	103	HIS	7.2

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Mol	Chain	Res	Type	RSRZ
2	D	1	MET	7.2
1	A	117	PHE	7.2
1	C	129	LEU	7.1
1	C	130	ALA	7.1
2	B	125	PRO	7.1
1	C	140	TYR	7.1
2	D	109	VAL	7.1
2	D	32	LEU	7.1
2	B	32	LEU	7.1
1	A	73	VAL	7.0
1	C	77	PRO	7.0
2	B	78	LEU	6.9
1	C	61	LYS	6.9
2	D	119	GLY	6.8
1	C	50	HIS	6.8
2	B	60	VAL	6.8
2	B	9	SER	6.8
1	A	76	MET	6.8
1	C	17	VAL	6.8
2	D	139	ASN	6.8
1	C	87	HIS	6.7
1	C	104	CYS	6.6
1	A	37	PRO	6.6
1	C	98	PHE	6.6
1	C	121	VAL	6.6
1	A	35	SER	6.5
1	A	80	LEU	6.5
2	B	75	LEU	6.5
1	A	103	HIS	6.5
2	B	17	LYS	6.5
2	D	128	ALA	6.5
1	C	141	ARG	6.5
2	D	79	ASP	6.5
1	A	9	ASN	6.5
1	A	60	LYS	6.4
2	D	81	LEU	6.4
1	A	136	LEU	6.4
2	D	11	VAL	6.4
2	D	68	LEU	6.4
2	B	115	ALA	6.3
1	A	14	TRP	6.3
2	B	11	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	HIS	6.3
1	A	33	PHE	6.3
2	B	61	LYS	6.3
1	A	120	ALA	6.3
1	C	41	THR	6.2
2	B	93	CYS	6.2
1	A	57	GLY	6.2
1	C	91	LEU	6.2
1	A	92	ARG	6.1
2	B	15	TRP	6.1
1	A	1	VAL	6.1
1	A	83	LEU	6.1
2	D	91	LEU	6.1
1	A	61	LYS	6.1
1	A	87	HIS	6.1
1	C	51	GLY	6.0
2	B	41	PHE	6.0
1	C	78	ASN	6.0
2	B	69	GLY	6.0
2	B	42	PHE	5.9
1	A	74	ASP	5.8
1	A	38	THR	5.8
2	D	63	HIS	5.8
2	B	19	ASN	5.8
1	C	70	VAL	5.8
2	D	23	VAL	5.8
2	D	28	LEU	5.8
1	A	114	PRO	5.8
2	B	4	THR	5.8
2	B	3	LEU	5.8
2	D	48	LEU	5.8
1	A	50	HIS	5.8
2	B	85	PHE	5.8
2	B	138	ALA	5.7
2	D	114	LEU	5.7
2	B	6	GLU	5.7
2	D	24	GLY	5.7
2	D	143	HIS	5.6
2	B	45	PHE	5.6
2	D	125	PRO	5.6
2	D	26	GLU	5.5
2	D	115	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	139	ASN	5.5
2	B	99	ASP	5.5
1	A	118	THR	5.5
1	A	130	ALA	5.5
2	B	134	VAL	5.5
2	D	67	VAL	5.5
1	C	108	THR	5.4
2	D	18	VAL	5.4
1	A	19	ALA	5.4
2	B	27	ALA	5.4
1	A	46	PHE	5.4
2	D	21	ASP	5.4
2	D	35	TYR	5.4
2	D	84	THR	5.4
1	C	80	LEU	5.3
1	C	134	THR	5.3
2	D	49	SER	5.3
2	D	52	ASP	5.3
2	D	65	LYS	5.3
2	D	97	HIS	5.3
1	C	118	THR	5.3
1	C	58	HIS	5.2
2	B	133	VAL	5.2
2	D	117	HIS	5.2
2	B	146	HIS	5.2
1	A	84	SER	5.2
2	B	113	VAL	5.2
1	C	2	LEU	5.2
1	A	5	ALA	5.2
2	B	35	TYR	5.1
1	A	55	VAL	5.1
1	C	101	LEU	5.1
1	C	102	SER	5.1
2	B	48	LEU	5.1
1	A	16	LYS	5.0
2	B	71	PHE	5.0
2	D	118	PHE	5.0
2	B	46	GLY	5.0
1	A	2	LEU	5.0
1	A	131	SER	5.0
2	B	119	GLY	5.0
1	A	68	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	103	PHE	5.0
1	A	91	LEU	4.9
1	C	3	SER	4.9
1	C	83	LEU	4.9
1	A	54	GLN	4.9
2	D	30	ARG	4.9
1	A	100	LEU	4.9
1	C	12	ALA	4.8
1	A	116	GLU	4.8
2	D	29	GLY	4.8
2	D	75	LEU	4.8
2	D	60	VAL	4.8
2	B	110	LEU	4.7
1	A	109	LEU	4.6
2	D	55	MET	4.6
1	C	44	PRO	4.6
1	A	53	ALA	4.6
2	D	83	GLY	4.6
1	C	117	PHE	4.6
2	D	12	THR	4.6
2	B	10	ALA	4.6
2	B	112	CYS	4.5
1	A	78	ASN	4.5
1	C	71	ALA	4.5
2	B	120	LYS	4.5
1	C	106	LEU	4.5
2	D	14	LEU	4.5
1	C	135	VAL	4.5
1	A	62	VAL	4.4
2	D	87	THR	4.4
2	B	86	ALA	4.4
2	B	140	ALA	4.4
2	D	5	PRO	4.4
1	A	122	HIS	4.4
2	D	72	SER	4.4
1	A	44	PRO	4.3
1	C	122	HIS	4.3
1	C	14	TRP	4.3
1	C	46	PHE	4.3
1	A	6	ASP	4.3
2	D	126	VAL	4.3
1	C	19	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	42	TYR	4.2
2	D	145	TYR	4.2
1	C	131	SER	4.2
2	D	9	SER	4.2
2	D	56	GLY	4.2
1	C	96	VAL	4.1
2	D	112	CYS	4.1
1	A	36	PHE	4.1
2	B	22	GLU	4.1
2	B	92	HIS	4.1
2	B	124	PRO	4.1
2	D	94	ASP	4.1
1	A	113	LEU	4.1
1	C	62	VAL	4.1
2	D	137	VAL	4.1
2	D	127	GLN	4.1
1	C	100	LEU	4.1
2	B	43	GLU	4.0
1	C	95	PRO	4.0
2	B	5	PRO	4.0
2	B	130	TYR	4.0
2	D	111	VAL	4.0
1	C	128	PHE	4.0
2	D	108	ASN	4.0
2	D	133	VAL	4.0
2	D	104	ARG	4.0
2	B	123	THR	4.0
1	C	116	GLU	4.0
2	D	86	ALA	4.0
1	A	64	ASP	3.9
1	C	27	GLU	3.9
2	B	89	SER	3.9
2	B	106	LEU	3.9
2	B	20	VAL	3.9
2	D	73	ASP	3.9
1	A	106	LEU	3.9
1	A	49	SER	3.9
2	B	7	GLU	3.9
2	D	4	THR	3.9
1	C	74	ASP	3.9
2	B	74	GLY	3.8
2	B	14	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	3	SER	3.8
2	B	94	ASP	3.8
1	C	63	ALA	3.8
2	B	12	THR	3.8
1	A	29	LEU	3.8
1	A	121	VAL	3.8
1	C	76	MET	3.8
2	B	50	THR	3.7
2	D	138	ALA	3.7
2	B	97	HIS	3.7
2	D	17	LYS	3.7
1	A	134	THR	3.7
1	A	45	HIS	3.7
1	C	107	VAL	3.7
1	C	109	LEU	3.7
1	A	110	ALA	3.7
1	A	125	LEU	3.7
1	C	39	THR	3.7
1	A	41	THR	3.7
1	C	123	ALA	3.7
1	C	49	SER	3.6
1	C	89	HIS	3.6
2	B	96	LEU	3.6
2	D	89	SER	3.6
2	D	47	ASP	3.6
1	A	132	VAL	3.6
2	B	77	HIS	3.6
1	C	115	ALA	3.6
2	D	106	LEU	3.6
2	D	146	HIS	3.6
1	C	126	ASP	3.6
2	B	79	ASP	3.6
2	B	111	VAL	3.6
1	A	81	SER	3.6
2	B	13	ALA	3.6
2	B	95	LYS	3.5
1	A	66	LEU	3.5
1	C	69	ALA	3.5
2	D	123	THR	3.5
1	A	139	LYS	3.5
1	A	48	LEU	3.5
1	C	31	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	129	ALA	3.4
2	D	107	GLY	3.4
1	C	21	ALA	3.4
2	B	65	LYS	3.4
2	B	118	PHE	3.4
1	A	108	THR	3.4
1	C	32	MET	3.4
1	C	94	ASP	3.4
2	B	47	ASP	3.4
1	C	37	PRO	3.4
1	C	114	PRO	3.4
2	B	18	VAL	3.4
1	C	105	LEU	3.4
2	D	116	HIS	3.4
2	D	57	ASN	3.4
2	B	37	TYR	3.4
2	B	126	VAL	3.4
1	A	56	LYS	3.4
2	B	59	LYS	3.4
2	D	51	PRO	3.4
2	B	145	TYR	3.3
1	C	66	LEU	3.3
1	C	79	ALA	3.3
2	D	25	GLY	3.3
2	D	130	TYR	3.3
1	C	11	LYS	3.3
2	B	84	THR	3.3
1	C	92	ARG	3.3
2	B	104	ARG	3.3
2	D	69	GLY	3.3
2	D	120	LYS	3.3
2	B	143	HIS	3.3
1	A	13	ALA	3.2
1	C	53	ALA	3.2
1	C	16	LYS	3.2
2	D	144	LYS	3.2
2	D	134	VAL	3.2
1	A	8	THR	3.2
2	B	24	GLY	3.2
1	A	82	ALA	3.2
1	C	139	LYS	3.2
2	D	19	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	99	LYS	3.2
2	D	62	ALA	3.2
2	D	20	VAL	3.1
1	C	29	LEU	3.1
2	B	30	ARG	3.1
2	B	129	ALA	3.1
1	A	127	LYS	3.1
2	B	40	ARG	3.1
2	D	6	GLU	3.1
1	A	77	PRO	3.1
2	D	8	LYS	3.1
1	C	8	THR	3.1
1	C	75	ASP	3.1
2	B	81	LEU	3.1
2	B	102	ASN	3.1
1	C	60	LYS	3.1
2	D	70	ALA	3.0
1	C	85	ASP	3.0
1	C	57	GLY	3.0
2	B	8	LYS	3.0
2	D	43	GLU	3.0
2	B	128	ALA	3.0
1	A	31	ARG	2.9
2	B	73	ASP	2.9
1	C	90	LYS	2.9
1	A	133	SER	2.9
2	D	58	PRO	2.9
2	D	95	LYS	2.9
1	A	4	PRO	2.9
1	A	7	LYS	2.9
1	A	90	LYS	2.9
1	C	127	LYS	2.8
1	C	40	LYS	2.8
2	B	107	GLY	2.8
2	D	50	THR	2.8
2	D	102	ASN	2.8
1	A	102	SER	2.7
1	C	64	ASP	2.7
2	B	131	GLN	2.7
2	B	82	LYS	2.7
2	B	51	PRO	2.7
1	C	9	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	88	LEU	2.7
2	B	55	MET	2.7
2	D	136	GLY	2.7
1	C	5	ALA	2.7
1	A	65	ALA	2.6
1	A	11	LYS	2.6
1	C	22	GLY	2.6
1	A	23	GLU	2.6
1	A	20	HIS	2.6
1	A	69	ALA	2.6
1	A	70	VAL	2.6
1	C	36	PHE	2.6
2	B	105	LEU	2.6
1	A	85	ASP	2.6
1	C	137	THR	2.6
2	B	56	GLY	2.6
2	D	10	ALA	2.6
1	C	56	LYS	2.6
1	A	72	HIS	2.6
1	C	72	HIS	2.6
1	C	65	ALA	2.5
2	B	114	LEU	2.5
1	C	7	LYS	2.5
1	A	141	ARG	2.5
2	B	90	GLU	2.5
2	D	101	GLU	2.5
1	A	96	VAL	2.5
1	C	54	GLN	2.4
2	B	21	ASP	2.4
1	C	18	GLY	2.4
1	C	86	LEU	2.4
1	A	32	MET	2.3
2	D	64	GLY	2.3
2	B	91	LEU	2.3
2	D	59	LYS	2.3
2	B	28	LEU	2.3
1	C	23	GLU	2.3
2	B	36	PRO	2.3
1	A	39	THR	2.3
1	C	59	GLY	2.2
2	B	117	HIS	2.2
2	B	67	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	39	GLN	2.2
1	A	89	HIS	2.2
1	A	21	ALA	2.2
1	C	110	ALA	2.1
2	D	99	ASP	2.1
1	A	71	ALA	2.1
2	D	131	GLN	2.1
1	C	124	SER	2.1
1	A	30	GLU	2.0
1	A	40	LYS	2.0
1	A	22	GLY	2.0
1	C	4	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	C	142	43/43	0.45	0.51	0.50	6,9,24,42	0
3	HEM	A	142	43/43	0.47	0.42	-0.18	9,14,30,49	0
3	HEM	B	147	43/43	0.65	0.34	-0.54	2,10,37,46	0
3	HEM	D	147	43/43	0.45	0.40	-0.60	10,18,51,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.