



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:57 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

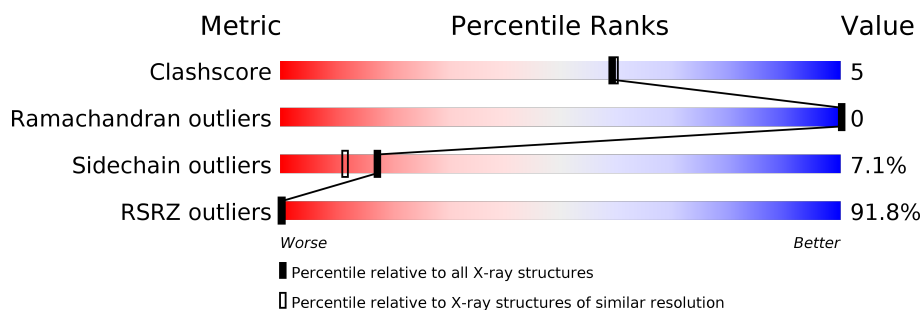
# 1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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  $\geq 3$ , 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>92%</div> <div>82%16%.</div> </div>
1	C	141	<div> <div>89%</div> <div>86%9%5%.</div> </div>
2	B	146	<div> <div>90%</div> <div>82%15%..</div> </div>
2	D	146	<div> <div>96%</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			

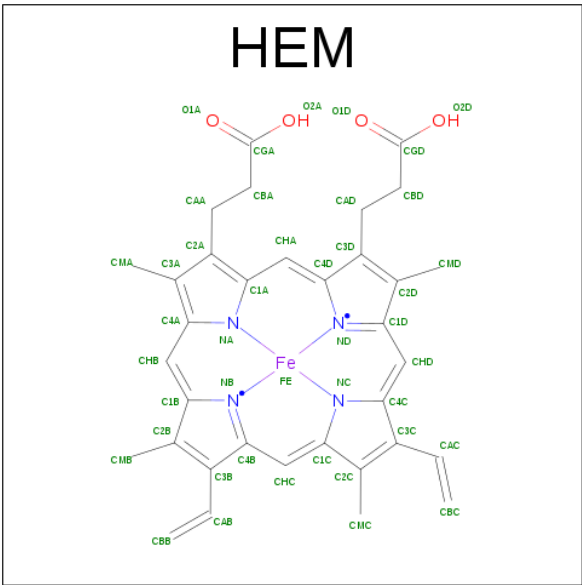
- Molecule 2 is a protein called HEMOGLOBIN (BETA CHAIN).

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

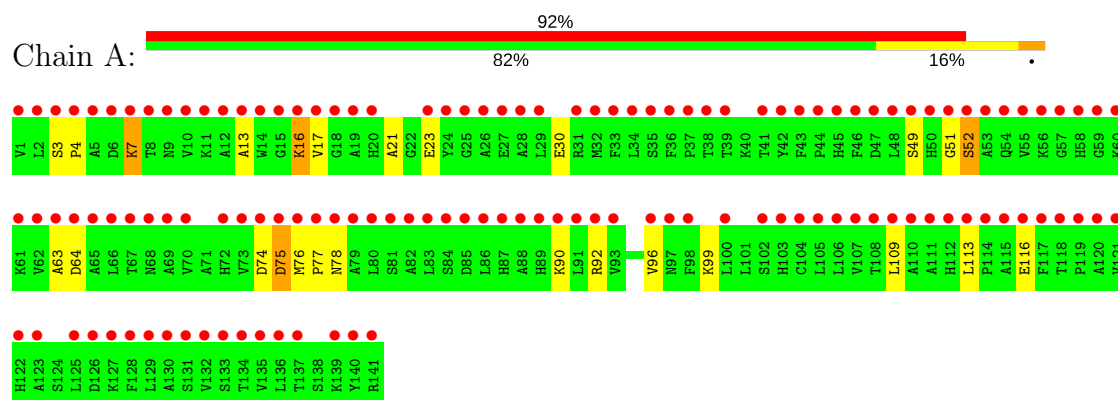
- Molecule 4 is water.

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		

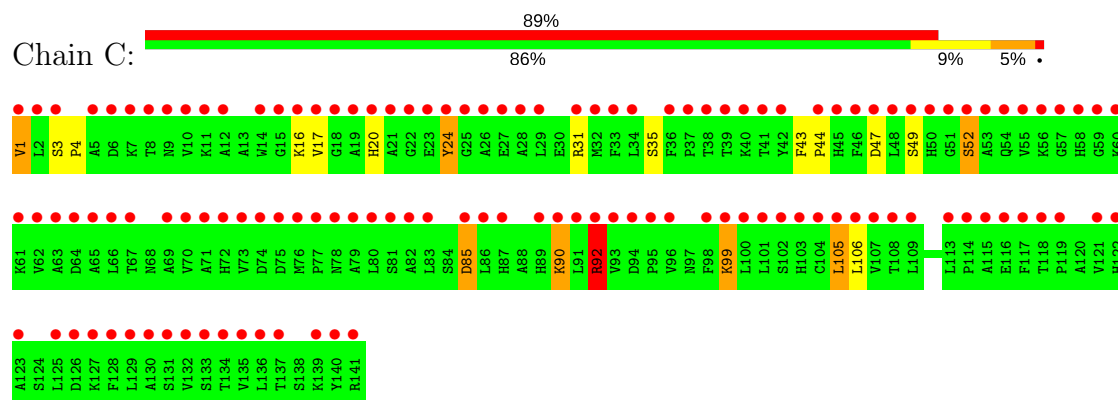
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

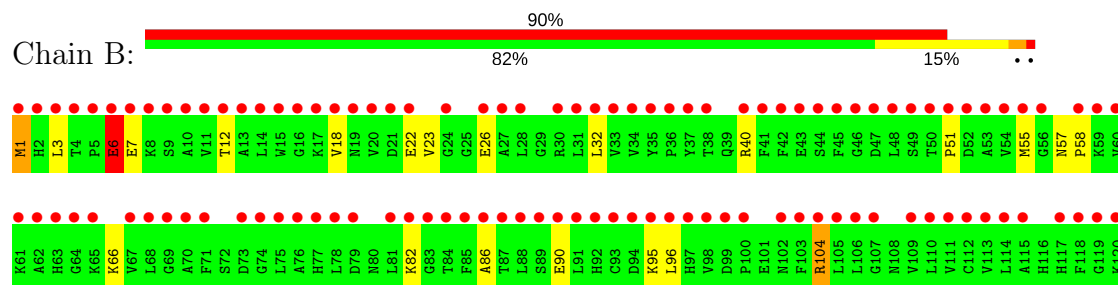
#### • Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

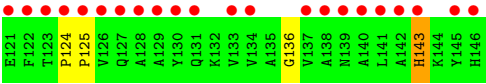


#### • Molecule 1: HEMOGLOBIN (ALPHA CHAIN)

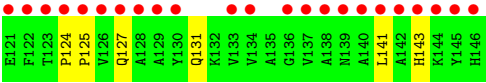
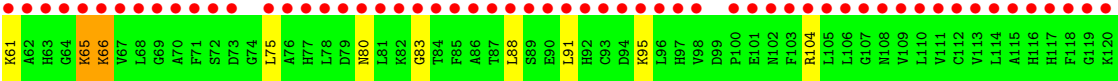
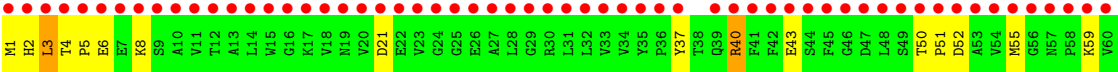
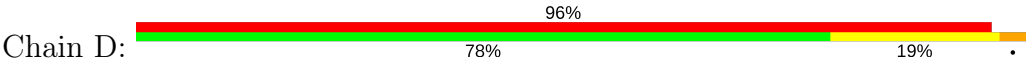


#### • Molecule 2: HEMOGLOBIN (BETA CHAIN)





● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.73Å)	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 <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 1496.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.40	EDS
Total number of atoms	4770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.99	0.44
2:D:51:PRO:O	2:D:55:MET:HG2	2.18	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:HA	2:B:95:LYS:HD3	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:76:MET:HB2	1:A:77:PRO:HD3	2.03	0.41
1:A:96:VAL:HB	1:A:99:LYS:HZ3	1.85	0.41
1:A:4:PRO:HD2	4:A:308:HOH:O	2.21	0.40
2:B:96:LEU:HD13	3:B:147:HEM:C3D	2.57	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

*Continued on next page...*

*Continued from previous page...*

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 ⓘ

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%)	33	28
1	C	113/113 (100%)	105 (93%)	8 (7%)	17	11
2	B	118/118 (100%)	110 (93%)	8 (7%)	18	13
2	D	118/118 (100%)	106 (90%)	12 (10%)	8	4
All	All	462/462 (100%)	429 (93%)	33 (7%)	17	11

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

*Continued on next page...*

*Continued from previous page...*

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	28,50,50	1.82	6 (21%)	17,82,82	1.97	6 (35%)
3	HEM	B	147	2	28,50,50	2.15	9 (32%)	17,82,82	1.87	5 (29%)
3	HEM	C	142	1	28,50,50	2.01	6 (21%)	17,82,82	1.90	7 (41%)
3	HEM	D	147	2	28,50,50	2.15	8 (28%)	17,82,82	1.55	6 (35%)

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	-	0/6/54/54	0/0/8/8
3	HEM	B	147	2	-	0/6/54/54	0/0/8/8
3	HEM	C	142	1	-	0/6/54/54	0/0/8/8
3	HEM	D	147	2	-	0/6/54/54	0/0/8/8

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3C-C2C	-5.39	1.33	1.40
3	D	147	HEM	C3C-C2C	-5.39	1.33	1.40
3	C	142	HEM	C3C-C2C	-5.13	1.33	1.40
3	A	142	HEM	C3C-C2C	-4.59	1.34	1.40
3	C	142	HEM	C3B-C2B	-4.26	1.34	1.40
3	D	147	HEM	C3B-C2B	-4.19	1.34	1.40
3	B	147	HEM	C3B-C2B	-4.00	1.35	1.40
3	A	142	HEM	C3B-C2B	-3.69	1.35	1.40
3	B	147	HEM	C1B-NB	2.07	1.39	1.36
3	B	147	HEM	CMA-C3A	2.08	1.55	1.51
3	D	147	HEM	CAA-C2A	2.13	1.55	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C4D-ND	2.27	1.39	1.36
3	D	147	HEM	CMB-C2B	2.27	1.56	1.51
3	A	142	HEM	C1B-NB	2.29	1.39	1.36
3	B	147	HEM	CMC-C2C	2.31	1.56	1.51
3	B	147	HEM	C4C-NC	2.45	1.39	1.36
3	D	147	HEM	CMA-C3A	2.45	1.56	1.51
3	C	142	HEM	C1B-NB	2.62	1.39	1.36
3	C	142	HEM	C4D-ND	2.72	1.40	1.36
3	B	147	HEM	C3B-CAB	2.72	1.53	1.47
3	B	147	HEM	CAA-C2A	2.85	1.56	1.52
3	A	142	HEM	C3C-CAC	3.06	1.53	1.47
3	A	142	HEM	C3B-CAB	3.07	1.54	1.47
3	D	147	HEM	C1C-NC	3.19	1.40	1.36
3	C	142	HEM	C3B-CAB	3.31	1.54	1.47
3	D	147	HEM	C3C-CAC	3.55	1.54	1.47
3	C	142	HEM	C3C-CAC	3.86	1.55	1.47
3	D	147	HEM	C3B-CAB	3.91	1.55	1.47
3	B	147	HEM	C3C-CAC	4.00	1.55	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CMA-C3A-C4A	-4.08	122.20	128.46
3	B	147	HEM	CMD-C2D-C1D	-3.79	122.64	128.46
3	A	142	HEM	CMD-C2D-C1D	-3.25	123.48	128.46
3	A	142	HEM	CMA-C3A-C4A	-3.23	123.50	128.46
3	D	147	HEM	CMD-C2D-C1D	-2.90	124.00	128.46
3	B	147	HEM	CMA-C3A-C4A	-2.88	124.03	128.46
3	C	142	HEM	CMD-C2D-C1D	-2.57	124.51	128.46
3	C	142	HEM	CBD-CAD-C3D	-2.29	108.11	112.47
3	D	147	HEM	CAD-CBD-CGD	-2.21	108.88	112.66
3	D	147	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
3	D	147	HEM	CMD-C2D-C3D	2.02	128.75	124.94
3	C	142	HEM	CMC-C2C-C3C	2.10	128.79	124.89
3	D	147	HEM	CMB-C2B-C3B	2.11	128.80	124.89
3	C	142	HEM	CMD-C2D-C3D	2.20	129.10	124.94
3	A	142	HEM	CMA-C3A-C2A	2.24	129.17	124.94
3	D	147	HEM	CAA-CBA-CGA	2.30	116.59	112.66
3	C	142	HEM	CBA-CAA-C2A	2.31	116.91	112.48
3	B	147	HEM	CMA-C3A-C2A	2.39	129.44	124.94
3	A	142	HEM	CMB-C2B-C3B	2.51	129.56	124.89
3	B	147	HEM	C4C-C3C-C2C	2.56	108.68	106.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CMD-C2D-C3D	2.59	129.82	124.94
3	B	147	HEM	CMD-C2D-C3D	2.85	130.31	124.94
3	C	142	HEM	CMA-C3A-C2A	3.10	130.78	124.94
3	A	142	HEM	CBA-CAA-C2A	4.22	120.56	112.48

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	141/141 (100%)	5.91	130 (92%) 0 0	8, 18, 45, 58	0
1	C	141/141 (100%)	5.10	126 (89%) 0 0	6, 13, 33, 47	0
2	B	146/146 (100%)	5.37	131 (89%) 0 0	7, 16, 49, 64	0
2	D	146/146 (100%)	6.33	140 (95%) 0 0	8, 19, 48, 103	0
All	All	574/574 (100%)	5.68	527 (91%) 0 0	6, 17, 45, 103	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	77	HIS	27.5
2	D	44	SER	27.0
1	A	34	LEU	25.5
1	A	79	ALA	23.4
2	D	33	VAL	21.6
2	B	44	SER	21.5
2	B	33	VAL	21.5
1	A	111	ALA	21.0
2	B	1	MET	20.9
1	A	52	SER	19.6
1	C	1	VAL	17.6
2	D	16	GLY	16.2
1	C	119	PRO	16.1
2	B	31	LEU	16.0
1	A	135	VAL	15.5
1	C	15	GLY	15.5
2	B	70	ALA	15.3
2	B	83	GLY	15.1
1	C	20	HIS	15.1
2	D	27	ALA	15.1
1	C	24	TYR	15.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	140	ALA	15.0
1	C	133	SER	14.8
2	D	42	PHE	14.8
1	A	12	ALA	14.5
2	B	38	THR	14.5
2	D	13	ALA	14.3
2	D	142	ALA	14.1
1	C	132	VAL	13.9
2	D	3	LEU	13.8
2	B	87	THR	13.7
1	A	97	ASN	13.7
2	B	26	GLU	13.4
1	C	82	ALA	13.2
2	B	137	VAL	13.1
2	B	141	LEU	13.0
1	C	55	VAL	13.0
2	B	53	ALA	12.9
2	D	36	PRO	12.8
2	B	64	GLY	12.6
1	A	42	TYR	12.3
1	A	115	ALA	12.2
2	D	31	LEU	12.0
1	A	26	ALA	12.0
1	A	140	TYR	11.8
1	C	73	VAL	11.8
2	D	37	TYR	11.5
1	A	107	VAL	11.5
2	D	71	PHE	11.5
1	A	28	ALA	11.4
2	D	40	ARG	11.3
2	D	88	LEU	11.2
1	A	59	GLY	11.0
2	D	66	LYS	11.0
1	C	113	LEU	11.0
2	D	2	HIS	11.0
2	B	34	VAL	11.0
2	D	15	TRP	10.8
1	A	67	THR	10.7
2	D	61	LYS	10.7
1	C	52	SER	10.6
1	C	25	GLY	10.5
1	A	123	ALA	10.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	93	CYS	10.4
1	A	15	GLY	10.4
2	D	82	LYS	10.2
1	A	17	VAL	10.2
1	A	58	HIS	10.2
2	B	63	HIS	10.2
2	D	53	ALA	10.1
1	A	86	LEU	9.9
1	C	34	LEU	9.9
2	D	96	LEU	9.8
2	B	142	ALA	9.7
2	D	85	PHE	9.7
2	B	109	VAL	9.7
2	B	122	PHE	9.7
2	D	76	ALA	9.7
1	C	81	SER	9.6
2	D	122	PHE	9.6
1	A	129	LEU	9.6
1	A	98	PHE	9.4
2	D	54	VAL	9.4
1	C	33	PHE	9.3
2	B	16	GLY	9.3
2	D	22	GLU	9.2
2	D	141	LEU	9.0
1	C	26	ALA	9.0
2	D	105	LEU	9.0
1	C	47	ASP	8.9
2	B	2	HIS	8.9
2	D	103	PHE	8.8
1	C	38	THR	8.6
2	B	54	VAL	8.6
2	D	46	GLY	8.5
2	D	34	VAL	8.4
2	D	7	GLU	8.4
1	C	136	LEU	8.4
1	C	48	LEU	8.3
1	A	24	TYR	8.3
1	A	27	GLU	8.3
2	B	100	PRO	8.3
1	A	128	PHE	8.2
2	B	62	ALA	8.2
2	B	52	ASP	8.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	25	GLY	8.1
1	A	43	PHE	8.1
2	D	124	PRO	8.1
2	D	121	GLU	8.1
1	A	126	ASP	8.1
2	B	49	SER	8.0
1	A	51	GLY	8.0
1	C	93	VAL	8.0
2	D	92	HIS	7.9
1	C	10	VAL	7.7
1	A	119	PRO	7.7
2	B	121	GLU	7.7
1	A	63	ALA	7.7
2	B	127	GLN	7.6
1	A	105	LEU	7.6
1	C	28	ALA	7.6
2	D	113	VAL	7.6
2	B	58	PRO	7.6
2	D	80	ASN	7.5
2	D	110	LEU	7.5
2	D	45	PHE	7.5
2	D	90	GLU	7.5
1	A	47	ASP	7.4
2	D	98	VAL	7.3
1	C	67	THR	7.3
2	D	78	LEU	7.3
2	D	100	PRO	7.3
2	B	76	ALA	7.3
1	C	125	LEU	7.2
1	A	104	CYS	7.2
1	A	10	VAL	7.2
2	D	41	PHE	7.2
1	A	88	ALA	7.2
1	A	18	GLY	7.1
1	C	6	ASP	7.1
2	B	68	LEU	7.1
1	A	93	VAL	7.1
1	A	137	THR	7.1
1	A	75	ASP	7.0
1	C	45	HIS	7.0
2	D	1	MET	7.0
1	C	103	HIS	7.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	98	VAL	7.0
1	C	140	TYR	6.9
2	B	125	PRO	6.9
1	C	129	LEU	6.8
1	A	117	PHE	6.8
1	C	130	ALA	6.8
2	B	32	LEU	6.8
2	D	32	LEU	6.8
1	C	77	PRO	6.7
2	D	109	VAL	6.7
1	C	61	LYS	6.7
1	C	50	HIS	6.7
2	B	78	LEU	6.6
1	A	76	MET	6.6
1	A	73	VAL	6.6
2	D	119	GLY	6.6
2	D	139	ASN	6.6
2	B	9	SER	6.5
1	C	87	HIS	6.5
2	B	60	VAL	6.4
1	A	37	PRO	6.4
1	C	104	CYS	6.4
1	C	17	VAL	6.4
1	A	103	HIS	6.3
1	A	35	SER	6.3
2	B	17	LYS	6.3
1	A	9	ASN	6.3
1	C	141	ARG	6.3
1	A	60	LYS	6.3
1	C	98	PHE	6.3
1	A	80	LEU	6.2
2	B	75	LEU	6.2
2	D	79	ASP	6.2
1	C	121	VAL	6.2
1	A	112	HIS	6.1
2	D	128	ALA	6.1
2	B	61	LYS	6.1
2	D	81	LEU	6.1
1	A	136	LEU	6.1
2	D	68	LEU	6.1
1	A	14	TRP	6.1
2	B	115	ALA	6.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	33	PHE	6.0
2	D	11	VAL	6.0
1	A	92	ARG	6.0
2	B	93	CYS	6.0
1	C	41	THR	6.0
2	B	11	VAL	6.0
1	A	120	ALA	5.9
1	A	61	LYS	5.9
1	A	57	GLY	5.9
1	C	91	LEU	5.9
1	A	87	HIS	5.9
2	B	15	TRP	5.9
2	D	91	LEU	5.8
1	A	83	LEU	5.8
1	C	78	ASN	5.8
1	A	1	VAL	5.8
1	C	51	GLY	5.8
2	B	41	PHE	5.7
2	B	69	GLY	5.7
2	B	19	ASN	5.7
2	D	63	HIS	5.7
2	B	42	PHE	5.6
1	A	74	ASP	5.6
1	A	38	THR	5.6
1	A	50	HIS	5.6
1	A	114	PRO	5.6
2	B	4	THR	5.6
2	B	6	GLU	5.6
2	B	3	LEU	5.5
2	D	28	LEU	5.5
2	D	48	LEU	5.5
2	B	85	PHE	5.5
2	D	143	HIS	5.5
1	C	70	VAL	5.5
2	D	23	VAL	5.5
2	D	114	LEU	5.5
2	B	138	ALA	5.4
2	D	24	GLY	5.4
2	D	26	GLU	5.4
2	D	125	PRO	5.4
2	B	139	ASN	5.4
2	B	45	PHE	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	99	ASP	5.3
1	A	118	THR	5.3
2	D	115	ALA	5.2
1	C	108	THR	5.2
2	D	35	TYR	5.2
1	A	130	ALA	5.2
2	D	21	ASP	5.2
1	A	46	PHE	5.2
2	D	84	THR	5.1
1	A	19	ALA	5.1
2	B	27	ALA	5.1
2	B	134	VAL	5.1
2	D	49	SER	5.1
2	D	67	VAL	5.1
2	D	65	LYS	5.1
2	D	97	HIS	5.1
1	C	134	THR	5.1
2	D	18	VAL	5.1
2	D	52	ASP	5.1
1	C	58	HIS	5.1
1	C	80	LEU	5.1
2	D	117	HIS	5.1
2	B	146	HIS	5.0
1	C	118	THR	5.0
1	A	84	SER	5.0
2	B	35	TYR	5.0
1	C	2	LEU	4.9
2	B	133	VAL	4.9
1	A	16	LYS	4.9
1	C	102	SER	4.9
1	A	5	ALA	4.9
2	B	113	VAL	4.9
1	A	68	ASN	4.8
1	C	101	LEU	4.8
2	B	48	LEU	4.8
1	A	55	VAL	4.8
2	B	71	PHE	4.8
1	A	131	SER	4.8
2	B	46	GLY	4.8
1	C	3	SER	4.8
2	B	119	GLY	4.8
1	A	2	LEU	4.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	118	PHE	4.7
2	D	30	ARG	4.7
1	A	54	GLN	4.7
1	A	91	LEU	4.7
2	B	103	PHE	4.7
1	A	116	GLU	4.7
1	A	100	LEU	4.6
1	C	83	LEU	4.6
1	C	12	ALA	4.6
2	D	29	GLY	4.5
2	D	75	LEU	4.5
2	D	55	MET	4.5
2	B	110	LEU	4.5
2	D	60	VAL	4.5
1	A	109	LEU	4.4
1	C	44	PRO	4.4
1	A	78	ASN	4.4
2	D	12	THR	4.4
2	D	83	GLY	4.4
2	B	112	CYS	4.4
2	B	120	LYS	4.4
1	C	117	PHE	4.3
1	A	53	ALA	4.3
2	B	10	ALA	4.3
1	C	71	ALA	4.3
1	A	122	HIS	4.3
2	D	5	PRO	4.3
1	C	106	LEU	4.3
2	D	14	LEU	4.2
2	D	87	THR	4.2
2	D	72	SER	4.2
1	C	122	HIS	4.2
1	A	44	PRO	4.2
1	C	135	VAL	4.2
2	B	86	ALA	4.2
2	B	140	ALA	4.2
1	A	62	VAL	4.2
1	A	6	ASP	4.1
1	C	14	TRP	4.1
1	C	42	TYR	4.1
2	D	145	TYR	4.1
1	C	46	PHE	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	131	SER	4.0
2	D	9	SER	4.0
1	C	19	ALA	4.0
2	D	126	VAL	4.0
2	B	22	GLU	4.0
2	D	112	CYS	4.0
2	D	56	GLY	4.0
2	B	92	HIS	4.0
2	B	124	PRO	3.9
2	D	127	GLN	3.9
2	B	43	GLU	3.9
1	A	36	PHE	3.9
2	D	94	ASP	3.9
2	B	130	TYR	3.9
2	D	108	ASN	3.9
1	C	95	PRO	3.9
2	B	5	PRO	3.9
1	C	116	GLU	3.9
2	D	104	ARG	3.9
1	C	96	VAL	3.9
1	A	113	LEU	3.9
1	C	100	LEU	3.8
1	C	27	GLU	3.8
1	C	128	PHE	3.8
2	B	123	THR	3.8
1	C	62	VAL	3.8
2	D	137	VAL	3.8
1	A	64	ASP	3.8
2	B	89	SER	3.8
2	D	111	VAL	3.8
2	D	133	VAL	3.8
2	D	86	ALA	3.8
2	B	7	GLU	3.7
2	D	73	ASP	3.7
2	B	106	LEU	3.7
1	A	49	SER	3.7
1	C	74	ASP	3.7
2	D	4	THR	3.7
1	A	106	LEU	3.7
2	B	94	ASP	3.6
1	C	76	MET	3.6
1	A	3	SER	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	74	GLY	3.6
2	B	20	VAL	3.6
2	B	14	LEU	3.6
2	B	97	HIS	3.6
2	B	12	THR	3.6
2	D	17	LYS	3.6
1	A	45	HIS	3.6
1	A	29	LEU	3.6
2	B	50	THR	3.6
1	C	63	ALA	3.6
1	A	134	THR	3.5
2	D	138	ALA	3.5
1	C	89	HIS	3.5
1	A	121	VAL	3.5
1	A	41	THR	3.5
1	C	39	THR	3.5
1	C	109	LEU	3.5
1	C	49	SER	3.5
2	B	77	HIS	3.5
1	A	125	LEU	3.5
1	A	110	ALA	3.5
2	D	89	SER	3.5
2	D	47	ASP	3.5
1	C	107	VAL	3.5
2	D	146	HIS	3.4
1	C	123	ALA	3.4
2	B	96	LEU	3.4
2	B	95	LYS	3.4
1	C	126	ASP	3.4
2	B	79	ASP	3.4
1	A	81	SER	3.4
2	D	106	LEU	3.4
1	A	132	VAL	3.4
1	C	115	ALA	3.4
1	A	139	LYS	3.4
2	B	13	ALA	3.3
1	A	66	LEU	3.3
1	C	31	ARG	3.3
2	D	123	THR	3.3
2	B	65	LYS	3.3
2	B	111	VAL	3.3
1	C	69	ALA	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	3.3
1	C	32	MET	3.3
2	D	116	HIS	3.3
1	C	37	PRO	3.3
1	C	114	PRO	3.3
2	D	57	ASN	3.3
1	C	94	ASP	3.2
2	B	47	ASP	3.2
2	D	107	GLY	3.2
1	A	56	LYS	3.2
2	B	59	LYS	3.2
1	A	108	THR	3.2
2	B	37	TYR	3.2
2	D	129	ALA	3.2
2	D	51	PRO	3.2
2	B	118	PHE	3.2
1	C	21	ALA	3.2
2	B	145	TYR	3.2
1	C	105	LEU	3.2
1	C	11	LYS	3.2
2	D	130	TYR	3.2
1	C	92	ARG	3.2
2	B	104	ARG	3.2
2	B	18	VAL	3.2
2	D	120	LYS	3.2
2	B	143	HIS	3.1
1	C	66	LEU	3.1
2	B	126	VAL	3.1
2	D	25	GLY	3.1
2	B	84	THR	3.1
1	C	16	LYS	3.1
2	D	144	LYS	3.1
1	C	79	ALA	3.1
2	D	69	GLY	3.1
1	C	139	LYS	3.1
2	D	19	ASN	3.1
1	A	8	THR	3.1
1	C	99	LYS	3.1
1	A	13	ALA	3.0
2	B	24	GLY	3.0
1	C	53	ALA	3.0
2	B	30	ARG	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	127	LYS	3.0
2	B	40	ARG	3.0
2	D	6	GLU	3.0
1	A	82	ALA	3.0
2	D	134	VAL	3.0
2	D	8	LYS	3.0
2	D	62	ALA	3.0
1	A	77	PRO	3.0
1	C	29	LEU	3.0
2	B	102	ASN	3.0
1	C	60	LYS	2.9
2	B	129	ALA	2.9
1	C	8	THR	2.9
1	C	75	ASP	2.9
2	D	20	VAL	2.9
2	B	81	LEU	2.9
2	B	8	LYS	2.9
2	D	43	GLU	2.9
2	D	70	ALA	2.9
1	C	85	ASP	2.9
1	C	90	LYS	2.9
1	A	31	ARG	2.8
1	C	57	GLY	2.8
2	D	95	LYS	2.8
2	B	73	ASP	2.8
1	A	133	SER	2.8
2	D	58	PRO	2.8
1	A	7	LYS	2.8
2	B	128	ALA	2.8
1	A	4	PRO	2.8
1	A	90	LYS	2.8
1	C	127	LYS	2.7
1	C	40	LYS	2.7
2	D	102	ASN	2.7
2	B	131	GLN	2.6
2	D	50	THR	2.6
2	B	82	LYS	2.6
2	B	107	GLY	2.6
1	A	102	SER	2.6
1	C	64	ASP	2.6
2	B	51	PRO	2.6
1	C	9	ASN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	55	MET	2.6
2	B	88	LEU	2.5
1	A	23	GLU	2.5
2	D	136	GLY	2.5
1	A	11	LYS	2.5
1	A	20	HIS	2.5
1	C	5	ALA	2.5
1	C	56	LYS	2.5
1	C	22	GLY	2.5
1	C	137	THR	2.5
1	A	72	HIS	2.5
1	C	72	HIS	2.5
1	A	85	ASP	2.5
2	B	56	GLY	2.5
1	A	65	ALA	2.5
1	A	69	ALA	2.4
1	C	36	PHE	2.4
2	B	105	LEU	2.4
2	D	10	ALA	2.4
1	A	70	VAL	2.4
1	C	7	LYS	2.4
2	B	90	GLU	2.4
1	C	65	ALA	2.4
2	D	101	GLU	2.4
1	A	141	ARG	2.4
2	B	114	LEU	2.3
1	C	54	GLN	2.3
2	B	21	ASP	2.3
1	A	96	VAL	2.3
1	C	18	GLY	2.3
1	A	32	MET	2.2
2	D	59	LYS	2.2
1	C	86	LEU	2.2
2	D	64	GLY	2.2
1	C	23	GLU	2.2
2	B	91	LEU	2.2
2	B	36	PRO	2.2
2	B	28	LEU	2.1
2	B	117	HIS	2.1
1	A	39	THR	2.1
1	C	59	GLY	2.1
2	D	39	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	89	HIS	2.1
2	B	67	VAL	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<sup>th</sup> 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 <sup>2</sup> )	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.