



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:46 PM GMT

PDB ID : 1QJS
Title : MAMMALIAN BLOOD SERUM HAEMOPEXIN GLYCOSYLATED-NATIVE PROTEIN AND IN COMPLEX WITH ITS LIGAND HAEM
Authors : Paoli, M.; Baker, H.M.; Morgan, W.T.; Smith, A.; Baker, E.N.
Deposited on : 1999-07-01
Resolution : 2.90 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

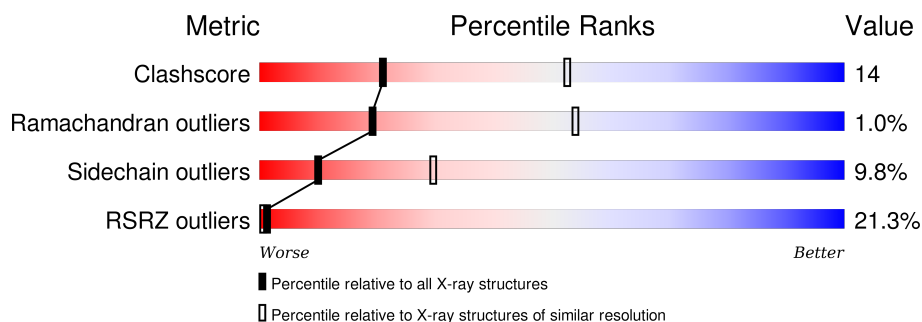
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	460	
1	B	460	

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
2	HEM	B	500	-	-	X	X
3	PO4	B	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	511	-	-	-	X
5	NA	A	512	-	-	-	X
5	NA	B	513	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6686 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 HEMOPEXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3289	2102	579	592	16			
1	B	408	Total	C	N	O	S	0	0	0
			3289	2102	579	592	16			

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		

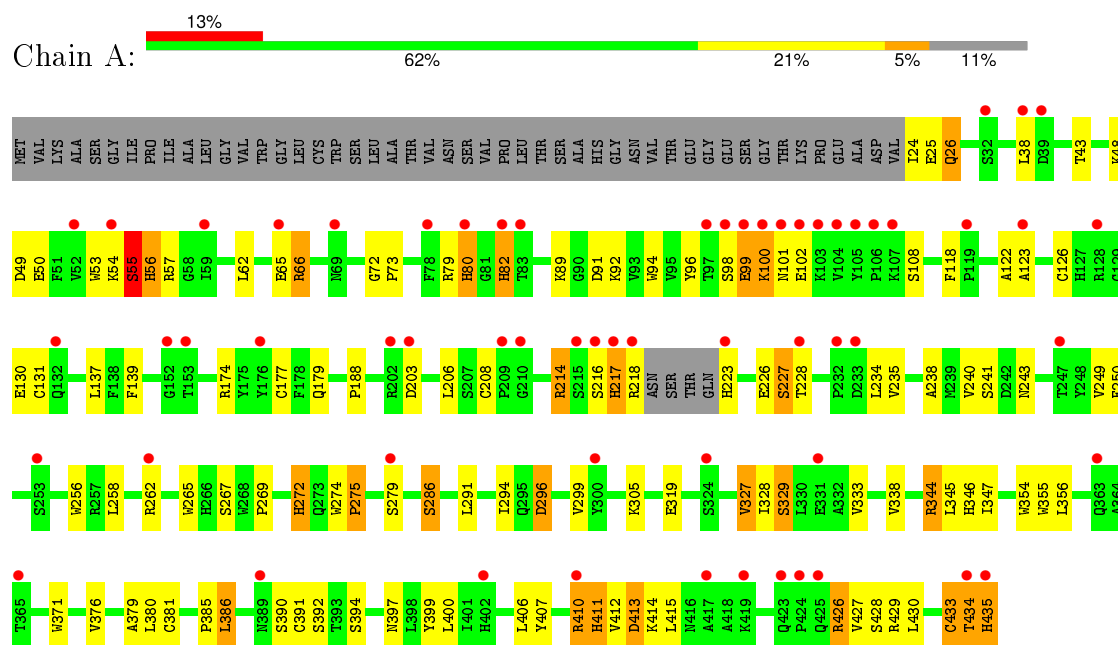
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	Na	0	0
			4	4		
5	A	4	Total	Na	0	0
			4	4		

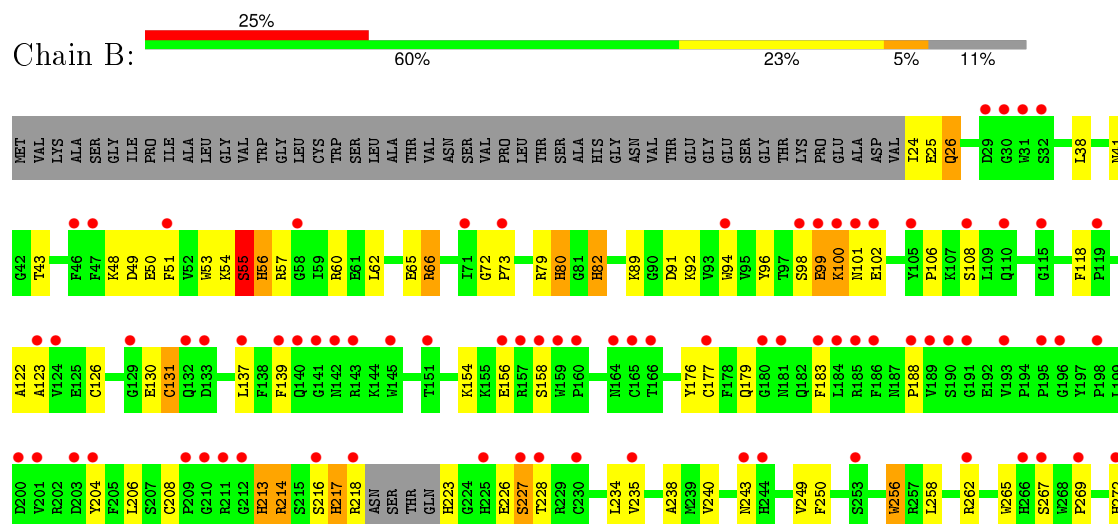
3 Residue-property plots

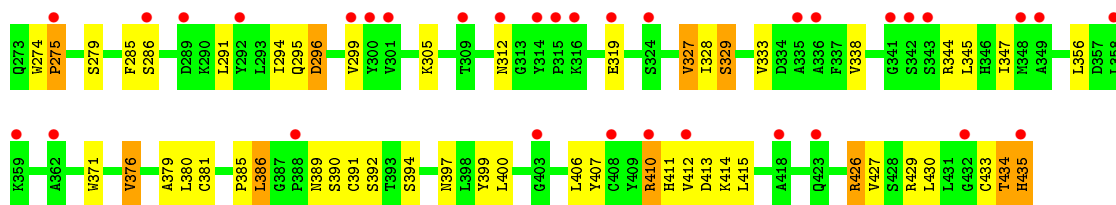
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HEMOPEXIN



• Molecule 1: HEMOPEXIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.90 Å 69.90 Å 151.81 Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.90 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.90) 96.3 (19.90-2.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.98 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.255 , 0.312 0.338 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 23.9	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20914 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6686	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, PO4, CL, NA

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	0.74	2/3400 (0.1%)	1.39	27/4624 (0.6%)
1	B	0.71	4/3400 (0.1%)	1.28	28/4624 (0.6%)
All	All	0.72	6/6800 (0.1%)	1.33	55/9248 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	HIS	N-CA	-19.25	1.07	1.46
1	B	435	HIS	N-CA	-10.09	1.26	1.46
1	A	434	THR	C-N	-9.07	1.13	1.34
1	B	434	THR	CA-C	-8.59	1.30	1.52
1	B	434	THR	C-N	-6.05	1.20	1.34
1	B	433	CYS	C-N	-5.19	1.22	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	THR	O-C-N	29.98	170.66	122.70
1	A	434	THR	CA-C-N	-25.70	60.66	117.20
1	A	434	THR	C-N-CA	9.55	145.57	121.70
1	B	126	CYS	CA-CB-SG	-9.34	97.19	114.00
1	A	126	CYS	CA-CB-SG	-9.23	97.39	114.00
1	B	434	THR	C-N-CA	-9.06	99.06	121.70
1	A	433	CYS	C-N-CA	-8.85	99.59	121.70
1	A	386	LEU	N-CA-C	-7.67	90.29	111.00
1	B	386	LEU	N-CA-C	-7.67	90.29	111.00
1	A	381	CYS	CA-CB-SG	-7.61	100.31	114.00
1	B	208	CYS	CA-CB-SG	-7.04	101.32	114.00
1	B	381	CYS	CA-CB-SG	-7.03	101.35	114.00
1	B	433	CYS	O-C-N	-7.03	111.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	SER	CA-CB-OG	6.51	128.78	111.20
1	B	433	CYS	C-N-CA	-6.27	106.04	121.70
1	B	79	ARG	CA-C-N	6.10	130.62	117.20
1	A	275	PRO	N-CA-C	6.10	127.95	112.10
1	B	275	PRO	N-CA-C	6.05	127.84	112.10
1	B	38	LEU	O-C-N	-5.95	113.18	122.70
1	A	427	VAL	CG1-CB-CG2	-5.87	101.50	110.90
1	A	80	HIS	CA-C-N	-5.87	104.46	116.20
1	B	338	VAL	N-CA-C	-5.86	95.17	111.00
1	A	38	LEU	O-C-N	-5.81	113.41	122.70
1	B	319	GLU	CA-C-N	-5.80	104.44	117.20
1	A	319	GLU	CA-C-N	-5.78	104.49	117.20
1	B	80	HIS	CA-C-N	-5.76	104.68	116.20
1	A	79	ARG	CA-C-N	5.71	129.76	117.20
1	A	413	ASP	O-C-N	-5.70	113.57	122.70
1	A	286	SER	CA-CB-OG	5.70	126.59	111.20
1	A	391	CYS	O-C-N	-5.70	113.58	122.70
1	B	391	CYS	O-C-N	-5.68	113.62	122.70
1	A	130	GLU	N-CA-C	-5.67	95.68	111.00
1	A	296	ASP	CA-C-N	5.66	129.66	117.20
1	B	227	SER	CA-CB-OG	5.58	126.28	111.20
1	A	208	CYS	CA-CB-SG	-5.52	104.06	114.00
1	B	130	GLU	N-CA-C	-5.46	96.27	111.00
1	B	413	ASP	O-C-N	-5.43	114.02	122.70
1	B	79	ARG	O-C-N	-5.42	114.02	122.70
1	A	338	VAL	N-CA-C	-5.42	96.37	111.00
1	B	296	ASP	CA-C-N	5.41	129.11	117.20
1	A	79	ARG	O-C-N	-5.40	114.06	122.70
1	B	131	CYS	O-C-N	-5.37	114.11	122.70
1	B	345	LEU	O-C-N	-5.32	114.18	122.70
1	A	179	GLN	N-CA-C	-5.22	96.91	111.00
1	B	427	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	A	235	VAL	CG1-CB-CG2	-5.20	102.57	110.90
1	A	345	LEU	O-C-N	-5.18	114.41	122.70
1	B	179	GLN	N-CA-C	-5.17	97.05	111.00
1	B	213	HIS	CA-C-N	-5.13	105.91	117.20
1	A	203	ASP	CA-C-N	-5.09	106.00	117.20
1	B	434	THR	N-CA-CB	5.07	119.94	110.30
1	B	235	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	A	241	SER	N-CA-C	-5.04	97.40	111.00
1	B	376	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	B	295	GLN	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3289	0	3120	93	0
1	B	3289	0	3121	110	12
2	A	43	0	30	7	0
2	B	43	0	30	24	0
3	A	5	0	0	1	0
3	B	5	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	6686	0	6301	185	12

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 14.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:HG23	1:A:435:HIS:CB	1.24	1.65
1:A:434:THR:CG2	1:A:435:HIS:HB3	1.54	1.37
1:A:434:THR:CG2	1:A:435:HIS:CB	2.04	1.30
1:A:411:HIS:CE1	1:B:100:LYS:NZ	2.04	1.25
1:A:411:HIS:HE1	1:B:100:LYS:NZ	1.39	1.15
1:A:411:HIS:CE1	1:B:100:LYS:HZ2	1.60	1.12
1:B:99:GLU:HB3	1:B:100:LYS:HE2	1.34	1.10
1:A:413:ASP:OD2	1:B:99:GLU:OE2	1.69	1.09
1:A:99:GLU:HB3	1:A:100:LYS:HE2	1.34	1.09
1:B:434:THR:HG23	1:B:434:THR:O	1.50	1.04
1:A:411:HIS:NE2	1:B:99:GLU:OE1	1.91	1.03
1:A:434:THR:HG23	1:A:435:HIS:HB2	1.05	1.03
1:A:380:LEU:HA	3:A:501:PO4:O2	1.58	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:HG23	1:A:435:HIS:HB3	1.00	0.99
1:B:380:LEU:HA	3:B:501:PO4:O2	1.67	0.94
1:A:434:THR:HG22	1:A:435:HIS:HB3	1.52	0.90
1:A:434:THR:CG2	1:A:435:HIS:HB2	1.87	0.90
1:B:213:HIS:HD2	2:B:500:HEM:C1D	1.90	0.89
1:A:385:PRO:HB3	1:A:390:SER:HB3	1.55	0.88
1:A:411:HIS:CE1	1:B:100:LYS:HZ3	1.90	0.88
1:B:204:TYR:HB3	2:B:500:HEM:C3A	2.10	0.87
1:B:214:ARG:HD2	2:B:500:HEM:C2C	2.10	0.86
1:B:213:HIS:CD2	2:B:500:HEM:C1D	2.65	0.85
1:B:434:THR:CG2	1:B:434:THR:O	2.17	0.83
1:B:385:PRO:HB3	1:B:390:SER:HB3	1.59	0.82
1:A:411:HIS:HE1	1:B:100:LYS:HZ2	0.89	0.81
1:B:380:LEU:HD23	1:B:386:LEU:HD22	1.62	0.80
1:B:213:HIS:HD2	2:B:500:HEM:ND	1.80	0.78
1:A:411:HIS:HE1	1:B:100:LYS:CE	1.96	0.78
1:B:213:HIS:HD2	2:B:500:HEM:C4D	2.02	0.78
1:A:411:HIS:CE1	1:B:100:LYS:CD	2.68	0.77
1:A:380:LEU:HD23	1:A:386:LEU:HD22	1.65	0.77
1:B:100:LYS:O	1:B:102:GLU:N	2.18	0.77
1:A:100:LYS:O	1:A:102:GLU:N	2.18	0.75
1:B:41:ASN:HD22	1:B:262:ARG:HH21	1.33	0.74
1:A:411:HIS:CE1	1:B:100:LYS:CE	2.70	0.74
1:A:413:ASP:CG	1:B:99:GLU:OE2	2.26	0.74
1:B:56:HIS:ND1	2:B:500:HEM:CBB	2.52	0.73
1:A:411:HIS:HE1	1:B:100:LYS:CD	2.03	0.72
1:B:94:TRP:HB3	1:B:96:TYR:CE2	2.25	0.71
1:B:214:ARG:HD2	2:B:500:HEM:C1C	2.26	0.71
1:B:213:HIS:CD2	2:B:500:HEM:C4D	2.79	0.71
1:A:411:HIS:CE1	1:B:99:GLU:OE1	2.45	0.69
1:A:94:TRP:HB3	1:A:96:TYR:CE2	2.27	0.68
1:A:413:ASP:HB2	1:B:99:GLU:OE2	1.94	0.68
1:A:82:HIS:CE1	1:A:262:ARG:HG2	2.28	0.68
1:B:183:PHE:HE2	2:B:500:HEM:CGA	2.07	0.68
1:A:428:SER:HB2	1:A:433:CYS:HB2	1.75	0.66
1:B:41:ASN:HD22	1:B:262:ARG:NH2	1.93	0.66
1:B:204:TYR:CD1	2:B:500:HEM:C1A	2.85	0.66
1:A:410:ARG:HG3	1:A:414:LYS:HD2	1.79	0.65
1:B:410:ARG:HG3	1:B:414:LYS:HD2	1.80	0.64
1:A:226:GLU:HG2	1:A:267:SER:H	1.63	0.63
1:A:413:ASP:CB	1:B:99:GLU:OE2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.81	0.62
1:B:226:GLU:HG2	1:B:267:SER:H	1.64	0.62
1:A:413:ASP:HB2	1:B:99:GLU:CD	2.20	0.61
1:A:411:HIS:CE1	1:B:100:LYS:HD3	2.35	0.61
1:A:56:HIS:CE1	2:A:500:HEM:CBB	2.84	0.60
1:B:204:TYR:HB3	2:B:500:HEM:C2A	2.37	0.59
1:B:49:ASP:HA	1:B:73:PRO:HB3	1.85	0.58
1:A:49:ASP:HA	1:A:73:PRO:HB3	1.86	0.58
1:A:434:THR:CB	1:A:435:HIS:HB2	2.34	0.57
1:B:56:HIS:CE1	2:B:500:HEM:CBB	2.88	0.57
1:B:183:PHE:CE2	2:B:500:HEM:CGA	2.88	0.57
1:A:406:LEU:HD22	1:A:430:LEU:HD23	1.87	0.56
1:B:286:SER:HB3	1:B:291:LEU:HD23	1.86	0.56
1:B:434:THR:O	1:B:435:HIS:CB	2.39	0.56
1:A:238:ALA:HB3	1:A:250:PHE:HB2	1.87	0.56
1:A:91:ASP:HB3	1:A:118:PHE:CE2	2.41	0.56
1:B:72:GLY:HA3	1:B:89:LYS:NZ	2.21	0.56
1:B:91:ASP:HB3	1:B:118:PHE:CE2	2.40	0.55
1:B:238:ALA:HB3	1:B:250:PHE:HB2	1.88	0.55
1:A:428:SER:HB2	1:A:433:CYS:CB	2.35	0.55
1:A:123:ALA:HA	1:A:137:LEU:O	2.07	0.55
1:A:56:HIS:CE1	2:A:500:HEM:HBB1	2.42	0.55
1:A:327:VAL:HG23	1:A:328:ILE:HD12	1.88	0.54
1:A:286:SER:HB3	1:A:291:LEU:HD23	1.88	0.54
1:A:269:PRO:HD2	1:A:272:HIS:CD2	2.43	0.54
1:A:82:HIS:NE2	1:A:262:ARG:HG2	2.21	0.54
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.89	0.54
1:B:183:PHE:HE2	2:B:500:HEM:O2A	1.91	0.54
1:B:410:ARG:CG	1:B:414:LYS:HD2	2.38	0.54
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.89	0.54
1:A:56:HIS:HE1	2:A:500:HEM:HBB1	1.74	0.53
1:A:410:ARG:CG	1:A:414:LYS:HD2	2.37	0.53
1:B:269:PRO:HD2	1:B:272:HIS:CD2	2.45	0.52
1:B:327:VAL:HG23	1:B:328:ILE:HD12	1.91	0.52
1:A:392:SER:HB3	1:A:410:ARG:HA	1.92	0.52
1:B:406:LEU:HD22	1:B:430:LEU:HD23	1.92	0.52
1:A:131:CYS:SG	1:A:188:PRO:HB2	2.51	0.51
1:A:413:ASP:CB	1:B:99:GLU:CD	2.79	0.51
1:B:123:ALA:HA	1:B:137:LEU:O	2.11	0.51
1:B:204:TYR:HD1	2:B:500:HEM:C1A	2.29	0.51
1:B:392:SER:HB3	1:B:410:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:HE1	2:B:500:HEM:O2A	1.94	0.50
1:B:214:ARG:HD2	2:B:500:HEM:C3C	2.46	0.50
1:A:294:ILE:HG12	1:A:299:VAL:HG22	1.92	0.50
1:B:328:ILE:HG22	1:B:329:SER:N	2.27	0.50
1:B:54:LYS:HZ1	1:B:66:ARG:HH21	1.59	0.50
1:B:216:SER:O	1:B:217:HIS:ND1	2.45	0.49
1:A:48:LYS:HB3	1:A:53:TRP:CZ3	2.47	0.49
1:B:412:VAL:O	1:B:415:LEU:HB3	2.12	0.49
1:B:434:THR:O	1:B:435:HIS:HB2	2.12	0.49
1:A:410:ARG:HG3	1:A:414:LYS:CD	2.43	0.48
1:B:294:ILE:HG12	1:B:299:VAL:HG22	1.94	0.48
1:A:216:SER:O	1:A:217:HIS:ND1	2.46	0.48
1:B:390:SER:HB2	1:B:397:ASN:ND2	2.29	0.47
1:B:333:VAL:HG21	1:B:347:ILE:HD11	1.96	0.47
1:A:379:ALA:HB2	1:A:400:LEU:HD23	1.94	0.47
1:A:328:ILE:HG22	1:A:329:SER:N	2.29	0.47
1:A:48:LYS:HB3	1:A:53:TRP:HZ3	1.79	0.47
1:B:379:ALA:HB2	1:B:400:LEU:HD23	1.95	0.47
1:A:411:HIS:CD2	1:B:99:GLU:OE1	2.63	0.47
1:B:24:ILE:HG23	1:B:25:GLU:H	1.78	0.47
1:B:48:LYS:HB3	1:B:53:TRP:CZ3	2.49	0.47
1:A:26:GLN:H	1:A:26:GLN:HE21	1.62	0.47
1:B:94:TRP:NE1	1:B:106:PRO:HG3	2.31	0.46
1:A:411:HIS:NE2	1:B:100:LYS:HD3	2.30	0.46
1:A:412:VAL:O	1:A:415:LEU:HB3	2.15	0.46
1:A:333:VAL:HG21	1:A:347:ILE:HD11	1.97	0.46
1:B:410:ARG:HG3	1:B:414:LYS:CD	2.44	0.46
1:B:243:ASN:ND2	1:B:243:ASN:H	2.14	0.46
1:B:26:GLN:H	1:B:26:GLN:HE21	1.62	0.46
1:B:214:ARG:HG3	2:B:500:HEM:CBC	2.45	0.46
1:A:390:SER:HB2	1:A:397:ASN:ND2	2.30	0.46
1:A:327:VAL:HG11	1:B:389:ASN:HB3	1.98	0.46
1:A:24:ILE:HG23	1:A:25:GLU:H	1.79	0.46
1:A:122:ALA:HB3	1:A:139:PHE:HB2	1.98	0.46
1:A:62:LEU:O	1:A:65:GLU:HB3	2.16	0.46
1:A:54:LYS:HE3	1:A:66:ARG:HH21	1.81	0.46
1:A:414:LYS:HG3	1:B:100:LYS:HD2	1.98	0.46
1:B:56:HIS:CD2	1:B:56:HIS:C	2.89	0.46
1:A:26:GLN:H	1:A:26:GLN:NE2	2.13	0.46
1:B:50:GLU:O	1:B:62:LEU:HD12	2.16	0.45
1:B:100:LYS:HA	1:B:100:LYS:HD3	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:H	1:A:243:ASN:ND2	2.14	0.45
1:B:426:ARG:HB3	1:B:426:ARG:HH11	1.81	0.45
1:B:122:ALA:HB3	1:B:139:PHE:HB2	1.99	0.45
1:B:48:LYS:HB3	1:B:53:TRP:HZ3	1.81	0.45
1:B:131:CYS:SG	1:B:188:PRO:HB2	2.57	0.45
1:B:100:LYS:HE2	1:B:100:LYS:N	2.32	0.45
1:B:62:LEU:O	1:B:65:GLU:HB3	2.17	0.44
1:A:100:LYS:N	1:A:100:LYS:HE2	2.32	0.44
1:B:390:SER:HB2	1:B:397:ASN:HD21	1.82	0.44
1:A:50:GLU:O	1:A:62:LEU:HD12	2.18	0.44
1:A:399:TYR:HA	1:A:407:TYR:O	2.16	0.44
1:B:214:ARG:CD	2:B:500:HEM:C3C	3.00	0.44
2:A:500:HEM:HBD2	2:A:500:HEM:HHA	1.99	0.44
1:B:55:SER:OG	1:B:57:ARG:HB2	2.18	0.44
1:B:72:GLY:HA3	1:B:89:LYS:HZ2	1.82	0.44
1:B:204:TYR:CD1	2:B:500:HEM:C2A	3.06	0.43
1:A:72:GLY:HA3	1:A:89:LYS:NZ	2.33	0.43
1:B:223:HIS:CD2	1:B:234:LEU:HD12	2.52	0.43
1:A:56:HIS:ND1	2:A:500:HEM:CBB	2.81	0.43
1:B:258:LEU:HD23	1:B:265:TRP:HZ3	1.82	0.43
1:A:214:ARG:HD3	1:A:214:ARG:N	2.33	0.43
1:B:214:ARG:HD3	1:B:214:ARG:N	2.33	0.43
1:A:56:HIS:CD2	1:A:56:HIS:C	2.92	0.43
1:B:26:GLN:NE2	1:B:26:GLN:H	2.15	0.43
1:A:55:SER:OG	1:A:57:ARG:HB2	2.19	0.43
1:A:174:ARG:HH22	1:A:272:HIS:CD2	2.37	0.43
1:B:386:LEU:HG	1:B:430:LEU:HD22	2.01	0.43
1:B:399:TYR:HA	1:B:407:TYR:O	2.18	0.42
1:B:204:TYR:CD1	2:B:500:HEM:CHA	3.02	0.42
1:A:426:ARG:HB3	1:A:426:ARG:HH11	1.84	0.42
1:A:386:LEU:HG	1:A:430:LEU:HD22	2.01	0.42
1:A:54:LYS:CE	1:A:66:ARG:HH21	2.33	0.42
1:B:24:ILE:HG23	1:B:25:GLU:N	2.34	0.42
1:A:223:HIS:CD2	1:A:234:LEU:HD12	2.54	0.42
1:A:274:TRP:HA	1:A:275:PRO:HD2	1.86	0.42
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.78	0.42
1:A:99:GLU:HB3	1:A:100:LYS:CE	2.25	0.42
1:A:344:ARG:HG2	1:A:355:TRP:CE3	2.55	0.42
1:A:346:HIS:HA	1:A:354:TRP:O	2.20	0.42
1:A:100:LYS:HD3	1:A:100:LYS:HA	1.44	0.41
1:B:54:LYS:NZ	1:B:66:ARG:HH21	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:HIS:ND1	1:B:82:HIS:O	2.53	0.41
1:B:256:TRP:CE2	1:B:267:SER:OG	2.72	0.41
1:B:94:TRP:CE2	1:B:106:PRO:HG3	2.55	0.41
1:A:258:LEU:HD23	1:A:265:TRP:HZ3	1.85	0.41
1:B:213:HIS:CD2	2:B:500:HEM:CHD	3.03	0.41
1:B:285:PHE:HA	3:B:501:PO4:O4	2.20	0.41
1:B:274:TRP:HA	1:B:275:PRO:HD2	1.85	0.40
1:A:100:LYS:C	1:A:102:GLU:N	2.75	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PHE:CZ	1:B:312:ASN:CG[4_556]	1.31	0.89
1:B:51:PHE:CE1	1:B:156:GLU:O[4_556]	1.44	0.76
1:B:118:PHE:CE1	1:B:312:ASN:ND2[4_556]	1.73	0.47
1:B:118:PHE:CZ	1:B:312:ASN:OD1[4_556]	1.80	0.40
1:B:118:PHE:CE2	1:B:312:ASN:CB[4_556]	1.88	0.32
1:B:118:PHE:CZ	1:B:312:ASN:CB[4_556]	1.92	0.28
1:B:118:PHE:CZ	1:B:312:ASN:ND2[4_556]	1.93	0.27
1:B:25:GLU:OE2	1:B:154:LYS:O[4_556]	1.98	0.22
1:B:118:PHE:CE1	1:B:312:ASN:CG[4_556]	2.11	0.09
1:B:51:PHE:CD1	1:B:156:GLU:O[4_556]	2.14	0.06
1:B:60:ARG:NH2	1:B:156:GLU:OE1[4_556]	2.16	0.04
1:B:62:LEU:CD1	1:B:158:SER:CB[4_556]	2.18	0.02

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	404/460 (88%)	370 (92%)	30 (7%)	4 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	404/460 (88%)	369 (91%)	31 (8%)	4 (1%)	19	54
All	All	808/920 (88%)	739 (92%)	61 (8%)	8 (1%)	19	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	296	ASP
1	B	101	ASN
1	B	296	ASP
1	A	55	SER
1	B	55	SER
1	B	82	HIS
1	A	82	HIS

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	352/393 (90%)	317 (90%)	35 (10%)	10	29
1	B	352/393 (90%)	318 (90%)	34 (10%)	10	30
All	All	704/786 (90%)	635 (90%)	69 (10%)	10	30

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	43	THR
1	A	55	SER
1	A	56	HIS
1	A	66	ARG
1	A	80	HIS
1	A	92	LYS
1	A	98	SER

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Mol	Chain	Res	Type
1	A	99	GLU
1	A	100	LYS
1	A	108	SER
1	A	177	CYS
1	A	206	LEU
1	A	214	ARG
1	A	217	HIS
1	A	218	ARG
1	A	227	SER
1	A	228	THR
1	A	240	VAL
1	A	249	VAL
1	A	256	TRP
1	A	272	HIS
1	A	279	SER
1	A	305	LYS
1	A	327	VAL
1	A	329	SER
1	A	344	ARG
1	A	356	LEU
1	A	371	TRP
1	A	376	VAL
1	A	394	SER
1	A	410	ARG
1	A	411	HIS
1	A	426	ARG
1	A	429	ARG
1	B	26	GLN
1	B	43	THR
1	B	55	SER
1	B	56	HIS
1	B	66	ARG
1	B	80	HIS
1	B	92	LYS
1	B	98	SER
1	B	99	GLU
1	B	100	LYS
1	B	108	SER
1	B	177	CYS
1	B	206	LEU
1	B	214	ARG
1	B	217	HIS

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Mol	Chain	Res	Type
1	B	218	ARG
1	B	227	SER
1	B	228	THR
1	B	240	VAL
1	B	249	VAL
1	B	256	TRP
1	B	279	SER
1	B	305	LYS
1	B	327	VAL
1	B	329	SER
1	B	344	ARG
1	B	356	LEU
1	B	371	TRP
1	B	376	VAL
1	B	394	SER
1	B	410	ARG
1	B	411	HIS
1	B	426	ARG
1	B	429	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	ASN
1	A	56	HIS
1	A	142	ASN
1	A	243	ASN
1	A	411	HIS
1	B	26	GLN
1	B	41	ASN
1	B	142	ASN
1	B	243	ASN
1	B	272	HIS
1	B	295	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	500	1	30,50,50	4.25	12 (40%)	24,82,82	2.38	7 (29%)
3	PO4	A	501	-	4,4,4	1.36	0	6,6,6	0.31	0
2	HEM	B	500	1	30,50,50	4.19	16 (53%)	24,82,82	2.97	13 (54%)
3	PO4	B	501	-	4,4,4	1.36	0	6,6,6	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	0/10/54/54	0/0/8/8
3	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	PO4	B	501	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-15.44	1.38	1.51
2	A	500	HEM	C3B-C4B	-14.84	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C4D	-8.75	1.40	1.51
2	A	500	HEM	C3B-CAB	-8.00	1.36	1.51
2	B	500	HEM	C3D-C4D	-7.57	1.41	1.51
2	A	500	HEM	C2C-C1C	-7.45	1.38	1.52
2	B	500	HEM	C2C-C1C	-6.20	1.40	1.52
2	A	500	HEM	C3C-CAC	-5.60	1.40	1.51
2	A	500	HEM	C2D-C3D	-5.19	1.39	1.54
2	B	500	HEM	C2D-C3D	-5.07	1.39	1.54
2	B	500	HEM	C2B-C1B	-4.29	1.37	1.51
2	A	500	HEM	C2D-C1D	-3.82	1.39	1.51
2	B	500	HEM	C3C-CAC	-3.62	1.44	1.51
2	B	500	HEM	C3B-CAB	-3.49	1.44	1.51
2	A	500	HEM	C2B-C1B	-2.76	1.42	1.51
2	B	500	HEM	C2D-C1D	-2.66	1.43	1.51
2	A	500	HEM	C1C-NC	-2.54	1.32	1.36
2	A	500	HEM	C4C-NC	-2.08	1.33	1.36
2	B	500	HEM	CHC-C1C	2.52	1.42	1.36
2	B	500	HEM	CHD-C1D	2.53	1.45	1.38
2	A	500	HEM	FE-NC	2.89	2.07	1.95
2	B	500	HEM	CBB-CAB	3.04	1.46	1.29
2	A	500	HEM	CBC-CAC	3.23	1.48	1.29
2	B	500	HEM	FE-NB	3.27	2.14	1.97
2	B	500	HEM	FE-NC	3.53	2.09	1.95
2	B	500	HEM	FE-ND	3.77	2.17	1.97
2	B	500	HEM	CBC-CAC	4.89	1.57	1.29
2	B	500	HEM	CHD-C4C	4.96	1.48	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C2C-C1C-CHC	-2.38	120.06	123.68
2	B	500	HEM	C3B-CAB-CBB	-2.18	121.11	124.46
2	B	500	HEM	CMA-C3A-C4A	-2.06	124.95	128.36
2	B	500	HEM	C1D-CHD-C4C	2.54	130.06	125.82
2	B	500	HEM	CAD-CBD-CGD	2.55	123.42	113.02
2	A	500	HEM	C3C-CAC-CBC	2.62	128.48	124.46
2	B	500	HEM	CMA-C3A-C2A	2.76	131.01	125.24
2	A	500	HEM	CBA-CAA-C2A	2.95	117.82	112.53
2	A	500	HEM	CMD-C2D-C3D	2.99	127.58	114.35
2	A	500	HEM	CAD-C3D-C4D	3.67	125.43	112.47
2	B	500	HEM	CBD-CAD-C3D	4.14	125.61	113.55
2	B	500	HEM	CMC-C2C-C3C	4.26	127.16	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAD-C3D-C2D	4.61	126.48	113.22
2	A	500	HEM	CMC-C2C-C3C	4.76	128.42	116.53
2	B	500	HEM	CMB-C2B-C3B	4.80	128.51	116.53
2	A	500	HEM	CMB-C2B-C3B	4.96	128.91	116.53
2	B	500	HEM	C3C-CAC-CBC	5.11	132.29	124.46
2	B	500	HEM	CAD-C3D-C4D	5.39	131.49	112.47
2	B	500	HEM	CBA-CAA-C2A	5.87	123.05	112.53
2	A	500	HEM	CAD-C3D-C2D	6.06	130.64	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	7	0
3	A	501	PO4	1	0
2	B	500	HEM	24	0
3	B	501	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	408/460 (88%)	1.06	61 (14%) 3 2	19, 39, 59, 70	0
1	B	408/460 (88%)	1.55	113 (27%) 1 0	18, 38, 59, 68	0
All	All	816/920 (88%)	1.31	174 (21%) 1 0	18, 38, 59, 70	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	GLY	10.0
1	B	101	ASN	7.4
1	A	217	HIS	7.3
1	A	101	ASN	7.2
1	A	423	GLN	7.2
1	B	32	SER	6.7
1	B	30	GLY	6.5
1	A	98	SER	6.0
1	B	210	GLY	5.9
1	B	216	SER	5.8
1	A	216	SER	5.7
1	B	119	PRO	5.4
1	B	142	ASN	5.1
1	A	435	HIS	4.9
1	B	180	GLY	4.7
1	B	141	GLY	4.7
1	B	195	PRO	4.6
1	B	343	SER	4.4
1	A	82	HIS	4.4
1	B	289	ASP	4.3
1	B	211	ARG	4.3
1	A	65	GLU	4.3
1	A	102	GLU	4.1
1	B	209	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	435	HIS	4.1
1	A	203	ASP	4.0
1	A	103	LYS	3.9
1	B	133	ASP	3.9
1	A	215	SER	3.7
1	A	105	TYR	3.7
1	A	32	SER	3.7
1	B	193	VAL	3.6
1	B	204	TYR	3.6
1	B	31	TRP	3.6
1	A	417	ALA	3.5
1	B	186	PHE	3.5
1	B	143	ARG	3.5
1	B	98	SER	3.5
1	B	312	ASN	3.4
1	A	100	LYS	3.4
1	B	188	PRO	3.4
1	A	80	HIS	3.4
1	A	99	GLU	3.3
1	A	69	ASN	3.3
1	A	389	ASN	3.3
1	B	243	ASN	3.2
1	B	29	ASP	3.2
1	B	269	PRO	3.2
1	A	107	LYS	3.1
1	B	362	ALA	3.1
1	B	272	HIS	3.1
1	B	286	SER	3.1
1	B	160	PRO	3.0
1	B	198	PRO	3.0
1	A	218	ARG	3.0
1	B	235	VAL	3.0
1	B	189	VAL	3.0
1	B	181	ASN	3.0
1	B	212	GLY	2.9
1	B	275	PRO	2.9
1	B	225	HIS	2.9
1	B	158	SER	2.9
1	B	183	PHE	2.9
1	B	200	ASP	2.9
1	B	123	ALA	2.9
1	B	403	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLN	2.8
1	B	418	ALA	2.8
1	B	100	LYS	2.8
1	A	410	ARG	2.8
1	B	99	GLU	2.8
1	B	359	LYS	2.7
1	B	51	PHE	2.7
1	B	184	LEU	2.7
1	A	232	PRO	2.7
1	B	73	PRO	2.7
1	B	124	VAL	2.7
1	B	314	TYR	2.7
1	A	253	SER	2.7
1	B	129	GLY	2.7
1	A	363	GLN	2.7
1	B	244	HIS	2.7
1	B	349	ALA	2.7
1	B	342	SER	2.6
1	B	267	SER	2.6
1	B	335	ALA	2.6
1	B	203	ASP	2.6
1	B	315	PRO	2.6
1	B	201	VAL	2.6
1	B	159	TRP	2.6
1	A	104	VAL	2.6
1	A	365	THR	2.6
1	B	228	THR	2.5
1	B	301	VAL	2.5
1	A	152	GLY	2.5
1	B	299	VAL	2.5
1	A	83	THR	2.5
1	A	106	PRO	2.5
1	B	177	CYS	2.5
1	B	47	PHE	2.5
1	B	348	MET	2.5
1	B	309	THR	2.4
1	B	139	PHE	2.4
1	B	196	GLY	2.4
1	A	223	HIS	2.4
1	A	38	LEU	2.4
1	A	54	LYS	2.4
1	A	324	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	TYR	2.4
1	B	108	SER	2.4
1	B	190	SER	2.4
1	B	157	ARG	2.4
1	A	300	TYR	2.4
1	B	166	THR	2.4
1	B	145	TRP	2.4
1	B	336	ALA	2.4
1	B	300	TYR	2.4
1	B	230	CYS	2.3
1	B	71	ILE	2.3
1	B	94	TRP	2.3
1	B	410	ARG	2.3
1	A	209	PRO	2.3
1	A	424	PRO	2.3
1	A	52	VAL	2.3
1	B	58	GLY	2.3
1	B	191	GLY	2.3
1	A	331	GLU	2.3
1	A	119	PRO	2.3
1	A	78	PHE	2.3
1	A	97	THR	2.3
1	B	140	GLN	2.3
1	B	316	LYS	2.3
1	A	247	THR	2.2
1	B	423	GLN	2.2
1	A	262	ARG	2.2
1	A	279	SER	2.2
1	B	227	SER	2.2
1	A	425	GLN	2.2
1	B	266	HIS	2.2
1	B	132	GLN	2.2
1	B	358	LEU	2.2
1	A	202	ARG	2.2
1	B	262	ARG	2.2
1	A	228	THR	2.2
1	B	164	ASN	2.2
1	B	115	GLY	2.2
1	B	218	ARG	2.2
1	B	102	GLU	2.2
1	A	153	THR	2.2
1	A	132	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	ARG	2.2
1	A	176	TYR	2.2
1	A	123	ALA	2.1
1	B	46	PHE	2.1
1	B	156	GLU	2.1
1	A	434	THR	2.1
1	B	151	THR	2.1
1	B	165	CYS	2.1
1	A	419	LYS	2.1
1	A	128	ARG	2.1
1	B	432	GLY	2.1
1	A	402	HIS	2.1
1	A	233	ASP	2.1
1	B	388	PRO	2.1
1	A	39	ASP	2.1
1	B	412	VAL	2.1
1	B	319	GLU	2.0
1	B	137	LEU	2.0
1	B	324	SER	2.0
1	B	253	SER	2.0
1	A	210	GLY	2.0
1	A	59	ILE	2.0
1	B	408	CYS	2.0
1	B	292	TYR	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
5	NA	A	512	1/1	0.78	0.48	4.18	33,33,33,33	0
4	CL	B	511	1/1	0.45	0.51	3.61	26,26,26,26	0
2	HEM	B	500	43/43	0.58	0.65	3.34	14,30,39,40	0
3	PO4	A	501	5/5	0.84	0.31	1.82	18,19,20,20	5
3	PO4	B	501	5/5	0.76	0.40	1.72	18,19,20,20	5
5	NA	B	513	1/1	0.37	0.41	1.34	32,32,32,32	0
4	CL	B	521	1/1	0.83	0.31	0.28	20,20,20,20	0
4	CL	A	521	1/1	0.84	0.23	0.26	20,20,20,20	0
5	NA	B	523	1/1	0.91	0.27	-0.15	27,27,27,27	0
5	NA	A	522	1/1	0.67	0.23	-0.47	26,26,26,26	0
5	NA	A	513	1/1	0.17	0.23	-0.60	32,32,32,32	0
2	HEM	A	500	43/43	0.89	0.23	-0.67	23,33,49,60	0
5	NA	B	512	1/1	0.49	0.25	-0.84	33,33,33,33	0
4	CL	A	511	1/1	0.90	0.16	-1.56	26,26,26,26	0
5	NA	A	523	1/1	0.89	0.15	-1.67	27,27,27,27	0
5	NA	B	522	1/1	0.58	0.17	-3.44	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.