Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:45 PM GMT

PDB ID	:	1QHU
Title	:	MAMMALIAN BLOOD SERUM HAEMOPEXIN DEGLYCOSYLATED AND IN COMPLEX WITH ITS LIGAND HAEM
Authors	:	Paoli, M.; Baker, H.M.; Morgan, W.T.; Smith, A.; Baker, E.N.
Deposited on	:	1999-05-27
Resolution	:	2.30 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:

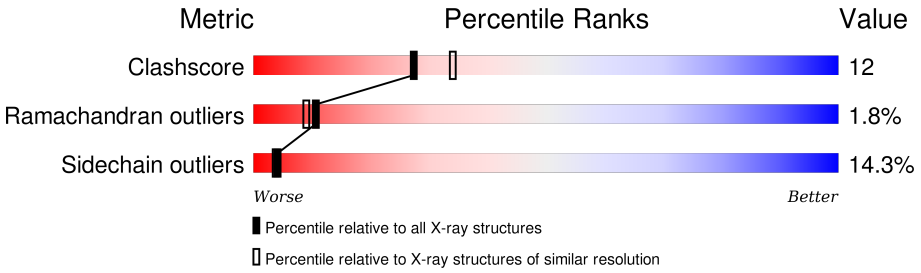
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	460	55% 22% 6% • 13%

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
4	PO4	A	441	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3463 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 PROTEIN (HEMOPEXIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3199	2047	561	575	16	1	0	0

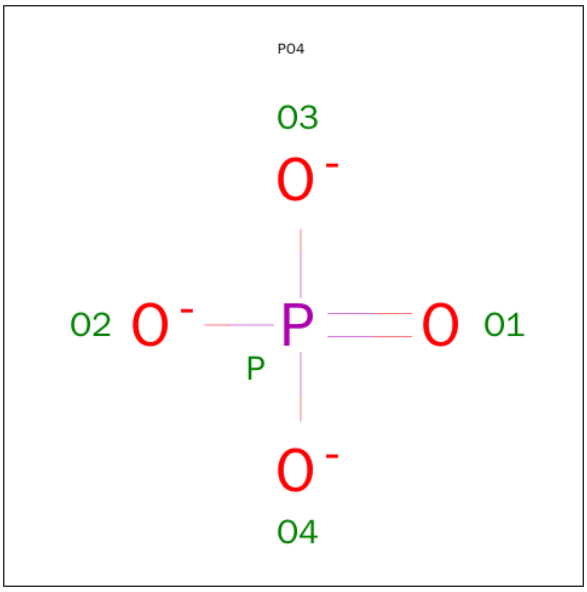
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

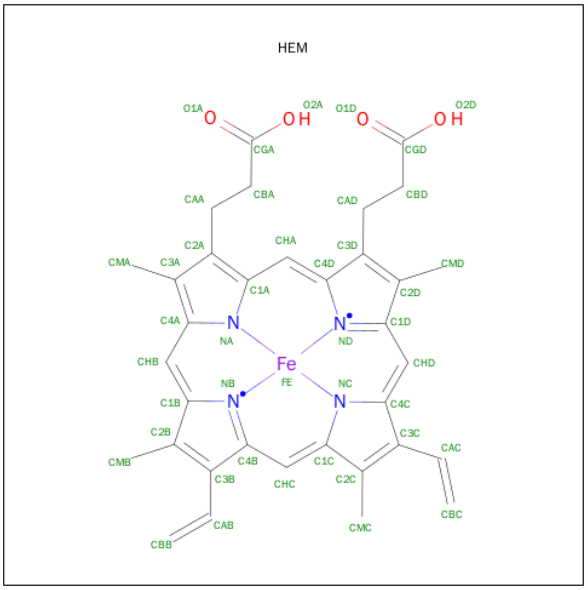
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	4	4	4	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0

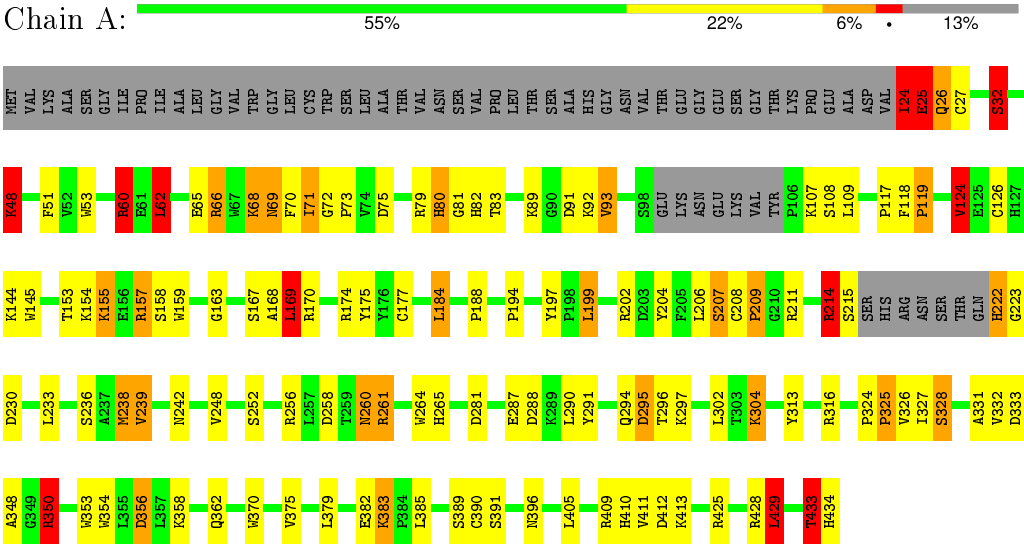
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: PROTEIN (HEMOPEXIN)

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.68Å 61.95Å 83.29Å 90.00° 93.21° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.7 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3463	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

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	0.88	11/3307 (0.3%)	2.05	97/4498 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	HIS	N-CA	8.78	1.64	1.46
1	A	223	GLY	N-CA	8.74	1.59	1.46
1	A	222	HIS	N-CA	-8.49	1.29	1.46
1	A	222	HIS	CA-C	6.54	1.70	1.52
1	A	223	GLY	CA-C	6.32	1.61	1.51
1	A	434	HIS	C-O	-5.97	1.12	1.23
1	A	214	ARG	CD-NE	5.75	1.56	1.46
1	A	434	HIS	C-OXT	-5.73	1.12	1.23
1	A	222	HIS	C-N	5.51	1.43	1.33
1	A	222	HIS	CA-CB	-5.46	1.42	1.53
1	A	223	GLY	C-N	5.03	1.45	1.34

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	ARG	NE-CZ-NH1	29.06	134.83	120.30
1	A	343	ARG	NE-CZ-NH2	-26.68	106.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	O-C-N	-26.26	80.69	122.70
1	A	214	ARG	CA-C-N	25.80	173.96	117.20
1	A	222	HIS	N-CA-CB	15.20	137.95	110.60
1	A	256	ARG	NE-CZ-NH2	-14.80	112.90	120.30
1	A	211	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	A	169	LEU	CA-CB-CG	13.40	146.12	115.30
1	A	128	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	A	214	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	A	128	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	350	ARG	CD-NE-CZ	9.77	137.28	123.60
1	A	214	ARG	CA-C-O	-9.32	100.53	120.10
1	A	60	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	A	428	ARG	CD-NE-CZ	8.89	136.05	123.60
1	A	256	ARG	NH1-CZ-NH2	8.74	129.01	119.40
1	A	197	TYR	CA-C-O	-8.65	101.94	120.10
1	A	79	ARG	NE-CZ-NH2	8.43	124.51	120.30
1	A	207	SER	N-CA-CB	8.37	123.05	110.50
1	A	288	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	167	SER	N-CA-CB	8.21	122.82	110.50
1	A	350	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	333	ASP	CB-CG-OD1	7.85	125.37	118.30
1	A	350	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	118	PHE	CA-C-O	-7.64	104.05	120.10
1	A	174	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	66	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	258	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	214	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
1	A	385	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	230	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	215	SER	CA-C-O	-7.05	105.30	120.10
1	A	428	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	126	CYS	CA-CB-SG	-6.91	101.57	114.00
1	A	325	PRO	O-C-N	6.88	133.71	122.70
1	A	66	ARG	CD-NE-CZ	6.86	133.20	123.60
1	A	239	VAL	CB-CA-C	-6.86	98.37	111.40
1	A	48	LYS	CA-CB-CG	6.71	128.16	113.40
1	A	425	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	343	ARG	CA-CB-CG	6.58	127.87	113.40
1	A	197	TYR	O-C-N	6.56	133.57	121.10
1	A	313	TYR	CA-C-O	-6.54	106.37	120.10
1	A	316	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	331	ALA	CA-C-O	6.23	133.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ALA	N-CA-CB	6.23	118.83	110.10
1	A	211	ARG	NH1-CZ-NH2	6.15	126.16	119.40
1	A	79	ARG	NE-CZ-NH1	-6.15	117.23	120.30
1	A	119	PRO	N-CA-CB	6.09	110.61	103.30
1	A	174	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	346	ILE	CB-CA-C	6.05	123.71	111.60
1	A	222	HIS	O-C-N	-6.05	112.92	123.20
1	A	91	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	204	TYR	CB-CG-CD2	6.04	124.62	121.00
1	A	39	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	429	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	118	PHE	O-C-N	5.99	132.48	121.10
1	A	40	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	124	VAL	CB-CA-C	-5.83	100.33	111.40
1	A	39	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	119	PRO	CA-N-CD	-5.78	103.41	111.50
1	A	429	LEU	N-CA-CB	5.76	121.93	110.40
1	A	170	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	214	ARG	N-CA-CB	-5.59	100.53	110.60
1	A	261	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	291	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	214	ARG	N-CA-C	5.51	125.88	111.00
1	A	288	ASP	OD1-CG-OD2	-5.50	112.84	123.30
1	A	258	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	291	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	412	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	287	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	A	356	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	385	LEU	N-CA-C	-5.40	96.42	111.00
1	A	356	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	62	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	47	PHE	CB-CG-CD1	-5.38	117.04	120.80
1	A	281	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	238	MET	CG-SD-CE	-5.32	91.68	100.20
1	A	24	ILE	CA-C-N	5.28	128.82	117.20
1	A	25	GLU	CB-CG-CD	5.28	128.46	114.20
1	A	410	HIS	CA-CB-CG	-5.28	104.63	113.60
1	A	199	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	295	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	410	HIS	O-C-N	5.20	131.02	122.70
1	A	214	ARG	CG-CD-NE	-5.20	100.89	111.80
1	A	328	SER	CB-CA-C	5.20	119.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	223	GLY	C-N-CA	5.18	134.65	121.70
1	A	433	THR	N-CA-C	5.16	124.94	111.00
1	A	197	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	197	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	202	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	343	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	24	ILE	CA-C-O	-5.05	109.50	120.10
1	A	32	SER	CA-CB-OG	-5.04	97.59	111.20
1	A	236	SER	CA-C-N	5.04	128.28	117.20
1	A	353	TRP	CA-CB-CG	5.02	123.23	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Mainchain,Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3199	0	3034	71	0
2	A	2	0	0	0	0
3	A	4	0	0	0	0
4	A	5	0	0	2	0
5	A	43	0	30	6	0
6	A	210	0	0	8	0
All	All	3463	0	3064	75	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 12.

All (75) 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:379:LEU:HA	4:A:441:PO4:O2	1.62	0.99
1:A:227:THR:HG22	1:A:233:LEU:HD13	1.56	0.85
1:A:26:GLN:HE21	1:A:26:GLN:H	1.27	0.81
1:A:326:VAL:HG23	1:A:327:ILE:HD12	1.65	0.78
1:A:302:LEU:HB3	1:A:304:LYS:HE2	1.70	0.72
1:A:68:LYS:O	1:A:69:ASN:HB3	1.90	0.69
1:A:214:ARG:HG2	5:A:500:HEM:CBC	2.23	0.69
1:A:326:VAL:CG2	1:A:327:ILE:HD12	2.23	0.68
1:A:73:PRO:HD2	1:A:89:LYS:HE3	1.75	0.68
1:A:324:PRO:HB2	1:A:326:VAL:HG22	1.76	0.68
1:A:383:LYS:HE2	6:A:709:HOH:O	1.93	0.67
1:A:326:VAL:HG23	1:A:327:ILE:HB	1.77	0.66
1:A:379:LEU:HD12	4:A:441:PO4:O2	1.95	0.66
1:A:214:ARG:HG2	5:A:500:HEM:HBC2	1.78	0.65
1:A:409:ARG:HD2	6:A:555:HOH:O	1.99	0.62
1:A:389:SER:HB3	1:A:396:ASN:HD21	1.67	0.60
1:A:26:GLN:NE2	1:A:26:GLN:H	1.96	0.59
5:A:500:HEM:HBB2	5:A:500:HEM:HMB2	1.85	0.59
1:A:328:SER:HB3	6:A:556:HOH:O	2.02	0.58
1:A:117:PRO:HG2	1:A:145:TRP:CH2	2.37	0.58
1:A:325:PRO:HD2	1:A:326:VAL:HG13	1.86	0.56
1:A:326:VAL:HG23	1:A:327:ILE:CD1	2.34	0.56
5:A:500:HEM:HBC2	5:A:500:HEM:HHD	1.88	0.55
1:A:222:HIS:CD2	1:A:224:HIS:H	2.26	0.54
1:A:326:VAL:HG23	1:A:327:ILE:CB	2.38	0.54
5:A:500:HEM:CMB	5:A:500:HEM:HBB2	2.39	0.52
1:A:80:HIS:HE1	1:A:135:GLY:O	1.94	0.51
1:A:390:CYS:O	1:A:409:ARG:HD3	2.13	0.48
1:A:68:LYS:HE3	6:A:627:HOH:O	2.13	0.48
1:A:124:VAL:HG22	1:A:168:ALA:HB1	1.95	0.48
1:A:177:CYS:HB3	1:A:184:LEU:HD12	1.96	0.47
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.79	0.47
1:A:326:VAL:HG23	1:A:327:ILE:CG1	2.44	0.47
1:A:68:LYS:O	1:A:69:ASN:CB	2.60	0.47
1:A:391:SER:H	1:A:396:ASN:ND2	2.13	0.47
1:A:32:SER:N	6:A:620:HOH:O	2.48	0.47
1:A:296:THR:HG22	1:A:296:THR:O	2.15	0.47
1:A:391:SER:H	1:A:396:ASN:HD21	1.64	0.46
1:A:343:ARG:HG2	1:A:354:TRP:CE3	2.51	0.46
1:A:24:ILE:O	1:A:27:CYS:HB2	2.16	0.46
1:A:82:HIS:CE1	1:A:261:ARG:HG2	2.51	0.45
1:A:51:PHE:CZ	1:A:62:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:HE21	1:A:297:LYS:NZ	2.15	0.45
1:A:124:VAL:HG22	1:A:168:ALA:CB	2.47	0.45
1:A:143:ARG:HH21	1:A:145:TRP:HZ2	1.65	0.45
1:A:325:PRO:CD	1:A:326:VAL:HG13	2.46	0.44
1:A:53:TRP:CE2	1:A:60:ARG:HG3	2.52	0.44
1:A:53:TRP:NE1	1:A:60:ARG:HG3	2.32	0.44
1:A:93:VAL:HG22	1:A:109:LEU:HD13	1.98	0.44
1:A:124:VAL:HG13	1:A:169:LEU:HA	2.00	0.44
1:A:60:ARG:HE	1:A:60:ARG:HB3	1.63	0.44
1:A:157:ARG:HG2	1:A:159:TRP:CE2	2.53	0.44
1:A:70:PHE:O	1:A:71:ILE:HD13	2.17	0.43
1:A:390:CYS:H	1:A:396:ASN:ND2	2.16	0.43
1:A:194:PRO:HG3	6:A:662:HOH:O	2.17	0.43
1:A:242:ASN:HD22	1:A:242:ASN:H	1.66	0.43
1:A:48:LYS:HZ2	1:A:48:LYS:HG2	1.66	0.43
1:A:153:THR:HB	1:A:155:LYS:NZ	2.33	0.43
1:A:75:ASP:OD2	1:A:119:PRO:HB3	2.19	0.43
1:A:383:LYS:HG2	6:A:509:HOH:O	2.19	0.43
1:A:260:ASN:HB2	1:A:264:TRP:CZ2	2.53	0.43
1:A:356:ASP:OD1	1:A:358:LYS:HB2	2.19	0.42
1:A:51:PHE:CE2	1:A:62:LEU:HD13	2.54	0.42
1:A:242:ASN:ND2	1:A:242:ASN:H	2.17	0.42
1:A:208:CYS:HA	1:A:209:PRO:HD3	1.70	0.42
1:A:405:LEU:HD22	1:A:429:LEU:HD23	2.01	0.42
1:A:175:TYR:CE1	1:A:188:PRO:HG3	2.54	0.42
5:A:500:HEM:HAD1	6:A:584:HOH:O	2.20	0.41
1:A:41:ASN:HD22	1:A:261:ARG:HH21	1.69	0.41
1:A:81:GLY:O	1:A:83:THR:HG23	2.19	0.41
1:A:70:PHE:C	1:A:71:ILE:HD13	2.40	0.41
1:A:222:HIS:NE2	1:A:224:HIS:HB3	2.36	0.40
1:A:71:ILE:HG22	1:A:72:GLY:N	2.35	0.40
1:A:222:HIS:CD2	1:A:224:HIS:N	2.89	0.40
1:A:175:TYR:CD1	1:A:188:PRO:HG3	2.56	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	392/460 (85%)	369 (94%)	16 (4%)	7 (2%)	11 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	THR
1	A	163	GLY
1	A	214	ARG
1	A	25	GLU
1	A	69	ASN
1	A	265	HIS
1	A	295	ASP

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	342/393 (87%)	293 (86%)	49 (14%)	4 4

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	25	GLU
1	A	26	GLN
1	A	32	SER

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Mol	Chain	Res	Type
1	A	48	LYS
1	A	60	ARG
1	A	62	LEU
1	A	65	GLU
1	A	66	ARG
1	A	68	LYS
1	A	71	ILE
1	A	80	HIS
1	A	92	LYS
1	A	93	VAL
1	A	107	LYS
1	A	108	SER
1	A	124	VAL
1	A	143	ARG
1	A	144	LYS
1	A	154	LYS
1	A	155	LYS
1	A	157	ARG
1	A	158	SER
1	A	169	LEU
1	A	184	LEU
1	A	199	LEU
1	A	206	LEU
1	A	207	SER
1	A	209	PRO
1	A	228	ARG
1	A	238	MET
1	A	239	VAL
1	A	248	VAL
1	A	252	SER
1	A	260	ASN
1	A	290	LEU
1	A	304	LYS
1	A	332	VAL
1	A	346	ILE
1	A	350	ARG
1	A	362	GLN
1	A	370	TRP
1	A	375	VAL
1	A	382	GLU
1	A	383	LYS
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	413	LYS
1	A	429	LEU
1	A	433	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	ASN
1	A	80	HIS
1	A	142	ASN
1	A	242	ASN
1	A	272	GLN
1	A	275	GLN
1	A	294	GLN
1	A	396	ASN
1	A	424	GLN

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

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	PO4	A	441	3	4,4,4	1.36	0	6,6,6	0.31	0
5	HEM	A	500	1	30,50,50	2.59	6 (20%)	24,82,82	2.59	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
4	PO4	A	441	3	-	0/0/0/0	0/0/0/0
5	HEM	A	500	1	-	0/10/54/54	0/0/8/8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEM	C3B-C4B	-8.20	1.44	1.51
5	A	500	HEM	C2D-C3D	-7.11	1.33	1.54
5	A	500	HEM	C3D-C4D	-4.83	1.45	1.51
5	A	500	HEM	C2C-C1C	-4.37	1.44	1.52
5	A	500	HEM	C2D-C1D	-2.07	1.45	1.51
5	A	500	HEM	C4C-NC	4.10	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	500	HEM	C3B-CAB-CBB	-3.02	119.82	124.46
5	A	500	HEM	CMA-C3A-C4A	-2.75	123.82	128.36
5	A	500	HEM	CMD-C2D-C3D	2.40	124.95	114.35
5	A	500	HEM	CAD-C3D-C4D	2.98	122.99	112.47
5	A	500	HEM	CBA-CAA-C2A	3.63	119.03	112.53
5	A	500	HEM	C3C-CAC-CBC	3.89	130.42	124.46
5	A	500	HEM	C2D-C3D-C4D	4.17	108.57	101.50
5	A	500	HEM	CMB-C2B-C3B	4.86	128.66	116.53
5	A	500	HEM	CMC-C2C-C3C	5.16	129.42	116.53
5	A	500	HEM	CAD-C3D-C2D	5.28	128.40	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	441	PO4	2	0
5	A	500	HEM	6	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.