Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JME
Title	:	Crystal Structure of Phe393His Cytochrome P450 BM3
Authors	:	Ost, T.W.B.; Munro, A.W.; Mowat, C.G.; Pesseguiero, A.; Fulco, A.J.; Cho, A.K.; Cheesman, M.A.; Walkinshaw, M.D.; Chapman, S.K.
Deposited on	:	2001-07-18
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:

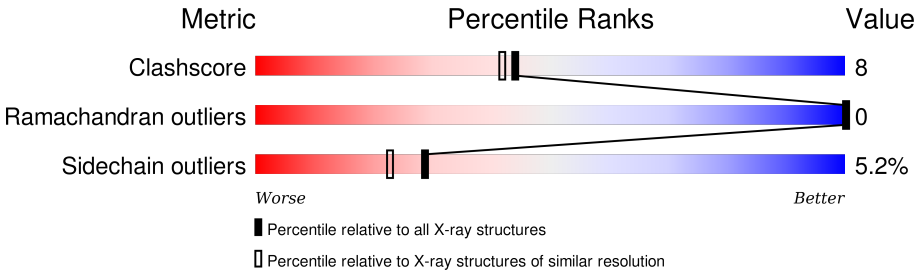
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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)

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	455	81% 13%
1	B	455	82% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8278 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.

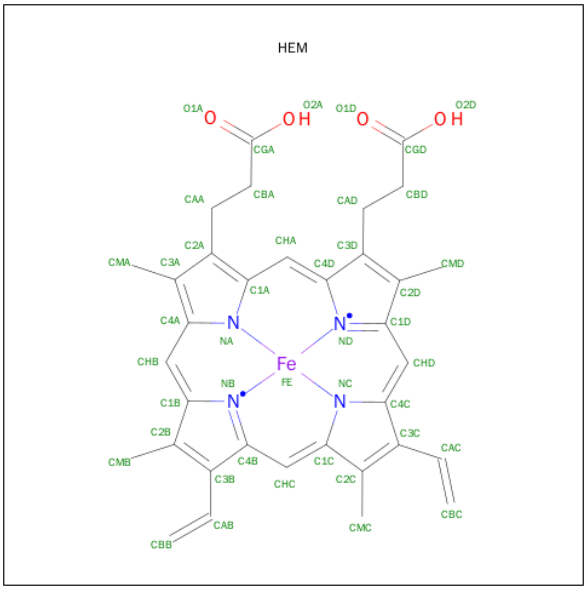
- Molecule 1 is a protein called BIFUNCTIONAL P-450:NADPH-P450 REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3496	2241	595	643	17			
1	B	441	Total	C	N	O	S	0	0	0
			3514	2252	596	649	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	HIS	PHE	ENGINEERED	UNP P14779
B	393	HIS	PHE	ENGINEERED	UNP P14779

- 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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	569	Total	O	0	0
			569	569		
3	B	613	Total	O	0	0
			613	613		

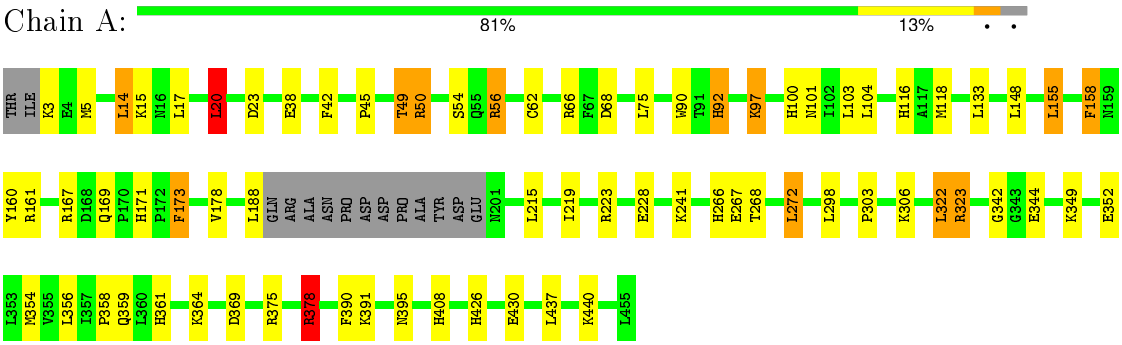
3 Residue-property plots (i)

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.

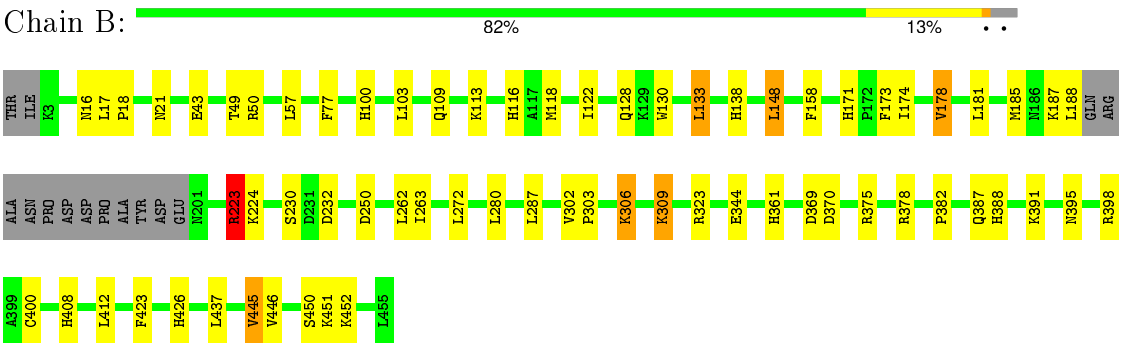
- Molecule 1: BIFUNCTIONAL P-450:NADPH-P450 REDUCTASE

Chain A:



- Molecule 1: BIFUNCTIONAL P-450:NADPH-P450 REDUCTASE

Chain B:



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	58.84Å 153.10Å 61.48Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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

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	0.35	0/3576	0.99	15/4841 (0.3%)
1	B	0.36	0/3595	0.97	7/4863 (0.1%)
All	All	0.36	0/7171	0.98	22/9704 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ARG	CG-CD-NE	8.67	130.00	111.80
1	A	56	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	223	ARG	CD-NE-CZ	7.97	134.76	123.60
1	B	223	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	323	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	161	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	20	LEU	CA-CB-CG	7.78	133.20	115.30
1	B	148	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	50	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	B	369	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	56	ARG	CD-NE-CZ	6.26	132.36	123.60
1	A	323	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	223	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	56	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	50	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	378	ARG	CA-CB-CG	5.75	126.04	113.40
1	A	68	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	250	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	66	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	398	ARG	CD-NE-CZ	5.16	130.82	123.60
1	A	323	ARG	CD-NE-CZ	5.02	130.63	123.60
1	A	173	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

There are no planarity outliers.

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	3496	0	3423	54	0
1	B	3514	0	3471	59	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	569	0	0	13	0
3	B	613	0	0	16	0
All	All	8278	0	6954	113	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 8.

All (113) 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:B:280:LEU:HB3	1:B:287:LEU:HD23	1.57	0.85
1:B:16:ASN:HD22	1:B:43:GLU:H	1.22	0.85
1:B:116:HIS:HD2	1:B:408:HIS:HE2	1.24	0.83
1:A:356:LEU:HD13	1:A:358:PRO:HD2	1.65	0.78
1:A:171:HIS:HD2	1:A:173:PHE:H	1.32	0.78
1:A:97:LYS:HB2	3:A:926:HOH:O	1.84	0.77
1:B:174:ILE:O	1:B:178:VAL:HG13	1.84	0.76
1:B:171:HIS:HD2	1:B:173:PHE:H	1.33	0.75
1:B:361:HIS:HE1	1:B:391:LYS:H	1.34	0.74
1:B:128:GLN:HG2	3:B:1060:HOH:O	1.89	0.73
1:A:272:LEU:HG	1:A:322:LEU:HD13	1.72	0.70
1:A:361:HIS:HE1	1:A:391:LYS:H	1.39	0.70
1:B:57:LEU:HD21	3:B:984:HOH:O	1.91	0.69
1:A:375:ARG:O	1:A:378:ARG:HG2	1.94	0.67
1:A:158:PHE:HE2	1:A:219:ILE:HD13	1.61	0.66
1:B:109:GLN:NE2	1:B:309:LYS:HZ3	1.94	0.66
1:B:109:GLN:HE22	1:B:309:LYS:HZ3	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:PRO:HD2	3:B:790:HOH:O	1.97	0.65
1:B:223:ARG:HH11	1:B:223:ARG:HG2	1.63	0.63
1:A:356:LEU:HD12	1:A:359:GLN:HG2	1.81	0.63
1:B:116:HIS:CD2	1:B:408:HIS:HE2	2.14	0.62
1:A:354:MET:HE1	3:A:677:HOH:O	1.99	0.62
1:A:158:PHE:CE2	1:A:219:ILE:HD13	2.35	0.61
1:B:130:TRP:HA	1:B:133:LEU:HD22	1.83	0.61
1:A:241:LYS:HD2	3:A:802:HOH:O	2.01	0.59
1:B:450:SER:O	1:B:452:LYS:HE2	2.03	0.59
1:A:97:LYS:HE2	1:A:101:ASN:OD1	2.03	0.58
1:B:100:HIS:HD2	3:B:710:HOH:O	1.86	0.58
1:B:21:ASN:HB2	3:B:741:HOH:O	2.03	0.58
1:B:223:ARG:HD2	3:B:1032:HOH:O	2.03	0.58
1:B:100:HIS:HE1	3:B:1014:HOH:O	1.87	0.58
1:A:352:GLU:HB2	3:A:806:HOH:O	2.04	0.57
1:A:100:HIS:HD2	3:A:686:HOH:O	1.90	0.55
1:B:109:GLN:HE22	1:B:309:LYS:NZ	2.04	0.55
1:A:223:ARG:HD3	1:A:228:GLU:HG2	1.87	0.55
1:B:223:ARG:HH22	1:B:230:SER:HB2	1.72	0.55
1:B:17:LEU:HB3	1:B:18:PRO:HD3	1.90	0.53
1:B:423:PHE:HD1	3:B:1055:HOH:O	1.91	0.53
1:B:185:MET:CE	1:B:437:LEU:HD13	2.39	0.53
1:A:267:GLU:HG2	3:A:970:HOH:O	2.09	0.52
1:B:280:LEU:CB	1:B:287:LEU:HD23	2.34	0.52
1:A:171:HIS:CD2	1:A:173:PHE:H	2.19	0.52
1:B:451:LYS:C	1:B:452:LYS:HE3	2.30	0.52
1:B:116:HIS:HE1	1:B:303:PRO:O	1.93	0.52
1:B:171:HIS:CD2	1:B:173:PHE:H	2.21	0.51
1:B:122:ILE:HG22	1:B:148:LEU:HD22	1.92	0.51
1:B:16:ASN:ND2	1:B:43:GLU:H	1.99	0.50
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.08	0.50
1:A:364:LYS:HD3	1:A:369:ASP:HA	1.93	0.50
1:A:342:GLY:O	1:A:344:GLU:HG3	2.12	0.49
1:A:266:HIS:CE1	1:A:267:GLU:HG3	2.48	0.49
1:A:178:VAL:HG22	3:A:792:HOH:O	2.11	0.49
1:B:323:ARG:HA	1:B:361:HIS:CD2	2.48	0.48
1:A:20:LEU:HD22	1:A:42:PHE:HZ	1.77	0.48
1:A:5:MET:SD	1:A:50:ARG:HG2	2.53	0.48
1:A:118:MET:SD	1:A:155:LEU:HD13	2.53	0.48
1:A:391:LYS:NZ	1:A:395:ASN:HD22	2.12	0.48
1:B:287:LEU:HD11	3:B:1055:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LYS:NZ	1:B:395:ASN:HD22	2.12	0.47
1:B:391:LYS:HZ3	1:B:395:ASN:HD22	1.60	0.47
1:A:356:LEU:HD12	1:A:359:GLN:CG	2.45	0.47
1:A:306:LYS:HG3	3:A:568:HOH:O	2.15	0.46
1:B:138:HIS:CD2	1:B:445:VAL:HG22	2.50	0.46
1:A:361:HIS:CE1	1:A:390:PHE:HA	2.50	0.46
1:A:49:THR:HG23	1:A:352:GLU:HB3	1.97	0.46
1:A:364:LYS:NZ	3:A:1004:HOH:O	2.48	0.46
1:B:375:ARG:O	1:B:378:ARG:HG3	2.15	0.46
1:B:426:HIS:HE1	3:B:676:HOH:O	1.98	0.46
1:A:437:LEU:HD23	3:A:1027:HOH:O	2.16	0.45
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.49	0.45
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.99	0.45
1:A:3:LYS:HA	1:A:3:LYS:HD3	1.73	0.45
1:A:426:HIS:HE1	3:A:690:HOH:O	2.00	0.45
1:B:50:ARG:NH1	3:B:643:HOH:O	2.50	0.45
1:B:50:ARG:NE	3:B:727:HOH:O	2.48	0.45
1:B:77:PHE:CE2	1:B:187:LYS:HB3	2.51	0.45
1:B:113:LYS:NZ	3:B:974:HOH:O	2.50	0.44
1:A:272:LEU:HG	1:A:322:LEU:CD1	2.43	0.44
1:B:370:ASP:OD2	1:B:375:ARG:NH2	2.49	0.44
1:A:215:LEU:O	1:A:219:ILE:HD12	2.18	0.44
1:A:20:LEU:HD22	1:A:42:PHE:CZ	2.52	0.44
1:A:116:HIS:HE1	1:A:303:PRO:O	2.00	0.44
1:B:303:PRO:HG2	1:B:412:LEU:CD1	2.48	0.44
1:B:185:MET:HE1	1:B:437:LEU:HD13	1.99	0.44
1:A:323:ARG:HA	1:A:361:HIS:CD2	2.53	0.43
1:B:387:GLN:HG2	1:B:388:HIS:ND1	2.34	0.43
1:A:62:CYS:HB3	1:A:395:ASN:ND2	2.34	0.43
1:A:241:LYS:HE3	3:A:542:HOH:O	2.18	0.43
1:B:370:ASP:OD2	1:B:375:ARG:NH1	2.50	0.43
1:B:391:LYS:HE2	1:B:395:ASN:HB2	2.01	0.43
1:B:426:HIS:H	1:B:426:HIS:CD2	2.36	0.43
1:B:388:HIS:HD2	1:B:391:LYS:HZ3	1.65	0.43
1:A:361:HIS:CE1	1:A:391:LYS:H	2.28	0.43
1:B:173:PHE:HE1	1:B:262:LEU:HD13	1.83	0.42
1:B:306:LYS:NZ	3:B:921:HOH:O	2.51	0.42
1:A:90:TRP:HB3	1:A:92:HIS:CE1	2.55	0.42
1:A:378:ARG:HD3	1:A:378:ARG:HH11	1.69	0.42
1:A:14:LEU:HA	1:A:14:LEU:HD12	1.86	0.42
1:A:268:THR:HB	2:A:460:HEM:C3B	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:OH	1:A:171:HIS:HE1	2.03	0.42
1:A:17:LEU:HD22	1:A:45:PRO:CD	2.50	0.42
1:B:138:HIS:HD2	1:B:445:VAL:HG22	1.83	0.42
1:B:50:ARG:NH2	3:B:817:HOH:O	2.52	0.42
1:B:128:GLN:NE2	3:B:491:HOH:O	2.52	0.41
1:A:118:MET:HB3	1:A:155:LEU:HD13	2.01	0.41
1:B:223:ARG:HH22	1:B:230:SER:CB	2.33	0.41
1:A:38:GLU:HB2	1:A:54:SER:HB3	2.03	0.41
1:A:440:LYS:NZ	3:A:1017:HOH:O	2.53	0.41
1:A:356:LEU:HD12	1:A:359:GLN:HB2	2.02	0.41
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.19	0.41
1:B:118:MET:HE3	1:B:118:MET:HB2	1.91	0.41
1:A:3:LYS:HE2	1:A:344:GLU:HA	2.02	0.40
1:B:400:CYS:HA	2:B:460:HEM:CHA	2.52	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	437/455 (96%)	423 (97%)	14 (3%)	0	100	100
1	B	437/455 (96%)	427 (98%)	10 (2%)	0	100	100
All	All	874/910 (96%)	850 (97%)	24 (3%)	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	369/399 (92%)	347 (94%)	22 (6%)	24 17
1	B	377/399 (94%)	360 (96%)	17 (4%)	34 29
All	All	746/798 (94%)	707 (95%)	39 (5%)	29 23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	15	LYS
1	A	20	LEU
1	A	23	ASP
1	A	49	THR
1	A	56	ARG
1	A	75	LEU
1	A	92	HIS
1	A	97	LYS
1	A	103	LEU
1	A	104	LEU
1	A	133	LEU
1	A	148	LEU
1	A	155	LEU
1	A	158	PHE
1	A	169	GLN
1	A	188	LEU
1	A	272	LEU
1	A	322	LEU
1	A	349	LYS
1	A	378	ARG
1	A	430	GLU
1	B	49	THR
1	B	103	LEU
1	B	133	LEU
1	B	158	PHE
1	B	178	VAL
1	B	181	LEU
1	B	188	LEU
1	B	223	ARG
1	B	224	LYS
1	B	263	ILE
1	B	272	LEU

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Mol	Chain	Res	Type
1	B	302	VAL
1	B	306	LYS
1	B	309	LYS
1	B	344	GLU
1	B	445	VAL
1	B	446	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	21	ASN
1	A	27	GLN
1	A	95	ASN
1	A	100	HIS
1	A	110	GLN
1	A	116	HIS
1	A	159	ASN
1	A	169	GLN
1	A	171	HIS
1	A	266	HIS
1	A	319	ASN
1	A	361	HIS
1	A	395	ASN
1	A	426	HIS
1	B	7	GLN
1	B	16	ASN
1	B	95	ASN
1	B	100	HIS
1	B	109	GLN
1	B	110	GLN
1	B	116	HIS
1	B	128	GLN
1	B	138	HIS
1	B	171	HIS
1	B	236	HIS
1	B	266	HIS
1	B	288	GLN
1	B	319	ASN
1	B	361	HIS
1	B	387	GLN
1	B	388	HIS

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Mol	Chain	Res	Type
1	B	395	ASN
1	B	403	GLN
1	B	426	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

2 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	$\#\|Z\| > 2$
2	HEM	A	460	1,3	30,50,50	2.72	9 (30%)	24,82,82	2.39	8 (33%)
2	HEM	B	460	1,3	30,50,50	2.70	9 (30%)	24,82,82	2.27	8 (33%)

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	460	1,3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	460	1,3	-	0/10/54/54	0/0/8/8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HEM	C3C-CAC	-6.56	1.39	1.51
2	A	460	HEM	C3B-CAB	-6.50	1.39	1.51
2	B	460	HEM	C3C-CAC	-6.47	1.39	1.51
2	A	460	HEM	C2D-C3D	-6.30	1.35	1.54
2	B	460	HEM	C2D-C3D	-6.17	1.36	1.54
2	B	460	HEM	C3B-CAB	-6.13	1.39	1.51
2	B	460	HEM	C3B-C4B	-5.53	1.46	1.51
2	A	460	HEM	C3B-C4B	-4.58	1.47	1.51
2	B	460	HEM	C3D-C4D	-4.58	1.45	1.51
2	A	460	HEM	C3D-C4D	-4.15	1.46	1.51
2	A	460	HEM	C2C-C1C	-3.97	1.45	1.52
2	B	460	HEM	C2C-C1C	-3.49	1.46	1.52
2	A	460	HEM	CBC-CAC	2.52	1.43	1.29
2	B	460	HEM	C1C-NC	2.57	1.39	1.36
2	A	460	HEM	CBB-CAB	2.62	1.44	1.29
2	B	460	HEM	CBC-CAC	2.72	1.45	1.29
2	B	460	HEM	CBB-CAB	2.76	1.45	1.29
2	A	460	HEM	C1C-NC	2.98	1.39	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	460	HEM	C3B-CAB-CBB	2.09	127.66	124.46
2	B	460	HEM	C3C-CAC-CBC	2.19	127.81	124.46
2	B	460	HEM	CAA-CBA-CGA	2.25	116.88	112.75
2	A	460	HEM	C2D-C3D-C4D	2.70	106.08	101.50
2	B	460	HEM	CMD-C2D-C3D	2.73	126.41	114.35
2	A	460	HEM	CMD-C2D-C3D	2.94	127.37	114.35
2	B	460	HEM	C2D-C3D-C4D	3.08	106.72	101.50
2	A	460	HEM	CAD-C3D-C4D	3.58	125.11	112.47
2	A	460	HEM	C3C-CAC-CBC	3.86	130.38	124.46
2	B	460	HEM	CAD-C3D-C2D	4.08	124.95	113.22
2	B	460	HEM	CAD-C3D-C4D	4.23	127.39	112.47
2	A	460	HEM	CMC-C2C-C3C	4.44	127.62	116.53
2	B	460	HEM	CMB-C2B-C3B	4.91	128.79	116.53
2	A	460	HEM	CAD-C3D-C2D	4.95	127.46	113.22
2	B	460	HEM	CMC-C2C-C3C	5.01	129.04	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	460	HEM	CMB-C2B-C3B	5.43	130.09	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	460	HEM	1	0
2	B	460	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.