



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 AM GMT

PDB ID : 2HPD
Title : CRYSTAL STRUCTURE OF HEMOPROTEIN DOMAIN OF P450BM-3, A
PROTOTYPE FOR MICROSOMAL P450'S
Authors : Ravichandran, K.G.; Boddupalli, S.S.; Hasemann, C.A.; Peterson, J.A.;
Deisenhofer, J.
Deposited on : 1993-09-16
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

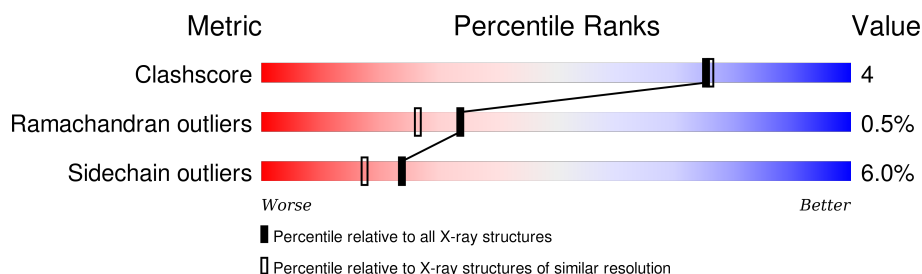
1 Overall quality at a glance

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	 76% 18% . .
1	B	471	 79% 15% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7897 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 CYTOCHROME P450 BM-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3678	2349	625	687	17			
1	B	457	Total	C	N	O	S	0	0	0
			3678	2349	625	687	17			

- 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 water.

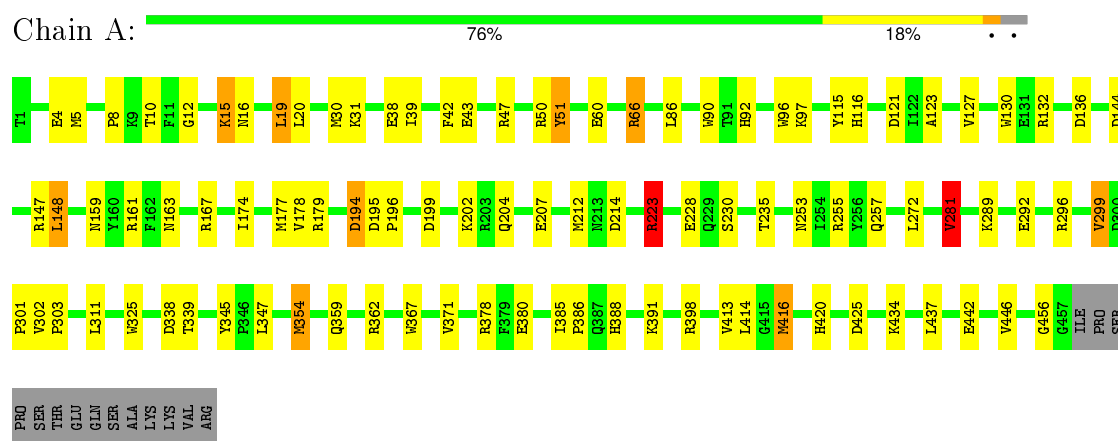
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total 233	O 233	0	0
3	B	222	Total 222	O 222	0	0

3 Residue-property plots

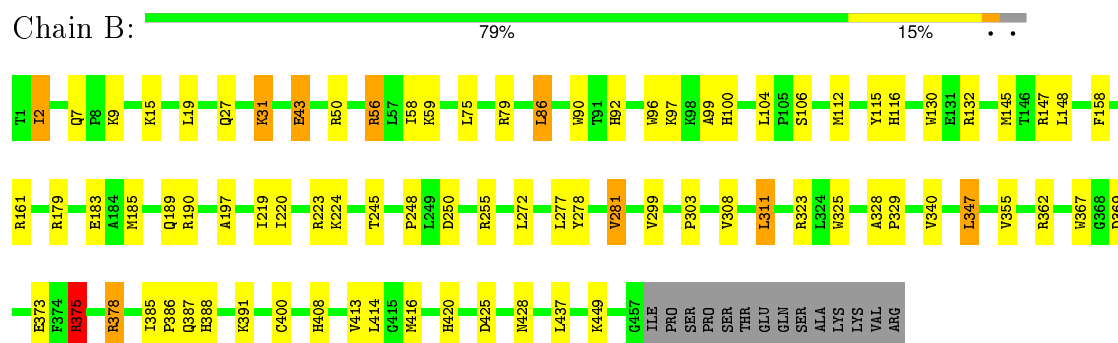
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: CYTOCHROME P450 BM-3



• Molecule 1: CYTOCHROME P450 BM-3



4 Data and refinement statistics

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	59.40Å 154.00Å 62.20Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7897	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	0.89	0/3763	1.63	56/5087 (1.1%)
1	B	0.89	0/3763	1.59	51/5087 (1.0%)
All	All	0.89	0/7526	1.61	107/10174 (1.1%)

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	1

There are no bond length outliers.

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	223	ARG	NE-CZ-NH2	-18.56	111.02	120.30
1	B	323	ARG	NE-CZ-NH1	14.38	127.49	120.30
1	A	398	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	A	223	ARG	NE-CZ-NH1	13.51	127.06	120.30
1	A	378	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	378	ARG	NE-CZ-NH2	-12.15	114.23	120.30
1	B	132	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	A	255	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	B	378	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	223	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	50	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	B	375	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	325	TRP	CD1-CG-CD2	9.36	113.79	106.30
1	B	132	ARG	NE-CZ-NH2	-8.99	115.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	MET	CG-SD-CE	-8.67	86.33	100.20
1	A	66	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	50	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	179	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	132	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	255	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	B	161	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	90	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	325	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	B	79	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	325	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	161	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	367	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	354	MET	CG-SD-CE	-7.38	88.40	100.20
1	B	325	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	B	56	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	223	ARG	CG-CD-NE	-7.24	96.60	111.80
1	B	362	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	223	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	323	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	214	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	96	TRP	CD1-CG-CD2	7.11	111.98	106.30
1	B	112	MET	CG-SD-CE	7.10	111.57	100.20
1	A	90	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	B	278	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	A	367	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	132	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	130	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	B	90	TRP	CD1-CG-CD2	6.82	111.76	106.30
1	A	296	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	96	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	96	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	66	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	4	GLU	N-CA-C	6.65	128.95	111.00
1	A	362	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	190	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	367	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	147	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	340	VAL	CG1-CB-CG2	-6.47	100.55	110.90
1	A	130	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	B	362	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	90	TRP	CE2-CD2-CG	-6.40	102.18	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	B	86	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	325	TRP	CG-CD1-NE1	-6.33	103.77	110.10
1	A	214	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	96	TRP	CG-CD2-CE3	6.15	139.44	133.90
1	A	96	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	B	223	ARG	CG-CD-NE	-6.14	98.90	111.80
1	A	127	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	A	161	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	367	TRP	CE2-CD2-CG	-6.06	102.45	107.30
1	A	147	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	255	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	296	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	43	GLU	CA-CB-CG	5.95	126.49	113.40
1	A	130	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	B	145	MET	CG-SD-CE	-5.79	90.93	100.20
1	A	325	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	A	299	VAL	N-CA-CB	-5.77	98.80	111.50
1	A	179	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	50	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	328	ALA	N-CA-C	-5.55	96.00	111.00
1	B	367	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	A	51	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	325	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	B	190	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	362	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	325	TRP	CG-CD2-CE3	5.46	138.81	133.90
1	B	75	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	177	MET	CG-SD-CE	-5.43	91.52	100.20
1	A	121	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	90	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	B	115	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	345	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	15	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	144	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	90	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	B	281	VAL	N-CA-CB	-5.28	99.89	111.50
1	A	47	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	115	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	B	90	TRP	CB-CG-CD1	-5.19	120.25	127.00
1	B	416	MET	CA-CB-CG	-5.17	104.52	113.30
1	A	212	MET	CA-CB-CG	-5.14	104.56	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LEU	N-CA-CB	-5.08	100.24	110.40
1	B	347	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	38	GLU	N-CA-C	5.08	124.71	111.00
1	B	373	GLU	CA-CB-CG	5.07	124.55	113.40
1	B	325	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	A	96	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	281	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	B	2	ILE	N-CA-C	-5.02	97.44	111.00
1	A	15	LYS	CA-C-N	5.02	128.25	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ASP	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	3678	0	3651	30	0
1	B	3678	0	3651	25	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	233	0	0	3	0
3	B	222	0	0	2	0
All	All	7897	0	7362	57	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 4.

All (57) 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:301:PRO:HB3	1:A:456:GLY:H	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:HIS:HE1	3:B:2182:HOH:O	1.81	0.62
1:B:400:CYS:HB2	2:B:472:HEM:NA	2.15	0.61
1:B:281:VAL:HG13	1:B:425:ASP:HB2	1.82	0.61
1:A:223:ARG:HH21	1:A:235:THR:HG23	1.68	0.59
1:A:15:LYS:HD3	1:A:43:GLU:HG2	1.84	0.58
1:B:92:HIS:HD2	3:B:2333:HOH:O	1.86	0.57
1:A:116:HIS:HE1	1:A:303:PRO:O	1.87	0.57
1:A:199:ASP:HA	1:A:202:LYS:HB3	1.86	0.56
1:A:20:LEU:HG	1:A:42:PHE:CZ	2.41	0.56
1:A:39:ILE:HA	1:A:51:TYR:O	2.06	0.56
1:A:230:SER:H	1:A:235:THR:HG21	1.71	0.56
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.04	0.55
1:A:97:LYS:HB3	3:A:1217:HOH:O	2.07	0.55
1:B:9:LYS:H	1:B:9:LYS:HD3	1.72	0.54
1:A:194:ASP:HA	1:A:202:LYS:NZ	2.23	0.54
1:A:123:ALA:HB1	1:A:416:MET:CE	2.38	0.54
1:A:8:PRO:HB2	1:A:19:LEU:HD21	1.90	0.53
1:A:60:GLU:HG2	1:A:66:ARG:HH12	1.73	0.52
1:B:375:ARG:HB2	1:B:378:ARG:NH1	2.25	0.52
1:A:174:ILE:O	1:A:178:VAL:HG23	2.10	0.51
1:A:281:VAL:HG13	1:A:425:ASP:HB2	1.93	0.49
1:A:30:MET:HG2	1:A:359:GLN:HE21	1.76	0.49
1:B:308:VAL:HA	1:B:311:LEU:HD22	1.93	0.49
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.95	0.48
1:A:388:HIS:HA	1:A:391:LYS:HE3	1.96	0.48
1:B:27:GLN:O	1:B:31:LYS:HD2	2.12	0.48
1:B:7:GLN:NE2	1:B:43:GLU:HG2	2.29	0.48
1:B:58:ILE:HD13	1:B:355:VAL:HG13	1.98	0.46
1:B:400:CYS:HB2	2:B:472:HEM:C1A	2.50	0.46
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.98	0.45
1:A:123:ALA:HB1	1:A:416:MET:HE1	1.98	0.45
1:B:158:PHE:HD2	1:B:219:ILE:HG21	1.82	0.44
1:A:194:ASP:HA	1:A:202:LYS:HZ1	1.81	0.44
1:B:388:HIS:HD2	1:B:391:LYS:HZ2	1.66	0.44
1:A:437:LEU:HD23	3:A:1165:HOH:O	2.17	0.44
1:A:223:ARG:NH2	1:A:235:THR:HG23	2.33	0.43
1:A:420:HIS:HE1	3:A:1182:HOH:O	2.01	0.43
1:B:116:HIS:HD2	1:B:408:HIS:NE2	2.17	0.43
1:A:434:LYS:HB2	1:A:442:GLU:HB2	2.00	0.43
1:B:185:MET:SD	1:B:437:LEU:HD13	2.58	0.43
1:B:7:GLN:HE22	1:B:43:GLU:HG2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:H	1:A:92:HIS:CD2	2.36	0.43
1:A:163:ASN:O	1:A:167:ARG:HG3	2.19	0.43
1:B:220:ILE:O	1:B:224:LYS:HG3	2.18	0.42
1:A:16:ASN:O	1:A:19:LEU:HB2	2.19	0.42
1:A:253:ASN:O	1:A:257:GLN:HG2	2.20	0.42
1:B:116:HIS:HE1	1:B:303:PRO:O	2.03	0.42
1:B:385:ILE:HA	1:B:386:PRO:HD3	1.89	0.42
2:A:472:HEM:HMC2	2:A:472:HEM:HBC2	2.01	0.42
1:A:385:ILE:HA	1:A:386:PRO:HD2	1.88	0.41
1:A:60:GLU:HG2	1:A:66:ARG:NH1	2.34	0.41
2:A:472:HEM:HAC	2:A:472:HEM:HHD	1.84	0.41
1:B:277:LEU:O	1:B:281:VAL:HB	2.21	0.41
1:B:86:LEU:HD13	1:B:99:ALA:HB3	2.03	0.40
1:B:100:HIS:O	1:B:104:LEU:HB2	2.21	0.40
1:B:59:LYS:HB3	1:B:59:LYS:HE2	1.91	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	455/471 (97%)	434 (95%)	17 (4%)	4 (1%)	21	13
1	B	455/471 (97%)	435 (96%)	19 (4%)	1 (0%)	52	48
All	All	910/942 (97%)	869 (96%)	36 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLY
1	A	196	PRO
1	A	194	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	5	MET
1	B	197	ALA

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	399/412 (97%)	373 (94%)	26 (6%)	21	15
1	B	399/412 (97%)	377 (94%)	22 (6%)	27	21
All	All	798/824 (97%)	750 (94%)	48 (6%)	24	17

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	19	LEU
1	A	31	LYS
1	A	86	LEU
1	A	136	ASP
1	A	148	LEU
1	A	159	ASN
1	A	204	GLN
1	A	207	GLU
1	A	223	ARG
1	A	228	GLU
1	A	272	LEU
1	A	281	VAL
1	A	289	LYS
1	A	292	GLU
1	A	299	VAL
1	A	302	VAL
1	A	311	LEU
1	A	338	ASP
1	A	339	THR
1	A	347	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	MET
1	A	371	VAL
1	A	380	GLU
1	A	414	LEU
1	A	446	VAL
1	B	2	ILE
1	B	19	LEU
1	B	31	LYS
1	B	56	ARG
1	B	97	LYS
1	B	106	SER
1	B	183	GLU
1	B	189	GLN
1	B	245	THR
1	B	248	PRO
1	B	250	ASP
1	B	272	LEU
1	B	299	VAL
1	B	311	LEU
1	B	329	PRO
1	B	347	LEU
1	B	369	ASP
1	B	375	ARG
1	B	387	GLN
1	B	414	LEU
1	B	428	ASN
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	92	HIS
1	A	116	HIS
1	A	125	GLN
1	A	128	GLN
1	A	159	ASN
1	A	201	ASN
1	A	359	GLN
1	A	388	HIS
1	A	420	HIS
1	A	426	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	7	GLN
1	B	116	HIS
1	B	125	GLN
1	B	128	GLN
1	B	189	GLN
1	B	359	GLN
1	B	388	HIS
1	B	420	HIS
1	B	426	HIS

5.3.3 RNA [i](#)

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](#)

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	472	1,3	30,50,50	2.48	8 (26%)	24,82,82	2.54	8 (33%)
2	HEM	B	472	1,3	30,50,50	2.73	9 (30%)	24,82,82	2.31	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	472	1,3	-	0/10/54/54	0/0/8/8
2	HEM	B	472	1,3	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	HEM	C2D-C3D	-6.63	1.34	1.54
2	B	472	HEM	C3B-CAB	-6.62	1.38	1.51
2	B	472	HEM	C3C-CAC	-6.27	1.39	1.51
2	A	472	HEM	C3B-CAB	-6.14	1.39	1.51
2	B	472	HEM	C2D-C3D	-6.04	1.36	1.54
2	A	472	HEM	C3C-CAC	-5.89	1.40	1.51
2	B	472	HEM	C3B-C4B	-5.58	1.46	1.51
2	B	472	HEM	C3D-C4D	-4.44	1.45	1.51
2	A	472	HEM	C3B-C4B	-3.83	1.48	1.51
2	A	472	HEM	C3D-C4D	-3.47	1.47	1.51
2	B	472	HEM	C2C-C1C	-3.00	1.46	1.52
2	A	472	HEM	C2C-C1C	-2.91	1.47	1.52
2	B	472	HEM	CBB-CAB	2.30	1.42	1.29
2	B	472	HEM	CBC-CAC	2.67	1.44	1.29
2	A	472	HEM	CBB-CAB	2.78	1.45	1.29
2	A	472	HEM	CBC-CAC	2.83	1.45	1.29
2	B	472	HEM	C1C-NC	3.83	1.40	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	HEM	C3B-CAB-CBB	-2.21	121.06	124.46
2	B	472	HEM	C3C-CAC-CBC	2.24	127.89	124.46
2	A	472	HEM	CMD-C2D-C3D	3.15	128.29	114.35
2	A	472	HEM	C2D-C3D-C4D	3.35	107.17	101.50
2	B	472	HEM	CAD-C3D-C4D	3.41	124.49	112.47
2	B	472	HEM	CMD-C2D-C3D	3.46	129.65	114.35
2	A	472	HEM	C3C-CAC-CBC	3.59	129.96	124.46
2	A	472	HEM	CAD-C3D-C4D	3.72	125.60	112.47
2	B	472	HEM	C2D-C3D-C4D	3.81	107.96	101.50
2	B	472	HEM	CMC-C2C-C3C	4.40	127.51	116.53
2	A	472	HEM	CMC-C2C-C3C	4.45	127.64	116.53
2	B	472	HEM	CMB-C2B-C3B	4.70	128.26	116.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	HEM	C3B-CAB-CBB	4.74	131.72	124.46
2	A	472	HEM	CAD-C3D-C2D	4.84	127.12	113.22
2	B	472	HEM	CAD-C3D-C2D	4.97	127.51	113.22
2	A	472	HEM	CMB-C2B-C3B	5.09	129.22	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	472	HEM	2	0
2	B	472	HEM	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 ⓘ

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.