



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:11 PM GMT

PDB ID : 4KEW
Title : structure of the A82F BM3 heme domain in complex with omeprazole
Authors : Leys, D.
Deposited on : 2013-04-26
Resolution : 1.89 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

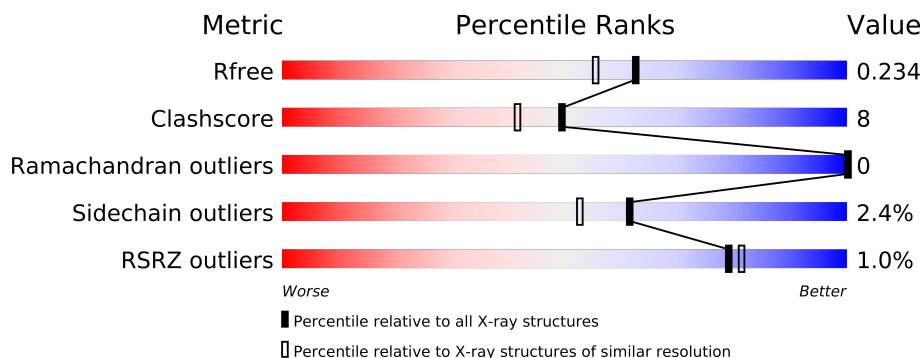
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.89 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))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	455	
1	B	455	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	1C6	A	502	-	X
3	1C6	B	502	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8159 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

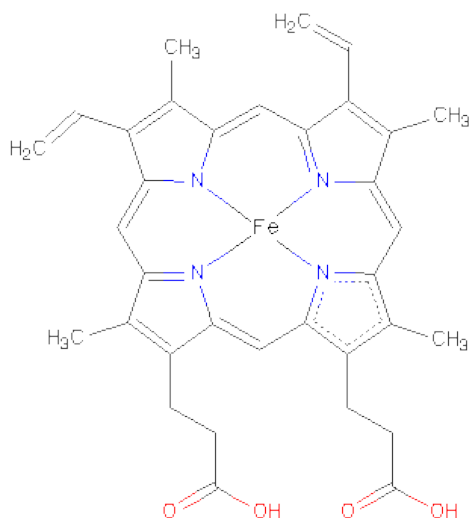
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	4	0
			3669	2348	621	683	17			
1	B	443	Total	C	N	O	S	0	3	0
			3611	2312	612	670	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
B	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779

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



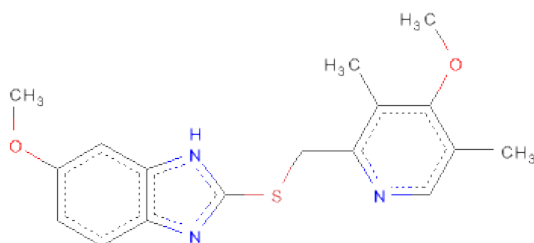
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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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 6-METHOXY-2-[[[(4-METHOXY-3,5-DIMETHYLPYRIDIN-2-YL)METHYL]SULFANYL]-1H-BENZIMIDAZOLE (three-letter code: 1C6) (formula: C₁₇H₁₉N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	17	3	2	1		
3	B	1	Total	C	N	O	S	0	0
			23	17	3	2	1		

- Molecule 4 is water.

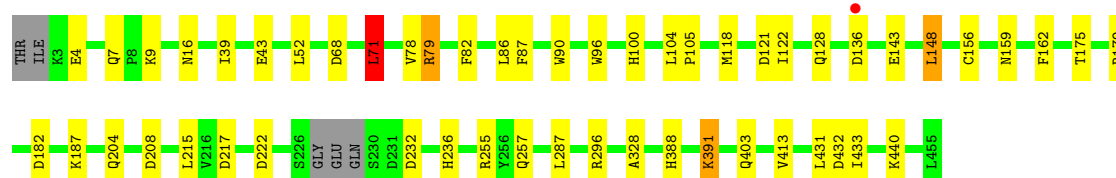
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	418	Total	O	0	0
			418	418		
4	B	329	Total	O	0	0
			329	329		

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.

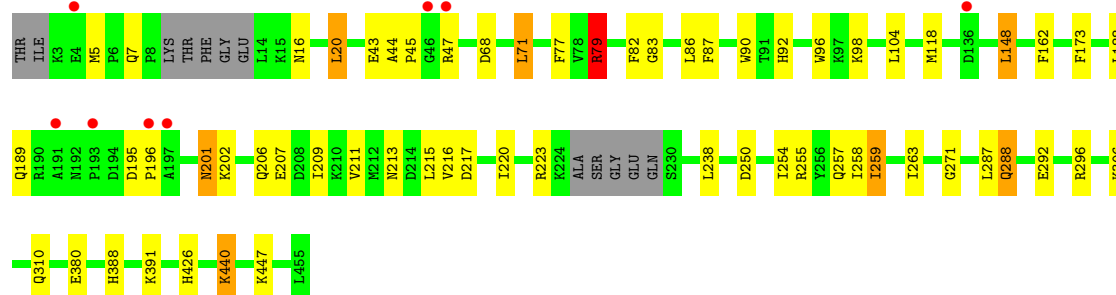
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase

Chain A: 



- Molecule 1: Bifunctional P-450/NADPH-P450 reductase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 129.51Å 145.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.75 – 1.89 64.75 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.75-1.89) 99.4 (64.75-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.237 0.192 , 0.234	Depositor DCC
R_{free} test set	4503 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 89901 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8159	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 1C6

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	1.06	2/3755 (0.1%)	0.97	14/5077 (0.3%)
1	B	0.97	1/3695 (0.0%)	0.90	8/4995 (0.2%)
All	All	1.02	3/7450 (0.0%)	0.94	22/10072 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	GLN	CG-CD	6.53	1.66	1.51
1	A	143	GLU	CG-CD	5.92	1.60	1.51
1	A	9	LYS	CE-NZ	5.31	1.62	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	CB-CG-OD1	8.16	125.64	118.30
1	A	79	ARG	CG-CD-NE	7.90	128.39	111.80
1	A	79	ARG	N-CA-CB	7.73	124.51	110.60
1	B	79	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	79	ARG	CB-CA-C	-6.96	96.49	110.40
1	A	68	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	79	ARG	CA-CB-CG	6.71	128.16	113.40
1	A	68	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	71	LEU	CB-CG-CD1	6.62	122.25	111.00
1	B	20	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	296	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	79	ARG	CA-CB-CG	6.14	126.90	113.40
1	B	287	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	68	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	432	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	296	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	79	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	B	96	TRP	CA-CB-CG	-5.11	104.00	113.70
1	A	96	TRP	CA-CB-CG	-5.08	104.05	113.70
1	B	250	ASP	CB-CG-OD1	5.02	122.81	118.30
1	A	391	LYS	CD-CE-NZ	-5.01	100.18	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3669	0	3614	46	0
1	B	3611	0	3565	59	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	23	0	19	12	0
3	B	23	0	19	6	0
4	A	418	0	0	11	0
4	B	329	0	0	14	0
All	All	8159	0	7277	112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:GLU:OE1	1:B:296:ARG:NH1	1.73	1.18
1:A:78:VAL:CG1	1:A:82:PHE:CD2	2.40	1.05
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.22	1.02
3:A:502:1C6:H10	4:A:756:HOH:O	1.59	1.01
1:A:217:ASP:OD1	1:A:255:ARG:NH1	1.98	0.96
1:B:20:LEU:HD23	4:B:651:HOH:O	1.62	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:502:1C6:H10	4:B:861:HOH:O	1.65	0.95
1:B:211:VAL:HG23	4:B:824:HOH:O	1.68	0.94
3:A:502:1C6:H8	3:A:502:1C6:H3	1.50	0.93
1:B:7:GLN:HE21	1:B:16:ASN:HD21	1.21	0.89
1:B:292:GLU:CD	1:B:296:ARG:NH1	2.27	0.87
1:A:78:VAL:CG1	1:A:82:PHE:HD2	1.86	0.87
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.08	0.86
1:A:7:GLN:HE21	1:A:16:ASN:HD21	1.25	0.84
1:B:217:ASP:OD1	1:B:255:ARG:NH1	2.11	0.83
1:B:310[A]:GLN:OE1	4:B:912:HOH:O	1.97	0.82
1:B:16:ASN:HD22	1:B:43:GLU:H	1.23	0.81
1:B:306:LYS:O	1:B:310[B]:GLN:HG2	1.80	0.81
1:B:86:LEU:H	1:B:257:GLN:HE22	1.29	0.81
1:A:118:MET:HE1	4:A:620:HOH:O	1.81	0.80
1:A:78:VAL:HG12	1:A:82:PHE:HD2	1.45	0.79
1:A:118:MET:HE2	4:A:645:HOH:O	1.82	0.79
1:B:207:GLU:O	4:B:824:HOH:O	2.01	0.78
1:A:16:ASN:HD22	1:A:43:GLU:H	1.32	0.76
1:B:92:HIS:HD2	4:B:665:HOH:O	1.68	0.75
1:A:78:VAL:HG12	1:A:82:PHE:CD2	2.20	0.75
3:A:502:1C6:C1	4:A:756:HOH:O	2.23	0.73
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.24	0.73
1:A:78:VAL:HG11	1:A:82:PHE:CD2	2.24	0.73
1:A:86:LEU:H	1:A:257:GLN:HE22	1.37	0.72
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.69	0.72
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.56	0.70
1:B:71:LEU:HD22	1:B:90:TRP:CE2	2.26	0.70
1:A:7:GLN:HE21	1:A:16:ASN:ND2	1.89	0.69
1:B:5:MET:HE3	4:B:688:HOH:O	1.92	0.69
1:A:136:ASP:OD1	4:A:989:HOH:O	2.13	0.66
1:A:179:ARG:NH1	1:A:204:GLN:OE1	2.28	0.65
1:B:82:PHE:HE1	1:B:263:ILE:HD12	1.62	0.65
1:A:175:THR:HG22	1:A:179:ARG:HH21	1.62	0.65
1:B:292:GLU:OE2	1:B:296:ARG:NH1	2.27	0.64
1:A:217:ASP:OD2	4:A:975:HOH:O	2.14	0.64
1:A:100:HIS:CE1	1:A:104:LEU:HD11	2.33	0.64
1:B:292:GLU:CD	1:B:296:ARG:HH11	2.00	0.60
1:B:209:ILE:CG2	1:B:213:ASN:HD21	2.13	0.60
1:A:78:VAL:HG11	1:A:82:PHE:CE2	2.36	0.60
1:A:87[A]:PHE:HZ	3:A:502:1C6:CE2	2.16	0.58
1:B:220:ILE:HD11	1:B:258:ILE:HD12	1.84	0.58
1:B:201:ASN:N	1:B:201:ASN:HD22	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209:ILE:HG22	1:B:213:ASN:ND2	2.19	0.57
1:B:271:GLY:HA2	1:B:440:LYS:HG3	1.85	0.57
1:A:78:VAL:HG13	1:A:82:PHE:CD2	2.38	0.57
1:A:87[A]:PHE:CZ	3:A:502:1C6:CE2	2.88	0.57
1:B:263:ILE:HG22	3:B:502:1C6:H6	1.85	0.56
1:B:173:PHE:CD1	1:B:215:LEU:HD23	2.40	0.56
1:A:162:PHE:HE1	1:A:215:LEU:CD2	2.19	0.56
3:A:502:1C6:C2	3:A:502:1C6:H3	2.31	0.56
1:A:128:GLN:HG2	4:A:684:HOH:O	2.07	0.55
1:A:71:LEU:HD22	1:A:90:TRP:CE2	2.42	0.54
1:A:182[A]:ASP:OD2	4:A:828:HOH:O	2.18	0.53
1:A:78:VAL:CG1	1:A:82:PHE:CE2	2.89	0.53
1:A:431:LEU:HD21	1:A:433:ILE:HD11	1.91	0.52
1:B:87[A]:PHE:CZ	3:B:502:1C6:CE2	2.94	0.51
1:A:87[A]:PHE:CE1	3:A:502:1C6:H11	2.46	0.51
1:B:86:LEU:N	1:B:257:GLN:HE22	2.06	0.51
1:A:87[A]:PHE:CE1	3:A:502:1C6:C1	2.94	0.51
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.44	0.50
1:B:195:ASP:CG	1:B:196:PRO:HD2	2.33	0.49
3:B:502:1C6:C1	4:B:861:HOH:O	2.38	0.49
1:A:104:LEU:N	1:A:105:PRO:CD	2.75	0.49
1:B:220:ILE:HD11	1:B:258:ILE:CD1	2.42	0.49
1:A:128:GLN:NE2	4:A:684:HOH:O	2.43	0.49
1:B:77:PHE:HE2	1:B:188:LEU:HD23	1.77	0.49
1:B:209:ILE:CG2	1:B:213:ASN:ND2	2.76	0.49
1:B:118:MET:CE	4:B:616:HOH:O	2.60	0.49
1:B:207:GLU:HG2	4:B:824:HOH:O	2.12	0.49
1:A:232:ASP:O	1:A:236:HIS:HD2	1.96	0.49
1:A:87[A]:PHE:HE1	3:A:502:1C6:C1	2.26	0.48
1:A:403:GLN:NE2	4:A:734:HOH:O	2.46	0.48
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.95	0.48
1:B:148:LEU:O	1:B:148:LEU:HG	2.14	0.48
1:A:87[A]:PHE:CE1	3:A:502:1C6:CZ	2.97	0.48
1:B:118:MET:HE1	4:B:616:HOH:O	2.13	0.48
1:B:77:PHE:CE2	1:B:188:LEU:HD23	2.49	0.47
1:A:118:MET:HE3	1:A:156:CYS:HA	1.95	0.47
1:B:209:ILE:HG23	1:B:213:ASN:HD21	1.79	0.47
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.44	0.47
1:A:39:ILE:HD12	1:A:52:LEU:CD2	2.46	0.46
1:B:195:ASP:OD2	1:B:196:PRO:HD2	2.16	0.46
1:A:87[A]:PHE:CZ	3:A:502:1C6:CZ	2.99	0.45
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:220:ILE:CD1	1:B:258:ILE:CD1	2.94	0.45
1:B:259:ILE:HD12	1:B:259:ILE:HG21	1.75	0.44
1:B:380:GLU:O	1:B:380:GLU:HG3	2.16	0.44
1:B:87[A]:PHE:HZ	3:B:502:1C6:CE2	2.29	0.44
1:B:16:ASN:ND2	1:B:43:GLU:H	2.02	0.44
1:A:328:ALA:HB1	3:A:502:1C6:N1	2.33	0.44
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.99	0.44
1:B:216:VAL:O	1:B:220:ILE:HG12	2.17	0.44
1:B:207:GLU:C	4:B:824:HOH:O	2.52	0.44
1:B:118:MET:HG2	4:B:841:HOH:O	2.17	0.44
1:B:209:ILE:O	1:B:213:ASN:ND2	2.51	0.43
1:A:79:ARG:HG3	4:A:746:HOH:O	2.17	0.43
1:B:79:ARG:HD3	1:B:83:GLY:O	2.18	0.43
1:B:306:LYS:O	1:B:310[B]:GLN:CG	2.61	0.43
1:B:426:HIS:CD2	1:B:447:LYS:HE3	2.54	0.42
1:B:44:ALA:HB1	1:B:45:PRO:CD	2.50	0.42
1:B:82:PHE:CE1	1:B:263:ILE:HD12	2.48	0.42
1:B:87[A]:PHE:CE1	3:B:502:1C6:C1	3.03	0.41
1:B:202:LYS:O	1:B:206:GLN:HG2	2.20	0.41
1:B:209:ILE:HG22	1:B:213:ASN:HD21	1.80	0.41
1:B:20:LEU:CD2	4:B:651:HOH:O	2.43	0.41
1:B:238:LEU:HD23	1:B:254:ILE:HD13	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	450/455 (99%)	439 (98%)	11 (2%)	0	100	100
1	B	440/455 (97%)	420 (96%)	20 (4%)	0	100	100
All	All	890/910 (98%)	859 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/400 (99%)	389 (98%)	8 (2%)	68	61
1	B	392/400 (98%)	381 (97%)	11 (3%)	56	45
All	All	789/800 (99%)	770 (98%)	19 (2%)	61	53

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	71	LEU
1	A	148	LEU
1	A	159	ASN
1	A	187	LYS
1	A	222	ASP
1	A	287	LEU
1	A	440	LYS
1	B	47	ARG
1	B	71	LEU
1	B	79	ARG
1	B	98	LYS
1	B	104	LEU
1	B	148	LEU
1	B	189	GLN
1	B	201	ASN
1	B	259	ILE
1	B	288	GLN
1	B	440	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	95	ASN
1	A	159	ASN
1	A	189	GLN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	236	HIS
1	A	253	ASN
1	A	257	GLN
1	A	388	HIS
1	A	403	GLN
1	B	16	ASN
1	B	73	GLN
1	B	95	ASN
1	B	159	ASN
1	B	213	ASN
1	B	253	ASN
1	B	257	GLN
1	B	283	ASN
1	B	288	GLN
1	B	381	ASN
1	B	388	HIS
1	B	403	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	501	1	49,50,50	2.63	18 (36%)	46,82,82	2.35	13 (28%)
3	1C6	A	502	-	25,25,25	3.42	7 (28%)	33,35,35	2.62	9 (27%)
2	HEM	B	501	1	49,50,50	2.47	18 (36%)	46,82,82	2.97	12 (26%)
3	1C6	B	502	-	25,25,25	3.87	8 (32%)	33,35,35	2.73	8 (24%)

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	501	1	-	0/14/114/114	0/0/8/8
3	1C6	A	502	-	-	0/8/9/9	0/1/3/3
2	HEM	B	501	1	-	0/14/114/114	0/0/8/8
3	1C6	B	502	-	-	1/8/9/9	0/1/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	1C6	CD1-CG	12.62	1.50	1.39
3	A	502	1C6	CD1-CG	11.99	1.50	1.39
2	A	501	HEM	C2D-C1D	-8.95	1.42	1.44
3	B	502	1C6	CB-S	-7.39	1.68	1.82
3	A	502	1C6	CE1-CD1	7.24	1.50	1.39
3	B	502	1C6	CE1-CD1	7.09	1.50	1.39
3	B	502	1C6	CE1-CZ	6.30	1.51	1.40
2	A	501	HEM	C3C-C2C	-6.18	1.33	1.43
2	B	501	HEM	C3D-C4D	5.94	1.46	1.44
3	A	502	1C6	CB-S	-5.87	1.71	1.82
2	A	501	HEM	C4A-C3A	5.61	1.47	1.40
3	B	502	1C6	CF1-S	-5.50	1.67	1.74
2	B	501	HEM	FE-ND	5.50	2.17	1.97
2	B	501	HEM	C4A-C3A	5.14	1.46	1.40
2	B	501	HEM	C3B-C2B	-5.04	1.35	1.43
2	B	501	HEM	C3C-CAC	5.03	1.56	1.40
3	A	502	1C6	CE1-CZ	4.91	1.49	1.40
2	B	501	HEM	C3D-C2D	4.83	1.52	1.43
2	A	501	HEM	C3B-C2B	-4.80	1.35	1.43
2	A	501	HEM	FE-NA	4.29	2.10	1.92
2	A	501	HEM	C3D-C2D	4.19	1.51	1.43
2	B	501	HEM	C3C-C2C	-4.07	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-CAB	3.92	1.52	1.40
2	A	501	HEM	C3D-C4D	-3.91	1.43	1.44
2	B	501	HEM	C3B-CAB	3.86	1.52	1.40
3	B	502	1C6	CE3-CZ3	3.86	1.43	1.37
2	B	501	HEM	CMD-C2D	3.35	1.57	1.47
2	B	501	HEM	CMB-C2B	3.15	1.57	1.47
2	B	501	HEM	FE-NA	3.07	2.05	1.92
2	A	501	HEM	C3C-CAC	3.05	1.49	1.40
2	B	501	HEM	CMC-C2C	2.96	1.56	1.47
2	A	501	HEM	C2B-C1B	2.87	1.45	1.44
3	A	502	1C6	CF1-S	-2.84	1.71	1.74
3	B	502	1C6	CX2-CS2	2.69	1.50	1.42
2	A	501	HEM	C1C-NC	-2.54	1.34	1.38
2	B	501	HEM	C2D-C1D	-2.52	1.43	1.44
2	A	501	HEM	CMD-C2D	2.52	1.55	1.47
2	B	501	HEM	FE-NC	2.48	2.07	1.97
2	A	501	HEM	CHC-C1C	2.35	1.40	1.36
2	A	501	HEM	O1A-CGA	2.33	1.30	1.22
3	B	502	1C6	CF1-NV	2.26	1.38	1.33
2	B	501	HEM	CHA-C4D	2.23	1.39	1.35
2	B	501	HEM	C1A-C2A	2.23	1.47	1.43
2	B	501	HEM	FE-NB	2.18	2.05	1.97
2	A	501	HEM	CAD-CBD	2.15	1.58	1.52
2	A	501	HEM	FE-NC	2.13	2.05	1.97
2	B	501	HEM	CAA-C2A	2.11	1.55	1.52
3	A	502	1C6	CZ2-CS2	-2.05	1.38	1.41
2	A	501	HEM	CHA-C4D	2.05	1.38	1.35
3	A	502	1C6	CE3-CZ3	2.03	1.40	1.37
2	A	501	HEM	FE-ND	2.03	2.05	1.97

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-C4B-NB	-12.15	105.31	114.00
3	B	502	1C6	CD1-CG-N1	-9.78	118.69	124.24
3	A	502	1C6	CD1-CG-N1	-9.16	119.05	124.24
2	A	501	HEM	C3B-C4B-NB	-8.90	107.63	114.00
2	B	501	HEM	C4D-ND-C1D	8.35	113.70	105.16
2	A	501	HEM	C4D-ND-C1D	6.20	111.51	105.16
3	A	502	1C6	CE2-N1-CG	5.82	124.80	117.85
2	B	501	HEM	CHC-C4B-NB	5.79	129.39	124.58
3	B	502	1C6	CE2-N1-CG	5.72	124.68	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	1C6	CZ-CE1-CD1	-5.32	117.16	121.74
2	B	501	HEM	C1B-NB-C4B	5.08	110.36	105.16
2	A	501	HEM	CBD-CAD-C3D	-4.98	103.50	114.37
3	A	502	1C6	CZ-CE1-CD1	-4.67	117.72	121.74
3	A	502	1C6	O2-CE1-CD1	4.64	125.06	118.77
2	B	501	HEM	CMA-C3A-C4A	-4.42	121.81	128.62
2	B	501	HEM	C4A-C3A-C2A	4.28	109.98	107.00
2	B	501	HEM	CBD-CAD-C3D	-4.26	105.06	114.37
2	A	501	HEM	CMA-C3A-C4A	-3.81	122.76	128.62
2	A	501	HEM	CBA-CAA-C2A	-3.77	106.05	112.69
2	A	501	HEM	CHA-C4D-ND	3.69	129.38	124.31
3	A	502	1C6	CZ-CE2-N1	-3.66	122.02	125.03
3	B	502	1C6	CE3-CX2-CS2	-3.65	115.53	122.33
3	B	502	1C6	CG-CB-S	3.31	116.92	109.79
3	B	502	1C6	CE1-CD1-CG	3.17	118.14	116.30
3	B	502	1C6	NV-CF1-NE1	3.13	115.32	111.96
2	B	501	HEM	C2D-C1D-ND	-3.12	109.25	112.93
2	A	501	HEM	C2D-C1D-ND	-3.00	109.39	112.93
3	A	502	1C6	CE2-CZ-CE1	2.75	118.99	116.08
2	B	501	HEM	CBA-CAA-C2A	-2.67	107.99	112.69
3	A	502	1C6	CE3-CX2-CS2	-2.62	117.44	122.33
2	A	501	HEM	O1A-CGA-CBA	-2.51	114.40	123.03
2	B	501	HEM	CHA-C4D-ND	2.50	127.75	124.31
3	B	502	1C6	CB-CG-N1	2.50	118.22	116.10
2	B	501	HEM	CHD-C1D-ND	2.47	126.64	124.58
2	A	501	HEM	C3A-C4A-NA	-2.46	107.55	109.41
2	B	501	HEM	C1A-C2A-C3A	-2.37	104.46	106.92
2	A	501	HEM	CMA-C3A-C2A	2.35	129.37	124.94
3	A	502	1C6	C4-O3-CZ3	2.31	123.16	117.54
2	A	501	HEM	C4C-NC-C1C	2.28	107.91	105.53
2	A	501	HEM	C1B-NB-C4B	2.28	107.49	105.16
3	A	502	1C6	C3-CD1-CG	-2.27	120.88	122.62
2	A	501	HEM	C1A-CHA-C4D	-2.18	124.60	127.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	1C6	NE1-CF1-S-CB

There are no ring outliers.

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 ⓘ

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	450/455 (98%)	-0.31	1 (0%) 93 94	10, 18, 36, 50	0
1	B	443/455 (97%)	-0.12	8 (1%) 65 67	14, 25, 53, 72	0
All	All	893/910 (98%)	-0.22	9 (1%) 79 81	10, 21, 47, 72	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	3.7
1	B	46	GLY	3.5
1	B	193	PRO	3.3
1	B	196	PRO	2.7
1	B	197	ALA	2.7
1	B	136	ASP	2.4
1	B	47	ARG	2.3
1	B	4	GLU	2.2
1	A	136	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	1C6	B	502	23/23	0.22	3.13	47,50,52,56	0
3	1C6	A	502	23/23	0.14	2.14	24,31,42,43	0
2	HEM	A	501	43/43	0.08	-0.28	6,10,13,14	0
2	HEM	B	501	43/43	0.08	-0.50	11,16,20,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.