



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:06 pm GMT

PDB ID : 1JRZ  
Title : Crystal structure of Arg402Tyr mutant flavocytochrome c3 from *Shewanella frigidimarina*  
Authors : Mowat, C.G.; Moysey, R.; Miles, C.S.; Leys, D.; Doherty, M.K.; Taylor, P.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.  
Deposited on : 2001-08-15  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

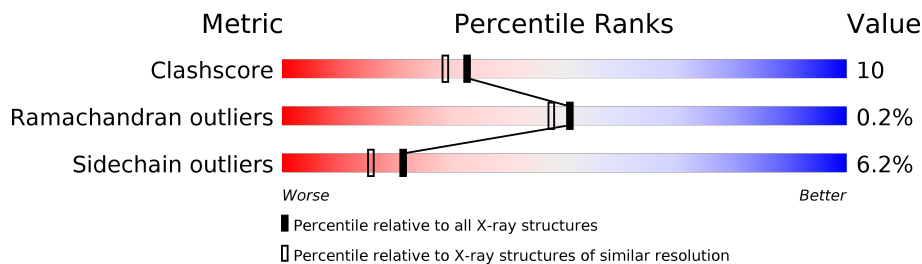
# 1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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  $\geq 3$ , 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	571	
1	B	571	

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	FAD	A	1805	X	-	-	-
4	FAD	B	2805	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10534 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 FLAVOCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4218	2618	741	834	25			
1	B	568	Total	C	N	O	S	0	0	0
			4218	2618	741	834	25			

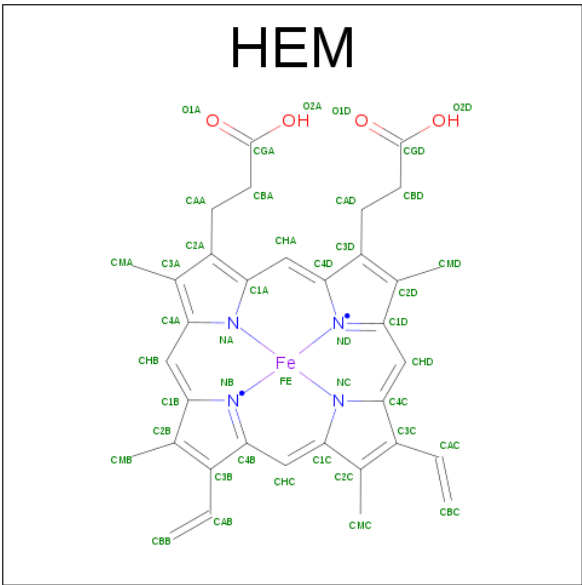
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	TYR	ARG	ENGINEERED	UNP Q02469
B	402	TYR	ARG	ENGINEERED	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



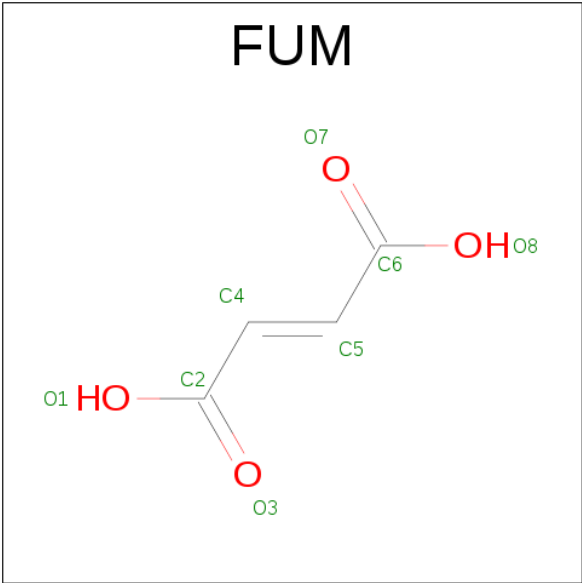
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

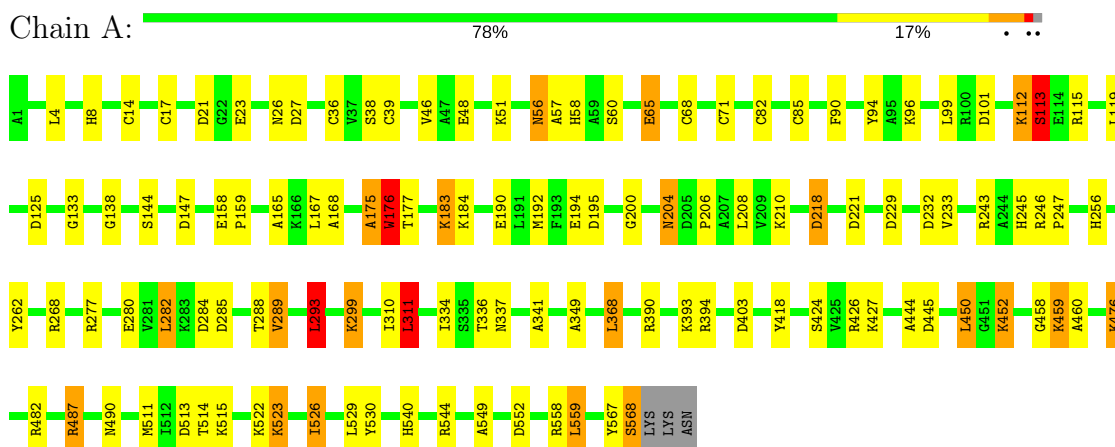
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	805	Total 805	O 805	0	0
6	B	825	Total 825	O 825	0	0

### 3 Residue-property plots

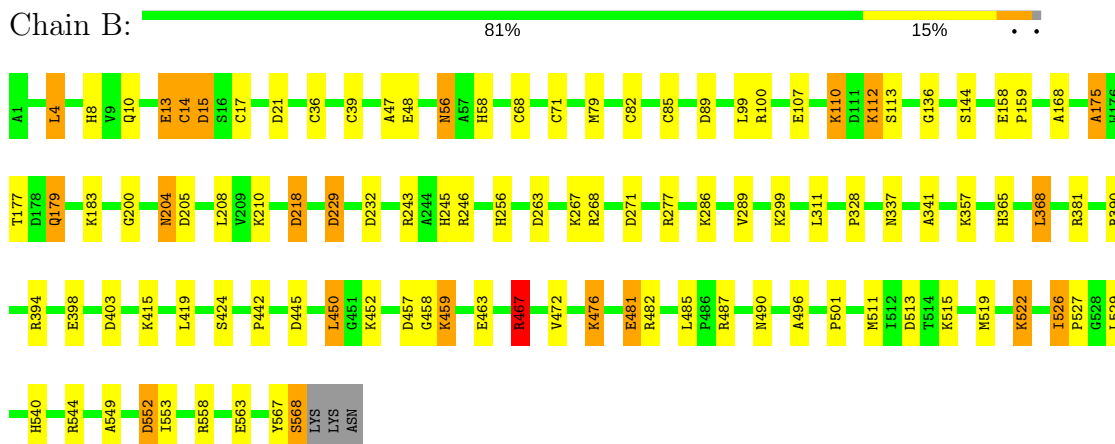
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: FLAVOCYTOCHROME C



#### • Molecule 1: FLAVOCYTOCHROME C



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.07Å 87.91Å 90.16Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.4 (20.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.176 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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, FUM, FAD, 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	2/4289 (0.0%)	1.56	52/5799 (0.9%)
1	B	0.71	0/4289	1.52	46/5799 (0.8%)
All	All	0.72	2/8578 (0.0%)	1.54	98/11598 (0.8%)

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
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	SER	CB-OG	-6.62	1.33	1.42
1	A	176	TRP	N-CA	-5.45	1.35	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	17.07	164.38	121.70
1	A	293	LEU	CA-CB-CG	17.03	154.47	115.30
1	B	218	ASP	CB-CG-OD1	-16.30	103.63	118.30
1	B	390	ARG	NE-CZ-NH2	-14.91	112.84	120.30
1	A	218	ASP	CB-CG-OD1	-13.49	106.16	118.30
1	A	277	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	A	243	ARG	NE-CZ-NH1	11.43	126.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ALA	O-C-N	-11.23	104.72	122.70
1	B	390	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	A	394	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	B	403	ASP	CB-CG-OD2	9.82	127.14	118.30
1	B	218	ASP	CB-CG-OD2	9.69	127.02	118.30
1	B	487	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	A	175	ALA	N-CA-CB	9.42	123.29	110.10
1	B	229	ASP	CB-CG-OD1	9.23	126.61	118.30
1	B	381	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	390	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	403	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	390	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	487	ARG	NE-CZ-NH2	8.65	124.62	120.30
1	B	558	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	487	ARG	CA-CB-CG	8.48	132.05	113.40
1	A	445	ASP	CB-CG-OD1	8.37	125.83	118.30
1	B	368	LEU	CA-CB-CG	8.20	134.17	115.30
1	A	94	TYR	CB-CG-CD1	-8.18	116.09	121.00
1	A	487	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	513	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	176	TRP	N-CA-CB	7.62	124.31	110.60
1	A	21	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	B	271	ASP	CB-CG-OD1	7.44	124.99	118.30
1	B	482	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	A	526	ILE	CA-CB-CG2	7.20	125.30	110.90
1	A	268	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	190	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	A	336	THR	CA-CB-CG2	6.87	122.02	112.40
1	A	558	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	125	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	558	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	567	TYR	C-N-CA	6.66	138.36	121.70
1	B	289	VAL	CA-CB-CG2	6.64	120.85	110.90
1	A	559	LEU	CA-CB-CG	6.50	130.24	115.30
1	A	21	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	394	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	513	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	284	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	65	GLU	CB-CG-CD	6.42	131.52	114.20
1	A	552	ASP	CB-CG-OD2	6.42	124.07	118.30
1	B	286	LYS	CD-CE-NZ	6.37	126.35	111.70
1	B	268	ARG	NE-CZ-NH2	-6.37	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	CD-NE-CZ	6.36	132.50	123.60
1	A	221	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	289	VAL	CA-CB-CG2	6.26	120.29	110.90
1	A	444	ALA	N-CA-CB	6.24	118.84	110.10
1	B	205	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	487	ARG	CG-CD-NE	-6.08	99.03	111.80
1	A	285	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	229	ASP	OD1-CG-OD2	-6.01	111.87	123.30
1	A	65	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	A	482	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	450	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	394	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	243	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	563	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	B	263	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	398	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	B	89	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	113	SER	N-CA-CB	-5.69	101.96	110.50
1	B	467	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	418	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	A	175	ALA	O-C-N	5.63	131.71	122.70
1	A	195	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	426	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	277	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	394	ARG	NH1-CZ-NH2	5.61	125.57	119.40
1	B	450	LEU	CB-CG-CD2	5.59	120.51	111.00
1	B	552	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	175	ALA	N-CA-CB	5.58	117.91	110.10
1	A	568	SER	N-CA-C	5.55	125.98	111.00
1	B	445	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	232	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	368	LEU	CA-CB-CG	5.49	127.94	115.30
1	A	112	LYS	C-N-CA	5.47	135.37	121.70
1	A	113	SER	CA-C-N	5.42	129.13	117.20
1	B	243	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	381	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	113	SER	C-N-CA	5.35	135.08	121.70
1	B	232	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	482	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	115	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	147	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	101	ASP	CB-CG-OD1	-5.19	113.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	13	GLU	CG-CD-OE1	5.12	128.55	118.30
1	A	311	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	424	SER	N-CA-CB	5.09	118.13	110.50
1	B	14	CYS	O-C-N	-5.07	114.60	122.70
1	A	450	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	27	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ALA	Peptide
1	B	175	ALA	Mainchain,Peptide

## 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	4218	0	4155	84	0
1	B	4218	0	4156	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	28	0
3	B	172	0	120	26	0
4	A	53	0	30	6	0
4	B	53	0	28	4	0
5	A	8	0	2	0	0
5	B	8	0	2	1	0
6	A	805	0	0	16	0
6	B	825	0	0	21	0
All	All	10534	0	8613	173	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 10.

All (173) 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:36:CYS:SG	3:A:802:HEM:CAB	2.45	1.04
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.48	1.02
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.50	1.00
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.50	0.99
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.53	0.97
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.53	0.96
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.54	0.95
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.54	0.95
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.55	0.95
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.54	0.95
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.55	0.94
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.57	0.93
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.57	0.92
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.60	0.90
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.59	0.90
1:A:229:ASP:H	1:A:256:HIS:HE1	1.18	0.88
1:A:14:CYS:HG	3:A:801:HEM:CAB	1.88	0.87
1:B:229:ASP:H	1:B:256:HIS:HE1	1.20	0.86
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.64	0.85
1:A:282:LEU:HD11	1:A:293:LEU:HD12	1.59	0.85
1:A:204:ASN:H	1:A:204:ASN:HD22	1.22	0.85
1:A:280:GLU:HB3	1:A:293:LEU:HD13	1.56	0.85
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.15	0.85
1:B:204:ASN:H	1:B:204:ASN:HD22	1.25	0.83
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.43	0.81
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.94	0.81
1:B:368:LEU:HB2	6:B:1693:HOH:O	1.82	0.80
1:B:229:ASP:H	1:B:256:HIS:CE1	1.99	0.79
1:A:515:LYS:HG3	6:A:2568:HOH:O	1.81	0.79
1:B:299:LYS:HB2	6:B:1879:HOH:O	1.81	0.78
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.96	0.78
1:B:48:GLU:HG3	6:B:2255:HOH:O	1.84	0.77
1:B:511:MET:HB2	6:B:2646:HOH:O	1.83	0.77
1:B:311:LEU:HD21	1:B:529:LEU:HD11	1.68	0.76
1:A:39:CYS:HG	3:A:802:HEM:CAC	1.99	0.76
1:A:229:ASP:H	1:A:256:HIS:CE1	2.05	0.74
1:B:179:GLN:H	1:B:179:GLN:HE21	1.36	0.72
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.55	0.71
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.29	0.70
1:B:515:LYS:HG3	6:B:2539:HOH:O	1.91	0.70
1:A:65:GLU:HG2	1:A:262:TYR:OH	1.92	0.69
1:B:4:LEU:HD22	1:B:8:HIS:CE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ILE:HG21	6:B:2357:HOH:O	1.93	0.68
1:A:452:LYS:HE2	6:A:2186:HOH:O	1.93	0.67
1:A:368:LEU:HB2	6:A:2108:HOH:O	1.95	0.66
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.35	0.66
1:A:218:ASP:HB3	6:A:2135:HOH:O	1.95	0.66
1:A:544:ARG:HD2	1:A:549:ALA:HB2	1.77	0.66
1:B:4:LEU:HD22	1:B:8:HIS:HE1	1.59	0.66
1:B:179:GLN:H	1:B:179:GLN:NE2	1.94	0.65
1:A:393:LYS:HE2	6:A:2107:HOH:O	1.97	0.64
1:A:427:LYS:HE3	1:B:328:PRO:HB3	1.80	0.64
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.36	0.64
1:A:334:ILE:HB	6:A:2309:HOH:O	1.97	0.63
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.39	0.63
1:A:183:LYS:O	1:A:184:LYS:HB2	1.98	0.62
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.39	0.62
1:B:210:LYS:HD2	1:B:210:LYS:O	1.99	0.61
1:A:368:LEU:HD22	6:A:2309:HOH:O	2.00	0.61
1:B:204:ASN:H	1:B:204:ASN:ND2	1.96	0.61
1:A:204:ASN:H	1:A:204:ASN:ND2	1.97	0.61
1:A:282:LEU:CD1	1:A:293:LEU:HD12	2.29	0.60
1:B:17:CYS:SG	3:B:801:HEM:HAC	2.42	0.59
1:A:459:LYS:HD2	1:A:460:ALA:N	2.17	0.59
1:B:481:GLU:HG3	6:B:1075:HOH:O	2.03	0.59
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.42	0.59
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.41	0.59
1:A:39:CYS:SG	3:A:802:HEM:HAC	2.43	0.58
1:A:183:LYS:CE	1:A:233:VAL:H	2.16	0.58
1:B:519:MET:SD	6:B:2657:HOH:O	2.57	0.58
1:B:567:TYR:O	1:B:568:SER:HB3	2.04	0.58
1:B:13:GLU:HB3	1:B:15:ASP:OD1	2.03	0.57
1:B:218:ASP:HB3	6:B:1918:HOH:O	2.05	0.57
1:B:136:GLY:HA3	1:B:553:ILE:HD12	1.85	0.57
1:B:112:LYS:HA	1:B:112:LYS:HE3	1.87	0.57
1:A:299:LYS:HB3	6:A:2596:HOH:O	2.04	0.57
1:A:311:LEU:HD23	1:A:349:ALA:HB2	1.88	0.56
1:B:467:ARG:HD2	6:B:2256:HOH:O	2.05	0.56
1:B:15:ASP:HB3	6:B:1861:HOH:O	2.06	0.56
1:B:168:ALA:HA	4:B:2805:FAD:N5	2.20	0.56
1:A:183:LYS:HE2	1:A:233:VAL:H	1.71	0.56
1:B:311:LEU:N	1:B:311:LEU:HD22	2.23	0.53
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:MET:HE1	1:A:523:LYS:HD2	1.91	0.53
1:A:476:LYS:N	1:A:476:LYS:HD3	2.24	0.53
1:B:476:LYS:HD3	1:B:476:LYS:N	2.23	0.53
1:B:158:GLU:HB3	1:B:159:PRO:HD2	1.90	0.52
1:A:194:GLU:HG2	1:A:194:GLU:O	2.08	0.52
1:B:85:CYS:SG	3:B:804:HEM:HAC	2.47	0.51
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.93	0.51
1:B:452:LYS:HD2	1:B:452:LYS:O	2.09	0.51
1:B:511:MET:HG2	6:B:2657:HOH:O	2.10	0.51
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.04	0.51
1:B:522:LYS:HD2	6:B:2380:HOH:O	2.12	0.50
1:B:183:LYS:HE2	6:B:1245:HOH:O	2.10	0.50
1:B:107:GLU:O	1:B:110:LYS:HG2	2.12	0.50
1:A:168:ALA:HA	4:A:1805:FAD:N5	2.27	0.50
1:A:424:SER:HB2	6:A:2301:HOH:O	2.11	0.50
1:A:85:CYS:SG	3:A:804:HEM:HAC	2.48	0.49
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.00	0.49
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.94	0.49
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.05	0.49
1:A:549:ALA:HB3	4:A:1805:FAD:N1	2.28	0.49
1:A:458:GLY:HA3	6:A:2459:HOH:O	2.13	0.49
1:B:168:ALA:HA	4:B:2805:FAD:C5X	2.43	0.48
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.94	0.48
1:B:79:MET:HE2	6:B:1876:HOH:O	2.13	0.48
1:A:26:ASN:HA	1:A:299:LYS:HE3	1.96	0.48
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.06	0.48
1:B:476:LYS:HD3	1:B:476:LYS:H	1.77	0.48
1:A:167:LEU:HB3	4:A:1805:FAD:HM72	1.95	0.48
1:B:549:ALA:HB3	4:B:2805:FAD:N1	2.28	0.48
1:B:229:ASP:N	1:B:256:HIS:HE1	2.00	0.47
1:A:119:LEU:HD11	1:A:293:LEU:HD11	1.96	0.47
1:A:168:ALA:HA	4:A:1805:FAD:C5X	2.44	0.47
1:B:17:CYS:SG	3:B:801:HEM:C3C	3.07	0.47
1:B:71:CYS:SG	3:B:803:HEM:C3C	3.08	0.47
1:A:204:ASN:N	1:A:204:ASN:HD22	2.03	0.47
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.06	0.47
1:A:82:CYS:SG	3:A:804:HEM:HAB	2.52	0.47
1:B:457:ASP:OD1	1:B:459:LYS:HE3	2.15	0.47
1:B:56:ASN:HD22	1:B:58:HIS:H	1.63	0.47
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.50	0.46
1:B:419:LEU:O	1:B:496:ALA:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:GLY:HA3	6:B:2671:HOH:O	2.14	0.46
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.81	0.46
1:B:10:GLN:HA	6:B:2659:HOH:O	2.15	0.46
1:B:82:CYS:SG	3:B:804:HEM:CBB	3.03	0.46
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.04	0.46
1:B:13:GLU:HG3	6:B:1618:HOH:O	2.16	0.46
1:B:311:LEU:HD21	1:B:529:LEU:CD1	2.43	0.46
1:B:357:LYS:HG2	6:B:2646:HOH:O	2.14	0.46
1:A:459:LYS:HD2	1:A:460:ALA:H	1.79	0.45
1:A:210:LYS:HD3	6:A:1871:HOH:O	2.16	0.45
1:A:56:ASN:HD22	1:A:58:HIS:H	1.64	0.45
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.98	0.45
1:A:168:ALA:HA	4:A:1805:FAD:C6	2.47	0.45
1:B:544:ARG:HD2	1:B:549:ALA:HB2	1.98	0.45
1:B:341:ALA:HA	6:B:1175:HOH:O	2.17	0.45
1:A:310:ILE:HG12	1:A:530:TYR:HB2	1.98	0.44
1:A:17:CYS:SG	3:A:801:HEM:HAC	2.51	0.44
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.11	0.44
1:B:311:LEU:CD2	1:B:529:LEU:HD11	2.44	0.44
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.11	0.44
1:A:57:ALA:HB2	1:A:90:PHE:CE2	2.53	0.44
1:A:177:THR:OG1	1:A:245:HIS:HE1	2.00	0.44
1:B:472:VAL:HG22	1:B:485:LEU:HB3	1.99	0.43
1:A:341:ALA:HA	6:A:1906:HOH:O	2.19	0.43
1:A:288:THR:HG22	6:A:1878:HOH:O	2.19	0.43
1:B:459:LYS:HE2	6:B:2650:HOH:O	2.17	0.43
1:A:204:ASN:O	1:A:206:PRO:HD3	2.18	0.43
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.53	0.43
1:B:442:PRO:HD2	1:B:496:ALA:O	2.19	0.42
1:A:192:MET:HG3	6:A:2598:HOH:O	2.18	0.42
1:A:246:ARG:HB2	1:A:247:PRO:HD2	2.01	0.42
3:A:801:HEM:CMC	3:A:801:HEM:HBC2	2.49	0.42
3:B:801:HEM:HBD2	3:B:801:HEM:HHA	2.01	0.42
4:B:2805:FAD:H9	4:B:2805:FAD:H1'1	1.77	0.42
1:B:47:ALA:HA	1:B:58:HIS:HB2	2.02	0.42
1:B:56:ASN:ND2	1:B:58:HIS:H	2.17	0.42
1:A:246:ARG:HB2	1:A:247:PRO:CD	2.50	0.42
1:B:365:HIS:O	1:B:501:PRO:HA	2.20	0.42
1:B:68:CYS:SG	3:B:803:HEM:C3B	3.13	0.42
1:B:36:CYS:SG	3:B:802:HEM:C3B	3.13	0.41
1:A:165:ALA:HA	4:A:1805:FAD:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:ARG:HH22	5:B:2806:FUM:C6	2.33	0.41
1:B:85:CYS:SG	3:B:804:HEM:CBC	3.05	0.41
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.12	0.41
1:A:514:THR:OG1	1:A:515:LYS:HE2	2.21	0.41
1:B:526:ILE:HA	1:B:527:PRO:HD3	1.89	0.41
1:A:183:LYS:HD3	6:A:2057:HOH:O	2.21	0.40
1:A:133:GLY:O	1:A:138:GLY:HA3	2.21	0.40
1:A:299:LYS:CB	6:A:2596:HOH:O	2.66	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	566/571 (99%)	544 (96%)	20 (4%)	2 (0%)	38	33
1	B	566/571 (99%)	546 (96%)	20 (4%)	0	100	100
All	All	1132/1142 (99%)	1090 (96%)	40 (4%)	2 (0%)	51	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	A	113	SER

### 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	442/445 (99%)	411 (93%)	31 (7%)	18	12
1	B	442/445 (99%)	418 (95%)	24 (5%)	26	20
All	All	884/890 (99%)	829 (94%)	55 (6%)	21	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	38	SER
1	A	48	GLU
1	A	51	LYS
1	A	56	ASN
1	A	96	LYS
1	A	99	LEU
1	A	112	LYS
1	A	113	SER
1	A	176	TRP
1	A	183	LYS
1	A	204	ASN
1	A	208	LEU
1	A	282	LEU
1	A	289	VAL
1	A	293	LEU
1	A	299	LYS
1	A	311	LEU
1	A	337	ASN
1	A	450	LEU
1	A	452	LYS
1	A	459	LYS
1	A	476	LYS
1	A	487	ARG
1	A	490	ASN
1	A	522	LYS
1	A	523	LYS
1	A	526	ILE
1	A	529	LEU
1	A	559	LEU
1	A	568	SER
1	B	4	LEU
1	B	15	ASP
1	B	21	ASP

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Mol	Chain	Res	Type
1	B	56	ASN
1	B	99	LEU
1	B	110	LYS
1	B	112	LYS
1	B	144	SER
1	B	179	GLN
1	B	204	ASN
1	B	208	LEU
1	B	267	LYS
1	B	337	ASN
1	B	415	LYS
1	B	450	LEU
1	B	459	LYS
1	B	463	GLU
1	B	467	ARG
1	B	476	LYS
1	B	481	GLU
1	B	490	ASN
1	B	522	LYS
1	B	526	ILE
1	B	568	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	490	ASN
1	A	540	HIS
1	B	56	ASN
1	B	179	GLN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	269	ASN
1	B	490	ASN
1	B	540	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 ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	FAD	A	1805	-	51,58,58	1.76	11 (21%)	54,89,89	2.90	16 (29%)
5	FUM	A	1806	-	1,7,7	1.32	0	0,8,8	0.00	-
3	HEM	A	801	1	28,50,50	2.29	7 (25%)	17,82,82	2.43	9 (52%)
3	HEM	A	802	1	28,50,50	2.15	8 (28%)	17,82,82	2.00	6 (35%)
3	HEM	A	803	1	28,50,50	2.10	9 (32%)	17,82,82	2.03	4 (23%)
3	HEM	A	804	1	28,50,50	2.09	6 (21%)	17,82,82	2.30	7 (41%)
4	FAD	B	2805	-	51,58,58	1.87	10 (19%)	54,89,89	2.54	18 (33%)
5	FUM	B	2806	-	1,7,7	1.41	0	0,8,8	0.00	-
3	HEM	B	801	1	28,50,50	2.37	9 (32%)	17,82,82	2.33	7 (41%)
3	HEM	B	802	1	28,50,50	1.80	6 (21%)	17,82,82	2.32	8 (47%)
3	HEM	B	803	1	28,50,50	2.28	9 (32%)	17,82,82	1.88	7 (41%)
3	HEM	B	804	1	28,50,50	2.17	7 (25%)	17,82,82	1.84	5 (29%)

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	FAD	A	1805	-	2/2/9/9	0/28/50/50	0/6/6/6
5	FUM	A	1806	-	-	0/0/5/5	0/0/0/0
3	HEM	A	801	1	-	0/6/54/54	0/0/8/8
3	HEM	A	802	1	-	0/6/54/54	0/0/8/8
3	HEM	A	803	1	-	0/6/54/54	0/0/8/8
3	HEM	A	804	1	-	0/6/54/54	0/0/8/8
4	FAD	B	2805	-	2/2/9/9	0/28/50/50	0/6/6/6
5	FUM	B	2806	-	-	0/0/5/5	0/0/0/0
3	HEM	B	801	1	-	0/6/54/54	0/0/8/8
3	HEM	B	802	1	-	0/6/54/54	0/0/8/8
3	HEM	B	803	1	-	0/6/54/54	0/0/8/8
3	HEM	B	804	1	-	0/6/54/54	0/0/8/8

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3B-C2B	-6.11	1.32	1.40
3	B	803	HEM	C3C-C2C	-6.03	1.32	1.40
3	B	801	HEM	C3B-C2B	-5.99	1.32	1.40
3	B	801	HEM	C3C-C2C	-5.88	1.32	1.40
3	B	804	HEM	C3B-C2B	-5.71	1.32	1.40
3	A	804	HEM	C3B-C2B	-5.56	1.33	1.40
3	A	802	HEM	C3B-C2B	-5.47	1.33	1.40
3	B	803	HEM	C3B-C2B	-5.36	1.33	1.40
3	A	804	HEM	C3C-C2C	-4.89	1.33	1.40
3	A	802	HEM	C3C-C2C	-4.75	1.34	1.40
3	A	803	HEM	C3B-C2B	-4.75	1.34	1.40
3	A	803	HEM	C3C-C2C	-4.72	1.34	1.40
3	B	804	HEM	C3C-C2C	-4.62	1.34	1.40
3	A	801	HEM	C3C-C2C	-4.57	1.34	1.40
3	B	802	HEM	C3B-C2B	-4.16	1.34	1.40
3	B	802	HEM	C3C-C2C	-3.73	1.35	1.40
4	B	2805	FAD	C10-N1	-3.08	1.28	1.33
4	A	1805	FAD	O4-C4	-2.73	1.17	1.24
4	B	2805	FAD	O4-C4	-2.69	1.17	1.24
4	A	1805	FAD	C10-N1	-2.37	1.29	1.33
4	A	1805	FAD	C8A-N7A	-2.37	1.30	1.34
4	B	2805	FAD	O2B-C2B	-2.15	1.38	1.43
4	A	1805	FAD	P-O2P	-2.00	1.45	1.55
3	B	801	HEM	C4C-NC	2.02	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	HEM	CAA-C2A	2.06	1.55	1.52
3	A	802	HEM	CMD-C2D	2.09	1.55	1.51
3	A	802	HEM	C1C-NC	2.10	1.39	1.36
3	B	801	HEM	CMA-C3A	2.14	1.56	1.51
3	B	804	HEM	C4A-NA	2.16	1.40	1.36
3	A	803	HEM	CMB-C2B	2.16	1.56	1.51
4	A	1805	FAD	C6-C5X	2.18	1.45	1.41
3	B	802	HEM	CMD-C2D	2.19	1.56	1.51
3	A	801	HEM	C1A-NA	2.25	1.40	1.36
3	A	804	HEM	C4D-ND	2.29	1.39	1.36
3	B	803	HEM	C1D-ND	2.32	1.41	1.36
3	A	803	HEM	CAA-C2A	2.38	1.56	1.52
3	B	804	HEM	C1C-NC	2.45	1.39	1.36
3	B	801	HEM	CAD-C3D	2.45	1.57	1.52
3	B	802	HEM	C4A-NA	2.46	1.41	1.36
4	A	1805	FAD	C9-C8	2.51	1.44	1.37
3	A	803	HEM	CAD-C3D	2.52	1.57	1.52
3	B	803	HEM	C4C-NC	2.54	1.39	1.36
3	A	803	HEM	C4D-ND	2.55	1.39	1.36
3	A	802	HEM	CAA-C2A	2.59	1.56	1.52
3	B	801	HEM	CMC-C2C	2.60	1.57	1.51
4	B	2805	FAD	C5'-C4'	2.62	1.55	1.51
4	B	2805	FAD	C6-C5X	2.68	1.45	1.41
4	B	2805	FAD	C2B-C1B	2.70	1.57	1.53
3	B	803	HEM	C1B-NB	2.70	1.40	1.36
3	B	803	HEM	CAD-C3D	2.71	1.57	1.52
3	B	802	HEM	C3B-CAB	2.78	1.53	1.47
4	B	2805	FAD	C9-C8	2.80	1.45	1.37
3	B	803	HEM	C3B-CAB	2.84	1.53	1.47
4	A	1805	FAD	C5'-C4'	2.89	1.56	1.51
3	A	801	HEM	C4C-NC	3.06	1.40	1.36
3	A	802	HEM	C3B-CAB	3.08	1.54	1.47
3	A	804	HEM	CAA-C2A	3.10	1.57	1.52
3	A	804	HEM	C3B-CAB	3.14	1.54	1.47
3	B	804	HEM	C3B-CAB	3.16	1.54	1.47
3	A	802	HEM	C4C-NC	3.17	1.40	1.36
3	A	803	HEM	C3B-CAB	3.20	1.54	1.47
3	A	801	HEM	CAA-C2A	3.21	1.57	1.52
3	B	801	HEM	C3C-CAC	3.27	1.54	1.47
3	B	804	HEM	CAA-C2A	3.32	1.57	1.52
3	A	803	HEM	C1B-NB	3.33	1.40	1.36
4	A	1805	FAD	C2B-C1B	3.56	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3C-CAC	3.57	1.54	1.47
4	A	1805	FAD	C4-N3	3.61	1.39	1.33
3	A	803	HEM	C3C-CAC	3.63	1.55	1.47
3	B	801	HEM	CAA-C2A	3.67	1.58	1.52
3	A	804	HEM	C3C-CAC	3.71	1.55	1.47
3	B	803	HEM	C3C-CAC	3.78	1.55	1.47
3	B	804	HEM	C3C-CAC	3.87	1.55	1.47
3	B	802	HEM	C3C-CAC	3.91	1.55	1.47
3	A	801	HEM	C3B-CAB	3.97	1.55	1.47
3	B	801	HEM	C3B-CAB	4.10	1.56	1.47
3	A	802	HEM	C3C-CAC	4.11	1.55	1.47
4	B	2805	FAD	C4-N3	4.54	1.41	1.33
4	B	2805	FAD	C4-C4X	4.93	1.50	1.41
4	A	1805	FAD	C4-C4X	5.12	1.51	1.41
4	A	1805	FAD	C1'-N10	5.62	1.54	1.48
4	B	2805	FAD	C1'-N10	6.21	1.54	1.48

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C4X-C4-N3	-8.97	110.70	123.48
4	B	2805	FAD	C4X-C4-N3	-7.70	112.53	123.48
3	A	801	HEM	CMD-C2D-C1D	-4.86	121.00	128.46
4	A	1805	FAD	C4X-C10-N10	-4.71	117.25	120.52
3	B	801	HEM	CMD-C2D-C1D	-4.51	121.53	128.46
3	A	802	HEM	CMD-C2D-C1D	-4.31	121.84	128.46
3	B	802	HEM	CMD-C2D-C1D	-4.25	121.93	128.46
4	B	2805	FAD	C4X-C10-N10	-4.08	117.69	120.52
3	B	804	HEM	CMD-C2D-C1D	-3.72	122.75	128.46
3	A	804	HEM	CMD-C2D-C1D	-3.48	123.12	128.46
3	A	801	HEM	CMA-C3A-C4A	-3.42	123.21	128.46
4	A	1805	FAD	C4-C4X-C10	-3.18	117.39	119.96
4	B	2805	FAD	N6A-C6A-N1A	-3.08	112.66	118.77
3	A	803	HEM	CBD-CAD-C3D	-2.95	106.85	112.47
3	B	801	HEM	CBD-CAD-C3D	-2.90	106.94	112.47
3	A	803	HEM	CMD-C2D-C1D	-2.83	124.11	128.46
3	B	801	HEM	CMA-C3A-C4A	-2.72	124.28	128.46
3	B	803	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
3	A	804	HEM	CMA-C3A-C4A	-2.50	124.63	128.46
4	A	1805	FAD	C5A-C6A-N1A	-2.41	112.40	119.70
3	A	802	HEM	CMA-C3A-C4A	-2.35	124.85	128.46
4	A	1805	FAD	O4'-C4'-C3'	-2.32	103.33	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2805	FAD	O4'-C4'-C3'	-2.28	103.43	109.09
3	B	803	HEM	CMD-C2D-C1D	-2.25	125.01	128.46
4	B	2805	FAD	C7M-C7-C8	-2.21	116.08	120.72
3	A	801	HEM	CBD-CAD-C3D	-2.11	108.44	112.47
4	A	1805	FAD	N6A-C6A-N1A	-2.02	114.77	118.77
3	A	802	HEM	C4A-C3A-C2A	2.00	108.39	107.00
4	A	1805	FAD	C5X-C9A-N10	2.03	119.16	117.66
3	A	801	HEM	CAA-CBA-CGA	2.04	116.14	112.66
3	B	803	HEM	C4C-C3C-C2C	2.05	108.33	106.90
4	B	2805	FAD	N3A-C2A-N1A	2.15	130.73	128.86
3	B	802	HEM	CAA-CBA-CGA	2.15	116.34	112.66
3	B	802	HEM	CMC-C2C-C3C	2.19	128.96	124.89
3	A	801	HEM	CMC-C2C-C3C	2.28	129.11	124.89
3	A	801	HEM	CMA-C3A-C2A	2.29	129.26	124.94
3	A	804	HEM	CMD-C2D-C3D	2.32	129.32	124.94
4	A	1805	FAD	O2'-C2'-C1'	2.33	115.18	109.79
3	B	803	HEM	CAA-CBA-CGA	2.36	116.69	112.66
3	B	803	HEM	CMB-C2B-C3B	2.39	129.33	124.89
4	A	1805	FAD	C10-C4X-N5	2.42	123.38	120.59
3	A	801	HEM	CAD-CBD-CGD	2.45	116.85	112.66
4	B	2805	FAD	O3'-C3'-C2'	2.46	114.90	108.82
3	B	804	HEM	CMC-C2C-C3C	2.48	129.49	124.89
3	B	804	HEM	CMD-C2D-C3D	2.54	129.72	124.94
3	A	802	HEM	C4C-C3C-C2C	2.56	108.68	106.90
4	A	1805	FAD	O4B-C4B-C5B	2.62	118.26	109.40
3	A	803	HEM	CMC-C2C-C3C	2.63	129.77	124.89
4	A	1805	FAD	N3A-C2A-N1A	2.69	131.20	128.86
4	A	1805	FAD	O5B-C5B-C4B	2.74	118.71	109.00
3	B	804	HEM	C4C-C3C-C2C	2.74	108.81	106.90
4	B	2805	FAD	O5B-C5B-C4B	2.76	118.79	109.00
3	A	804	HEM	C4C-C3C-C2C	2.77	108.83	106.90
3	A	802	HEM	CMD-C2D-C3D	2.81	130.24	124.94
3	B	802	HEM	CMB-C2B-C3B	2.84	130.17	124.89
3	A	802	HEM	CAA-CBA-CGA	2.85	117.53	112.66
3	B	802	HEM	CMD-C2D-C3D	2.90	130.41	124.94
3	B	802	HEM	CBD-CAD-C3D	2.94	118.07	112.47
4	B	2805	FAD	C10-C4X-N5	3.01	124.05	120.59
3	B	803	HEM	CMC-C2C-C3C	3.02	130.50	124.89
3	A	804	HEM	CMB-C2B-C3B	3.08	130.61	124.89
4	B	2805	FAD	C5X-C9A-N10	3.14	119.99	117.66
3	B	801	HEM	CMB-C2B-C3B	3.18	130.79	124.89
3	B	801	HEM	CMC-C2C-C3C	3.19	130.81	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2805	FAD	C1'-N10-C10	3.34	121.92	118.50
3	B	802	HEM	CBA-CAA-C2A	3.38	118.94	112.48
3	B	801	HEM	CAA-CBA-CGA	3.41	118.49	112.66
4	B	2805	FAD	O2'-C2'-C1'	3.50	117.89	109.79
3	A	804	HEM	CMC-C2C-C3C	3.69	131.74	124.89
4	B	2805	FAD	C5A-C6A-N6A	3.73	128.07	120.47
3	B	804	HEM	CMB-C2B-C3B	3.83	132.00	124.89
3	B	803	HEM	CAD-CBD-CGD	3.84	119.22	112.66
3	A	801	HEM	CMD-C2D-C3D	3.88	132.26	124.94
3	B	801	HEM	CMD-C2D-C3D	3.88	132.26	124.94
4	B	2805	FAD	O3'-C3'-C4'	4.01	118.74	108.82
4	B	2805	FAD	O4B-C4B-C5B	4.06	123.11	109.40
3	B	802	HEM	CAD-CBD-CGD	4.09	119.65	112.66
3	A	801	HEM	CMB-C2B-C3B	4.10	132.49	124.89
4	B	2805	FAD	C4'-C3'-C2'	4.33	122.74	113.41
4	A	1805	FAD	O3'-C3'-C4'	4.63	120.28	108.82
4	B	2805	FAD	C1'-C2'-C3'	4.64	123.08	109.82
3	A	804	HEM	CBD-CAD-C3D	5.08	122.15	112.47
3	A	803	HEM	CAD-CBD-CGD	5.40	121.89	112.66
4	A	1805	FAD	C4'-C3'-C2'	5.85	126.00	113.41
4	A	1805	FAD	C5A-C6A-N6A	6.07	132.84	120.47
4	B	2805	FAD	C4-N3-C2	8.66	122.73	115.16
4	A	1805	FAD	C4-N3-C2	12.39	125.99	115.16

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1805	FAD	C4'
4	A	1805	FAD	C3'
4	B	2805	FAD	C4'
4	B	2805	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1805	FAD	6	0
3	A	801	HEM	7	0
3	A	802	HEM	6	0
3	A	803	HEM	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	HEM	9	0
4	B	2805	FAD	4	0
5	B	2806	FUM	1	0
3	B	801	HEM	6	0
3	B	802	HEM	5	0
3	B	803	HEM	6	0
3	B	804	HEM	9	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.