



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:07 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 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>

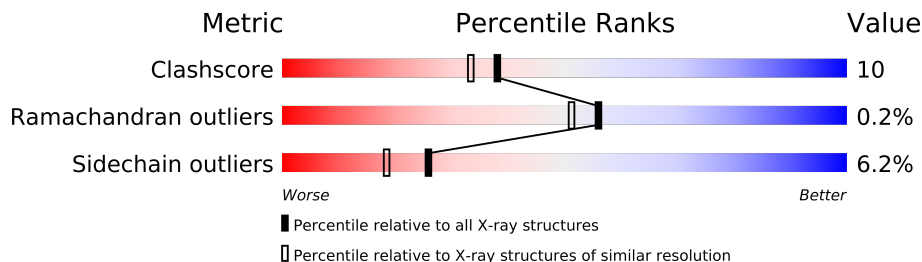
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10534 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 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: C₃₄H₃₂FeN₄O₄).



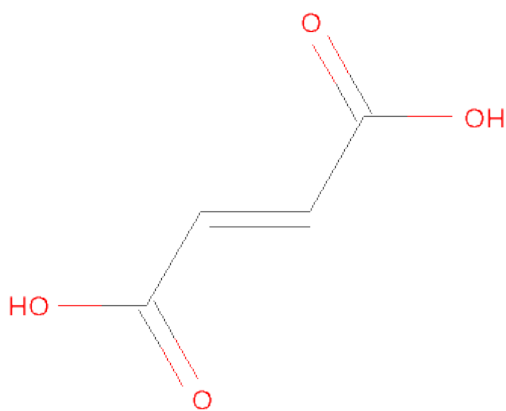
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).



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

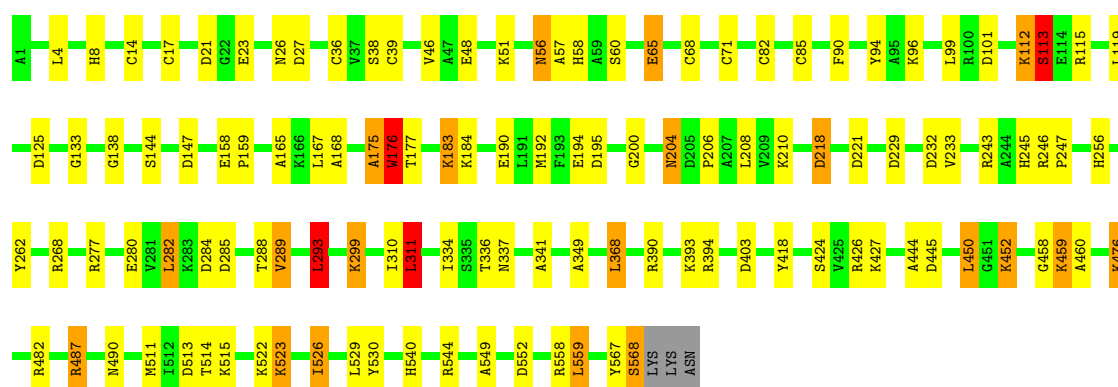
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

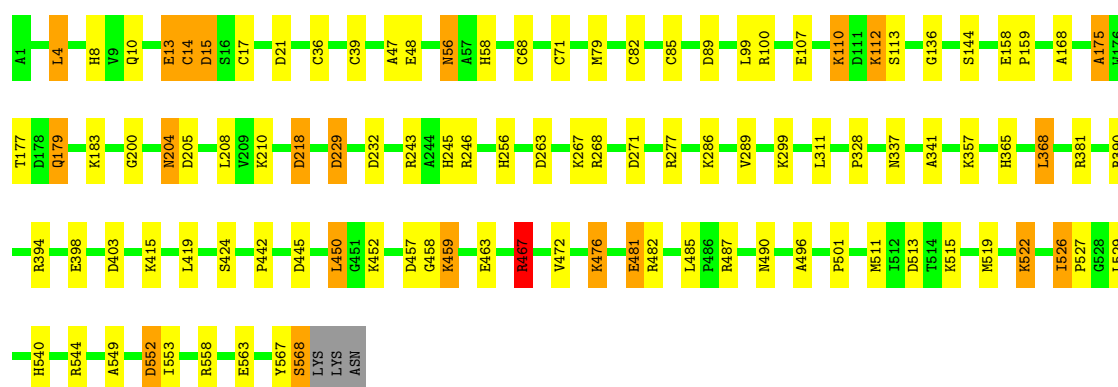
• Molecule 1: FLAVOCYTOCHROME C

Chain A:



• Molecule 1: FLAVOCYTOCHROME C

Chain B:



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	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 ²)	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 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	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

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 10.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:280:GLU:HB3	1:A:293:LEU:HD13	1.56	0.85
1:A:204:ASN:H	1:A:204:ASN:HD22	1.22	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	Distance(Å)	Clash(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:B:204:ASN:H	1:B:204:ASN:ND2	1.96	0.61
1:A:368:LEU:HD22	6:A:2309:HOH:O	2.00	0.61
1:A:204:ASN:ND2	1:A:204:ASN:H	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:B:82:CYS:SG	3:B:804:HEM:HAB	2.41	0.59
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.42	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
1:A:511:MET:HE1	1:A:523:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:476:LYS:HD3	1:A:476:LYS:N	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:511:MET:HG2	6:B:2657:HOH:O	2.10	0.51
1:B:452:LYS:HD2	1:B:452:LYS:O	2.09	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:39:CYS:SG	3:B:802:HEM:C3C	3.05	0.49
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.94	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:B:79:MET:HE2	6:B:1876:HOH:O	2.13	0.48
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.94	0.48
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.06	0.48
1:A:26:ASN:HA	1:A:299:LYS:HE3	1.96	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:B:17:CYS:SG	3:B:801:HEM:C3C	3.07	0.47
1:A:168:ALA:HA	4:A:1805:FAD:C5X	2.44	0.47
1:B:71:CYS:SG	3:B:803:HEM:C3C	3.08	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:A:204:ASN:N	1:A:204:ASN:HD22	2.03	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
1:B:458:GLY:HA3	6:B:2671:HOH:O	2.14	0.46
1:B:10:GLN:HA	6:B:2659:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.81	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:B:459:LYS:HE2	6:B:2650:HOH:O	2.17	0.43
1:A:288:THR:HG22	6:A:1878:HOH:O	2.19	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:246:ARG:HB2	1:A:247:PRO:HD2	2.01	0.42
1:A:192:MET:HG3	6:A:2598:HOH:O	2.18	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:68:CYS:SG	3:B:803:HEM:C3B	3.13	0.42
1:B:365:HIS:O	1:B:501:PRO:HA	2.20	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:299:LYS:CB	6:A:2596:HOH:O	2.66	0.40
1:A:133:GLY:O	1:A:138:GLY:HA3	2.21	0.40

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	566/571 (99%)	544 (96%)	20 (4%)	2 (0%)	43	36
1	B	566/571 (99%)	546 (96%)	20 (4%)	0	100	100
All	All	1132/1142 (99%)	1090 (96%)	40 (4%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

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

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	442/445 (99%)	411 (93%)	31 (7%)	21	14
1	B	442/445 (99%)	418 (95%)	24 (5%)	31	24
All	All	884/890 (99%)	829 (94%)	55 (6%)	26	18

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
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

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Mol	Chain	Res	Type
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 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

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	-	58,58,58	1.79	11 (18%)	85,89,89	2.23	21 (24%)
5	FUM	A	1806	-	7,7,7	1.88	3 (42%)	8,8,8	1.77	3 (37%)
3	HEM	A	801	1	49,50,50	3.24	17 (34%)	46,82,82	2.13	11 (23%)
3	HEM	A	802	1	49,50,50	2.66	14 (28%)	46,82,82	2.09	12 (26%)
3	HEM	A	803	1	49,50,50	2.42	15 (30%)	46,82,82	1.78	7 (15%)
3	HEM	A	804	1	49,50,50	2.86	14 (28%)	46,82,82	1.70	7 (15%)
4	FAD	B	2805	-	58,58,58	1.92	14 (24%)	85,89,89	1.97	22 (25%)
5	FUM	B	2806	-	7,7,7	2.37	4 (57%)	8,8,8	1.63	2 (25%)
3	HEM	B	801	1	49,50,50	3.86	15 (30%)	46,82,82	1.94	12 (26%)
3	HEM	B	802	1	49,50,50	2.87	12 (24%)	46,82,82	2.04	13 (28%)
3	HEM	B	803	1	49,50,50	2.41	12 (24%)	46,82,82	1.70	4 (8%)
3	HEM	B	804	1	49,50,50	3.05	15 (30%)	46,82,82	1.40	5 (10%)

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	0/34/50/50	0/1/6/6
5	FUM	A	1806	-	-	0/5/5/5	0/0/0/0
3	HEM	A	801	1	-	0/14/114/114	0/0/8/8
3	HEM	A	802	1	-	0/14/114/114	0/0/8/8
3	HEM	A	803	1	-	0/14/114/114	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	804	1	-	0/14/114/114	0/0/8/8
4	FAD	B	2805	-	2/2/9/9	0/34/50/50	0/1/6/6
5	FUM	B	2806	-	-	0/5/5/5	0/0/0/0
3	HEM	B	801	1	-	0/14/114/114	0/0/8/8
3	HEM	B	802	1	-	0/14/114/114	0/0/8/8
3	HEM	B	803	1	-	0/14/114/114	0/0/8/8
3	HEM	B	804	1	-	0/14/114/114	0/0/8/8

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	HEM	C2D-C1D	15.67	1.48	1.44
3	B	801	HEM	C2B-C1B	14.42	1.48	1.44
3	A	801	HEM	C2D-C1D	12.15	1.47	1.44
3	B	802	HEM	C2B-C1B	11.90	1.47	1.44
3	A	801	HEM	C2B-C1B	9.31	1.46	1.44
3	A	804	HEM	C2D-C1D	9.21	1.46	1.44
3	B	804	HEM	C2D-C1D	8.78	1.46	1.44
3	A	804	HEM	C2B-C1B	8.74	1.46	1.44
3	B	804	HEM	C2B-C1B	8.26	1.46	1.44
3	B	804	HEM	C3D-C4D	7.79	1.46	1.44
3	A	803	HEM	C2B-C1B	-7.52	1.42	1.44
3	A	802	HEM	C2B-C1B	7.06	1.46	1.44
3	A	801	HEM	C3B-C2B	-6.56	1.32	1.43
3	B	803	HEM	C3C-C2C	-6.50	1.32	1.43
3	B	803	HEM	C3D-C4D	6.50	1.46	1.44
3	B	801	HEM	C3B-C2B	-6.47	1.32	1.43
3	B	801	HEM	C3C-C2C	-6.39	1.32	1.43
3	B	804	HEM	C3D-C2D	-6.31	1.32	1.43
3	A	801	HEM	C3D-C2D	-6.30	1.32	1.43
3	B	804	HEM	C3B-C2B	-6.26	1.32	1.43
3	B	802	HEM	C3D-C2D	-6.18	1.33	1.43
3	A	804	HEM	C3B-C2B	-6.15	1.33	1.43
3	A	802	HEM	C3D-C2D	-6.10	1.33	1.43
3	A	802	HEM	C3B-C2B	-6.08	1.33	1.43
4	A	1805	FAD	C4-C4X	6.04	1.51	1.41
3	B	803	HEM	C3B-C2B	-5.99	1.33	1.43
3	B	801	HEM	C3D-C2D	-5.92	1.33	1.43
3	A	804	HEM	C3D-C2D	-5.85	1.33	1.43
4	B	2805	FAD	C1'-N10	5.85	1.54	1.48
4	B	2805	FAD	C4-C4X	5.82	1.50	1.41
3	B	803	HEM	C3D-C2D	-5.80	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	HEM	C3D-C4D	5.78	1.46	1.44
3	A	804	HEM	C3C-C2C	-5.64	1.33	1.43
3	A	802	HEM	C3D-C4D	5.57	1.45	1.44
3	A	802	HEM	C2D-C1D	5.56	1.45	1.44
3	A	802	HEM	C3C-C2C	-5.54	1.34	1.43
3	A	803	HEM	C3B-C2B	-5.54	1.34	1.43
3	A	803	HEM	C3C-C2C	-5.51	1.34	1.43
3	B	804	HEM	C3C-C2C	-5.44	1.34	1.43
3	A	801	HEM	C3C-C2C	-5.40	1.34	1.43
4	A	1805	FAD	C1'-N10	5.32	1.54	1.48
3	A	803	HEM	C3D-C2D	-5.27	1.34	1.43
3	B	804	HEM	C4A-C3A	5.19	1.46	1.40
3	B	802	HEM	C3B-C2B	-5.09	1.34	1.43
3	B	801	HEM	C3B-CAB	4.95	1.56	1.40
3	A	802	HEM	C3C-CAC	4.92	1.55	1.40
3	A	801	HEM	C3B-CAB	4.87	1.55	1.40
3	B	802	HEM	C3C-CAC	4.79	1.55	1.40
3	B	804	HEM	C3C-CAC	4.77	1.55	1.40
3	B	802	HEM	C2D-C1D	4.77	1.45	1.44
3	B	802	HEM	C3C-C2C	-4.77	1.35	1.43
3	A	803	HEM	C4A-C3A	4.73	1.46	1.40
3	B	803	HEM	C3C-CAC	4.71	1.55	1.40
3	A	804	HEM	C3C-CAC	4.67	1.55	1.40
3	A	803	HEM	C3C-CAC	4.62	1.55	1.40
3	A	801	HEM	C4A-C3A	4.59	1.45	1.40
3	A	801	HEM	C3C-CAC	4.58	1.54	1.40
3	A	801	HEM	C3D-C4D	4.49	1.45	1.44
3	A	803	HEM	C3B-CAB	4.40	1.54	1.40
3	B	801	HEM	C3C-CAC	4.39	1.54	1.40
3	B	804	HEM	C3B-CAB	4.37	1.54	1.40
3	A	804	HEM	C3B-CAB	4.36	1.54	1.40
3	A	802	HEM	C3B-CAB	4.32	1.54	1.40
3	A	804	HEM	C3D-C4D	4.31	1.45	1.44
3	B	803	HEM	C4A-C3A	4.20	1.45	1.40
3	B	801	HEM	C4A-C3A	4.18	1.45	1.40
3	B	803	HEM	C3B-CAB	4.17	1.53	1.40
3	B	802	HEM	C3B-CAB	4.14	1.53	1.40
4	A	1805	FAD	C2B-C1B	4.12	1.59	1.53
5	B	2806	FUM	O8-C6	-4.09	1.18	1.30
4	B	2805	FAD	C1'-C2'	-4.00	1.47	1.51
3	B	802	HEM	C4A-C3A	3.94	1.45	1.40
3	A	802	HEM	C4A-C3A	3.92	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2805	FAD	C10-N1	-3.79	1.28	1.35
3	B	801	HEM	CAA-C2A	3.55	1.58	1.52
4	A	1805	FAD	O4-C4	-3.50	1.17	1.24
4	B	2805	FAD	O4-C4	-3.44	1.17	1.24
4	B	2805	FAD	C6-C5X	3.43	1.45	1.41
3	A	804	HEM	C4A-C3A	3.25	1.44	1.40
4	A	1805	FAD	C10-N1	-3.23	1.29	1.35
3	B	804	HEM	CAA-C2A	3.21	1.57	1.52
3	B	801	HEM	CHA-C4D	3.21	1.40	1.35
4	B	2805	FAD	C2B-C1B	3.15	1.57	1.53
3	B	801	HEM	CMC-C2C	3.12	1.57	1.47
3	A	801	HEM	CAA-C2A	3.10	1.57	1.52
5	A	1806	FUM	O7-C6	3.06	1.31	1.23
3	A	804	HEM	CAA-C2A	3.00	1.57	1.52
3	A	803	HEM	CMB-C2B	2.82	1.56	1.47
3	B	802	HEM	CMD-C2D	2.80	1.56	1.47
4	A	1805	FAD	C6-C5X	2.79	1.45	1.41
4	A	1805	FAD	C5'-C4'	2.77	1.56	1.51
3	A	802	HEM	CMD-C2D	2.73	1.55	1.47
3	B	803	HEM	CHA-C4D	2.71	1.39	1.35
3	A	804	HEM	CMB-C2B	2.70	1.55	1.47
4	B	2805	FAD	C9-C8	2.69	1.45	1.37
3	A	802	HEM	CMC-C2C	2.66	1.55	1.47
3	A	801	HEM	CMD-C2D	2.61	1.55	1.47
3	A	803	HEM	CMD-C2D	2.56	1.55	1.47
3	A	801	HEM	CMC-C2C	2.55	1.55	1.47
5	B	2806	FUM	O7-C6	2.54	1.30	1.23
4	B	2805	FAD	C5'-C4'	2.52	1.55	1.51
3	B	803	HEM	CMD-C2D	2.52	1.55	1.47
5	B	2806	FUM	O3-C2	2.51	1.30	1.23
3	A	802	HEM	CAA-C2A	2.49	1.56	1.52
3	B	803	HEM	CMB-C2B	2.49	1.55	1.47
3	B	801	HEM	CMB-C2B	2.49	1.55	1.47
3	B	804	HEM	CMD-C2D	2.48	1.55	1.47
3	A	801	HEM	CMB-C2B	2.47	1.55	1.47
3	B	802	HEM	C4A-NA	2.46	1.41	1.36
3	A	803	HEM	FE-NA	2.45	2.02	1.92
3	B	801	HEM	CMD-C2D	2.44	1.55	1.47
4	B	2805	FAD	C4-N3	2.41	1.41	1.37
4	A	1805	FAD	C9-C8	2.41	1.44	1.37
4	A	1805	FAD	C4X-N5	-2.40	1.31	1.36
3	B	802	HEM	CHA-C4D	2.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEM	CMB-C2B	2.33	1.54	1.47
3	B	804	HEM	CMC-C2C	2.33	1.54	1.47
3	B	801	HEM	C3D-C4D	2.31	1.45	1.44
3	A	803	HEM	CAA-C2A	2.29	1.56	1.52
3	B	804	HEM	CMB-C2B	2.27	1.54	1.47
3	A	804	HEM	FE-NA	2.26	2.02	1.92
3	A	803	HEM	C3D-C4D	-2.25	1.44	1.44
3	A	804	HEM	CMD-C2D	2.24	1.54	1.47
3	A	801	HEM	C1A-NA	2.23	1.40	1.36
4	A	1805	FAD	P-O2P	-2.23	1.45	1.55
4	A	1805	FAD	C8A-N7A	-2.22	1.30	1.34
5	A	1806	FUM	O8-C6	-2.21	1.23	1.30
3	A	801	HEM	CHA-C4D	2.21	1.39	1.35
4	B	2805	FAD	P-O2P	-2.21	1.45	1.55
5	A	1806	FUM	O3-C2	2.20	1.29	1.23
3	B	804	HEM	FE-NA	2.20	2.01	1.92
3	B	803	HEM	CMC-C2C	2.18	1.54	1.47
3	A	803	HEM	CMC-C2C	2.15	1.54	1.47
3	B	804	HEM	C4A-NA	2.13	1.40	1.36
3	B	803	HEM	FE-NA	2.12	2.01	1.92
5	B	2806	FUM	C5-C6	2.08	1.53	1.48
3	B	801	HEM	CMA-C3A	2.07	1.56	1.51
3	A	802	HEM	CHA-C4D	2.07	1.38	1.35
3	A	803	HEM	CHA-C4D	2.06	1.38	1.35
3	A	804	HEM	CMC-C2C	2.06	1.53	1.47
3	A	801	HEM	FE-NA	2.06	2.01	1.92
3	A	803	HEM	CHB-C1B	2.05	1.38	1.35
4	B	2805	FAD	O2B-C2B	-2.05	1.38	1.43
4	B	2805	FAD	C4X-N5	-2.02	1.31	1.36
3	A	801	HEM	CHB-C1B	2.02	1.38	1.35
4	B	2805	FAD	O2-C2	-2.01	1.19	1.23

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C3B-C4B-NB	-8.73	107.75	114.00
3	A	802	HEM	C3B-C4B-NB	-8.33	108.04	114.00
3	B	802	HEM	C3B-C4B-NB	-7.60	108.56	114.00
3	B	801	HEM	C3B-C4B-NB	-7.52	108.62	114.00
3	A	803	HEM	C3B-C4B-NB	-7.21	108.84	114.00
3	B	803	HEM	C3B-C4B-NB	-6.92	109.05	114.00
3	A	804	HEM	C3B-C4B-NB	-6.83	109.11	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C2'-C1'-N10	-6.81	103.41	112.45
4	A	1805	FAD	C4X-C10-N10	-6.53	117.25	120.51
4	A	1805	FAD	C4X-C10-N1	5.96	128.69	122.73
4	A	1805	FAD	O4B-C1B-C2B	-5.88	97.76	106.77
4	B	2805	FAD	C4X-C10-N10	-5.66	117.69	120.51
4	A	1805	FAD	C4'-C3'-C2'	5.64	126.00	113.25
3	B	804	HEM	C3B-C4B-NB	-5.57	110.02	114.00
4	A	1805	FAD	C5A-C6A-N6A	5.36	132.84	120.72
4	B	2805	FAD	C5'-C4'-C3'	-5.32	102.01	112.06
4	B	2805	FAD	C2'-C1'-N10	-5.30	105.42	112.45
4	A	1805	FAD	C5'-C4'-C3'	-5.22	102.22	112.06
3	A	802	HEM	C4A-CHB-C1B	-5.15	120.70	127.47
3	B	802	HEM	C4A-CHB-C1B	-5.00	120.89	127.47
4	B	2805	FAD	C1'-C2'-C3'	4.64	123.08	109.82
4	A	1805	FAD	O3'-C3'-C4'	4.57	120.28	108.74
4	B	2805	FAD	C4'-C3'-C2'	4.20	122.74	113.25
4	B	2805	FAD	O4B-C1B-C2B	-4.19	100.35	106.77
3	A	802	HEM	C2D-C1D-ND	-4.11	108.08	112.93
4	B	2805	FAD	O3'-C3'-C4'	3.96	118.74	108.74
3	B	803	HEM	C1A-CHA-C4D	-3.93	122.30	127.47
4	B	2805	FAD	O4B-C4B-C5B	3.85	123.11	109.36
3	B	802	HEM	C2D-C1D-ND	-3.78	108.47	112.93
3	B	801	HEM	C4A-CHB-C1B	-3.74	122.55	127.47
3	A	802	HEM	CHC-C1C-NC	-3.66	121.55	124.73
4	A	1805	FAD	O4B-C1B-N9A	-3.62	105.07	108.44
3	B	801	HEM	C2D-C1D-ND	-3.59	108.69	112.93
3	A	801	HEM	C2D-C1D-ND	-3.57	108.71	112.93
3	A	804	HEM	CBD-CAD-C3D	3.56	122.15	114.37
3	B	802	HEM	CBA-CAA-C2A	3.55	118.94	112.69
3	A	801	HEM	CMA-C3A-C4A	-3.52	123.21	128.62
3	A	804	HEM	C2D-C1D-ND	-3.50	108.80	112.93
3	A	803	HEM	O2A-CGA-O1A	3.48	132.14	123.30
3	A	803	HEM	CBD-CAD-C3D	-3.45	106.85	114.37
4	B	2805	FAD	N6A-C6A-N1A	-3.41	112.66	119.36
3	B	801	HEM	CBD-CAD-C3D	-3.40	106.94	114.37
3	A	802	HEM	C1B-NB-C4B	3.33	108.57	105.16
3	B	804	HEM	C2D-C1D-ND	-3.33	109.00	112.93
3	A	803	HEM	C2D-C1D-ND	-3.32	109.02	112.93
4	B	2805	FAD	O2'-C2'-C1'	3.30	117.89	109.71
4	B	2805	FAD	C5A-C6A-N6A	3.25	128.07	120.72
4	B	2805	FAD	C5X-C9A-N10	3.23	119.99	116.80
3	A	801	HEM	C1B-NB-C4B	3.19	108.42	105.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2805	FAD	C4X-C10-N1	3.17	125.90	122.73
4	A	1805	FAD	C2A-N3A-C4A	-3.09	105.22	114.01
3	A	801	HEM	CHC-C4B-NB	3.06	127.13	124.58
3	A	801	HEM	C4A-CHB-C1B	-3.03	123.48	127.47
4	A	1805	FAD	N3A-C2A-N1A	2.98	131.20	128.71
4	B	2805	FAD	C10-C4X-N5	2.96	124.05	120.45
3	B	801	HEM	CMD-C2D-C3D	2.94	132.26	125.60
3	A	801	HEM	CMD-C2D-C3D	2.94	132.26	125.60
3	B	801	HEM	CMA-C3A-C4A	-2.82	124.28	128.62
3	B	801	HEM	C1B-NB-C4B	2.80	108.03	105.16
3	B	802	HEM	C1B-NB-C4B	2.75	107.97	105.16
3	A	802	HEM	C4D-ND-C1D	2.73	107.95	105.16
3	A	801	HEM	CBD-CAD-C3D	-2.72	108.44	114.37
3	A	803	HEM	CAD-CBD-CGD	2.69	121.89	113.48
3	B	803	HEM	CMA-C3A-C4A	-2.69	124.48	128.62
3	A	801	HEM	CMB-C2B-C3B	2.69	132.49	126.16
4	B	2805	FAD	O5B-C5B-C4B	2.68	118.79	108.94
3	B	802	HEM	C4D-ND-C1D	2.66	107.89	105.16
4	A	1805	FAD	O5B-C5B-C4B	2.66	118.71	108.94
4	A	1805	FAD	C3B-C2B-C1B	-2.64	96.78	100.91
3	A	804	HEM	CMA-C3A-C4A	-2.60	124.63	128.62
3	B	802	HEM	CHC-C1C-NC	-2.58	122.49	124.73
3	B	802	HEM	O1A-CGA-CBA	-2.56	114.21	123.03
4	A	1805	FAD	C2B-C1B-N9A	-2.54	106.74	113.27
3	A	804	HEM	O1D-CGD-CBD	-2.54	114.29	123.03
5	B	2806	FUM	O7-C6-C5	-2.50	112.70	120.75
4	A	1805	FAD	O4B-C4B-C5B	2.49	118.26	109.36
3	B	801	HEM	CHD-C1D-ND	2.49	126.65	124.58
3	A	803	HEM	C1A-CHA-C4D	-2.48	124.20	127.47
3	A	802	HEM	O1D-CGD-CBD	-2.48	114.49	123.03
3	B	804	HEM	CMB-C2B-C3B	2.48	132.00	126.16
5	A	1806	FUM	O3-C2-C4	-2.48	112.77	120.75
3	A	802	HEM	CMA-C3A-C4A	-2.45	124.85	128.62
4	B	2805	FAD	O3'-C3'-C2'	2.44	114.90	108.74
4	B	2805	FAD	N3A-C2A-N1A	2.42	130.73	128.71
4	A	1805	FAD	C10-C4X-N5	2.41	123.38	120.45
4	A	1805	FAD	C5X-C9A-N10	2.40	119.16	116.80
3	A	804	HEM	CMC-C2C-C3C	2.37	131.74	126.16
5	B	2806	FUM	C4-C5-C6	-2.35	116.22	127.28
4	A	1805	FAD	N6A-C6A-N1A	-2.34	114.77	119.36
3	B	801	HEM	O2D-CGD-CBD	2.32	122.43	114.22
4	A	1805	FAD	O4'-C4'-C3'	-2.30	103.33	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	CMA-C3A-C2A	2.29	129.26	124.94
4	B	2805	FAD	O4'-C4'-C3'	-2.26	103.43	109.05
3	A	802	HEM	C3A-C4A-NA	-2.24	107.72	109.41
3	B	802	HEM	C1A-CHA-C4D	-2.24	124.53	127.47
3	A	802	HEM	CHC-C4B-NB	2.22	126.43	124.58
4	A	1805	FAD	O2'-C2'-C1'	2.21	115.18	109.71
3	B	801	HEM	C1A-CHA-C4D	-2.18	124.60	127.47
3	B	804	HEM	C1A-C2A-C3A	2.18	109.17	106.92
3	B	802	HEM	C4C-NC-C1C	2.17	107.79	105.53
3	B	801	HEM	C4D-ND-C1D	2.17	107.38	105.16
5	A	1806	FUM	C4-C5-C6	-2.17	117.08	127.28
3	B	803	HEM	C1A-C2A-C3A	2.16	109.15	106.92
3	B	802	HEM	O2A-CGA-O1A	2.15	128.77	123.30
3	A	804	HEM	CBA-CAA-C2A	-2.14	108.92	112.69
5	A	1806	FUM	O7-C6-C5	-2.13	113.87	120.75
3	B	802	HEM	CMD-C2D-C3D	2.12	130.41	125.60
3	A	803	HEM	C4C-NC-C1C	2.12	107.74	105.53
3	A	801	HEM	CHD-C1D-ND	2.09	126.32	124.58
3	B	802	HEM	CMA-C3A-C4A	-2.07	125.43	128.62
4	B	2805	FAD	C9A-N10-C10	-2.07	119.73	121.77
3	B	801	HEM	CHC-C1C-NC	-2.07	122.94	124.73
3	B	804	HEM	CHD-C4C-NC	-2.06	122.94	124.73
3	A	802	HEM	CMD-C2D-C3D	2.05	130.24	125.60
4	B	2805	FAD	C2B-C1B-N9A	-2.05	108.01	113.27
4	A	1805	FAD	C5A-C6A-N1A	-2.05	112.40	119.27
4	B	2805	FAD	C3B-C2B-C1B	-2.04	97.72	100.91
4	B	2805	FAD	C7M-C7-C8	-2.02	116.08	120.74
3	A	802	HEM	C4A-C3A-C2A	2.00	108.39	107.00

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.

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.