Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:19 PM GMT

PDB ID	:	1JRX
Title	:	Crystal structure of Arg402Ala 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

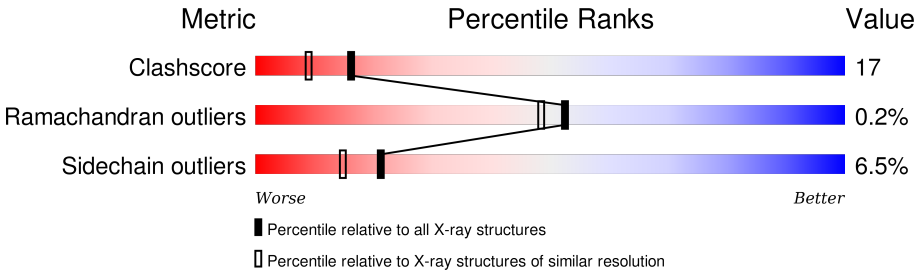
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	68% 27%
1	B	571	68% 26% 5%

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	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10555 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
			4207	2609	740	833	25			
1	B	568	Total	C	N	O	S	0	0	0
			4204	2609	741	829	25			

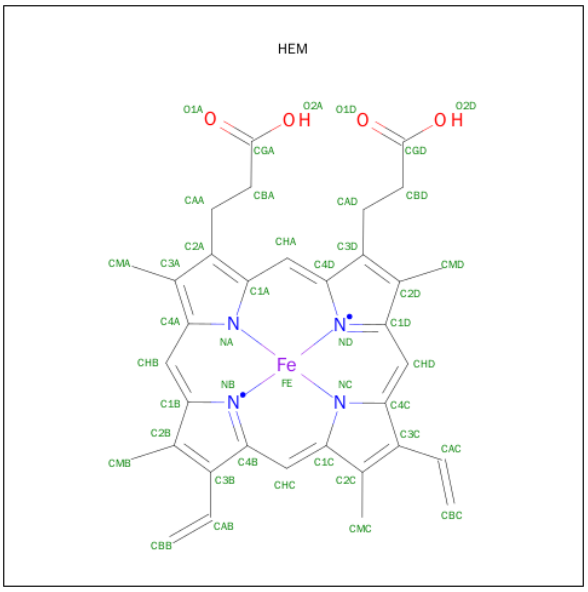
There are 2 discrepancies between the modelled and reference sequences:

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

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

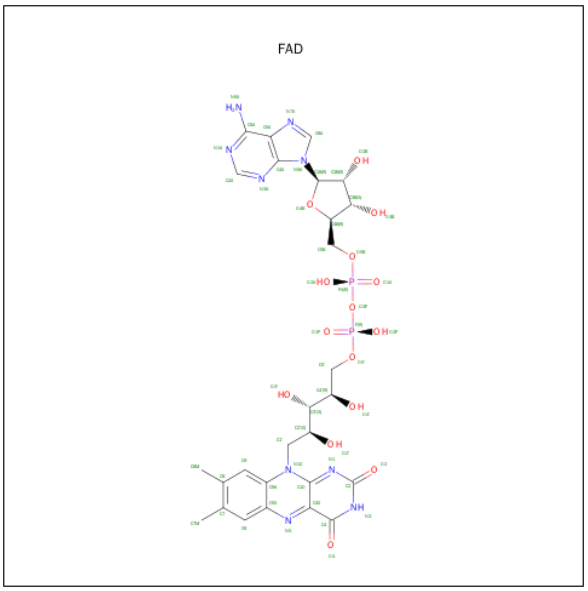
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



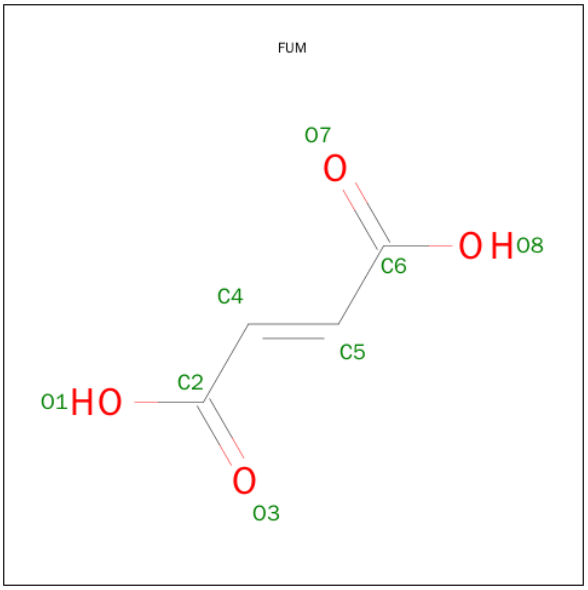
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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: $C_4H_4O_4$).



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	822	Total O 822 822	0	0
6	B	854	Total O 854 854	0	0

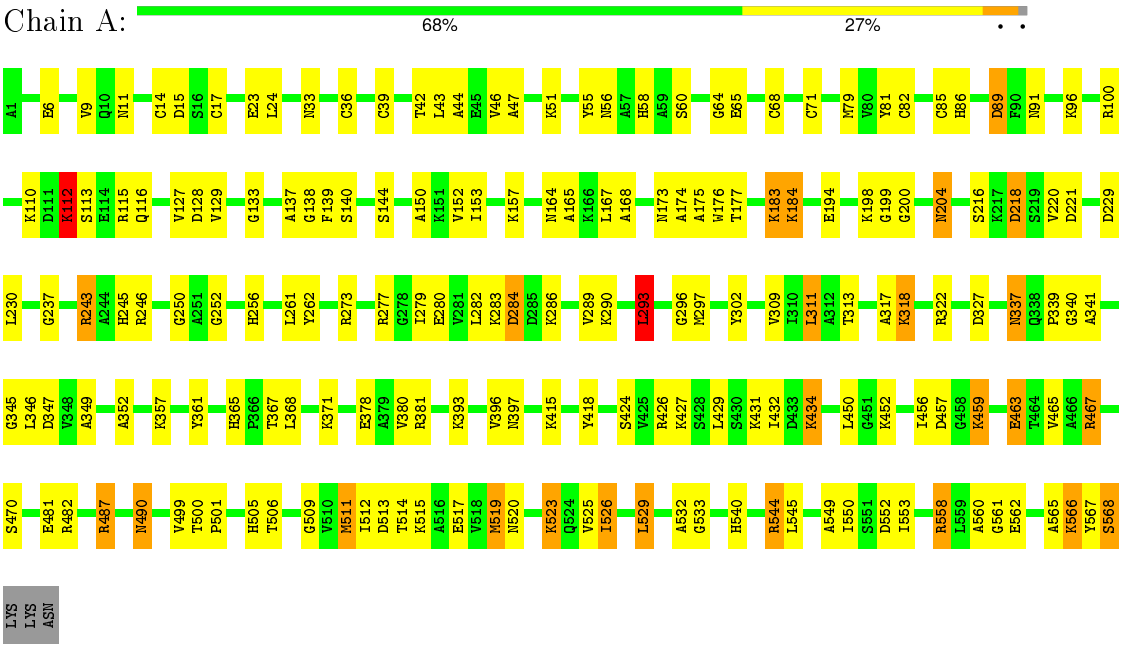
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

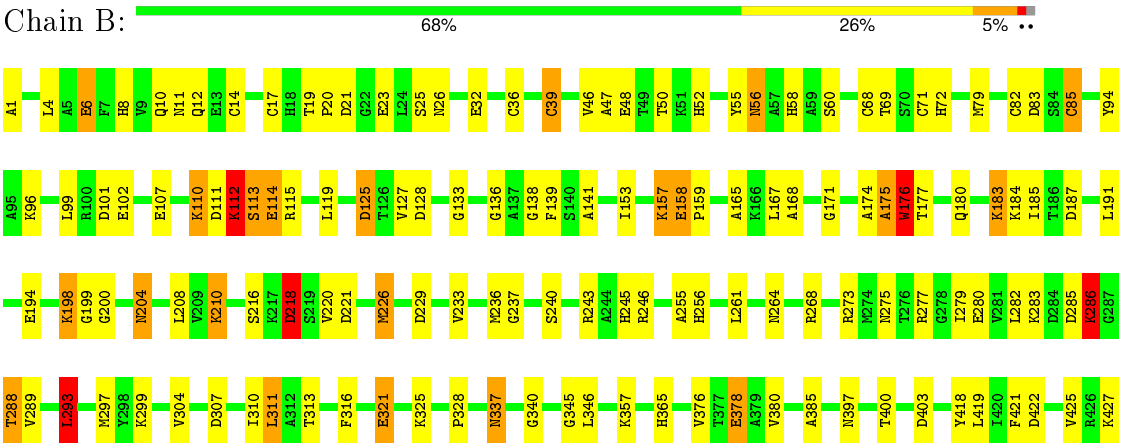
- Molecule 1: FLAVOCYTOCHROME C

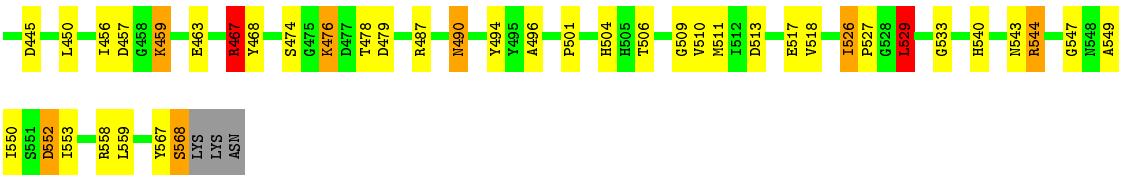
Chain A:



- Molecule 1: FLAVOCYTOCHROME C

Chain B:




D445
L450
T456
D457
G458
K459
E463
R467
Y468
S474
G475
K476
D477
T478
D479
R487
N490
Y494
Y495
A496
P501
H504
H505
T506
G509
Y510
M511
I512
D513
E517
V518
T526
P527
G528
L529
G533
H540
N543
R544
G547
N548
A549
I550
S551
D552
I553
R558
L559
Y567
S568
LYS
LYS
ASN

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.97Å 85.93Å 88.32Å 90.00° 104.74° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.4 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10555	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	0.71	1/4277 (0.0%)	1.65	57/5784 (1.0%)
1	B	0.71	0/4274	1.66	61/5779 (1.1%)
All	All	0.71	1/8551 (0.0%)	1.66	118/11563 (1.0%)

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	B	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-6.01	1.34	1.46

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	487	ARG	CD-NE-CZ	29.39	164.75	123.60
1	A	175	ALA	C-N-CA	21.93	176.52	121.70
1	A	277	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	B	176	TRP	N-CA-CB	14.29	136.31	110.60
1	B	273	ARG	NE-CZ-NH1	-14.23	113.18	120.30
1	B	175	ALA	C-N-CA	12.87	153.88	121.70
1	B	277	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	218	ASP	CB-CG-OD2	-12.42	107.12	118.30
1	B	293	LEU	CA-CB-CG	12.32	143.63	115.30
1	A	487	ARG	NE-CZ-NH1	12.20	126.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LYS	CA-CB-CG	12.12	140.07	113.40
1	A	293	LEU	CA-CB-CG	10.85	140.26	115.30
1	A	482	ARG	NE-CZ-NH2	-10.81	114.89	120.30
1	A	487	ARG	CD-NE-CZ	10.55	138.38	123.60
1	B	494	TYR	CB-CG-CD2	-10.38	114.77	121.00
1	A	567	TYR	C-N-CA	10.20	147.20	121.70
1	A	115	ARG	NE-CZ-NH2	10.07	125.33	120.30
1	A	273	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	A	284	ASP	CB-CG-OD1	9.92	127.23	118.30
1	B	268	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	221	ASP	CB-CG-OD2	9.77	127.10	118.30
1	B	422	ASP	CB-CG-OD2	9.13	126.52	118.30
1	A	175	ALA	N-CA-CB	8.98	122.67	110.10
1	A	487	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	B	378	GLU	OE1-CD-OE2	-8.71	112.85	123.30
1	B	115	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	A	511	MET	CA-CB-CG	8.21	127.26	113.30
1	B	403	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	125	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	B	286	LYS	CD-CE-NZ	7.71	129.44	111.70
1	B	427	LYS	CD-CE-NZ	7.70	129.40	111.70
1	B	175	ALA	CB-CA-C	-7.65	98.62	110.10
1	A	218	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	175	ALA	N-CA-CB	7.55	120.67	110.10
1	A	176	TRP	N-CA-CB	7.54	124.18	110.60
1	A	381	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	286	LYS	CA-CB-CG	7.51	129.93	113.40
1	A	322	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	566	LYS	CA-CB-CG	7.28	129.42	113.40
1	B	558	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	15	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	B	445	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	246	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	426	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	A	552	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	445	ASP	CB-CG-OD1	6.74	124.37	118.30
1	B	487	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	B	468	TYR	CB-CG-CD1	-6.66	117.01	121.00
1	A	322	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	B	293	LEU	CB-CG-CD2	6.55	122.13	111.00
1	B	289	VAL	CA-CB-CG2	6.50	120.65	110.90
1	A	567	TYR	O-C-N	-6.48	112.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	347	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	322	ARG	NH1-CZ-NH2	6.36	126.40	119.40
1	A	361	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	B	273	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	B	494	TYR	CB-CG-CD1	6.26	124.75	121.00
1	B	286	LYS	N-CA-CB	6.22	121.80	110.60
1	B	39	CYS	CA-CB-SG	-6.21	102.82	114.00
1	A	110	LYS	CD-CE-NZ	6.19	125.94	111.70
1	B	112	LYS	CA-CB-CG	6.15	126.92	113.40
1	A	327	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	B	422	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	246	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	221	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	221	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	B	467	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	175	ALA	CA-C-N	-5.87	104.29	117.20
1	B	187	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	100	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	B	218	ASP	OD1-CG-OD2	5.80	134.32	123.30
1	A	519	MET	CA-CB-CG	-5.80	103.44	113.30
1	B	552	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	567	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	B	544	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	112	LYS	CB-CG-CD	5.73	126.50	111.60
1	B	83	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	346	LEU	CB-CA-C	-5.73	99.31	110.20
1	B	101	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	560	ALA	CB-CA-C	-5.70	101.56	110.10
1	B	307	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	112	LYS	C-N-CA	5.63	135.78	121.70
1	B	268	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	B	558	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	504	HIS	N-CA-CB	-5.57	100.58	110.60
1	A	506	THR	CA-CB-CG2	-5.56	104.62	112.40
1	B	94	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	463	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	558	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	32	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	B	283	LYS	CB-CG-CD	5.49	125.86	111.60
1	A	113	SER	N-CA-CB	-5.47	102.29	110.50
1	A	277	ARG	NH1-CZ-NH2	5.45	125.40	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	CYS	CA-CB-SG	-5.43	104.23	114.00
1	B	220	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	B	286	LYS	CA-CB-CG	5.41	125.31	113.40
1	B	463	GLU	CB-CG-CD	5.36	128.67	114.20
1	A	424	SER	N-CA-CB	5.29	118.43	110.50
1	B	226	MET	CA-CB-CG	-5.29	104.32	113.30
1	B	243	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	A	220	VAL	CA-CB-CG2	-5.27	102.99	110.90
1	A	567	TYR	CA-C-O	5.27	131.17	120.10
1	A	243	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	81	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	B	285	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	296	GLY	N-CA-C	-5.18	100.14	113.10
1	B	509	GLY	O-C-N	5.16	130.96	122.70
1	B	243	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	111	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	544	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	33	ASN	CA-CB-CG	-5.08	102.23	113.40
1	A	89	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	A	514	THR	CA-CB-CG2	-5.06	105.31	112.40
1	A	532	ALA	N-CA-CB	5.06	117.18	110.10
1	B	529	LEU	CB-CG-CD2	5.06	119.60	111.00
1	B	128	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	465	VAL	CA-CB-CG2	-5.04	103.34	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	GLU	Mainchain
1	B	175	ALA	Mainchain,Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4207	0	4139	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4204	0	4145	141	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	41	0
3	B	172	0	120	32	0
4	A	53	0	31	6	0
4	B	53	0	31	7	0
5	A	8	0	2	0	0
5	B	8	0	2	1	0
6	A	822	0	0	20	0
6	B	854	0	0	21	0
All	All	10555	0	8590	293	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 17.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:HA	6:B:3035:HOH:O	1.57	1.04
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.46	1.03
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.47	1.03
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.49	1.01
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.48	1.01
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.50	0.99
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.51	0.99
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.51	0.99
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.50	0.98
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.54	0.96
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.53	0.96
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.56	0.93
1:B:279:ILE:HB	1:B:293:LEU:HD13	1.47	0.93
1:B:204:ASN:HD22	1:B:204:ASN:H	1.15	0.92
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.83	0.91
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.59	0.90
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.59	0.90
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.60	0.90
1:A:280:GLU:HB3	1:A:293:LEU:HD11	1.53	0.90
1:B:229:ASP:H	1:B:256:HIS:HE1	1.22	0.87
1:B:183:LYS:HD3	6:B:1812:HOH:O	1.73	0.86
1:A:280:GLU:HB3	1:A:293:LEU:CD1	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HB2	6:B:1852:HOH:O	1.78	0.83
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.68	0.82
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.67	0.82
1:B:1:ALA:HB1	1:B:6:GLU:HB3	1.61	0.81
1:A:431:LYS:HA	1:A:434:LYS:HD3	1.63	0.81
1:A:229:ASP:H	1:A:256:HIS:HE1	1.30	0.79
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.94	0.79
1:B:14:CYS:HG	3:B:801:HEM:CAB	1.95	0.79
1:A:279:ILE:HB	1:A:293:LEU:HD13	1.66	0.78
1:B:229:ASP:H	1:B:256:HIS:CE1	2.03	0.77
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.50	0.76
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.26	0.75
1:B:286:LYS:HE3	6:B:3107:HOH:O	1.85	0.74
1:A:204:ASN:HD22	1:A:204:ASN:H	1.36	0.74
1:A:229:ASP:H	1:A:256:HIS:CE1	2.05	0.74
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.27	0.73
4:B:2805:FAD:O2'	4:B:2805:FAD:C9A	2.36	0.72
1:A:14:CYS:HG	3:A:801:HEM:CAB	2.00	0.72
1:B:279:ILE:HB	1:B:293:LEU:CD1	2.18	0.72
1:B:180:GLN:HB3	1:B:185:ILE:HB	1.74	0.69
1:A:311:LEU:HD23	1:A:349:ALA:HB2	1.74	0.69
1:A:39:CYS:HG	3:A:802:HEM:CAC	2.05	0.69
1:A:427:LYS:HG3	1:B:328:PRO:HB2	1.74	0.68
1:A:157:LYS:HZ1	1:A:340:GLY:HA3	1.59	0.68
1:A:218:ASP:HB3	6:A:2029:HOH:O	1.94	0.66
1:B:204:ASN:H	1:B:204:ASN:ND2	1.91	0.65
1:B:21:ASP:OD1	1:B:23:GLU:HB3	1.97	0.65
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.61	0.65
1:A:174:ALA:HA	1:A:216:SER:HB2	1.77	0.64
1:B:280:GLU:HB3	1:B:293:LEU:CD1	2.28	0.64
1:B:568:SER:HA	6:B:1293:HOH:O	1.97	0.64
1:A:139:PHE:HB3	1:A:261:LEU:HB3	1.80	0.64
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.79	0.63
1:A:565:ALA:O	1:A:568:SER:HA	1.98	0.63
1:B:567:TYR:O	1:B:568:SER:HB2	1.98	0.63
1:A:427:LYS:HG3	1:B:328:PRO:CB	2.28	0.63
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.39	0.62
3:A:801:HEM:HMC2	3:A:801:HEM:HBC2	1.83	0.61
1:A:431:LYS:HD3	1:A:434:LYS:HD3	1.83	0.60
1:B:168:ALA:HA	4:B:2805:FAD:N5	2.17	0.60
1:A:39:CYS:SG	3:A:802:HEM:C3C	2.95	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:HA	4:A:1805:FAD:N5	2.17	0.59
1:A:204:ASN:ND2	1:A:204:ASN:H	2.00	0.59
1:B:286:LYS:HD3	6:B:3421:HOH:O	2.02	0.59
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.41	0.58
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.43	0.58
1:A:357:LYS:HB3	1:A:511:MET:HE3	1.85	0.58
1:B:418:TYR:CG	1:B:456:ILE:HD11	2.39	0.57
1:B:174:ALA:HA	1:B:216:SER:HB2	1.85	0.57
1:A:183:LYS:HD3	6:A:2375:HOH:O	2.03	0.57
1:A:60:SER:HB3	3:A:804:HEM:HBB2	1.86	0.57
1:B:36:CYS:SG	3:B:802:HEM:C3B	2.97	0.57
1:A:17:CYS:SG	3:A:801:HEM:CBC	2.92	0.57
1:A:293:LEU:HB2	6:A:2201:HOH:O	2.04	0.57
1:A:427:LYS:CG	1:B:328:PRO:HB2	2.34	0.57
1:A:140:SER:O	1:A:144:SER:HB2	2.05	0.57
1:A:230:LEU:HB3	1:A:245:HIS:HB3	1.86	0.57
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.87	0.57
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.40	0.57
1:B:8:HIS:O	1:B:12:GLN:HG2	2.04	0.57
1:A:533:GLY:HA2	1:A:553:ILE:HG22	1.86	0.57
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.44	0.57
1:A:133:GLY:O	1:A:138:GLY:HA3	2.05	0.57
1:B:71:CYS:SG	3:B:803:HEM:C3C	2.98	0.56
1:B:17:CYS:SG	3:B:801:HEM:CBC	2.94	0.56
1:A:144:SER:HB3	1:A:561:GLY:HA3	1.87	0.56
1:A:302:TYR:HA	6:A:2308:HOH:O	2.06	0.56
1:B:112:LYS:HE2	6:B:3268:HOH:O	2.05	0.56
1:A:17:CYS:SG	3:A:801:HEM:C3C	2.98	0.56
1:B:311:LEU:HD22	1:B:529:LEU:HD21	1.87	0.56
1:B:158:GLU:HB3	1:B:159:PRO:HD2	1.88	0.56
1:B:107:GLU:O	1:B:110:LYS:HB2	2.06	0.55
1:A:463:GLU:HG2	6:A:2070:HOH:O	2.05	0.55
1:B:167:LEU:HB3	4:B:2805:FAD:HM72	1.87	0.55
1:B:17:CYS:SG	3:B:801:HEM:C3C	2.98	0.55
1:B:280:GLU:N	1:B:293:LEU:HD12	2.22	0.55
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.88	0.55
1:B:157:LYS:NZ	1:B:340:GLY:HA3	2.21	0.55
1:B:180:GLN:HG2	1:B:233:VAL:HG11	1.88	0.54
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.47	0.54
1:B:194:GLU:HG2	6:B:1685:HOH:O	2.06	0.54
1:B:112:LYS:HA	1:B:112:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HE3	6:A:2573:HOH:O	2.07	0.54
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.91	0.53
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.00	0.53
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.01	0.53
3:A:801:HEM:CMC	3:A:801:HEM:HBC2	2.38	0.53
1:B:419:LEU:O	1:B:496:ALA:HA	2.07	0.53
1:A:280:GLU:CB	1:A:293:LEU:HD11	2.33	0.53
1:B:457:ASP:OD1	1:B:459:LYS:HG3	2.08	0.53
1:A:91:ASN:HB2	6:A:2321:HOH:O	2.08	0.53
1:B:139:PHE:HB3	1:B:261:LEU:HB3	1.90	0.53
1:A:168:ALA:HA	4:A:1805:FAD:C5X	2.39	0.52
1:B:107:GLU:HB3	6:B:1540:HOH:O	2.09	0.52
1:A:85:CYS:SG	3:A:804:HEM:HAC	2.47	0.52
1:A:167:LEU:HB3	4:A:1805:FAD:HM72	1.91	0.52
1:B:365:HIS:O	1:B:501:PRO:HA	2.09	0.52
1:B:191:LEU:HD21	1:B:240:SER:HB2	1.92	0.52
1:B:337:ASN:HD22	1:B:337:ASN:N	2.08	0.52
1:A:415:LYS:HD3	6:A:2560:HOH:O	2.08	0.52
1:A:68:CYS:SG	3:A:803:HEM:C3B	3.03	0.52
1:B:47:ALA:HA	1:B:58:HIS:HB2	1.93	0.51
1:B:85:CYS:SG	3:B:804:HEM:CBC	2.97	0.51
1:B:157:LYS:HZ1	1:B:340:GLY:HA3	1.74	0.51
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.04	0.51
1:B:540:HIS:CD2	1:B:544:ARG:HG3	2.46	0.51
1:A:237:GLY:N	1:A:378:GLU:OE2	2.32	0.51
1:B:133:GLY:O	1:B:138:GLY:HA3	2.10	0.51
1:A:157:LYS:NZ	1:A:340:GLY:HA3	2.24	0.51
1:B:183:LYS:O	1:B:184:LYS:HB2	2.11	0.51
1:A:157:LYS:HZ1	1:A:340:GLY:CA	2.23	0.51
1:A:280:GLU:HB3	1:A:293:LEU:HD12	1.91	0.50
1:B:550:ILE:HD11	6:B:3035:HOH:O	2.10	0.50
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.01	0.50
1:B:113:SER:O	1:B:114:GLU:CB	2.59	0.50
1:B:313:THR:OG1	1:B:345:GLY:HA3	2.11	0.50
1:A:293:LEU:CB	6:A:2201:HOH:O	2.60	0.50
1:B:85:CYS:SG	3:B:804:HEM:HAC	2.44	0.50
1:B:11:ASN:HB2	6:B:3063:HOH:O	2.12	0.50
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.48	0.49
1:B:236:MET:HB3	1:B:378:GLU:OE2	2.12	0.49
1:A:481:GLU:HG3	6:A:2061:HOH:O	2.11	0.49
1:A:393:LYS:HD3	6:A:2231:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.48	0.49
1:B:210:LYS:HD3	6:B:1521:HOH:O	2.11	0.49
1:B:68:CYS:SG	3:B:803:HEM:C3B	3.05	0.49
1:A:365:HIS:O	1:A:501:PRO:HA	2.12	0.49
1:A:112:LYS:O	1:A:116:GLN:HB2	2.12	0.49
1:B:198:LYS:HG2	6:B:1728:HOH:O	2.13	0.49
1:A:313:THR:OG1	1:A:345:GLY:HA3	2.13	0.49
1:B:204:ASN:N	1:B:204:ASN:HD22	1.94	0.49
1:B:136:GLY:HA3	1:B:553:ILE:HD12	1.94	0.48
1:A:457:ASP:OD1	1:A:459:LYS:HG3	2.13	0.48
1:A:39:CYS:SG	3:A:802:HEM:CBC	3.01	0.48
1:B:56:ASN:HD22	1:B:58:HIS:H	1.61	0.48
1:A:519:MET:HE2	1:A:523:LYS:O	2.14	0.48
1:A:558:ARG:O	1:A:562:GLU:HG3	2.13	0.48
1:B:380:VAL:HG12	1:B:385:ALA:HB2	1.94	0.48
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.06	0.48
1:B:540:HIS:HD2	6:B:1162:HOH:O	1.96	0.48
1:B:513:ASP:OD2	1:B:517:GLU:OE1	2.32	0.48
1:A:44:ALA:O	1:A:47:ALA:HB3	2.14	0.48
1:A:368:LEU:HB3	1:A:500:THR:O	2.13	0.48
1:A:65:GLU:HG3	1:A:262:TYR:CE2	2.49	0.48
1:B:476:LYS:HG2	1:B:478:THR:HG23	1.96	0.48
1:A:418:TYR:CG	1:A:456:ILE:HD11	2.49	0.48
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.07	0.47
1:B:25:SER:O	1:B:26:ASN:HB3	2.14	0.47
1:B:79:MET:CE	1:B:96:LYS:HE3	2.44	0.47
1:B:226:MET:HB3	1:B:264:ASN:ND2	2.29	0.47
1:A:164:ASN:HB2	4:A:1805:FAD:H4'	1.95	0.47
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.00	0.47
1:A:297:MET:HE1	6:A:2116:HOH:O	2.15	0.47
1:B:46:VAL:HG21	3:B:803:HEM:HMB3	1.97	0.47
1:B:280:GLU:HB3	1:B:293:LEU:HD12	1.96	0.47
1:A:183:LYS:HD2	6:A:1944:HOH:O	2.15	0.47
1:B:380:VAL:HG12	1:B:385:ALA:CB	2.44	0.47
1:B:559:LEU:C	1:B:559:LEU:HD13	2.36	0.47
1:A:517:GLU:HB3	1:A:525:VAL:HG13	1.96	0.47
1:B:50:THR:HG21	1:B:58:HIS:CE1	2.49	0.46
1:A:431:LYS:NZ	1:A:434:LYS:HE2	2.30	0.46
1:B:19:THR:HB	1:B:20:PRO:HD2	1.98	0.46
1:A:47:ALA:HA	1:A:58:HIS:HB2	1.97	0.46
1:A:318:LYS:HE3	1:A:339:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HD23	1:A:432:ILE:HG13	1.98	0.46
1:A:24:LEU:HG	3:A:801:HEM:HBA1	1.98	0.46
1:A:431:LYS:HA	1:A:434:LYS:CD	2.41	0.46
1:B:490:ASN:C	1:B:490:ASN:HD22	2.19	0.46
1:A:86:HIS:CD2	3:A:804:HEM:NB	2.84	0.46
1:B:280:GLU:HB3	1:B:293:LEU:HD11	1.97	0.45
1:B:229:ASP:N	1:B:256:HIS:HE1	2.02	0.45
1:A:165:ALA:HB2	4:A:1805:FAD:O4'	2.16	0.45
1:B:79:MET:HE2	1:B:96:LYS:HE3	1.97	0.45
1:A:60:SER:CB	3:A:804:HEM:HBB2	2.46	0.45
4:B:2805:FAD:C2	5:B:2806:FUM:O7	2.64	0.45
1:A:6:GLU:HA	1:A:9:VAL:HG22	1.99	0.45
1:A:79:MET:HE2	1:A:96:LYS:HE3	1.98	0.45
1:B:218:ASP:HB2	6:B:1321:HOH:O	2.17	0.45
1:A:42:THR:O	1:A:46:VAL:HG23	2.16	0.45
1:A:229:ASP:N	1:A:256:HIS:HE1	2.08	0.45
1:B:14:CYS:SG	3:B:801:HEM:C3B	3.10	0.45
1:A:520:ASN:HB2	6:A:1871:HOH:O	2.16	0.45
4:B:2805:FAD:H1'1	6:B:1141:HOH:O	2.16	0.45
4:B:2805:FAD:O2'	4:B:2805:FAD:C9	2.65	0.45
1:A:174:ALA:HA	1:A:216:SER:CB	2.47	0.45
1:B:518:VAL:HG21	1:B:529:LEU:HD13	1.99	0.44
1:B:48:GLU:HG3	6:B:1998:HOH:O	2.15	0.44
1:B:526:ILE:HD13	1:B:529:LEU:HD12	1.99	0.44
1:B:60:SER:HB3	3:B:804:HEM:HMB1	1.99	0.44
1:A:396:VAL:HG22	1:A:397:ASN:N	2.32	0.44
1:B:357:LYS:HB3	1:B:511:MET:HE2	2.00	0.44
1:A:252:GLY:H	1:A:434:LYS:NZ	2.15	0.44
1:B:474:SER:OG	1:B:476:LYS:NZ	2.37	0.44
1:A:199:GLY:HA3	1:A:545:LEU:HD21	2.00	0.44
1:B:255:ALA:HB1	6:B:1913:HOH:O	2.15	0.44
1:A:82:CYS:SG	3:A:804:HEM:CBB	3.03	0.44
1:B:544:ARG:CZ	1:B:549:ALA:HB2	2.46	0.44
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.98	0.44
1:A:367:THR:HA	1:A:499:VAL:HB	2.00	0.44
1:A:64:GLY:HA2	1:A:262:TYR:CD2	2.53	0.43
1:B:237:GLY:N	1:B:378:GLU:OE2	2.33	0.43
1:B:199:GLY:O	1:B:543:ASN:HB3	2.18	0.43
1:B:99:LEU:HD12	6:B:1879:HOH:O	2.16	0.43
3:B:803:HEM:HBC1	3:B:804:HEM:HBB1	1.99	0.43
1:A:60:SER:HB3	3:A:804:HEM:CMB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HE2	1:A:183:LYS:HB3	1.78	0.43
1:B:510:VAL:CG1	1:B:518:VAL:HG13	2.49	0.43
1:A:526:ILE:CD1	1:A:529:LEU:HD12	2.47	0.43
1:B:4:LEU:HD21	3:B:802:HEM:HMB3	2.00	0.43
3:A:803:HEM:HBB2	3:A:803:HEM:CMB	2.48	0.43
1:B:112:LYS:HA	1:B:112:LYS:CE	2.49	0.43
1:A:513:ASP:OD2	1:A:517:GLU:OE1	2.37	0.43
1:B:125:ASP:HB2	1:B:304:VAL:HG13	2.00	0.43
1:A:127:VAL:HG11	1:A:153:ILE:HG13	2.00	0.43
1:B:316:PHE:CE2	1:B:506:THR:HB	2.53	0.43
1:A:371:LYS:HE2	6:A:2408:HOH:O	2.18	0.43
1:A:82:CYS:HG	3:A:804:HEM:CBB	2.30	0.43
1:A:14:CYS:SG	3:A:801:HEM:C3B	3.10	0.43
1:A:380:VAL:HG22	1:A:432:ILE:HG12	2.01	0.43
1:A:55:TYR:OH	1:A:89:ASP:HB3	2.19	0.43
1:B:321:GLU:O	1:B:325:LYS:HG3	2.19	0.43
1:A:194:GLU:HB2	6:A:2458:HOH:O	2.18	0.43
1:B:293:LEU:CB	6:B:1852:HOH:O	2.54	0.43
1:B:68:CYS:SG	3:B:803:HEM:CBB	3.06	0.43
3:A:804:HEM:HMB1	3:A:804:HEM:HBB2	1.99	0.43
1:A:341:ALA:HA	6:A:1831:HOH:O	2.19	0.43
1:A:284:ASP:HA	1:A:290:LYS:HD3	2.01	0.42
1:A:487:ARG:HD3	6:A:2316:HOH:O	2.19	0.42
1:B:397:ASN:O	1:B:400:THR:HG22	2.20	0.42
1:A:434:LYS:HG3	6:A:2259:HOH:O	2.19	0.42
1:A:68:CYS:SG	3:A:803:HEM:CBB	3.06	0.42
1:A:540:HIS:CG	1:A:544:ARG:HG3	2.54	0.42
1:B:141:ALA:HB1	1:B:310:ILE:HD13	2.01	0.42
1:A:283:LYS:NZ	1:A:352:ALA:O	2.44	0.42
1:B:288:THR:HB	1:B:527:PRO:HB2	2.02	0.42
1:B:280:GLU:H	1:B:293:LEU:HD12	1.84	0.42
1:A:317:ALA:HB3	1:A:337:ASN:OD1	2.20	0.42
1:B:102:GLU:OE2	1:B:157:LYS:HE2	2.19	0.42
1:B:467:ARG:NE	1:B:479:ASP:OD2	2.53	0.42
1:A:129:VAL:O	1:A:152:VAL:HA	2.19	0.42
1:A:137:ALA:HA	1:A:553:ILE:O	2.19	0.42
1:B:168:ALA:HA	4:B:2805:FAD:C5X	2.49	0.42
1:A:36:CYS:SG	3:A:802:HEM:CBB	3.06	0.42
1:B:421:PHE:HB2	1:B:425:VAL:HB	2.01	0.41
1:B:113:SER:O	1:B:114:GLU:HB2	2.21	0.41
1:B:69:THR:HA	1:B:72:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ILE:HA	1:A:517:GLU:O	2.20	0.41
1:A:544:ARG:HD2	1:A:549:ALA:HB2	2.03	0.41
1:B:52:HIS:HB2	1:B:55:TYR:O	2.20	0.41
1:A:184:LYS:HA	1:A:184:LYS:HD2	1.87	0.41
1:A:346:LEU:HD21	1:A:509:GLY:HA2	2.02	0.41
1:B:533:GLY:HA2	1:B:553:ILE:HG22	2.02	0.41
1:A:79:MET:CE	1:A:96:LYS:HE3	2.50	0.41
1:A:490:ASN:C	1:A:490:ASN:HD22	2.23	0.41
1:A:279:ILE:HB	1:A:293:LEU:CD1	2.44	0.41
1:A:431:LYS:O	1:A:434:LYS:HB2	2.20	0.41
1:B:286:LYS:HE2	1:B:286:LYS:HB2	1.28	0.41
1:A:550:ILE:HG12	4:A:1805:FAD:C2	2.51	0.41
1:B:127:VAL:HG11	1:B:153:ILE:HG13	2.03	0.41
1:B:10:GLN:HG3	6:B:1489:HOH:O	2.20	0.41
1:A:505:HIS:CG	1:A:544:ARG:HE	2.39	0.40
1:A:43:LEU:HD23	6:A:2300:HOH:O	2.21	0.40
1:A:337:ASN:N	1:A:337:ASN:HD22	2.18	0.40
1:A:289:VAL:HG21	1:A:309:VAL:HG23	2.03	0.40
1:B:171:GLY:O	1:B:547:GLY:HA2	2.21	0.40
1:A:173:ASN:HA	1:A:243:ARG:O	2.20	0.40
1:B:4:LEU:CD2	3:B:802:HEM:HMB3	2.52	0.40
1:B:376:VAL:HG11	1:B:419:LEU:CD1	2.52	0.40
1:A:250:GLY:HA3	1:A:429:LEU:HD12	2.03	0.40
1:B:275:ASN:HB3	1:B:297:MET:HB3	2.03	0.40
1:A:128:ASP:HB2	1:A:150:ALA:HB1	2.03	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%)	543 (96%)	23 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	566/571 (99%)	544 (96%)	20 (4%)	2 (0%)	39 33
All	All	1132/1142 (99%)	1087 (96%)	43 (4%)	2 (0%)	52 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	GLU
1	B	176	TRP

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	440/444 (99%)	413 (94%)	27 (6%)	23 17
1	B	439/444 (99%)	409 (93%)	30 (7%)	20 13
All	All	879/888 (99%)	822 (94%)	57 (6%)	21 15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	23	GLU
1	A	51	LYS
1	A	56	ASN
1	A	112	LYS
1	A	183	LYS
1	A	184	LYS
1	A	198	LYS
1	A	204	ASN
1	A	282	LEU
1	A	293	LEU
1	A	311	LEU
1	A	318	LYS
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	434	LYS
1	A	450	LEU
1	A	452	LYS
1	A	459	LYS
1	A	467	ARG
1	A	470	SER
1	A	490	ASN
1	A	515	LYS
1	A	523	LYS
1	A	526	ILE
1	A	529	LEU
1	A	566	LYS
1	A	568	SER
1	B	6	GLU
1	B	56	ASN
1	B	110	LYS
1	B	112	LYS
1	B	113	SER
1	B	119	LEU
1	B	157	LYS
1	B	176	TRP
1	B	183	LYS
1	B	198	LYS
1	B	204	ASN
1	B	208	LEU
1	B	210	LYS
1	B	218	ASP
1	B	282	LEU
1	B	286	LYS
1	B	288	THR
1	B	293	LEU
1	B	299	LYS
1	B	311	LEU
1	B	321	GLU
1	B	337	ASN
1	B	450	LEU
1	B	459	LYS
1	B	467	ARG
1	B	476	LYS
1	B	490	ASN
1	B	526	ILE
1	B	529	LEU

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Mol	Chain	Res	Type
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	10	GLN
1	A	35	GLN
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	204	ASN
1	B	245	HIS
1	B	256	HIS
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	-	48,58,58	1.78	10 (20%)	54,89,89	2.78	23 (42%)
5	FUM	A	1806	-	1,7,7	0.62	0	0,8,8	0.00	-
3	HEM	A	801	1	30,50,50	2.74	8 (26%)	24,82,82	2.98	11 (45%)
3	HEM	A	802	1	30,50,50	2.58	10 (33%)	24,82,82	2.70	10 (41%)
3	HEM	A	803	1	30,50,50	2.51	8 (26%)	24,82,82	3.44	13 (54%)
3	HEM	A	804	1	30,50,50	2.74	8 (26%)	24,82,82	2.97	10 (41%)
4	FAD	B	2805	-	48,58,58	2.10	13 (27%)	54,89,89	2.55	20 (37%)
5	FUM	B	2806	-	1,7,7	0.94	0	0,8,8	0.00	-
3	HEM	B	801	1	30,50,50	2.43	7 (23%)	24,82,82	2.75	10 (41%)
3	HEM	B	802	1	30,50,50	2.33	8 (26%)	24,82,82	3.05	12 (50%)
3	HEM	B	803	1	30,50,50	2.40	7 (23%)	24,82,82	3.41	12 (50%)
3	HEM	B	804	1	30,50,50	2.39	9 (30%)	24,82,82	2.95	11 (45%)

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	-	1/1/9/9	0/30/50/50	0/6/6/6
5	FUM	A	1806	-	-	0/0/5/5	0/0/0/0
3	HEM	A	801	1	-	0/10/54/54	0/0/8/8
3	HEM	A	802	1	-	0/10/54/54	0/0/8/8
3	HEM	A	803	1	-	0/10/54/54	0/0/8/8
3	HEM	A	804	1	-	0/10/54/54	0/0/8/8
4	FAD	B	2805	-	-	0/30/50/50	0/6/6/6
5	FUM	B	2806	-	-	0/0/5/5	0/0/0/0
3	HEM	B	801	1	-	0/10/54/54	0/0/8/8
3	HEM	B	802	1	-	0/10/54/54	0/0/8/8
3	HEM	B	803	1	-	0/10/54/54	0/0/8/8
3	HEM	B	804	1	-	0/10/54/54	0/0/8/8

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3B-C4B	-9.33	1.43	1.51
3	A	804	HEM	C3B-C4B	-9.23	1.43	1.51
3	A	802	HEM	C3B-C4B	-8.31	1.44	1.51
3	B	802	HEM	C3B-C4B	-8.00	1.44	1.51
3	A	803	HEM	C3B-C4B	-7.74	1.45	1.51
3	B	803	HEM	C3B-C4B	-7.54	1.45	1.51
3	B	801	HEM	C3B-C4B	-7.46	1.45	1.51
3	A	802	HEM	C2D-C3D	-7.22	1.32	1.54
3	A	804	HEM	C2D-C3D	-7.18	1.33	1.54
3	B	804	HEM	C2D-C3D	-6.97	1.33	1.54
3	B	803	HEM	C2D-C3D	-6.92	1.33	1.54
3	B	802	HEM	C2D-C3D	-6.90	1.33	1.54
3	B	801	HEM	C2D-C3D	-6.86	1.33	1.54
3	A	801	HEM	C2D-C3D	-6.81	1.34	1.54
3	A	803	HEM	C2D-C3D	-6.73	1.34	1.54
3	B	804	HEM	C3B-C4B	-5.86	1.46	1.51
3	A	803	HEM	C3D-C4D	-5.32	1.44	1.51
3	A	804	HEM	C3D-C4D	-5.01	1.45	1.51
3	B	804	HEM	C3D-C4D	-4.99	1.45	1.51
3	B	803	HEM	C3D-C4D	-4.83	1.45	1.51
3	A	801	HEM	C3D-C4D	-4.55	1.45	1.51
3	B	801	HEM	C3D-C4D	-4.38	1.46	1.51
3	A	801	HEM	C2C-C1C	-4.25	1.44	1.52
3	A	802	HEM	C3D-C4D	-4.22	1.46	1.51
3	B	804	HEM	C2C-C1C	-4.07	1.44	1.52
3	B	801	HEM	C2C-C1C	-3.75	1.45	1.52
3	A	802	HEM	C2C-C1C	-3.72	1.45	1.52
4	A	1805	FAD	C10-N1	-3.70	1.29	1.35
3	A	804	HEM	C2C-C1C	-3.68	1.45	1.52
4	A	1805	FAD	O4-C4	-3.64	1.16	1.24
3	A	803	HEM	C2C-C1C	-3.58	1.45	1.52
4	B	2805	FAD	C10-N1	-3.54	1.29	1.35
4	B	2805	FAD	O4-C4	-3.17	1.17	1.24
3	B	802	HEM	C3D-C4D	-2.69	1.48	1.51
3	B	802	HEM	C2C-C1C	-2.67	1.47	1.52
4	A	1805	FAD	C4X-N5	-2.61	1.29	1.33
3	B	803	HEM	C2D-C1D	-2.55	1.43	1.51
3	B	802	HEM	C2B-C1B	-2.47	1.43	1.51
3	B	803	HEM	C2C-C1C	-2.41	1.48	1.52
4	B	2805	FAD	O4B-C4B	-2.40	1.39	1.45
3	A	802	HEM	C2D-C1D	-2.37	1.44	1.51
3	A	802	HEM	C2B-C1B	-2.20	1.44	1.51
4	B	2805	FAD	P-O2P	-2.17	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	HEM	C2B-C1B	-2.15	1.44	1.51
4	B	2805	FAD	PA-O1A	-2.07	1.43	1.51
3	B	802	HEM	C2D-C1D	-2.04	1.45	1.51
3	A	803	HEM	C2D-C1D	-2.03	1.45	1.51
3	B	802	HEM	C3C-CAC	2.00	1.55	1.51
3	B	804	HEM	C1C-NC	2.01	1.38	1.36
3	B	804	HEM	C3C-CAC	2.03	1.55	1.51
3	A	802	HEM	C1C-NC	2.11	1.38	1.36
4	B	2805	FAD	C4'-C3'	2.16	1.57	1.53
3	A	801	HEM	C3B-CAB	2.16	1.55	1.51
3	A	802	HEM	C3C-CAC	2.20	1.55	1.51
3	B	803	HEM	C4C-NC	2.22	1.38	1.36
4	B	2805	FAD	C6-C5X	2.26	1.45	1.41
3	B	801	HEM	CAA-C2A	2.26	1.55	1.52
3	B	801	HEM	C1C-NC	2.28	1.38	1.36
3	A	802	HEM	CMA-C3A	2.29	1.56	1.51
3	B	804	HEM	C4C-NC	2.29	1.38	1.36
3	B	804	HEM	C3B-CAB	2.33	1.55	1.51
3	B	801	HEM	CMA-C3A	2.34	1.56	1.51
3	A	803	HEM	CAA-C2A	2.35	1.56	1.52
3	B	803	HEM	C3B-CAB	2.36	1.55	1.51
3	A	802	HEM	C4C-NC	2.45	1.39	1.36
3	A	804	HEM	CAA-C2A	2.46	1.56	1.52
3	A	804	HEM	C1C-NC	2.49	1.39	1.36
3	A	803	HEM	C3B-CAB	2.52	1.56	1.51
3	B	802	HEM	C4C-NC	2.56	1.39	1.36
3	A	801	HEM	CMA-C3A	2.62	1.57	1.51
3	A	804	HEM	C3B-CAB	2.70	1.56	1.51
3	B	804	HEM	CAA-C2A	2.70	1.56	1.52
4	A	1805	FAD	C2'-C3'	2.76	1.59	1.53
4	A	1805	FAD	C9-C8	2.87	1.45	1.37
3	A	801	HEM	C3C-CAC	2.91	1.56	1.51
3	A	804	HEM	C4C-NC	2.96	1.39	1.36
4	B	2805	FAD	C9-C8	3.09	1.46	1.37
3	A	801	HEM	C1C-NC	3.09	1.39	1.36
4	A	1805	FAD	C2A-N3A	3.11	1.37	1.32
4	A	1805	FAD	C1'-N10	3.16	1.51	1.48
4	B	2805	FAD	C2'-C3'	3.65	1.60	1.53
4	A	1805	FAD	C4-C4X	3.75	1.48	1.41
4	B	2805	FAD	C4-C4X	3.99	1.49	1.41
4	A	1805	FAD	C5'-C4'	4.03	1.57	1.51
4	A	1805	FAD	C4-N3	4.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2805	FAD	C2A-N3A	4.36	1.39	1.32
4	B	2805	FAD	C4-N3	4.52	1.41	1.33
4	B	2805	FAD	C1'-N10	7.38	1.56	1.48

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	803	HEM	CAA-C2A-C1A	-7.77	118.57	127.01
3	A	803	HEM	CAA-C2A-C1A	-7.34	119.04	127.01
3	A	803	HEM	C3B-CAB-CBB	-7.15	113.49	124.46
4	A	1805	FAD	C4-C4X-C10	-6.91	115.52	119.94
4	A	1805	FAD	C4X-C10-N10	-6.10	116.92	120.52
4	B	2805	FAD	C4X-C4-N3	-6.02	115.36	123.59
4	B	2805	FAD	C4-C4X-C10	-5.44	116.46	119.94
3	B	804	HEM	CAA-C2A-C1A	-5.24	121.32	127.01
3	B	802	HEM	CAA-C2A-C1A	-5.22	121.34	127.01
4	A	1805	FAD	C4X-C4-N3	-5.07	116.66	123.59
3	B	803	HEM	C3C-CAC-CBC	-4.90	116.94	124.46
3	B	801	HEM	CAA-C2A-C1A	-4.78	121.82	127.01
4	B	2805	FAD	N3A-C2A-N1A	-4.69	125.30	128.89
3	B	803	HEM	C3B-CAB-CBB	-4.56	117.46	124.46
3	A	801	HEM	C3B-CAB-CBB	-4.52	117.52	124.46
3	A	804	HEM	CMA-C3A-C4A	-4.43	121.03	128.36
3	A	802	HEM	CAA-C2A-C1A	-4.43	122.20	127.01
3	A	803	HEM	C3C-CAC-CBC	-4.41	117.70	124.46
3	B	804	HEM	C3C-CAC-CBC	-4.37	117.75	124.46
4	B	2805	FAD	C1B-N9A-C4A	-4.36	120.37	126.94
3	A	801	HEM	CAA-C2A-C1A	-4.30	122.33	127.01
4	A	1805	FAD	C2B-C1B-N9A	-4.26	107.79	114.29
3	B	804	HEM	CMA-C3A-C4A	-4.05	121.67	128.36
4	B	2805	FAD	O4'-C4'-C3'	-3.78	99.50	109.02
4	A	1805	FAD	O2'-C2'-C3'	-3.78	99.51	109.02
3	A	804	HEM	CAA-C2A-C1A	-3.63	123.07	127.01
4	B	2805	FAD	O2'-C2'-C1'	-3.57	101.18	109.94
3	B	803	HEM	CAA-CBA-CGA	-3.49	106.35	112.75
3	A	804	HEM	C3C-CAC-CBC	-3.47	119.13	124.46
3	A	801	HEM	CBA-CAA-C2A	-3.39	106.45	112.53
3	A	802	HEM	CMA-C3A-C4A	-3.34	122.84	128.36
4	B	2805	FAD	C2B-C1B-N9A	-3.01	109.70	114.29
4	A	1805	FAD	C1B-N9A-C4A	-2.97	122.46	126.94
4	B	2805	FAD	O4B-C1B-N9A	-2.86	102.11	108.10
4	A	1805	FAD	C5X-C9A-N10	-2.80	115.49	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	HEM	C3B-CAB-CBB	-2.79	120.18	124.46
4	A	1805	FAD	O4B-C1B-N9A	-2.59	102.67	108.10
3	B	803	HEM	CBD-CAD-C3D	-2.59	106.02	113.55
4	B	2805	FAD	O3'-C3'-C4'	-2.58	102.25	108.75
3	A	803	HEM	CBD-CAD-C3D	-2.54	106.15	113.55
3	B	802	HEM	C3B-C4B-NB	-2.51	106.83	111.63
4	A	1805	FAD	C9A-C5X-N5	-2.41	118.78	122.36
4	B	2805	FAD	C8M-C8-C9	-2.39	113.78	120.28
4	A	1805	FAD	C8M-C8-C9	-2.37	113.82	120.28
4	B	2805	FAD	C5B-C4B-C3B	-2.37	105.80	115.21
4	A	1805	FAD	O3B-C3B-C4B	-2.30	104.16	111.05
3	A	803	HEM	CAA-CBA-CGA	-2.20	108.71	112.75
4	A	1805	FAD	C5B-C4B-C3B	-2.20	106.48	115.21
3	A	801	HEM	C3C-CAC-CBC	-2.18	121.11	124.46
3	A	802	HEM	C3B-C4B-NB	-2.07	107.67	111.63
3	B	802	HEM	C2C-C1C-NC	-2.07	106.72	110.21
4	A	1805	FAD	O4'-C4'-C5'	-2.05	105.72	110.19
4	B	2805	FAD	C4X-C10-N10	-2.04	119.32	120.52
4	A	1805	FAD	O2A-PA-O5B	-2.02	98.28	108.46
3	B	801	HEM	CAA-CBA-CGA	2.01	116.44	112.75
3	A	802	HEM	C3B-C4B-CHC	2.02	126.00	123.16
4	A	1805	FAD	O4B-C4B-C5B	2.02	116.55	109.32
4	A	1805	FAD	O2A-PA-O1A	2.06	123.69	112.53
4	A	1805	FAD	C7M-C7-C6	2.13	126.08	120.28
3	B	801	HEM	C2C-C1C-CHC	2.18	127.00	123.68
3	B	804	HEM	C3B-C4B-CHC	2.30	126.40	123.16
3	A	801	HEM	C1D-CHD-C4C	2.36	129.76	125.82
3	A	803	HEM	C3B-C4B-CHC	2.37	126.50	123.16
4	A	1805	FAD	O2'-C2'-C1'	2.38	115.79	109.94
3	A	803	HEM	C2C-C1C-CHC	2.53	127.53	123.68
3	B	801	HEM	C1D-CHD-C4C	2.57	130.11	125.82
3	A	801	HEM	CAD-C3D-C4D	2.64	121.77	112.47
3	B	801	HEM	CAD-C3D-C4D	2.68	121.93	112.47
3	B	804	HEM	CMA-C3A-C2A	2.76	131.01	125.24
3	B	802	HEM	CAD-C3D-C4D	2.76	122.21	112.47
3	A	804	HEM	CMA-C3A-C2A	2.94	131.39	125.24
4	B	2805	FAD	C4X-N5-C5X	2.95	120.15	116.76
4	B	2805	FAD	O3B-C3B-C2B	3.00	121.57	111.83
3	A	804	HEM	CAD-C3D-C4D	3.00	123.04	112.47
3	A	802	HEM	CAD-C3D-C4D	3.04	123.20	112.47
3	A	802	HEM	CMD-C2D-C3D	3.04	127.82	114.35
4	A	1805	FAD	C6-C5X-N5	3.13	122.99	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	HEM	CAD-C3D-C4D	3.14	123.55	112.47
3	B	802	HEM	C2C-C1C-CHC	3.15	128.47	123.68
3	B	804	HEM	CAD-C3D-C4D	3.22	123.84	112.47
4	B	2805	FAD	C4-C4X-N5	3.32	122.75	118.72
4	B	2805	FAD	C4B-O4B-C1B	3.34	113.39	109.72
4	B	2805	FAD	C2A-N1A-C6A	3.45	124.92	118.77
3	B	803	HEM	CAD-C3D-C4D	3.65	125.35	112.47
3	A	801	HEM	CMD-C2D-C3D	3.65	130.51	114.35
3	B	804	HEM	CMD-C2D-C3D	3.66	130.54	114.35
3	A	803	HEM	CMD-C2D-C3D	3.70	130.72	114.35
3	B	802	HEM	CMD-C2D-C3D	3.70	130.73	114.35
3	B	803	HEM	CMD-C2D-C3D	3.73	130.83	114.35
3	B	803	HEM	C2D-C3D-C4D	3.75	107.86	101.50
3	A	804	HEM	CMD-C2D-C3D	3.79	131.12	114.35
3	B	802	HEM	C2D-C3D-C4D	3.83	107.99	101.50
4	B	2805	FAD	O4B-C4B-C5B	3.86	123.13	109.32
3	B	804	HEM	C2D-C3D-C4D	3.88	108.07	101.50
3	B	801	HEM	CMD-C2D-C3D	3.94	131.78	114.35
4	A	1805	FAD	O5B-C5B-C4B	3.95	123.68	109.12
3	A	803	HEM	C2D-C3D-C4D	3.98	108.25	101.50
3	A	802	HEM	C2D-C3D-C4D	4.08	108.41	101.50
3	B	803	HEM	CBA-CAA-C2A	4.13	119.93	112.53
3	A	804	HEM	C2D-C3D-C4D	4.36	108.88	101.50
3	A	801	HEM	C2D-C3D-C4D	4.40	108.97	101.50
3	B	801	HEM	C2D-C3D-C4D	4.41	108.98	101.50
3	B	803	HEM	CAD-C3D-C2D	4.62	126.51	113.22
3	B	802	HEM	C3B-C4B-CHC	4.63	129.69	123.16
3	A	803	HEM	CMC-C2C-C3C	4.98	128.95	116.53
3	A	803	HEM	CAD-C3D-C2D	5.06	127.77	113.22
3	A	802	HEM	CMC-C2C-C3C	5.08	129.21	116.53
4	B	2805	FAD	O5B-C5B-C4B	5.14	128.06	109.12
3	B	804	HEM	CAD-C3D-C2D	5.16	128.05	113.22
3	A	804	HEM	CAD-C3D-C2D	5.17	128.07	113.22
3	B	804	HEM	CMC-C2C-C3C	5.18	129.47	116.53
3	A	801	HEM	CMC-C2C-C3C	5.21	129.53	116.53
3	A	802	HEM	CAD-C3D-C2D	5.25	128.31	113.22
3	A	802	HEM	CMB-C2B-C3B	5.35	129.89	116.53
3	B	801	HEM	CMC-C2C-C3C	5.37	129.94	116.53
3	B	801	HEM	CMB-C2B-C3B	5.38	129.97	116.53
3	B	803	HEM	CMB-C2B-C3B	5.40	130.01	116.53
3	B	801	HEM	CAD-C3D-C2D	5.50	129.04	113.22
3	A	801	HEM	CAD-C3D-C2D	5.54	129.14	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	HEM	CMB-C2B-C3B	5.54	130.36	116.53
3	B	803	HEM	CMC-C2C-C3C	5.56	130.40	116.53
3	B	804	HEM	CMB-C2B-C3B	5.65	130.62	116.53
3	B	802	HEM	CAD-C3D-C2D	5.65	129.47	113.22
3	A	803	HEM	CMB-C2B-C3B	5.84	131.11	116.53
3	A	804	HEM	CMC-C2C-C3C	5.88	131.21	116.53
3	B	802	HEM	CMC-C2C-C3C	5.98	131.45	116.53
3	A	804	HEM	CMB-C2B-C3B	6.00	131.50	116.53
4	A	1805	FAD	C4-N3-C2	6.27	120.67	115.25
3	A	801	HEM	CMB-C2B-C3B	6.41	132.53	116.53
4	A	1805	FAD	C4-C4X-N5	6.62	126.75	118.72
4	B	2805	FAD	C4-N3-C2	7.18	121.45	115.25
4	A	1805	FAD	C4X-N5-C5X	7.87	125.81	116.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1805	FAD	C4'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1805	FAD	6	0
3	A	801	HEM	10	0
3	A	802	HEM	7	0
3	A	803	HEM	9	0
3	A	804	HEM	15	0
4	B	2805	FAD	7	0
5	B	2806	FUM	1	0
3	B	801	HEM	7	0
3	B	802	HEM	7	0
3	B	803	HEM	9	0
3	B	804	HEM	10	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.