Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:47 PM GMT

PDB ID	:	1QO8
Title	:	THE STRUCTURE OF THE OPEN CONFORMATION OF A FLAVOCY-TOCHROME C3 FUMARATE REDUCTASE
Authors	:	Bamford, V.; Dobbin, P.S.; Richardson, D.J.; Hemmings, A.M.
Deposited on	:	1999-11-04
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

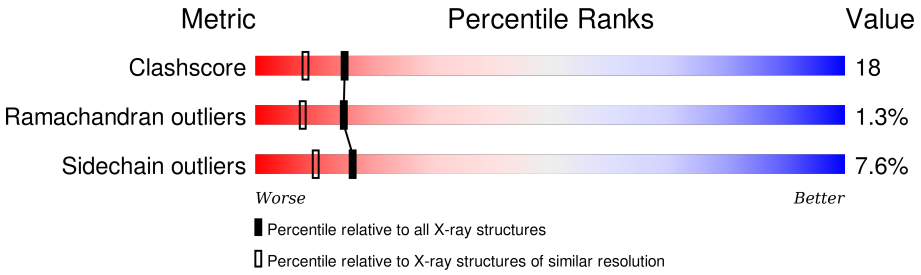
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)

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	566	68% 23% 6%
1	D	566	63% 30% 6%

2 Entry composition

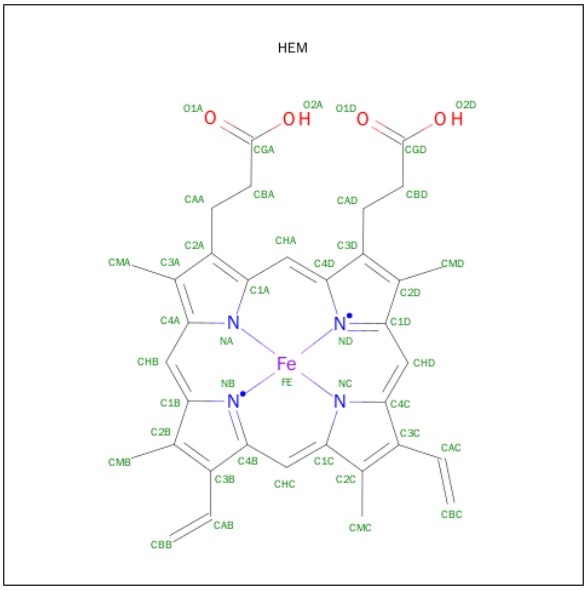
There are 4 unique types of molecules in this entry. The entry contains 9425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C3 FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4234	2627	753	826	28			
1	D	564	Total	C	N	O	S	0	0	0
			4234	2627	753	826	28			

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



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

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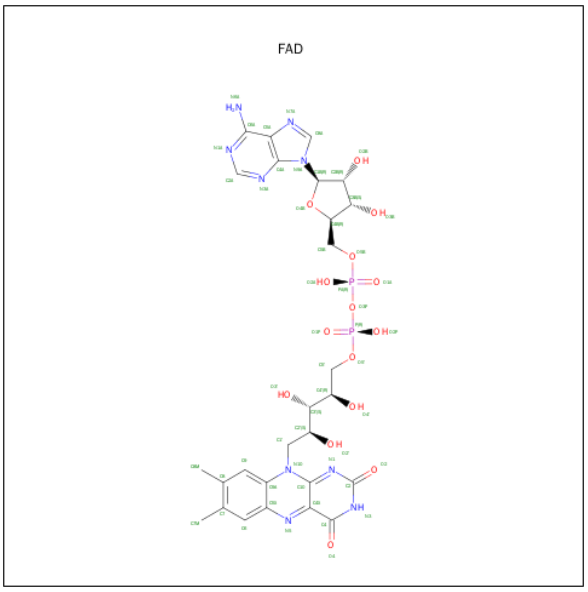
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	358	Total	O	0	0
			358	358		
4	D	149	Total	O	0	0
			149	149		

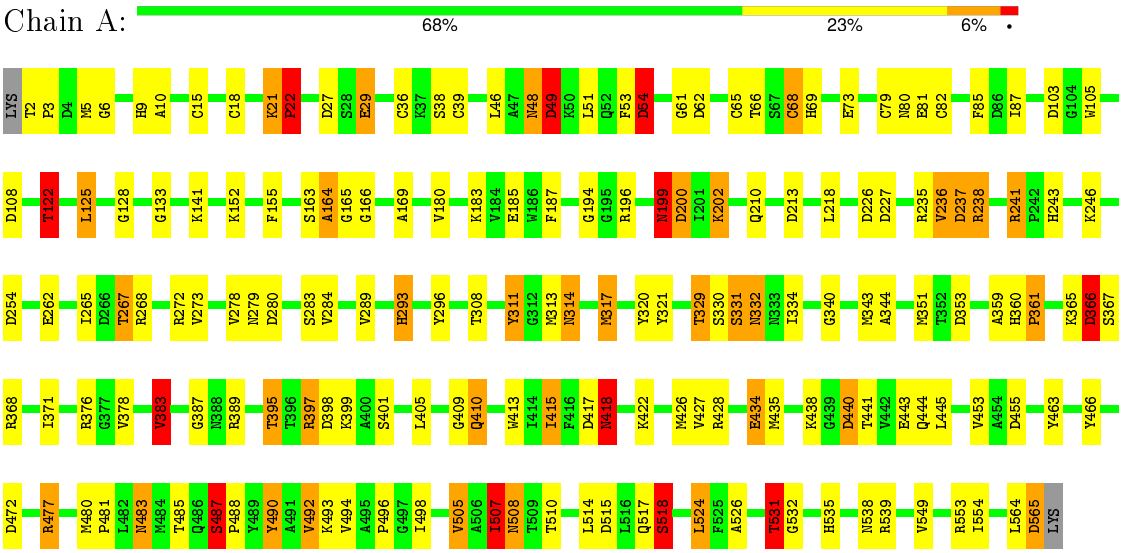
3 Residue-property plots (i)

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.

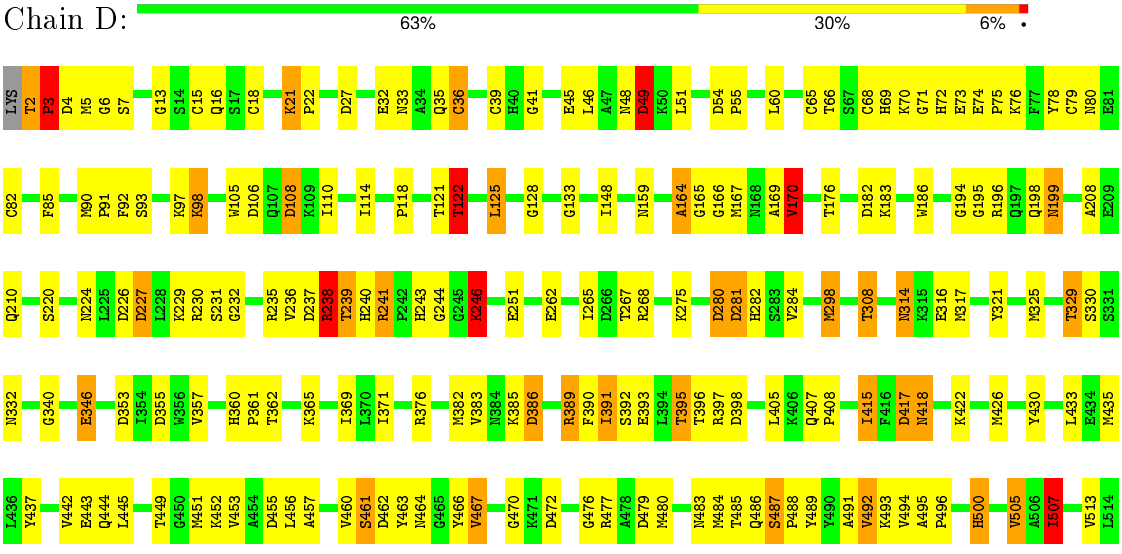
• Molecule 1: FLAVOCYTOCHROME C3 FUMARATE REDUCTASE

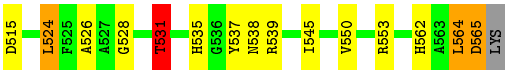
Chain A:



• Molecule 1: FLAVOCYTOCHROME C3 FUMARATE REDUCTASE

Chain D:




D515
L524
F525
A526
A527
G528
T531
H535
G536
Y537
N538
R539
I545
V550
R553
H562
A563
L564
D565
LYS1

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.77Å 109.69Å 227.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15	Depositor
% Data completeness (in resolution range)	93.4 (20.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9425	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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, FAD

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	0.94	4/4312 (0.1%)	1.94	119/5820 (2.0%)
1	D	0.61	0/4312	1.47	49/5820 (0.8%)
All	All	0.79	4/8624 (0.0%)	1.72	168/11640 (1.4%)

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	10
1	D	0	2
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ALA	CA-CB	6.30	1.65	1.52
1	A	330	SER	CB-OG	5.81	1.49	1.42
1	A	61	GLY	CA-C	5.12	1.60	1.51
1	A	330	SER	CA-CB	5.09	1.60	1.52

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	376	ARG	NE-CZ-NH2	23.64	132.12	120.30
1	A	428	ARG	NE-CZ-NH1	18.82	129.71	120.30
1	D	196	ARG	NE-CZ-NH2	-16.45	112.08	120.30
1	A	368	ARG	NE-CZ-NH1	16.34	128.47	120.30
1	A	241	ARG	NE-CZ-NH1	16.24	128.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	PRO	CA-N-CD	-14.71	90.90	111.50
1	A	415	ILE	CA-CB-CG2	13.91	138.72	110.90
1	D	196	ARG	NE-CZ-NH1	12.97	126.79	120.30
1	A	164	ALA	N-CA-CB	-12.46	92.66	110.10
1	A	389	ARG	NE-CZ-NH1	-12.35	114.13	120.30
1	D	196	ARG	CD-NE-CZ	11.78	140.09	123.60
1	A	428	ARG	CD-NE-CZ	11.33	139.46	123.60
1	D	565	ASP	CA-CB-CG	11.10	137.82	113.40
1	A	21	LYS	C-N-CD	-11.06	96.28	120.60
1	A	565	ASP	CB-CG-OD2	11.05	128.24	118.30
1	D	241	ARG	NE-CZ-NH1	-10.69	114.95	120.30
1	A	62	ASP	CB-CG-OD1	10.62	127.85	118.30
1	A	428	ARG	CA-CB-CG	9.92	135.22	113.40
1	A	21	LYS	C-N-CA	9.59	162.26	122.00
1	A	368	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	238	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	492	VAL	CB-CA-C	-9.41	93.51	111.40
1	A	254	ASP	CB-CG-OD1	9.25	126.62	118.30
1	A	163	SER	C-N-CA	8.98	144.15	121.70
1	A	539	ARG	NE-CZ-NH1	-8.80	115.90	120.30
1	A	515	ASP	CB-CG-OD1	8.78	126.20	118.30
1	D	108	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	238	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	A	22	PRO	N-CD-CG	8.65	116.17	103.20
1	D	268	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	73	GLU	OE1-CD-OE2	-8.59	113.00	123.30
1	A	487	SER	CA-C-O	-8.58	102.08	120.10
1	A	418	ASN	OD1-CG-ND2	-8.56	102.20	121.90
1	A	376	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	A	226	ASP	CB-CG-OD1	8.47	125.92	118.30
1	A	434	GLU	OE1-CD-OE2	-8.44	113.18	123.30
1	A	488	PRO	N-CA-CB	8.29	113.25	103.30
1	D	227	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	477	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	D	321	TYR	CB-CG-CD2	7.98	125.79	121.00
1	A	54	ASP	N-CA-CB	7.78	124.61	110.60
1	A	553	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	D	353	ASP	CB-CG-OD2	7.67	125.20	118.30
1	D	355	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	A	213	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	346	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	49	ASP	CB-CG-OD1	7.45	125.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	PRO	N-CA-CB	7.36	112.13	103.30
1	D	238	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	415	ILE	CA-CB-CG1	-7.27	97.18	111.00
1	D	426	MET	CA-CB-CG	7.27	125.66	113.30
1	A	267	THR	CA-CB-CG2	-7.26	102.24	112.40
1	A	518	SER	CB-CA-C	7.24	123.86	110.10
1	A	565	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	A	268	ARG	CA-CB-CG	7.14	129.12	113.40
1	A	532	GLY	CA-C-N	7.10	130.41	116.20
1	D	227	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	D	389	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	488	PRO	N-CD-CG	7.03	113.74	103.20
1	A	29	GLU	OE1-CD-OE2	-7.00	114.89	123.30
1	A	376	ARG	NH1-CZ-NH2	-6.92	111.79	119.40
1	A	122	THR	CB-CA-C	-6.88	93.03	111.60
1	D	565	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	481	PRO	N-CA-CB	6.75	111.40	103.30
1	A	241	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	213	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	426	MET	O-C-N	-6.71	111.97	122.70
1	A	463	TYR	CD1-CE1-CZ	-6.70	113.78	119.80
1	A	155	PHE	N-CA-CB	6.67	122.61	110.60
1	A	488	PRO	CA-N-CD	-6.64	102.20	111.50
1	D	505	VAL	N-CA-CB	-6.57	97.04	111.50
1	A	455	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	27	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	417	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	49	ASP	CA-CB-CG	6.49	127.69	113.40
1	A	397	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	A	311	TYR	CB-CG-CD2	6.45	124.87	121.00
1	A	227	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	428	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
1	D	553	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	331	SER	N-CA-CB	-6.27	101.10	110.50
1	D	164	ALA	N-CA-CB	-6.20	101.42	110.10
1	D	507	ILE	CA-CB-CG2	6.20	123.30	110.90
1	A	383	VAL	CA-CB-CG1	6.18	120.17	110.90
1	A	505	VAL	N-CA-CB	-6.17	97.93	111.50
1	A	401	SER	CB-CA-C	-6.17	98.39	110.10
1	A	565	ASP	CA-CB-CG	6.14	126.90	113.40
1	A	108	ASP	CB-CA-C	6.13	122.67	110.40
1	D	505	VAL	CA-CB-CG1	6.12	120.07	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	ALA	N-CA-CB	6.10	118.64	110.10
1	A	293	HIS	CA-CB-CG	-6.08	103.27	113.60
1	A	361	PRO	O-C-N	-6.05	113.02	122.70
1	A	254	ASP	OD1-CG-OD2	-5.99	111.92	123.30
1	A	108	ASP	CB-CG-OD2	5.97	123.68	118.30
1	D	125	LEU	CA-CB-CG	5.96	129.02	115.30
1	A	321	TYR	CB-CG-CD2	5.94	124.56	121.00
1	D	78	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	D	492	VAL	CB-CA-C	-5.94	100.12	111.40
1	D	241	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	D	122	THR	N-CA-CB	5.89	121.49	110.30
1	A	227	ASP	CA-CB-CG	5.84	126.25	113.40
1	D	170	VAL	CB-CA-C	-5.81	100.37	111.40
1	D	281	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	505	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	A	466	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	A	366	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	418	ASN	CB-CG-OD1	5.70	132.99	121.60
1	D	564	LEU	CA-C-N	5.69	129.71	117.20
1	A	235	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	D	500	HIS	N-CA-CB	-5.66	100.42	110.60
1	D	280	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	531	THR	N-CA-CB	-5.64	99.58	110.30
1	D	238	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	353	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	417	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	316	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	A	21	LYS	O-C-N	5.55	131.64	121.10
1	A	236	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	D	98	LYS	CA-CB-CG	5.54	125.59	113.40
1	A	200	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	532	GLY	O-C-N	-5.51	113.83	123.20
1	A	490	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	164	ALA	CB-CA-C	-5.50	101.85	110.10
1	A	125	LEU	CB-CG-CD2	5.50	120.34	111.00
1	A	320	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	D	208	ALA	N-CA-CB	5.47	117.76	110.10
1	A	321	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	313	MET	CG-SD-CE	5.43	108.89	100.20
1	A	440	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	238	ARG	O-C-N	-5.41	114.05	122.70
1	D	32	GLU	OE1-CD-OE2	-5.40	116.83	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	78	TYR	CB-CG-CD2	5.39	124.23	121.00
1	D	167	MET	CG-SD-CE	5.39	108.82	100.20
1	A	383	VAL	N-CA-CB	-5.34	99.75	111.50
1	A	196	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	515	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	27	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	48	ASN	O-C-N	-5.30	114.21	122.70
1	A	483	ASN	CA-CB-CG	-5.30	101.73	113.40
1	A	498	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	A	507	ILE	CA-CB-CG2	5.28	121.47	110.90
1	D	49	ASP	N-CA-CB	5.28	120.10	110.60
1	A	237	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	A	103	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	268	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	A	272	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	346	GLU	CA-CB-CG	5.19	124.81	113.40
1	D	386	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	483	ASN	CB-CG-ND2	5.17	129.10	116.70
1	A	351	MET	CA-CB-CG	5.14	122.04	113.30
1	A	238	ARG	N-CA-CB	-5.12	101.38	110.60
1	A	427	VAL	N-CA-CB	-5.10	100.28	111.50
1	A	38	SER	N-CA-CB	5.10	118.15	110.50
1	A	199	ASN	N-CA-CB	5.08	119.75	110.60
1	A	164	ALA	N-CA-C	5.08	124.72	111.00
1	A	466	TYR	C-N-CA	-5.08	109.01	121.70
1	A	81	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	A	317	MET	CG-SD-CE	5.07	108.31	100.20
1	D	235	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	344	ALA	N-CA-CB	5.06	117.18	110.10
1	A	311	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	483	ASN	OD1-CG-ND2	-5.05	110.29	121.90
1	A	508	ASN	CB-CG-OD1	5.03	131.66	121.60
1	D	505	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	A	262	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	A	472	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	492	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	D	531	THR	N-CA-CB	-5.00	100.79	110.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	LYS	Peptide
1	A	246	LYS	Peptide
1	A	311	TYR	Mainchain
1	A	331	SER	Mainchain
1	A	334	ILE	Mainchain
1	A	359	ALA	Mainchain
1	A	487	SER	Mainchain,Peptide
1	A	5	MET	Mainchain
1	A	68	CYS	Mainchain
1	D	246	LYS	Peptide
1	D	486	GLN	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	4234	0	4153	138	0
1	D	4234	0	4154	157	0
2	A	172	0	120	42	0
2	D	172	0	120	33	0
3	A	53	0	30	1	0
3	D	53	0	31	0	0
4	A	358	0	0	17	1
4	D	149	0	0	11	1
All	All	9425	0	8608	307	1

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 18.

All (307) 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:65:CYS:SG	2:A:602:HEM:CAB	2.34	1.15
1:A:36:CYS:SG	2:A:603:HEM:CAB	2.35	1.13
1:A:82:CYS:SG	2:A:601:HEM:CAC	2.39	1.11
1:A:79:CYS:SG	2:A:601:HEM:CAB	2.39	1.10
1:A:68:CYS:SG	2:A:602:HEM:CAC	2.41	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:CYS:SG	2:A:604:HEM:CAC	2.44	1.06
1:A:508:ASN:ND2	1:A:510:THR:H	1.59	0.98
1:A:308:THR:HG21	1:A:340:GLY:HA3	1.45	0.98
1:A:15:CYS:SG	2:A:604:HEM:CAB	2.53	0.97
1:A:36:CYS:SG	2:A:603:HEM:HAB	2.01	0.95
1:A:564:LEU:O	1:A:565:ASP:HB3	1.65	0.95
1:A:378:VAL:HB	4:A:2247:HOH:O	1.67	0.95
1:A:79:CYS:HG	2:A:601:HEM:CAB	1.80	0.94
1:A:39:CYS:SG	2:A:603:HEM:CAC	2.56	0.92
1:D:79:CYS:SG	2:D:601:HEM:CAB	2.58	0.91
1:D:82:CYS:SG	2:D:601:HEM:CAC	2.58	0.91
1:D:80:ASN:HD21	1:D:85:PHE:H	1.19	0.90
1:A:507:ILE:HD11	1:A:526:ALA:HB3	1.51	0.90
1:D:365:LYS:HD3	1:D:493:LYS:HD3	1.57	0.87
1:A:2:THR:N	1:A:3:PRO:HD3	1.89	0.86
1:A:65:CYS:SG	2:A:602:HEM:HAB	2.15	0.86
1:D:21:LYS:HB3	1:D:22:PRO:HD3	1.58	0.85
1:A:236:VAL:HG12	1:A:237:ASP:H	1.41	0.83
1:A:371:ILE:HD13	1:A:494:VAL:HG12	1.61	0.83
1:A:68:CYS:HG	2:A:602:HEM:CAC	1.91	0.81
1:A:418:ASN:ND2	1:A:422:LYS:HG3	1.97	0.80
1:A:65:CYS:HG	2:A:602:HEM:CAB	1.92	0.79
1:A:15:CYS:HG	2:A:604:HEM:CAB	1.95	0.79
1:A:308:THR:HG23	4:A:2217:HOH:O	1.82	0.78
1:A:15:CYS:SG	2:A:604:HEM:HAB	2.22	0.78
1:D:472:ASP:HB2	1:D:480:MET:HE3	1.66	0.78
1:D:308:THR:HG21	1:D:340:GLY:HA3	1.64	0.78
1:A:82:CYS:HG	2:A:601:HEM:CAC	1.93	0.78
1:A:199:ASN:H	1:A:199:ASN:HD22	1.32	0.77
1:D:65:CYS:SG	2:D:602:HEM:CAB	2.72	0.77
1:A:508:ASN:HD21	1:A:510:THR:H	1.30	0.77
1:D:48:ASN:O	1:D:49:ASP:HB3	1.84	0.77
1:A:180:VAL:HG13	1:A:236:VAL:HG11	1.65	0.77
1:A:564:LEU:O	1:A:565:ASP:CB	2.30	0.76
1:D:82:CYS:HG	2:D:601:HEM:CAC	1.98	0.76
1:A:483:ASN:ND2	1:A:485:THR:OG1	2.18	0.75
1:A:483:ASN:HD22	1:A:485:THR:HG23	1.51	0.74
1:D:437:TYR:HB2	1:D:491:ALA:HB3	1.70	0.74
1:D:80:ASN:ND2	1:D:85:PHE:H	1.86	0.73
1:A:22:PRO:HD2	4:A:2014:HOH:O	1.88	0.73
1:A:308:THR:HG21	1:A:340:GLY:CA	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:OE1	1:D:477:ARG:HD2	1.89	0.73
1:A:18:CYS:SG	2:A:604:HEM:HAC	2.30	0.72
1:A:68:CYS:SG	2:A:602:HEM:HAC	2.28	0.72
1:D:36:CYS:SG	2:D:603:HEM:CAB	2.78	0.71
1:D:507:ILE:HD11	1:D:526:ALA:HB3	1.70	0.71
1:D:68:CYS:SG	2:D:602:HEM:CAC	2.77	0.71
1:D:79:CYS:SG	2:D:601:HEM:HAB	2.30	0.71
1:D:118:PRO:HA	1:D:298:MET:HG2	1.71	0.71
1:D:18:CYS:SG	2:D:604:HEM:CAC	2.78	0.71
1:A:82:CYS:SG	2:A:601:HEM:HAC	2.30	0.70
1:D:80:ASN:HD21	1:D:85:PHE:N	1.88	0.70
1:D:430:TYR:HA	1:D:435:MET:HE3	1.74	0.69
1:A:79:CYS:SG	2:A:601:HEM:CBB	2.79	0.69
1:A:483:ASN:HD22	1:A:485:THR:CG2	2.07	0.67
2:D:602:HEM:HAA2	2:D:603:HEM:HBA1	1.77	0.67
1:D:21:LYS:HB3	1:D:22:PRO:CD	2.24	0.67
1:A:236:VAL:HG12	1:A:237:ASP:N	2.10	0.67
1:A:267:THR:HG21	4:A:2119:HOH:O	1.93	0.67
1:A:507:ILE:HD13	1:A:531:THR:OG1	1.95	0.67
1:A:2:THR:N	1:A:3:PRO:CD	2.57	0.66
1:D:4:ASP:OD1	1:D:72:HIS:HA	1.94	0.66
1:D:376:ARG:HD3	1:D:382:MET:HE2	1.77	0.66
1:D:122:THR:HG21	1:D:148:ILE:HG13	1.78	0.65
1:A:180:VAL:HG13	1:A:236:VAL:CG1	2.27	0.65
1:D:122:THR:CG2	1:D:148:ILE:HG13	2.27	0.65
1:D:371:ILE:HD13	1:D:494:VAL:HG12	1.78	0.65
1:A:122:THR:HG23	4:A:2010:HOH:O	1.97	0.65
1:D:407:GLN:HB3	1:D:408:PRO:HD2	1.78	0.64
1:D:531:THR:HG21	4:D:2144:HOH:O	1.95	0.64
1:D:199:ASN:HD22	1:D:199:ASN:H	1.43	0.64
1:D:360:HIS:CD2	1:D:362:THR:H	2.15	0.64
2:D:603:HEM:HBB2	2:D:603:HEM:HMB1	1.79	0.63
1:D:114:ILE:HD11	1:D:275:LYS:HD3	1.81	0.62
1:D:18:CYS:HA	1:D:35:GLN:HG3	1.81	0.62
1:D:229:LYS:HG2	1:D:230:ARG:H	1.65	0.62
1:A:82:CYS:SG	2:A:601:HEM:C3C	2.93	0.61
1:D:231:SER:OG	1:D:239:THR:HG21	1.99	0.61
1:D:2:THR:N	1:D:3:PRO:CD	2.63	0.61
1:A:418:ASN:HD21	1:A:422:LYS:HG3	1.65	0.61
1:A:308:THR:CG2	1:A:340:GLY:HA3	2.24	0.60
1:A:383:VAL:HG13	1:A:387:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:OE2	1:A:293:HIS:HE1	1.85	0.59
1:D:462:ASP:HB3	1:D:466:TYR:CZ	2.38	0.58
1:D:4:ASP:HB3	1:D:7:SER:H	1.68	0.58
1:A:518:SER:HB2	4:A:2225:HOH:O	2.01	0.58
1:A:80:ASN:HD21	1:A:85:PHE:H	1.50	0.58
1:A:371:ILE:HD13	1:A:494:VAL:CG1	2.33	0.57
2:D:601:HEM:HBB1	2:D:602:HEM:CBC	2.34	0.57
1:A:169:ALA:O	1:A:238:ARG:HG2	2.04	0.57
1:A:293:HIS:HD2	2:A:604:HEM:O2A	1.88	0.57
1:A:405:LEU:HA	1:A:410:GLN:HG3	1.86	0.57
1:A:443:GLU:HG3	1:A:453:VAL:HG13	1.85	0.57
1:A:361:PRO:HG3	1:A:397:ARG:HB3	1.86	0.57
1:D:246:LYS:HD3	1:D:251:GLU:HA	1.87	0.57
1:D:229:LYS:NZ	1:D:241:ARG:NH1	2.52	0.56
1:A:441:THR:HG23	1:A:444:GLN:NE2	2.20	0.56
1:D:418:ASN:ND2	1:D:422:LYS:HG3	2.20	0.56
1:D:74:GLU:OE1	1:D:97:LYS:HB3	2.06	0.56
1:A:51:LEU:HD23	1:A:54:ASP:HA	1.88	0.56
1:A:367:SER:HB2	4:A:2084:HOH:O	2.05	0.56
1:D:15:CYS:SG	2:D:604:HEM:CAB	2.94	0.56
1:D:467:VAL:HG23	4:D:2113:HOH:O	2.05	0.56
1:D:390:PHE:O	1:D:391:ILE:HB	2.06	0.56
1:D:60:LEU:HD21	2:D:601:HEM:HMC3	1.88	0.56
1:A:218:LEU:HD11	1:A:549:VAL:HG21	1.87	0.56
1:A:531:THR:HG21	4:A:2344:HOH:O	2.05	0.56
1:D:464:ASN:OD1	1:D:483:ASN:HB2	2.05	0.56
1:A:165:GLY:HA2	1:A:241:ARG:HH21	1.71	0.56
1:D:389:ARG:NH1	1:D:463:TYR:HD2	2.04	0.55
1:A:418:ASN:CG	4:A:2269:HOH:O	2.44	0.55
1:A:477:ARG:HD3	1:A:480:MET:HG2	1.89	0.55
2:A:602:HEM:HAA2	2:A:603:HEM:HBA2	1.88	0.55
1:D:18:CYS:SG	2:D:604:HEM:HAC	2.46	0.55
1:D:314:ASN:ND2	1:D:317:MET:H	2.04	0.55
1:A:483:ASN:CG	4:A:2314:HOH:O	2.44	0.55
1:A:508:ASN:HD21	1:A:510:THR:N	2.02	0.55
1:A:141:LYS:HE3	1:A:265:ILE:HG12	1.89	0.54
1:A:65:CYS:SG	2:A:602:HEM:C3B	3.00	0.54
1:A:508:ASN:ND2	1:A:510:THR:N	2.43	0.54
1:A:53:PHE:HE2	1:A:434:GLU:OE2	1.90	0.54
1:D:284:VAL:HG21	1:D:524:LEU:HG	1.90	0.54
1:A:440:ASP:HB2	1:A:444:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:LEU:HD12	1:D:456:LEU:O	2.08	0.54
1:A:65:CYS:SG	2:A:602:HEM:CBB	2.95	0.53
1:D:463:TYR:O	1:D:467:VAL:HG12	2.08	0.53
1:D:443:GLU:HG3	1:D:453:VAL:CG1	2.39	0.53
1:D:495:ALA:HB1	1:D:496:PRO:HD2	1.91	0.53
1:D:169:ALA:O	1:D:238:ARG:HB2	2.08	0.53
1:A:9:HIS:HB2	2:A:604:HEM:HMC3	1.91	0.53
1:D:365:LYS:HD3	1:D:493:LYS:CD	2.34	0.52
1:D:165:GLY:HA2	1:D:241:ARG:NE	2.25	0.52
1:A:332:ASN:N	1:A:332:ASN:HD22	2.06	0.52
1:D:487:SER:O	1:D:488:PRO:C	2.48	0.52
1:D:6:GLY:O	2:D:604:HEM:HMC3	2.10	0.51
1:D:443:GLU:HG3	1:D:453:VAL:HG11	1.91	0.51
1:D:464:ASN:HA	1:D:467:VAL:CG1	2.39	0.51
1:D:66:THR:HA	1:D:69:HIS:O	2.10	0.51
1:D:507:ILE:HD13	1:D:531:THR:OG1	2.11	0.51
1:D:229:LYS:HZ3	1:D:241:ARG:NH1	2.06	0.51
1:A:367:SER:HB3	1:A:435:MET:HG2	1.91	0.51
1:D:415:ILE:HD11	1:D:451:MET:CE	2.40	0.51
1:A:395:THR:HG22	1:A:399:LYS:HD2	1.93	0.51
2:D:602:HEM:HBB2	2:D:602:HEM:HMB1	1.91	0.51
1:A:128:GLY:O	1:A:133:GLY:HA3	2.11	0.51
1:A:210:GLN:HE22	1:A:554:ILE:HD11	1.74	0.51
1:D:36:CYS:SG	2:D:603:HEM:HAB	2.50	0.51
1:D:166:GLY:HA3	1:D:240:HIS:O	2.11	0.51
1:D:51:LEU:HD23	1:D:55:PRO:HD2	1.93	0.51
1:A:79:CYS:SG	2:A:601:HEM:HAB	2.45	0.51
1:A:68:CYS:SG	2:A:602:HEM:C3C	3.03	0.50
1:D:70:LYS:HB2	1:D:73:GLU:O	2.12	0.50
2:A:601:HEM:HBB1	2:A:602:HEM:CBC	2.41	0.50
1:A:483:ASN:N	1:A:483:ASN:OD1	2.35	0.50
1:D:227:ASP:HB3	1:D:241:ARG:HB2	1.93	0.50
1:D:325:MET:HE1	1:D:357:VAL:CG1	2.41	0.50
1:D:33:ASN:HA	1:D:36:CYS:SG	2.52	0.50
1:D:361:PRO:HG3	1:D:397:ARG:HA	1.93	0.50
1:D:165:GLY:HA2	1:D:241:ARG:HE	1.77	0.50
1:A:18:CYS:HG	2:A:604:HEM:CAC	2.22	0.50
1:A:66:THR:HA	1:A:69:HIS:O	2.12	0.50
1:D:483:ASN:ND2	1:D:485:THR:HG23	2.28	0.49
1:A:200:ASP:OD1	1:A:202:LYS:HE2	2.12	0.49
1:A:314:ASN:ND2	1:A:317:MET:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ILE:CD1	1:D:494:VAL:HG12	2.42	0.49
1:D:229:LYS:HZ3	1:D:241:ARG:HH12	1.60	0.49
1:D:106:ASP:O	1:D:110:ILE:HG13	2.12	0.49
1:A:185:GLU:CD	1:A:185:GLU:H	2.16	0.49
1:D:545:ILE:HG13	4:D:2050:HOH:O	2.11	0.49
1:A:36:CYS:SG	2:A:603:HEM:CBB	2.98	0.49
1:D:21:LYS:CB	1:D:22:PRO:HD3	2.38	0.49
1:D:170:VAL:HG12	1:D:182:ASP:CG	2.32	0.49
1:D:405:LEU:HG	1:D:496:PRO:HG3	1.93	0.49
1:D:433:LEU:HD21	2:D:601:HEM:C2A	2.47	0.49
1:A:273:VAL:HG12	1:A:343:MET:SD	2.53	0.49
1:A:46:LEU:HD11	2:A:602:HEM:CMB	2.43	0.48
1:A:418:ASN:ND2	1:A:422:LYS:HE2	2.28	0.48
1:A:183:LYS:HB3	1:A:185:GLU:OE2	2.13	0.48
1:A:79:CYS:SG	2:A:601:HEM:C3B	2.97	0.48
1:A:51:LEU:CD2	1:A:54:ASP:HA	2.43	0.48
1:A:18:CYS:HG	2:A:604:HEM:HAC	1.76	0.48
1:D:476:GLY:O	1:D:477:ARG:C	2.51	0.48
1:D:369:ILE:CD1	1:D:433:LEU:HD13	2.43	0.48
1:A:314:ASN:C	1:A:314:ASN:HD22	2.16	0.48
1:D:6:GLY:HA2	2:D:604:HEM:C2C	2.49	0.48
2:D:601:HEM:HBB1	2:D:602:HEM:HBC1	1.95	0.48
1:D:65:CYS:SG	2:D:602:HEM:HAB	2.54	0.48
1:D:415:ILE:HD11	1:D:451:MET:HE1	1.95	0.48
1:D:72:HIS:N	2:D:604:HEM:O2D	2.47	0.47
1:A:80:ASN:HD21	1:A:85:PHE:N	2.12	0.47
1:A:82:CYS:SG	2:A:601:HEM:CBC	2.99	0.47
1:D:21:LYS:CB	1:D:22:PRO:CD	2.92	0.47
1:D:382:MET:O	1:D:389:ARG:HG2	2.14	0.47
1:D:564:LEU:O	1:D:565:ASP:OD1	2.32	0.47
1:A:199:ASN:H	1:A:199:ASN:ND2	2.06	0.47
1:D:68:CYS:HB3	1:D:76:LYS:O	2.14	0.47
2:D:602:HEM:HBC2	2:D:602:HEM:HMC2	1.97	0.47
1:D:243:HIS:HB3	4:D:2048:HOH:O	2.15	0.47
1:A:39:CYS:SG	2:A:603:HEM:CBC	3.03	0.47
1:A:39:CYS:SG	2:A:603:HEM:C3C	3.08	0.47
1:A:18:CYS:SG	2:A:604:HEM:C3C	3.06	0.47
1:A:152:LYS:HE2	3:A:605:FAD:C8A	2.44	0.47
1:A:565:ASP:HA	4:A:2347:HOH:O	2.14	0.47
1:A:507:ILE:CD1	1:A:526:ALA:HB3	2.34	0.47
1:D:71:GLY:HA3	2:D:604:HEM:C2D	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG21	1:A:524:LEU:HG	1.95	0.47
1:D:39:CYS:SG	2:D:603:HEM:CAC	3.03	0.46
1:D:41:GLY:HA3	1:D:45:GLU:HG2	1.97	0.46
1:D:195:GLY:HA3	1:D:199:ASN:HD21	1.81	0.46
1:D:472:ASP:HB2	1:D:480:MET:CE	2.43	0.46
1:D:417:ASP:HB3	1:D:484:MET:HG2	1.97	0.46
1:D:82:CYS:SG	2:D:601:HEM:C3C	3.08	0.46
1:D:198:GLN:HG3	1:D:537:TYR:CE2	2.50	0.46
2:A:603:HEM:HBC2	2:A:603:HEM:HMC1	1.98	0.46
1:D:360:HIS:O	1:D:496:PRO:HA	2.16	0.46
1:A:535:HIS:HD2	4:A:2340:HOH:O	1.99	0.46
1:D:418:ASN:HD22	1:D:422:LYS:HG3	1.80	0.45
1:A:236:VAL:CG1	1:A:237:ASP:H	2.21	0.45
1:D:275:LYS:NZ	4:D:2056:HOH:O	2.50	0.45
1:D:314:ASN:C	1:D:314:ASN:HD22	2.19	0.45
1:D:325:MET:HE1	1:D:357:VAL:HG11	1.97	0.45
1:A:164:ALA:HB2	4:A:2128:HOH:O	2.16	0.45
1:D:329:THR:HG22	1:D:330:SER:H	1.81	0.45
1:A:194:GLY:O	1:A:538:ASN:HB3	2.16	0.45
1:D:16:GLN:NE2	1:D:21:LYS:O	2.50	0.45
1:D:391:ILE:HD11	1:D:395:THR:HG21	1.98	0.45
1:D:199:ASN:HD22	1:D:199:ASN:N	2.13	0.45
1:D:5:MET:HG3	1:D:92:PHE:CE2	2.52	0.45
1:A:68:CYS:SG	2:A:602:HEM:CBC	3.02	0.45
1:A:53:PHE:CE2	1:A:434:GLU:OE2	2.68	0.45
1:D:164:ALA:HB2	4:D:2035:HOH:O	2.16	0.45
1:A:395:THR:HG23	4:A:2112:HOH:O	2.17	0.44
1:D:183:LYS:HE3	1:D:186:TRP:CZ2	2.51	0.44
1:D:224:ASN:ND2	1:D:226:ASP:OD2	2.50	0.44
1:D:308:THR:HG23	4:D:2063:HOH:O	2.16	0.44
1:D:449:THR:OG1	1:D:451:MET:HG3	2.17	0.44
1:D:396:THR:O	1:D:397:ARG:C	2.56	0.44
1:D:75:PRO:CD	1:D:93:SER:HA	2.47	0.44
1:A:267:THR:HG22	1:A:267:THR:H	1.47	0.44
1:D:528:GLY:O	1:D:531:THR:HB	2.18	0.44
1:D:128:GLY:O	1:D:133:GLY:HA3	2.17	0.44
1:D:71:GLY:HA3	2:D:604:HEM:C1D	2.52	0.44
2:D:602:HEM:CMC	2:D:602:HEM:HBC2	2.48	0.43
1:A:483:ASN:CB	4:A:2314:HOH:O	2.66	0.43
1:A:514:LEU:HB3	1:A:518:SER:HA	2.00	0.43
2:D:602:HEM:HAA2	2:D:603:HEM:CBA	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ALA:O	1:D:461:SER:OG	2.36	0.43
1:D:194:GLY:O	1:D:538:ASN:HB3	2.18	0.43
1:D:391:ILE:HG23	1:D:392:SER:O	2.19	0.43
1:A:6:GLY:HA2	2:A:604:HEM:C2C	2.54	0.43
1:D:246:LYS:HD3	1:D:251:GLU:CA	2.48	0.43
1:A:508:ASN:CG	1:A:510:THR:H	2.18	0.43
1:A:18:CYS:SG	2:A:604:HEM:CBC	3.03	0.43
1:D:122:THR:HG23	1:D:148:ILE:HG13	1.99	0.42
1:D:229:LYS:HZ2	1:D:241:ARG:HH11	1.66	0.42
1:D:466:TYR:O	1:D:470:GLY:N	2.51	0.42
1:A:279:ASN:ND2	1:A:283:SER:HB2	2.33	0.42
1:A:51:LEU:HD23	1:A:54:ASP:H	1.84	0.42
1:D:452:LYS:NZ	1:D:455:ASP:OD2	2.52	0.42
1:A:48:ASN:OD1	1:A:49:ASP:N	2.41	0.42
1:A:360:HIS:O	1:A:496:PRO:HA	2.20	0.42
1:A:438:LYS:HE2	1:A:490:TYR:HE1	1.85	0.42
1:A:278:VAL:HA	1:A:283:SER:O	2.20	0.42
1:D:389:ARG:NH1	4:D:2102:HOH:O	2.53	0.42
1:A:366:ASP:OD1	1:A:366:ASP:N	2.42	0.42
1:A:418:ASN:HD21	1:A:422:LYS:CG	2.32	0.42
1:A:289:VAL:O	1:A:296:TYR:HA	2.20	0.42
1:D:68:CYS:SG	2:D:602:HEM:CBC	3.07	0.42
1:A:409:GLY:O	1:A:410:GLN:CB	2.66	0.42
1:A:418:ASN:CB	4:A:2269:HOH:O	2.66	0.42
1:D:75:PRO:HD3	1:D:93:SER:HA	2.02	0.42
1:D:90:MET:HB3	1:D:91:PRO:HD2	2.01	0.42
1:D:430:TYR:CD1	1:D:435:MET:HE1	2.55	0.41
1:A:441:THR:H	1:A:444:GLN:HE21	1.66	0.41
1:D:487:SER:HB3	1:D:488:PRO:HD3	2.01	0.41
1:D:90:MET:HG3	4:D:2019:HOH:O	2.18	0.41
1:D:308:THR:HG21	1:D:340:GLY:CA	2.43	0.41
1:D:265:ILE:HA	4:D:2054:HOH:O	2.20	0.41
1:D:159:ASN:HD21	1:D:332:ASN:ND2	2.18	0.41
1:D:82:CYS:SG	2:D:601:HEM:CBC	3.07	0.41
1:A:438:LYS:HE2	1:A:490:TYR:CE1	2.55	0.41
1:D:442:VAL:HG23	1:D:489:TYR:CE2	2.55	0.41
1:D:227:ASP:O	1:D:240:HIS:HA	2.19	0.41
1:D:46:LEU:HD11	2:D:602:HEM:CMB	2.50	0.41
1:A:141:LYS:HE3	1:A:265:ILE:CG1	2.49	0.41
1:D:464:ASN:HA	1:D:467:VAL:HG13	2.03	0.41
1:D:70:LYS:HG3	1:D:73:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TRP:CZ3	1:A:493:LYS:HB2	2.56	0.41
1:D:386:ASP:HB3	1:D:452:LYS:HE3	2.01	0.41
1:D:210:GLN:NE2	1:D:550:VAL:HG13	2.36	0.41
1:A:187:PHE:CD2	1:A:238:ARG:HD3	2.56	0.41
1:D:535:HIS:HB3	1:D:539:ARG:HA	2.03	0.41
1:D:281:ASP:O	1:D:282:HIS:HB2	2.21	0.40
1:D:562:HIS:HE1	4:D:2129:HOH:O	2.03	0.40
1:D:433:LEU:CD1	1:D:435:MET:HE2	2.52	0.40
1:D:407:GLN:HB3	1:D:408:PRO:CD	2.48	0.40
1:A:397:ARG:HH11	1:A:397:ARG:HD3	1.51	0.40
1:D:500:HIS:CG	1:D:539:ARG:HD3	2.56	0.40
1:A:517:GLN:HG2	4:A:2329:HOH:O	2.21	0.40
2:D:604:HEM:HHA	2:D:604:HEM:HAA1	1.97	0.40
1:D:460:VAL:HG12	1:D:464:ASN:ND2	2.36	0.40
1:D:505:VAL:HG13	1:D:513:VAL:HG13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2135:HOH:O	4:D:2105:HOH:O[3_655]	2.19	0.01

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	562/566 (99%)	523 (93%)	33 (6%)	6 (1%)	17 10
1	D	562/566 (99%)	511 (91%)	42 (8%)	9 (2%)	12 5
All	All	1124/1132 (99%)	1034 (92%)	75 (7%)	15 (1%)	15 8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	PRO
1	D	3	PRO
1	D	391	ILE
1	D	487	SER
1	A	49	ASP
1	A	243	HIS
1	D	49	ASP
1	A	329	THR
1	D	54	ASP
1	D	13	GLY
1	D	244	GLY
1	A	54	ASP
1	A	166	GLY
1	D	21	LYS
1	D	232	GLY

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	446/448 (100%)	420 (94%)	26 (6%)	25 19
1	D	446/448 (100%)	404 (91%)	42 (9%)	11 5
All	All	892/896 (100%)	824 (92%)	68 (8%)	16 10

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ILE
1	A	105	TRP
1	A	122	THR
1	A	125	LEU
1	A	199	ASN
1	A	202	LYS
1	A	280	ASP
1	A	314	ASN
1	A	329	THR

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Mol	Chain	Res	Type
1	A	332	ASN
1	A	365	LYS
1	A	366	ASP
1	A	383	VAL
1	A	395	THR
1	A	398	ASP
1	A	410	GLN
1	A	415	ILE
1	A	418	ASN
1	A	445	LEU
1	A	487	SER
1	A	492	VAL
1	A	505	VAL
1	A	507	ILE
1	A	518	SER
1	A	524	LEU
1	A	531	THR
1	D	2	THR
1	D	3	PRO
1	D	36	CYS
1	D	49	ASP
1	D	98	LYS
1	D	105	TRP
1	D	108	ASP
1	D	121	THR
1	D	122	THR
1	D	125	LEU
1	D	170	VAL
1	D	176	THR
1	D	199	ASN
1	D	220	SER
1	D	236	VAL
1	D	237	ASP
1	D	238	ARG
1	D	239	THR
1	D	246	LYS
1	D	262	GLU
1	D	267	THR
1	D	280	ASP
1	D	298	MET
1	D	308	THR
1	D	314	ASN

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Mol	Chain	Res	Type
1	D	329	THR
1	D	346	GLU
1	D	383	VAL
1	D	385	LYS
1	D	395	THR
1	D	398	ASP
1	D	415	ILE
1	D	418	ASN
1	D	444	GLN
1	D	445	LEU
1	D	461	SER
1	D	467	VAL
1	D	479	ASP
1	D	492	VAL
1	D	507	ILE
1	D	524	LEU
1	D	531	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	199	ASN
1	A	210	GLN
1	A	293	HIS
1	A	314	ASN
1	A	418	ASN
1	A	419	GLN
1	A	444	GLN
1	A	483	ASN
1	A	508	ASN
1	D	80	ASN
1	D	197	GLN
1	D	199	ASN
1	D	210	GLN
1	D	282	HIS
1	D	314	ASN
1	D	332	ASN
1	D	360	HIS
1	D	388	ASN
1	D	444	GLN
1	D	517	GLN

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

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	601	1	30,50,50	2.76	8 (26%)	24,82,82	3.04	14 (58%)
2	HEM	A	602	1	30,50,50	2.84	9 (30%)	24,82,82	3.06	12 (50%)
2	HEM	A	603	1	30,50,50	2.55	9 (30%)	24,82,82	2.92	13 (54%)
2	HEM	A	604	1	30,50,50	2.54	10 (33%)	24,82,82	3.55	12 (50%)
3	FAD	A	605	-	48,58,58	2.06	12 (25%)	54,89,89	1.95	16 (29%)
2	HEM	D	601	1	30,50,50	2.46	9 (30%)	24,82,82	2.61	11 (45%)
2	HEM	D	602	1	30,50,50	2.51	7 (23%)	24,82,82	2.74	11 (45%)
2	HEM	D	603	1	30,50,50	2.69	8 (26%)	24,82,82	3.10	14 (58%)
2	HEM	D	604	1	30,50,50	2.55	8 (26%)	24,82,82	4.49	14 (58%)
3	FAD	D	605	-	48,58,58	1.78	11 (22%)	54,89,89	2.28	15 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1	-	0/10/54/54	0/0/8/8
2	HEM	A	602	1	-	0/10/54/54	0/0/8/8
2	HEM	A	603	1	-	0/10/54/54	0/0/8/8
2	HEM	A	604	1	-	0/10/54/54	0/0/8/8
3	FAD	A	605	-	-	0/30/50/50	0/6/6/6
2	HEM	D	601	1	-	0/10/54/54	0/0/8/8
2	HEM	D	602	1	-	0/10/54/54	0/0/8/8
2	HEM	D	603	1	-	0/10/54/54	0/0/8/8
2	HEM	D	604	1	-	0/10/54/54	0/0/8/8
3	FAD	D	605	-	-	0/30/50/50	0/6/6/6

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	HEM	C3B-C4B	-9.04	1.43	1.51
2	A	603	HEM	C2D-C3D	-8.56	1.28	1.54
2	D	603	HEM	C3B-C4B	-8.49	1.44	1.51
2	A	601	HEM	C3B-C4B	-8.43	1.44	1.51
2	A	604	HEM	C3B-C4B	-7.58	1.45	1.51
2	D	602	HEM	C3B-C4B	-7.42	1.45	1.51
2	A	604	HEM	C2D-C3D	-7.31	1.32	1.54
2	A	601	HEM	C2D-C3D	-7.27	1.32	1.54
2	D	604	HEM	C3B-C4B	-7.16	1.45	1.51
2	D	602	HEM	C2D-C3D	-7.14	1.33	1.54
2	A	602	HEM	C2D-C3D	-7.10	1.33	1.54
2	D	603	HEM	C2D-C3D	-7.04	1.33	1.54
2	D	601	HEM	C3B-C4B	-6.85	1.45	1.51
2	D	604	HEM	C2D-C3D	-6.83	1.34	1.54
2	D	601	HEM	C2D-C3D	-6.75	1.34	1.54
2	A	603	HEM	C3B-C4B	-6.37	1.46	1.51
2	D	604	HEM	C3D-C4D	-6.34	1.43	1.51
2	D	603	HEM	C3D-C4D	-6.02	1.43	1.51
2	A	602	HEM	C3D-C4D	-5.78	1.44	1.51
2	D	601	HEM	C3D-C4D	-5.75	1.44	1.51
2	D	602	HEM	C3D-C4D	-5.46	1.44	1.51
2	A	601	HEM	C3D-C4D	-4.88	1.45	1.51
3	D	605	FAD	C10-N10	-4.82	1.33	1.39
3	D	605	FAD	PA-O2A	-4.51	1.35	1.54
3	A	605	FAD	PA-O2A	-4.45	1.36	1.54
3	A	605	FAD	C10-N10	-3.90	1.34	1.39
2	D	604	HEM	C2C-C1C	-3.84	1.45	1.52
2	A	604	HEM	C2C-C1C	-3.82	1.45	1.52
2	D	603	HEM	C2C-C1C	-3.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	FAD	P-O2P	-3.54	1.39	1.54
2	D	602	HEM	C2C-C1C	-3.45	1.46	1.52
2	A	603	HEM	C2C-C1C	-3.36	1.46	1.52
2	A	601	HEM	C2C-C1C	-3.32	1.46	1.52
2	A	604	HEM	C3D-C4D	-3.32	1.47	1.51
2	A	602	HEM	C2B-C1B	-3.16	1.41	1.51
2	A	603	HEM	C3D-C4D	-3.12	1.47	1.51
2	A	602	HEM	C2C-C1C	-3.09	1.46	1.52
2	D	601	HEM	C2C-C1C	-2.89	1.47	1.52
3	A	605	FAD	O3B-C3B	-2.87	1.36	1.43
2	A	602	HEM	C2D-C1D	-2.77	1.42	1.51
2	A	603	HEM	C2B-C1B	-2.73	1.42	1.51
3	D	605	FAD	P-O2P	-2.58	1.43	1.54
2	A	602	HEM	C2A-C3A	-2.45	1.30	1.37
2	D	604	HEM	C2D-C1D	-2.41	1.44	1.51
2	D	601	HEM	C2B-C1B	-2.31	1.44	1.51
2	D	603	HEM	C2D-C1D	-2.28	1.44	1.51
2	A	604	HEM	C2D-C1D	-2.27	1.44	1.51
2	D	603	HEM	C2B-C1B	-2.25	1.44	1.51
2	D	601	HEM	C2D-C1D	-2.21	1.44	1.51
2	D	602	HEM	C2D-C1D	-2.10	1.45	1.51
2	A	604	HEM	FE-NB	2.01	2.08	1.97
2	D	604	HEM	C3C-CAC	2.01	1.55	1.51
2	D	604	HEM	CAD-C3D	2.06	1.58	1.54
2	D	604	HEM	C4C-NC	2.06	1.38	1.36
3	D	605	FAD	C4-C4X	2.07	1.45	1.41
2	A	602	HEM	CAD-C3D	2.14	1.58	1.54
2	A	604	HEM	CAA-C2A	2.15	1.55	1.52
2	D	603	HEM	C1C-NC	2.15	1.38	1.36
3	A	605	FAD	C2A-N1A	2.19	1.38	1.33
2	D	601	HEM	FE-NC	2.21	2.04	1.95
3	D	605	FAD	C2A-N1A	2.24	1.38	1.33
2	A	603	HEM	CMA-C3A	2.24	1.56	1.51
2	A	603	HEM	CBC-CAC	2.24	1.42	1.29
2	A	601	HEM	C4C-NC	2.25	1.38	1.36
3	D	605	FAD	C3B-C4B	2.31	1.59	1.53
2	A	604	HEM	C4C-NC	2.38	1.38	1.36
2	D	601	HEM	CAA-C2A	2.40	1.56	1.52
2	D	602	HEM	CAA-C2A	2.41	1.56	1.52
2	D	603	HEM	C4C-NC	2.43	1.39	1.36
3	D	605	FAD	C4-N3	2.44	1.37	1.33
3	D	605	FAD	O5'-C5'	2.49	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	HEM	C4C-NC	2.49	1.39	1.36
2	A	603	HEM	C3C-CAC	2.58	1.56	1.51
2	A	602	HEM	CMA-C3A	2.61	1.57	1.51
3	A	605	FAD	C4-C4X	2.65	1.46	1.41
2	A	604	HEM	C1C-NC	2.72	1.39	1.36
2	A	601	HEM	CAA-C2A	2.78	1.56	1.52
3	A	605	FAD	O4B-C4B	2.81	1.51	1.45
3	D	605	FAD	C4X-C10	2.83	1.46	1.41
2	D	601	HEM	C3C-CAC	2.88	1.56	1.51
3	A	605	FAD	O5'-C5'	2.92	1.56	1.44
2	A	604	HEM	C3C-CAC	2.96	1.56	1.51
3	D	605	FAD	C9A-N10	2.97	1.42	1.38
3	A	605	FAD	C5B-C4B	3.04	1.61	1.51
2	A	603	HEM	C4C-NC	3.24	1.40	1.36
2	A	601	HEM	C3C-CAC	3.37	1.57	1.51
3	A	605	FAD	C4-N3	3.48	1.39	1.33
3	A	605	FAD	C5'-C4'	3.82	1.57	1.51
2	A	601	HEM	C3B-CAB	4.28	1.59	1.51
3	D	605	FAD	O4B-C1B	5.01	1.47	1.41
3	A	605	FAD	O4B-C1B	5.98	1.48	1.41

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	604	HEM	CBD-CAD-C3D	-9.02	87.30	113.55
3	D	605	FAD	N3A-C2A-N1A	-6.76	123.72	128.89
2	D	603	HEM	CBD-CAD-C3D	-6.33	95.14	113.55
2	A	602	HEM	CMA-C3A-C4A	-5.36	119.50	128.36
3	D	605	FAD	C4X-C10-N10	-5.34	117.37	120.52
3	D	605	FAD	C4-C4X-C10	-5.28	116.56	119.94
2	A	603	HEM	C3C-CAC-CBC	-4.98	116.81	124.46
2	A	602	HEM	CAA-C2A-C1A	-4.77	121.82	127.01
3	A	605	FAD	N3A-C2A-N1A	-4.66	125.33	128.89
2	A	603	HEM	C4B-CHC-C1C	-4.63	118.08	125.82
2	D	603	HEM	CAA-C2A-C1A	-4.58	122.03	127.01
2	D	604	HEM	CAA-C2A-C1A	-4.51	122.11	127.01
2	A	604	HEM	CMA-C3A-C4A	-4.37	121.13	128.36
3	A	605	FAD	O3'-C3'-C4'	-4.20	98.16	108.75
2	D	602	HEM	CMA-C3A-C4A	-4.09	121.59	128.36
2	D	604	HEM	CMA-C3A-C4A	-4.07	121.63	128.36
3	D	605	FAD	C4X-C4-N3	-4.03	118.08	123.59
3	A	605	FAD	C4X-C10-N10	-3.91	118.22	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CMA-C3A-C4A	-3.85	121.99	128.36
2	D	601	HEM	CAA-C2A-C1A	-3.70	122.99	127.01
2	D	602	HEM	CBD-CAD-C3D	-3.67	102.88	113.55
3	A	605	FAD	O2'-C2'-C1'	-3.58	101.14	109.94
3	D	605	FAD	O4B-C1B-N9A	-3.57	100.62	108.10
3	A	605	FAD	C4B-O4B-C1B	-3.32	106.08	109.72
2	A	602	HEM	C4B-CHC-C1C	-3.29	120.32	125.82
2	A	601	HEM	CAA-C2A-C1A	-3.23	123.50	127.01
2	A	604	HEM	C3C-CAC-CBC	-3.15	119.63	124.46
3	D	605	FAD	O5B-PA-O1A	-3.07	97.71	109.62
2	A	603	HEM	CBD-CAD-C3D	-3.02	104.77	113.55
2	A	603	HEM	CAA-C2A-C1A	-2.98	123.78	127.01
2	D	601	HEM	CMA-C3A-C4A	-2.97	123.45	128.36
3	D	605	FAD	O2'-C2'-C1'	-2.92	102.78	109.94
3	A	605	FAD	O4B-C1B-N9A	-2.84	102.16	108.10
2	A	603	HEM	C3B-C4B-NB	-2.72	106.42	111.63
2	D	603	HEM	CMA-C3A-C4A	-2.60	124.06	128.36
3	A	605	FAD	C4-C4X-C10	-2.43	118.39	119.94
2	A	601	HEM	C3B-CAB-CBB	-2.40	120.77	124.46
2	D	603	HEM	C3B-CAB-CBB	-2.37	120.82	124.46
2	A	604	HEM	CBD-CAD-C3D	-2.31	106.84	113.55
3	D	605	FAD	C6-C5X-N5	-2.28	116.02	118.96
2	A	602	HEM	CBD-CAD-C3D	-2.28	106.92	113.55
3	A	605	FAD	C1B-N9A-C4A	-2.25	123.54	126.94
2	D	603	HEM	C1D-CHD-C4C	-2.19	122.16	125.82
3	A	605	FAD	O4'-C4'-C3'	-2.18	103.53	109.02
3	A	605	FAD	O5B-PA-O1A	-2.16	101.25	109.62
2	A	601	HEM	C3B-C4B-NB	-2.12	107.58	111.63
2	A	603	HEM	CBA-CAA-C2A	-2.09	108.79	112.53
2	D	603	HEM	C3B-C4B-NB	-2.07	107.67	111.63
3	D	605	FAD	C4B-O4B-C1B	-2.01	107.51	109.72
2	A	604	HEM	CAD-C3D-C4D	2.09	119.83	112.47
3	D	605	FAD	C6-C5X-C9A	2.09	121.73	118.98
2	A	602	HEM	C3B-C4B-CHC	2.11	126.13	123.16
2	D	603	HEM	C2C-C1C-CHC	2.13	126.91	123.68
3	A	605	FAD	O2A-PA-O3P	2.13	114.74	105.09
2	A	601	HEM	C4B-CHC-C1C	2.15	129.41	125.82
2	D	604	HEM	CMA-C3A-C2A	2.17	129.77	125.24
3	A	605	FAD	O3P-PA-O5B	2.20	108.77	102.94
2	D	604	HEM	C3B-C4B-CHC	2.21	126.27	123.16
2	D	601	HEM	CAA-CBA-CGA	2.23	116.83	112.75
2	A	603	HEM	C1D-CHD-C4C	2.26	129.60	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	HEM	CAA-CBA-CGA	2.33	117.02	112.75
3	D	605	FAD	O2B-C2B-C3B	2.34	119.43	111.83
3	D	605	FAD	C2A-N1A-C6A	2.34	122.94	118.77
2	D	601	HEM	C3B-C4B-CHC	2.48	126.65	123.16
2	D	601	HEM	C3B-CAB-CBB	2.51	128.30	124.46
3	D	605	FAD	O3P-PA-O5B	2.52	109.63	102.94
2	D	602	HEM	CAD-C3D-C4D	2.53	121.41	112.47
2	D	602	HEM	CMA-C3A-C2A	2.59	130.65	125.24
2	D	604	HEM	CAD-C3D-C4D	2.60	121.66	112.47
3	D	605	FAD	P-O3P-PA	2.63	140.12	132.73
3	A	605	FAD	C2A-N1A-C6A	2.73	123.65	118.77
3	A	605	FAD	O3B-C3B-C2B	2.74	120.72	111.83
2	D	602	HEM	CAD-CBD-CGD	2.76	124.29	113.02
3	A	605	FAD	O3B-C3B-C4B	2.79	119.41	111.05
2	A	601	HEM	CAD-C3D-C4D	2.88	122.63	112.47
2	A	601	HEM	CMA-C3A-C2A	2.89	131.28	125.24
2	A	603	HEM	CAD-C3D-C4D	2.90	122.71	112.47
2	A	601	HEM	C2C-C1C-CHC	2.93	128.14	123.68
2	A	602	HEM	CMD-C2D-C3D	2.95	127.41	114.35
2	D	603	HEM	CAD-C3D-C4D	3.08	123.34	112.47
2	A	602	HEM	CMA-C3A-C2A	3.09	131.69	125.24
2	D	602	HEM	CMD-C2D-C3D	3.22	128.59	114.35
2	D	601	HEM	CAD-C3D-C4D	3.30	124.10	112.47
2	D	603	HEM	CMD-C2D-C3D	3.37	129.27	114.35
2	D	604	HEM	CAA-CBA-CGA	3.40	118.97	112.75
2	A	602	HEM	CAD-C3D-C4D	3.43	124.58	112.47
2	D	601	HEM	CMD-C2D-C3D	3.44	129.54	114.35
2	D	604	HEM	CMD-C2D-C3D	3.47	129.70	114.35
2	A	601	HEM	C3B-C4B-CHC	3.50	128.09	123.16
3	A	605	FAD	C4X-N5-C5X	3.59	120.89	116.76
2	A	604	HEM	CMD-C2D-C3D	3.61	130.31	114.35
2	A	601	HEM	CMD-C2D-C3D	3.66	130.55	114.35
2	D	603	HEM	C3B-C4B-CHC	3.75	128.44	123.16
2	A	603	HEM	CMD-C2D-C3D	3.86	131.44	114.35
2	A	603	HEM	C2D-C3D-C4D	3.88	108.08	101.50
2	D	604	HEM	CAD-C3D-C2D	4.02	124.78	113.22
2	D	601	HEM	C2D-C3D-C4D	4.04	108.34	101.50
2	A	603	HEM	CMB-C2B-C3B	4.05	126.63	116.53
2	A	604	HEM	C2D-C3D-C4D	4.26	108.72	101.50
2	D	603	HEM	CAD-C3D-C2D	4.32	125.64	113.22
2	D	601	HEM	CMB-C2B-C3B	4.38	127.47	116.53
2	A	602	HEM	CAD-C3D-C2D	4.40	125.86	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	HEM	CMB-C2B-C3B	4.51	127.79	116.53
2	A	602	HEM	C2D-C3D-C4D	4.53	109.19	101.50
2	A	604	HEM	CMB-C2B-C3B	4.56	127.91	116.53
2	D	602	HEM	C2D-C3D-C4D	4.63	109.35	101.50
2	A	601	HEM	C2D-C3D-C4D	4.65	109.39	101.50
2	D	604	HEM	CMC-C2C-C3C	4.69	128.25	116.53
2	D	604	HEM	CMB-C2B-C3B	4.86	128.67	116.53
2	A	604	HEM	CMC-C2C-C3C	4.94	128.86	116.53
2	D	601	HEM	CAD-C3D-C2D	4.99	127.55	113.22
2	A	604	HEM	C3B-CAB-CBB	5.03	132.17	124.46
2	A	601	HEM	CAD-C3D-C2D	5.13	127.97	113.22
2	D	603	HEM	CMB-C2B-C3B	5.13	129.34	116.53
2	D	603	HEM	C2D-C3D-C4D	5.14	110.21	101.50
2	D	603	HEM	CMC-C2C-C3C	5.20	129.51	116.53
2	A	603	HEM	CMC-C2C-C3C	5.21	129.53	116.53
2	A	602	HEM	CMB-C2B-C3B	5.27	129.69	116.53
2	D	602	HEM	CAD-C3D-C2D	5.48	128.97	113.22
2	A	603	HEM	CAD-C3D-C2D	5.55	129.19	113.22
2	D	601	HEM	CMC-C2C-C3C	5.64	130.60	116.53
2	D	602	HEM	CMC-C2C-C3C	5.71	130.79	116.53
2	A	601	HEM	CMC-C2C-C3C	5.78	130.95	116.53
2	D	604	HEM	C2D-C3D-C4D	5.84	111.40	101.50
2	A	601	HEM	CMB-C2B-C3B	6.06	131.66	116.53
2	A	604	HEM	CAD-C3D-C2D	6.33	131.41	113.22
2	A	602	HEM	CMC-C2C-C3C	6.74	133.34	116.53
2	A	604	HEM	CAA-CBA-CGA	7.05	125.66	112.75
3	D	605	FAD	C4-N3-C2	7.39	121.63	115.25
2	A	604	HEM	CBA-CAA-C2A	7.48	125.93	112.53
2	D	604	HEM	CAD-CBD-CGD	9.89	153.35	113.02
2	D	604	HEM	CBA-CAA-C2A	10.92	132.10	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	11	0
2	A	602	HEM	13	0
2	A	603	HEM	8	0
2	A	604	HEM	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	FAD	1	0
2	D	601	HEM	10	0
2	D	602	HEM	12	0
2	D	603	HEM	6	0
2	D	604	HEM	9	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.