



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:54 PM GMT

PDB ID : 1D4E  
Title : CRYSTAL STRUCTURE OF THE FLAVOCYTOCHROME C FUMARATE  
REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1 COM-  
PLEXED WITH FUMARATE  
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.  
Deposited on : 1999-10-03  
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

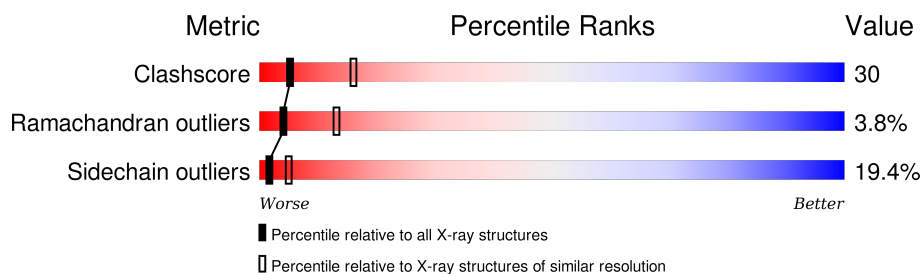
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	

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
3	FAD	A	600	X	-	-	-
4	FUM	A	700	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4254 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 FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			3965	2462	710	774	19			

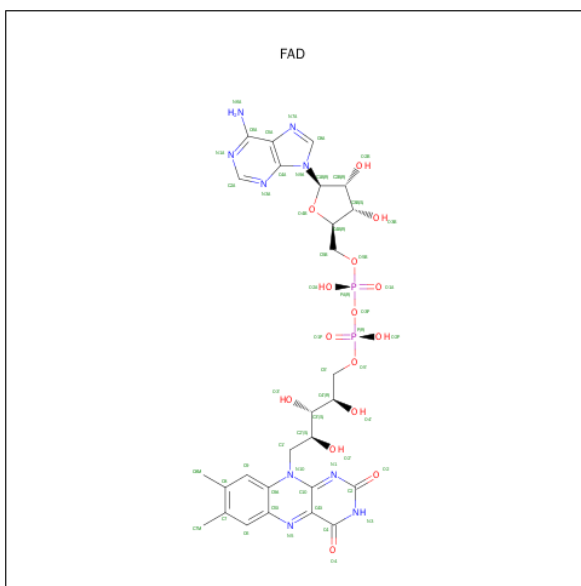
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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		

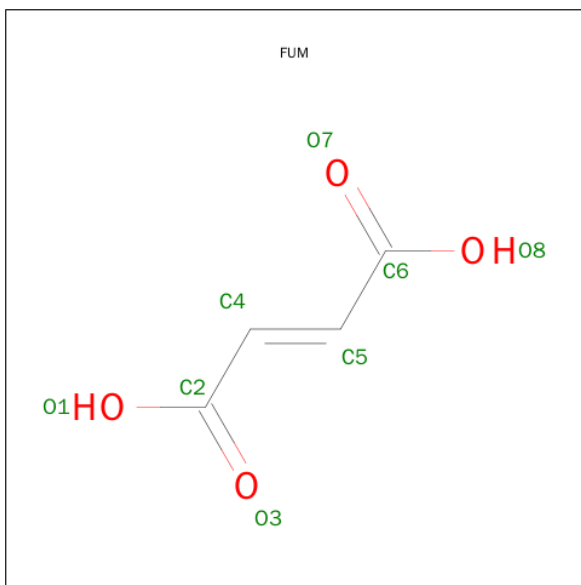
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

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



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

- Molecule 5 is water.

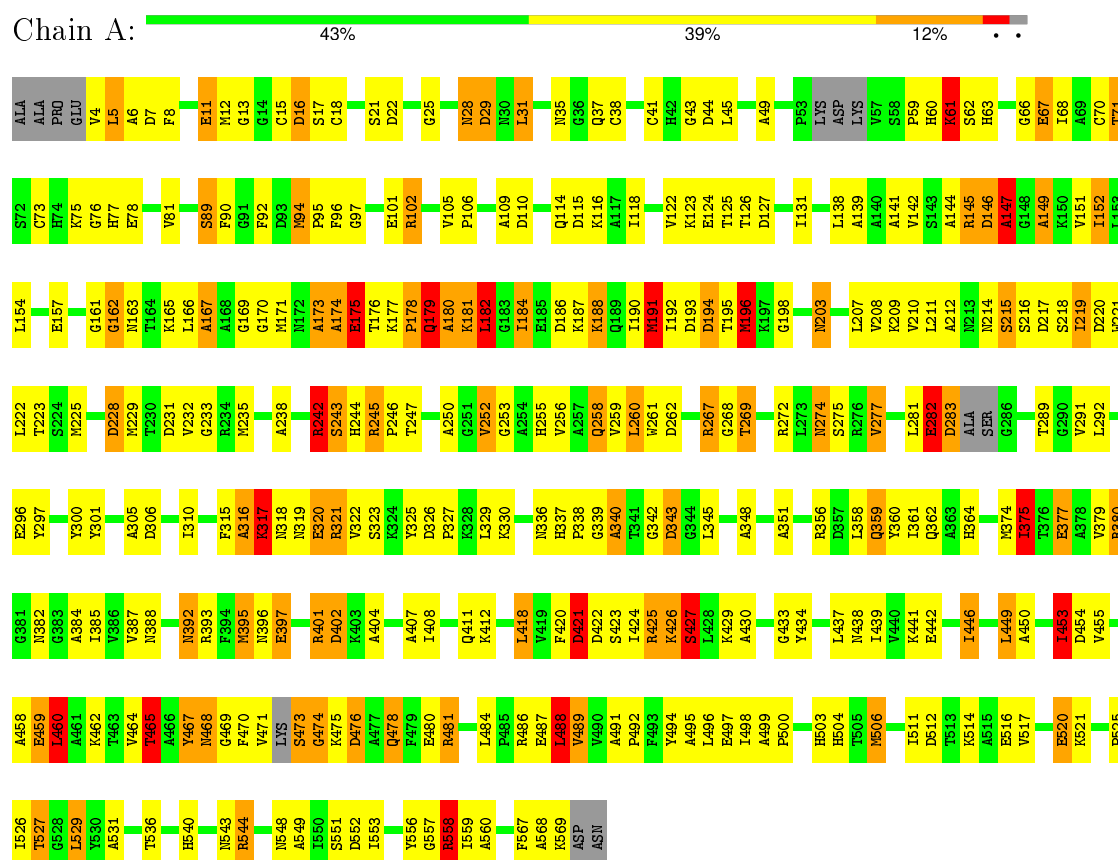
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		

### 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 FUMARATE REDUCTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.08Å 73.08Å 216.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.243 , 0.311	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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

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	0.66	0/4029	2.03	138/5478 (2.5%)

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	2

There are no bond length outliers.

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	356	ARG	NE-CZ-NH1	-15.26	112.67	120.30
1	A	267	ARG	NE-CZ-NH2	12.20	126.40	120.30
1	A	175	GLU	C-N-CA	11.91	151.47	121.70
1	A	272	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	A	558	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	A	558	ARG	CD-NE-CZ	11.32	139.45	123.60
1	A	321	ARG	NE-CZ-NH1	-11.21	114.69	120.30
1	A	321	ARG	NE-CZ-NH2	11.00	125.80	120.30
1	A	242	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	A	242	ARG	NE-CZ-NH1	-9.92	115.34	120.30
1	A	499	ALA	CB-CA-C	9.55	124.42	110.10
1	A	283	ASP	CA-C-O	9.24	139.50	120.10
1	A	262	ASP	CB-CG-OD1	9.23	126.60	118.30
1	A	191	MET	CA-CB-CG	9.12	128.80	113.30
1	A	356	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	147	ALA	CB-CA-C	8.38	122.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	401	ARG	CD-NE-CZ	8.31	135.23	123.60
1	A	174	ALA	CA-C-N	-8.27	99.02	117.20
1	A	44	ASP	CB-CG-OD2	8.22	125.70	118.30
1	A	173	ALA	N-CA-CB	8.11	121.45	110.10
1	A	267	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	A	360	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	A	422	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	481	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	343	ASP	CB-CG-OD1	7.67	125.21	118.30
1	A	16	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	320	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	A	375	ILE	N-CA-CB	7.38	127.78	110.80
1	A	122	VAL	N-CA-CB	7.29	127.54	111.50
1	A	377	GLU	OE1-CD-OE2	7.16	131.89	123.30
1	A	326	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	A	174	ALA	CA-C-O	7.06	134.92	120.10
1	A	316	ALA	CA-C-N	7.02	132.64	117.20
1	A	494	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	A	491	ALA	CA-C-O	-6.94	105.52	120.10
1	A	468	ASN	CA-CB-CG	-6.89	98.23	113.40
1	A	29	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	171	MET	CG-SD-CE	6.85	111.16	100.20
1	A	421	ASP	N-CA-CB	-6.77	98.42	110.60
1	A	325	TYR	CB-CG-CD2	6.64	124.99	121.00
1	A	61	LYS	CA-CB-CG	6.63	127.99	113.40
1	A	169	GLY	N-CA-C	6.63	129.68	113.10
1	A	326	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	281	LEU	C-N-CA	6.50	137.95	121.70
1	A	181	LYS	CA-C-N	6.50	131.50	117.20
1	A	67	GLU	OE1-CD-OE2	-6.50	115.51	123.30
1	A	418	LEU	N-CA-CB	6.48	123.35	110.40
1	A	228	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	427	SER	N-CA-CB	6.39	120.08	110.50
1	A	169	GLY	CA-C-N	6.34	128.88	116.20
1	A	325	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	13	GLY	N-CA-C	6.33	128.91	113.10
1	A	425	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	220	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	29	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	A	425	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	360	TYR	CB-CG-CD2	6.20	124.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	HIS	N-CA-CB	-6.20	99.45	110.60
1	A	325	TYR	CB-CA-C	-6.18	98.04	110.40
1	A	426	LYS	CA-C-O	-6.18	107.12	120.10
1	A	178	PRO	C-N-CA	6.17	137.13	121.70
1	A	167	ALA	N-CA-CB	6.16	118.73	110.10
1	A	182	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	144	ALA	CA-C-O	6.14	133.00	120.10
1	A	196	MET	CB-CA-C	6.11	122.63	110.40
1	A	506	MET	CB-CA-C	-6.08	98.24	110.40
1	A	426	LYS	CA-C-N	6.06	130.54	117.20
1	A	252	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	317	LYS	N-CA-CB	6.05	121.48	110.60
1	A	161	GLY	N-CA-C	6.02	128.15	113.10
1	A	544	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	A	146	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	402	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	11	GLU	CA-CB-CG	5.96	126.50	113.40
1	A	481	ARG	NH1-CZ-NH2	5.96	125.95	119.40
1	A	421	ASP	CB-CA-C	-5.95	98.49	110.40
1	A	544	ARG	CD-NE-CZ	5.95	131.94	123.60
1	A	551	SER	N-CA-CB	5.95	119.42	110.50
1	A	282	GLU	CB-CG-CD	5.93	130.20	114.20
1	A	474	GLY	N-CA-C	5.92	127.90	113.10
1	A	147	ALA	N-CA-C	-5.89	95.08	111.00
1	A	520	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	173	ALA	CA-C-N	-5.83	104.37	117.20
1	A	467	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	397	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	A	486	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	556	TYR	CA-CB-CG	-5.81	102.35	113.40
1	A	318	ASN	OD1-CG-ND2	5.81	135.26	121.90
1	A	465	THR	N-CA-CB	5.80	121.33	110.30
1	A	175	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	272	ARG	NH1-CZ-NH2	5.80	125.78	119.40
1	A	31	LEU	N-CA-CB	-5.72	98.96	110.40
1	A	492	PRO	N-CA-CB	5.69	110.13	103.30
1	A	16	ASP	N-CA-CB	-5.66	100.41	110.60
1	A	459	GLU	CG-CD-OE1	5.64	129.59	118.30
1	A	194	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	144	ALA	O-C-N	-5.61	113.73	122.70
1	A	245	ARG	CA-CB-CG	5.59	125.71	113.40
1	A	222	LEU	CB-CA-C	5.59	120.82	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	425	ARG	CG-CD-NE	5.55	123.47	111.80
1	A	267	ARG	CA-C-N	5.52	127.24	116.20
1	A	382	ASN	CA-C-N	5.50	127.19	116.20
1	A	453	ILE	N-CA-CB	-5.48	98.20	110.80
1	A	147	ALA	CA-C-N	-5.48	105.24	116.20
1	A	481	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	A	81	VAL	CB-CA-C	-5.39	101.16	111.40
1	A	247	THR	CA-CB-CG2	-5.37	104.88	112.40
1	A	486	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	228	ASP	CA-C-N	-5.36	105.41	117.20
1	A	395	MET	CA-CB-CG	5.35	122.39	113.30
1	A	45	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	425	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	179	GLN	CB-CG-CD	5.32	125.44	111.60
1	A	558	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	193	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	89	SER	CB-CA-C	5.29	120.16	110.10
1	A	149	ALA	CA-C-O	5.27	131.17	120.10
1	A	220	ASP	CA-CB-CG	5.27	125.00	113.40
1	A	281	LEU	CA-C-O	5.26	131.14	120.10
1	A	277	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	A	536	THR	N-CA-CB	5.20	120.18	110.30
1	A	77	HIS	CA-CB-CG	-5.20	104.76	113.60
1	A	468	ASN	N-CA-CB	-5.19	101.25	110.60
1	A	43	GLY	CA-C-O	5.18	129.93	120.60
1	A	551	SER	O-C-N	5.17	130.97	122.70
1	A	362	GLN	OE1-CD-NE2	-5.14	110.07	121.90
1	A	446	ILE	CB-CG1-CD1	-5.13	99.52	113.90
1	A	385	ILE	CA-C-O	-5.11	109.36	120.10
1	A	152	ILE	CB-CG1-CD1	5.11	128.20	113.90
1	A	527	THR	CA-C-O	5.11	130.82	120.10
1	A	258	GLN	CG-CD-OE1	-5.09	111.42	121.60
1	A	229	MET	N-CA-CB	-5.09	101.44	110.60
1	A	489	VAL	O-C-N	-5.06	114.60	122.70
1	A	476	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	323	SER	CB-CA-C	5.04	119.67	110.10
1	A	149	ALA	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	VAL	Mainchain
1	A	421	ASP	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3965	0	3738	233	0
2	A	172	0	120	25	0
3	A	53	0	31	11	0
4	A	8	0	2	7	0
5	A	56	0	0	5	0
All	All	4254	0	3891	243	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 30.

All (243) 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:15:CYS:SG	2:A:603:HEM:HAB	1.19	1.70
1:A:18:CYS:SG	2:A:603:HEM:HAC	1.15	1.68
3:A:600:FAD:C2'	3:A:600:FAD:C1'	1.80	1.53
1:A:73:CYS:SG	2:A:602:HEM:HAC	1.54	1.44
1:A:41:CYS:SG	2:A:604:HEM:CAC	2.14	1.35
1:A:41:CYS:SG	2:A:604:HEM:HAC	1.73	1.26
1:A:412:LYS:HD2	1:A:412:LYS:H	1.29	0.96
1:A:73:CYS:HG	2:A:602:HEM:CAC	1.60	0.95
1:A:41:CYS:HG	2:A:604:HEM:HAC	1.19	0.90
1:A:392:ASN:HD22	1:A:393:ARG:H	1.23	0.86
1:A:246:PRO:HG2	1:A:250:ALA:HB3	1.55	0.86
1:A:35:ASN:HD21	1:A:71:THR:H	1.26	0.82
1:A:73:CYS:HG	2:A:602:HEM:HAC	0.74	0.81
1:A:145:ARG:HD2	1:A:268:GLY:H	1.45	0.81
1:A:49:ALA:HB1	1:A:61:LYS:HD3	1.63	0.81
1:A:393:ARG:HD3	1:A:478:GLN:HE22	1.48	0.78
1:A:392:ASN:ND2	1:A:393:ARG:H	1.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:ND2	1:A:487:GLU:HG2	2.00	0.77
1:A:245:ARG:HB2	1:A:246:PRO:HD2	1.68	0.76
1:A:154:LEU:HD23	1:A:275:SER:HB3	1.67	0.76
1:A:322:VAL:HG22	1:A:361:ILE:HD13	1.66	0.74
1:A:114:GLN:O	1:A:118:ILE:HG13	1.87	0.74
1:A:453:ILE:HG23	1:A:455:VAL:HG13	1.68	0.73
3:A:600:FAD:C3'	3:A:600:FAD:C1'	2.65	0.73
1:A:337:HIS:HB2	1:A:338:PRO:HD2	1.69	0.73
1:A:319:ASN:HD21	1:A:330:LYS:HA	1.51	0.73
1:A:514:LYS:HD3	1:A:516:GLU:OE2	1.89	0.73
1:A:170:GLY:HA3	1:A:243:SER:OG	1.89	0.73
1:A:434:TYR:HB3	1:A:439:ILE:HD11	1.72	0.72
1:A:41:CYS:SG	2:A:604:HEM:C3C	2.82	0.72
1:A:377:GLU:N	4:A:700:FUM:O1	2.17	0.72
1:A:198:GLY:O	1:A:543:ASN:HB3	1.90	0.71
1:A:388:ASN:HD22	1:A:412:LYS:HZ3	1.39	0.70
1:A:28:ASN:H	1:A:28:ASN:HD22	1.39	0.70
1:A:62:SER:CB	2:A:601:HEM:HBB2	2.22	0.70
1:A:235:MET:CE	4:A:700:FUM:H5	2.21	0.69
1:A:146:ASP:O	1:A:147:ALA:HB3	1.93	0.68
1:A:467:TYR:CZ	1:A:484:LEU:HD23	2.27	0.68
1:A:388:ASN:ND2	1:A:412:LYS:HZ3	1.91	0.68
1:A:359:GLN:HE21	1:A:359:GLN:N	1.92	0.67
3:A:600:FAD:O2'	3:A:600:FAD:C1'	2.41	0.67
1:A:66:GLY:H	1:A:258:GLN:HE22	1.40	0.67
1:A:245:ARG:HB2	1:A:246:PRO:CD	2.25	0.66
1:A:517:VAL:HB	1:A:529:LEU:HD13	1.77	0.65
1:A:393:ARG:HH11	1:A:478:GLN:NE2	1.95	0.65
1:A:18:CYS:SG	2:A:603:HEM:C3C	2.90	0.65
1:A:359:GLN:HE21	1:A:359:GLN:H	1.43	0.64
1:A:252:VAL:O	1:A:256:VAL:HG23	1.98	0.63
1:A:345:LEU:HD11	1:A:358:LEU:HD21	1.80	0.63
1:A:15:CYS:SG	2:A:603:HEM:C3B	2.91	0.63
1:A:426:LYS:O	1:A:427:SER:HB3	1.96	0.63
1:A:465:THR:O	1:A:468:ASN:HB2	1.99	0.63
1:A:467:TYR:OH	1:A:484:LEU:HD23	1.98	0.63
1:A:393:ARG:HD3	1:A:478:GLN:NE2	2.14	0.62
1:A:395:MET:CE	1:A:407:ALA:HB3	2.30	0.62
1:A:364:HIS:O	1:A:500:PRO:HA	2.00	0.62
1:A:196:MET:HE3	1:A:196:MET:HA	1.82	0.62
1:A:190:ILE:O	1:A:194:ASP:OD1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.18	0.61
1:A:8:PHE:O	1:A:11:GLU:HG2	2.00	0.61
1:A:188:LYS:O	1:A:191:MET:HB3	2.00	0.61
1:A:73:CYS:SG	2:A:602:HEM:C3C	2.93	0.61
1:A:146:ASP:O	1:A:147:ALA:CB	2.49	0.61
1:A:167:ALA:HB3	1:A:253:GLY:CA	2.31	0.60
3:A:600:FAD:C2'	3:A:600:FAD:N10	2.59	0.60
1:A:28:ASN:HD22	1:A:28:ASN:N	1.99	0.60
1:A:235:MET:HE3	4:A:700:FUM:H5	1.83	0.60
1:A:316:ALA:O	1:A:317:LYS:CB	2.46	0.60
1:A:567:PHE:O	1:A:568:ALA:HB3	2.02	0.59
1:A:165:LYS:HG3	1:A:166:LEU:HD23	1.83	0.59
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.00	0.59
1:A:337:HIS:HB2	1:A:338:PRO:CD	2.32	0.59
1:A:395:MET:HE2	1:A:407:ALA:HB3	1.84	0.59
1:A:170:GLY:HA2	1:A:244:HIS:O	2.02	0.59
1:A:392:ASN:HD22	1:A:393:ARG:N	1.97	0.59
1:A:506:MET:HG3	1:A:540:HIS:HB2	1.85	0.59
1:A:453:ILE:HD11	1:A:495:ALA:CB	2.34	0.58
1:A:106:PRO:HG2	1:A:109:ALA:HB2	1.84	0.58
1:A:377:GLU:CB	4:A:700:FUM:O1	2.52	0.57
1:A:177:LYS:O	1:A:179:GLN:N	2.37	0.57
1:A:167:ALA:HB3	1:A:253:GLY:HA3	1.87	0.57
1:A:393:ARG:HH11	1:A:478:GLN:HE21	1.52	0.57
1:A:433:GLY:HA3	2:A:601:HEM:HBA2	1.87	0.56
1:A:421:ASP:HB3	1:A:424:ILE:H	1.70	0.56
1:A:348:ALA:O	1:A:351:ALA:HB3	2.06	0.55
1:A:228:ASP:N	1:A:255:HIS:NE2	2.47	0.55
1:A:388:ASN:ND2	1:A:412:LYS:NZ	2.54	0.55
3:A:600:FAD:O3'	3:A:600:FAD:H1'1	2.06	0.55
1:A:182:LEU:HD13	1:A:184:ILE:HD11	1.89	0.55
1:A:127:ASP:HB2	1:A:149:ALA:HB1	1.89	0.55
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.37	0.54
3:A:600:FAD:O3'	3:A:600:FAD:C1'	2.56	0.54
1:A:412:LYS:H	1:A:412:LYS:CD	2.09	0.54
1:A:255:HIS:O	1:A:259:VAL:HG13	2.06	0.54
1:A:359:GLN:NE2	1:A:359:GLN:H	2.06	0.54
1:A:450:ALA:HB1	1:A:455:VAL:O	2.08	0.54
1:A:154:LEU:HD12	1:A:154:LEU:N	2.23	0.54
1:A:196:MET:CE	1:A:203:ASN:HB2	2.38	0.53
1:A:142:VAL:HG11	1:A:225:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLY:O	1:A:470:PHE:C	2.44	0.53
1:A:426:LYS:O	1:A:427:SER:CB	2.57	0.53
1:A:411:GLN:O	1:A:412:LYS:C	2.48	0.52
1:A:127:ASP:CB	1:A:149:ALA:HB1	2.39	0.52
1:A:102:ARG:NH2	1:A:157:GLU:OE1	2.43	0.52
1:A:195:THR:HG21	1:A:208:VAL:HG13	1.92	0.52
1:A:380:ARG:HA	1:A:384:ALA:HB3	1.92	0.51
1:A:421:ASP:HB2	1:A:424:ILE:HG12	1.92	0.51
1:A:131:ILE:HD11	1:A:277:VAL:HG11	1.92	0.51
1:A:407:ALA:O	1:A:411:GLN:HG2	2.10	0.51
1:A:151:VAL:HB	1:A:269:THR:HG23	1.92	0.51
1:A:498:ILE:HD12	1:A:498:ILE:O	2.10	0.51
1:A:141:ALA:O	1:A:145:ARG:HB2	2.11	0.51
1:A:190:ILE:H	1:A:190:ILE:HD12	1.76	0.51
1:A:214:ASN:O	1:A:215:SER:C	2.48	0.51
1:A:392:ASN:ND2	1:A:393:ARG:N	2.56	0.51
1:A:175:GLU:OE2	1:A:187:LYS:HA	2.10	0.51
1:A:145:ARG:HG2	1:A:151:VAL:HG23	1.92	0.51
1:A:467:TYR:O	1:A:471:VAL:HG23	2.11	0.50
1:A:511:ILE:HD12	1:A:512:ASP:O	2.12	0.50
1:A:300:TYR:O	1:A:301:TYR:HB3	2.11	0.50
1:A:59:PRO:HD3	1:A:92:PHE:CE2	2.46	0.50
1:A:449:LEU:HD13	1:A:453:ILE:HD12	1.92	0.50
1:A:142:VAL:HG11	1:A:225:MET:HE2	1.93	0.50
1:A:559:ILE:O	1:A:560:ALA:C	2.50	0.49
1:A:145:ARG:HD2	1:A:268:GLY:N	2.22	0.49
1:A:337:HIS:CE1	1:A:339:GLY:HA3	2.47	0.49
1:A:343:ASP:HB2	5:A:704:HOH:O	2.13	0.49
1:A:511:ILE:HA	1:A:516:GLU:O	2.11	0.49
1:A:228:ASP:O	1:A:246:PRO:HA	2.13	0.49
1:A:29:ASP:O	1:A:274:ASN:ND2	2.41	0.49
1:A:62:SER:OG	2:A:601:HEM:HBB2	2.13	0.49
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.77	0.49
1:A:221:TRP:CZ2	1:A:558:ARG:HG3	2.47	0.49
1:A:412:LYS:HD2	1:A:412:LYS:N	2.13	0.49
1:A:252:VAL:HG12	1:A:256:VAL:HG23	1.94	0.48
1:A:329:LEU:O	1:A:330:LYS:C	2.50	0.48
1:A:310:ILE:O	1:A:531:ALA:HA	2.13	0.48
1:A:105:VAL:HG13	1:A:106:PRO:HD2	1.94	0.48
1:A:481:ARG:HD3	1:A:484:LEU:HG	1.95	0.48
1:A:4:VAL:O	1:A:5:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:CB	1:A:246:PRO:CD	2.91	0.48
1:A:395:MET:HE1	1:A:404:ALA:HA	1.96	0.47
1:A:62:SER:HB3	2:A:601:HEM:HBB2	1.91	0.47
1:A:90:PHE:HB2	5:A:747:HOH:O	2.15	0.47
1:A:66:GLY:H	1:A:258:GLN:NE2	2.12	0.47
1:A:179:GLN:O	1:A:180:ALA:C	2.53	0.47
1:A:106:PRO:HG2	1:A:109:ALA:CB	2.44	0.46
1:A:217:ASP:O	1:A:218:SER:C	2.54	0.46
1:A:245:ARG:CB	1:A:246:PRO:HD2	2.44	0.46
1:A:162:GLY:O	1:A:165:LYS:HG2	2.15	0.46
1:A:379:VAL:HG11	1:A:418:LEU:HD13	1.97	0.46
1:A:173:ALA:O	1:A:242:ARG:HD3	2.16	0.46
1:A:377:GLU:HB2	4:A:700:FUM:O1	2.16	0.46
1:A:517:VAL:CB	1:A:529:LEU:HD13	2.44	0.46
1:A:238:ALA:HB2	5:A:712:HOH:O	2.15	0.46
1:A:420:PHE:HE1	1:A:496:LEU:HD11	1.81	0.46
1:A:404:ALA:O	1:A:408:ILE:HG13	2.16	0.46
1:A:145:ARG:HG2	1:A:151:VAL:CG2	2.47	0.45
1:A:316:ALA:O	1:A:317:LYS:HB3	2.16	0.45
1:A:437:LEU:O	1:A:438:ASN:HB2	2.15	0.45
1:A:221:TRP:CH2	1:A:558:ARG:HG3	2.51	0.45
1:A:487:GLU:O	1:A:488:LEU:HB2	2.16	0.45
1:A:235:MET:HE3	4:A:700:FUM:C5	2.46	0.45
1:A:395:MET:HE1	1:A:407:ALA:HB3	1.98	0.45
1:A:374:MET:HE1	3:A:600:FAD:H6	1.98	0.45
1:A:186:ASP:OD1	1:A:187:LYS:N	2.49	0.45
1:A:166:LEU:O	1:A:167:ALA:C	2.54	0.45
1:A:25:GLY:H	2:A:603:HEM:CHB	2.29	0.45
1:A:219:ILE:HD13	1:A:244:HIS:CD2	2.52	0.45
1:A:375:ILE:O	1:A:375:ILE:HG13	2.16	0.45
1:A:449:LEU:HD11	1:A:495:ALA:HB2	1.97	0.45
1:A:296:GLU:HG2	1:A:297:TYR:CE2	2.52	0.45
1:A:245:ARG:HA	1:A:252:VAL:HG22	1.98	0.44
1:A:568:ALA:O	1:A:569:LYS:C	2.56	0.44
1:A:163:ASN:OD1	1:A:336:ASN:HA	2.17	0.44
1:A:549:ALA:O	1:A:553:ILE:HG23	2.18	0.44
3:A:600:FAD:O2'	3:A:600:FAD:C9	2.65	0.44
3:A:600:FAD:O2'	3:A:600:FAD:C9A	2.66	0.44
1:A:420:PHE:HE1	1:A:496:LEU:CD1	2.30	0.44
1:A:458:ALA:O	1:A:462:LYS:HG3	2.17	0.44
1:A:433:GLY:CA	2:A:601:HEM:HBA2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:PHE:O	1:A:568:ALA:CB	2.64	0.44
1:A:139:ALA:HA	1:A:260:LEU:HD22	1.99	0.44
1:A:59:PRO:HG3	2:A:602:HEM:HMD3	1.98	0.44
1:A:170:GLY:HA2	1:A:252:VAL:HG21	2.00	0.44
1:A:480:GLU:O	1:A:481:ARG:C	2.55	0.44
1:A:380:ARG:HD2	1:A:397:GLU:O	2.17	0.44
1:A:402:ASP:HB3	5:A:735:HOH:O	2.18	0.44
1:A:315:PHE:CD1	1:A:321:ARG:HG2	2.53	0.44
1:A:126:THR:OG1	1:A:127:ASP:N	2.51	0.44
1:A:35:ASN:ND2	1:A:70:CYS:N	2.66	0.44
1:A:151:VAL:HG12	1:A:152:ILE:N	2.32	0.44
1:A:429:LYS:O	1:A:430:ALA:C	2.54	0.44
1:A:467:TYR:CE2	1:A:484:LEU:HD23	2.52	0.43
1:A:289:THR:O	1:A:305:ALA:O	2.36	0.43
1:A:421:ASP:CB	1:A:424:ILE:HG12	2.49	0.43
2:A:604:HEM:HHA	2:A:604:HEM:HAA1	1.91	0.43
1:A:315:PHE:O	1:A:316:ALA:C	2.55	0.43
1:A:468:ASN:OD1	1:A:487:GLU:O	2.36	0.43
1:A:402:ASP:OD1	1:A:402:ASP:N	2.50	0.43
3:A:600:FAD:H3B	5:A:701:HOH:O	2.19	0.42
1:A:453:ILE:HD11	1:A:495:ALA:HB1	2.01	0.42
1:A:469:GLY:O	1:A:473:SER:HB2	2.19	0.42
1:A:115:ASP:O	1:A:116:LYS:C	2.57	0.42
1:A:127:ASP:O	1:A:305:ALA:HB1	2.19	0.42
1:A:207:LEU:O	1:A:209:LYS:N	2.53	0.42
1:A:35:ASN:HD22	1:A:70:CYS:H	1.66	0.42
1:A:557:GLY:O	1:A:558:ARG:C	2.58	0.42
1:A:4:VAL:O	1:A:6:ALA:N	2.53	0.42
1:A:138:LEU:HD13	1:A:261:TRP:HA	2.02	0.42
1:A:215:SER:O	1:A:216:SER:C	2.57	0.42
1:A:94:MET:HA	1:A:95:PRO:HD2	1.84	0.42
1:A:235:MET:HE1	4:A:700:FUM:O3	2.20	0.42
1:A:191:MET:HG2	1:A:212:ALA:CA	2.50	0.42
1:A:7:ASP:O	1:A:8:PHE:C	2.56	0.41
1:A:174:ALA:O	1:A:175:GLU:CB	2.68	0.41
1:A:460:LEU:O	1:A:464:VAL:HG23	2.19	0.41
1:A:487:GLU:O	1:A:488:LEU:CB	2.68	0.41
1:A:517:VAL:O	1:A:525:PRO:HA	2.20	0.41
1:A:109:ALA:O	1:A:110:ASP:HB3	2.19	0.41
1:A:437:LEU:O	1:A:438:ASN:CB	2.68	0.41
1:A:306:ASP:CB	1:A:568:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:HD22	1:A:340:ALA:CB	2.32	0.41
1:A:282:GLU:HG3	1:A:282:GLU:H	1.22	0.41
1:A:437:LEU:HD11	2:A:601:HEM:HAA1	2.00	0.41
1:A:196:MET:HE1	1:A:203:ASN:HB2	2.03	0.41
1:A:232:VAL:HG12	1:A:233:GLY:N	2.35	0.41
1:A:421:ASP:H	1:A:424:ILE:HG12	1.86	0.41
1:A:37:GLN:O	1:A:38:CYS:C	2.58	0.41
1:A:71:THR:HG21	2:A:603:HEM:HMD3	2.03	0.41
1:A:453:ILE:HG22	1:A:455:VAL:H	1.85	0.41
1:A:470:PHE:HB3	1:A:476:ASP:HA	2.02	0.41
1:A:63:HIS:CD2	2:A:601:HEM:NA	2.89	0.41
1:A:208:VAL:O	1:A:208:VAL:HG12	2.20	0.41
1:A:4:VAL:HA	1:A:96:PHE:HB3	2.03	0.41
1:A:252:VAL:H	1:A:252:VAL:HG23	1.57	0.41
1:A:60:HIS:HD2	2:A:602:HEM:C1C	2.40	0.40
1:A:317:LYS:HD3	1:A:337:HIS:O	2.22	0.40
1:A:63:HIS:HE1	2:A:601:HEM:NC	2.18	0.40
1:A:342:GLY:O	1:A:343:ASP:C	2.60	0.40
1:A:343:ASP:HB3	3:A:600:FAD:H61A	1.86	0.40
1:A:35:ASN:ND2	1:A:70:CYS:H	2.19	0.40
1:A:231:ASP:O	1:A:245:ARG:HG2	2.20	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	552/572 (96%)	470 (85%)	61 (11%)	21 (4%)	4	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	175	GLU
1	A	178	PRO
1	A	181	LYS
1	A	474	GLY
1	A	5	LEU
1	A	147	ALA
1	A	180	ALA
1	A	215	SER
1	A	317	LYS
1	A	427	SER
1	A	489	VAL
1	A	97	GLY
1	A	521	LYS
1	A	179	GLN
1	A	340	ALA
1	A	488	LEU
1	A	192	ILE
1	A	162	GLY
1	A	76	GLY
1	A	327	PRO

### 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	377/429 (88%)	304 (81%)	73 (19%)	<b>2</b> <b>5</b>

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	SER
1	A	21	SER
1	A	22	ASP
1	A	28	ASN
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	61	LYS
1	A	67	GLU
1	A	68	ILE
1	A	71	THR
1	A	75	LYS
1	A	78	GLU
1	A	89	SER
1	A	94	MET
1	A	101	GLU
1	A	102	ARG
1	A	123	LYS
1	A	124	GLU
1	A	125	THR
1	A	145	ARG
1	A	175	GLU
1	A	176	THR
1	A	182	LEU
1	A	184	ILE
1	A	188	LYS
1	A	191	MET
1	A	196	MET
1	A	203	ASN
1	A	211	LEU
1	A	219	ILE
1	A	223	THR
1	A	242	ARG
1	A	243	SER
1	A	260	LEU
1	A	267	ARG
1	A	269	THR
1	A	274	ASN
1	A	282	GLU
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	320	GLU
1	A	359	GLN
1	A	375	ILE
1	A	387	VAL
1	A	392	ASN
1	A	396	ASN
1	A	401	ARG

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Mol	Chain	Res	Type
1	A	421	ASP
1	A	423	SER
1	A	425	ARG
1	A	427	SER
1	A	441	LYS
1	A	442	GLU
1	A	446	ILE
1	A	449	LEU
1	A	453	ILE
1	A	454	ASP
1	A	459	GLU
1	A	460	LEU
1	A	465	THR
1	A	473	SER
1	A	475	LYS
1	A	478	GLN
1	A	488	LEU
1	A	497	GLU
1	A	520	GLU
1	A	526	ILE
1	A	527	THR
1	A	529	LEU
1	A	548	ASN
1	A	552	ASP
1	A	558	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	35	ASN
1	A	114	GLN
1	A	172	ASN
1	A	189	GLN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	359	GLN
1	A	388	ASN
1	A	392	ASN
1	A	411	GLN
1	A	468	ASN

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Mol	Chain	Res	Type
1	A	478	GLN
1	A	543	ASN
1	A	548	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
3	FAD	A	600	-	48,58,58	1.83	10 (20%)	54,89,89	3.71	24 (44%)
2	HEM	A	601	1	30,50,50	2.43	6 (20%)	24,82,82	3.32	12 (50%)
2	HEM	A	602	1	30,50,50	2.70	10 (33%)	24,82,82	3.23	13 (54%)
2	HEM	A	603	1	30,50,50	2.61	10 (33%)	24,82,82	3.16	11 (45%)
2	HEM	A	604	1	30,50,50	2.68	7 (23%)	24,82,82	4.13	16 (66%)
4	FUM	A	700	-	1,7,7	1.13	0	0,8,8	0.00	-

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
3	FAD	A	600	-	2/2/9/9	0/30/50/50	0/6/6/6
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
4	FUM	A	700	-	-	0/0/5/5	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	HEM	C3B-C4B	-9.32	1.43	1.51
2	A	602	HEM	C3B-C4B	-8.74	1.44	1.51
2	A	603	HEM	C3B-C4B	-7.74	1.45	1.51
2	A	604	HEM	C2D-C3D	-7.15	1.33	1.54
2	A	603	HEM	C2D-C3D	-6.93	1.33	1.54
2	A	601	HEM	C2D-C3D	-6.93	1.33	1.54
2	A	601	HEM	C3B-C4B	-6.77	1.45	1.51
2	A	602	HEM	C2D-C3D	-6.72	1.34	1.54
2	A	603	HEM	C3D-C4D	-5.31	1.44	1.51
2	A	601	HEM	C3D-C4D	-5.00	1.45	1.51
2	A	604	HEM	C2C-C1C	-4.14	1.44	1.52
2	A	602	HEM	C2C-C1C	-3.93	1.45	1.52
2	A	602	HEM	C3D-C4D	-3.92	1.46	1.51
2	A	603	HEM	C2C-C1C	-3.80	1.45	1.52
2	A	604	HEM	C3D-C4D	-3.72	1.46	1.51
2	A	601	HEM	C2C-C1C	-3.69	1.45	1.52
3	A	600	FAD	C5'-C4'	-3.01	1.47	1.51
2	A	603	HEM	C2D-C1D	-2.49	1.43	1.51
3	A	600	FAD	PA-O2A	-2.45	1.44	1.54
2	A	604	HEM	C2B-C1B	-2.37	1.44	1.51
3	A	600	FAD	O4'-C4'	-2.36	1.38	1.43
2	A	602	HEM	C2D-C1D	-2.34	1.44	1.51
3	A	600	FAD	C8A-N7A	-2.13	1.30	1.34
2	A	602	HEM	C2B-C1B	-2.12	1.44	1.51
3	A	600	FAD	P-O1P	-2.08	1.43	1.51
2	A	603	HEM	C2B-C1B	-2.04	1.45	1.51
2	A	603	HEM	C4C-NC	2.02	1.38	1.36
2	A	604	HEM	C3C-CAC	2.36	1.55	1.51
2	A	601	HEM	C3B-CAB	2.36	1.55	1.51
2	A	603	HEM	C3B-CAB	2.68	1.56	1.51
2	A	602	HEM	C3C-CAC	2.70	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	HEM	C3C-CAC	2.72	1.56	1.51
2	A	604	HEM	C3B-CAB	2.82	1.56	1.51
2	A	602	HEM	C1C-NC	2.84	1.39	1.36
2	A	603	HEM	C1C-NC	2.97	1.39	1.36
2	A	601	HEM	C3C-CAC	3.05	1.57	1.51
3	A	600	FAD	C4-N3	3.07	1.38	1.33
3	A	600	FAD	O4B-C1B	3.09	1.45	1.41
2	A	602	HEM	C4C-NC	3.29	1.40	1.36
3	A	600	FAD	C4-C4X	3.84	1.48	1.41
2	A	602	HEM	C3B-CAB	3.88	1.58	1.51
3	A	600	FAD	C1'-C2'	4.58	1.80	1.51
3	A	600	FAD	C5B-C4B	6.39	1.72	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	C5B-C4B-C3B	-10.50	73.52	115.21
3	A	600	FAD	O4B-C1B-N9A	-8.01	91.33	108.10
2	A	604	HEM	CAA-C2A-C1A	-7.84	118.50	127.01
3	A	600	FAD	C4B-O4B-C1B	-7.46	101.53	109.72
2	A	601	HEM	C3C-CAC-CBC	-6.00	115.26	124.46
2	A	602	HEM	CAA-C2A-C1A	-5.92	120.58	127.01
2	A	603	HEM	CMA-C3A-C4A	-5.78	118.80	128.36
2	A	603	HEM	C3B-CAB-CBB	-5.76	115.63	124.46
3	A	600	FAD	O2'-C2'-C1'	-5.62	96.14	109.94
2	A	601	HEM	C3B-CAB-CBB	-5.53	115.98	124.46
2	A	602	HEM	C3C-CAC-CBC	-5.31	116.30	124.46
2	A	602	HEM	C3B-CAB-CBB	-5.13	116.59	124.46
3	A	600	FAD	C2B-C1B-N9A	-4.95	106.72	114.29
2	A	604	HEM	C3C-CAC-CBC	-4.28	117.89	124.46
3	A	600	FAD	C5X-C9A-N10	-4.15	114.47	117.62
2	A	604	HEM	CAA-CBA-CGA	-4.10	105.23	112.75
2	A	604	HEM	C3B-CAB-CBB	-4.03	118.27	124.46
2	A	602	HEM	CBA-CAA-C2A	-3.87	105.59	112.53
3	A	600	FAD	C1B-N9A-C4A	-3.86	121.12	126.94
3	A	600	FAD	O4'-C4'-C3'	-3.85	99.35	109.02
3	A	600	FAD	C4-C4X-C10	-3.79	117.51	119.94
2	A	601	HEM	CAA-C2A-C1A	-3.78	122.90	127.01
2	A	603	HEM	C3C-CAC-CBC	-3.23	119.51	124.46
2	A	604	HEM	CMA-C3A-C4A	-3.16	123.13	128.36
3	A	600	FAD	C6-C5X-N5	-3.09	114.99	118.96
3	A	600	FAD	C9A-C5X-N5	-3.07	117.81	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEM	C4B-CHC-C1C	-3.05	120.72	125.82
2	A	602	HEM	CMA-C3A-C4A	-2.92	123.53	128.36
2	A	602	HEM	C4B-CHC-C1C	-2.52	121.60	125.82
3	A	600	FAD	O4B-C4B-C3B	-2.49	100.14	105.15
2	A	601	HEM	CMA-C3A-C4A	-2.29	124.58	128.36
2	A	601	HEM	C1D-CHD-C4C	-2.12	122.28	125.82
2	A	602	HEM	CBD-CAD-C3D	2.08	119.60	113.55
2	A	604	HEM	CMA-C3A-C2A	2.11	129.66	125.24
3	A	600	FAD	O2A-PA-O3P	2.23	115.21	105.09
3	A	600	FAD	C2A-N1A-C6A	2.29	122.86	118.77
2	A	601	HEM	CBD-CAD-C3D	2.64	121.22	113.55
2	A	603	HEM	CAD-C3D-C4D	2.64	121.80	112.47
2	A	603	HEM	CBA-CAA-C2A	2.66	117.30	112.53
2	A	604	HEM	C2D-C3D-C4D	2.68	106.04	101.50
2	A	604	HEM	C3B-C4B-CHC	2.69	126.96	123.16
2	A	602	HEM	CAD-C3D-C4D	2.71	122.02	112.47
3	A	600	FAD	N6A-C6A-N1A	2.88	125.38	119.20
2	A	604	HEM	CAD-C3D-C4D	3.00	123.04	112.47
2	A	601	HEM	CMD-C2D-C3D	3.01	127.66	114.35
2	A	603	HEM	CMD-C2D-C3D	3.15	128.28	114.35
3	A	600	FAD	O3'-C3'-C4'	3.21	116.83	108.75
2	A	601	HEM	C3B-C4B-CHC	3.27	127.77	123.16
3	A	600	FAD	P-O3P-PA	3.32	142.06	132.73
2	A	602	HEM	CMD-C2D-C3D	3.37	129.24	114.35
2	A	602	HEM	CMB-C2B-C3B	3.48	125.21	116.53
2	A	602	HEM	C2D-C3D-C4D	3.52	107.46	101.50
2	A	604	HEM	CMD-C2D-C3D	3.60	130.25	114.35
3	A	600	FAD	O2B-C2B-C3B	3.70	123.86	111.83
3	A	600	FAD	C6-C5X-C9A	3.86	124.06	118.98
2	A	603	HEM	C2D-C3D-C4D	3.92	108.15	101.50
2	A	601	HEM	C2D-C3D-C4D	4.06	108.39	101.50
2	A	603	HEM	CMA-C3A-C2A	4.30	134.22	125.24
2	A	604	HEM	CMB-C2B-C3B	4.42	127.56	116.53
2	A	603	HEM	CMC-C2C-C3C	4.57	127.94	116.53
2	A	604	HEM	CMC-C2C-C3C	4.58	127.97	116.53
3	A	600	FAD	C4-C4X-N5	4.62	124.32	118.72
3	A	600	FAD	C4X-N5-C5X	5.05	122.58	116.76
2	A	602	HEM	CMC-C2C-C3C	5.68	130.71	116.53
2	A	603	HEM	CMB-C2B-C3B	5.84	131.11	116.53
2	A	603	HEM	CAD-C3D-C2D	5.86	130.06	113.22
2	A	601	HEM	CMC-C2C-C3C	5.98	131.45	116.53
2	A	602	HEM	CAD-C3D-C2D	6.01	130.51	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CMB-C2B-C3B	6.04	131.62	116.53
2	A	604	HEM	CAD-C3D-C2D	6.14	130.86	113.22
2	A	604	HEM	CBD-CAD-C3D	6.60	132.76	113.55
2	A	601	HEM	CAD-C3D-C2D	6.62	132.24	113.22
3	A	600	FAD	O4B-C4B-C5B	7.03	134.46	109.32
3	A	600	FAD	O5B-C5B-C4B	7.72	137.58	109.12
2	A	604	HEM	CBA-CAA-C2A	10.11	130.64	112.53
3	A	600	FAD	C1'-N10-C9A	10.26	130.38	118.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C4'
3	A	600	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	11	0
2	A	601	HEM	8	0
2	A	602	HEM	6	0
2	A	603	HEM	6	0
2	A	604	HEM	5	0
4	A	700	FUM	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section 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.