



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:21 pm GMT

PDB ID : 2WS3  
Title : Crystal structure of the E. coli succinate:quinone oxidoreductase (SQR) SdhD Tyr83Phe mutant  
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.  
Deposited on : 2009-09-03  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

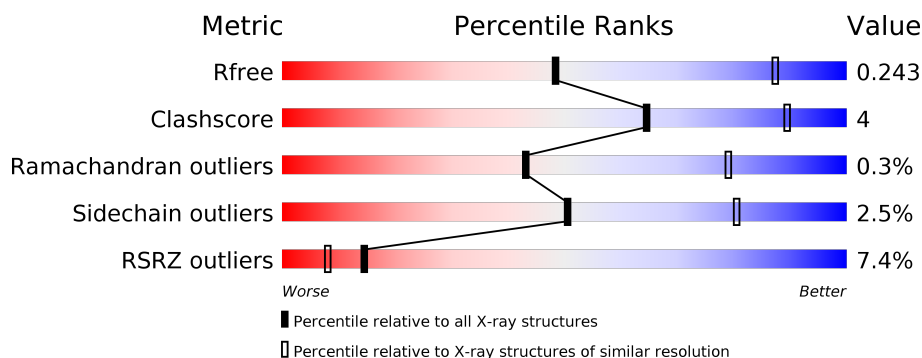
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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.

Mol	Chain	Length	Quality of chain
1	A	588	<div> <div>0%</div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	E	588	<div> <div>4%</div> <div>88%</div> <div>12%</div> <div>•</div> </div>
1	I	588	<div> <div>21%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
2	B	238	<div> <div>3%</div> <div>87%</div> <div>12%</div> </div>
2	F	238	<div> <div>3%</div> <div>87%</div> <div>13%</div> </div>
2	J	238	<div> <div>13%</div> <div>88%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
3	K	129	
4	D	115	
4	H	115	
4	L	115	

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
10	F3S	F	304	-	-	X	-
7	TEO	E	1590	-	-	X	-
7	TEO	I	1590	-	-	X	-
9	SF4	J	303	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24900 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 SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	E	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	I	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called SUCCINATE DEHYDROGENASE IRON-SULFUR SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			
2	F	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			
2	J	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			
3	G	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			
3	K	121	Total	C	N	O	S	0	0	0
			933	619	151	158	5			

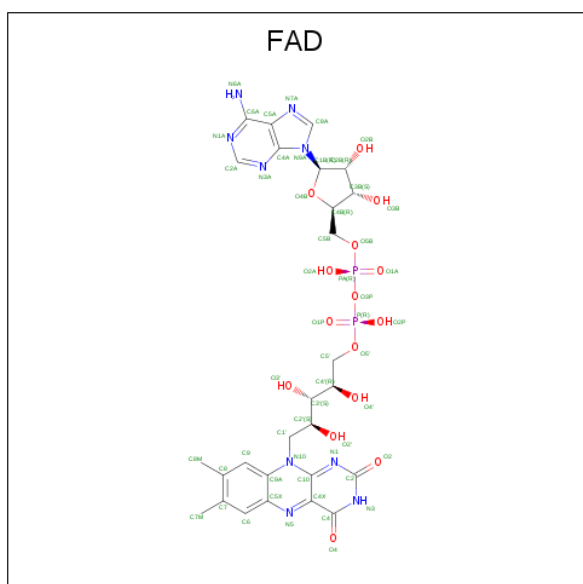
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	H	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	L	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	83	PHE	TYR	engineered mutation	UNP P0AC44
H	83	PHE	TYR	engineered mutation	UNP P0AC44
L	83	PHE	TYR	engineered mutation	UNP P0AC44

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

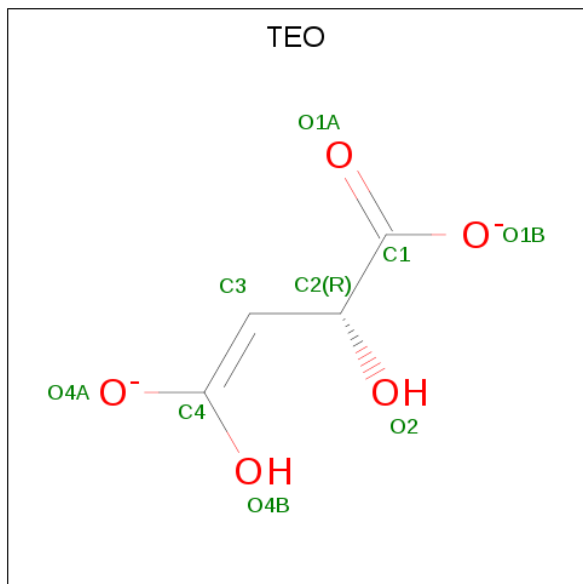


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

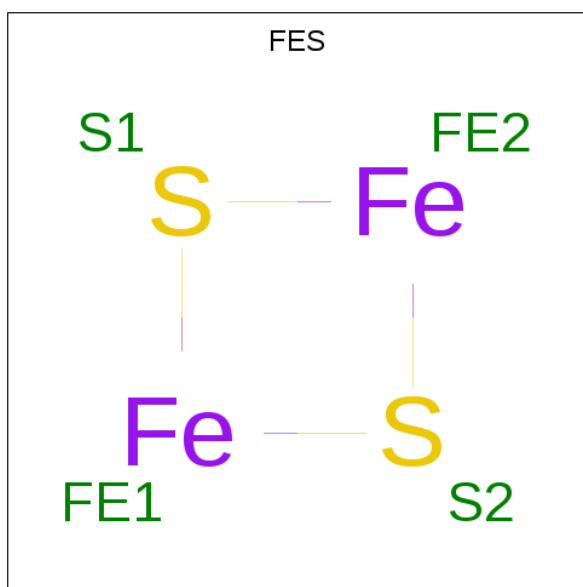
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		

- Molecule 7 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula:  $C_4H_4O_5$ ).



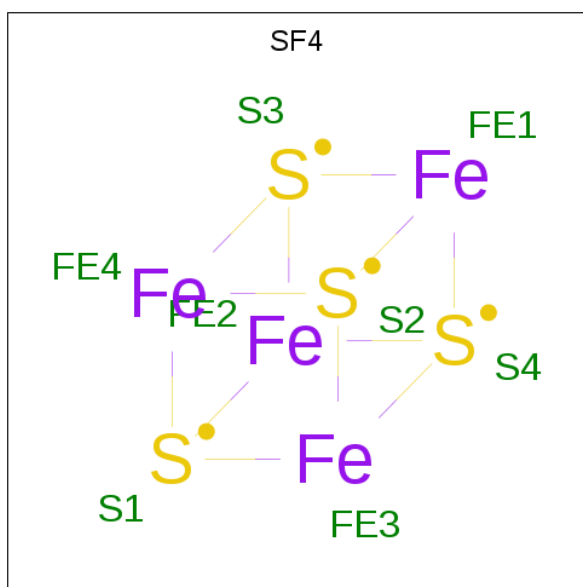
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	4	5		
7	E	1	Total	C	O	0	0
			9	4	5		
7	I	1	Total	C	O	0	0
			9	4	5		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		
8	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



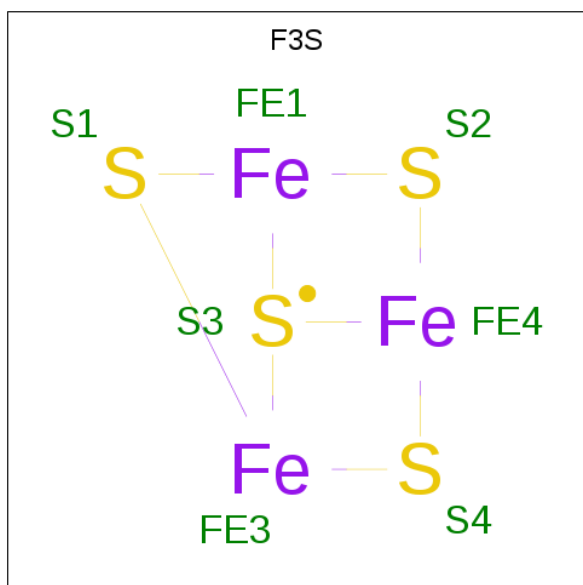
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	J	1	Total	Fe	S	0	0
			8	4	4		

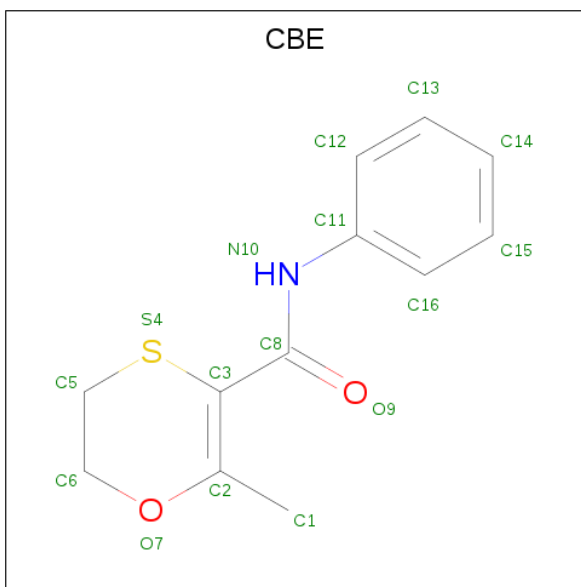
- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		
10	F	1	Total	Fe	S	0	0
			7	3	4		
10	J	1	Total	Fe	S	0	0
			7	3	4		

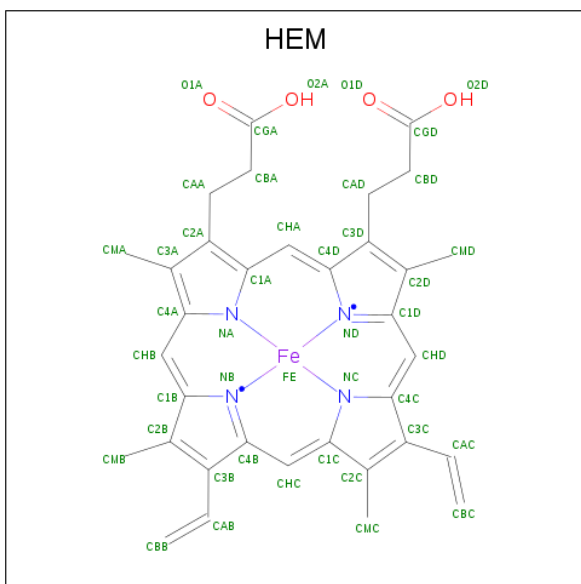
- Molecule 11 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula:  $\text{C}_{12}\text{H}_{13}\text{NO}_2\text{S}$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
11	G	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
11	K	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

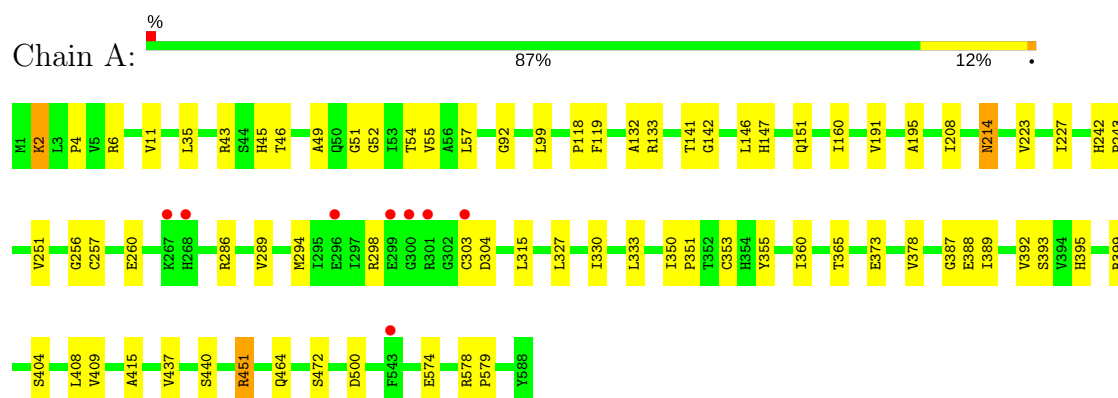


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

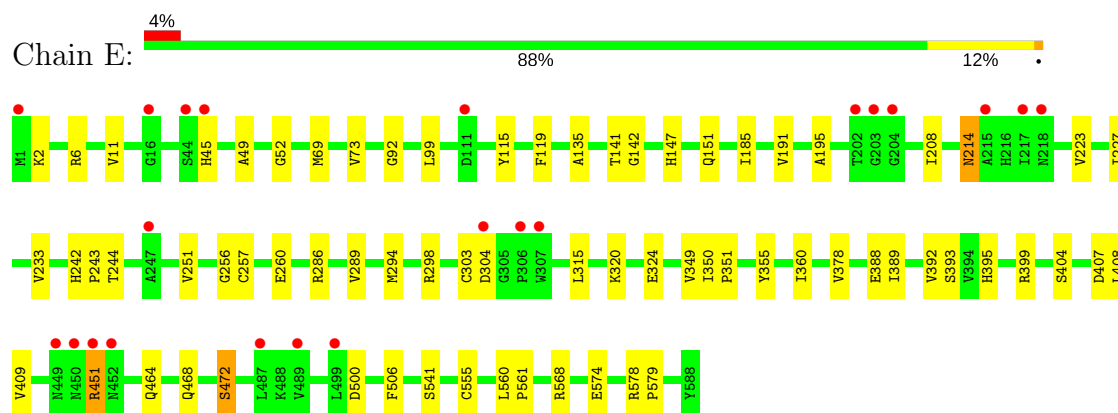
### 3 Residue-property plots [i](#)

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

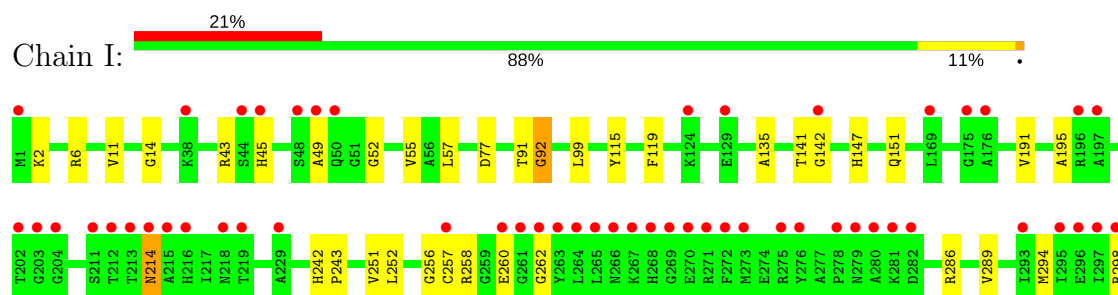
#### • Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

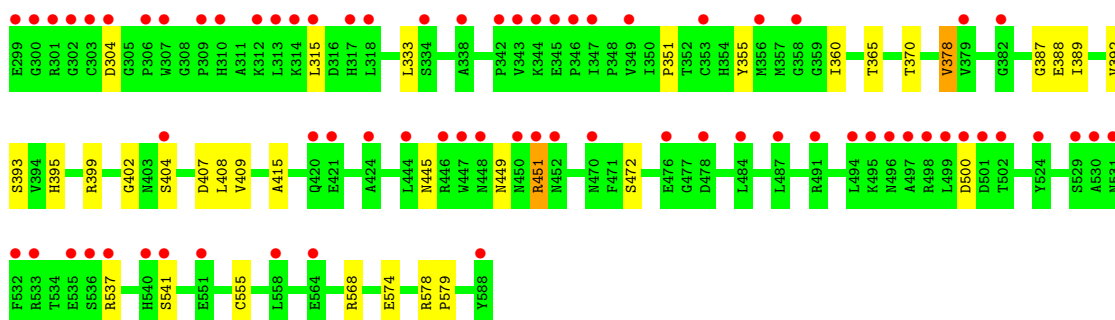


#### • Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

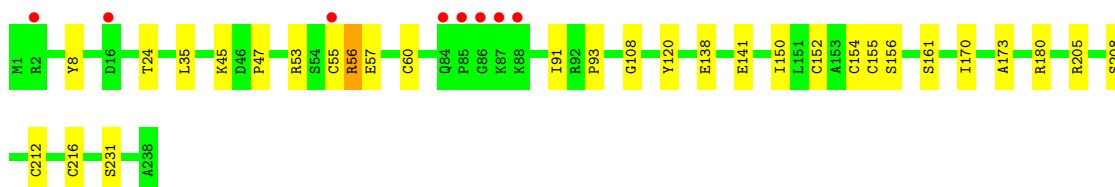
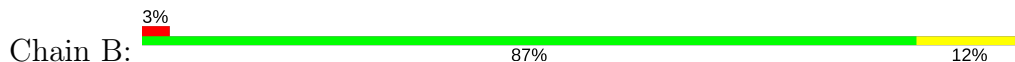


#### • Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

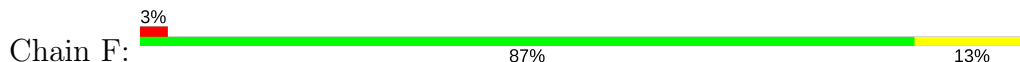




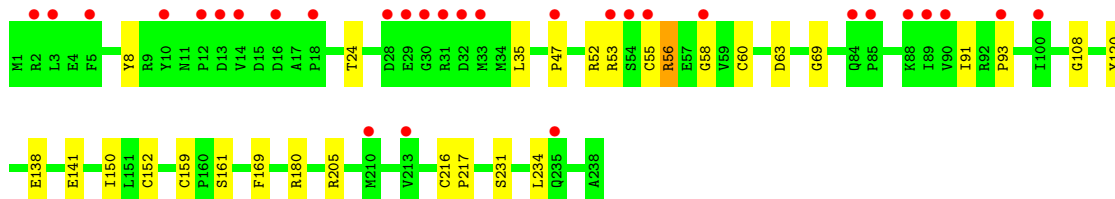
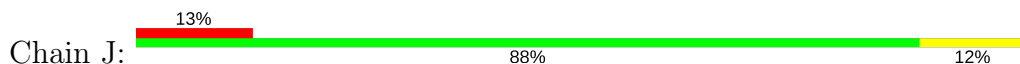
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



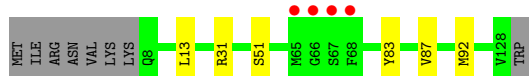
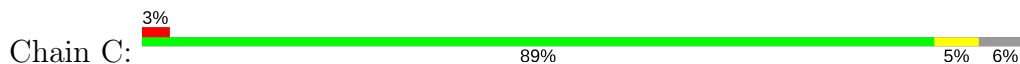
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



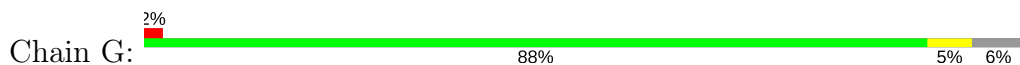
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT

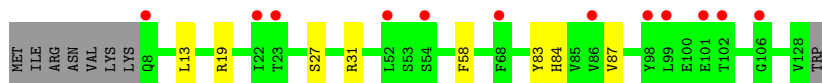
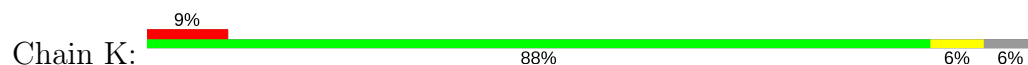


• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT

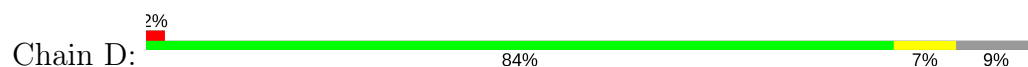




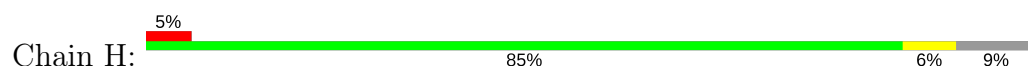
● Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT



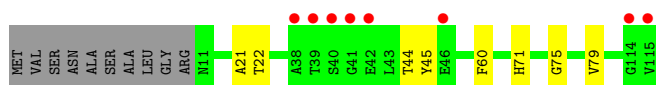
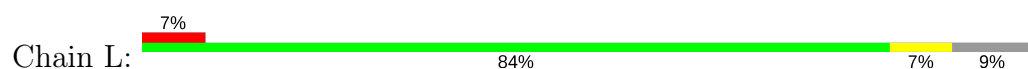
● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.85Å 184.71Å 203.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.20 49.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.03-3.20) 99.8 (49.01-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.219 , 0.253 0.210 , 0.243	Depositor DCC
$R_{free}$ test set	3797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TEO, NA, SF4, CBE, F3S, FES, 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	0.65	1/4611 (0.0%)	0.67	0/6237
1	E	0.59	0/4611	0.64	0/6237
1	I	0.46	0/4611	0.58	0/6237
2	B	0.72	2/1908 (0.1%)	0.69	0/2578
2	F	0.61	0/1908	0.68	0/2578
2	J	0.51	0/1908	0.61	0/2578
3	C	0.66	0/953	0.62	0/1293
3	G	0.62	0/953	0.61	1/1293 (0.1%)
3	K	0.55	0/953	0.56	0/1293
4	D	0.68	0/858	0.59	0/1173
4	H	0.64	0/858	0.59	0/1173
4	L	0.61	0/858	0.58	0/1173
All	All	0.59	3/24990 (0.0%)	0.63	1/33843 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	154	CYS	CB-SG	-5.44	1.73	1.81
1	A	353	CYS	CB-SG	-5.42	1.73	1.81
2	B	216	CYS	CB-SG	-5.39	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	19	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4522	0	4426	52	0
1	E	4522	0	4426	43	0
1	I	4522	0	4426	46	0
2	B	1869	0	1850	12	0
2	F	1869	0	1850	14	0
2	J	1869	0	1850	15	0
3	C	933	0	979	4	0
3	G	933	0	979	3	0
3	K	933	0	979	6	0
4	D	835	0	875	6	0
4	H	835	0	875	5	0
4	L	835	0	875	6	0
5	A	53	0	31	9	0
5	E	53	0	31	10	0
5	I	53	0	31	17	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
7	A	9	0	3	3	0
7	E	9	0	3	5	0
7	I	9	0	3	6	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	1	0
9	B	8	0	0	0	0
9	F	8	0	0	0	0
9	J	8	0	0	3	0
10	B	7	0	0	1	0
10	F	7	0	0	2	0
10	J	7	0	0	1	0
11	C	16	0	13	2	0
11	G	16	0	13	0	0
11	K	16	0	13	2	0
12	C	43	0	30	7	0
12	G	43	0	30	6	0
12	K	43	0	30	12	0
All	All	24900	0	24621	223	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 4.

All (223) 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:E:45:HIS:NE2	5:E:601:FAD:HM82	1.36	1.38
1:A:45:HIS:NE2	5:A:601:FAD:C8M	1.94	1.30
1:A:45:HIS:NE2	5:A:601:FAD:HM82	1.42	1.30
1:E:45:HIS:NE2	5:E:601:FAD:C8M	2.08	1.15
1:A:45:HIS:CE1	5:A:601:FAD:HM82	1.88	1.08
1:A:45:HIS:NE2	5:A:601:FAD:HM81	1.78	0.98
1:I:45:HIS:NE2	5:I:601:FAD:HM82	1.82	0.94
1:E:45:HIS:CE1	5:E:601:FAD:HM82	2.08	0.89
1:I:45:HIS:NE2	5:I:601:FAD:C8M	2.38	0.86
12:C:1130:HEM:HBB2	12:C:1130:HEM:HHC	1.58	0.83
1:A:451:ARG:NH1	1:A:451:ARG:HG2	1.95	0.81
12:K:1130:HEM:HBC2	12:K:1130:HEM:HHD	1.62	0.80
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.49	0.77
12:K:1130:HEM:CBA	12:K:1130:HEM:HHA	2.16	0.74
3:C:31:ARG:HB2	11:C:1129:CBE:H52	1.70	0.74
5:I:601:FAD:H9	5:I:601:FAD:O2'	1.88	0.73
12:G:1130:HEM:HHC	12:G:1130:HEM:HBB2	1.73	0.71
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.72	0.71
1:I:45:HIS:CE1	5:I:601:FAD:HM82	2.25	0.70
2:J:159:CYS:HB2	10:J:304:F3S:S2	2.30	0.70
12:K:1130:HEM:HBA2	12:K:1130:HEM:HHA	1.73	0.70
2:J:35:LEU:HD11	2:J:91:ILE:HD11	1.74	0.69
1:A:49:ALA:HA	5:A:601:FAD:C6	2.23	0.69
1:A:408:LEU:HD11	5:A:601:FAD:H4'	1.73	0.69
1:A:355:TYR:CE1	1:A:388:GLU:HG3	2.28	0.68
2:J:217:PRO:HD2	9:J:303:SF4:S3	2.34	0.67
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.75	0.67
1:A:147:HIS:O	1:A:151:GLN:HG3	1.95	0.67
3:C:31:ARG:CZ	11:C:1129:CBE:H62	2.25	0.66
2:F:35:LEU:HD11	2:F:91:ILE:HD11	1.78	0.66
1:I:286:ARG:HH22	7:I:1590:TEO:C3	2.10	0.65
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.78	0.65
1:E:147:HIS:O	1:E:151:GLN:HG3	1.97	0.65
3:K:27:SER:OG	11:K:1129:CBE:H51	1.97	0.65
1:E:45:HIS:NE2	5:E:601:FAD:HM81	2.09	0.64
12:K:1130:HEM:HAA1	4:L:75:GLY:CA	2.27	0.64
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.80	0.64
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.81	0.63
1:I:294:MET:O	1:I:298:ARG:HB2	1.99	0.63
1:A:294:MET:O	1:A:298:ARG:HB2	1.99	0.63
12:G:1130:HEM:HMC1	4:H:26:LEU:HB3	1.79	0.63
5:I:601:FAD:N5	7:I:1590:TEO:H2	2.13	0.63
1:A:451:ARG:CG	1:A:451:ARG:HH11	2.11	0.63
1:I:408:LEU:HD11	5:I:601:FAD:H4'	1.81	0.62
1:I:6:ARG:HD2	1:I:191:VAL:HG11	1.82	0.61
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.84	0.60
1:I:500:ASP:HB3	2:J:47:PRO:HG2	1.83	0.60
1:I:45:HIS:NE2	5:I:601:FAD:HM81	2.15	0.60
3:K:31:ARG:NH1	11:K:1129:CBE:H12A	2.17	0.60
1:I:147:HIS:O	1:I:151:GLN:HG3	2.02	0.59
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.33	0.58
12:C:1130:HEM:HBC2	12:C:1130:HEM:HHD	1.85	0.58
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.85	0.58
1:E:286:ARG:HH22	7:E:1590:TEO:C3	2.16	0.57
1:A:286:ARG:HH22	7:A:1590:TEO:C3	2.18	0.57
1:E:392:VAL:N	1:E:393:SER:HA	2.18	0.57
2:J:69:GLY:HA3	3:K:19:ARG:HG2	1.87	0.56
12:K:1130:HEM:HHC	12:K:1130:HEM:HBB2	1.87	0.56
1:E:294:MET:O	1:E:298:ARG:HB2	2.06	0.56
1:I:355:TYR:CE1	1:I:388:GLU:HG3	2.41	0.55
1:I:392:VAL:N	1:I:393:SER:HA	2.21	0.55
1:A:4:PRO:HB2	1:A:191:VAL:HG22	1.88	0.55
1:I:49:ALA:HA	5:I:601:FAD:C6	2.37	0.55
1:A:6:ARG:HD2	1:A:191:VAL:HG11	1.88	0.54
4:L:22:THR:OG1	4:L:71:HIS:HB2	2.07	0.54
5:I:601:FAD:C10	7:I:1590:TEO:O4B	2.56	0.54
1:E:214:ASN:N	1:E:214:ASN:HD22	2.06	0.54
12:K:1130:HEM:HBA1	12:K:1130:HEM:CHA	2.37	0.54
12:C:1130:HEM:HHC	12:C:1130:HEM:CBB	2.33	0.53
1:I:404:SER:HG	5:I:601:FAD:HO3'	1.50	0.53
12:K:1130:HEM:CHA	12:K:1130:HEM:CBA	2.82	0.53
1:A:214:ASN:HD22	1:A:214:ASN:N	2.07	0.52
12:C:1130:HEM:HBB2	12:C:1130:HEM:CHC	2.31	0.52
1:I:43:ARG:HD3	2:J:60:CYS:O	2.10	0.52
12:G:1130:HEM:HBA2	12:G:1130:HEM:HHA	1.91	0.52
1:E:395:HIS:ND1	1:E:399:ARG:HG3	2.24	0.51
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.45	0.51
12:K:1130:HEM:HBA1	12:K:1130:HEM:HHA	1.92	0.51
1:I:214:ASN:HD22	1:I:214:ASN:N	2.07	0.51
1:I:242:HIS:O	1:I:351:PRO:HA	2.11	0.51
2:B:55:CYS:O	2:B:56:ARG:HG3	2.10	0.51
1:A:242:HIS:O	1:A:351:PRO:HA	2.11	0.50
1:A:51:GLY:N	7:A:1590:TEO:O1A	2.35	0.50
3:K:84:HIS:CD2	12:K:1130:HEM:NC	2.80	0.49
1:E:6:ARG:HD2	1:E:191:VAL:HG11	1.93	0.49
12:K:1130:HEM:HAA1	4:L:75:GLY:HA2	1.93	0.49
2:B:208:SER:HA	10:B:304:F3S:S4	2.52	0.49
2:J:150:ILE:HG12	9:J:303:SF4:S1	2.53	0.49
1:E:408:LEU:HD11	5:E:601:FAD:H4'	1.95	0.49
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.93	0.49
2:J:150:ILE:HG13	2:J:152:CYS:HB3	1.95	0.49
1:A:350:ILE:HG13	1:A:351:PRO:HD2	1.95	0.49
1:E:555:CYS:SG	1:E:568:ARG:HD2	2.53	0.48
1:E:256:GLY:O	1:E:260:GLU:HG2	2.13	0.48
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.48	0.48
4:D:95:LEU:HD13	4:L:21:ALA:HB1	1.95	0.48
1:E:49:ALA:HA	5:E:601:FAD:C6	2.43	0.48
1:I:256:GLY:O	1:I:260:GLU:HG2	2.14	0.48
1:E:578:ARG:NH1	1:E:579:PRO:O	2.47	0.47
1:I:404:SER:OG	5:I:601:FAD:O3'	2.15	0.47
1:I:445:ASN:O	1:I:449:ASN:ND2	2.48	0.47
5:E:601:FAD:C4	7:E:1590:TEO:C3	2.92	0.47
1:E:355:TYR:CE1	1:E:388:GLU:HG3	2.50	0.47
1:E:115:TYR:O	1:E:135:ALA:HA	2.15	0.47
1:I:402:GLY:N	7:I:1590:TEO:O4A	2.38	0.47
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.45	0.47
12:G:1130:HEM:HMC1	4:H:26:LEU:CB	2.44	0.47
4:D:87:LEU:HD21	2:J:234:LEU:HB3	1.96	0.47
1:I:14:GLY:HA2	5:I:601:FAD:H1B	1.96	0.47
1:A:256:GLY:O	1:A:260:GLU:HG2	2.15	0.46
1:A:243:PRO:HB3	1:A:289:VAL:HG12	1.98	0.46
1:E:500:ASP:HB3	2:F:47:PRO:HG2	1.97	0.46
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.98	0.46
1:E:320:LYS:HE2	1:E:324:GLU:OE2	2.15	0.46
2:F:208:SER:HA	10:F:304:F3S:S4	2.55	0.46
5:E:601:FAD:N5	7:E:1590:TEO:H2	2.30	0.46
3:G:92:MET:HG2	4:H:20:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:243:PRO:HB3	1:I:289:VAL:HG12	1.96	0.46
1:I:365:THR:O	1:I:415:ALA:HA	2.16	0.46
1:I:404:SER:O	1:I:407:ASP:HB3	2.16	0.46
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.98	0.46
1:E:185:ILE:O	1:E:506:PHE:HA	2.16	0.46
1:I:578:ARG:NH1	1:I:579:PRO:O	2.49	0.46
1:A:392:VAL:N	1:A:393:SER:HA	2.30	0.46
4:D:22:THR:OG1	4:D:71:HIS:HB2	2.16	0.46
1:I:387:GLY:HA2	1:I:408:LEU:HD23	1.98	0.46
1:E:451:ARG:HH11	1:E:451:ARG:HA	1.81	0.45
1:I:251:VAL:HG11	1:I:333:LEU:HD22	1.99	0.45
2:F:150:ILE:HG13	2:F:152:CYS:HB3	1.99	0.45
2:F:207:HIS:ND1	12:G:1130:HEM:O1D	2.48	0.45
1:A:365:THR:O	1:A:415:ALA:HA	2.16	0.45
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.99	0.45
1:I:555:CYS:SG	1:I:568:ARG:HD2	2.56	0.45
2:F:159:CYS:HB2	10:F:304:F3S:S2	2.57	0.45
2:B:150:ILE:HG13	2:B:152:CYS:HB3	1.99	0.45
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.52	0.44
2:J:216:CYS:HA	9:J:303:SF4:S3	2.57	0.44
1:A:52:GLY:HA2	1:A:141:THR:HG21	1.99	0.44
4:H:22:THR:OG1	4:H:71:HIS:HB2	2.18	0.44
5:I:601:FAD:O2'	5:I:601:FAD:C9	2.60	0.44
12:C:1130:HEM:HBC2	4:D:23:ALA:HB1	1.99	0.44
1:I:99:LEU:HD11	1:I:409:VAL:HG21	2.00	0.44
1:I:115:TYR:O	1:I:135:ALA:HA	2.18	0.44
1:I:52:GLY:HA2	1:I:141:THR:HG21	1.99	0.44
5:I:601:FAD:C4X	7:I:1590:TEO:C4	2.96	0.44
1:I:451:ARG:HH11	1:I:451:ARG:HA	1.82	0.44
2:B:155:CYS:SG	2:B:156:SER:N	2.91	0.44
1:A:360:ILE:HD12	1:A:389:ILE:HG13	2.00	0.44
1:E:243:PRO:HB3	1:E:289:VAL:HG12	1.98	0.44
1:A:2:LYS:O	1:A:2:LYS:HD3	2.17	0.44
5:E:601:FAD:H1'1	5:E:601:FAD:H9	1.69	0.43
1:A:223:VAL:HG12	1:A:227:ILE:HD12	2.00	0.43
1:A:408:LEU:HD11	5:A:601:FAD:C4'	2.45	0.43
1:A:43:ARG:HD3	2:B:60:CYS:O	2.18	0.43
1:E:468:GLN:O	1:E:472:SER:HB2	2.18	0.43
1:E:560:LEU:HA	1:E:561:PRO:HD3	1.91	0.43
1:E:69:MET:O	1:E:73:VAL:HG23	2.17	0.43
1:E:223:VAL:HG13	1:E:233:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:360:ILE:HD12	1:I:389:ILE:HG13	2.00	0.43
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.32	0.43
1:A:437:VAL:O	1:A:440:SER:HB2	2.18	0.43
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.54	0.43
1:E:251:VAL:HG13	2:F:57:GLU:OE1	2.18	0.43
3:C:92:MET:HG2	4:D:20:ARG:HG2	2.00	0.43
12:C:1130:HEM:CBC	4:D:23:ALA:HB1	2.49	0.43
2:B:170:ILE:HD13	2:B:170:ILE:HA	1.89	0.42
1:E:52:GLY:HA2	1:E:141:THR:HG21	2.01	0.42
1:A:35:LEU:HD23	1:A:160:ILE:HG12	2.00	0.42
2:J:52:ARG:O	2:J:63:ASP:HB3	2.19	0.42
1:E:208:ILE:O	1:E:464:GLN:HA	2.19	0.42
1:I:258:ARG:HA	1:I:262:GLY:O	2.19	0.42
1:A:387:GLY:HA2	1:A:408:LEU:HD23	2.01	0.42
12:C:1130:HEM:CBC	12:C:1130:HEM:HHD	2.48	0.42
1:I:370:THR:HG23	1:I:378:VAL:HG22	2.02	0.42
1:A:99:LEU:HD11	1:A:409:VAL:HG21	2.00	0.42
2:B:138:GLU:O	2:B:138:GLU:HG3	2.16	0.42
1:E:242:HIS:CD2	7:E:1590:TEO:O2	2.72	0.42
1:I:252:LEU:HD22	5:I:601:FAD:HM73	2.02	0.42
1:A:118:PRO:HA	1:A:132:ALA:HA	2.02	0.42
1:E:350:ILE:HG13	1:E:351:PRO:HD2	2.01	0.42
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.55	0.42
1:E:404:SER:O	1:E:407:ASP:HB3	2.19	0.42
12:G:1130:HEM:CHA	12:G:1130:HEM:HBA2	2.50	0.42
5:I:601:FAD:C5X	7:I:1590:TEO:H2	2.49	0.42
1:A:46:THR:HB	1:A:146:LEU:HD13	2.02	0.41
1:A:286:ARG:NH2	7:A:1590:TEO:O2	2.53	0.41
1:A:251:VAL:HG13	2:B:57:GLU:OE1	2.19	0.41
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.54	0.41
12:K:1130:HEM:CBC	12:K:1130:HEM:HHD	2.41	0.41
2:B:155:CYS:SG	2:B:173:ALA:HB2	2.60	0.41
3:K:58:PHE:CB	4:L:45:TYR:HD1	2.34	0.41
1:A:327:LEU:O	1:A:330:ILE:HG13	2.21	0.41
1:A:578:ARG:NH1	1:A:579:PRO:O	2.54	0.41
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.56	0.41
1:A:54:THR:HG23	1:A:133:ARG:HG3	2.02	0.41
1:E:404:SER:O	1:E:408:LEU:HG	2.21	0.41
1:I:395:HIS:ND1	1:I:399:ARG:HG3	2.35	0.41
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.51	0.41
1:A:251:VAL:HG11	1:A:333:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:O	1:A:464:GLN:HA	2.21	0.41
1:E:360:ILE:HD12	1:E:389:ILE:HG13	2.03	0.41
3:G:31:ARG:O	3:G:35:VAL:HG23	2.20	0.41
1:I:404:SER:O	1:I:408:LEU:HG	2.20	0.41
1:E:223:VAL:HG12	1:E:227:ILE:HD12	2.02	0.41
2:F:77:THR:HA	2:F:78:PRO:HD3	1.91	0.41
1:E:244:THR:HG22	1:E:349:VAL:HG21	2.03	0.41
1:I:55:VAL:HG13	1:I:57:LEU:HG	2.03	0.41
2:J:55:CYS:O	2:J:56:ARG:HG3	2.21	0.41
2:F:55:CYS:HB3	2:F:60:CYS:HB3	2.02	0.41
1:E:286:ARG:HH12	7:E:1590:TEO:C4	2.32	0.40
2:F:222:PRO:O	2:F:226:ILE:HG13	2.20	0.40
1:A:404:SER:HB3	5:A:601:FAD:N1	2.36	0.40
12:K:1130:HEM:O2A	4:L:79:VAL:HG23	2.21	0.40
1:A:389:ILE:O	1:A:389:ILE:HG13	2.21	0.40
1:A:500:ASP:HB3	2:B:47:PRO:HG2	2.02	0.40
1:A:451:ARG:CA	1:A:451:ARG:HH11	2.33	0.40
2:F:170:ILE:HA	2:F:170:ILE:HD13	1.91	0.40
2:J:58:GLY:HA2	8:J:302:FES:S1	2.62	0.40
2:F:95:PRO:O	2:F:157:THR:HB	2.22	0.40
1:I:77:ASP:HB3	1:I:537:ARG:HG2	2.04	0.40
1:I:91:THR:O	1:I:92:GLY:C	2.60	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	586/588 (100%)	560 (96%)	24 (4%)	2 (0%)	43	79
1	E	586/588 (100%)	558 (95%)	26 (4%)	2 (0%)	43	79
1	I	586/588 (100%)	561 (96%)	23 (4%)	2 (0%)	43	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	236/238 (99%)	223 (94%)	12 (5%)	1 (0%)	36	74
2	F	236/238 (99%)	220 (93%)	15 (6%)	1 (0%)	36	74
2	J	236/238 (99%)	223 (94%)	12 (5%)	1 (0%)	36	74
3	C	119/129 (92%)	114 (96%)	5 (4%)	0	100	100
3	G	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
3	K	119/129 (92%)	116 (98%)	3 (2%)	0	100	100
4	D	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	H	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	L	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
All	All	3132/3210 (98%)	2984 (95%)	139 (4%)	9 (0%)	43	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLY
1	E	92	GLY
1	I	92	GLY
1	A	472	SER
1	E	472	SER
1	I	472	SER
2	F	108	GLY
2	J	108	GLY
2	B	108	GLY

### 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	473/473 (100%)	464 (98%)	9 (2%)	60	84
1	E	473/473 (100%)	464 (98%)	9 (2%)	60	84
1	I	473/473 (100%)	465 (98%)	8 (2%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	208/208 (100%)	197 (95%)	11 (5%)	25	62
2	F	208/208 (100%)	198 (95%)	10 (5%)	28	65
2	J	208/208 (100%)	199 (96%)	9 (4%)	32	68
3	C	101/109 (93%)	99 (98%)	2 (2%)	58	83
3	G	101/109 (93%)	100 (99%)	1 (1%)	78	92
3	K	101/109 (93%)	100 (99%)	1 (1%)	78	92
4	D	88/96 (92%)	86 (98%)	2 (2%)	53	81
4	H	88/96 (92%)	86 (98%)	2 (2%)	53	81
4	L	88/96 (92%)	86 (98%)	2 (2%)	53	81
All	All	2610/2658 (98%)	2544 (98%)	66 (2%)	50	80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	119	PHE
1	A	214	ASN
1	A	303	CYS
1	A	304	ASP
1	A	373	GLU
1	A	378	VAL
1	A	451	ARG
1	A	574	GLU
2	B	24	THR
2	B	45	LYS
2	B	53	ARG
2	B	56	ARG
2	B	120	TYR
2	B	141	GLU
2	B	161	SER
2	B	180	ARG
2	B	205	ARG
2	B	212	CYS
2	B	231	SER
3	C	13	LEU
3	C	51	SER
4	D	44	THR
4	D	60	PHE
1	E	2	LYS

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Mol	Chain	Res	Type
1	E	119	PHE
1	E	214	ASN
1	E	303	CYS
1	E	304	ASP
1	E	378	VAL
1	E	451	ARG
1	E	541	SER
1	E	574	GLU
2	F	24	THR
2	F	53	ARG
2	F	56	ARG
2	F	120	TYR
2	F	138	GLU
2	F	141	GLU
2	F	161	SER
2	F	180	ARG
2	F	212	CYS
2	F	231	SER
3	G	13	LEU
4	H	44	THR
4	H	60	PHE
1	I	2	LYS
1	I	119	PHE
1	I	214	ASN
1	I	304	ASP
1	I	378	VAL
1	I	451	ARG
1	I	541	SER
1	I	574	GLU
2	J	24	THR
2	J	53	ARG
2	J	56	ARG
2	J	120	TYR
2	J	138	GLU
2	J	141	GLU
2	J	161	SER
2	J	180	ARG
2	J	231	SER
3	K	13	LEU
4	L	44	THR
4	L	60	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	449	ASN
4	D	14	HIS
4	D	78	GLN
1	E	449	ASN
4	H	78	GLN
1	I	449	ASN
4	L	78	GLN

### 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](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\# Z  > 2$
7	TEO	A	1590	-	1,8,8	0.10	0	0,10,10	0.00	-
5	FAD	A	601	-	51,58,58	1.41	8 (15%)	57,89,89	2.29	11 (19%)
8	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CBE	C	1129	-	15,17,17	1.55	1 (6%)	15,22,22	2.66	2 (13%)
12	HEM	C	1130	3,4	27,50,50	2.18	5 (18%)	17,82,82	1.83	5 (29%)
7	TEO	E	1590	-	1,8,8	0.50	0	0,10,10	0.00	-
5	FAD	E	601	-	51,58,58	1.50	8 (15%)	57,89,89	2.24	13 (22%)
8	FES	F	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	F	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	F	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	CBE	G	1129	-	15,17,17	1.50	2 (13%)	15,22,22	2.56	3 (20%)
12	HEM	G	1130	3,4	27,50,50	2.37	8 (29%)	17,82,82	1.28	3 (17%)
7	TEO	I	1590	-	1,8,8	0.85	0	0,10,10	0.00	-
5	FAD	I	601	-	51,58,58	1.44	6 (11%)	57,89,89	2.07	7 (12%)
8	FES	J	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	J	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	J	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	CBE	K	1129	-	15,17,17	1.76	3 (20%)	15,22,22	2.21	2 (13%)
12	HEM	K	1130	3,4	27,50,50	2.41	7 (25%)	17,82,82	2.11	6 (35%)

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
7	TEO	A	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	A	601	-	-	0/28/50/50	0/6/6/6
8	FES	B	302	2	-	0/0/4/4	0/1/1/1
9	SF4	B	303	2	-	0/0/48/48	0/6/5/5
10	F3S	B	304	2	-	0/0/24/24	0/3/3/3
11	CBE	C	1129	-	-	0/6/19/19	0/1/2/2
12	HEM	C	1130	3,4	-	0/6/54/54	0/0/8/8
7	TEO	E	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	E	601	-	-	0/28/50/50	0/6/6/6
8	FES	F	302	2	-	0/0/4/4	0/1/1/1
9	SF4	F	303	2	-	0/0/48/48	0/6/5/5
10	F3S	F	304	2	-	0/0/24/24	0/3/3/3
11	CBE	G	1129	-	-	0/6/19/19	0/1/2/2
12	HEM	G	1130	3,4	-	0/6/54/54	0/0/8/8
7	TEO	I	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	I	601	-	-	0/28/50/50	0/6/6/6
8	FES	J	302	2	-	0/0/4/4	0/1/1/1
9	SF4	J	303	2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	F3S	J	304	2	-	0/0/24/24	0/3/3/3
11	CBE	K	1129	-	-	0/6/19/19	0/1/2/2
12	HEM	K	1130	3,4	-	0/6/54/54	0/0/8/8

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	1130	HEM	C3C-C2C	-5.17	1.33	1.40
12	C	1130	HEM	C3C-C2C	-4.95	1.33	1.40
12	C	1130	HEM	C3B-C2B	-4.86	1.33	1.40
12	G	1130	HEM	C3B-C2B	-4.76	1.33	1.40
12	K	1130	HEM	C3B-C2B	-4.68	1.33	1.40
12	G	1130	HEM	C3C-C2C	-4.36	1.34	1.40
11	C	1129	CBE	C11-N10	-3.81	1.34	1.41
11	G	1129	CBE	C11-N10	-3.15	1.35	1.41
11	K	1129	CBE	C11-N10	-3.10	1.35	1.41
5	A	601	FAD	O4B-C4B	-2.07	1.40	1.45
5	E	601	FAD	O4B-C4B	-2.06	1.40	1.45
12	G	1130	HEM	CMC-C2C	2.00	1.56	1.51
12	G	1130	HEM	CMD-C2D	2.08	1.55	1.51
5	E	601	FAD	C2A-N1A	2.10	1.37	1.33
12	G	1130	HEM	C1C-C2C	2.11	1.47	1.42
5	A	601	FAD	C2A-N1A	2.11	1.37	1.33
12	K	1130	HEM	C1C-C2C	2.27	1.47	1.42
11	K	1129	CBE	C8-C3	2.33	1.54	1.49
5	A	601	FAD	C1'-N10	2.35	1.50	1.48
5	I	601	FAD	C5X-N5	2.49	1.39	1.35
5	A	601	FAD	C4-N3	2.54	1.37	1.33
5	I	601	FAD	C1'-N10	2.76	1.51	1.48
5	E	601	FAD	C4-N3	2.82	1.38	1.33
5	A	601	FAD	C5X-N5	2.87	1.39	1.35
12	C	1130	HEM	C3C-CAC	2.92	1.53	1.47
5	E	601	FAD	C5X-N5	2.95	1.39	1.35
11	G	1129	CBE	C1-C2	3.00	1.55	1.49
5	E	601	FAD	C1'-N10	3.13	1.51	1.48
12	C	1130	HEM	C3B-CAB	3.21	1.54	1.47
5	A	601	FAD	C2A-N3A	3.35	1.37	1.32
11	K	1129	CBE	C3-S4	3.46	1.81	1.74
5	I	601	FAD	C4-N3	3.53	1.39	1.33
12	K	1130	HEM	CAA-C2A	3.57	1.58	1.52
12	K	1130	HEM	C3C-CAC	3.58	1.54	1.47
5	I	601	FAD	C4X-N5	3.85	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	FAD	C2A-N3A	3.90	1.38	1.32
5	E	601	FAD	C10-N1	3.91	1.38	1.33
12	G	1130	HEM	C3B-CAB	4.00	1.55	1.47
5	A	601	FAD	C4X-N5	4.03	1.39	1.33
5	E	601	FAD	C2A-N3A	4.15	1.38	1.32
12	G	1130	HEM	C3C-CAC	4.26	1.56	1.47
12	K	1130	HEM	C3B-CAB	4.46	1.56	1.47
5	I	601	FAD	C10-N1	4.50	1.39	1.33
5	A	601	FAD	C10-N1	4.52	1.39	1.33
5	E	601	FAD	C4X-N5	4.88	1.40	1.33
12	C	1130	HEM	C3D-C2D	4.97	1.52	1.37
12	K	1130	HEM	C3D-C2D	5.57	1.54	1.37
12	G	1130	HEM	C3D-C2D	5.81	1.54	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	N3A-C2A-N1A	-11.29	119.20	128.86
5	I	601	FAD	N3A-C2A-N1A	-10.65	119.75	128.86
5	E	601	FAD	N3A-C2A-N1A	-10.40	119.96	128.86
11	C	1129	CBE	C3-C8-N10	-4.62	107.47	115.94
12	K	1130	HEM	C1D-C2D-C3D	-4.00	104.21	107.00
12	C	1130	HEM	C1D-C2D-C3D	-3.65	104.46	107.00
12	C	1130	HEM	CAD-CBD-CGD	-3.57	106.56	112.66
12	K	1130	HEM	CBA-CAA-C2A	-3.15	106.46	112.48
5	I	601	FAD	C4X-C4-N3	-3.15	118.99	123.47
5	A	601	FAD	C4X-C4-N3	-3.11	119.05	123.47
5	E	601	FAD	C4'-C3'-C2'	-2.79	107.53	113.40
5	A	601	FAD	C1B-N9A-C4A	-2.48	122.35	126.64
5	A	601	FAD	P-O3P-PA	-2.46	124.35	132.63
12	G	1130	HEM	CBA-CAA-C2A	-2.46	107.78	112.48
12	G	1130	HEM	C1D-C2D-C3D	-2.45	105.29	107.00
5	A	601	FAD	C4A-C5A-N7A	-2.40	107.09	109.41
12	C	1130	HEM	CBA-CAA-C2A	-2.39	107.92	112.48
5	E	601	FAD	C4X-C4-N3	-2.37	120.10	123.47
12	G	1130	HEM	CAA-CBA-CGA	-2.29	108.75	112.66
11	G	1129	CBE	C3-C8-N10	-2.29	111.75	115.94
12	K	1130	HEM	CBD-CAD-C3D	-2.28	108.11	112.47
12	C	1130	HEM	CMA-C3A-C4A	-2.26	125.00	128.46
5	E	601	FAD	C10-C4X-N5	-2.21	118.05	120.59
12	K	1130	HEM	CAD-CBD-CGD	-2.19	108.92	112.66
5	A	601	FAD	O2'-C2'-C3'	-2.02	104.11	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C1'-C2'-C3'	2.03	115.63	109.82
5	E	601	FAD	C4B-O4B-C1B	2.08	111.99	109.83
11	K	1129	CBE	C5-S4-C3	2.17	106.54	100.84
5	E	601	FAD	O4'-C4'-C3'	2.27	114.71	109.10
5	E	601	FAD	C6-C5X-N5	2.38	121.68	118.95
12	C	1130	HEM	C4C-C3C-C2C	2.59	108.71	106.90
11	G	1129	CBE	C5-S4-C3	2.66	107.83	100.84
5	E	601	FAD	C1'-C2'-C3'	2.76	117.70	109.82
5	E	601	FAD	C5X-C9A-N10	2.76	119.82	117.71
12	K	1130	HEM	C4C-C3C-C2C	2.85	108.89	106.90
5	I	601	FAD	C5X-C9A-N10	2.96	119.97	117.71
5	A	601	FAD	C1'-N10-C9A	3.00	120.98	118.31
5	I	601	FAD	C1'-C2'-C3'	3.12	118.73	109.82
5	I	601	FAD	C1'-N10-C10	3.18	121.64	118.46
5	A	601	FAD	C4-C4X-N5	3.28	122.38	118.70
5	I	601	FAD	C4X-N5-C5X	3.64	120.58	116.76
5	E	601	FAD	C4X-N5-C5X	3.74	120.67	116.76
5	E	601	FAD	C1'-N10-C10	3.94	122.39	118.46
5	E	601	FAD	C4-C4X-N5	4.21	123.43	118.70
12	K	1130	HEM	CAA-CBA-CGA	4.47	120.30	112.66
5	A	601	FAD	C4X-N5-C5X	4.68	121.67	116.76
5	I	601	FAD	C4-N3-C2	6.11	120.34	115.14
5	E	601	FAD	C4-N3-C2	6.34	120.54	115.14
5	A	601	FAD	C4-N3-C2	7.21	121.28	115.14
11	K	1129	CBE	O7-C2-C1	7.89	118.95	109.44
11	C	1129	CBE	O7-C2-C1	8.57	119.78	109.44
11	G	1129	CBE	O7-C2-C1	8.62	119.83	109.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1590	TEO	3	0
5	A	601	FAD	9	0
10	B	304	F3S	1	0
11	C	1129	CBE	2	0
12	C	1130	HEM	7	0
7	E	1590	TEO	5	0
5	E	601	FAD	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	304	F3S	2	0
12	G	1130	HEM	6	0
7	I	1590	TEO	6	0
5	I	601	FAD	17	0
8	J	302	FES	1	0
9	J	303	SF4	3	0
10	J	304	F3S	1	0
11	K	1129	CBE	2	0
12	K	1130	HEM	12	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	588/588 (100%)	-0.05	8 (1%) 75 63	45, 63, 84, 97	0
1	E	588/588 (100%)	0.05	22 (3%) 41 27	53, 72, 95, 112	0
1	I	588/588 (100%)	1.09	125 (21%) 1 0	91, 124, 168, 190	0
2	B	238/238 (100%)	-0.01	8 (3%) 45 30	45, 61, 88, 107	0
2	F	238/238 (100%)	-0.00	6 (2%) 57 43	54, 72, 104, 123	0
2	J	238/238 (100%)	0.45	30 (12%) 3 2	75, 96, 165, 189	0
3	C	121/129 (93%)	-0.07	4 (3%) 46 30	62, 76, 107, 120	0
3	G	121/129 (93%)	0.18	3 (2%) 57 43	71, 94, 119, 126	0
3	K	121/129 (93%)	0.50	12 (9%) 7 4	93, 118, 135, 144	0
4	D	105/115 (91%)	-0.12	2 (1%) 66 53	55, 75, 109, 124	0
4	H	105/115 (91%)	0.14	6 (5%) 24 13	63, 79, 137, 155	0
4	L	105/115 (91%)	0.10	8 (7%) 14 7	73, 90, 142, 165	0
All	All	3156/3210 (98%)	0.26	234 (7%) 14 8	45, 80, 147, 190	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	48	SER	6.8
1	I	499	LEU	6.8
1	I	500	ASP	6.4
1	I	203	GLY	6.1
1	I	268	HIS	5.8
1	I	262	GLY	5.8
1	I	265	LEU	5.6
1	I	266	ASN	5.3
1	I	1	MET	5.1
1	I	494	LEU	4.9
1	I	282	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	307	TRP	4.9
1	I	306	PRO	4.8
1	I	45	HIS	4.8
1	I	300	GLY	4.7
4	H	115	VAL	4.6
1	I	204	GLY	4.6
1	I	214	ASN	4.5
1	I	212	THR	4.5
1	I	216	HIS	4.4
1	A	268	HIS	4.4
1	I	312	LYS	4.3
2	J	29	GLU	4.3
1	I	303	CYS	4.3
1	E	452	ASN	4.3
1	I	44	SER	4.3
1	I	269	GLY	4.2
1	I	345	GLU	4.2
1	I	470	ASN	4.2
1	I	491	ARG	4.1
1	I	273	MET	4.1
1	I	270	GLU	4.0
1	I	478	ASP	4.0
1	I	267	LYS	4.0
1	I	420	GLN	4.0
1	I	263	TYR	3.9
1	I	175	GLY	3.9
1	I	450	ASN	3.9
1	I	310	HIS	3.9
1	I	50	GLN	3.9
1	I	301	ARG	3.9
1	I	529	SER	3.9
4	L	42	GLU	3.9
1	I	497	ALA	3.9
1	I	502	THR	3.9
1	I	295	ILE	3.8
2	J	31	ARG	3.8
1	I	496	ASN	3.8
1	I	275	ARG	3.8
4	H	114	GLY	3.8
4	L	115	VAL	3.8
1	I	218	ASN	3.8
2	J	100	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	444	LEU	3.7
1	I	299	GLU	3.7
1	I	452	ASN	3.6
1	I	272	PHE	3.6
1	I	176	ALA	3.6
1	I	541	SER	3.6
1	I	302	GLY	3.6
1	I	297	ILE	3.6
1	I	49	ALA	3.6
1	I	495	LYS	3.5
3	K	68	PHE	3.5
2	J	18	PRO	3.5
1	I	202	THR	3.5
2	J	54	SER	3.5
1	A	301	ARG	3.5
4	H	42	GLU	3.4
4	L	38	ALA	3.4
2	J	5	PHE	3.4
1	I	313	LEU	3.3
3	G	68	PHE	3.3
1	I	314	LYS	3.3
1	I	476	GLU	3.2
1	I	451	ARG	3.2
1	I	501	ASP	3.2
1	I	271	ARG	3.2
1	I	304	ASP	3.2
1	I	338	ALA	3.1
4	L	40	SER	3.1
2	B	16	ASP	3.1
1	I	260	GLU	3.1
1	I	276	TYR	3.1
1	E	306	PRO	3.1
1	I	535	GLU	3.1
1	I	213	THR	3.1
2	J	88	LYS	3.1
1	I	530	ALA	3.1
2	J	235	GLN	3.0
1	I	280	ALA	3.0
1	E	203	GLY	3.0
2	J	32	ASP	3.0
1	I	356	MET	3.0
1	E	202	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	197	ALA	3.0
4	L	39	THR	3.0
1	I	447	TRP	3.0
1	I	142	GLY	3.0
4	L	114	GLY	3.0
1	E	307	TRP	3.0
2	J	30	GLY	3.0
1	I	540	HIS	2.9
1	E	16	GLY	2.9
1	I	379	VAL	2.9
3	C	68	PHE	2.9
1	A	267	LYS	2.9
1	E	450	ASN	2.9
3	K	99	LEU	2.9
1	A	300	GLY	2.9
1	I	318	LEU	2.8
2	B	85	PRO	2.8
3	K	23	THR	2.8
3	K	98	TYR	2.8
2	J	14	VAL	2.8
1	I	296	GLU	2.8
1	I	38	LYS	2.8
1	I	346	PRO	2.8
1	I	279	ASN	2.8
1	A	543	PHE	2.8
1	E	44	SER	2.7
2	J	12	PRO	2.7
1	I	421	GLU	2.7
3	C	67	SER	2.7
1	I	309	PRO	2.7
1	I	524	TYR	2.7
2	B	2	ARG	2.7
3	C	66	GLY	2.7
1	I	215	ALA	2.7
1	I	588	TYR	2.7
1	I	129	GLU	2.7
1	I	344	LYS	2.7
1	I	293	ILE	2.6
1	I	342	PRO	2.6
3	K	22	ILE	2.6
1	I	353	CYS	2.6
3	K	8	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	K	102	THR	2.6
1	E	218	ASN	2.6
2	J	84	GLN	2.6
1	I	551	GLU	2.6
3	K	86	VAL	2.6
4	D	43	LEU	2.6
2	J	89	ILE	2.5
2	F	26	GLU	2.5
1	I	487	LEU	2.5
2	F	18	PRO	2.5
1	E	215	ALA	2.5
1	I	261	GLY	2.5
1	I	532	PHE	2.5
2	J	210	MET	2.5
3	K	101	GLU	2.5
2	J	55	CYS	2.5
1	E	111	ASP	2.5
2	J	58	GLY	2.5
2	J	16	ASP	2.5
1	I	498	ARG	2.5
2	J	10	TYR	2.5
1	E	45	HIS	2.5
1	I	382	GLY	2.5
2	F	54	SER	2.5
2	J	3	LEU	2.4
4	L	46	GLU	2.4
1	I	448	ASN	2.4
1	I	533	ARG	2.4
1	I	537	ARG	2.4
3	K	52	LEU	2.4
2	J	28	ASP	2.4
1	I	317	HIS	2.4
2	J	2	ARG	2.4
1	I	278	PRO	2.4
2	J	13	ASP	2.4
2	J	33	MET	2.4
2	F	15	ASP	2.3
1	I	347	ILE	2.3
4	D	42	GLU	2.3
2	J	85	PRO	2.3
1	I	343	VAL	2.3
1	I	169	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	10	TYR	2.3
3	C	65	MET	2.3
3	G	8	GLN	2.3
3	K	106	GLY	2.3
1	I	219	THR	2.3
1	I	536	SER	2.2
4	L	41	GLY	2.2
1	I	264	LEU	2.2
2	B	55	CYS	2.2
1	I	424	ALA	2.2
2	J	53	ARG	2.2
1	I	334	SER	2.2
1	E	1	MET	2.2
1	I	281	LYS	2.2
1	E	247	ALA	2.2
1	E	449	ASN	2.2
4	H	43	LEU	2.2
3	K	54	SER	2.2
1	I	196	ARG	2.2
1	A	303	CYS	2.2
1	E	487	LEU	2.1
2	B	84	GLN	2.1
1	E	489	VAL	2.1
1	I	298	ARG	2.1
3	G	56	GLU	2.1
1	E	304	ASP	2.1
1	I	349	VAL	2.1
1	I	211	SER	2.1
2	J	93	PRO	2.1
2	F	8	TYR	2.1
1	A	299	GLU	2.1
1	E	217	ILE	2.1
1	I	358	GLY	2.1
1	I	558	LEU	2.1
1	I	531	ASN	2.1
1	I	315	LEU	2.1
4	H	41	GLY	2.1
1	I	229	ALA	2.1
1	E	451	ARG	2.1
2	B	87	LYS	2.1
1	A	296	GLU	2.1
2	B	86	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	446	ARG	2.1
2	J	90	VAL	2.1
2	J	213	VAL	2.1
1	I	257	CYS	2.1
1	I	124	LYS	2.1
1	I	564	GLU	2.1
1	E	204	GLY	2.1
2	B	88	LYS	2.0
1	I	404	SER	2.0
4	H	40	SER	2.0
1	I	484	LEU	2.0
1	E	499	LEU	2.0
2	J	47	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TEO	I	1590	9/9	0.88	0.31	109,112,114,114	0
6	NA	I	1589	1/1	0.91	0.47	53,53,53,53	0
11	CBE	K	1129	16/16	0.91	0.36	85,91,97,97	0
5	FAD	I	601	53/53	0.91	0.47	106,112,121,125	0
8	FES	J	302	4/4	0.94	0.26	108,110,116,117	0
6	NA	A	1589	1/1	0.94	0.27	27,27,27,27	0
5	FAD	E	601	53/53	0.95	0.33	46,61,71,73	0
11	CBE	G	1129	16/16	0.96	0.29	56,60,62,62	0
11	CBE	C	1129	16/16	0.96	0.20	53,55,56,56	0
12	HEM	K	1130	43/43	0.96	0.29	50,54,72,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TEO	E	1590	9/9	0.97	0.16	50,52,53,55	0
12	HEM	G	1130	43/43	0.98	0.27	55,61,71,75	0
12	HEM	C	1130	43/43	0.98	0.25	40,48,62,67	0
9	SF4	J	303	8/8	0.98	0.18	83,87,90,91	0
6	NA	E	1589	1/1	0.98	0.33	45,45,45,45	0
7	TEO	A	1590	9/9	0.98	0.26	50,52,53,53	0
5	FAD	A	601	53/53	0.98	0.24	38,42,53,54	0
9	SF4	B	303	8/8	0.99	0.23	38,40,40,41	0
9	SF4	F	303	8/8	0.99	0.20	55,58,59,59	0
10	F3S	J	304	7/7	0.99	0.13	88,90,92,93	0
8	FES	F	302	4/4	0.99	0.25	54,55,56,58	0
10	F3S	F	304	7/7	0.99	0.13	64,69,72,75	0
8	FES	B	302	4/4	1.00	0.27	38,41,43,44	0
10	F3S	B	304	7/7	1.00	0.16	49,54,58,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.