Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:16 AM GMT

PDB ID	:	2WDV
Title	:	E. COLI SUCCINATE:QUINONE OXIDOREDUCTASE (SQR) WITH AN EMPTY QUINONE-BINDING POCKET
Authors	:	Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on	:	2009-03-26
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

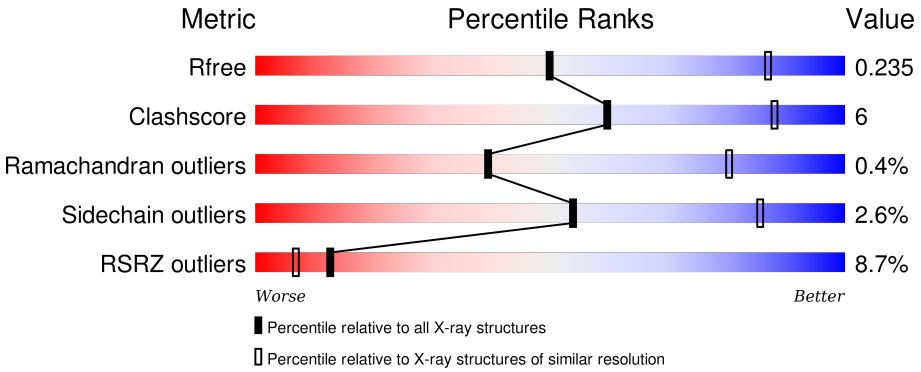
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	588	2% 88% 12%
1	E	588	3% 87% 12%
1	I	588	22% 84% 15%
2	B	238	4% 83% 15%
2	F	238	4% 85% 13%

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Mol	Chain	Length	Quality of chain
2	J	238	12% 82% 16%
3	C	129	4% 88% 6% 6%
3	G	129	11% 85% 8% 6%
3	K	129	19% 87% 7% 6%
4	D	115	4% 78% 11% 9%
4	H	115	7% 78% 11% 9%
4	L	115	7% 77% 11% 9%

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
6	TEO	E	1589	-	-	X	-
6	TEO	I	1589	-	-	X	-
8	FES	J	302	-	-	X	-
9	SF4	F	303	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24855 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 SUBUNIT.

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 SUBUNIT.

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			

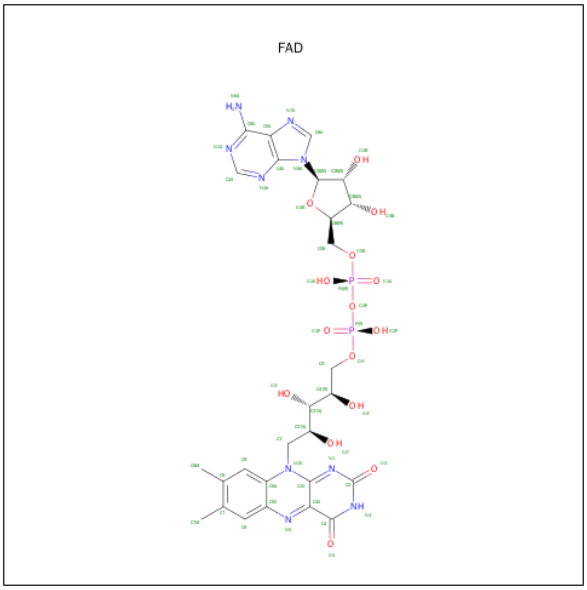
- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

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 PROTEIN.

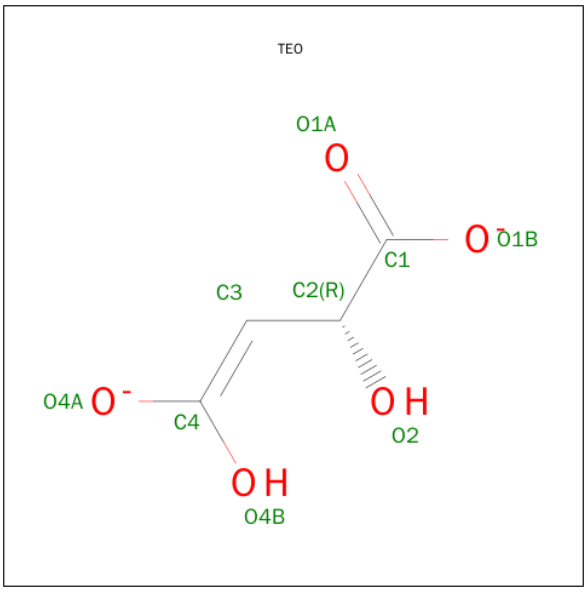
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	H	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			
4	L	105	Total	C	N	O	S	0	0	0
			836	577	123	133	3			

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

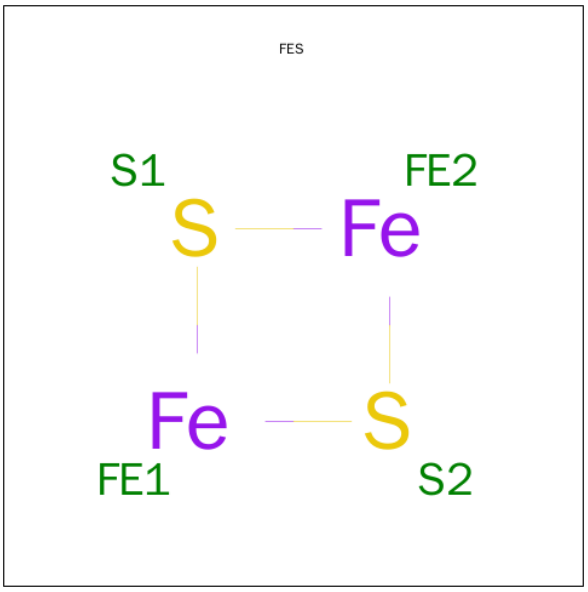


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

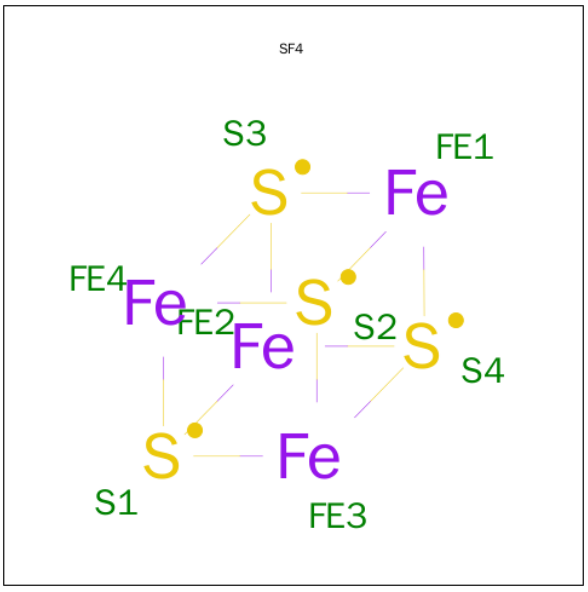
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Na 1 1	0	0
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

- 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 4 2 2	0	0
8	F	1	Total Fe S 4 2 2	0	0
8	J	1	Total Fe S 4 2 2	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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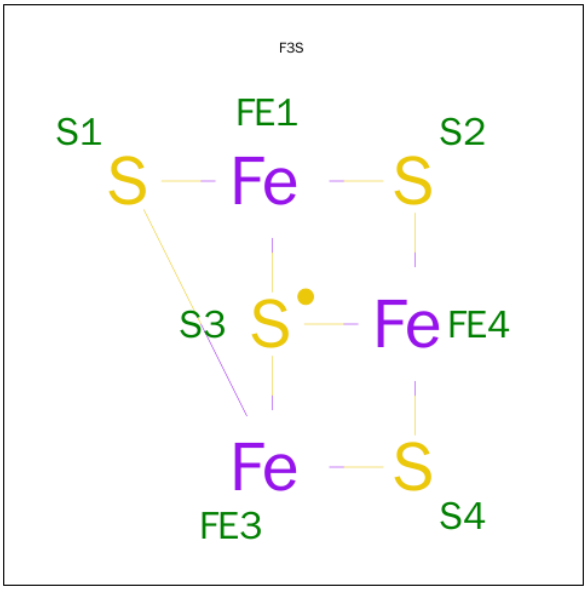
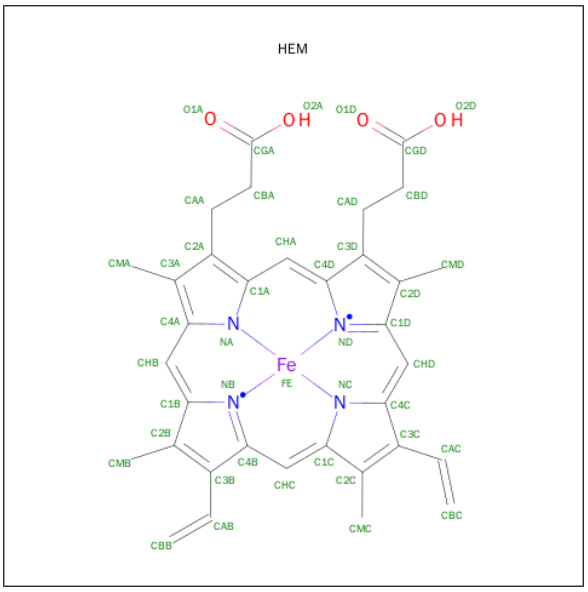
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Fe S 8 4 4	0	0
9	J	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



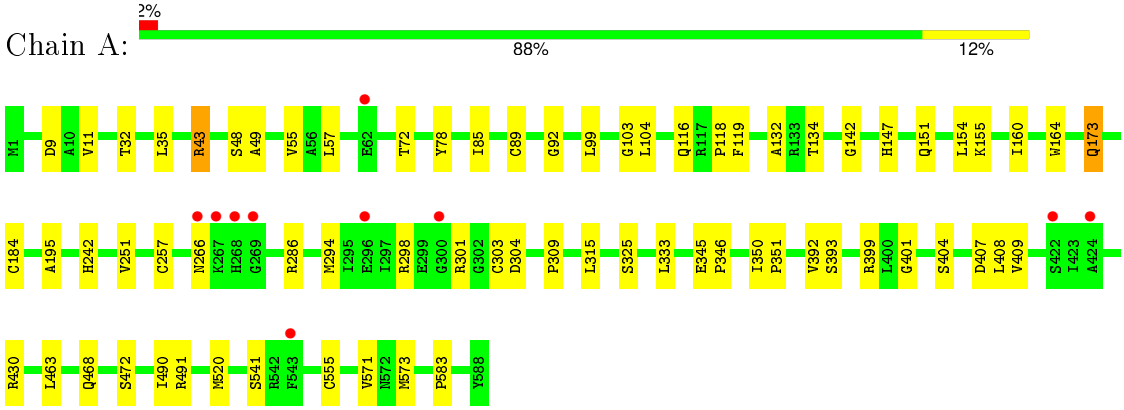
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.

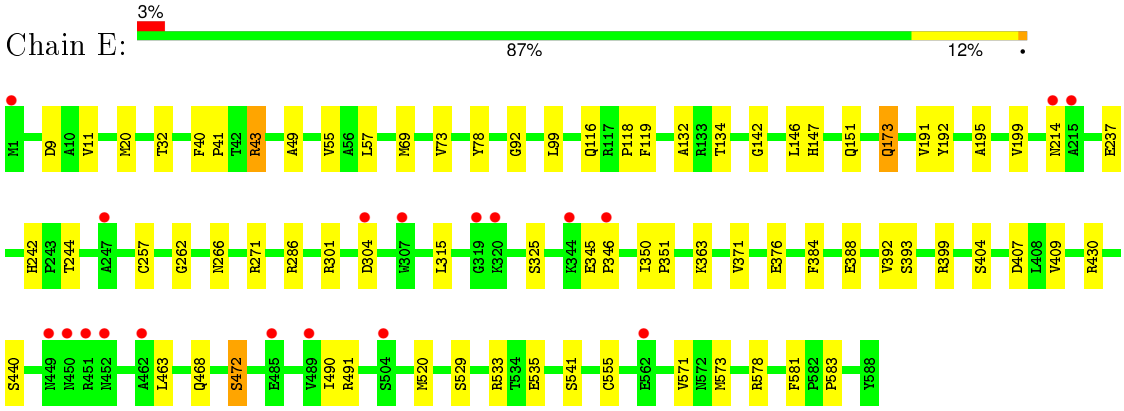
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain A:



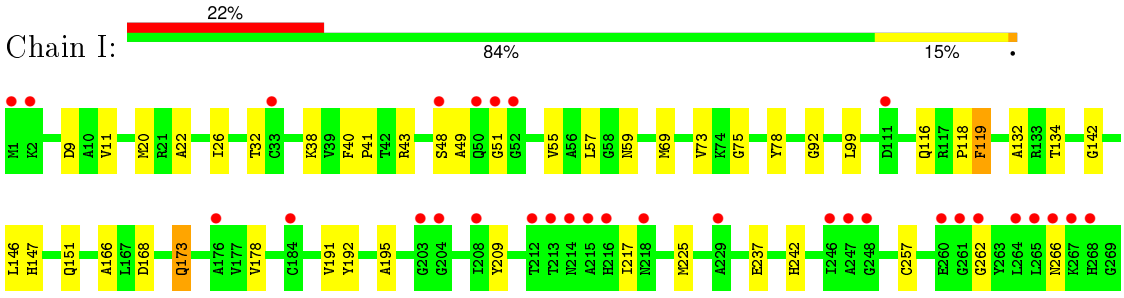
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

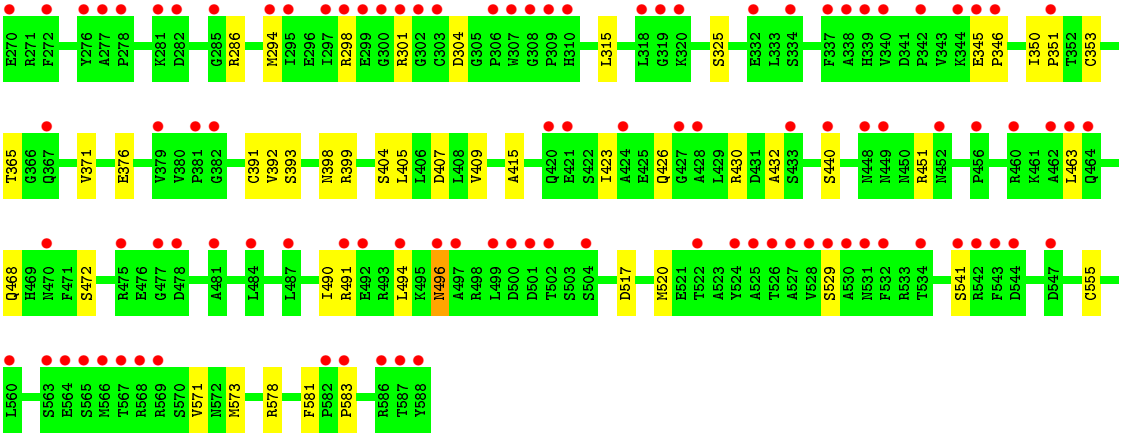
Chain E:



- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

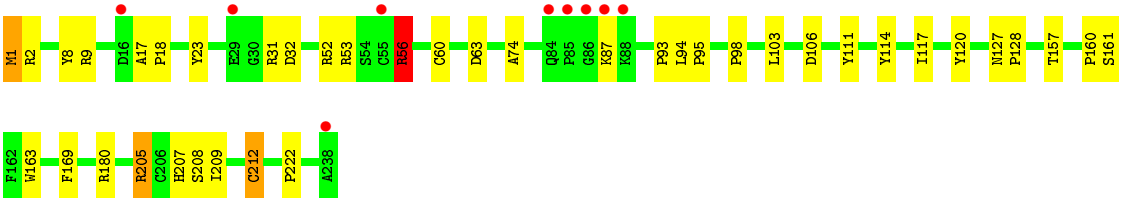
Chain I:





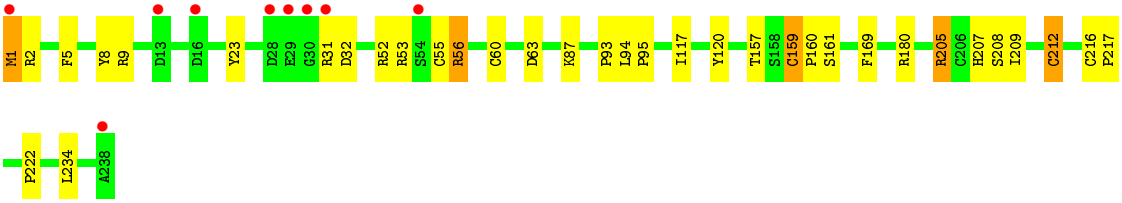
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B:



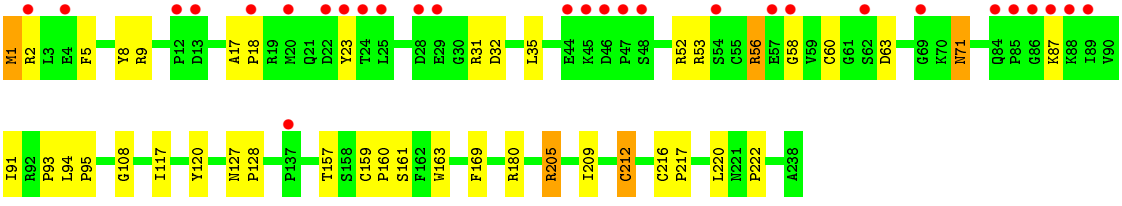
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F:



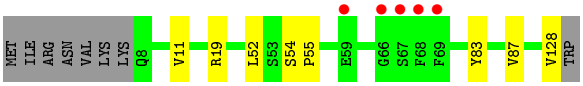
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J:



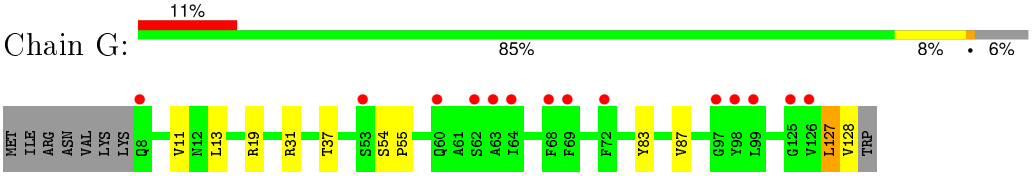
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C:



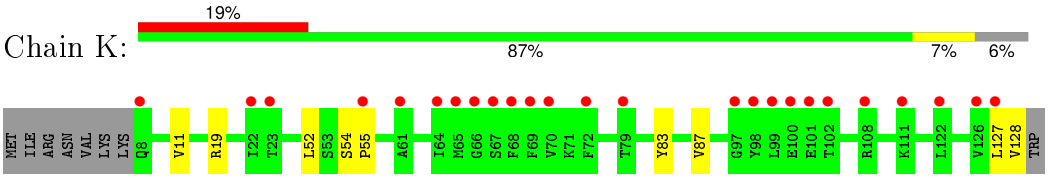
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G:



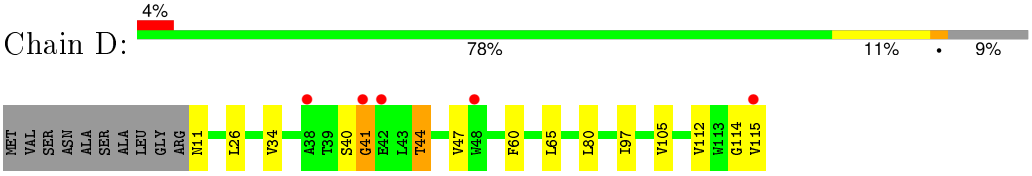
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:



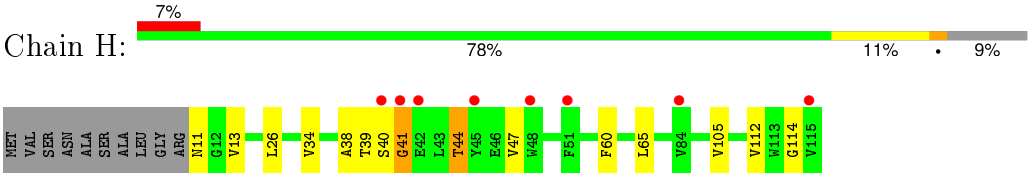
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN

Chain D:



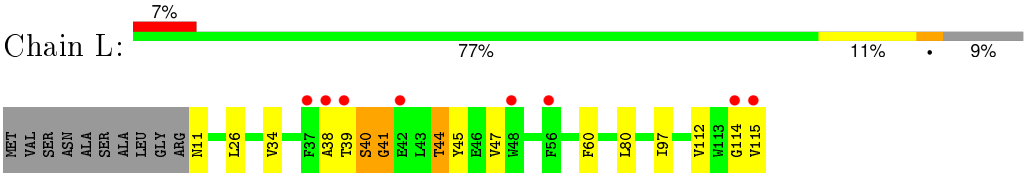
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN

Chain H:



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	120.34Å 184.85Å 204.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.85 – 3.20 49.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.85-3.20) 99.7 (49.95-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.205 , 0.233 0.207 , 0.235	Depositor DCC
R_{free} test set	3844 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 93.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 75707 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24855	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TEO, NA, SF4, 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	0.62	2/4611 (0.0%)	0.64	0/6237
1	E	0.52	1/4611 (0.0%)	0.61	0/6237
1	I	0.43	1/4611 (0.0%)	0.56	0/6237
2	B	0.66	0/1908	0.67	0/2578
2	F	0.59	1/1908 (0.1%)	0.66	0/2578
2	J	0.47	1/1908 (0.1%)	0.60	0/2578
3	C	0.54	0/953	0.57	0/1293
3	G	0.52	0/953	0.56	0/1293
3	K	0.44	0/953	0.50	0/1293
4	D	0.50	0/859	0.53	0/1175
4	H	0.50	0/859	0.53	0/1175
4	L	0.47	0/859	0.53	0/1175
All	All	0.53	6/24993 (0.0%)	0.60	0/33849

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	159	CYS	CB-SG	-6.16	1.71	1.82
1	I	173	GLN	CD-NE2	-5.74	1.18	1.32
1	E	173	GLN	CD-NE2	-5.73	1.18	1.32
2	J	71	ASN	CG-ND2	-5.45	1.19	1.32
1	A	89	CYS	CB-SG	-5.36	1.73	1.81
1	A	173	GLN	CD-NE2	-5.28	1.19	1.32

There are no bond angle outliers.

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	44	0
1	E	4522	0	4426	50	0
1	I	4522	0	4426	61	0
2	B	1869	0	1850	22	0
2	F	1869	0	1850	20	0
2	J	1869	0	1850	23	0
3	C	933	0	979	6	0
3	G	933	0	979	9	0
3	K	933	0	979	8	0
4	D	836	0	875	9	0
4	H	836	0	875	10	0
4	L	836	0	875	11	0
5	A	53	0	30	6	0
5	E	53	0	30	4	0
5	I	53	0	29	7	0
6	A	9	0	3	2	0
6	E	9	0	3	4	0
6	I	9	0	3	4	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	2	0
9	B	8	0	0	0	0
9	F	8	0	0	2	0
9	J	8	0	0	1	0
10	B	7	0	0	0	0
10	F	7	0	0	1	0
10	J	7	0	0	1	0
11	C	43	0	30	4	0
11	G	43	0	30	5	0
11	K	43	0	30	8	0
All	All	24855	0	24578	280	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 6.

All (280) 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)
11:C:1129:HEM:HBC2	11:C:1129:HEM:HHD	1.39	1.04
11:K:1129:HEM:HBA2	11:K:1129:HEM:HHA	1.39	1.02
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.50	0.94
11:K:1129:HEM:HBB2	4:L:26:LEU:HD13	1.51	0.90
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.52	0.88
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.58	0.84
11:G:1129:HEM:HHD	11:G:1129:HEM:HBC2	1.61	0.83
1:E:345:GLU:HG2	1:E:346:PRO:HD2	1.61	0.83
1:I:51:GLY:HA3	6:I:1589:TEO:O1A	1.83	0.78
2:J:58:GLY:HA2	8:J:302:FES:S1	2.26	0.76
1:I:345:GLU:HG2	1:I:346:PRO:HD2	1.68	0.76
11:K:1129:HEM:HBC2	11:K:1129:HEM:HHD	1.66	0.75
1:I:490:ILE:HG22	1:I:520:MET:CE	2.16	0.74
1:A:147:HIS:O	1:A:151:GLN:HG3	1.88	0.74
1:E:388:GLU:OE1	5:E:601:FAD:O3'	2.03	0.74
2:B:1:MET:O	2:B:1:MET:HG3	1.88	0.72
1:A:345:GLU:HG2	1:A:346:PRO:HD2	1.69	0.72
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.70	0.72
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.70	0.72
1:E:490:ILE:HG22	1:E:520:MET:CE	2.21	0.71
1:I:147:HIS:O	1:I:151:GLN:HG3	1.91	0.71
1:A:408:LEU:HD21	5:A:601:FAD:H5'2	1.73	0.69
1:I:490:ILE:HG22	1:I:520:MET:HE3	1.76	0.68
1:I:392:VAL:N	1:I:393:SER:HA	2.09	0.67
1:A:490:ILE:HG22	1:A:520:MET:CE	2.25	0.67
11:G:1129:HEM:HBB2	11:G:1129:HEM:HHC	1.77	0.66
1:A:49:ALA:HA	5:A:601:FAD:N5	2.12	0.65
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.32	0.65
2:J:160:PRO:HG2	2:J:209:ILE:HD13	1.77	0.65
1:E:490:ILE:HG22	1:E:520:MET:HE3	1.78	0.64
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.79	0.64
11:C:1129:HEM:HBC2	11:C:1129:HEM:CHD	2.17	0.63
1:A:350:ILE:HG13	1:A:351:PRO:HD2	1.80	0.63
1:E:392:VAL:N	1:E:393:SER:HA	2.12	0.63
3:G:31:ARG:NE	11:G:1129:HEM:O1A	2.32	0.62
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.13	0.62
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.35	0.62
1:A:392:VAL:N	1:A:393:SER:HA	2.13	0.62
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.35	0.62
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HG22	1:A:520:MET:HE1	1.82	0.61
1:E:147:HIS:O	1:E:151:GLN:HG3	2.01	0.60
2:F:160:PRO:HG2	2:F:209:ILE:HD13	1.83	0.60
3:K:128:VAL:O	3:K:128:VAL:HG12	2.02	0.60
1:E:286:ARG:HH12	6:E:1589:TEO:C4	2.14	0.59
2:J:212:CYS:HB2	2:J:222:PRO:HG2	1.83	0.59
1:E:345:GLU:HG2	1:E:346:PRO:CD	2.31	0.59
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.85	0.58
1:A:242:HIS:O	1:A:351:PRO:HA	2.03	0.58
1:I:350:ILE:HG13	1:I:351:PRO:HD2	1.86	0.58
1:E:350:ILE:HG13	1:E:351:PRO:HD2	1.84	0.58
1:I:490:ILE:HG22	1:I:520:MET:HE1	1.83	0.58
4:H:44:THR:HG23	4:H:47:VAL:HG13	1.85	0.58
11:K:1129:HEM:HHA	11:K:1129:HEM:CBA	2.24	0.58
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.34	0.58
1:I:209:TYR:CD2	1:I:353:CYS:SG	2.97	0.57
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.86	0.56
1:I:242:HIS:O	1:I:351:PRO:HA	2.04	0.56
3:G:128:VAL:HG12	3:G:128:VAL:O	2.05	0.56
1:I:49:ALA:HA	5:I:601:FAD:N5	2.21	0.56
1:E:173:GLN:CD	1:E:430:ARG:HH11	2.09	0.56
2:F:159:CYS:HB2	10:F:304:F3S:S2	2.46	0.55
4:L:44:THR:HG23	4:L:47:VAL:HG13	1.88	0.55
1:E:242:HIS:HD1	1:E:244:THR:H	1.52	0.55
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.88	0.55
11:K:1129:HEM:HBA2	11:K:1129:HEM:CHA	2.19	0.55
1:I:173:GLN:CD	1:I:430:ARG:HH11	2.09	0.55
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.88	0.55
1:A:49:ALA:HA	5:A:601:FAD:C6	2.38	0.54
1:I:345:GLU:HG2	1:I:346:PRO:CD	2.36	0.53
2:J:58:GLY:CA	8:J:302:FES:S1	2.97	0.53
2:B:31:ARG:HG2	2:B:32:ASP:N	2.23	0.53
11:C:1129:HEM:HHD	11:C:1129:HEM:CBC	2.24	0.53
3:G:54:SER:HB2	3:G:55:PRO:CD	2.39	0.53
2:J:159:CYS:HB2	10:J:304:F3S:S2	2.48	0.53
2:F:31:ARG:HG2	2:F:32:ASP:N	2.22	0.53
2:B:9:ARG:NH1	2:B:23:TYR:OH	2.42	0.53
3:K:127:LEU:HD23	3:K:127:LEU:O	2.09	0.53
1:I:51:GLY:CA	6:I:1589:TEO:O1A	2.55	0.53
3:K:128:VAL:O	3:K:128:VAL:CG1	2.56	0.53
3:C:128:VAL:HG12	3:C:128:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HD3	2:B:60:CYS:O	2.10	0.52
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.44	0.52
1:I:116:GLN:HA	1:I:134:THR:O	2.09	0.52
1:I:468:GLN:O	1:I:472:SER:HB2	2.10	0.52
11:G:1129:HEM:HBB2	4:H:26:LEU:HD13	1.91	0.52
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.92	0.52
4:D:44:THR:HG23	4:D:47:VAL:HG13	1.91	0.52
2:J:1:MET:O	2:J:1:MET:HG3	2.09	0.52
1:E:490:ILE:HG22	1:E:520:MET:HE1	1.89	0.52
1:I:371:VAL:HA	1:I:376:GLU:O	2.09	0.52
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.23	0.51
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.92	0.51
1:A:78:TYR:CD1	1:A:583:PRO:HA	2.45	0.51
1:I:43:ARG:HD3	2:J:60:CYS:O	2.10	0.51
1:A:463:LEU:C	1:A:463:LEU:HD23	2.31	0.51
1:A:345:GLU:HG2	1:A:346:PRO:CD	2.37	0.51
3:C:54:SER:HB2	3:C:55:PRO:CD	2.40	0.51
1:I:391:CYS:SG	1:I:393:SER:HB2	2.51	0.51
1:A:490:ILE:HG22	1:A:520:MET:HE3	1.92	0.51
2:J:95:PRO:O	2:J:157:THR:HB	2.10	0.51
2:F:217:PRO:HD2	9:F:303:SF4:S2	2.51	0.51
2:F:212:CYS:HB2	2:F:222:PRO:HG2	1.93	0.51
1:I:578:ARG:NH1	1:I:581:PHE:CZ	2.79	0.51
1:E:463:LEU:C	1:E:463:LEU:HD23	2.31	0.51
2:F:1:MET:HG3	2:F:1:MET:O	2.10	0.51
2:J:9:ARG:NH1	2:J:23:TYR:OH	2.43	0.51
1:I:119:PHE:HZ	6:I:1589:TEO:O1A	1.94	0.50
1:E:20:MET:CE	1:E:146:LEU:CD1	2.89	0.50
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.93	0.50
2:B:160:PRO:HG2	2:B:209:ILE:HD13	1.93	0.50
1:A:173:GLN:CD	1:A:430:ARG:HH11	2.14	0.50
1:I:237:GLU:OE1	1:I:529:SER:HB3	2.12	0.50
1:E:242:HIS:O	1:E:351:PRO:HA	2.10	0.50
2:F:55:CYS:O	2:F:56:ARG:HD2	2.12	0.50
3:K:52:LEU:HB3	4:L:115:VAL:HG21	1.93	0.50
11:K:1129:HEM:CBB	4:L:26:LEU:HD13	2.34	0.49
1:A:408:LEU:HD11	5:A:601:FAD:H4'	1.94	0.49
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.47	0.49
1:A:35:LEU:HD23	1:A:160:ILE:HG12	1.93	0.49
3:G:128:VAL:CG1	3:G:128:VAL:O	2.60	0.49
2:F:95:PRO:O	2:F:157:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HB3	5:A:601:FAD:HM72	1.95	0.49
4:D:112:VAL:C	4:D:114:GLY:H	2.15	0.49
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.94	0.48
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.48	0.48
1:E:199:VAL:HG22	1:E:384:PHE:HB2	1.96	0.48
1:I:166:ALA:N	5:I:601:FAD:N1A	2.50	0.48
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.95	0.48
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.95	0.48
2:J:5:PHE:HB2	2:J:23:TYR:HB2	1.96	0.48
1:E:371:VAL:HA	1:E:376:GLU:O	2.14	0.48
1:A:294:MET:O	1:A:298:ARG:HB2	2.13	0.48
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.49	0.48
2:J:52:ARG:O	2:J:63:ASP:HB3	2.13	0.47
1:I:69:MET:O	1:I:73:VAL:HG23	2.14	0.47
2:J:217:PRO:HD2	9:J:303:SF4:S3	2.54	0.47
1:E:350:ILE:CG1	1:E:351:PRO:HD2	2.44	0.47
1:A:350:ILE:CG1	1:A:351:PRO:HD2	2.44	0.47
1:A:118:PRO:HA	1:A:132:ALA:HA	1.96	0.47
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.96	0.47
2:J:31:ARG:HG2	2:J:32:ASP:N	2.28	0.47
1:E:468:GLN:O	1:E:472:SER:HB2	2.13	0.47
1:I:266:ASN:HB2	1:I:301:ARG:O	2.14	0.47
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.50	0.47
1:I:405:LEU:HG	5:I:601:FAD:C2	2.44	0.47
1:A:9:ASP:HB2	1:A:32:THR:O	2.15	0.47
4:D:11:ASN:OD1	4:D:11:ASN:C	2.53	0.47
3:K:55:PRO:HA	4:L:45:TYR:CE1	2.50	0.47
11:K:1129:HEM:CHA	11:K:1129:HEM:CBA	2.89	0.46
11:K:1129:HEM:CBC	11:K:1129:HEM:HHD	2.40	0.46
1:E:271:ARG:O	1:E:271:ARG:HG2	2.15	0.46
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.97	0.46
1:E:20:MET:CE	1:E:146:LEU:HD11	2.45	0.46
3:K:54:SER:HB2	3:K:55:PRO:CD	2.45	0.46
2:J:117:ILE:C	2:J:117:ILE:HD12	2.35	0.46
1:E:78:TYR:CD1	1:E:583:PRO:HA	2.51	0.46
1:I:294:MET:O	1:I:298:ARG:HB2	2.16	0.46
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.97	0.46
1:A:401:GLY:HA2	6:A:1589:TEO:O4A	2.16	0.46
2:F:52:ARG:O	2:F:63:ASP:HB3	2.15	0.46
1:A:468:GLN:O	1:A:472:SER:HB2	2.16	0.46
3:G:127:LEU:O	3:G:127:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:GLN:HA	1:E:134:THR:O	2.16	0.46
1:I:286:ARG:HH12	6:I:1589:TEO:C4	2.29	0.45
4:D:80:LEU:HD11	4:D:97:ILE:HD12	1.97	0.45
1:I:490:ILE:CG2	1:I:520:MET:HE1	2.47	0.45
1:I:178:VAL:HG21	1:I:432:ALA:HB2	1.99	0.45
2:F:117:ILE:C	2:F:117:ILE:HD12	2.36	0.45
1:I:496:ASN:O	1:I:496:ASN:ND2	2.48	0.45
2:F:216:CYS:HA	9:F:303:SF4:S2	2.57	0.45
2:B:17:ALA:HB1	2:B:18:PRO:CD	2.46	0.45
1:E:214:ASN:N	1:E:214:ASN:HD22	2.13	0.45
4:H:112:VAL:C	4:H:114:GLY:H	2.20	0.45
1:E:40:PHE:CD1	1:E:41:PRO:HD2	2.51	0.45
1:E:404:SER:O	1:E:407:ASP:HB3	2.16	0.45
1:I:9:ASP:HB2	1:I:32:THR:O	2.16	0.45
11:C:1129:HEM:HBB2	11:C:1129:HEM:HHC	1.97	0.45
1:I:399:ARG:CZ	1:I:404:SER:HB2	2.47	0.45
4:L:112:VAL:C	4:L:114:GLY:H	2.18	0.45
4:H:38:ALA:O	4:H:39:THR:HG23	2.16	0.45
2:F:9:ARG:NH1	2:F:23:TYR:OH	2.50	0.45
3:C:128:VAL:CG1	3:C:128:VAL:O	2.65	0.45
1:A:490:ILE:CG2	1:A:520:MET:HE1	2.46	0.45
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.99	0.45
1:E:20:MET:HE2	1:E:146:LEU:HD11	1.98	0.44
1:E:242:HIS:CD2	6:E:1589:TEO:O2	2.71	0.44
1:E:49:ALA:HA	5:E:601:FAD:N5	2.32	0.44
1:E:69:MET:O	1:E:73:VAL:HG23	2.17	0.44
4:H:11:ASN:C	4:H:11:ASN:OD1	2.55	0.44
1:E:266:ASN:HB2	1:E:301:ARG:O	2.17	0.44
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.99	0.44
1:A:116:GLN:HA	1:A:134:THR:O	2.17	0.44
2:B:212:CYS:HB2	2:B:222:PRO:HG2	1.99	0.44
1:E:533:ARG:NH1	1:E:535:GLU:OE2	2.47	0.44
1:E:9:ASP:HB2	1:E:32:THR:O	2.17	0.44
1:I:168:ASP:HA	1:I:225:MET:HG2	1.99	0.44
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.48	0.44
1:I:404:SER:HB3	5:I:601:FAD:N1	2.33	0.44
4:L:44:THR:HG23	4:L:47:VAL:HG22	1.99	0.44
2:J:35:LEU:HD11	2:J:91:ILE:HD11	2.00	0.44
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.99	0.44
4:L:80:LEU:HD11	4:L:97:ILE:HD12	1.99	0.44
1:I:463:LEU:C	1:I:463:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:GLY:HA3	1:I:315:LEU:HD23	2.00	0.43
2:B:160:PRO:HA	2:B:163:TRP:CE3	2.54	0.43
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.48	0.43
4:L:38:ALA:O	4:L:39:THR:HG23	2.19	0.43
1:I:48:SER:HB3	5:I:601:FAD:HM72	2.00	0.43
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.49	0.43
4:H:44:THR:CG2	4:H:47:VAL:HG13	2.48	0.43
2:J:17:ALA:HB1	2:J:18:PRO:CD	2.49	0.43
1:I:22:ALA:O	1:I:26:ILE:HG13	2.19	0.43
2:B:63:ASP:OD2	2:B:74:ALA:HB3	2.19	0.43
2:B:56:ARG:C	2:B:56:ARG:HD2	2.39	0.43
2:B:127:ASN:N	2:B:128:PRO:CD	2.82	0.43
1:I:404:SER:O	1:I:407:ASP:HB3	2.19	0.43
4:L:11:ASN:C	4:L:11:ASN:OD1	2.57	0.43
1:I:40:PHE:CD1	1:I:41:PRO:HD2	2.54	0.43
5:I:601:FAD:H1'1	5:I:601:FAD:H9	1.80	0.42
1:E:237:GLU:OE1	1:E:529:SER:HB3	2.19	0.42
1:E:578:ARG:NH1	1:E:581:PHE:CZ	2.87	0.42
2:F:8:TYR:CG	2:F:93:PRO:HD3	2.54	0.42
2:B:111:TYR:O	2:B:114:TYR:HB3	2.20	0.42
1:I:75:GLY:O	1:I:398:ASN:HB3	2.19	0.42
2:F:5:PHE:HB2	2:F:23:TYR:HB2	2.01	0.42
2:B:52:ARG:O	2:B:63:ASP:HB3	2.20	0.42
4:L:40:SER:O	4:L:41:GLY:C	2.58	0.42
1:I:78:TYR:CD1	1:I:583:PRO:HA	2.54	0.42
4:D:65:LEU:HB3	4:D:105:VAL:HG22	2.00	0.42
2:J:160:PRO:HA	2:J:163:TRP:CE3	2.55	0.42
1:I:59:ASN:HB2	1:I:116:GLN:OE1	2.20	0.42
1:A:404:SER:O	1:A:407:ASP:HB3	2.19	0.42
2:J:71:ASN:OD1	2:J:94:LEU:HD23	2.20	0.42
3:G:13:LEU:HA	3:G:13:LEU:HD12	1.86	0.42
2:F:94:LEU:HA	2:F:95:PRO:HD3	1.91	0.42
2:J:35:LEU:HD11	2:J:91:ILE:CD1	2.50	0.42
3:G:37:THR:HG22	11:G:1129:HEM:HMB3	2.01	0.42
1:A:154:LEU:O	1:A:155:LYS:C	2.57	0.42
1:E:191:VAL:HG12	1:E:192:TYR:N	2.35	0.42
5:E:601:FAD:C4	6:E:1589:TEO:C3	2.98	0.41
1:E:399:ARG:CZ	1:E:404:SER:HB2	2.49	0.41
1:A:266:ASN:HB2	1:A:301:ARG:O	2.20	0.41
2:J:127:ASN:N	2:J:128:PRO:CD	2.84	0.41
4:D:26:LEU:HD23	4:D:26:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:HG11	1:A:333:LEU:HD22	2.02	0.41
1:I:494:LEU:HD21	1:I:517:ASP:HA	2.02	0.41
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.03	0.41
2:B:98:PRO:HB2	2:B:106:ASP:HB3	2.02	0.41
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.87	0.41
1:I:451:ARG:HD3	1:I:451:ARG:HA	1.89	0.41
3:C:52:LEU:HB3	4:D:115:VAL:HG21	2.02	0.41
2:J:216:CYS:SG	2:J:220:LEU:N	2.80	0.41
1:E:43:ARG:HD3	2:F:60:CYS:O	2.20	0.41
2:F:207:HIS:O	2:F:208:SER:HB2	2.20	0.41
1:I:20:MET:CE	1:I:146:LEU:CD1	2.99	0.41
2:B:117:ILE:HD12	2:B:117:ILE:C	2.41	0.41
1:I:350:ILE:CG1	1:I:351:PRO:HD2	2.48	0.41
1:E:262:GLY:HA3	1:E:315:LEU:HD23	2.03	0.41
4:H:65:LEU:HB3	4:H:105:VAL:HG22	2.03	0.41
1:I:191:VAL:CG1	1:I:192:TYR:N	2.84	0.41
1:I:118:PRO:HA	1:I:132:ALA:HA	2.02	0.41
1:A:303:CYS:O	1:A:309:PRO:HA	2.21	0.41
1:I:49:ALA:HB3	1:I:142:GLY:CA	2.50	0.41
2:B:31:ARG:CG	2:B:32:ASP:N	2.84	0.41
1:E:20:MET:HE2	1:E:146:LEU:CD1	2.51	0.41
1:E:118:PRO:HA	1:E:132:ALA:HA	2.03	0.41
4:D:40:SER:O	4:D:41:GLY:C	2.59	0.41
4:H:40:SER:O	4:H:41:GLY:C	2.59	0.41
2:B:207:HIS:O	2:B:208:SER:HB2	2.20	0.41
1:I:423:ILE:O	1:I:426:GLN:HG2	2.20	0.40
2:B:95:PRO:O	2:B:157:THR:HB	2.20	0.40
1:A:72:THR:HG22	1:A:85:ILE:HD13	2.04	0.40
1:A:103:GLY:O	1:A:104:LEU:C	2.59	0.40
1:I:365:THR:O	1:I:415:ALA:HA	2.22	0.40
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.57	0.40
2:F:1:MET:HB2	2:F:1:MET:HE3	1.85	0.40
1:E:191:VAL:CG1	1:E:192:TYR:N	2.84	0.40
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.92	0.40
1:I:38:LYS:HE3	1:I:217:ILE:HB	2.04	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%)	567 (97%)	18 (3%)	1 (0%)	52	88
1	E	586/588 (100%)	563 (96%)	21 (4%)	2 (0%)	46	85
1	I	586/588 (100%)	562 (96%)	23 (4%)	1 (0%)	52	88
2	B	236/238 (99%)	221 (94%)	14 (6%)	1 (0%)	39	80
2	F	236/238 (99%)	220 (93%)	16 (7%)	0	100	100
2	J	236/238 (99%)	220 (93%)	14 (6%)	2 (1%)	24	69
3	C	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
3	G	119/129 (92%)	115 (97%)	3 (2%)	1 (1%)	24	69
3	K	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
4	D	103/115 (90%)	94 (91%)	8 (8%)	1 (1%)	19	65
4	H	103/115 (90%)	95 (92%)	7 (7%)	1 (1%)	19	65
4	L	103/115 (90%)	95 (92%)	6 (6%)	2 (2%)	10	50
All	All	3132/3210 (98%)	2982 (95%)	138 (4%)	12 (0%)	39	80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	56	ARG
2	B	56	ARG
4	H	41	GLY
4	L	41	GLY
4	D	41	GLY
1	E	92	GLY
1	E	472	SER
3	G	127	LEU
1	I	92	GLY
4	L	40	SER
1	A	92	GLY
2	J	108	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	473/473 (100%)	466 (98%)	7 (2%)	72	91
1	E	473/473 (100%)	464 (98%)	9 (2%)	65	89
1	I	473/473 (100%)	465 (98%)	8 (2%)	68	90
2	B	208/208 (100%)	198 (95%)	10 (5%)	31	72
2	F	208/208 (100%)	198 (95%)	10 (5%)	31	72
2	J	208/208 (100%)	198 (95%)	10 (5%)	31	72
3	C	101/109 (93%)	99 (98%)	2 (2%)	63	88
3	G	101/109 (93%)	99 (98%)	2 (2%)	63	88
3	K	101/109 (93%)	99 (98%)	2 (2%)	63	88
4	D	88/96 (92%)	85 (97%)	3 (3%)	44	80
4	H	88/96 (92%)	85 (97%)	3 (3%)	44	80
4	L	88/96 (92%)	85 (97%)	3 (3%)	44	80
All	All	2610/2658 (98%)	2541 (97%)	69 (3%)	54	85

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	119	PHE
1	A	304	ASP
1	A	325	SER
1	A	491	ARG
1	A	541	SER
1	A	573	MET
2	B	1	MET
2	B	2	ARG
2	B	53	ARG
2	B	56	ARG
2	B	87	LYS
2	B	120	TYR
2	B	161	SER

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Mol	Chain	Res	Type
2	B	180	ARG
2	B	205	ARG
2	B	212	CYS
3	C	11	VAL
3	C	19	ARG
4	D	34	VAL
4	D	44	THR
4	D	60	PHE
1	E	43	ARG
1	E	119	PHE
1	E	304	ASP
1	E	325	SER
1	E	363	LYS
1	E	440	SER
1	E	491	ARG
1	E	541	SER
1	E	573	MET
2	F	1	MET
2	F	2	ARG
2	F	53	ARG
2	F	56	ARG
2	F	87	LYS
2	F	120	TYR
2	F	161	SER
2	F	180	ARG
2	F	205	ARG
2	F	212	CYS
3	G	11	VAL
3	G	19	ARG
4	H	34	VAL
4	H	44	THR
4	H	60	PHE
1	I	119	PHE
1	I	304	ASP
1	I	325	SER
1	I	440	SER
1	I	491	ARG
1	I	496	ASN
1	I	541	SER
1	I	573	MET
2	J	1	MET
2	J	2	ARG

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Mol	Chain	Res	Type
2	J	53	ARG
2	J	56	ARG
2	J	87	LYS
2	J	120	TYR
2	J	161	SER
2	J	180	ARG
2	J	205	ARG
2	J	212	CYS
3	K	11	VAL
3	K	19	ARG
4	L	34	VAL
4	L	44	THR
4	L	60	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\#\|Z\|>2$
6	TEO	A	1589	-	0,8,8	0.00	-	1,10,10	0.96	0
5	FAD	A	601	1	48,58,58	1.42	7 (14%)	54,89,89	2.25	13 (24%)
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	-
11	HEM	C	1129	3,4	30,50,50	2.11	6 (20%)	24,82,82	2.32	7 (29%)
6	TEO	E	1589	-	0,8,8	0.00	-	1,10,10	2.07	1 (100%)
5	FAD	E	601	1	48,58,58	1.35	6 (12%)	54,89,89	2.20	10 (18%)
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	HEM	G	1129	3,4	30,50,50	2.11	8 (26%)	24,82,82	2.00	6 (25%)
6	TEO	I	1589	-	0,8,8	0.00	-	1,10,10	0.58	0
5	FAD	I	601	1	48,58,58	1.27	5 (10%)	54,89,89	1.95	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	HEM	K	1129	3,4	30,50,50	2.18	6 (20%)	24,82,82	2.34	9 (37%)

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
6	TEO	A	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	A	601	1	-	0/30/50/50	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	0/0/3/3
11	HEM	C	1129	3,4	-	0/10/54/54	0/0/8/8
6	TEO	E	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	E	601	1	-	0/30/50/50	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	0/0/3/3
11	HEM	G	1129	3,4	-	0/10/54/54	0/0/8/8
6	TEO	I	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	I	601	1	-	0/30/50/50	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	0/0/3/3
11	HEM	K	1129	3,4	-	0/10/54/54	0/0/8/8

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	1129	HEM	C3B-C4B	-7.13	1.45	1.51
11	K	1129	HEM	C3B-C4B	-6.79	1.45	1.51
11	C	1129	HEM	C3B-C4B	-6.54	1.46	1.51
11	C	1129	HEM	C3D-C4D	-5.93	1.44	1.51
11	K	1129	HEM	C3D-C4D	-5.36	1.44	1.51
11	G	1129	HEM	C3D-C4D	-5.19	1.44	1.51
11	K	1129	HEM	C2C-C1C	-3.51	1.45	1.52
11	C	1129	HEM	C2C-C1C	-3.47	1.46	1.52
11	G	1129	HEM	C2C-C1C	-3.41	1.46	1.52
5	A	601	FAD	O4B-C4B	-2.27	1.39	1.45
11	C	1129	HEM	C2D-C1D	-2.23	1.44	1.51
5	A	601	FAD	C10-N10	-2.19	1.36	1.39
11	G	1129	HEM	C2D-C1D	-2.14	1.44	1.51
11	G	1129	HEM	C2B-C1B	-2.04	1.45	1.51
11	C	1129	HEM	CAA-C2A	2.06	1.55	1.52
11	G	1129	HEM	C3B-CAB	2.21	1.55	1.51
5	I	601	FAD	C2A-N1A	2.24	1.38	1.33
11	G	1129	HEM	C1C-NC	2.25	1.38	1.36
11	G	1129	HEM	C3C-CAC	2.27	1.55	1.51
11	K	1129	HEM	C1C-NC	2.33	1.38	1.36
11	K	1129	HEM	FE-ND	2.34	2.09	1.97
5	E	601	FAD	C10-N1	2.41	1.39	1.35
5	E	601	FAD	C2A-N1A	2.57	1.38	1.33
5	E	601	FAD	C5X-N5	2.58	1.39	1.35
5	A	601	FAD	C4-N3	2.62	1.38	1.33
5	E	601	FAD	C4-N3	2.68	1.38	1.33
5	I	601	FAD	C5X-N5	2.80	1.39	1.35
11	C	1129	HEM	C1C-NC	2.84	1.39	1.36
5	A	601	FAD	C2A-N1A	2.84	1.39	1.33
5	I	601	FAD	C4-N3	3.02	1.38	1.33
5	A	601	FAD	C5X-N5	3.12	1.40	1.35
11	K	1129	HEM	FE-NC	3.20	2.08	1.95
5	E	601	FAD	C2A-N3A	3.66	1.38	1.32
5	I	601	FAD	C4X-N5	3.74	1.39	1.33
5	A	601	FAD	C2A-N3A	3.86	1.39	1.32
5	I	601	FAD	C2A-N3A	4.21	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	601	FAD	C4X-N5	4.43	1.40	1.33
5	A	601	FAD	C4X-N5	4.74	1.40	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	601	FAD	N3A-C2A-N1A	-11.21	120.31	128.89
5	A	601	FAD	N3A-C2A-N1A	-10.29	121.01	128.89
5	I	601	FAD	N3A-C2A-N1A	-10.27	121.03	128.89
5	A	601	FAD	C4-C4X-C10	-4.20	117.26	119.94
11	C	1129	HEM	C3B-CAB-CBB	-4.03	118.27	124.46
5	E	601	FAD	P-O3P-PA	-3.44	123.06	132.73
11	K	1129	HEM	CBA-CAA-C2A	-3.44	106.37	112.53
11	C	1129	HEM	C3C-CAC-CBC	-3.15	119.63	124.46
11	K	1129	HEM	C3B-CAB-CBB	-2.94	119.94	124.46
5	A	601	FAD	P-O3P-PA	-2.94	124.48	132.73
5	A	601	FAD	O3B-C3B-C4B	-2.78	102.71	111.05
5	E	601	FAD	C4-C4X-C10	-2.68	118.22	119.94
5	A	601	FAD	O2'-C2'-C3'	-2.40	102.97	109.02
5	E	601	FAD	O3B-C3B-C4B	-2.36	103.96	111.05
5	A	601	FAD	C1B-N9A-C4A	-2.24	123.56	126.94
11	K	1129	HEM	CAA-C2A-C1A	-2.22	124.60	127.01
5	E	601	FAD	C1B-N9A-C4A	-2.14	123.70	126.94
5	I	601	FAD	C4X-C4-N3	-2.12	120.69	123.59
5	I	601	FAD	C4A-C5A-N7A	-2.07	107.58	109.48
5	I	601	FAD	O3'-C3'-C4'	2.01	113.81	108.75
6	E	1589	TEO	O2-C2-C3	2.07	113.84	109.53
5	A	601	FAD	O3P-PA-O5B	2.10	108.51	102.94
5	E	601	FAD	C5X-C9A-N10	2.18	119.28	117.62
5	A	601	FAD	C2B-C3B-C4B	2.31	107.36	102.61
11	G	1129	HEM	C2D-C3D-C4D	2.43	105.62	101.50
5	I	601	FAD	C4-C4X-N5	2.49	121.75	118.72
11	K	1129	HEM	C3B-C4B-CHC	2.59	126.80	123.16
11	C	1129	HEM	CMB-C2B-C3B	2.66	123.18	116.53
11	G	1129	HEM	CMD-C2D-C3D	2.75	126.51	114.35
11	G	1129	HEM	CMB-C2B-C3B	2.79	123.50	116.53
11	K	1129	HEM	CMD-C2D-C3D	2.91	127.22	114.35
5	E	601	FAD	C6-C5X-N5	2.95	122.75	118.96
11	K	1129	HEM	CMB-C2B-C3B	2.96	123.91	116.53
5	A	601	FAD	C4X-N5-C5X	3.12	120.35	116.76
11	C	1129	HEM	CMD-C2D-C3D	3.13	128.21	114.35
5	A	601	FAD	C4X-C10-N10	3.20	122.41	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	1129	HEM	CMC-C2C-C3C	3.29	124.74	116.53
5	I	601	FAD	C4X-N5-C5X	3.55	120.85	116.76
11	K	1129	HEM	CMC-C2C-C3C	3.70	125.76	116.53
5	A	601	FAD	C1'-N10-C9A	3.73	123.05	118.86
11	C	1129	HEM	CMC-C2C-C3C	3.84	126.12	116.53
11	C	1129	HEM	CAD-C3D-C4D	4.18	127.20	112.47
11	G	1129	HEM	CAD-C3D-C2D	4.27	125.49	113.22
5	E	601	FAD	C4-C4X-N5	4.33	123.98	118.72
11	K	1129	HEM	CAD-C3D-C2D	4.41	125.88	113.22
5	E	601	FAD	C4X-N5-C5X	4.44	121.86	116.76
5	E	601	FAD	C4-N3-C2	4.51	119.15	115.25
11	G	1129	HEM	CAD-C3D-C4D	4.65	128.87	112.47
11	K	1129	HEM	CAD-C3D-C4D	4.82	129.46	112.47
5	A	601	FAD	C4-N3-C2	5.02	119.59	115.25
5	A	601	FAD	C4-C4X-N5	5.03	124.82	118.72
11	C	1129	HEM	CAD-C3D-C2D	5.45	128.89	113.22
5	I	601	FAD	C4-N3-C2	5.47	119.98	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1589	TEO	2	0
5	A	601	FAD	6	0
11	C	1129	HEM	4	0
6	E	1589	TEO	4	0
5	E	601	FAD	4	0
9	F	303	SF4	2	0
10	F	304	F3S	1	0
11	G	1129	HEM	5	0
6	I	1589	TEO	4	0
5	I	601	FAD	7	0
8	J	302	FES	2	0
9	J	303	SF4	1	0
10	J	304	F3S	1	0
11	K	1129	HEM	8	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

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^{th} 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^2)	Q<0.9
1	A	588/588 (100%)	0.18	10 (1%) 73 60	54, 55, 56, 58	0
1	E	588/588 (100%)	0.26	19 (3%) 51 36	54, 55, 56, 58	0
1	I	588/588 (100%)	1.19	132 (22%) 1 1	54, 55, 56, 58	0
2	B	238/238 (100%)	0.24	9 (3%) 44 29	53, 55, 56, 57	0
2	F	238/238 (100%)	0.29	9 (3%) 44 29	54, 55, 56, 57	0
2	J	238/238 (100%)	0.71	29 (12%) 5 3	54, 55, 56, 57	0
3	C	121/129 (93%)	0.29	5 (4%) 41 27	54, 55, 56, 56	0
3	G	121/129 (93%)	0.49	14 (11%) 6 4	54, 55, 56, 56	0
3	K	121/129 (93%)	1.07	25 (20%) 1 1	54, 55, 56, 56	0
4	D	105/115 (91%)	0.10	5 (4%) 34 21	54, 55, 56, 57	0
4	H	105/115 (91%)	0.27	8 (7%) 17 9	54, 55, 56, 57	0
4	L	105/115 (91%)	0.13	8 (7%) 17 9	54, 55, 56, 57	0
All	All	3156/3210 (98%)	0.49	273 (8%) 13 7	53, 55, 56, 58	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	MET	8.1
1	I	338	ALA	7.6
1	I	334	SER	6.4
1	I	268	HIS	5.6
1	I	525	ALA	5.5
1	I	382	GLY	5.4
1	I	295	ILE	5.4
3	K	68	PHE	5.2
1	I	448	ASN	5.1
3	K	69	PHE	5.1
1	I	337	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
3	K	65	MET	5.0
3	G	68	PHE	5.0
2	J	87	LYS	4.8
2	J	89	ILE	4.8
1	I	565	SER	4.7
2	J	86	GLY	4.6
4	D	42	GLU	4.6
4	H	41	GLY	4.5
3	K	8	GLN	4.4
1	I	319	GLY	4.4
3	K	97	GLY	4.4
2	J	24	THR	4.3
2	J	88	LYS	4.3
1	I	463	LEU	4.3
3	C	68	PHE	4.2
1	I	588	TYR	4.2
1	I	563	SER	4.1
3	K	98	TYR	4.1
1	I	424	ALA	4.1
1	I	261	GLY	4.1
1	I	266	ASN	4.1
1	I	381	PRO	4.1
1	I	298	ARG	4.1
1	E	452	ASN	4.0
2	J	29	GLU	4.0
1	I	307	TRP	4.0
1	I	294	MET	4.0
1	I	524	TYR	4.0
1	I	345	GLU	3.9
1	I	583	PRO	3.8
3	C	66	GLY	3.8
4	H	42	GLU	3.8
1	I	501	ASP	3.8
1	I	320	LYS	3.8
1	I	541	SER	3.7
1	I	302	GLY	3.7
1	I	379	VAL	3.6
3	K	22	ILE	3.6
1	I	184	CYS	3.6
1	I	306	PRO	3.6
1	I	267	LYS	3.6
1	I	470	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	567	THR	3.6
1	I	213	THR	3.6
1	I	499	LEU	3.6
4	H	40	SER	3.6
3	K	101	GLU	3.5
1	I	428	ALA	3.5
1	I	529	SER	3.5
3	G	99	LEU	3.5
1	I	478	ASP	3.5
2	J	47	PRO	3.5
1	A	268	HIS	3.4
3	K	100	GLU	3.4
2	J	28	ASP	3.4
1	I	282	ASP	3.4
3	C	69	PHE	3.4
4	L	42	GLU	3.4
2	B	84	GLN	3.4
2	J	48	SER	3.4
3	C	67	SER	3.3
4	D	41	GLY	3.3
1	I	176	ALA	3.3
1	I	531	ASN	3.3
3	K	79	THR	3.3
2	J	2	ARG	3.3
1	I	300	GLY	3.3
1	I	452	ASN	3.3
1	I	427	GLY	3.3
1	I	270	GLU	3.2
1	I	527	ALA	3.2
1	I	2	LYS	3.2
3	G	64	ILE	3.2
2	J	4	GLU	3.2
3	K	127	LEU	3.2
1	I	421	GLU	3.2
1	I	500	ASP	3.2
2	J	45	LYS	3.2
3	G	53	SER	3.1
1	I	456	PRO	3.1
1	I	309	PRO	3.1
2	J	85	PRO	3.1
1	I	204	GLY	3.1
1	I	214	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	115	VAL	3.1
1	I	216	HIS	3.1
2	F	1	MET	3.1
1	E	489	VAL	3.1
1	I	420	GLN	3.1
3	K	67	SER	3.0
4	L	114	GLY	3.0
1	I	491	ARG	3.0
1	I	310	HIS	3.0
1	I	433	SER	3.0
1	I	301	ARG	3.0
1	I	582	PRO	3.0
3	K	126	VAL	3.0
3	G	98	TYR	3.0
1	I	526	THR	3.0
1	I	534	THR	2.9
1	I	569	ARG	2.9
1	I	277	ALA	2.9
1	I	264	LEU	2.9
2	B	16	ASP	2.9
1	E	450	ASN	2.9
2	B	86	GLY	2.9
1	I	497	ALA	2.9
1	I	208	ILE	2.9
1	I	342	PRO	2.9
1	I	460	ARG	2.9
1	I	346	PRO	2.8
1	E	562	GLU	2.8
1	I	544	ASP	2.8
3	K	66	GLY	2.8
2	F	28	ASP	2.8
4	L	39	THR	2.8
1	I	48	SER	2.8
1	I	276	TYR	2.8
1	I	299	GLU	2.8
1	I	481	ALA	2.8
2	B	87	LYS	2.8
1	I	462	ALA	2.8
2	J	84	GLN	2.7
1	I	528	VAL	2.7
2	J	18	PRO	2.7
1	I	464	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	30	GLY	2.7
2	F	29	GLU	2.7
3	G	8	GLN	2.7
4	D	38	ALA	2.7
4	L	38	ALA	2.7
1	I	566	MET	2.7
1	I	50	GLN	2.7
1	I	587	THR	2.7
1	A	267	LYS	2.7
2	F	54	SER	2.7
1	A	269	GLY	2.7
1	I	260	GLU	2.7
1	I	564	GLU	2.7
1	I	484	LEU	2.7
2	J	12	PRO	2.7
1	E	451	ARG	2.7
1	E	449	ASN	2.6
1	I	487	LEU	2.6
2	J	58	GLY	2.6
2	B	85	PRO	2.6
1	I	475	ARG	2.6
1	I	203	GLY	2.6
1	I	449	ASN	2.6
1	I	530	ALA	2.6
3	G	97	GLY	2.6
1	E	344	LYS	2.6
4	D	48	TRP	2.6
2	F	31	ARG	2.6
2	B	55	CYS	2.6
1	I	248	GLY	2.5
1	I	278	PRO	2.5
1	I	340	VAL	2.5
2	J	137	PRO	2.5
3	K	64	ILE	2.5
1	I	218	ASN	2.5
1	A	543	PHE	2.5
1	I	339	HIS	2.5
2	J	54	SER	2.5
3	G	60	GLN	2.5
1	E	462	ALA	2.5
4	H	45	TYR	2.5
2	J	25	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	214	ASN	2.5
4	H	115	VAL	2.5
3	K	70	VAL	2.4
1	I	492	GLU	2.4
3	K	61	ALA	2.4
1	E	307	TRP	2.4
3	G	62	SER	2.4
1	I	543	PHE	2.4
1	I	281	LYS	2.4
4	D	115	VAL	2.4
1	I	496	ASN	2.4
3	K	55	PRO	2.4
2	J	13	ASP	2.4
2	J	46	ASP	2.4
4	H	48	TRP	2.4
1	I	522	THR	2.4
1	I	502	THR	2.3
1	A	300	GLY	2.3
1	I	477	GLY	2.3
2	B	238	ALA	2.3
1	I	262	GLY	2.3
3	G	126	VAL	2.3
2	J	23	TYR	2.3
1	I	344	LYS	2.3
1	I	318	LEU	2.3
2	J	69	GLY	2.3
4	L	37	PHE	2.3
1	E	304	ASP	2.3
3	C	59	GLU	2.3
2	J	44	GLU	2.3
1	I	33	CYS	2.3
1	I	560	LEU	2.3
3	G	72	PHE	2.3
3	K	122	LEU	2.3
1	I	586	ARG	2.3
3	K	99	LEU	2.3
1	E	320	LYS	2.3
1	I	285	GLY	2.2
1	I	351	PRO	2.2
2	B	88	LYS	2.2
3	G	69	PHE	2.2
1	I	297	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	303	CYS	2.2
1	I	440	SER	2.2
2	J	62	SER	2.2
3	K	23	THR	2.2
2	F	238	ALA	2.2
1	I	51	GLY	2.2
1	A	62	GLU	2.2
1	I	212	THR	2.2
1	I	494	LEU	2.2
2	F	13	ASP	2.2
1	I	265	LEU	2.2
1	E	504	SER	2.2
1	I	547	ASP	2.2
1	I	367	GLN	2.1
3	G	125	GLY	2.1
4	L	48	TRP	2.1
1	I	246	ILE	2.1
1	I	542	ARG	2.1
1	I	308	GLY	2.1
2	F	16	ASP	2.1
2	J	22	ASP	2.1
4	H	51	PHE	2.1
1	E	215	ALA	2.1
3	K	108	ARG	2.1
4	H	84	VAL	2.1
1	I	532	PHE	2.1
1	E	1	MET	2.1
4	L	56	PHE	2.1
1	I	52	GLY	2.1
1	I	229	ALA	2.1
3	G	63	ALA	2.1
1	E	247	ALA	2.1
1	E	319	GLY	2.1
1	I	247	ALA	2.1
1	I	504	SER	2.1
1	A	424	ALA	2.1
1	A	422	SER	2.1
1	A	266	ASN	2.1
1	I	111	ASP	2.1
3	K	72	PHE	2.1
2	J	20	MET	2.1
3	K	102	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	29	GLU	2.0
2	J	57	GLU	2.0
1	E	346	PRO	2.0
1	I	215	ALA	2.0
3	K	111	LYS	2.0
1	I	568	ARG	2.0
1	I	272	PHE	2.0
1	A	296	GLU	2.0
1	E	485	GLU	2.0
1	I	332	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
11	HEM	G	1129	43/43	0.97	0.23	1.05	55,59,63,65	0
6	TEO	E	1589	9/9	0.90	0.28	0.51	43,45,47,48	0
11	HEM	K	1129	43/43	0.96	0.23	0.21	54,55,65,65	0
6	TEO	I	1589	9/9	0.89	0.26	-0.89	122,123,124,124	0
11	HEM	C	1129	43/43	0.97	0.17	-1.00	43,46,55,58	0
5	FAD	I	601	53/53	0.90	0.23	-1.09	70,80,90,93	0
6	TEO	A	1589	9/9	0.94	0.18	-2.08	33,35,35,38	0
10	F3S	F	304	7/7	0.98	0.09	-2.34	47,48,50,53	0
10	F3S	J	304	7/7	0.98	0.10	-2.41	61,64,66,69	0
8	FES	J	302	4/4	0.94	0.10	-2.51	70,71,72,73	0
8	FES	F	302	4/4	0.99	0.10	-2.54	32,33,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NA	I	1590	1/1	0.93	0.13	-2.62	41,41,41,41	0
5	FAD	E	601	53/53	0.96	0.14	-2.67	26,40,50,53	0
9	SF4	J	303	8/8	0.97	0.07	-3.26	60,61,64,64	0
5	FAD	A	601	53/53	0.97	0.12	-3.56	17,21,30,40	0
9	SF4	B	303	8/8	0.99	0.10	-4.01	28,28,30,33	0
8	FES	B	302	4/4	0.99	0.14	-4.02	30,31,34,35	0
7	NA	E	1590	1/1	0.96	0.11	-4.19	9,9,9,9	0
10	F3S	B	304	7/7	0.97	0.08	-4.94	43,45,49,49	0
9	SF4	F	303	8/8	0.99	0.07	-5.16	37,38,41,42	0
7	NA	A	1590	1/1	0.98	0.08	-5.68	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.