



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:03 am GMT

PDB ID : 2WU5
Title : CRYSTAL STRUCTURE OF THE E. COLI SUCCINATE:QUINONE OXIDOREDUCTASE (SQR) SDHD HIS71MET MUTANT
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-09-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

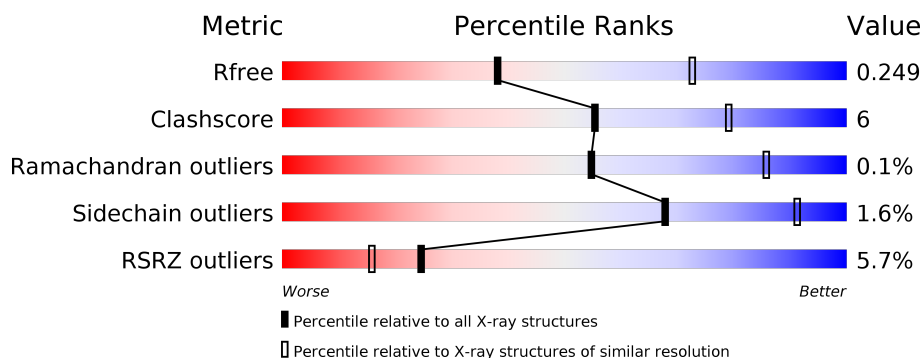
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



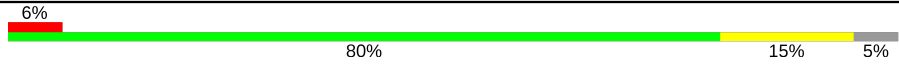

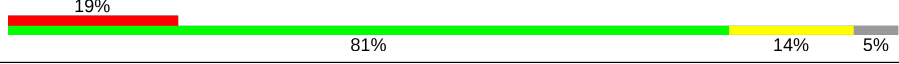

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 85%, yellow 85%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 15% </div> </div>
1	E	588	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 86%, yellow 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 14% </div> </div>
1	I	588	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 10%, orange 10%, orange 85%, yellow 85%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 15% </div> </div>
2	B	238	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 85%, yellow 85%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 14% </div> </div>
2	F	238	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 86%, yellow 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 14% </div> </div>
2	J	238	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 86%, yellow 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 14% </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
6	TEO	I	1589	-	-	X	-
7	NA	A	1590	-	-	-	X
7	NA	E	1590	-	-	-	X
7	NA	I	1590	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25164 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 B556 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			
3	G	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			
3	K	122	Total	C	N	O	S	0	0	0
			948	630	153	160	5			

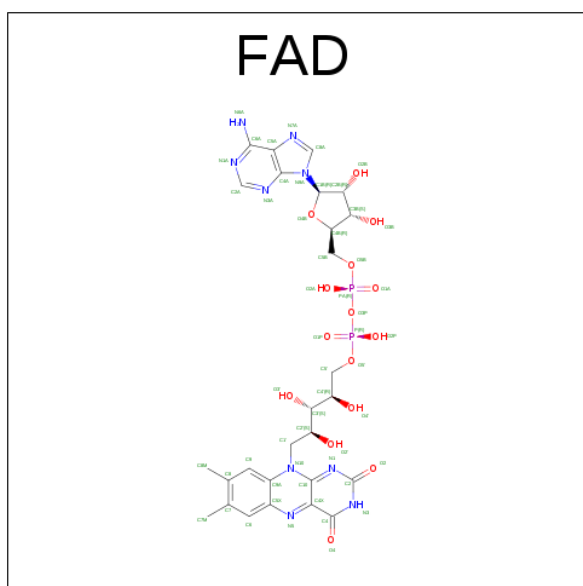
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			834	576	121	133	4			
4	H	105	Total	C	N	O	S	0	0	0
			834	576	121	133	4			
4	L	105	Total	C	N	O	S	0	0	0
			834	576	121	133	4			

There are 3 discrepancies between the modelled and reference sequences:

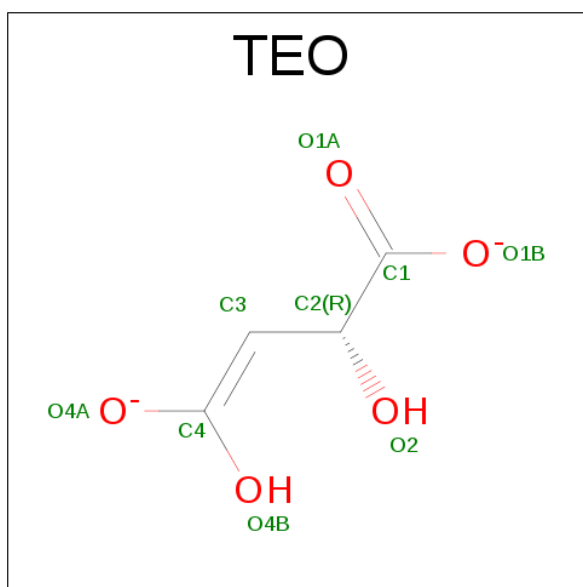
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44
H	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44
L	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44

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

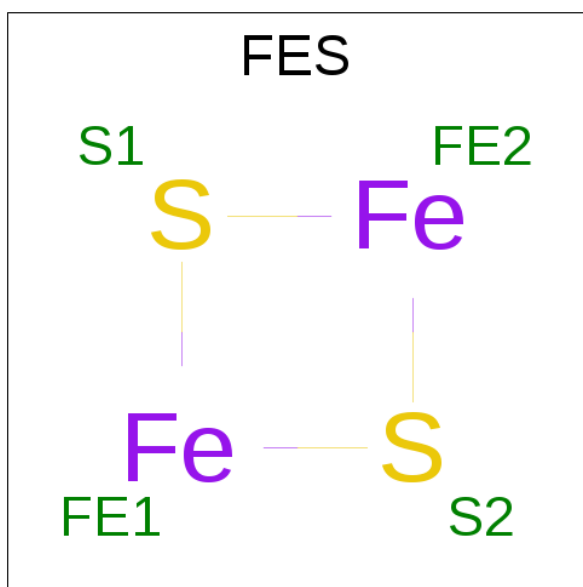


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	E	1	Total	C	O	0	0
			9	4	5		
6	I	1	Total	C	O	0	0
			9	4	5		

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

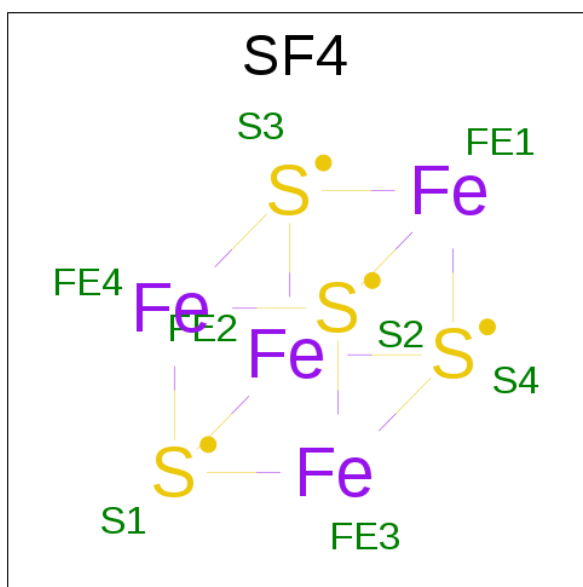
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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: Fe₄S₄).



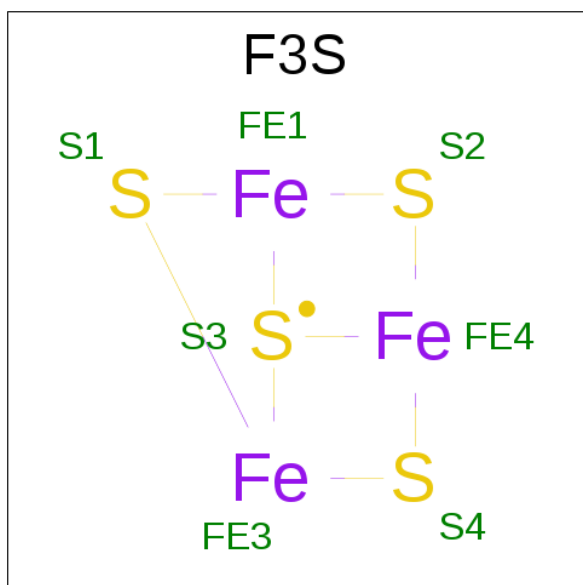
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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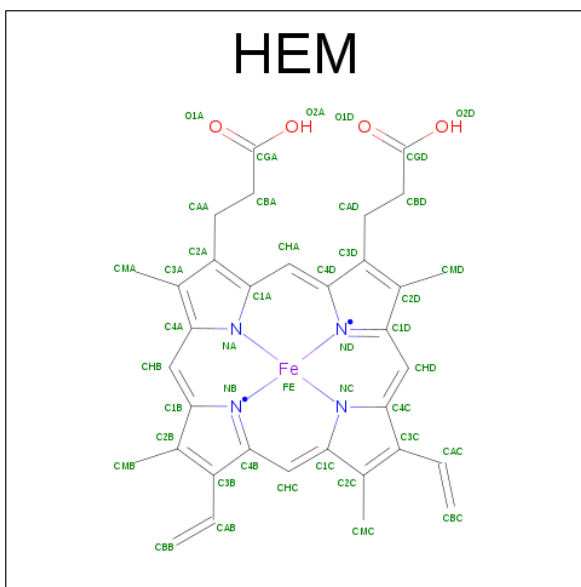
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	J	1	Total	Fe	S	0	0
			8	4	4		

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



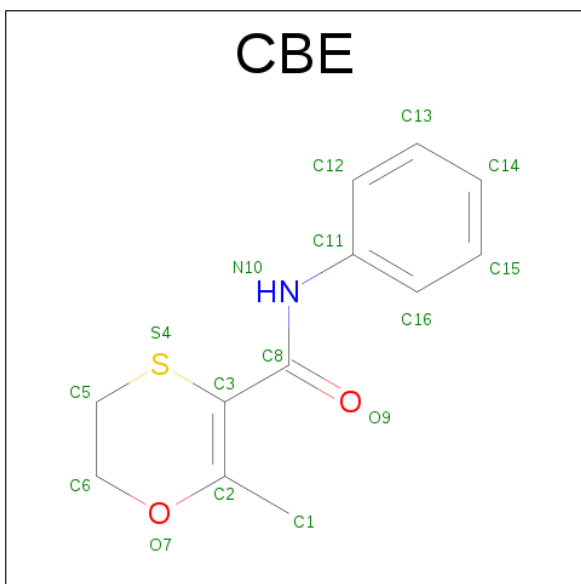
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		
10	F	1	Total	Fe	S	0	0
			7	3	4		
10	J	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 12 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula: $C_{12}H_{13}NO_2S$).



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

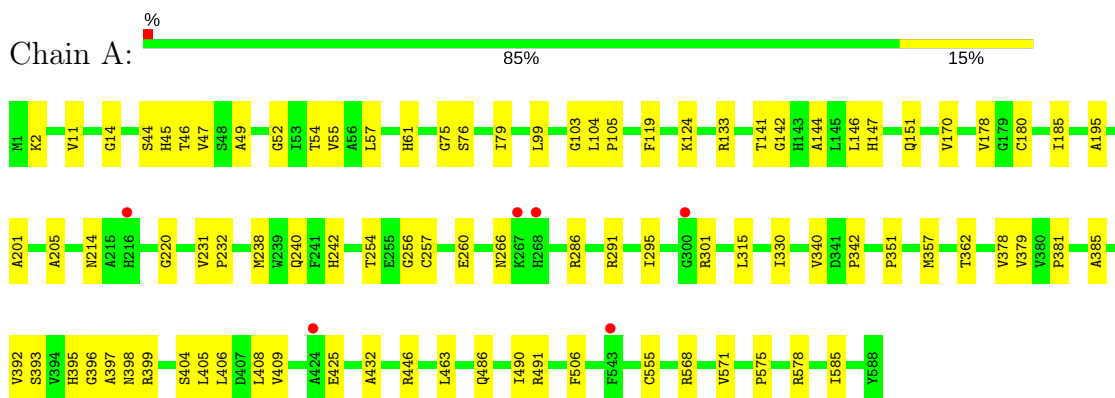
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	66	Total	O	0	0
			66	66		
13	B	33	Total	O	0	0
			33	33		
13	C	6	Total	O	0	0
			6	6		
13	D	2	Total	O	0	0
			2	2		
13	E	36	Total	O	0	0
			36	36		
13	F	28	Total	O	0	0
			28	28		
13	G	8	Total	O	0	0
			8	8		
13	H	2	Total	O	0	0
			2	2		
13	I	23	Total	O	0	0
			23	23		
13	J	15	Total	O	0	0
			15	15		
13	K	2	Total	O	0	0
			2	2		
13	L	1	Total	O	0	0
			1	1		

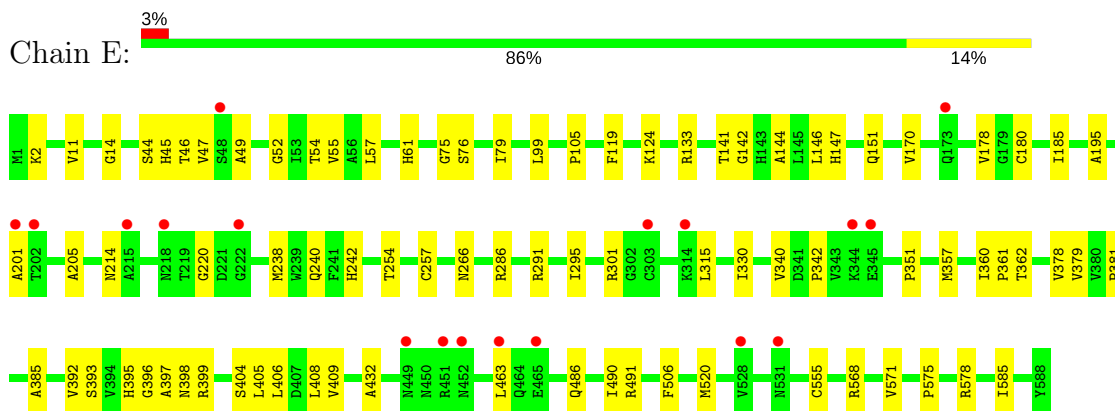
3 Residue-property plots [i](#)

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.

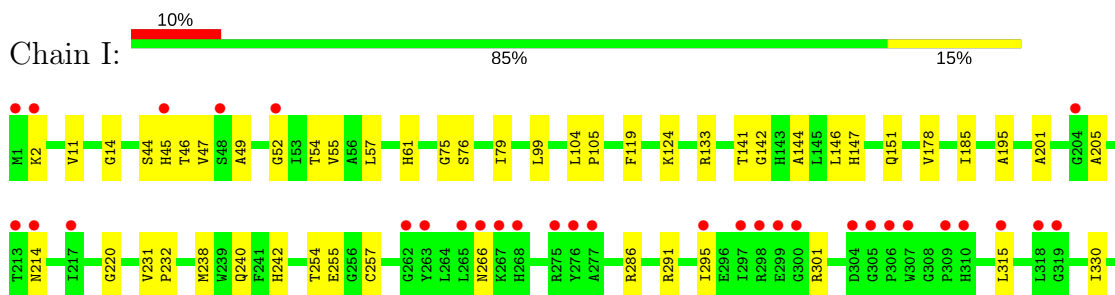
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

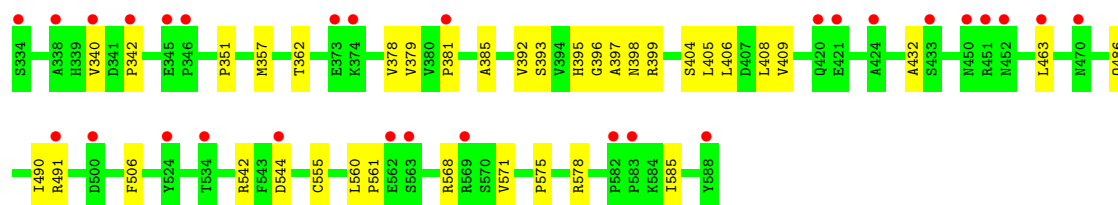


• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

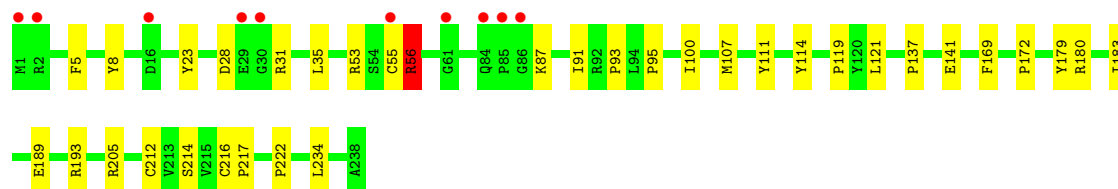
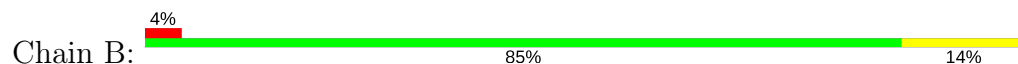


• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

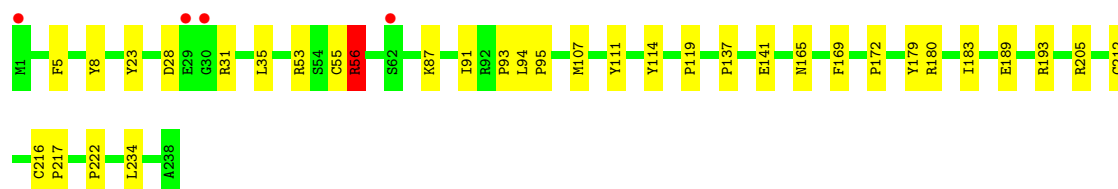
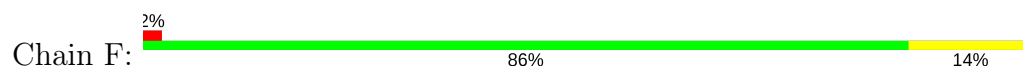




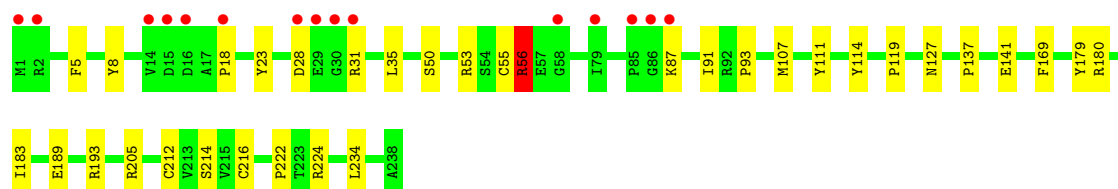
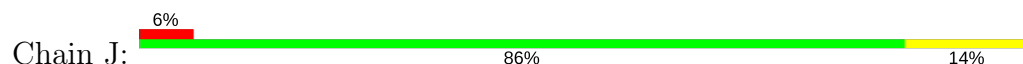
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



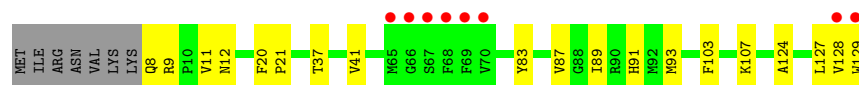
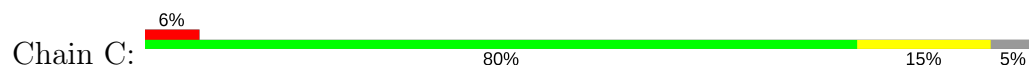
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



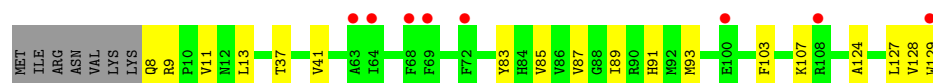
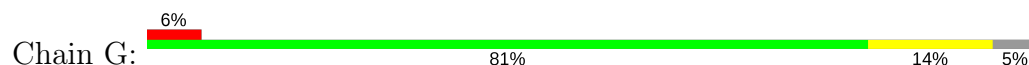
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



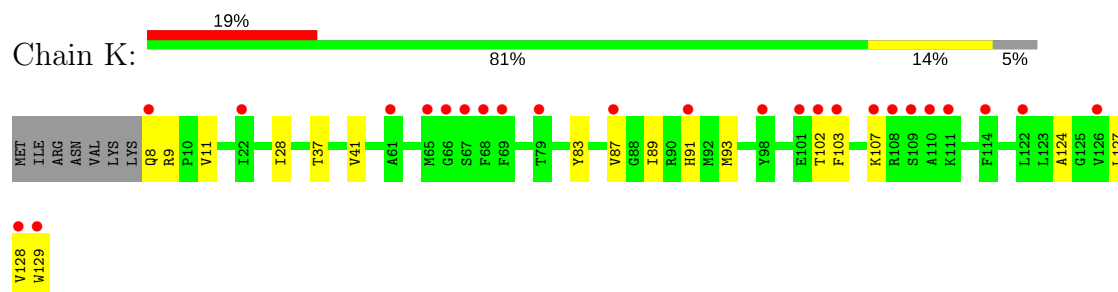
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



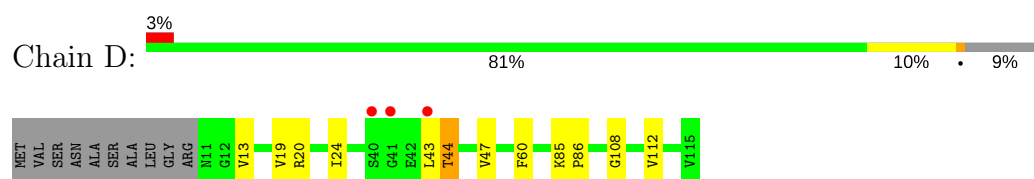
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



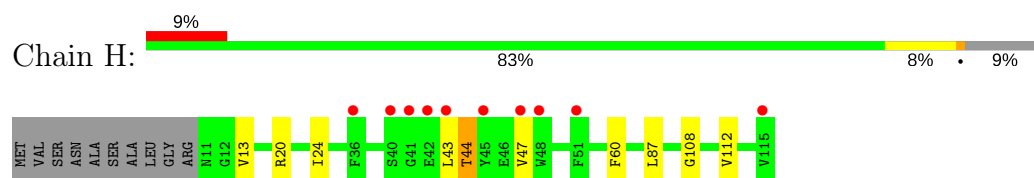
● Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



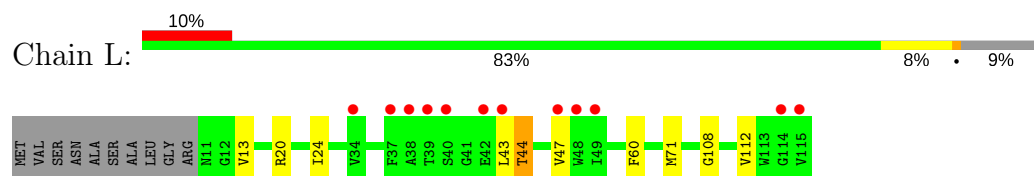
● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.06Å 183.82Å 203.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 2.80 48.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.83-2.80) 99.8 (48.79-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.252 0.213 , 0.249	Depositor DCC
R_{free} test set	10652 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25164	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CBE, NA, SF4, TEO, 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	0.21	0/4611	0.38	0/6237
1	E	0.21	0/4611	0.38	0/6237
1	I	0.21	0/4611	0.38	0/6237
2	B	0.21	0/1908	0.37	0/2578
2	F	0.21	0/1908	0.37	0/2578
2	J	0.21	0/1908	0.37	0/2578
3	C	0.22	0/970	0.36	0/1316
3	G	0.22	0/970	0.36	0/1316
3	K	0.22	0/970	0.36	0/1316
4	D	0.23	0/856	0.35	0/1170
4	H	0.23	0/856	0.35	0/1170
4	L	0.27	0/856	0.36	0/1170
All	All	0.22	0/25035	0.37	0/33903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	4426	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4522	0	4426	54	0
1	I	4522	0	4426	55	0
2	B	1869	0	1850	22	0
2	F	1869	0	1850	19	0
2	J	1869	0	1850	21	0
3	C	948	0	989	12	0
3	G	948	0	989	10	0
3	K	948	0	989	12	0
4	D	834	0	877	6	0
4	H	834	0	877	5	0
4	L	834	0	877	5	0
5	A	53	0	30	8	0
5	E	53	0	29	7	0
5	I	53	0	29	8	0
6	A	9	0	2	3	0
6	E	9	0	3	3	0
6	I	9	0	3	5	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	0	0
9	B	8	0	0	0	0
9	F	8	0	0	0	0
9	J	8	0	0	1	0
10	B	7	0	0	1	0
10	F	7	0	0	1	0
10	J	7	0	0	0	0
11	C	43	0	30	6	0
11	G	43	0	30	4	0
11	K	43	0	30	4	0
12	C	16	0	13	2	0
12	G	16	0	13	1	0
12	K	16	0	13	3	0
13	A	66	0	0	3	0
13	B	33	0	0	0	0
13	C	6	0	0	0	0
13	D	2	0	0	0	0
13	E	36	0	0	0	0
13	F	28	0	0	1	0
13	G	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	H	2	0	0	0	0
13	I	23	0	0	1	0
13	J	15	0	0	2	0
13	K	2	0	0	1	0
13	L	1	0	0	0	0
All	All	25164	0	24651	292	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 (292) 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:G:305:HEM:HHD	11:G:305:HEM:HBC2	1.49	0.93
11:C:305:HEM:HHD	11:C:305:HEM:HBC2	1.52	0.90
11:K:305:HEM:HBC2	11:K:305:HEM:HHD	1.53	0.89
11:K:305:HEM:HBB2	11:K:305:HEM:HHC	1.54	0.89
11:G:305:HEM:HBB2	11:G:305:HEM:HHC	1.53	0.88
11:C:305:HEM:HBB2	11:C:305:HEM:HHC	1.53	0.87
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.63	0.81
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.63	0.80
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.63	0.80
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.69	0.75
1:I:49:ALA:HB3	1:I:142:GLY:HA3	1.69	0.74
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.69	0.73
2:J:50:SER:HA	13:J:2002:HOH:O	1.92	0.69
2:B:55:CYS:O	2:B:56:ARG:HD3	1.94	0.68
2:F:55:CYS:O	2:F:56:ARG:HD3	1.94	0.67
12:K:1130:CBE:O9	12:K:1130:CBE:H16	1.94	0.67
1:I:392:VAL:N	1:I:393:SER:HA	2.10	0.67
2:J:55:CYS:O	2:J:56:ARG:HD3	1.94	0.67
1:E:392:VAL:N	1:E:393:SER:HA	2.10	0.66
1:E:76:SER:HB2	1:E:396:GLY:HA3	1.77	0.66
1:E:555:CYS:SG	1:E:568:ARG:HD2	2.36	0.66
1:A:76:SER:HB2	1:A:396:GLY:HA3	1.78	0.66
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.09	0.66
1:A:555:CYS:SG	1:A:568:ARG:HD2	2.36	0.65
1:I:76:SER:HB2	1:I:396:GLY:HA3	1.77	0.65
1:I:408:LEU:HD11	5:I:601:FAD:H4'	1.78	0.65
1:I:555:CYS:SG	1:I:568:ARG:HD2	2.36	0.65
1:A:392:VAL:N	1:A:393:SER:HA	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:PRO:HD2	1:E:144:ALA:HB1	1.80	0.64
1:I:105:PRO:HD2	1:I:144:ALA:HB1	1.80	0.64
2:J:114:TYR:O	2:J:119:PRO:HG3	1.99	0.63
1:A:105:PRO:HD2	1:A:144:ALA:HB1	1.80	0.63
2:B:114:TYR:O	2:B:119:PRO:HG3	1.99	0.62
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.35	0.62
2:J:169:PHE:CD1	2:J:205:ARG:HB2	2.35	0.62
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.81	0.62
2:F:114:TYR:O	2:F:119:PRO:HG3	1.99	0.61
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.35	0.61
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.81	0.61
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.81	0.61
3:K:127:LEU:HD23	3:K:127:LEU:O	2.01	0.60
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.82	0.60
3:G:127:LEU:O	3:G:127:LEU:HD23	2.01	0.60
1:E:408:LEU:HD11	5:E:601:FAD:H4'	1.82	0.60
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.31	0.60
1:A:2:LYS:O	1:A:2:LYS:HD3	2.02	0.60
3:C:127:LEU:O	3:C:127:LEU:HD23	2.01	0.59
1:E:2:LYS:HD3	1:E:2:LYS:O	2.02	0.59
1:I:2:LYS:O	1:I:2:LYS:HD3	2.03	0.59
2:F:56:ARG:O	2:F:56:ARG:HG2	2.03	0.59
2:J:56:ARG:HG2	2:J:56:ARG:O	2.02	0.59
1:I:286:ARG:HH22	6:I:1589:TEO:C3	2.16	0.59
2:B:56:ARG:O	2:B:56:ARG:HG2	2.02	0.59
5:I:601:FAD:N5	6:I:1589:TEO:H2	2.18	0.59
2:B:172:PRO:HG3	10:B:304:F3S:S3	2.43	0.58
1:A:405:LEU:HG	5:A:601:FAD:C2	2.34	0.57
12:C:1130:CBE:O9	12:C:1130:CBE:H16	2.04	0.57
2:J:127:ASN:HA	13:J:2007:HOH:O	2.04	0.57
2:F:172:PRO:HG3	10:F:304:F3S:S3	2.45	0.56
1:I:49:ALA:HA	5:I:601:FAD:N5	2.21	0.56
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.18	0.56
1:I:49:ALA:HB3	1:I:142:GLY:CA	2.36	0.56
2:J:28:ASP:HB3	2:J:31:ARG:HB3	1.88	0.56
1:A:408:LEU:HD11	5:A:601:FAD:H4'	1.88	0.55
2:F:28:ASP:HB3	2:F:31:ARG:HB3	1.88	0.55
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.89	0.55
2:B:28:ASP:HB3	2:B:31:ARG:HB3	1.88	0.54
5:I:601:FAD:C4	6:I:1589:TEO:C3	2.86	0.54
1:A:49:ALA:HB3	1:A:142:GLY:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.89	0.54
1:E:575:PRO:HB2	1:E:578:ARG:O	2.08	0.54
1:A:425:GLU:HG2	13:A:2049:HOH:O	2.06	0.54
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.89	0.54
1:A:379:VAL:O	1:A:381:PRO:HD3	2.08	0.54
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.89	0.54
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.23	0.54
1:E:49:ALA:HB3	1:E:142:GLY:CA	2.36	0.54
1:I:379:VAL:O	1:I:381:PRO:HD3	2.08	0.54
1:E:286:ARG:HH22	6:E:1589:TEO:C4	2.21	0.54
1:E:49:ALA:HA	5:E:601:FAD:N5	2.24	0.53
1:A:575:PRO:HB2	1:A:578:ARG:O	2.08	0.53
1:E:379:VAL:O	1:E:381:PRO:HD3	2.08	0.53
2:F:35:LEU:HD11	2:F:91:ILE:HD11	1.90	0.53
2:J:35:LEU:HD11	2:J:91:ILE:HD11	1.90	0.53
1:I:575:PRO:HB2	1:I:578:ARG:O	2.08	0.53
1:E:486:GLN:O	1:E:490:ILE:HG13	2.10	0.52
1:I:486:GLN:O	1:I:490:ILE:HG13	2.10	0.52
2:J:5:PHE:HB2	2:J:23:TYR:HB2	1.91	0.52
1:I:405:LEU:HG	5:I:601:FAD:C2	2.40	0.51
2:B:5:PHE:HB2	2:B:23:TYR:HB2	1.91	0.51
2:F:5:PHE:HB2	2:F:23:TYR:HB2	1.91	0.51
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.40	0.51
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.40	0.51
1:A:178:VAL:HG21	1:A:432:ALA:HB2	1.93	0.50
1:A:486:GLN:O	1:A:490:ILE:HG13	2.10	0.50
4:D:44:THR:HG23	4:D:47:VAL:HG22	1.93	0.50
2:F:212:CYS:HB2	2:F:222:PRO:HG2	1.94	0.50
1:I:178:VAL:HG21	1:I:432:ALA:HB2	1.93	0.50
1:A:238:MET:O	1:A:357:MET:HB2	2.12	0.50
2:B:212:CYS:HB2	2:B:222:PRO:HG2	1.94	0.50
11:C:305:HEM:HBB2	11:C:305:HEM:CHC	2.30	0.50
1:E:238:MET:O	1:E:357:MET:HB2	2.12	0.50
1:E:178:VAL:HG21	1:E:432:ALA:HB2	1.93	0.50
2:B:100:ILE:HG12	3:C:9:ARG:NH1	2.26	0.49
4:L:44:THR:HG23	4:L:47:VAL:HG22	1.94	0.49
3:C:103:PHE:CE2	3:C:107:LYS:HE3	2.47	0.49
4:H:44:THR:HG23	4:H:47:VAL:HG22	1.93	0.49
1:I:45:HIS:CE1	1:I:214:ASN:HA	2.47	0.49
2:J:212:CYS:HB2	2:J:222:PRO:HG2	1.93	0.49
2:B:95:PRO:HA	3:C:12:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	5:A:601:FAD:N5	2.27	0.49
1:E:240:GLN:HB2	1:E:357:MET:SD	2.53	0.49
1:I:147:HIS:O	1:I:151:GLN:HG3	2.13	0.49
11:K:305:HEM:CHC	11:K:305:HEM:HBB2	2.32	0.49
1:E:45:HIS:CE1	1:E:214:ASN:HA	2.47	0.49
1:A:240:GLN:HB2	1:A:357:MET:SD	2.53	0.49
3:C:128:VAL:HG12	3:C:128:VAL:O	2.12	0.49
5:E:601:FAD:C4	6:E:1589:TEO:C3	2.91	0.49
1:E:242:HIS:O	1:E:351:PRO:HA	2.13	0.49
1:E:79:ILE:HD11	1:E:397:ALA:HB2	1.95	0.49
1:A:147:HIS:O	1:A:151:GLN:HG3	2.12	0.48
1:A:242:HIS:O	1:A:351:PRO:HA	2.13	0.48
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.47	0.48
1:I:238:MET:O	1:I:357:MET:HB2	2.12	0.48
1:E:185:ILE:O	1:E:506:PHE:HA	2.14	0.48
3:K:37:THR:O	3:K:41:VAL:HG23	2.13	0.48
1:A:46:THR:HB	1:A:146:LEU:HD13	1.96	0.48
1:A:185:ILE:O	1:A:506:PHE:HA	2.13	0.48
3:G:103:PHE:CE2	3:G:107:LYS:HE3	2.48	0.48
12:G:1130:CBE:O9	12:G:1130:CBE:H16	2.12	0.48
1:I:242:HIS:O	1:I:351:PRO:HA	2.13	0.48
3:K:103:PHE:CE2	3:K:107:LYS:HE3	2.47	0.48
3:K:128:VAL:O	3:K:128:VAL:HG12	2.12	0.48
2:J:234:LEU:HD23	4:L:13:VAL:HG13	1.95	0.48
3:C:37:THR:O	3:C:41:VAL:HG23	2.13	0.48
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.48	0.48
1:A:79:ILE:HD11	1:A:397:ALA:HB2	1.96	0.48
3:G:85:VAL:HG22	11:G:305:HEM:HMC3	1.94	0.48
1:A:446:ARG:NE	13:A:2053:HOH:O	2.46	0.48
2:F:179:TYR:O	2:F:183:ILE:HG13	2.14	0.48
1:I:240:GLN:HB2	1:I:357:MET:SD	2.53	0.48
12:K:1130:CBE:O9	12:K:1130:CBE:C16	2.55	0.48
3:G:37:THR:O	3:G:41:VAL:HG23	2.13	0.48
1:I:185:ILE:O	1:I:506:PHE:HA	2.13	0.48
3:G:128:VAL:HG12	3:G:128:VAL:O	2.12	0.48
2:J:179:TYR:O	2:J:183:ILE:HG13	2.14	0.48
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.48	0.48
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.48	0.48
1:I:52:GLY:HA2	1:I:141:THR:HG21	1.96	0.48
2:B:179:TYR:O	2:B:183:ILE:HG13	2.14	0.47
1:E:147:HIS:O	1:E:151:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:HB3	5:A:601:FAD:N1	2.29	0.47
1:E:405:LEU:HG	5:E:601:FAD:C2	2.44	0.47
1:A:446:ARG:NH2	13:A:2053:HOH:O	2.48	0.47
1:I:46:THR:HB	1:I:146:LEU:HD13	1.97	0.47
1:I:79:ILE:HD11	1:I:397:ALA:HB2	1.95	0.47
1:E:52:GLY:HA2	1:E:141:THR:HG21	1.96	0.47
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.30	0.46
1:E:46:THR:HB	1:E:146:LEU:HD13	1.96	0.46
5:A:601:FAD:C4	6:A:1589:TEO:C3	2.93	0.46
1:E:395:HIS:ND1	1:E:399:ARG:HG3	2.30	0.46
12:C:1130:CBE:O9	12:C:1130:CBE:C16	2.63	0.46
1:E:14:GLY:HA3	1:E:201:ALA:O	2.16	0.46
6:I:1589:TEO:O2	6:I:1589:TEO:O4B	2.28	0.46
1:A:14:GLY:HA3	1:A:201:ALA:O	2.16	0.46
11:G:305:HEM:HBB2	11:G:305:HEM:CHC	2.32	0.46
5:A:601:FAD:H1'1	5:A:601:FAD:H9	1.76	0.46
1:A:52:GLY:HA2	1:A:141:THR:HG21	1.96	0.46
11:C:305:HEM:CHD	11:C:305:HEM:HBC2	2.31	0.46
1:E:14:GLY:HA2	5:E:601:FAD:H1B	1.98	0.46
1:I:14:GLY:HA3	1:I:201:ALA:O	2.16	0.46
4:L:108:GLY:O	4:L:112:VAL:HG22	2.17	0.45
1:I:395:HIS:ND1	1:I:399:ARG:HG3	2.30	0.45
3:K:107:LYS:HD2	13:K:2001:HOH:O	2.16	0.45
3:C:8:GLN:HG2	3:C:9:ARG:N	2.32	0.45
1:A:54:THR:HG23	1:A:133:ARG:HG3	1.98	0.45
4:D:108:GLY:O	4:D:112:VAL:HG22	2.16	0.45
3:G:8:GLN:HG2	3:G:9:ARG:N	2.32	0.45
1:E:54:THR:HG23	1:E:133:ARG:HG3	1.98	0.45
1:E:214:ASN:N	1:E:214:ASN:HD22	2.14	0.45
3:G:13:LEU:HA	3:G:13:LEU:HD12	1.87	0.45
1:I:254:THR:HG22	1:I:330:ILE:HG21	1.99	0.45
2:B:234:LEU:HB3	4:H:87:LEU:HD21	1.99	0.45
4:H:108:GLY:O	4:H:112:VAL:HG22	2.16	0.45
1:A:214:ASN:HD22	1:A:214:ASN:N	2.14	0.44
1:I:231:VAL:HA	1:I:232:PRO:HD3	1.84	0.44
2:J:216:CYS:HA	9:J:303:SF4:S4	2.57	0.44
3:K:28:ILE:HA	12:K:1130:CBE:S4	2.57	0.44
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.99	0.44
2:B:107:MET:HB2	2:B:111:TYR:CE2	2.52	0.44
1:I:54:THR:HG23	1:I:133:ARG:HG3	1.98	0.44
1:E:266:ASN:HB2	1:E:301:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:O	1:A:408:LEU:HG	2.18	0.44
2:J:107:MET:HB2	2:J:111:TYR:CE2	2.53	0.44
2:J:214:SER:HB3	3:K:103:PHE:CZ	2.52	0.44
1:A:254:THR:HG22	1:A:330:ILE:HG21	2.00	0.43
1:I:266:ASN:HB2	1:I:301:ARG:O	2.18	0.43
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.53	0.43
3:K:8:GLN:HG2	3:K:9:ARG:N	2.32	0.43
1:E:55:VAL:HG13	1:E:57:LEU:HG	1.99	0.43
1:I:404:SER:O	1:I:408:LEU:HG	2.18	0.43
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.78	0.43
1:I:214:ASN:HD22	1:I:214:ASN:N	2.14	0.43
1:E:61:HIS:CE1	1:E:124:LYS:HE2	2.54	0.43
1:E:404:SER:O	1:E:408:LEU:HG	2.18	0.43
1:I:340:VAL:O	1:I:342:PRO:HD3	2.19	0.43
1:I:55:VAL:HG13	1:I:57:LEU:HG	1.99	0.43
2:B:216:CYS:HA	2:B:217:PRO:HD2	1.91	0.43
1:E:254:THR:HG22	1:E:330:ILE:HG21	1.99	0.43
2:F:107:MET:HB2	2:F:111:TYR:CE2	2.53	0.43
2:B:214:SER:HB3	3:C:103:PHE:CZ	2.52	0.43
1:E:340:VAL:O	1:E:342:PRO:HD3	2.19	0.43
2:F:8:TYR:CG	2:F:93:PRO:HD3	2.54	0.43
1:I:286:ARG:HH22	6:I:1589:TEO:C4	2.31	0.43
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.01	0.43
1:A:340:VAL:O	1:A:342:PRO:HD3	2.18	0.43
1:E:75:GLY:O	1:E:398:ASN:HB3	2.19	0.43
1:I:75:GLY:O	1:I:398:ASN:HB3	2.18	0.43
1:A:61:HIS:CE1	1:A:124:LYS:HE2	2.54	0.43
1:A:362:THR:HG21	1:A:385:ALA:HB3	2.01	0.43
1:A:54:THR:O	1:A:406:LEU:HD22	2.19	0.43
2:B:189:GLU:O	2:B:193:ARG:HG3	2.19	0.43
11:C:305:HEM:HAD1	4:D:19:VAL:HG11	2.01	0.43
1:A:103:GLY:HA2	2:B:121:LEU:HD22	2.00	0.43
1:I:61:HIS:CE1	1:I:124:LYS:HE2	2.54	0.43
1:I:463:LEU:C	1:I:463:LEU:HD23	2.40	0.43
1:A:266:ASN:HB2	1:A:301:ARG:O	2.18	0.42
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.54	0.42
1:E:257:CYS:HB3	1:E:315:LEU:HD21	2.01	0.42
3:G:89:ILE:O	3:G:93:MET:HG3	2.19	0.42
1:A:75:GLY:O	1:A:398:ASN:HB3	2.19	0.42
1:I:255:GLU:HA	13:I:2015:HOH:O	2.20	0.42
1:I:362:THR:HG21	1:I:385:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:THR:O	1:I:406:LEU:HD22	2.19	0.42
2:J:189:GLU:O	2:J:193:ARG:HG3	2.19	0.42
1:A:205:ALA:HB2	1:A:220:GLY:CA	2.49	0.42
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.84	0.42
1:E:463:LEU:C	1:E:463:LEU:HD23	2.39	0.42
1:I:291:ARG:O	1:I:295:ILE:HG13	2.19	0.42
3:K:89:ILE:O	3:K:93:MET:HG3	2.19	0.42
1:E:205:ALA:HB2	1:E:220:GLY:HA3	2.02	0.42
2:F:189:GLU:O	2:F:193:ARG:HG3	2.19	0.42
1:I:104:LEU:HA	1:I:105:PRO:HD3	1.77	0.42
3:K:124:ALA:O	3:K:128:VAL:HG23	2.19	0.42
1:E:54:THR:O	1:E:406:LEU:HD22	2.19	0.42
4:H:20:ARG:O	4:H:24:ILE:HG13	2.20	0.42
1:I:205:ALA:HB2	1:I:220:GLY:CA	2.49	0.42
1:I:399:ARG:CZ	1:I:404:SER:HB2	2.50	0.42
1:E:205:ALA:HB2	1:E:220:GLY:CA	2.49	0.42
3:G:124:ALA:O	3:G:128:VAL:HG23	2.20	0.42
1:I:205:ALA:HB2	1:I:220:GLY:HA3	2.02	0.42
1:I:257:CYS:HB3	1:I:315:LEU:HD21	2.01	0.42
4:D:20:ARG:O	4:D:24:ILE:HG13	2.19	0.42
2:F:94:LEU:HA	2:F:95:PRO:HD3	1.85	0.42
1:A:463:LEU:C	1:A:463:LEU:HD23	2.39	0.42
1:I:44:SER:O	1:I:47:VAL:HG12	2.20	0.42
2:B:234:LEU:HD23	4:D:13:VAL:HG13	2.02	0.41
2:F:55:CYS:O	2:F:56:ARG:CD	2.66	0.41
4:L:20:ARG:O	4:L:24:ILE:HG13	2.20	0.41
1:E:520:MET:HB2	1:E:520:MET:HE2	1.94	0.41
11:K:305:HEM:C4B	4:L:71:MET:HG2	2.55	0.41
2:B:55:CYS:O	2:B:56:ARG:CD	2.66	0.41
1:E:408:LEU:HD11	5:E:601:FAD:C4'	2.49	0.41
11:C:305:HEM:CBC	11:C:305:HEM:HHD	2.38	0.41
1:E:362:THR:HG21	1:E:385:ALA:HB3	2.01	0.41
1:A:205:ALA:HB2	1:A:220:GLY:HA3	2.02	0.41
1:E:291:ARG:O	1:E:295:ILE:HG13	2.20	0.41
5:I:601:FAD:H9	5:I:601:FAD:H1'1	1.78	0.41
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.50	0.41
3:C:89:ILE:O	3:C:93:MET:HG3	2.19	0.41
1:E:399:ARG:CZ	1:E:404:SER:HB2	2.50	0.41
2:F:165:ASN:HB2	13:F:2022:HOH:O	2.20	0.41
1:I:49:ALA:HA	5:I:601:FAD:C6	2.50	0.41
1:A:291:ARG:O	1:A:295:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:CYS:O	2:J:56:ARG:CD	2.66	0.41
1:E:44:SER:O	1:E:47:VAL:HG12	2.21	0.41
3:C:124:ALA:O	3:C:128:VAL:HG23	2.20	0.41
2:J:224:ARG:NH2	3:K:102:THR:HG22	2.36	0.41
1:A:170:VAL:HG23	1:A:180:CYS:HA	2.03	0.41
1:A:44:SER:O	1:A:47:VAL:HG12	2.20	0.41
2:J:137:PRO:O	2:J:141:GLU:HG3	2.21	0.41
1:A:256:GLY:O	1:A:260:GLU:HG2	2.21	0.40
1:E:360:ILE:HA	1:E:361:PRO:HD2	1.90	0.40
2:F:137:PRO:O	2:F:141:GLU:HG3	2.21	0.40
4:D:85:LYS:HB2	4:D:86:PRO:HD3	2.03	0.40
3:C:20:PHE:HA	3:C:21:PRO:HD3	1.90	0.40
1:I:542:ARG:HB3	1:I:544:ASP:OD1	2.22	0.40
1:I:560:LEU:HA	1:I:561:PRO:HD3	1.85	0.40
1:E:170:VAL:HG23	1:E:180:CYS:HA	2.03	0.40
2:J:8:TYR:CZ	2:J:18:PRO:HB3	2.56	0.40
2:B:137:PRO:O	2:B:141:GLU:HG3	2.21	0.40
2:F:216:CYS:HA	2:F:217:PRO:HD2	1.91	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%)	565 (96%)	21 (4%)	0	100	100
1	E	586/588 (100%)	565 (96%)	21 (4%)	0	100	100
1	I	586/588 (100%)	566 (97%)	20 (3%)	0	100	100
2	B	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	38	72
2	F	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	38	72
2	J	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	38	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	120/129 (93%)	120 (100%)	0	0	100	100
3	G	120/129 (93%)	120 (100%)	0	0	100	100
3	K	120/129 (93%)	120 (100%)	0	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	3135/3210 (98%)	3025 (96%)	107 (3%)	3 (0%)	55	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	ARG
2	F	56	ARG
2	J	56	ARG

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%)	469 (99%)	4 (1%)	85	96
1	E	473/473 (100%)	469 (99%)	4 (1%)	85	96
1	I	473/473 (100%)	469 (99%)	4 (1%)	85	96
2	B	208/208 (100%)	204 (98%)	4 (2%)	62	89
2	F	208/208 (100%)	204 (98%)	4 (2%)	62	89
2	J	208/208 (100%)	204 (98%)	4 (2%)	62	89
3	C	102/109 (94%)	99 (97%)	3 (3%)	48	81
3	G	102/109 (94%)	99 (97%)	3 (3%)	48	81
3	K	102/109 (94%)	99 (97%)	3 (3%)	48	81
4	D	88/96 (92%)	85 (97%)	3 (3%)	42	76
4	H	88/96 (92%)	85 (97%)	3 (3%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	88/96 (92%)	85 (97%)	3 (3%)	42 76
All	All	2613/2658 (98%)	2571 (98%)	42 (2%)	68 91

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	378	VAL
1	A	491	ARG
1	A	585	ILE
2	B	53	ARG
2	B	56	ARG
2	B	87	LYS
2	B	180	ARG
3	C	11	VAL
3	C	91	HIS
3	C	129	TRP
4	D	43	LEU
4	D	44	THR
4	D	60	PHE
1	E	119	PHE
1	E	378	VAL
1	E	491	ARG
1	E	585	ILE
2	F	53	ARG
2	F	56	ARG
2	F	87	LYS
2	F	180	ARG
3	G	11	VAL
3	G	91	HIS
3	G	129	TRP
4	H	43	LEU
4	H	44	THR
4	H	60	PHE
1	I	119	PHE
1	I	378	VAL
1	I	491	ARG
1	I	585	ILE
2	J	53	ARG
2	J	56	ARG
2	J	87	LYS
2	J	180	ARG

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Mol	Chain	Res	Type
3	K	11	VAL
3	K	91	HIS
3	K	129	TRP
4	L	43	LEU
4	L	44	THR
4	L	60	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	78	GLN
3	G	30	HIS
4	H	78	GLN
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
6	TEO	A	1589	-	1,8,8	0.80	0	0,10,10	0.00	-
5	FAD	A	601	1	51,58,58	1.29	6 (11%)	54,89,89	1.92	6 (11%)
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	-
12	CBE	C	1130	-	15,17,17	1.11	1 (6%)	17,22,22	1.79	2 (11%)
11	HEM	C	305	3,4	28,50,50	2.30	6 (21%)	17,82,82	1.45	2 (11%)
6	TEO	E	1589	-	1,8,8	0.43	0	0,10,10	0.00	-
5	FAD	E	601	1	51,58,58	1.29	6 (11%)	54,89,89	1.91	6 (11%)
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	-
12	CBE	G	1130	-	15,17,17	1.21	1 (6%)	17,22,22	1.89	1 (5%)
11	HEM	G	305	3,4	28,50,50	2.28	6 (21%)	17,82,82	1.40	1 (5%)
6	TEO	I	1589	-	1,8,8	0.51	0	0,10,10	0.00	-
5	FAD	I	601	1	51,58,58	1.29	6 (11%)	54,89,89	1.88	6 (11%)
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	-
12	CBE	K	1130	-	15,17,17	1.21	2 (13%)	17,22,22	1.58	2 (11%)
11	HEM	K	305	3,4	28,50,50	2.28	6 (21%)	17,82,82	1.41	2 (11%)

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	-	0/28/50/50	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	0/0/3/3
12	CBE	C	1130	-	-	0/6/19/19	0/1/2/2
11	HEM	C	305	3,4	-	0/6/54/54	0/0/8/8
6	TEO	E	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	E	601	1	-	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	0/0/3/3
12	CBE	G	1130	-	-	0/6/19/19	0/1/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	G	305	3,4	-	0/6/54/54	0/0/8/8
6	TEO	I	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	I	601	1	-	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
10	F3S	J	304	2	-	0/0/24/24	0/0/3/3
12	CBE	K	1130	-	-	0/6/19/19	0/1/2/2
11	HEM	K	305	3,4	-	0/6/54/54	0/0/8/8

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	305	HEM	C3B-C2B	-5.05	1.33	1.40
11	C	305	HEM	C3C-C2C	-4.98	1.33	1.40
11	K	305	HEM	C3C-C2C	-4.92	1.33	1.40
11	G	305	HEM	C3B-C2B	-4.90	1.33	1.40
11	G	305	HEM	C3C-C2C	-4.89	1.33	1.40
11	K	305	HEM	C3B-C2B	-4.85	1.33	1.40
12	G	1130	CBE	C11-N10	-3.57	1.34	1.41
12	K	1130	CBE	C11-N10	-3.32	1.35	1.41
12	C	1130	CBE	C11-N10	-2.87	1.36	1.41
5	A	601	FAD	C5X-N5	2.05	1.38	1.35
5	I	601	FAD	C5X-N5	2.09	1.38	1.35
5	E	601	FAD	C5X-N5	2.25	1.38	1.35
12	K	1130	CBE	C1-C2	2.26	1.54	1.49
5	E	601	FAD	C2A-N1A	2.42	1.38	1.33
11	K	305	HEM	C4D-ND	2.43	1.39	1.36
5	I	601	FAD	C2A-N1A	2.47	1.38	1.33
11	C	305	HEM	C4D-ND	2.50	1.39	1.36
11	G	305	HEM	C4D-ND	2.54	1.39	1.36
5	A	601	FAD	C2A-N1A	2.62	1.38	1.33
5	E	601	FAD	C4-N3	2.91	1.38	1.33
5	A	601	FAD	C4-N3	2.94	1.38	1.33
5	I	601	FAD	C4-N3	2.98	1.38	1.33
11	K	305	HEM	C3B-CAB	3.41	1.54	1.47
11	C	305	HEM	C3B-CAB	3.51	1.54	1.47
11	G	305	HEM	C3B-CAB	3.53	1.54	1.47
5	I	601	FAD	C4X-N5	3.56	1.38	1.33
5	A	601	FAD	C10-N1	3.60	1.38	1.33
5	E	601	FAD	C2A-N3A	3.64	1.38	1.32
5	E	601	FAD	C4X-N5	3.67	1.38	1.33
5	A	601	FAD	C4X-N5	3.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	C2A-N3A	3.72	1.38	1.32
5	I	601	FAD	C10-N1	3.73	1.38	1.33
5	E	601	FAD	C10-N1	3.77	1.38	1.33
5	I	601	FAD	C2A-N3A	3.80	1.38	1.32
11	G	305	HEM	C3C-CAC	3.82	1.55	1.47
11	K	305	HEM	C3C-CAC	3.85	1.55	1.47
11	C	305	HEM	C3C-CAC	3.93	1.55	1.47
11	G	305	HEM	C3D-C2D	5.49	1.53	1.37
11	C	305	HEM	C3D-C2D	5.53	1.54	1.37
11	K	305	HEM	C3D-C2D	5.58	1.54	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	N3A-C2A-N1A	-10.43	119.77	128.86
5	E	601	FAD	N3A-C2A-N1A	-10.25	119.94	128.86
5	I	601	FAD	N3A-C2A-N1A	-10.22	119.96	128.86
12	K	1130	CBE	C11-N10-C8	-3.94	120.87	127.58
12	C	1130	CBE	C11-N10-C8	-3.38	121.82	127.58
5	A	601	FAD	C4'-C3'-C2'	-2.55	107.92	113.41
5	A	601	FAD	C4X-C4-N3	-2.49	119.93	123.48
5	I	601	FAD	C4X-C4-N3	-2.48	119.96	123.48
5	E	601	FAD	C4X-C4-N3	-2.43	120.02	123.48
11	C	305	HEM	C1D-C2D-C3D	-2.40	105.32	107.00
5	E	601	FAD	C4'-C3'-C2'	-2.29	108.48	113.41
11	C	305	HEM	CAD-CBD-CGD	-2.25	108.82	112.66
11	K	305	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
5	I	601	FAD	C4'-C3'-C2'	-2.17	108.74	113.41
11	G	305	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
11	K	305	HEM	CAD-CBD-CGD	-2.10	109.06	112.66
5	A	601	FAD	C5X-C9A-N10	2.78	119.73	117.66
5	I	601	FAD	C5X-C9A-N10	2.89	119.80	117.66
5	E	601	FAD	C5X-C9A-N10	2.94	119.84	117.66
5	I	601	FAD	C4X-N5-C5X	3.18	120.12	116.76
5	A	601	FAD	C4X-N5-C5X	3.21	120.15	116.76
5	E	601	FAD	C4X-N5-C5X	3.26	120.21	116.76
12	K	1130	CBE	O7-C2-C1	4.61	114.93	109.46
12	C	1130	CBE	O7-C2-C1	5.59	116.09	109.46
5	I	601	FAD	C4-N3-C2	5.71	120.15	115.16
5	E	601	FAD	C4-N3-C2	5.79	120.23	115.16
5	A	601	FAD	C4-N3-C2	5.80	120.23	115.16
12	G	1130	CBE	O7-C2-C1	6.23	116.85	109.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1589	TEO	3	0
5	A	601	FAD	8	0
10	B	304	F3S	1	0
12	C	1130	CBE	2	0
11	C	305	HEM	6	0
6	E	1589	TEO	3	0
5	E	601	FAD	7	0
10	F	304	F3S	1	0
12	G	1130	CBE	1	0
11	G	305	HEM	4	0
6	I	1589	TEO	5	0
5	I	601	FAD	8	0
9	J	303	SF4	1	0
12	K	1130	CBE	3	0
11	K	305	HEM	4	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, 95th 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%)	0.03	6 (1%) 82 77	36, 60, 102, 151	0
1	E	588/588 (100%)	0.14	18 (3%) 49 38	41, 67, 107, 155	0
1	I	588/588 (100%)	0.51	61 (10%) 7 4	53, 77, 117, 170	0
2	B	238/238 (100%)	0.00	10 (4%) 37 26	36, 58, 108, 157	0
2	F	238/238 (100%)	-0.08	4 (1%) 70 63	44, 62, 110, 158	0
2	J	238/238 (100%)	0.19	15 (6%) 21 13	56, 71, 116, 159	0
3	C	122/129 (94%)	0.14	8 (6%) 19 11	54, 83, 120, 171	0
3	G	122/129 (94%)	0.30	8 (6%) 19 11	54, 87, 121, 173	0
3	K	122/129 (94%)	0.98	25 (20%) 1 1	69, 93, 124, 170	0
4	D	105/115 (91%)	0.03	3 (2%) 52 41	52, 74, 125, 186	0
4	H	105/115 (91%)	0.20	10 (9%) 9 5	52, 74, 125, 184	0
4	L	105/115 (91%)	0.32	12 (11%) 6 3	61, 80, 126, 182	0
All	All	3159/3210 (98%)	0.21	180 (5%) 24 16	36, 71, 117, 186	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	129	TRP	12.3
3	G	129	TRP	8.2
3	G	68	PHE	7.5
3	C	129	TRP	6.9
1	I	1	MET	6.7
4	D	41	GLY	5.5
3	K	101	GLU	5.5
4	L	115	VAL	5.4
3	C	68	PHE	5.2
3	K	69	PHE	5.1
3	K	68	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	I	338	ALA	5.1
1	I	346	PRO	4.9
1	I	266	ASN	4.9
4	L	38	ALA	4.8
1	I	268	HIS	4.7
1	E	449	ASN	4.6
1	I	298	ARG	4.5
2	F	29	GLU	4.3
4	H	41	GLY	4.3
1	I	276	TYR	4.2
4	L	37	PHE	4.1
2	J	29	GLU	4.1
2	J	2	ARG	4.1
1	I	267	LYS	4.1
3	C	69	PHE	4.1
2	J	28	ASP	4.0
1	I	340	VAL	4.0
4	H	42	GLU	4.0
1	I	452	ASN	3.9
1	E	202	THR	3.8
2	J	16	ASP	3.8
1	I	204	GLY	3.8
2	J	58	GLY	3.7
1	I	381	PRO	3.6
1	I	213	THR	3.6
4	H	47	VAL	3.6
3	K	8	GLN	3.6
1	I	297	ILE	3.6
2	J	31	ARG	3.6
1	E	528	VAL	3.6
3	K	108	ARG	3.6
1	E	452	ASN	3.5
3	K	126	VAL	3.5
2	B	1	MET	3.5
3	K	103	PHE	3.5
3	K	67	SER	3.4
1	I	534	THR	3.4
3	K	98	TYR	3.4
4	H	115	VAL	3.4
1	I	500	ASP	3.4
1	I	588	TYR	3.4
2	B	86	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	K	102	THR	3.3
2	B	2	ARG	3.2
3	K	128	VAL	3.2
3	K	65	MET	3.2
1	I	582	PRO	3.2
1	E	451	ARG	3.1
1	E	463	LEU	3.1
1	I	334	SER	3.1
1	I	463	LEU	3.1
2	B	84	GLN	3.1
3	G	64	ILE	3.1
1	A	300	GLY	3.0
1	I	345	GLU	3.0
1	I	307	TRP	3.0
1	E	344	LYS	3.0
3	G	69	PHE	3.0
1	I	374	LYS	3.0
2	J	15	ASP	3.0
1	I	562	GLU	3.0
4	H	51	PHE	3.0
1	I	421	GLU	2.9
1	I	262	GLY	2.9
1	I	563	SER	2.9
3	G	63	ALA	2.9
3	C	70	VAL	2.9
1	I	306	PRO	2.9
1	I	295	ILE	2.8
1	I	420	GLN	2.8
2	B	30	GLY	2.8
1	I	315	LEU	2.8
4	L	39	THR	2.8
3	K	110	ALA	2.8
2	J	86	GLY	2.8
3	C	66	GLY	2.7
3	K	111	LYS	2.7
1	I	544	ASP	2.7
2	J	14	VAL	2.7
1	E	345	GLU	2.7
4	L	49	ILE	2.7
1	E	48	SER	2.6
2	J	79	ILE	2.6
4	H	40	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	43	LEU	2.6
3	K	107	LYS	2.6
1	I	373	GLU	2.6
4	D	40	SER	2.6
1	I	309	PRO	2.6
4	H	48	TRP	2.6
2	B	29	GLU	2.5
1	I	277	ALA	2.5
1	I	424	ALA	2.5
2	F	30	GLY	2.5
4	L	114	GLY	2.5
1	A	424	ALA	2.5
1	I	304	ASP	2.5
1	I	310	HIS	2.5
3	C	128	VAL	2.5
1	I	451	ARG	2.5
1	I	265	LEU	2.5
3	K	66	GLY	2.5
4	L	43	LEU	2.5
2	B	55	CYS	2.4
3	K	79	THR	2.4
1	I	275	ARG	2.4
3	G	72	PHE	2.4
1	I	433	SER	2.4
3	G	108	ARG	2.4
1	I	48	SER	2.4
3	G	100	GLU	2.4
2	B	85	PRO	2.4
1	A	543	PHE	2.3
1	I	305	GLY	2.3
3	K	87	VAL	2.3
3	K	122	LEU	2.3
4	L	42	GLU	2.3
4	H	36	PHE	2.3
1	A	268	HIS	2.3
1	E	215	ALA	2.3
2	F	1	MET	2.3
3	K	61	ALA	2.3
1	E	222	GLY	2.3
1	E	531	ASN	2.3
1	I	470	ASN	2.3
1	I	491	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	67	SER	2.3
4	L	34	VAL	2.3
2	J	18	PRO	2.3
1	E	303	CYS	2.2
1	E	218	ASN	2.2
3	K	109	SER	2.2
4	L	40	SER	2.2
1	E	201	ALA	2.2
1	I	263	TYR	2.2
4	L	48	TRP	2.2
1	I	299	GLU	2.2
4	D	43	LEU	2.2
3	K	91	HIS	2.2
2	J	87	LYS	2.2
3	K	22	ILE	2.2
4	L	47	VAL	2.2
1	I	583	PRO	2.1
2	J	85	PRO	2.1
1	I	569	ARG	2.1
1	I	52	GLY	2.1
2	J	1	MET	2.1
1	A	216	HIS	2.1
1	I	300	GLY	2.1
1	I	319	GLY	2.1
1	E	465	GLU	2.1
1	I	318	LEU	2.1
2	B	16	ASP	2.1
2	B	61	GLY	2.1
1	I	524	TYR	2.1
3	C	65	MET	2.1
1	E	314	LYS	2.0
1	I	2	LYS	2.0
1	I	214	ASN	2.0
1	I	450	ASN	2.0
1	I	217	ILE	2.0
4	H	45	TYR	2.0
1	A	267	LYS	2.0
2	F	62	SER	2.0
2	J	30	GLY	2.0
1	E	173	GLN	2.0
1	I	342	PRO	2.0
1	I	45	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	K	114	PHE	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, 95th 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
7	NA	I	1590	1/1	0.88	0.68	9.41	64,64,64,64	0
7	NA	E	1590	1/1	0.86	0.47	5.28	39,39,39,39	0
7	NA	A	1590	1/1	0.95	0.40	5.08	35,35,35,35	0
6	TEO	I	1589	9/9	0.87	0.31	1.26	66,86,104,126	0
11	HEM	C	305	43/43	0.97	0.20	1.04	40,71,82,87	0
12	CBE	K	1130	16/16	0.95	0.23	0.57	46,84,107,110	0
12	CBE	G	1130	16/16	0.99	0.18	0.46	33,54,81,87	0
6	TEO	A	1589	9/9	0.98	0.25	0.46	31,44,56,57	0
11	HEM	G	305	43/43	0.97	0.19	0.38	22,78,110,118	0
5	FAD	I	601	53/53	0.95	0.28	0.34	53,83,120,218	0
5	FAD	E	601	53/53	0.96	0.26	-0.06	30,59,90,95	0
5	FAD	A	601	53/53	0.97	0.23	-0.15	22,50,74,93	0
11	HEM	K	305	43/43	0.98	0.18	-0.17	58,89,128,156	0
12	CBE	C	1130	16/16	0.97	0.15	-0.30	26,42,64,67	0
8	FES	F	302	4/4	0.99	0.22	-0.33	44,51,54,58	0
6	TEO	E	1589	9/9	0.96	0.17	-0.33	44,53,63,81	0
8	FES	J	302	4/4	0.98	0.21	-0.48	90,91,92,92	0
9	SF4	F	303	8/8	0.99	0.15	-0.49	47,51,53,53	0
9	SF4	B	303	8/8	0.99	0.18	-0.51	40,46,51,52	0
9	SF4	J	303	8/8	0.98	0.14	-0.98	65,72,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	F3S	J	304	7/7	0.99	0.12	-1.10	64,70,84,87	0
8	FES	B	302	4/4	0.99	0.21	-1.10	35,38,43,52	0
10	F3S	B	304	7/7	0.99	0.13	-1.56	42,45,53,57	0
10	F3S	F	304	7/7	1.00	0.11	-1.99	54,56,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.