



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:42 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 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/ValidationPDFNotes.html>

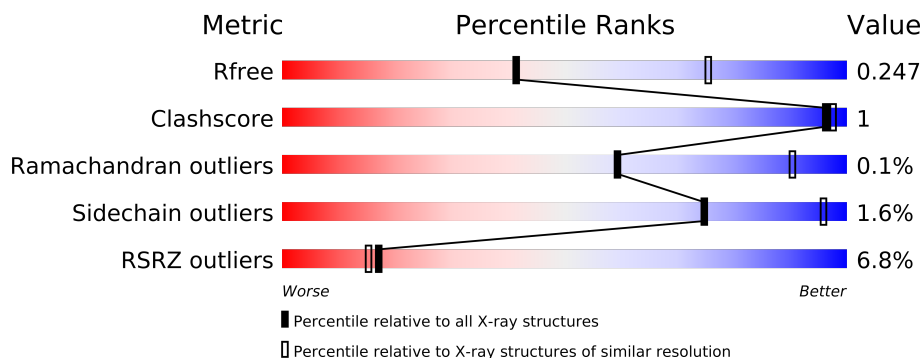
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	588	
1	E	588	
1	I	588	
2	B	238	
2	F	238	
2	J	238	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
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 hydrogen and 0 are deuterium.

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			

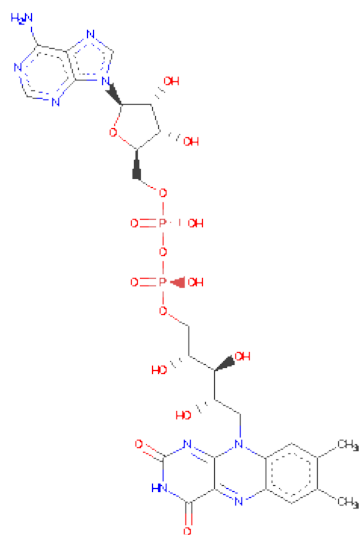
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT.

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:

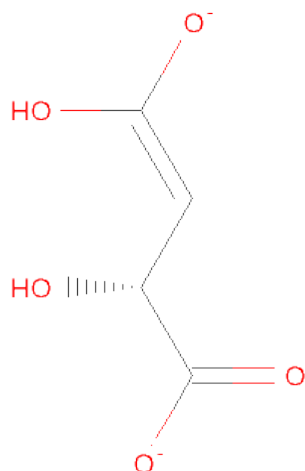
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44
H	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44
L	71	MET	HIS	ENGINEERED MUTATION	UNP P0AC44

- 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: $C_4H_4O_5$).

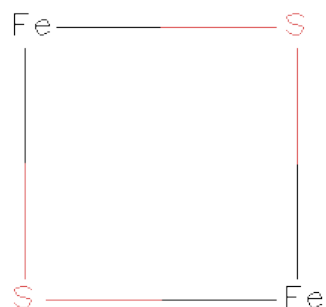


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	E	1	Total	C	O	0	0
			9	4	5		
6	I	1	Total	C	O	0	0
			9	4	5		

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

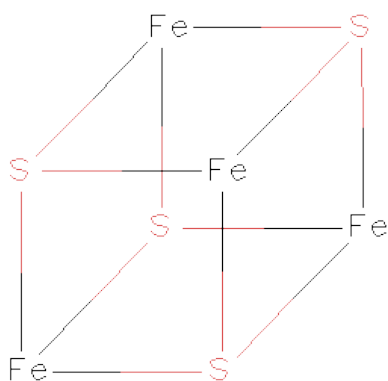
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		

- 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: Fe_4S_4).



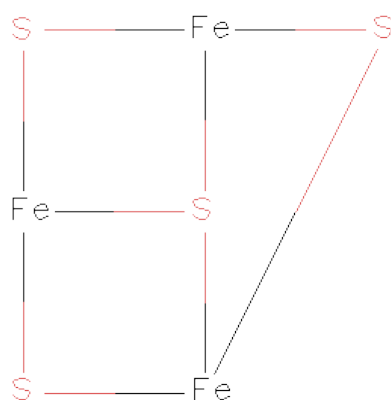
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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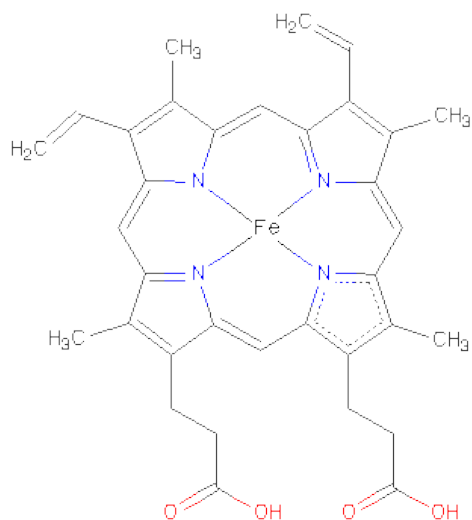
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	J	1	Total	Fe	S	0	0
			8	4	4		

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



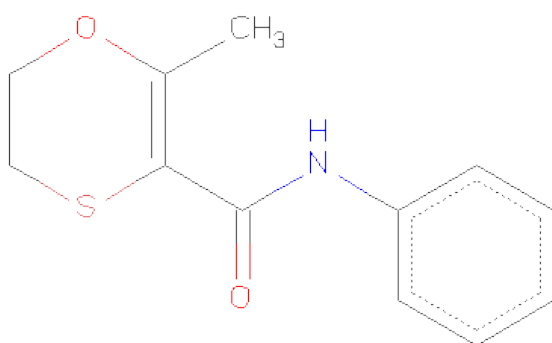
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		
10	F	1	Total	Fe	S	0	0
			7	3	4		
10	J	1	Total	Fe	S	0	0
			7	3	4		

- 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	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		

- 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.

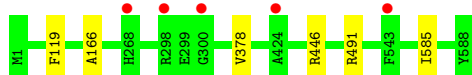
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	66	Total	O	0	0
			66	66		
13	B	33	Total	O	0	0
			33	33		
13	C	6	Total	O	0	0
			6	6		
13	D	2	Total	O	0	0
			2	2		
13	E	36	Total	O	0	0
			36	36		
13	F	28	Total	O	0	0
			28	28		
13	G	8	Total	O	0	0
			8	8		
13	H	2	Total	O	0	0
			2	2		
13	I	23	Total	O	0	0
		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

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.

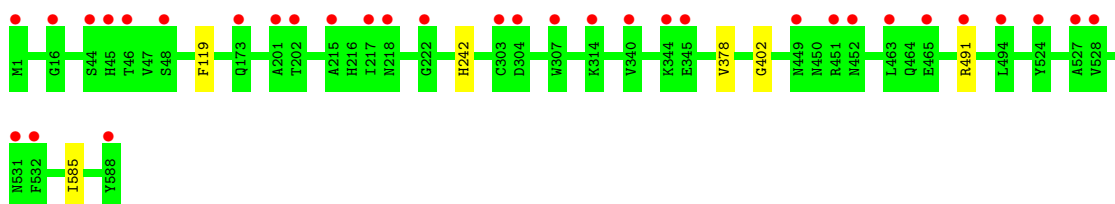
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain A: 



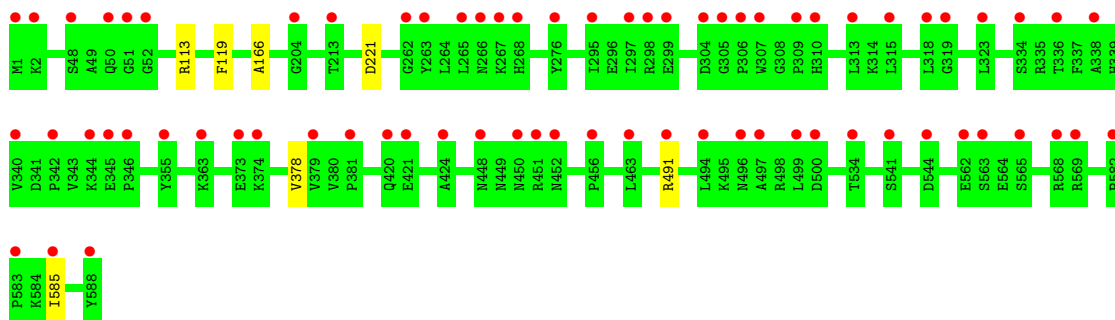
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain E: 



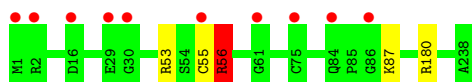
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain I: 



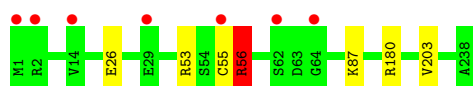
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain B: 



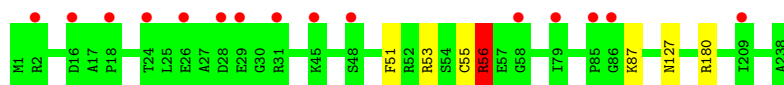
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain F: 



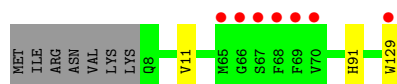
- Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT

Chain J:



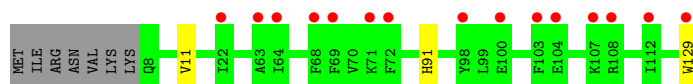
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain C:



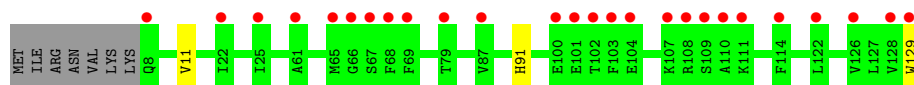
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain G:



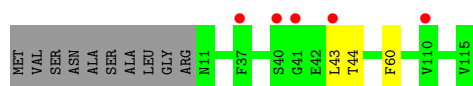
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:



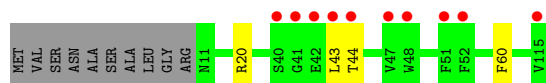
- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT

Chain D:



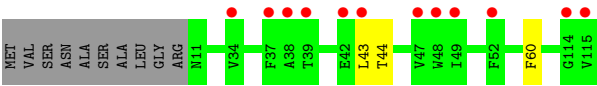
- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT

Chain H:



- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR PROTEIN SUBUNIT

Chain L:



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 0.212 , 0.247	Depositor DCC
R_{free} test set	5608 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 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 110643 reflections	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.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	0	3	0
1	E	4522	0	0	2	0
1	I	4522	0	0	3	0
2	B	1869	0	0	1	0
2	F	1869	0	0	3	0
2	J	1869	0	0	3	0
3	C	948	0	0	0	0
3	G	948	0	0	0	0
3	K	948	0	0	0	0
4	D	834	0	0	0	0
4	H	834	0	0	1	0
4	L	834	0	0	0	0
5	A	53	0	0	3	0
5	E	53	0	0	1	0
5	I	53	0	0	3	0
6	A	9	0	2	2	0
6	E	9	0	3	3	0
6	I	9	0	3	3	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	0	0
10	B	7	0	0	0	0
10	F	7	0	0	0	0
10	J	7	0	0	0	0
11	C	43	0	0	0	0
11	G	43	0	0	0	0
11	K	43	0	0	0	0
12	C	16	0	13	2	0
12	G	16	0	13	1	0
12	K	16	0	13	2	0
13	A	66	0	0	2	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	2	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	1	0
13	I	23	0	0	2	0
13	J	15	0	0	2	0
13	K	2	0	0	0	0
13	L	1	0	0	0	0
All	All	25164	0	47	27	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:K:1130:CBE:O9	12:K:1130:CBE:H16	1.94	0.67
2:J:51:PHE:N	13:J:2002:HOH:O	2.32	0.61
5:I:601:FAD:N5	6:I:1589:TEO:H2	2.18	0.59
12:C:1130:CBE:O9	12:C:1130:CBE:H16	2.04	0.57
4:H:20:ARG:NH1	13:H:2001:HOH:O	2.36	0.57
1:I:113:ARG:NH1	13:I:2004:HOH:O	2.38	0.56
5:I:601:FAD:C4	6:I:1589:TEO:C3	2.86	0.54
2:F:26:GLU:N	13:F:2002:HOH:O	2.40	0.54
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.23	0.54
1:I:221:ASP:N	13:I:2014:HOH:O	2.43	0.51
5:E:601:FAD:C4	6:E:1589:TEO:C3	2.91	0.49
12:G:1130:CBE:O9	12:G:1130:CBE:H16	2.12	0.48
12:K:1130:CBE:C16	12:K:1130:CBE:O9	2.55	0.48
1:A:446:ARG:NE	13:A:2053:HOH:O	2.46	0.48
1:A:446:ARG:NH2	13:A:2053:HOH:O	2.48	0.47
2:F:203:VAL:N	13:F:2026:HOH:O	2.48	0.47
5:A:601:FAD:C4	6:A:1589:TEO:C3	2.93	0.46
12:C:1130:CBE:C16	12:C:1130:CBE:O9	2.63	0.46
6:I:1589:TEO:O2	6:I:1589:TEO:O4B	2.28	0.46
1:A:166:ALA:N	5:A:601:FAD:N1A	2.65	0.45
2:J:55:CYS:O	2:J:56:ARG:CD	2.66	0.43
2:F:55:CYS:O	2:F:56:ARG:CD	2.66	0.43
2:B:55:CYS:O	2:B:56:ARG:CD	2.66	0.43
1:E:402:GLY:N	6:E:1589:TEO:O4A	2.53	0.42
2:J:127:ASN:CA	13:J:2007:HOH:O	2.67	0.42
1:I:166:ALA:N	5:I:601:FAD:N1A	2.68	0.41
1:E:242:HIS:NE2	6:E:1589:TEO:O1B	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	43	80
2	F	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	43	80
2	J	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	43	80
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%)	59	90

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%)	89	98
1	E	473/473 (100%)	469 (99%)	4 (1%)	89	98
1	I	473/473 (100%)	469 (99%)	4 (1%)	89	98
2	B	208/208 (100%)	204 (98%)	4 (2%)	69	94
2	F	208/208 (100%)	204 (98%)	4 (2%)	69	94
2	J	208/208 (100%)	204 (98%)	4 (2%)	69	94
3	C	102/109 (94%)	99 (97%)	3 (3%)	55	88
3	G	102/109 (94%)	99 (97%)	3 (3%)	55	88
3	K	102/109 (94%)	99 (97%)	3 (3%)	55	88
4	D	88/96 (92%)	85 (97%)	3 (3%)	49	84
4	H	88/96 (92%)	85 (97%)	3 (3%)	49	84
4	L	88/96 (92%)	85 (97%)	3 (3%)	49	84
All	All	2613/2658 (98%)	2571 (98%)	42 (2%)	75	96

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

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Mol	Chain	Res	Type
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
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 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	-	5,8,8	0.65	0	3,10,10	1.04	0
5	FAD	A	601	1	58,58,58	0.98	3 (5%)	85,89,89	1.90	14 (16%)
8	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	B	303	2	12,12,12	4.08	12 (100%)	0,24,24	0.00	-
10	F3S	B	304	2	3,9,9	18.94	3 (100%)	0,15,15	0.00	-
12	CBE	C	1130	-	17,17,17	1.06	1 (5%)	22,22,22	1.34	2 (9%)
11	HEM	C	305	3,4	49,50,50	2.29	14 (28%)	46,82,82	2.02	6 (13%)
6	TEO	E	1589	-	5,8,8	1.07	0	3,10,10	1.13	0
5	FAD	E	601	1	58,58,58	0.98	3 (5%)	85,89,89	1.93	14 (16%)
8	FES	F	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	F	303	2	12,12,12	4.07	12 (100%)	0,24,24	0.00	-
10	F3S	F	304	2	3,9,9	18.94	3 (100%)	0,15,15	0.00	-
12	CBE	G	1130	-	17,17,17	1.12	1 (5%)	22,22,22	1.38	1 (4%)
11	HEM	G	305	3,4	49,50,50	2.26	15 (30%)	46,82,82	2.04	7 (15%)
6	TEO	I	1589	-	5,8,8	1.07	0	3,10,10	1.85	1 (33%)
5	FAD	I	601	1	58,58,58	0.97	3 (5%)	85,89,89	1.86	13 (15%)
8	FES	J	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	J	303	2	12,12,12	4.13	12 (100%)	0,24,24	0.00	-
10	F3S	J	304	2	3,9,9	18.54	3 (100%)	0,15,15	0.00	-
12	CBE	K	1130	-	17,17,17	1.18	2 (11%)	22,22,22	1.16	2 (9%)
11	HEM	K	305	3,4	49,50,50	2.28	15 (30%)	46,82,82	2.04	6 (13%)

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	-	-	0/2/8/8	0/0/0/0
5	FAD	A	601	1	-	0/34/50/50	0/1/6/6
8	FES	B	302	2	-	0/0/4/4	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	303	2	-	0/0/48/48	0/0/5/5
10	F3S	B	304	2	-	0/0/24/24	0/0/3/3
12	CBE	C	1130	-	-	0/8/19/19	0/2/2/2
11	HEM	C	305	3,4	-	0/14/114/114	0/0/8/8
6	TEO	E	1589	-	-	0/2/8/8	0/0/0/0
5	FAD	E	601	1	-	0/34/50/50	0/1/6/6
8	FES	F	302	2	-	0/0/4/4	0/0/1/1
9	SF4	F	303	2	-	0/0/48/48	0/0/5/5
10	F3S	F	304	2	-	0/0/24/24	0/0/3/3
12	CBE	G	1130	-	-	0/8/19/19	0/2/2/2
11	HEM	G	305	3,4	-	0/14/114/114	0/0/8/8
6	TEO	I	1589	-	-	0/2/8/8	0/0/0/0
5	FAD	I	601	1	-	0/34/50/50	0/1/6/6
8	FES	J	302	2	-	0/0/4/4	0/0/1/1
9	SF4	J	303	2	-	0/0/48/48	0/0/5/5
10	F3S	J	304	2	-	0/0/24/24	0/0/3/3
12	CBE	K	1130	-	-	0/8/19/19	0/2/2/2
11	HEM	K	305	3,4	-	0/14/114/114	0/0/8/8

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	304	F3S	S3-FE4	-19.35	2.20	2.33
10	F	304	F3S	S3-FE4	-19.23	2.20	2.33
10	B	304	F3S	S3-FE1	-19.06	2.20	2.33
10	J	304	F3S	S3-FE3	-18.93	2.20	2.33
10	F	304	F3S	S3-FE1	-18.85	2.20	2.33
10	F	304	F3S	S3-FE3	-18.73	2.20	2.33
10	J	304	F3S	S3-FE1	-18.48	2.20	2.33
10	B	304	F3S	S3-FE3	-18.41	2.20	2.33
10	J	304	F3S	S3-FE4	-18.19	2.21	2.33
11	K	305	HEM	C3D-C2D	5.96	1.54	1.43
11	C	305	HEM	C3D-C2D	5.89	1.54	1.43
11	G	305	HEM	C3D-C2D	5.82	1.53	1.43
11	C	305	HEM	C3B-C2B	-5.76	1.33	1.43
11	C	305	HEM	C3C-C2C	-5.71	1.33	1.43
11	K	305	HEM	C3C-C2C	-5.66	1.33	1.43
11	G	305	HEM	C3B-C2B	-5.65	1.33	1.43
11	G	305	HEM	C3C-C2C	-5.64	1.33	1.43
11	K	305	HEM	C3B-C2B	-5.61	1.33	1.43
11	C	305	HEM	C3C-CAC	4.80	1.55	1.40
11	K	305	HEM	C3C-CAC	4.76	1.55	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	305	HEM	C3C-CAC	4.74	1.55	1.40
9	J	303	SF4	S2-FE1	-4.70	2.30	2.33
11	G	305	HEM	C3B-CAB	4.60	1.54	1.40
11	C	305	HEM	C3B-CAB	4.58	1.54	1.40
9	F	303	SF4	S3-FE2	-4.58	2.30	2.33
11	K	305	HEM	C3B-CAB	4.53	1.54	1.40
9	B	303	SF4	S4-FE1	-4.50	2.30	2.33
9	F	303	SF4	S2-FE1	-4.41	2.30	2.33
9	J	303	SF4	S2-FE3	-4.33	2.30	2.33
9	J	303	SF4	S1-FE2	-4.30	2.30	2.33
9	J	303	SF4	S1-FE4	-4.28	2.30	2.33
9	B	303	SF4	S2-FE4	-4.27	2.30	2.33
9	J	303	SF4	S3-FE1	-4.21	2.30	2.33
9	F	303	SF4	S1-FE3	-4.21	2.30	2.33
9	F	303	SF4	S2-FE3	-4.21	2.30	2.33
9	B	303	SF4	S1-FE4	-4.20	2.30	2.33
9	J	303	SF4	S3-FE2	-4.19	2.30	2.33
9	F	303	SF4	S1-FE4	-4.19	2.30	2.33
9	B	303	SF4	S4-FE3	-4.16	2.30	2.33
9	B	303	SF4	S4-FE2	-4.16	2.30	2.33
9	B	303	SF4	S2-FE1	-4.12	2.30	2.33
9	F	303	SF4	S2-FE4	-4.11	2.30	2.33
9	J	303	SF4	S2-FE4	-4.09	2.30	2.33
11	K	305	HEM	C4A-C3A	4.08	1.45	1.40
9	B	303	SF4	S3-FE2	-4.08	2.30	2.33
11	C	305	HEM	C4A-C3A	4.07	1.45	1.40
11	G	305	HEM	C4A-C3A	4.07	1.45	1.40
9	B	303	SF4	S1-FE2	-4.07	2.30	2.33
9	J	303	SF4	S4-FE2	-4.04	2.30	2.33
9	J	303	SF4	S1-FE3	-4.03	2.30	2.33
9	B	303	SF4	S3-FE4	-3.96	2.30	2.33
9	B	303	SF4	S2-FE3	-3.96	2.30	2.33
9	J	303	SF4	S4-FE3	-3.95	2.30	2.33
9	F	303	SF4	S4-FE3	-3.94	2.30	2.33
9	B	303	SF4	S1-FE3	-3.91	2.30	2.33
9	F	303	SF4	S3-FE1	-3.88	2.30	2.33
9	F	303	SF4	S4-FE1	-3.85	2.30	2.33
9	F	303	SF4	S1-FE2	-3.83	2.30	2.33
9	J	303	SF4	S3-FE4	-3.81	2.30	2.33
9	F	303	SF4	S3-FE4	-3.79	2.30	2.33
9	F	303	SF4	S4-FE2	-3.76	2.30	2.33
12	G	1130	CBE	C11-N10	-3.64	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	303	SF4	S3-FE1	-3.55	2.30	2.33
9	J	303	SF4	S4-FE1	-3.55	2.30	2.33
12	K	1130	CBE	C11-N10	-3.39	1.35	1.41
11	C	305	HEM	FE-ND	3.33	2.09	1.97
11	K	305	HEM	C2B-C1B	3.27	1.45	1.44
11	K	305	HEM	FE-NA	3.26	2.06	1.92
11	C	305	HEM	C2B-C1B	3.25	1.45	1.44
11	C	305	HEM	FE-NA	3.23	2.06	1.92
5	I	601	FAD	C2A-N3A	3.21	1.38	1.32
11	K	305	HEM	FE-ND	3.15	2.09	1.97
5	A	601	FAD	C2A-N3A	3.13	1.38	1.32
11	G	305	HEM	C2B-C1B	3.07	1.45	1.44
5	E	601	FAD	C2A-N3A	3.07	1.38	1.32
11	G	305	HEM	FE-NA	3.06	2.05	1.92
12	C	1130	CBE	C11-N10	-2.94	1.36	1.41
11	G	305	HEM	FE-ND	2.82	2.08	1.97
11	C	305	HEM	FE-NB	2.77	2.07	1.97
11	K	305	HEM	FE-NB	2.62	2.07	1.97
11	G	305	HEM	FE-NB	2.56	2.07	1.97
11	K	305	HEM	CMD-C2D	2.52	1.55	1.47
11	C	305	HEM	CMD-C2D	2.51	1.55	1.47
5	A	601	FAD	C2A-N1A	2.49	1.38	1.33
11	G	305	HEM	CMD-C2D	2.44	1.55	1.47
11	K	305	HEM	CMC-C2C	2.40	1.54	1.47
11	G	305	HEM	CMC-C2C	2.37	1.54	1.47
11	K	305	HEM	CMB-C2B	2.37	1.54	1.47
5	I	601	FAD	C2A-N1A	2.35	1.38	1.33
11	C	305	HEM	FE-NC	2.35	2.06	1.97
11	C	305	HEM	CMC-C2C	2.35	1.54	1.47
11	K	305	HEM	FE-NC	2.34	2.06	1.97
11	G	305	HEM	CMB-C2B	2.31	1.54	1.47
5	E	601	FAD	C2A-N1A	2.30	1.38	1.33
11	C	305	HEM	CMB-C2B	2.29	1.54	1.47
12	K	1130	CBE	C1-C2	2.27	1.54	1.49
11	G	305	HEM	FE-NC	2.26	2.06	1.97
5	E	601	FAD	C5X-N5	2.26	1.38	1.35
11	G	305	HEM	C3D-C4D	2.25	1.45	1.44
5	I	601	FAD	C5X-N5	2.10	1.38	1.35
5	A	601	FAD	C5X-N5	2.06	1.38	1.35
11	K	305	HEM	C2D-C1D	2.01	1.45	1.44

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	N3A-C2A-N1A	-10.69	119.77	128.71
5	E	601	FAD	N3A-C2A-N1A	-10.49	119.94	128.71
5	I	601	FAD	N3A-C2A-N1A	-10.47	119.96	128.71
11	C	305	HEM	C3B-C4B-NB	-8.55	107.89	114.00
11	K	305	HEM	C3B-C4B-NB	-8.49	107.93	114.00
11	G	305	HEM	C3B-C4B-NB	-8.36	108.02	114.00
11	K	305	HEM	C4D-ND-C1D	6.55	111.86	105.16
11	G	305	HEM	C4D-ND-C1D	6.51	111.82	105.16
5	E	601	FAD	C2'-C1'-N10	-6.45	103.90	112.45
11	C	305	HEM	C4D-ND-C1D	6.33	111.64	105.16
5	A	601	FAD	C2'-C1'-N10	-5.87	104.66	112.45
5	E	601	FAD	C2-N1-C10	5.22	120.24	114.98
5	I	601	FAD	C2'-C1'-N10	-5.21	105.54	112.45
5	A	601	FAD	C2-N1-C10	5.19	120.21	114.98
5	I	601	FAD	C2-N1-C10	5.11	120.13	114.98
12	G	1130	CBE	O7-C2-C1	4.23	116.85	109.71
12	C	1130	CBE	O7-C2-C1	3.78	116.09	109.71
11	K	305	HEM	C2D-C1D-ND	-3.69	108.57	112.93
12	K	1130	CBE	C11-N10-C8	-3.66	120.87	127.54
11	G	305	HEM	C2D-C1D-ND	-3.65	108.62	112.93
5	E	601	FAD	N3A-C4A-N9A	3.64	132.01	125.43
5	I	601	FAD	N3A-C4A-N9A	3.64	132.00	125.43
5	E	601	FAD	P-O3P-PA	-3.62	121.07	131.68
5	E	601	FAD	O4B-C1B-N9A	3.57	111.76	108.44
5	A	601	FAD	N3A-C4A-N9A	3.54	131.83	125.43
11	C	305	HEM	C2D-C1D-ND	-3.52	108.77	112.93
5	A	601	FAD	P-O3P-PA	-3.50	121.43	131.68
5	I	601	FAD	P-O3P-PA	-3.49	121.44	131.68
12	C	1130	CBE	C11-N10-C8	-3.14	121.82	127.54
5	E	601	FAD	C4X-N5-C5X	3.13	120.21	116.69
12	K	1130	CBE	O7-C2-C1	3.10	114.93	109.71
5	A	601	FAD	O4B-C1B-N9A	3.09	111.31	108.44
5	E	601	FAD	C5X-C9A-N10	3.08	119.84	116.80
5	A	601	FAD	C4X-N5-C5X	3.08	120.15	116.69
5	I	601	FAD	C4X-N5-C5X	3.05	120.12	116.69
5	I	601	FAD	C5X-C9A-N10	3.05	119.80	116.80
6	I	1589	TEO	C2-C3-C4	-3.01	117.13	124.92
5	I	601	FAD	O4B-C1B-N9A	3.00	111.23	108.44
5	A	601	FAD	C5X-C9A-N10	2.97	119.73	116.80
11	K	305	HEM	C4C-NC-C1C	2.79	108.44	105.53
5	E	601	FAD	C4X-C10-N1	-2.75	119.98	122.73
5	I	601	FAD	C4X-C10-N1	-2.73	120.00	122.73
11	C	305	HEM	C4C-NC-C1C	2.67	108.31	105.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	305	HEM	C4C-NC-C1C	2.67	108.31	105.53
11	K	305	HEM	C1B-NB-C4B	2.66	107.89	105.16
5	A	601	FAD	C4X-C10-N1	-2.64	120.09	122.73
11	C	305	HEM	C1B-NB-C4B	2.60	107.82	105.16
11	G	305	HEM	C1B-NB-C4B	2.56	107.78	105.16
5	I	601	FAD	C4-N3-C2	-2.55	120.15	125.39
5	E	601	FAD	C4-N3-C2	-2.52	120.23	125.39
5	A	601	FAD	C4-N3-C2	-2.51	120.23	125.39
5	A	601	FAD	C4'-C3'-C2'	-2.36	107.92	113.25
11	G	305	HEM	CBD-CAD-C3D	-2.27	109.43	114.37
5	E	601	FAD	C5A-C4A-N3A	-2.26	120.78	125.70
5	I	601	FAD	C5A-C4A-N3A	-2.25	120.81	125.70
5	A	601	FAD	C5A-C4A-N3A	-2.23	120.84	125.70
11	G	305	HEM	CHD-C1D-ND	2.22	126.42	124.58
5	A	601	FAD	C2A-N3A-C4A	2.21	120.31	114.01
11	C	305	HEM	CBD-CAD-C3D	-2.20	109.56	114.37
5	I	601	FAD	N7A-C8A-N9A	-2.20	108.14	114.36
5	E	601	FAD	C2A-N3A-C4A	2.18	120.21	114.01
5	I	601	FAD	C2A-N3A-C4A	2.13	120.09	114.01
5	E	601	FAD	N7A-C8A-N9A	-2.13	108.35	114.36
5	A	601	FAD	N7A-C8A-N9A	-2.13	108.35	114.36
5	E	601	FAD	C4'-C3'-C2'	-2.11	108.48	113.25
11	K	305	HEM	CBD-CAD-C3D	-2.10	109.78	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	5 (0%) 81 81	36, 60, 102, 151	0
1	E	588/588 (100%)	0.13	33 (5%) 24 23	41, 67, 107, 155	0
1	I	588/588 (100%)	0.52	71 (12%) 5 4	53, 77, 117, 170	0
2	B	238/238 (100%)	-0.07	10 (4%) 35 35	36, 58, 108, 157	0
2	F	238/238 (100%)	-0.12	7 (2%) 49 50	44, 62, 110, 158	0
2	J	238/238 (100%)	0.16	15 (6%) 19 18	56, 71, 116, 159	0
3	C	122/129 (94%)	0.18	7 (5%) 23 23	54, 83, 120, 171	0
3	G	122/129 (94%)	0.42	15 (12%) 5 4	54, 87, 121, 173	0
3	K	122/129 (94%)	1.10	26 (21%) 1 1	69, 93, 124, 170	0
4	D	105/115 (91%)	0.04	5 (4%) 29 30	52, 74, 125, 186	0
4	H	105/115 (91%)	0.31	10 (9%) 8 7	52, 74, 125, 184	0
4	L	105/115 (91%)	0.36	12 (11%) 6 4	61, 80, 126, 182	0
All	All	3159/3210 (98%)	0.20	216 (6%) 17 15	36, 71, 117, 186	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	129	TRP	13.5
3	G	129	TRP	9.8
1	I	1	MET	9.4
3	G	68	PHE	8.5
3	C	129	TRP	6.6
4	L	115	VAL	5.9
3	K	69	PHE	5.9
3	C	68	PHE	5.7
1	I	338	ALA	5.6
3	K	101	GLU	5.6
2	J	2	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
3	K	68	PHE	5.2
3	C	69	PHE	5.1
1	I	346	PRO	5.0
1	I	298	ARG	4.9
1	I	268	HIS	4.8
4	L	38	ALA	4.8
3	K	103	PHE	4.8
1	I	500	ASP	4.8
1	I	452	ASN	4.7
4	H	115	VAL	4.7
2	J	31	ARG	4.6
3	K	126	VAL	4.6
4	H	47	VAL	4.5
1	I	340	VAL	4.4
1	E	528	VAL	4.3
1	I	334	SER	4.2
1	I	267	LYS	4.2
1	E	449	ASN	4.2
2	J	28	ASP	4.1
4	L	37	PHE	4.1
1	E	344	LYS	4.1
1	I	266	ASN	4.1
1	I	381	PRO	4.1
3	G	69	PHE	4.0
4	H	51	PHE	4.0
1	E	345	GLU	4.0
4	L	42	GLU	4.0
4	D	41	GLY	4.0
4	H	41	GLY	4.0
4	H	42	GLU	4.0
1	I	213	THR	3.9
3	K	67	SER	3.8
4	H	48	TRP	3.8
2	J	58	GLY	3.8
2	F	29	GLU	3.7
3	K	128	VAL	3.7
1	I	463	LEU	3.7
3	K	102	THR	3.7
2	B	2	ARG	3.6
3	C	70	VAL	3.5
1	I	562	GLU	3.5
1	I	306	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	588	TYR	3.5
1	I	582	PRO	3.5
2	B	86	GLY	3.5
1	A	300	GLY	3.4
1	E	452	ASN	3.4
1	I	262	GLY	3.4
1	I	491	ARG	3.4
3	K	108	ARG	3.4
2	J	29	GLU	3.4
3	G	108	ARG	3.4
1	A	543	PHE	3.3
1	I	297	ILE	3.3
3	K	65	MET	3.3
1	E	451	ARG	3.2
1	I	204	GLY	3.2
3	K	110	ALA	3.2
2	J	86	GLY	3.2
4	L	49	ILE	3.2
2	B	1	MET	3.1
1	I	307	TRP	3.1
1	E	202	THR	3.1
1	E	463	LEU	3.1
3	K	114	PHE	3.1
1	I	276	TYR	3.1
1	I	345	GLU	3.1
1	I	2	LYS	3.0
4	H	52	PHE	3.0
1	E	531	ASN	3.0
1	I	315	LEU	3.0
1	I	420	GLN	3.0
1	I	563	SER	2.9
1	I	544	ASP	2.9
3	G	103	PHE	2.9
1	I	534	THR	2.9
1	I	451	ARG	2.9
1	I	309	PRO	2.9
1	I	583	PRO	2.9
3	K	122	LEU	2.9
4	D	43	LEU	2.9
1	I	421	GLU	2.9
3	G	107	LYS	2.9
3	K	111	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	55	CYS	2.9
2	B	55	CYS	2.8
3	C	66	GLY	2.8
3	K	22	ILE	2.8
2	J	16	ASP	2.8
3	K	66	GLY	2.8
1	I	456	PRO	2.8
4	L	47	VAL	2.8
1	E	48	SER	2.8
2	B	29	GLU	2.8
4	H	44	THR	2.8
1	I	568	ARG	2.7
1	I	318	LEU	2.7
3	K	61	ALA	2.7
1	I	295	ILE	2.7
2	J	45	LYS	2.7
4	H	43	LEU	2.7
4	L	48	TRP	2.7
1	A	298	ARG	2.7
1	A	424	ALA	2.7
3	K	8	GLN	2.7
2	B	30	GLY	2.7
3	G	72	PHE	2.7
1	E	532	PHE	2.6
1	I	374	LYS	2.6
1	I	52	GLY	2.6
1	I	319	GLY	2.6
1	I	363	LYS	2.6
1	E	173	GLN	2.6
2	J	26	GLU	2.6
1	E	465	GLU	2.5
4	H	40	SER	2.5
3	G	112	ILE	2.5
3	K	107	LYS	2.5
4	L	43	LEU	2.5
1	I	424	ALA	2.5
2	B	84	GLN	2.5
1	E	215	ALA	2.5
2	F	1	MET	2.5
4	D	37	PHE	2.5
1	I	448	ASN	2.5
1	I	305	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	379	VAL	2.5
3	G	64	ILE	2.5
3	G	100	GLU	2.5
4	D	40	SER	2.5
1	I	373	GLU	2.4
1	I	265	LEU	2.4
1	E	524	TYR	2.4
3	G	98	TYR	2.4
3	K	104	GLU	2.4
2	J	24	THR	2.4
1	I	51	GLY	2.4
4	L	114	GLY	2.4
1	I	304	ASP	2.4
2	F	64	GLY	2.4
2	J	18	PRO	2.4
1	E	303	CYS	2.4
1	E	16	GLY	2.4
2	F	2	ARG	2.3
4	L	52	PHE	2.3
3	C	67	SER	2.3
2	J	85	PRO	2.3
1	I	565	SER	2.3
1	I	494	LEU	2.3
4	L	39	THR	2.3
1	I	263	TYR	2.3
1	I	569	ARG	2.3
3	K	87	VAL	2.3
1	I	497	ALA	2.3
1	E	491	ARG	2.3
1	I	336	THR	2.3
1	E	304	ASP	2.2
2	J	209	ILE	2.2
2	F	62	SER	2.2
1	I	450	ASN	2.2
1	I	499	LEU	2.2
3	K	109	SER	2.2
1	E	307	TRP	2.2
2	J	79	ILE	2.2
3	K	25	ILE	2.2
1	A	268	HIS	2.2
1	I	310	HIS	2.2
1	E	314	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	355	TYR	2.2
1	E	46	THR	2.2
1	E	340	VAL	2.2
1	I	496	ASN	2.2
1	E	222	GLY	2.1
1	E	527	ALA	2.1
3	G	104	GLU	2.1
2	J	48	SER	2.1
3	G	71	LYS	2.1
2	B	75	CYS	2.1
3	G	22	ILE	2.1
1	E	45	HIS	2.1
1	I	299	GLU	2.1
1	I	585	ILE	2.1
1	I	50	GLN	2.1
4	L	34	VAL	2.1
1	I	48	SER	2.1
3	K	79	THR	2.1
2	F	14	VAL	2.1
1	I	323	LEU	2.1
1	I	342	PRO	2.1
4	D	110	VAL	2.1
1	E	217	ILE	2.0
2	B	61	GLY	2.0
1	I	541	SER	2.0
3	C	65	MET	2.0
1	I	344	LYS	2.0
1	E	588	TYR	2.0
1	E	218	ASN	2.0
3	K	100	GLU	2.0
1	I	313	LEU	2.0
1	E	44	SER	2.0
3	G	63	ALA	2.0
1	E	494	LEU	2.0
2	B	16	ASP	2.0
1	E	1	MET	2.0
1	E	201	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NA	I	1590	1/1	0.61	8.25	64,64,64,64	0
7	NA	E	1590	1/1	0.43	4.27	39,39,39,39	0
7	NA	A	1590	1/1	0.35	4.17	35,35,35,35	0
6	TEO	A	1589	9/9	0.28	1.61	31,44,56,57	0
6	TEO	I	1589	9/9	0.33	1.33	66,86,104,126	0
12	CBE	K	1130	16/16	0.26	0.89	46,84,107,110	0
12	CBE	G	1130	16/16	0.20	0.58	33,54,81,87	0
11	HEM	G	305	43/43	0.19	0.49	22,78,110,118	0
9	SF4	B	303	8/8	0.19	0.47	40,46,51,52	0
5	FAD	I	601	53/53	0.27	0.36	53,83,120,218	0
6	TEO	E	1589	9/9	0.18	0.28	44,53,63,81	0
11	HEM	K	305	43/43	0.18	0.25	58,89,128,156	0
9	SF4	F	303	8/8	0.17	0.22	47,51,53,53	0
5	FAD	E	601	53/53	0.26	0.17	30,59,90,95	0
5	FAD	A	601	53/53	0.23	0.14	22,50,74,93	0
11	HEM	C	305	43/43	0.18	0.13	40,71,82,87	0
9	SF4	J	303	8/8	0.15	-0.19	65,72,76,80	0
8	FES	F	302	4/4	0.24	-0.26	44,51,54,58	0
8	FES	J	302	4/4	0.23	-0.27	90,91,92,92	0
12	CBE	C	1130	16/16	0.14	-0.36	26,42,64,67	0
10	F3S	J	304	7/7	0.12	-0.79	64,70,84,87	0
8	FES	B	302	4/4	0.21	-0.85	35,38,43,52	0
10	F3S	B	304	7/7	0.12	-1.25	42,45,53,57	0
10	F3S	F	304	7/7	0.11	-1.67	54,56,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.