



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:46 PM GMT

PDB ID : 2WS3
Title : CRYSTAL STRUCTURE OF THE E. COLI SUCCINATE:QUINONE OXIDOREDUCTASE (SQR) SDHD TYR83PHE MUTANT
Authors : Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on : 2009-09-03
Resolution : 3.20 Å(reported)

This is a full wwPDB 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>

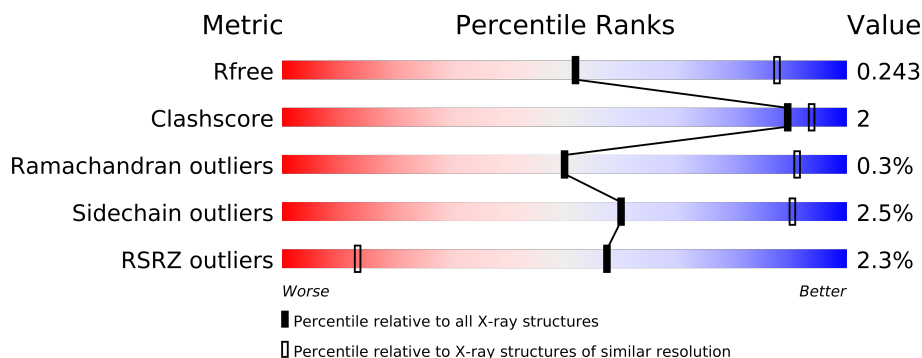
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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
11	CBE	K	1129	-	X
12	HEM	C	1130	-	X
6	NA	E	1589	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24900 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 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 B-556 SUBUNIT.

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

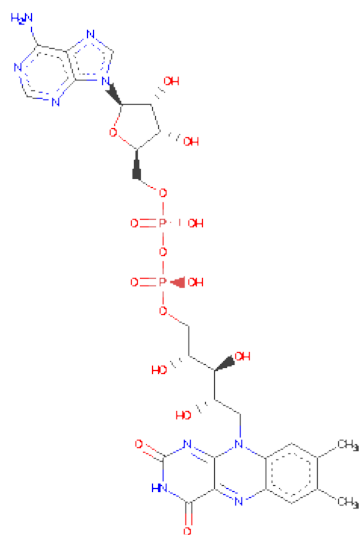
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	83	PHE	TYR	ENGINEERED MUTATION	UNP P0AC44
H	83	PHE	TYR	ENGINEERED MUTATION	UNP P0AC44
L	83	PHE	TYR	ENGINEERED MUTATION	UNP P0AC44

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

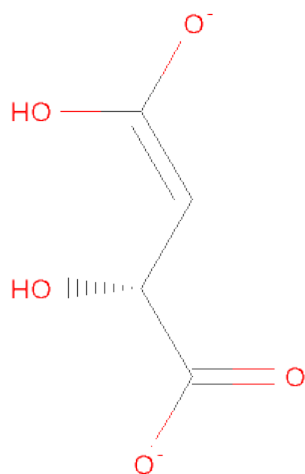


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

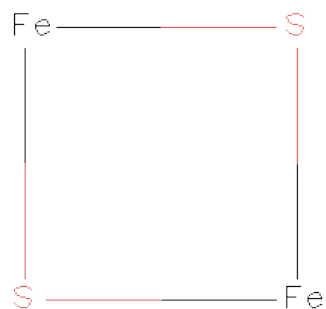
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		

- Molecule 7 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: C₄H₄O₅).



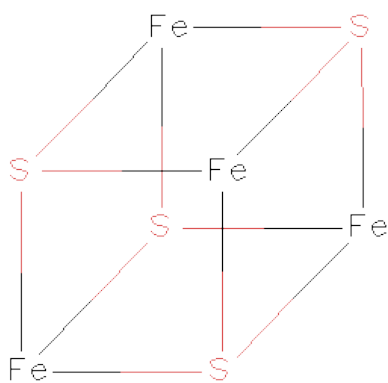
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	4	5		
7	E	1	Total	C	O	0	0
			9	4	5		
7	I	1	Total	C	O	0	0
			9	4	5		

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



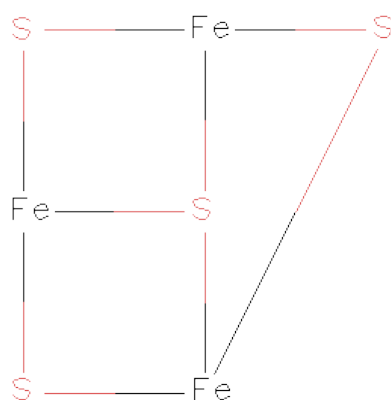
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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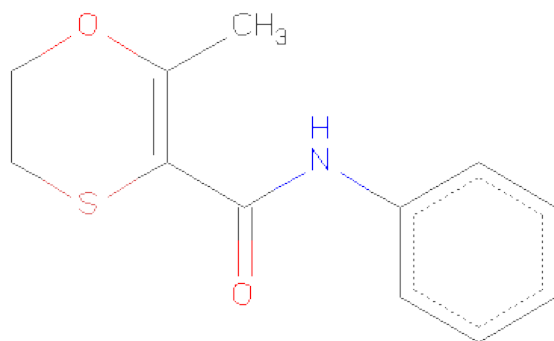
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	J	1	Total	Fe	S	0	0
			8	4	4		

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



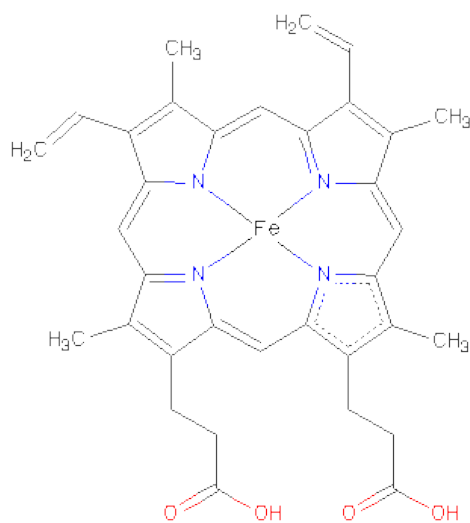
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		
10	F	1	Total	Fe	S	0	0
			7	3	4		
10	J	1	Total	Fe	S	0	0
			7	3	4		

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



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

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



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

3 Residue-property plots

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: 



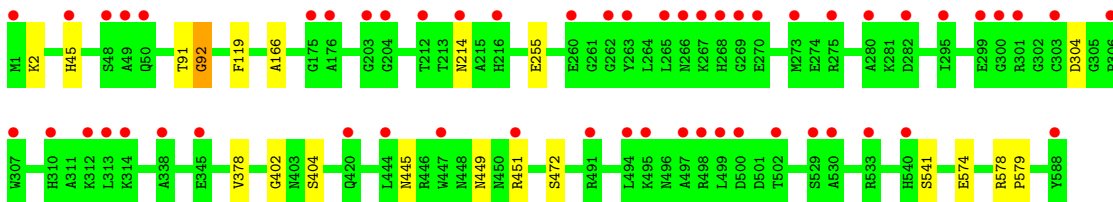
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain E: 



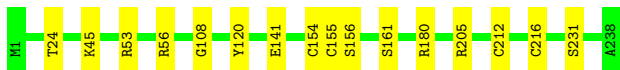
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

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: 



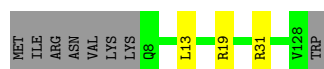
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT

Chain C:



- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT

Chain G:



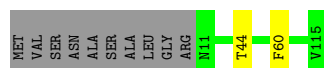
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B-556 SUBUNIT

Chain K:



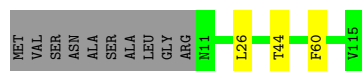
- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain D:



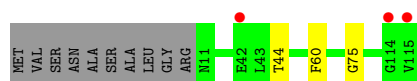
- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain H:



- Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR 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	119.85Å 184.71Å 203.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.20 49.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.03-3.20) 99.8 (49.01-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.219 , 0.253 0.210 , 0.243	Depositor DCC
R_{free} test set	3797 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 74902 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24900	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

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

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: TEO, NA, SF4, CBE, F3S, FES, HEM, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	1/4611 (0.0%)	0.67	0/6237
1	E	0.59	0/4611	0.64	0/6237
1	I	0.46	0/4611	0.58	0/6237
2	B	0.72	2/1908 (0.1%)	0.69	0/2578
2	F	0.61	0/1908	0.68	0/2578
2	J	0.51	0/1908	0.61	0/2578
3	C	0.66	0/953	0.62	0/1293
3	G	0.62	0/953	0.61	1/1293 (0.1%)
3	K	0.55	0/953	0.56	0/1293
4	D	0.68	0/858	0.59	0/1173
4	H	0.64	0/858	0.59	0/1173
4	L	0.61	0/858	0.58	0/1173
All	All	0.59	3/24990 (0.0%)	0.63	1/33843 (0.0%)

All (3) bond length outliers are listed below:

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

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 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	9	0
1	E	4522	0	0	6	0
1	I	4522	0	0	8	0
2	B	1869	0	0	1	0
2	F	1869	0	0	1	0
2	J	1869	0	0	1	0
3	C	933	0	0	2	0
3	G	933	0	0	1	0
3	K	933	0	0	3	0
4	D	835	0	0	0	0
4	H	835	0	0	1	0
4	L	835	0	0	1	0
5	A	53	0	0	2	0
5	E	53	0	0	3	0
5	I	53	0	0	8	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
7	A	9	0	3	4	0
7	E	9	0	3	5	0
7	I	9	0	3	6	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	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	1	0
11	C	16	0	13	1	0
11	G	16	0	13	0	0
11	K	16	0	13	2	0
12	C	43	0	30	5	0
12	G	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	43	0	30	10	0
All	All	24900	0	138	56	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 2.

All (56) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:HIS:NE2	5:A:601:FAD:C8M	1.94	1.30
1:E:45:HIS:NE2	5:E:601:FAD:C8M	2.08	1.16
1:I:45:HIS:NE2	5:I:601:FAD:C8M	2.38	0.87
12:C:1130:HEM:HBB2	12:C:1130:HEM:HHC	1.58	0.83
12:K:1130:HEM:HBC2	12:K:1130:HEM:HHH	1.62	0.80
12:K:1130:HEM:HHA	12:K:1130:HEM:CBA	2.16	0.74
12:G:1130:HEM:HHC	12:G:1130:HEM:HBB2	1.73	0.71
12:K:1130:HEM:HBA2	12:K:1130:HEM:HHA	1.73	0.70
3:C:31:ARG:CZ	11:C:1129:CBE:H62	2.25	0.66
1:I:404:SER:OG	5:I:601:FAD:O3'	2.15	0.65
1:A:45:HIS:CE1	5:A:601:FAD:C8M	2.76	0.65
3:K:27:SER:OG	11:K:1129:CBE:H51	1.97	0.65
12:K:1130:HEM:HAA1	4:L:75:GLY:CA	2.27	0.64
5:I:601:FAD:N5	7:I:1590:TEO:H2	2.13	0.63
3:K:31:ARG:NH1	11:K:1129:CBE:H12A	2.17	0.60
1:A:51:GLY:N	7:A:1590:TEO:O1A	2.35	0.59
12:C:1130:HEM:HHH	12:C:1130:HEM:HBC2	1.85	0.58
1:E:399:ARG:NH2	7:E:1590:TEO:O4B	2.37	0.58
12:K:1130:HEM:HHC	12:K:1130:HEM:HBB2	1.87	0.56
1:I:402:GLY:N	7:I:1590:TEO:O4A	2.38	0.55
5:I:601:FAD:C10	7:I:1590:TEO:O4B	2.56	0.54
12:K:1130:HEM:CHA	12:K:1130:HEM:HBA1	2.37	0.54
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.67	0.54
12:C:1130:HEM:CBB	12:C:1130:HEM:HHC	2.33	0.53
12:K:1130:HEM:CHA	12:K:1130:HEM:CBA	2.82	0.53
1:A:402:GLY:N	7:A:1590:TEO:O4A	2.42	0.53
12:C:1130:HEM:HBB2	12:C:1130:HEM:CHC	2.31	0.52
3:G:31:ARG:NE	12:G:1130:HEM:O1A	2.42	0.52
12:G:1130:HEM:HHA	12:G:1130:HEM:HBA2	1.91	0.52
12:K:1130:HEM:HHA	12:K:1130:HEM:HBA1	1.92	0.51
3:K:84:HIS:CD2	12:K:1130:HEM:NC	2.80	0.49
5:I:601:FAD:C9	5:I:601:FAD:O2'	2.60	0.49
12:G:1130:HEM:HMC1	4:H:26:LEU:CB	2.44	0.48
1:E:578:ARG:NH1	1:E:579:PRO:O	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:445:ASN:O	1:I:449:ASN:ND2	2.48	0.47
5:E:601:FAD:C4	7:E:1590:TEO:C3	2.92	0.47
5:E:601:FAD:N5	7:E:1590:TEO:H2	2.30	0.46
2:F:207:HIS:ND1	12:G:1130:HEM:O1D	2.48	0.46
1:I:578:ARG:NH1	1:I:579:PRO:O	2.49	0.46
2:J:159:CYS:CB	10:J:304:F3S:S2	3.04	0.45
1:A:399:ARG:NH2	7:A:1590:TEO:O4B	2.50	0.45
5:I:601:FAD:C4X	7:I:1590:TEO:C4	2.96	0.44
1:I:166:ALA:N	5:I:601:FAD:N1A	2.65	0.44
2:B:155:CYS:SG	2:B:156:SER:N	2.91	0.44
1:E:402:GLY:N	7:E:1590:TEO:O4A	2.51	0.43
1:E:86:GLU:OE2	1:E:577:LEU:N	2.52	0.43
1:A:186:GLU:OE2	3:C:9:ARG:NH2	2.52	0.43
12:C:1130:HEM:HHD	12:C:1130:HEM:CBC	2.48	0.42
1:E:242:HIS:CD2	7:E:1590:TEO:O2	2.72	0.42
5:I:601:FAD:C5X	7:I:1590:TEO:H2	2.49	0.42
12:G:1130:HEM:CHA	12:G:1130:HEM:HBA2	2.50	0.42
12:K:1130:HEM:CBC	12:K:1130:HEM:HHD	2.41	0.41
1:A:286:ARG:NH2	7:A:1590:TEO:O2	2.53	0.41
1:A:578:ARG:NH1	1:A:579:PRO:O	2.54	0.41
1:I:255:GLU:N	7:I:1590:TEO:O1B	2.55	0.40
1:I:91:THR:O	1:I:92:GLY:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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%)	560 (96%)	24 (4%)	2 (0%)	50	91
1	E	586/588 (100%)	558 (95%)	26 (4%)	2 (0%)	50	91
1	I	586/588 (100%)	561 (96%)	23 (4%)	2 (0%)	50	91
2	B	236/238 (99%)	223 (94%)	12 (5%)	1 (0%)	43	88
2	F	236/238 (99%)	220 (93%)	15 (6%)	1 (0%)	43	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	236/238 (99%)	223 (94%)	12 (5%)	1 (0%)	43	88
3	C	119/129 (92%)	114 (96%)	5 (4%)	0	100	100
3	G	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
3	K	119/129 (92%)	116 (98%)	3 (2%)	0	100	100
4	D	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	H	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
4	L	103/115 (90%)	98 (95%)	5 (5%)	0	100	100
All	All	3132/3210 (98%)	2984 (95%)	139 (4%)	9 (0%)	50	91

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	473/473 (100%)	464 (98%)	9 (2%)	69	93
1	E	473/473 (100%)	464 (98%)	9 (2%)	69	93
1	I	473/473 (100%)	465 (98%)	8 (2%)	73	94
2	B	208/208 (100%)	197 (95%)	11 (5%)	32	75
2	F	208/208 (100%)	198 (95%)	10 (5%)	35	79
2	J	208/208 (100%)	199 (96%)	9 (4%)	40	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	101/109 (93%)	99 (98%)	2 (2%)	68	92
3	G	101/109 (93%)	100 (99%)	1 (1%)	85	97
3	K	101/109 (93%)	100 (99%)	1 (1%)	85	97
4	D	88/96 (92%)	86 (98%)	2 (2%)	63	91
4	H	88/96 (92%)	86 (98%)	2 (2%)	63	91
4	L	88/96 (92%)	86 (98%)	2 (2%)	63	91
All	All	2610/2658 (98%)	2544 (98%)	66 (2%)	60	90

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

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

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 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$
7	TEO	A	1590	-	5,8,8	1.11	1 (20%)	3,10,10	0.96	0
5	FAD	A	601	-	58,58,58	1.24	7 (12%)	85,89,89	2.08	15 (17%)
8	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	B	303	2	12,12,12	8.00	12 (100%)	0,24,24	0.00	-
10	F3S	B	304	2	3,9,9	19.99	3 (100%)	0,15,15	0.00	-
11	CBE	C	1129	-	17,17,17	1.45	1 (5%)	22,22,22	1.84	2 (9%)
12	HEM	C	1130	3,4	49,50,50	2.41	13 (26%)	46,82,82	2.11	10 (21%)
7	TEO	E	1590	-	5,8,8	1.14	0	3,10,10	0.80	0
5	FAD	E	601	-	58,58,58	1.17	5 (8%)	85,89,89	2.12	17 (20%)
8	FES	F	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	F	303	2	12,12,12	7.18	11 (91%)	0,24,24	0.00	-
10	F3S	F	304	2	3,9,9	17.54	3 (100%)	0,15,15	0.00	-
11	CBE	G	1129	-	17,17,17	1.40	3 (17%)	22,22,22	1.79	4 (18%)
12	HEM	G	1130	3,4	49,50,50	2.57	16 (32%)	46,82,82	1.82	9 (19%)
7	TEO	I	1590	-	5,8,8	1.13	0	3,10,10	1.71	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	I	601	-	58,58,58	1.28	6 (10%)	85,89,89	2.00	16 (18%)
8	FES	J	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	J	303	2	12,12,12	4.94	10 (83%)	0,24,24	0.00	-
10	F3S	J	304	2	3,9,9	18.84	3 (100%)	0,15,15	0.00	-
11	CBE	K	1129	-	17,17,17	1.61	3 (17%)	22,22,22	1.69	3 (13%)
12	HEM	K	1130	3,4	49,50,50	2.95	17 (34%)	46,82,82	2.23	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TEO	A	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	A	601	-	-	0/34/50/50	0/1/6/6
8	FES	B	302	2	-	0/0/4/4	0/0/1/1
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
11	CBE	C	1129	-	-	0/8/19/19	0/2/2/2
12	HEM	C	1130	3,4	-	0/14/114/114	0/0/8/8
7	TEO	E	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	E	601	-	-	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
11	CBE	G	1129	-	-	0/8/19/19	0/2/2/2
12	HEM	G	1130	3,4	-	0/14/114/114	0/0/8/8
7	TEO	I	1590	-	-	0/2/8/8	0/0/0/0
5	FAD	I	601	-	-	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
11	CBE	K	1129	-	-	0/8/19/19	0/2/2/2
12	HEM	K	1130	3,4	-	0/14/114/114	0/0/8/8

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	304	F3S	S3-FE4	-25.26	2.16	2.33
10	J	304	F3S	S3-FE1	-24.53	2.16	2.33
10	F	304	F3S	S3-FE4	-19.81	2.19	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	304	F3S	S3-FE1	-19.73	2.20	2.33
10	F	304	F3S	S3-FE1	-17.61	2.21	2.33
10	J	304	F3S	S3-FE4	-16.12	2.22	2.33
10	F	304	F3S	S3-FE3	-14.84	2.23	2.33
10	J	304	F3S	S3-FE3	-14.24	2.23	2.33
10	B	304	F3S	S3-FE3	-13.08	2.24	2.33
9	B	303	SF4	S4-FE2	-12.00	2.25	2.33
9	F	303	SF4	S2-FE4	-10.08	2.26	2.33
9	B	303	SF4	S3-FE1	-10.00	2.26	2.33
9	B	303	SF4	S1-FE3	-9.54	2.26	2.33
9	B	303	SF4	S4-FE3	-9.54	2.26	2.33
9	F	303	SF4	S4-FE3	-9.48	2.26	2.33
12	K	1130	HEM	C2D-C1D	8.94	1.46	1.44
9	J	303	SF4	S4-FE2	-8.70	2.27	2.33
9	B	303	SF4	S2-FE4	-8.64	2.27	2.33
9	F	303	SF4	S3-FE2	-8.56	2.27	2.33
9	F	303	SF4	S2-FE3	-8.31	2.27	2.33
9	F	303	SF4	S3-FE1	-8.22	2.27	2.33
9	F	303	SF4	S4-FE1	-8.14	2.27	2.33
9	B	303	SF4	S4-FE1	-7.48	2.28	2.33
9	B	303	SF4	S3-FE2	-7.44	2.28	2.33
9	F	303	SF4	S1-FE2	-7.37	2.28	2.33
9	J	303	SF4	S3-FE1	-6.84	2.28	2.33
9	B	303	SF4	S1-FE4	-6.77	2.28	2.33
12	G	1130	HEM	C3D-C2D	6.37	1.54	1.43
12	C	1130	HEM	C2B-C1B	6.36	1.46	1.44
9	J	303	SF4	S4-FE3	-6.32	2.29	2.33
9	J	303	SF4	S2-FE4	-6.27	2.29	2.33
12	K	1130	HEM	C2B-C1B	6.21	1.46	1.44
9	F	303	SF4	S1-FE4	-6.11	2.29	2.33
9	F	303	SF4	S3-FE4	-6.08	2.29	2.33
12	K	1130	HEM	C3C-C2C	-6.04	1.33	1.43
9	B	303	SF4	S1-FE2	-5.97	2.29	2.33
12	K	1130	HEM	C3D-C2D	5.96	1.54	1.43
12	C	1130	HEM	C3C-C2C	-5.86	1.33	1.43
12	C	1130	HEM	C3B-C2B	-5.79	1.33	1.43
12	G	1130	HEM	C3B-C2B	-5.71	1.33	1.43
12	K	1130	HEM	FE-NB	5.69	2.18	1.97
12	K	1130	HEM	C3B-C2B	-5.64	1.33	1.43
9	B	303	SF4	S2-FE3	-5.61	2.29	2.33
12	G	1130	HEM	C3C-C2C	-5.39	1.34	1.43
12	G	1130	HEM	C2D-C1D	5.28	1.45	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	1130	HEM	C3B-CAB	5.18	1.56	1.40
12	K	1130	HEM	C4A-C3A	5.12	1.46	1.40
12	G	1130	HEM	C4A-C3A	5.11	1.46	1.40
12	G	1130	HEM	C3C-CAC	5.01	1.56	1.40
12	C	1130	HEM	C3D-C2D	4.94	1.52	1.43
12	G	1130	HEM	C3B-CAB	4.90	1.55	1.40
12	C	1130	HEM	C4A-C3A	4.71	1.46	1.40
9	B	303	SF4	S2-FE1	-4.69	2.30	2.33
9	J	303	SF4	S1-FE3	-4.66	2.30	2.33
9	B	303	SF4	S3-FE4	-4.64	2.30	2.33
5	I	601	FAD	C1'-C2'	4.59	1.56	1.51
12	K	1130	HEM	C3C-CAC	4.59	1.54	1.40
9	J	303	SF4	S3-FE2	-4.45	2.30	2.33
12	C	1130	HEM	C3B-CAB	4.40	1.54	1.40
12	C	1130	HEM	C2D-C1D	4.40	1.45	1.44
12	G	1130	HEM	C3D-C4D	4.24	1.45	1.44
12	C	1130	HEM	C3C-CAC	4.18	1.53	1.40
5	A	601	FAD	C1'-C2'	4.10	1.55	1.51
12	G	1130	HEM	FE-NA	3.99	2.09	1.92
11	C	1129	CBE	C11-N10	-3.98	1.34	1.41
12	G	1130	HEM	C2B-C1B	3.83	1.45	1.44
9	J	303	SF4	S2-FE1	-3.81	2.30	2.33
9	F	303	SF4	S4-FE2	-3.72	2.30	2.33
9	J	303	SF4	S1-FE4	-3.67	2.30	2.33
9	J	303	SF4	S1-FE2	-3.66	2.30	2.33
12	K	1130	HEM	CAA-C2A	3.41	1.58	1.52
12	K	1130	HEM	FE-NA	3.40	2.07	1.92
5	E	601	FAD	C2A-N3A	3.40	1.38	1.32
11	K	1129	CBE	C3-S4	3.39	1.81	1.74
12	C	1130	HEM	FE-NA	3.34	2.06	1.92
11	G	1129	CBE	C11-N10	-3.30	1.35	1.41
11	K	1129	CBE	C11-N10	-3.25	1.35	1.41
5	I	601	FAD	C2A-N3A	3.19	1.38	1.32
5	A	601	FAD	C2B-C1B	-3.06	1.49	1.53
5	E	601	FAD	C1'-N10	3.06	1.51	1.48
11	G	1129	CBE	C1-C2	2.96	1.55	1.49
5	E	601	FAD	C5X-N5	2.95	1.39	1.35
5	A	601	FAD	C5X-N5	2.88	1.39	1.35
12	G	1130	HEM	CMC-C2C	2.87	1.56	1.47
12	K	1130	HEM	C3B-C4B	2.84	1.47	1.44
12	C	1130	HEM	CMB-C2B	2.80	1.56	1.47
9	F	303	SF4	S1-FE3	-2.80	2.31	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	1130	HEM	FE-NB	2.75	2.07	1.97
5	A	601	FAD	C2A-N3A	2.74	1.37	1.32
12	G	1130	HEM	CMD-C2D	2.72	1.55	1.47
5	I	601	FAD	C1'-N10	2.72	1.51	1.48
12	K	1130	HEM	CMC-C2C	2.71	1.55	1.47
12	C	1130	HEM	CMC-C2C	2.70	1.55	1.47
12	K	1130	HEM	CMB-C2B	2.71	1.55	1.47
5	I	601	FAD	P-O3P	2.69	1.64	1.59
12	G	1130	HEM	CMB-C2B	2.66	1.55	1.47
5	E	601	FAD	C1'-C2'	2.52	1.54	1.51
12	C	1130	HEM	CMD-C2D	2.51	1.55	1.47
5	I	601	FAD	C5X-N5	2.49	1.39	1.35
9	J	303	SF4	S3-FE4	-2.45	2.31	2.33
12	K	1130	HEM	CMD-C2D	2.44	1.55	1.47
12	K	1130	HEM	FE-ND	2.37	2.06	1.97
5	A	601	FAD	C1'-N10	2.34	1.50	1.48
12	K	1130	HEM	CHC-C1C	2.33	1.40	1.36
12	C	1130	HEM	FE-NB	2.18	2.05	1.97
11	K	1129	CBE	C8-C3	2.16	1.54	1.50
7	A	1590	TEO	O4A-C4	2.15	1.25	1.22
12	G	1130	HEM	CHB-C1B	2.05	1.38	1.35
5	E	601	FAD	C4X-N5	2.05	1.40	1.36
12	G	1130	HEM	C3B-C4B	2.05	1.46	1.44
5	A	601	FAD	C10-N1	2.04	1.39	1.35
11	G	1129	CBE	C16-C11	2.04	1.42	1.39
5	I	601	FAD	C10-N1	2.03	1.39	1.35
5	A	601	FAD	C2A-N1A	2.01	1.37	1.33

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	N3A-C2A-N1A	-11.38	119.20	128.71
5	I	601	FAD	N3A-C2A-N1A	-10.72	119.75	128.71
5	E	601	FAD	N3A-C2A-N1A	-10.47	119.96	128.71
12	C	1130	HEM	C3B-C4B-NB	-10.05	106.81	114.00
12	K	1130	HEM	C3B-C4B-NB	-9.65	107.10	114.00
5	A	601	FAD	C2'-C1'-N10	-8.41	101.29	112.45
12	G	1130	HEM	C3B-C4B-NB	-8.09	108.21	114.00
5	E	601	FAD	C2'-C1'-N10	-7.21	102.89	112.45
5	E	601	FAD	C2-N1-C10	6.59	121.62	114.98
12	K	1130	HEM	C4D-ND-C1D	6.47	111.78	105.16
5	I	601	FAD	C2-N1-C10	6.01	121.03	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	1129	CBE	O7-C2-C1	6.00	119.83	109.71
11	C	1129	CBE	O7-C2-C1	5.97	119.78	109.71
5	I	601	FAD	C2'-C1'-N10	-5.74	104.83	112.45
11	K	1129	CBE	O7-C2-C1	5.48	118.95	109.71
12	G	1130	HEM	C4D-ND-C1D	5.03	110.31	105.16
12	C	1130	HEM	C4D-ND-C1D	4.94	110.22	105.16
5	A	601	FAD	C4X-N5-C5X	4.43	121.67	116.69
5	I	601	FAD	C4X-C10-N1	-4.36	118.37	122.73
11	C	1129	CBE	C3-C8-N10	-4.34	107.47	115.62
5	A	601	FAD	C2-N1-C10	4.01	119.02	114.98
5	E	601	FAD	N3A-C4A-N9A	3.76	132.23	125.43
12	C	1130	HEM	CHC-C4B-NB	3.72	127.68	124.58
5	I	601	FAD	N3A-C4A-N9A	3.59	131.92	125.43
5	E	601	FAD	C4X-N5-C5X	3.55	120.67	116.69
12	K	1130	HEM	CBA-CAA-C2A	-3.54	106.46	112.69
5	I	601	FAD	C4X-N5-C5X	3.46	120.58	116.69
11	K	1129	CBE	C8-C3-S4	3.43	119.86	111.06
12	K	1130	HEM	C4C-NC-C1C	3.40	109.07	105.53
5	E	601	FAD	C4X-C10-N1	-3.39	119.34	122.73
5	I	601	FAD	C5X-C9A-N10	3.22	119.97	116.80
12	K	1130	HEM	C2D-C1D-ND	-3.20	109.15	112.93
5	I	601	FAD	C1'-C2'-C3'	3.12	118.73	109.82
5	E	601	FAD	C5X-C9A-N10	3.07	119.82	116.80
12	K	1130	HEM	C1B-NB-C4B	2.96	108.19	105.16
12	K	1130	HEM	CHD-C1D-ND	-2.93	122.15	124.58
12	K	1130	HEM	CBD-CAD-C3D	-2.87	108.11	114.37
5	A	601	FAD	C4A-C5A-N7A	-2.84	107.09	109.52
7	I	1590	TEO	O2-C2-C3	2.80	115.86	110.17
12	G	1130	HEM	CBA-CAA-C2A	-2.79	107.78	112.69
12	G	1130	HEM	C2D-C1D-ND	-2.77	109.66	112.93
5	E	601	FAD	C1'-C2'-C3'	2.76	117.70	109.82
5	A	601	FAD	N3A-C4A-N9A	2.73	130.37	125.43
12	C	1130	HEM	CBA-CAA-C2A	-2.71	107.92	112.69
5	E	601	FAD	C5A-C4A-N3A	-2.71	119.81	125.70
5	I	601	FAD	C4-C4X-C10	2.56	121.09	116.95
5	E	601	FAD	C2A-N3A-C4A	2.55	121.26	114.01
12	C	1130	HEM	C2D-C1D-ND	-2.54	109.93	112.93
5	E	601	FAD	C4'-C3'-C2'	-2.53	107.53	113.25
5	A	601	FAD	P-O3P-PA	-2.50	124.35	131.68
5	A	601	FAD	C1B-N9A-C4A	-2.48	122.35	126.64
5	I	601	FAD	C4-N3-C2	-2.46	120.34	125.39
12	G	1130	HEM	O1D-CGD-CBD	-2.44	114.62	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	FAD	C9A-N10-C10	-2.43	119.38	121.77
12	C	1130	HEM	C4A-CHB-C1B	-2.42	124.28	127.47
12	G	1130	HEM	CHB-C1B-NB	2.42	127.63	124.31
5	I	601	FAD	N7A-C8A-N9A	-2.41	107.55	114.36
11	G	1129	CBE	C5-S4-C3	2.39	107.83	101.25
5	E	601	FAD	C4-N3-C2	-2.37	120.54	125.39
12	C	1130	HEM	CMA-C3A-C4A	-2.36	125.00	128.62
5	E	601	FAD	C6-C5X-N5	2.32	121.68	118.97
12	G	1130	HEM	C1B-NB-C4B	2.31	107.52	105.16
5	E	601	FAD	C1'-N10-C10	2.27	122.39	119.17
5	E	601	FAD	O4'-C4'-C3'	2.27	114.71	109.05
5	I	601	FAD	C2A-N3A-C4A	2.26	120.45	114.01
12	C	1130	HEM	CAD-CBD-CGD	-2.22	106.56	113.48
5	A	601	FAD	C2A-N3A-C4A	2.22	120.33	114.01
5	I	601	FAD	C5A-C4A-N3A	-2.20	120.90	125.70
12	C	1130	HEM	C1B-NB-C4B	2.18	107.39	105.16
5	I	601	FAD	C4A-C5A-N7A	-2.17	107.66	109.52
5	A	601	FAD	C1'-N10-C9A	2.17	120.98	118.87
5	A	601	FAD	N7A-C8A-N9A	-2.16	108.24	114.36
5	E	601	FAD	C4A-C5A-N7A	-2.16	107.68	109.52
12	G	1130	HEM	O2D-CGD-CBD	2.15	121.83	114.22
5	A	601	FAD	C4X-C10-N1	-2.15	120.58	122.73
11	G	1129	CBE	C2-C3-S4	-2.14	118.43	123.11
12	K	1130	HEM	CAA-CBA-CGA	2.13	120.30	113.47
5	I	601	FAD	C8A-N9A-C4A	2.08	108.48	106.90
5	E	601	FAD	C4B-O4B-C1B	2.07	111.99	109.75
11	G	1129	CBE	C3-C8-N10	-2.06	111.75	115.62
12	C	1130	HEM	O1A-CGA-CBA	-2.05	115.96	123.03
12	G	1130	HEM	CAD-C3D-C4D	2.05	128.22	124.53
11	K	1129	CBE	O7-C2-C3	-2.03	119.72	123.22
5	A	601	FAD	C1'-C2'-C3'	2.03	115.63	109.82
5	A	601	FAD	C5A-C4A-N3A	-2.02	121.31	125.70
5	A	601	FAD	C4-N3-C2	-2.00	121.28	125.39

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%)	-0.09	2 (0%) 91 58	45, 63, 84, 97	0
1	E	588/588 (100%)	-0.01	2 (0%) 91 58	53, 72, 95, 112	0
1	I	588/588 (100%)	0.64	55 (9%) 9 2	91, 124, 168, 190	0
2	B	238/238 (100%)	-0.05	0 100 100	45, 61, 88, 107	0
2	F	238/238 (100%)	-0.02	0 100 100	54, 72, 104, 123	0
2	J	238/238 (100%)	0.18	3 (1%) 74 24	75, 96, 165, 189	0
3	C	121/129 (93%)	-0.03	1 (0%) 83 35	62, 76, 107, 120	0
3	G	121/129 (93%)	0.12	0 100 100	71, 94, 119, 126	0
3	K	121/129 (93%)	0.28	2 (1%) 67 19	93, 118, 135, 144	0
4	D	105/115 (91%)	-0.13	0 100 100	55, 75, 109, 124	0
4	H	105/115 (91%)	-0.04	0 100 100	63, 79, 137, 155	0
4	L	105/115 (91%)	0.02	3 (2%) 49 10	73, 90, 142, 165	0
All	All	3156/3210 (98%)	0.12	68 (2%) 57 14	45, 80, 147, 190	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	499	LEU	5.0
1	I	500	ASP	4.1
1	I	268	HIS	4.1
1	I	265	LEU	3.9
1	I	1	MET	3.8
1	I	312	LYS	3.6
1	I	203	GLY	3.5
1	I	45	HIS	3.5
1	I	494	LEU	3.4
1	I	303	CYS	3.4
4	L	42	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	267	LYS	3.3
1	I	451	ARG	3.2
1	I	491	ARG	3.2
1	I	262	GLY	3.1
1	I	495	LYS	3.1
1	I	260	GLU	3.1
1	I	444	LEU	3.1
1	I	204	GLY	3.0
1	I	263	TYR	2.9
1	I	282	ASP	2.9
1	I	48	SER	2.8
1	I	266	ASN	2.8
1	I	313	LEU	2.7
1	I	216	HIS	2.7
1	I	420	GLN	2.6
1	I	314	LYS	2.6
1	I	269	GLY	2.6
1	I	310	HIS	2.6
1	I	50	GLN	2.6
2	J	18	PRO	2.6
1	I	502	THR	2.6
1	A	268	HIS	2.5
1	I	270	GLU	2.5
1	I	49	ALA	2.5
4	L	115	VAL	2.5
1	I	345	GLU	2.4
1	I	530	ALA	2.4
4	L	114	GLY	2.4
1	I	273	MET	2.4
1	A	301	ARG	2.4
3	K	22	ILE	2.3
2	J	29	GLU	2.3
1	I	275	ARG	2.3
1	I	588	TYR	2.3
1	E	491	ARG	2.3
1	I	175	GLY	2.3
1	I	307	TRP	2.2
1	I	295	ILE	2.2
1	I	306	PRO	2.2
1	I	212	THR	2.2
1	I	301	ARG	2.1
1	I	176	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	338	ALA	2.1
1	I	498	ARG	2.1
1	I	529	SER	2.1
1	I	299	GLU	2.1
1	I	447	TRP	2.1
1	I	280	ALA	2.1
1	I	214	ASN	2.1
3	K	111	LYS	2.1
1	I	533	ARG	2.0
3	C	65	MET	2.0
1	E	1	MET	2.0
1	I	300	GLY	2.0
1	I	497	ALA	2.0
1	I	540	HIS	2.0
2	J	53	ARG	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
6	NA	E	1589	1/1	0.45	2.21	45,45,45,45	0
12	HEM	C	1130	43/43	0.25	2.14	40,48,62,67	0
11	CBE	K	1129	16/16	0.40	2.05	85,91,97,97	0
7	TEO	A	1590	9/9	0.29	1.55	50,52,53,53	0
6	NA	A	1589	1/1	0.28	1.39	27,27,27,27	0
11	CBE	G	1129	16/16	0.38	0.91	56,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NA	I	1589	1/1	0.47	0.86	53,53,53,53	0
9	SF4	B	303	8/8	0.25	0.76	38,40,40,41	0
7	TEO	I	1590	9/9	0.45	0.76	109,112,114,114	0
12	HEM	G	1130	43/43	0.26	0.74	55,61,71,75	0
11	CBE	C	1129	16/16	0.23	0.65	53,55,56,56	0
12	HEM	K	1130	43/43	0.28	0.53	50,54,72,82	0
5	FAD	I	601	53/53	0.50	0.45	106,112,121,125	0
7	TEO	E	1590	9/9	0.22	0.35	50,52,53,55	0
5	FAD	E	601	53/53	0.34	0.33	46,61,71,73	0
9	SF4	F	303	8/8	0.20	0.22	55,58,59,59	0
5	FAD	A	601	53/53	0.25	0.08	38,42,53,54	0
8	FES	F	302	4/4	0.26	-0.14	54,55,56,58	0
9	SF4	J	303	8/8	0.20	-0.28	83,87,90,91	0
8	FES	B	302	4/4	0.28	-0.60	38,41,43,44	0
8	FES	J	302	4/4	0.29	-0.89	108,110,116,117	0
10	F3S	J	304	7/7	0.13	-0.95	88,90,92,93	0
10	F3S	B	304	7/7	0.16	-0.97	49,54,58,59	0
10	F3S	F	304	7/7	0.13	-1.30	64,69,72,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.