



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:47 PM GMT

PDB ID : 4YSZ
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with 2-iodo-N-[3-(1-methylethoxy)phenyl]benzamide
Authors : Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on : 2015-03-17
Resolution : 3.30 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

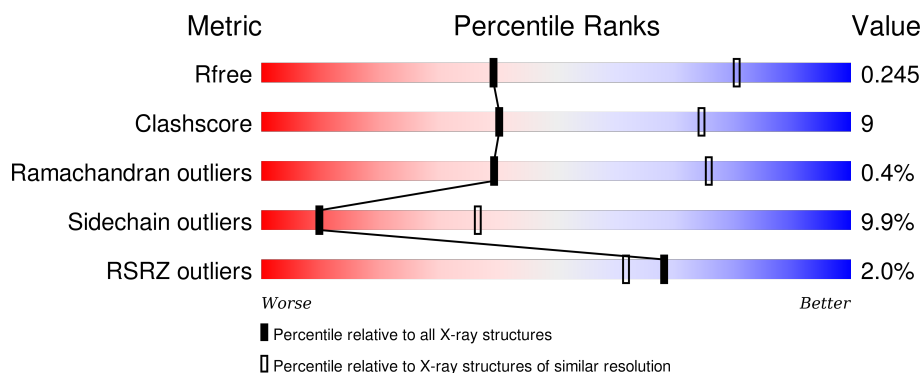
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	645	<div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	E	645	<div> <div>%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
2	B	282	<div> <div>71%</div> <div>16%</div> <div>• 11%</div> </div>
2	F	282	<div> <div>2%</div> <div>72%</div> <div>13%</div> <div>• 11%</div> </div>
3	C	188	<div> <div>3%</div> <div>64%</div> <div>14%</div> <div>• 19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	188	
4	D	156	
4	H	156	

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
12	EPH	D	201	-	-	-	X
12	EPH	H	201	-	-	-	X
5	MLI	E	701	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18361 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			
1	E	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			
2	F	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			

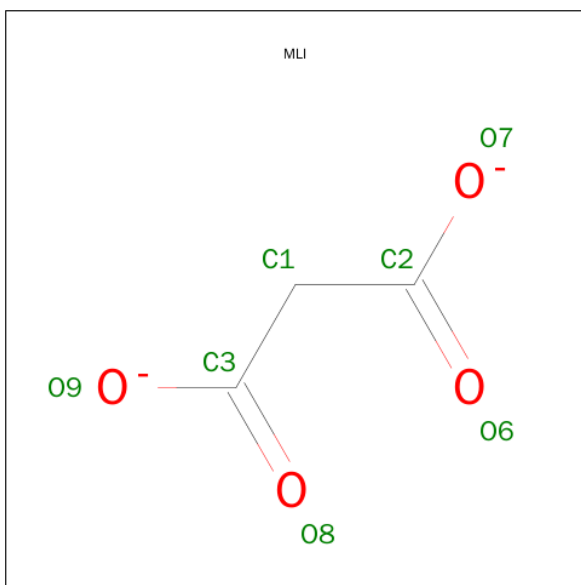
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

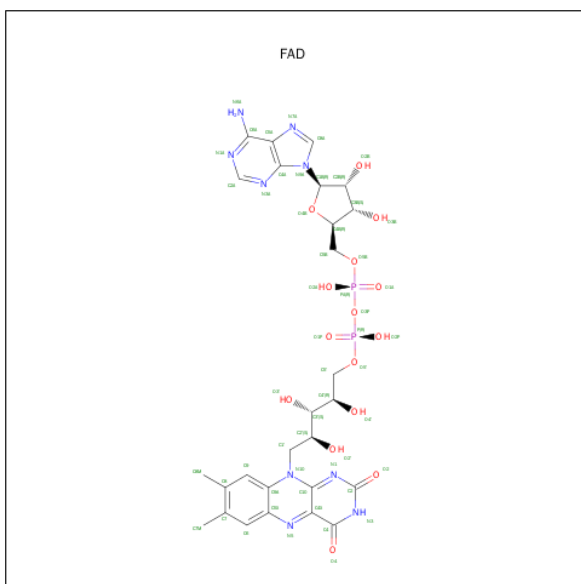
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



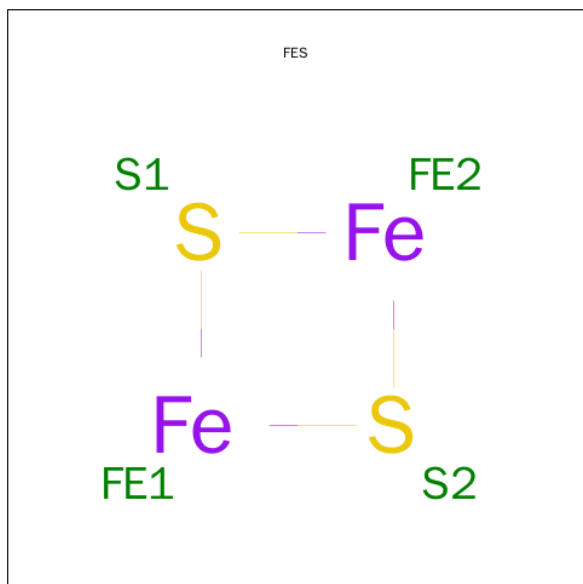
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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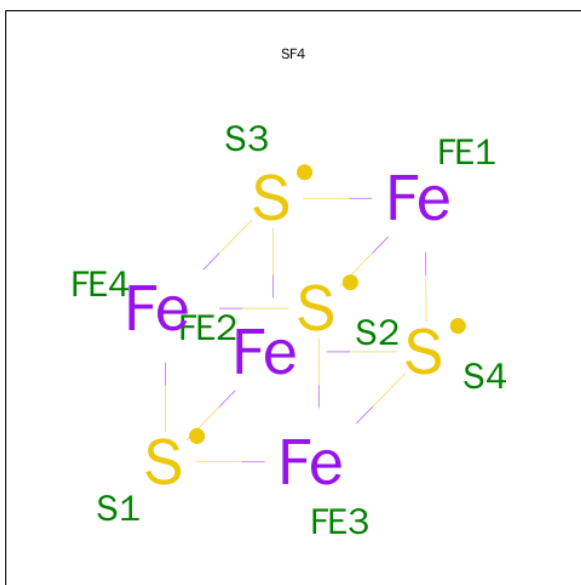
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



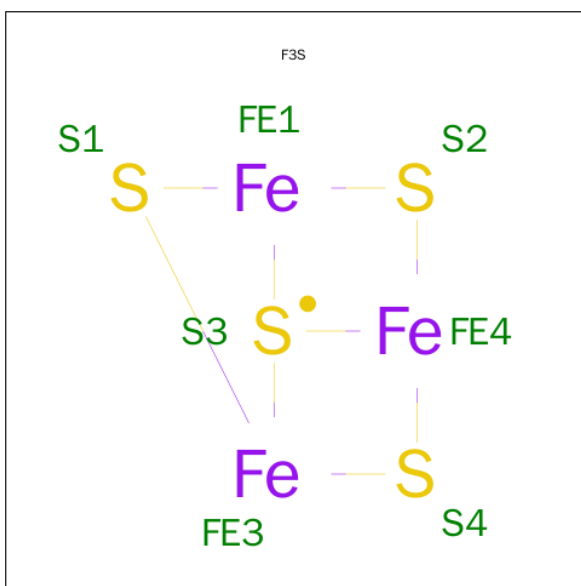
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



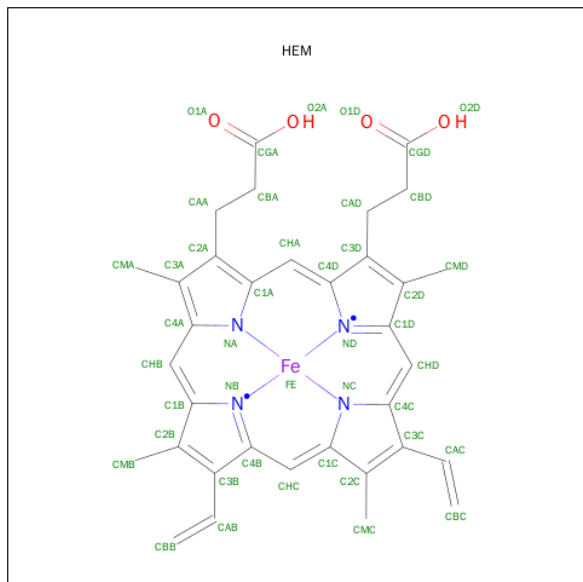
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



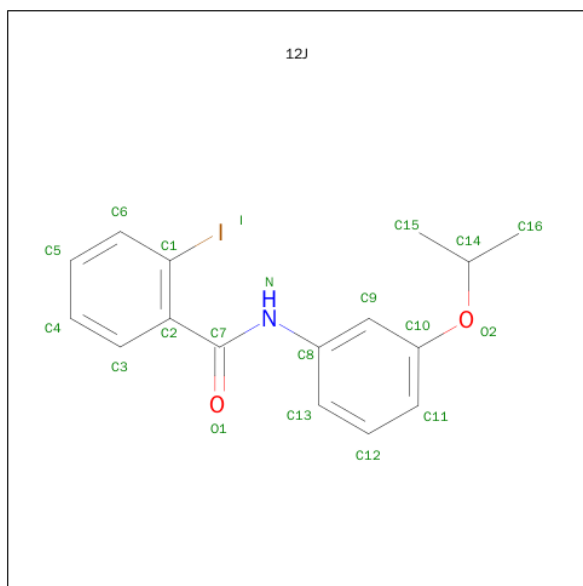
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



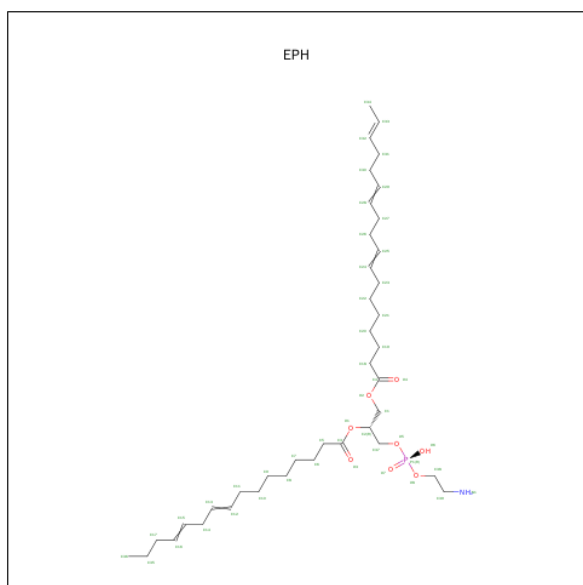
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 2-iodo-N-[3-(1-methylethoxy)phenyl]benzamide (three-letter code: 12J) (formula: $C_{16}H_{16}INO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	I	N	O	0	0
			20	16	1	1	2		
11	G	1	Total	C	I	N	O	0	0
			20	16	1	1	2		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	O	0	0
			4	4		
13	B	2	Total	O	0	0
			2	2		
13	C	1	Total	O	0	0
			1	1		
13	D	1	Total	O	0	0
			1	1		
13	E	6	Total	O	0	0
			6	6		

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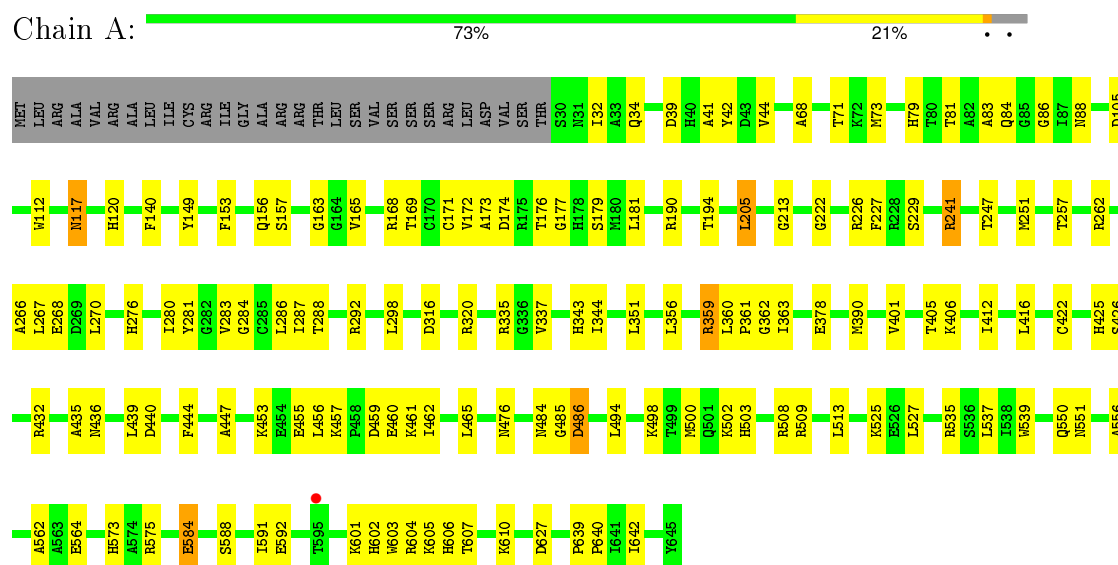
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	1	Total	O	0	0
			1	1		

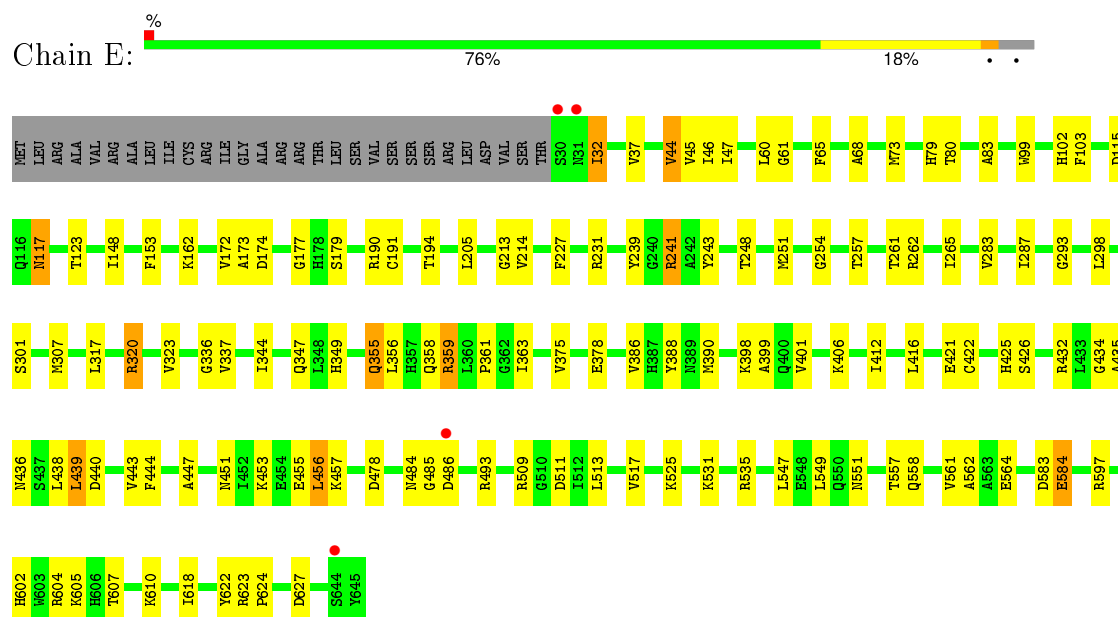
3 Residue-property plots

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.

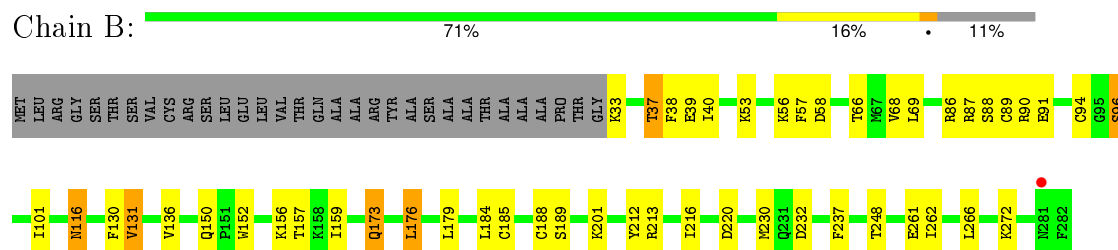
• Molecule 1: Succinate dehydrogenase flavoprotein



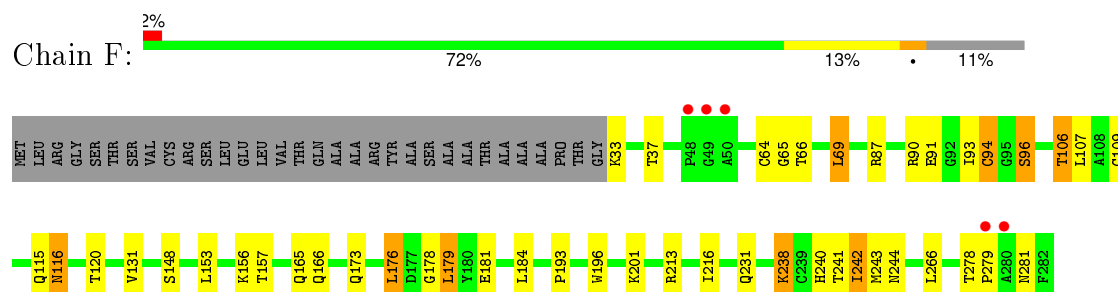
• Molecule 1: Succinate dehydrogenase flavoprotein



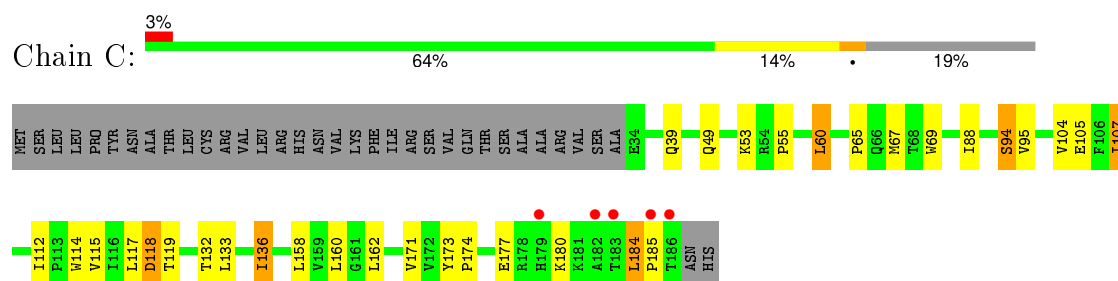
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



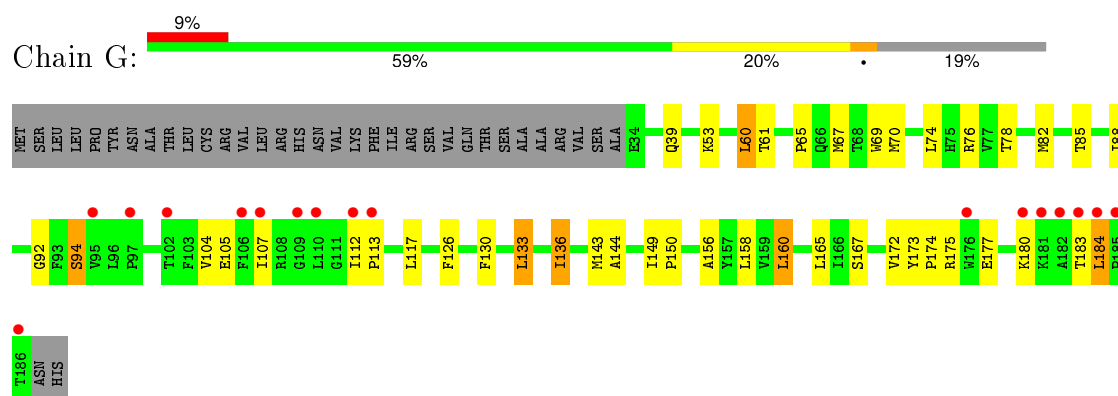
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Cytochrome b-large subunit

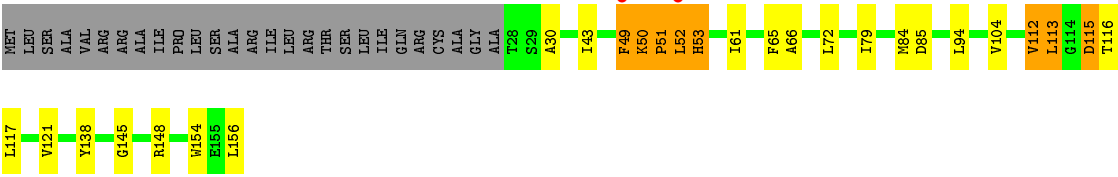


- Molecule 3: Cytochrome b-large subunit

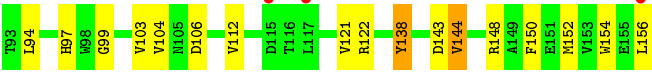
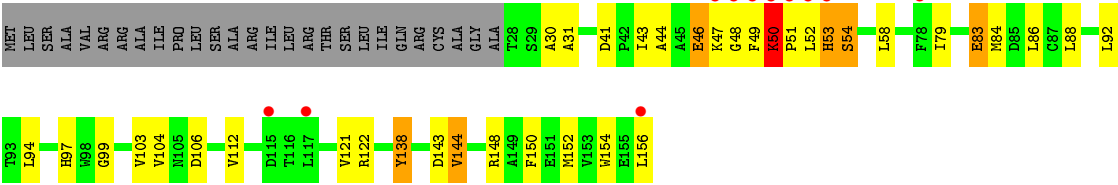


- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.93Å 126.97Å 219.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.30 29.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.82-3.30) 97.5 (29.82-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.250 0.180 , 0.245	Depositor DCC
R_{free} test set	2624 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.3	EDS
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 51446 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18361	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MLI, F3S, FES, EPH, HEM, 12J, 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	0.45	0/4889	0.68	0/6605
1	E	0.45	0/4889	0.68	0/6605
2	B	0.43	0/2029	0.66	0/2739
2	F	0.47	1/2029 (0.0%)	0.64	0/2739
3	C	0.43	0/1255	0.62	0/1709
3	G	0.44	0/1255	0.63	0/1709
4	D	0.51	0/1030	0.65	0/1406
4	H	0.51	0/1030	0.64	0/1406
All	All	0.45	1/18406 (0.0%)	0.66	0/24918

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	H	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	CYS	C-N	5.55	1.43	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	ALA	Peptide
4	H	30	ALA	Peptide
4	H	50	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4787	0	4720	71	0
1	E	4787	0	4720	77	0
2	B	1985	0	2001	19	0
2	F	1985	0	2001	21	0
3	C	1217	0	1265	25	0
3	G	1217	0	1265	23	0
4	D	998	0	985	44	0
4	H	998	0	985	47	0
5	A	7	0	2	1	0
5	E	7	0	2	2	0
6	A	53	0	31	4	0
6	E	53	0	31	5	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	6	0
10	G	43	0	30	5	0
11	C	20	0	16	4	0
11	G	20	0	16	4	0
12	D	44	0	53	0	0
12	H	44	0	53	2	0
13	A	4	0	0	0	0
13	B	2	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
All	All	18361	0	18206	318	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 9.

All (318) 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)
4:D:112:VAL:C	4:D:113:LEU:HD23	1.39	1.39
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.48	1.28
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.52	1.23
4:D:112:VAL:HG12	4:D:113:LEU:CD2	1.77	1.13
4:H:50:LYS:N	4:H:50:LYS:HD2	1.59	1.12
4:D:112:VAL:HG12	4:D:113:LEU:HD21	1.14	1.11
4:D:113:LEU:N	4:D:113:LEU:HD23	1.50	1.11
4:D:50:LYS:N	4:D:51:PRO:CD	2.15	1.09
4:H:46:GLU:OE2	4:H:46:GLU:HA	1.47	1.06
4:H:52:LEU:C	4:H:53:HIS:CD2	2.30	1.05
1:A:172:VAL:O	1:A:172:VAL:HG12	1.55	1.04
4:D:50:LYS:H	4:D:51:PRO:CD	1.68	1.03
4:H:50:LYS:N	4:H:51:PRO:HD3	1.73	1.01
4:D:52:LEU:C	4:D:53:HIS:HD2	1.64	1.00
4:D:112:VAL:C	4:D:113:LEU:CD2	2.31	0.99
4:D:112:VAL:CG1	4:D:113:LEU:HD21	1.92	0.98
4:D:50:LYS:N	4:D:51:PRO:HD2	1.77	0.98
4:D:50:LYS:H	4:D:51:PRO:HD3	1.27	0.98
4:H:51:PRO:HB2	4:H:53:HIS:NE2	1.78	0.97
4:H:51:PRO:CB	4:H:53:HIS:NE2	2.30	0.95
4:D:113:LEU:N	4:D:113:LEU:CD2	2.30	0.94
4:H:50:LYS:N	4:H:51:PRO:CD	2.30	0.94
4:D:53:HIS:CD2	4:D:53:HIS:N	2.30	0.94
4:D:52:LEU:C	4:D:53:HIS:CD2	2.41	0.94
4:D:52:LEU:CA	4:D:53:HIS:HD2	1.80	0.94
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.29	0.93
4:H:50:LYS:N	4:H:50:LYS:CD	2.30	0.93
2:F:94:CYS:SG	2:F:96:SER:OG	2.32	0.87
1:E:79:HIS:CD2	6:E:702:FAD:HM82	2.10	0.87
4:H:49:PHE:CD1	4:H:49:PHE:O	2.30	0.84
4:D:49:PHE:O	4:D:49:PHE:CD1	2.30	0.84
4:H:51:PRO:C	4:H:53:HIS:NE2	2.32	0.82
4:H:52:LEU:C	4:H:53:HIS:HD2	1.80	0.81
4:D:112:VAL:CG1	4:D:113:LEU:CD2	2.56	0.80
4:D:52:LEU:CA	4:D:53:HIS:CD2	2.65	0.80
2:F:242:ILE:O	2:F:243:MET:HB2	1.82	0.78
4:D:112:VAL:O	4:D:113:LEU:HD23	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:GLU:OE2	4:H:46:GLU:CA	2.30	0.74
1:A:172:VAL:O	1:A:173:ALA:HB3	1.87	0.73
4:H:49:PHE:CG	4:H:49:PHE:O	2.38	0.72
1:A:172:VAL:O	1:A:172:VAL:CG1	2.30	0.72
4:H:49:PHE:C	4:H:51:PRO:HD2	2.10	0.72
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.71	0.72
4:H:53:HIS:CD2	4:H:53:HIS:N	2.57	0.72
4:H:49:PHE:C	4:H:51:PRO:CD	2.59	0.71
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.04	0.71
1:A:604:ARG:NH1	1:A:627:ASP:OD2	2.23	0.71
10:C:201:HEM:HHA	10:C:201:HEM:HBD1	1.72	0.71
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.73	0.70
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.44	0.70
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.72	0.70
4:H:52:LEU:N	4:H:53:HIS:CD2	2.59	0.69
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.75	0.69
4:H:50:LYS:H	4:H:50:LYS:CD	2.03	0.68
2:F:240:HIS:O	2:F:241:THR:OG1	2.12	0.68
3:G:74:LEU:HD23	3:G:130:PHE:CE1	2.29	0.68
1:A:205:LEU:HD23	1:A:465:LEU:HD21	1.75	0.67
1:E:47:ILE:HD11	1:E:214:VAL:CG2	2.25	0.67
4:D:112:VAL:O	4:D:113:LEU:CD2	2.42	0.66
2:F:116:ASN:C	2:F:116:ASN:HD22	1.97	0.66
2:B:94:CYS:SG	2:B:96:SER:OG	2.53	0.66
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.42	0.65
4:D:115:ASP:N	4:D:115:ASP:OD2	2.29	0.65
4:D:51:PRO:O	4:D:53:HIS:NE2	2.30	0.65
4:H:52:LEU:O	4:H:53:HIS:HD2	1.79	0.64
4:D:52:LEU:N	4:D:53:HIS:HD2	1.95	0.64
2:F:240:HIS:C	2:F:241:THR:OG1	2.35	0.64
4:H:50:LYS:H	4:H:51:PRO:HD3	1.63	0.64
1:E:262:ARG:HH22	1:E:551:ASN:HD21	1.45	0.63
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.81	0.63
11:C:202:12J:O1	11:C:202:12J:I	2.87	0.63
3:C:69:TRP:CE3	11:C:202:12J:H14	2.34	0.62
1:A:267:LEU:HD12	1:A:270:LEU:HD11	1.81	0.62
4:H:51:PRO:HB2	4:H:53:HIS:CE1	2.34	0.62
2:B:68:VAL:HG11	2:B:101:ILE:HD13	1.80	0.62
1:E:190:ARG:HG3	4:H:43:ILE:HD11	1.81	0.62
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.82	0.62
1:A:425:HIS:N	1:A:426:SER:HA	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:PHE:CE1	2:B:266:LEU:HD23	2.35	0.61
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.82	0.61
1:E:356:LEU:HD23	1:E:375:VAL:HG23	1.82	0.61
1:E:103:PHE:HA	1:E:123:THR:HG21	1.82	0.61
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.81	0.60
2:F:231:GLN:HB3	4:H:54:SER:HA	1.83	0.60
1:E:583:ASP:O	1:E:597:ARG:NH2	2.34	0.60
4:D:52:LEU:N	4:D:53:HIS:CD2	2.70	0.60
1:E:47:ILE:HD11	1:E:214:VAL:HG21	1.84	0.59
1:A:42:TYR:O	1:A:229:SER:HA	2.01	0.59
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.15	0.59
1:A:602:HIS:O	1:A:605:LYS:HE2	2.02	0.59
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.84	0.59
1:A:584:GLU:OE2	1:A:604:ARG:NH2	2.36	0.59
1:E:425:HIS:N	1:E:426:SER:HA	2.18	0.59
4:H:52:LEU:CA	4:H:53:HIS:CD2	2.86	0.58
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.02	0.58
2:B:188:CYS:SG	2:B:189:SER:N	2.77	0.58
4:H:88:LEU:O	4:H:92:LEU:HB2	2.04	0.57
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.85	0.57
4:H:52:LEU:O	4:H:53:HIS:CD2	2.57	0.57
4:H:41:ASP:HB3	4:H:44:ALA:HB3	1.87	0.57
1:E:485:GLY:O	1:E:531:LYS:HB2	2.05	0.56
1:A:603:TRP:HA	1:A:605:LYS:HE2	1.88	0.55
4:D:104:VAL:HG13	4:D:121:VAL:HG12	1.88	0.55
1:E:32:ILE:HG13	1:E:32:ILE:O	2.07	0.55
3:C:112:ILE:HD11	3:C:117:LEU:CD2	2.37	0.54
4:D:49:PHE:C	4:D:49:PHE:CD1	2.80	0.54
1:A:588:SER:HB3	1:A:642:ILE:HD11	1.89	0.54
2:F:238:LYS:HE3	4:H:106:ASP:OD1	2.08	0.54
3:C:60:LEU:HA	11:C:202:12J:H15A	1.89	0.54
11:G:202:12J:I	11:G:202:12J:O1	2.96	0.54
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.90	0.54
1:A:174:ASP:OD2	1:A:362:GLY:N	2.41	0.54
2:F:242:ILE:O	2:F:243:MET:CB	2.50	0.53
1:E:117:ASN:HD22	1:E:117:ASN:N	2.06	0.53
2:F:242:ILE:HG22	2:F:244:ASN:H	1.73	0.53
2:F:116:ASN:ND2	2:F:116:ASN:C	2.62	0.53
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.09	0.53
1:A:213:GLY:HA3	1:A:227:PHE:O	2.08	0.53
1:A:117:ASN:HD22	1:A:117:ASN:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.91	0.53
1:E:47:ILE:HD11	1:E:214:VAL:HG22	1.90	0.52
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.91	0.52
1:E:557:THR:O	1:E:561:VAL:HG13	2.09	0.52
4:H:83:GLU:CD	4:H:83:GLU:H	2.11	0.52
3:G:112:ILE:HD11	3:G:117:LEU:HD21	1.91	0.52
1:A:41:ALA:HB1	1:A:462:ILE:HD13	1.92	0.52
4:H:51:PRO:C	4:H:53:HIS:CD2	2.83	0.52
1:E:401:VAL:HG21	1:E:416:LEU:HG	1.91	0.52
1:A:174:ASP:OD2	1:A:363:ILE:N	2.41	0.52
4:D:51:PRO:C	4:D:53:HIS:CD2	2.84	0.51
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.92	0.51
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.35	0.51
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.92	0.51
1:E:172:VAL:O	1:E:173:ALA:C	2.47	0.51
3:G:74:LEU:HD23	3:G:130:PHE:CZ	2.45	0.51
1:E:172:VAL:O	1:E:172:VAL:HG12	2.09	0.51
1:A:117:ASN:N	1:A:117:ASN:HD22	2.08	0.51
1:E:486:ASP:OD2	1:E:486:ASP:N	2.30	0.51
1:A:172:VAL:O	1:A:173:ALA:CB	2.54	0.51
1:E:301:SER:HB3	1:E:336:GLY:O	2.10	0.51
1:A:84:GLN:OE1	1:A:288:THR:HB	2.10	0.51
3:G:133:LEU:O	3:G:136:ILE:HG23	2.11	0.51
3:G:94:SER:HA	4:H:138:TYR:CZ	2.46	0.51
3:G:126:PHE:HA	3:G:167:SER:OG	2.11	0.51
3:G:104:VAL:HG13	4:H:156:LEU:HD21	1.93	0.51
1:A:486:ASP:OD2	1:A:486:ASP:N	2.44	0.50
1:E:174:ASP:OD1	1:E:174:ASP:O	2.30	0.50
4:D:51:PRO:C	4:D:53:HIS:HE2	2.13	0.50
3:G:60:LEU:HD12	3:G:61:THR:HG23	1.94	0.50
1:A:591:ILE:N	1:A:591:ILE:HD12	2.27	0.50
1:E:73:MET:SD	1:E:251:MET:HG3	2.51	0.50
4:D:112:VAL:HG12	4:D:113:LEU:HD23	1.78	0.50
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.47	0.50
3:C:95:VAL:O	3:C:95:VAL:HG12	2.11	0.49
4:H:46:GLU:O	4:H:48:GLY:O	2.30	0.49
1:E:493:ARG:HB2	1:E:549:LEU:HD13	1.94	0.49
4:H:94:LEU:O	4:H:97:HIS:HB3	2.11	0.49
1:A:105:ASP:OD2	1:A:157:SER:N	2.39	0.49
2:F:153:LEU:HD21	2:F:166:GLN:HE22	1.77	0.49
1:A:247:THR:HG22	1:A:284:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:158:LEU:C	3:G:158:LEU:HD23	2.33	0.49
3:C:158:LEU:CD2	3:C:162:LEU:HD12	2.43	0.49
1:E:45:VAL:HG21	1:E:227:PHE:HB3	1.95	0.49
2:B:86:ARG:CZ	2:B:136:VAL:HG13	2.43	0.49
1:E:307:MET:CE	1:E:323:VAL:HG22	2.43	0.48
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.95	0.48
3:G:173:TYR:HB3	3:G:174:PRO:HD3	1.93	0.48
1:A:359:ARG:O	1:A:360:LEU:HD23	2.13	0.48
1:A:73:MET:SD	1:A:251:MET:HG3	2.53	0.48
4:D:51:PRO:C	4:D:53:HIS:NE2	2.67	0.48
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.95	0.48
3:C:180:LYS:O	3:C:184:LEU:HB3	2.13	0.48
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.96	0.48
3:C:184:LEU:HD22	3:C:185:PRO:O	2.14	0.47
1:A:500:MET:HE1	1:A:556:ALA:O	2.14	0.47
1:A:86:GLY:HA2	1:A:176:THR:HG21	1.95	0.47
3:G:69:TRP:CE2	11:G:202:12J:H14	2.49	0.47
1:A:42:TYR:CD2	1:A:68:ALA:HB2	2.49	0.47
1:E:355:GLN:O	1:E:359:ARG:HB2	2.14	0.47
2:B:130:PHE:CD2	3:C:49:GLN:HB3	2.50	0.47
2:B:37:THR:HB	2:B:58:ASP:OD2	2.15	0.47
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.97	0.47
4:D:50:LYS:N	4:D:51:PRO:HD3	1.96	0.47
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.48	0.47
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.96	0.47
1:E:293:GLY:CA	1:E:317:LEU:HD21	2.45	0.47
1:E:44:VAL:HB	1:E:231:ARG:HB2	1.97	0.47
1:E:509:ARG:NH1	1:E:511:ASP:OD2	2.39	0.47
2:F:69:LEU:HD12	2:F:109:CYS:HB3	1.97	0.46
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.97	0.46
2:B:230:MET:HE1	2:B:262:ILE:HD13	1.96	0.46
2:F:193:PRO:O	2:F:196:TRP:HB2	2.15	0.46
1:E:451:ASN:N	1:E:451:ASN:HD22	2.14	0.46
3:C:69:TRP:CZ3	11:C:202:12J:H14	2.51	0.46
1:E:602:HIS:O	1:E:605:LYS:NZ	2.44	0.46
1:E:241:ARG:HD2	1:E:241:ARG:HA	1.77	0.46
10:G:201:HEM:HBC2	10:G:201:HEM:HHD	1.98	0.46
3:C:136:ILE:HD12	3:C:136:ILE:C	2.37	0.46
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.46	0.46
1:E:584:GLU:HA	1:E:602:HIS:CD2	2.50	0.46
1:A:169:THR:HG23	1:A:435:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:THR:HG23	2:F:107:LEU:N	2.31	0.46
1:A:459:ASP:OD1	1:A:460:GLU:N	2.49	0.46
1:A:476:ASN:HD21	1:A:550:GLN:NE2	2.10	0.46
10:G:201:HEM:HAD1	4:H:99:GLY:CA	2.46	0.46
3:C:112:ILE:HD11	3:C:117:LEU:HD23	1.98	0.46
2:F:64:CYS:SG	2:F:65:GLY:N	2.89	0.46
1:E:243:TYR:CD2	1:E:386:VAL:HG21	2.51	0.46
2:B:40:ILE:HD12	2:B:57:PHE:CD1	2.51	0.46
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.98	0.45
2:F:173:GLN:O	2:F:176:LEU:HB2	2.17	0.45
3:C:158:LEU:HD21	3:C:162:LEU:HD12	1.99	0.45
1:E:451:ASN:ND2	1:E:451:ASN:N	2.64	0.45
3:C:94:SER:HA	4:D:138:TYR:CZ	2.51	0.45
10:C:201:HEM:CBD	10:C:201:HEM:HHA	2.45	0.45
1:A:584:GLU:CD	1:A:604:ARG:NH2	2.69	0.45
10:C:201:HEM:HHD	10:C:201:HEM:HBC2	1.97	0.45
1:E:99:TRP:O	1:E:102:HIS:HB3	2.16	0.45
1:E:347:GLN:HG3	1:E:349:HIS:CE1	2.50	0.45
2:B:116:ASN:ND2	2:B:116:ASN:C	2.69	0.45
1:A:262:ARG:HH22	1:A:551:ASN:ND2	2.14	0.45
2:B:38:PHE:O	2:B:56:LYS:HA	2.16	0.45
4:D:116:THR:OG1	4:D:117:LEU:N	2.48	0.45
3:G:180:LYS:O	3:G:184:LEU:HB3	2.16	0.45
4:H:51:PRO:HB3	4:H:53:HIS:NE2	2.26	0.45
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.52	0.45
2:B:220:ASP:O	2:B:272:LYS:NZ	2.49	0.45
3:G:69:TRP:CD2	11:G:202:12J:H14	2.52	0.45
1:E:241:ARG:NH2	1:E:248:THR:O	2.50	0.45
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.98	0.44
2:B:150:GLN:HA	2:B:152:TRP:CZ3	2.52	0.44
3:C:118:ASP:HB3	3:C:171:VAL:CG1	2.47	0.44
4:D:52:LEU:HA	4:D:53:HIS:CD2	2.52	0.44
1:A:190:ARG:HG3	4:D:43:ILE:HD11	2.00	0.44
1:E:439:LEU:HD22	1:E:443:VAL:HG23	1.98	0.44
3:C:104:VAL:HG13	4:D:156:LEU:HD21	1.99	0.44
1:E:558:GLN:HA	1:E:618:ILE:HD13	1.99	0.44
1:A:476:ASN:ND2	1:A:550:GLN:HE22	2.12	0.44
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.99	0.44
4:H:51:PRO:CA	4:H:53:HIS:NE2	2.81	0.44
1:E:605:LYS:HD2	1:E:622:TYR:HB3	2.00	0.44
3:G:76:ARG:CZ	4:H:103:VAL:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.98	0.44
1:A:508:ARG:HB3	1:A:513:LEU:HD11	1.99	0.44
10:G:201:HEM:HAD1	4:H:99:GLY:HA3	1.99	0.44
4:H:144:VAL:HG11	4:H:152:MET:SD	2.58	0.44
3:C:107:ILE:HD11	4:D:156:LEU:CD1	2.48	0.43
1:E:172:VAL:O	1:E:173:ALA:HB3	2.18	0.43
1:A:494:LEU:HG	1:A:498:LYS:HD2	2.00	0.43
1:E:438:LEU:HG	6:E:702:FAD:C2	2.48	0.43
1:A:174:ASP:OD2	1:A:362:GLY:CA	2.65	0.43
1:A:267:LEU:CD1	1:A:270:LEU:HD11	2.48	0.43
1:E:46:ILE:HD11	1:E:60:LEU:HD12	2.01	0.43
4:H:52:LEU:N	4:H:53:HIS:HD2	2.15	0.43
1:E:517:VAL:HG13	1:E:561:VAL:HG12	2.00	0.43
3:C:173:TYR:HB3	3:C:174:PRO:HD3	1.99	0.43
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.01	0.43
2:B:39:GLU:HG2	2:B:56:LYS:HD2	1.99	0.43
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.52	0.43
1:E:45:VAL:HG22	1:E:68:ALA:HB3	2.00	0.43
1:E:439:LEU:HD22	1:E:443:VAL:CG2	2.49	0.43
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.93	0.43
4:D:50:LYS:H	4:D:51:PRO:HD2	1.48	0.43
1:A:584:GLU:CD	1:A:604:ARG:HH21	2.22	0.43
1:E:65:PHE:CE2	1:E:456:LEU:HD13	2.53	0.43
1:A:573:HIS:CE1	1:A:575:ARG:HG2	2.54	0.42
1:E:623:ARG:HG3	1:E:624:PRO:HD2	2.02	0.42
4:H:49:PHE:C	4:H:50:LYS:HD2	2.32	0.42
1:E:307:MET:HE2	1:E:323:VAL:HG22	2.01	0.42
1:E:604:ARG:HH22	1:E:627:ASP:CG	2.22	0.42
1:E:320:ARG:NH1	5:E:701:MLI:C2	2.79	0.42
2:B:262:ILE:O	2:B:266:LEU:HB2	2.19	0.42
3:G:156:ALA:O	3:G:160:LEU:HD22	2.20	0.42
4:D:72:LEU:HD23	4:D:72:LEU:O	2.20	0.42
3:C:132:THR:HG23	10:C:201:HEM:CBB	2.50	0.42
3:C:136:ILE:HD12	3:C:136:ILE:O	2.20	0.42
4:H:46:GLU:O	4:H:47:LYS:C	2.56	0.41
1:E:561:VAL:HG21	1:E:618:ILE:HG21	2.02	0.41
4:D:65:PHE:CE2	4:D:94:LEU:HD23	2.55	0.41
2:B:173:GLN:O	2:B:176:LEU:HB2	2.20	0.41
3:G:78:THR:O	3:G:82:MET:HG3	2.20	0.41
1:A:149:TYR:CD2	1:A:171:CYS:SG	3.13	0.41
1:E:115:ASP:HB3	1:E:117:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.55	0.41
1:A:639:PRO:HA	1:A:640:PRO:HD3	1.97	0.41
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.56	0.41
1:A:292:ARG:HD2	1:A:316:ASP:O	2.21	0.41
3:C:114:TRP:CE2	3:C:115:VAL:HG23	2.56	0.41
10:C:201:HEM:HMB2	4:D:66:ALA:HB1	2.02	0.41
1:A:401:VAL:HG21	1:A:416:LEU:HG	2.02	0.41
2:F:178:GLY:N	2:F:181:GLU:OE1	2.52	0.41
1:A:444:PHE:HA	1:A:447:ALA:HB3	2.03	0.41
1:E:61:GLY:HA3	1:E:191:CYS:HB2	2.03	0.41
1:E:213:GLY:HA3	1:E:227:PHE:O	2.21	0.41
1:E:623:ARG:CG	1:E:624:PRO:HD2	2.51	0.41
4:H:150:PHE:HB3	12:H:201:EPH:H2	2.03	0.41
1:A:268:GLU:HG3	1:A:606:HIS:HB3	2.03	0.41
1:E:398:LYS:O	1:E:399:ALA:HB3	2.21	0.41
4:D:112:VAL:CG1	4:D:113:LEU:HD23	2.40	0.41
1:A:81:THR:HB	1:A:181:LEU:HD23	2.03	0.41
1:A:502:LYS:HD3	1:A:503:HIS:CE1	2.55	0.41
1:E:434:GLY:O	1:E:435:ALA:HB3	2.21	0.41
3:G:149:ILE:HB	3:G:150:PRO:HD3	2.03	0.41
1:E:37:VAL:HB	4:H:31:ALA:HB2	2.03	0.41
1:E:432:ARG:HH21	1:E:435:ALA:H	1.70	0.41
1:E:148:ILE:H	2:F:165:GLN:HE22	1.68	0.41
1:E:32:ILE:HG23	1:E:478:ASP:OD1	2.21	0.40
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.56	0.40
1:A:280:ILE:HD11	1:A:287:ILE:HD11	2.02	0.40
3:G:88:ILE:O	3:G:92:GLY:HA3	2.21	0.40
3:G:143:MET:O	3:G:144:ALA:HB3	2.21	0.40
1:E:287:ILE:HG23	1:E:363:ILE:HD13	2.03	0.40
2:F:193:PRO:HG3	11:G:202:12J:H16A	2.03	0.40
3:C:115:VAL:O	3:C:119:THR:OG1	2.32	0.40
3:G:65:PRO:HA	3:G:69:TRP:CZ2	2.56	0.40
3:G:85:THR:HG21	12:H:201:EPH:C27	2.51	0.40
1:A:281:TYR:CD1	1:A:343:HIS:HB3	2.57	0.40
4:D:85:ASP:OD1	4:D:145:GLY:HA3	2.21	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	614/645 (95%)	573 (93%)	39 (6%)	2 (0%)	46	81
1	E	614/645 (95%)	583 (95%)	30 (5%)	1 (0%)	52	85
2	B	248/282 (88%)	232 (94%)	14 (6%)	2 (1%)	24	62
2	F	248/282 (88%)	231 (93%)	16 (6%)	1 (0%)	39	76
3	C	151/188 (80%)	142 (94%)	9 (6%)	0	100	100
3	G	151/188 (80%)	140 (93%)	10 (7%)	1 (1%)	26	66
4	D	127/156 (81%)	120 (94%)	6 (5%)	1 (1%)	24	62
4	H	127/156 (81%)	123 (97%)	4 (3%)	0	100	100
All	All	2280/2542 (90%)	2144 (94%)	128 (6%)	8 (0%)	39	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY
1	E	80	THR
2	B	88	SER
2	B	232	ASP
3	G	113	PRO
4	D	50	LYS
1	A	163	GLY
2	F	279	PRO

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	502/527 (95%)	456 (91%)	46 (9%)	11	40
1	E	502/527 (95%)	465 (93%)	37 (7%)	17	52
2	B	220/242 (91%)	197 (90%)	23 (10%)	8	33
2	F	220/242 (91%)	194 (88%)	26 (12%)	6	27
3	C	127/158 (80%)	114 (90%)	13 (10%)	9	35
3	G	127/158 (80%)	112 (88%)	15 (12%)	6	27
4	D	98/119 (82%)	86 (88%)	12 (12%)	6	26
4	H	98/119 (82%)	82 (84%)	16 (16%)	3	14
All	All	1894/2092 (90%)	1706 (90%)	188 (10%)	10	37

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	34	GLN
1	A	44	VAL
1	A	71	THR
1	A	117	ASN
1	A	120	HIS
1	A	153	PHE
1	A	165	VAL
1	A	179	SER
1	A	194	THR
1	A	205	LEU
1	A	241	ARG
1	A	257	THR
1	A	283	VAL
1	A	298	LEU
1	A	335	ARG
1	A	337	VAL
1	A	344	ILE
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	378	GLU
1	A	390	MET
1	A	405	THR
1	A	406	LYS
1	A	412	ILE
1	A	422	CYS

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Mol	Chain	Res	Type
1	A	432	ARG
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP
1	A	453	LYS
1	A	455	GLU
1	A	456	LEU
1	A	457	LYS
1	A	461	LYS
1	A	484	ASN
1	A	486	ASP
1	A	509	ARG
1	A	525	LYS
1	A	527	LEU
1	A	535	ARG
1	A	539	TRP
1	A	584	GLU
1	A	592	GLU
1	A	601	LYS
2	B	33	LYS
2	B	37	THR
2	B	53	LYS
2	B	66	THR
2	B	69	LEU
2	B	87	ARG
2	B	89	CYS
2	B	90	ARG
2	B	91	GLU
2	B	96	SER
2	B	116	ASN
2	B	131	VAL
2	B	156	LYS
2	B	157	THR
2	B	159	ILE
2	B	173	GLN
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	185	CYS
2	B	213	ARG
2	B	216	ILE
2	B	248	THR

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Mol	Chain	Res	Type
3	C	53	LYS
3	C	60	LEU
3	C	67	MET
3	C	88	ILE
3	C	94	SER
3	C	105	GLU
3	C	107	ILE
3	C	118	ASP
3	C	133	LEU
3	C	136	ILE
3	C	160	LEU
3	C	177	GLU
3	C	184	LEU
4	D	49	PHE
4	D	51	PRO
4	D	52	LEU
4	D	53	HIS
4	D	61	ILE
4	D	79	ILE
4	D	84	MET
4	D	112	VAL
4	D	113	LEU
4	D	115	ASP
4	D	148	ARG
4	D	154	TRP
1	E	32	ILE
1	E	44	VAL
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	179	SER
1	E	194	THR
1	E	205	LEU
1	E	241	ARG
1	E	257	THR
1	E	261	THR
1	E	283	VAL
1	E	298	LEU
1	E	320	ARG
1	E	337	VAL
1	E	344	ILE
1	E	355	GLN

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Mol	Chain	Res	Type
1	E	358	GLN
1	E	359	ARG
1	E	378	GLU
1	E	390	MET
1	E	406	LYS
1	E	412	ILE
1	E	422	CYS
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	455	GLU
1	E	456	LEU
1	E	457	LYS
1	E	484	ASN
1	E	525	LYS
1	E	535	ARG
1	E	547	LEU
1	E	584	GLU
1	E	610	LYS
2	F	33	LYS
2	F	37	THR
2	F	66	THR
2	F	69	LEU
2	F	87	ARG
2	F	90	ARG
2	F	91	GLU
2	F	93	ILE
2	F	96	SER
2	F	106	THR
2	F	115	GLN
2	F	116	ASN
2	F	120	THR
2	F	131	VAL
2	F	148	SER
2	F	156	LYS
2	F	157	THR
2	F	176	LEU
2	F	179	LEU
2	F	184	LEU
2	F	213	ARG
2	F	238	LYS

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Mol	Chain	Res	Type
2	F	242	ILE
2	F	266	LEU
2	F	278	THR
2	F	281	ASN
3	G	53	LYS
3	G	60	LEU
3	G	67	MET
3	G	70	MET
3	G	94	SER
3	G	105	GLU
3	G	133	LEU
3	G	136	ILE
3	G	160	LEU
3	G	165	LEU
3	G	172	VAL
3	G	175	ARG
3	G	177	GLU
3	G	183	THR
3	G	184	LEU
4	H	46	GLU
4	H	50	LYS
4	H	53	HIS
4	H	54	SER
4	H	58	LEU
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	112	VAL
4	H	122	ARG
4	H	138	TYR
4	H	143	ASP
4	H	144	VAL
4	H	148	ARG
4	H	154	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	250	HIS
1	A	355	GLN
1	A	358	GLN
1	A	436	ASN
1	A	497	GLN
1	A	503	HIS
1	A	550	GLN
1	A	551	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	116	ASN
2	B	145	GLN
2	B	150	GLN
4	D	53	HIS
4	D	140	ASN
1	E	88	ASN
1	E	95	ASN
1	E	117	ASN
1	E	349	HIS
1	E	358	GLN
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	503	HIS
1	E	551	ASN
1	E	573	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
4	H	140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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$
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	A	702	-	52,58,58	1.22	5 (9%)	52,89,89	2.54	15 (28%)
7	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	C	201	3,4	24,50,50	0.93	2 (8%)	16,82,82	1.87	3 (18%)
11	12J	C	202	-	21,21,21	1.52	2 (9%)	28,28,28	1.19	2 (7%)
12	EPH	D	201	-	42,43,48	1.09	2 (4%)	43,48,53	1.16	4 (9%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	-	52,58,58	1.33	5 (9%)	52,89,89	2.62	15 (28%)
7	FES	F	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	G	201	3,4	24,50,50	1.04	2 (8%)	16,82,82	2.00	3 (18%)
11	12J	G	202	-	21,21,21	1.35	2 (9%)	28,28,28	2.03	1 (3%)
12	EPH	H	201	-	42,43,48	1.16	2 (4%)	43,48,53	1.29	4 (9%)

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
5	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FAD	A	702	-	-	0/30/50/50	0/6/6/6
7	FES	B	301	2	-	0/0/4/4	0/1/1/1
8	SF4	B	302	2	-	0/0/48/48	0/6/5/5
9	F3S	B	303	2	-	0/0/24/24	0/0/3/3
10	HEM	C	201	3,4	-	2/6/54/54	0/0/8/8
11	12J	C	202	-	-	0/12/12/12	0/2/2/2
12	EPH	D	201	-	-	0/47/47/52	0/0/0/0
5	MLI	E	701	-	-	0/0/4/4	0/0/0/0
6	FAD	E	702	-	-	0/30/50/50	0/6/6/6
7	FES	F	301	2	-	0/0/4/4	0/1/1/1
8	SF4	F	302	2	-	0/0/48/48	0/6/5/5
9	F3S	F	303	2	-	0/0/24/24	0/0/3/3
10	HEM	G	201	3,4	-	0/6/54/54	0/0/8/8
11	12J	G	202	-	-	0/12/12/12	0/2/2/2
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	202	12J	C2-C7	-4.57	1.40	1.50
11	C	202	12J	C8-N	-4.53	1.33	1.41
11	G	202	12J	C2-C7	-4.28	1.40	1.50
10	G	201	HEM	C3B-C2B	-3.33	1.36	1.40
11	G	202	12J	C8-N	-3.22	1.35	1.41
10	C	201	HEM	C3B-C2B	-2.35	1.37	1.40
10	G	201	HEM	C1B-NB	-2.24	1.33	1.36
10	C	201	HEM	C1B-NB	-2.09	1.34	1.36
6	A	702	FAD	C5A-C4A	2.47	1.46	1.40
6	E	702	FAD	C5A-C4A	2.87	1.47	1.40
6	A	702	FAD	C4-C4X	2.88	1.47	1.41
6	A	702	FAD	C8-C7	2.98	1.49	1.41
6	A	702	FAD	C9A-C5X	3.15	1.49	1.42
6	E	702	FAD	C8-C7	3.24	1.49	1.41
6	A	702	FAD	C4X-C10	3.33	1.47	1.40
6	E	702	FAD	C4-C4X	3.37	1.48	1.41
6	E	702	FAD	C9A-C5X	3.52	1.50	1.42
6	E	702	FAD	C4X-C10	3.92	1.48	1.40
12	D	201	EPH	O1-C3	4.19	1.46	1.34
12	H	201	EPH	O1-C3	4.41	1.47	1.34
12	D	201	EPH	O2-C4	4.42	1.46	1.33
12	H	201	EPH	O2-C4	4.83	1.47	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	N3A-C2A-N1A	-8.52	122.18	128.87
6	E	702	FAD	C4-C4X-C10	-7.71	115.01	119.94
6	E	702	FAD	N3A-C2A-N1A	-7.61	122.89	128.87
6	A	702	FAD	C4-C4X-C10	-6.25	115.94	119.94
6	A	702	FAD	C1B-N9A-C4A	-5.31	120.88	126.81
6	E	702	FAD	C4X-C4-N3	-3.91	118.41	123.52
6	A	702	FAD	N3-C2-N1	-3.64	121.56	127.69
6	A	702	FAD	C4X-C4-N3	-3.56	118.87	123.52
6	E	702	FAD	N3-C2-N1	-3.50	121.79	127.69
6	E	702	FAD	C8M-C8-C9	-3.21	111.26	120.33
6	E	702	FAD	C1B-N9A-C4A	-3.11	123.33	126.81
12	H	201	EPH	O2-C4-O4	-3.07	115.45	123.51
10	G	201	HEM	CAD-C3D-C2D	-2.73	121.20	129.00
12	D	201	EPH	O2-C4-O4	-2.58	116.75	123.51
10	C	201	HEM	CAD-C3D-C2D	-2.44	122.04	129.00
12	D	201	EPH	O1-C3-O3	-2.42	117.09	123.67
11	C	202	12J	C8-N-C7	-2.34	120.91	126.78
10	G	201	HEM	C3C-C4C-NC	-2.17	106.84	110.94
6	A	702	FAD	C2B-C1B-N9A	-2.09	107.88	113.47
6	A	702	FAD	N6A-C6A-N1A	2.11	122.05	118.52
6	E	702	FAD	O2A-PA-O1A	2.20	124.02	112.56
6	E	702	FAD	C1'-C2'-C3'	2.24	116.22	109.82
6	A	702	FAD	O2A-PA-O1A	2.24	124.22	112.56
6	A	702	FAD	C5X-C9A-N10	2.31	119.31	117.58
6	E	702	FAD	C4X-N5-C5X	2.34	119.48	116.72
6	A	702	FAD	C2A-N1A-C6A	2.38	123.02	118.77
6	A	702	FAD	C4X-N5-C5X	3.01	120.26	116.72
6	E	702	FAD	O4B-C1B-N9A	3.02	113.81	108.11
12	H	201	EPH	C1-O2-C4	3.15	126.37	117.00
6	A	702	FAD	C4-C4X-N5	3.17	122.55	118.70
10	C	201	HEM	CAD-CBD-CGD	3.19	118.99	112.78
12	D	201	EPH	O2-C4-C18	3.29	121.97	111.85
6	E	702	FAD	C1'-N10-C9A	3.43	122.81	118.83
6	A	702	FAD	O4B-C1B-N9A	3.53	114.77	108.11
6	E	702	FAD	C8M-C8-C7	3.55	128.36	120.73
6	E	702	FAD	C4-C4X-N5	3.69	123.18	118.70
6	A	702	FAD	C1'-N10-C9A	3.80	123.23	118.83
12	H	201	EPH	O2-C4-C18	4.09	124.43	111.85
11	C	202	12J	C10-O2-C14	4.18	124.70	119.41
12	D	201	EPH	O1-C3-C5	4.24	120.45	111.53
12	H	201	EPH	O1-C3-C5	4.35	120.70	111.53
6	E	702	FAD	C5X-C9A-N10	4.91	121.26	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	201	HEM	CBD-CAD-C3D	5.44	122.01	112.47
10	G	201	HEM	CBD-CAD-C3D	6.25	123.43	112.47
6	A	702	FAD	C4-N3-C2	8.66	122.38	115.16
6	E	702	FAD	C4-N3-C2	8.96	122.63	115.16
11	G	202	12J	C10-O2-C14	9.28	131.15	119.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	1	0
6	A	702	FAD	4	0
10	C	201	HEM	6	0
11	C	202	12J	4	0
5	E	701	MLI	2	0
6	E	702	FAD	5	0
10	G	201	HEM	5	0
11	G	202	12J	4	0
12	H	201	EPH	2	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(Å²)	Q<0.9	
1	A	616/645 (95%)	-0.49	1 (0%)	95	95	34, 55, 80, 108	1 (0%)
1	E	616/645 (95%)	-0.43	4 (0%)	90	88	34, 57, 83, 112	1 (0%)
2	B	250/282 (88%)	-0.53	1 (0%)	93	92	35, 53, 78, 94	0
2	F	250/282 (88%)	-0.47	5 (2%)	68	62	39, 55, 79, 109	0
3	C	153/188 (81%)	-0.27	5 (3%)	50	43	46, 62, 104, 151	0
3	G	153/188 (81%)	0.31	17 (11%)	7	6	48, 68, 136, 211	0
4	D	129/156 (82%)	-0.36	2 (1%)	74	69	54, 66, 104, 141	0
4	H	129/156 (82%)	-0.13	11 (8%)	13	10	52, 72, 120, 154	0
All	All	2296/2542 (90%)	-0.38	46 (2%)	68	62	34, 58, 93, 211	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	185	PRO	13.0
3	G	186	THR	8.7
3	G	184	LEU	8.1
3	G	183	THR	5.2
3	G	107	ILE	3.9
3	G	106	PHE	3.7
3	G	110	LEU	3.7
2	F	49	GLY	3.5
3	C	186	THR	3.5
4	H	52	LEU	3.5
1	E	644	SER	3.4
3	G	109	GLY	3.3
1	E	30	SER	3.3
1	E	31	ASN	3.2
3	G	182	ALA	3.2
3	C	183	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	48	PRO	3.0
4	H	78	PHE	2.9
4	H	48	GLY	2.8
4	H	156	LEU	2.8
3	G	102	THR	2.8
4	H	115	ASP	2.8
3	G	181	LYS	2.7
4	H	50	LYS	2.7
2	F	50	ALA	2.7
4	H	49	PHE	2.6
3	C	179	HIS	2.6
1	E	486	ASP	2.6
4	D	49	PHE	2.5
2	B	281	ASN	2.5
3	G	113	PRO	2.5
3	G	176	TRP	2.5
3	G	97	PRO	2.5
4	H	47	LYS	2.4
4	D	52	LEU	2.4
2	F	279	PRO	2.3
4	H	51	PRO	2.3
1	A	595	THR	2.2
4	H	117	LEU	2.2
3	G	112	ILE	2.2
4	H	53	HIS	2.2
3	C	182	ALA	2.1
2	F	280	ALA	2.1
3	C	185	PRO	2.0
3	G	180	LYS	2.0
3	G	95	VAL	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	EPH	H	201	44/49	0.75	0.38	4.77	72,121,165,169	0
12	EPH	D	201	44/49	0.85	0.31	3.02	66,95,128,141	0
10	HEM	C	201	43/43	0.97	0.17	0.94	56,68,77,89	0
5	MLI	E	701	7/7	0.97	0.21	0.45	51,54,55,55	0
10	HEM	G	201	43/43	0.98	0.16	0.38	49,68,81,85	0
11	12J	G	202	20/20	0.98	0.18	0.30	56,59,66,70	0
11	12J	C	202	20/20	0.97	0.19	0.19	61,70,76,77	0
8	SF4	B	302	8/8	0.99	0.15	0.14	35,38,43,44	0
6	FAD	E	702	53/53	0.98	0.15	-0.27	37,45,51,53	0
6	FAD	A	702	53/53	0.97	0.14	-0.38	33,40,43,44	0
9	F3S	F	303	7/7	0.99	0.14	-0.48	46,55,57,58	0
8	SF4	F	302	8/8	0.99	0.13	-0.51	36,40,41,41	0
9	F3S	B	303	7/7	0.99	0.15	-0.65	40,47,53,56	0
5	MLI	A	701	7/7	0.98	0.13	-1.22	46,48,51,51	0
7	FES	F	301	4/4	0.99	0.11	-1.28	42,45,45,50	0
7	FES	B	301	4/4	0.99	0.11	-1.40	44,46,48,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.