



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:01 am GMT

PDB ID : 4YTM  
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with N-biphenyl-3-yl-2-(trifluoromethyl)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 : 2015-03-18  
Resolution : 3.40 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

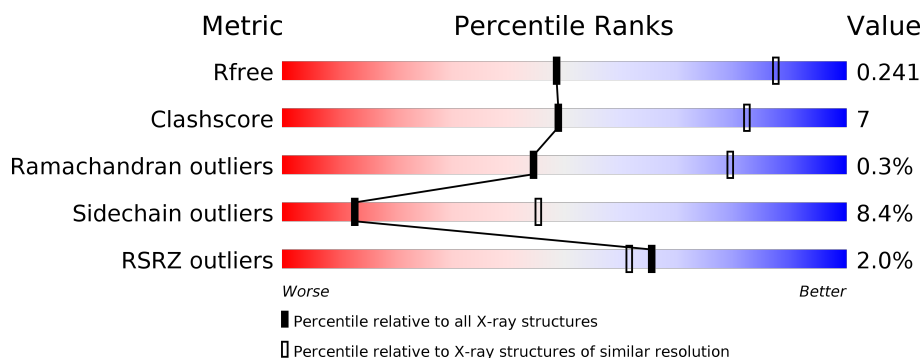
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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  $\geq 3$ , 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 74%, yellow 20%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>74%</span> <span>20%</span> <span>• •</span> </div> </div>
1	E	645	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 78%, yellow 17%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>17%</span> <span>•</span> </div> </div>
2	B	282	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 71%, yellow 15%, orange 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>71%</span> <span>15%</span> <span>•</span> <span>11%</span> </div> </div>
2	F	282	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 74%, yellow 13%, orange 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>74%</span> <span>13%</span> <span>•</span> <span>11%</span> </div> </div>
3	C	188	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 68%, yellow 12%, orange 5%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>68%</span> <span>12%</span> <span>•</span> <span>19%</span> </div> </div>
3	G	188	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 70%, yellow 10%, orange 5%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>70%</span> <span>10%</span> <span>•</span> <span>20%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	156	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
4	H	156	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>16%</div> <div>•</div> <div>17%</div> </div> </div>

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
11	F6A	C	202	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18300 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	252	Total	C	N	O	S	0	0	0
			1994	1268	340	363	23			

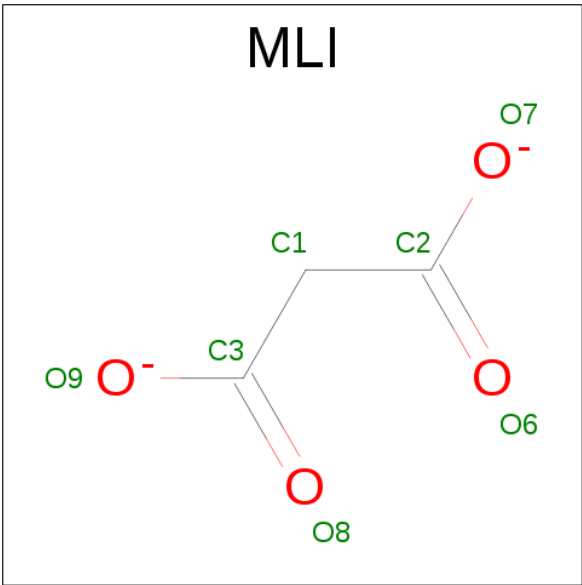
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	152	Total	C	N	O	S	0	0	0
			1210	809	203	192	6			
3	G	151	Total	C	N	O	S	0	0	0
			1203	804	202	191	6			

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

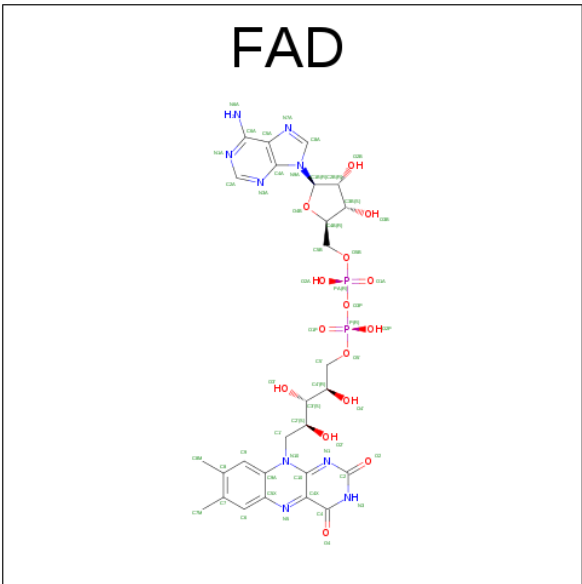
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



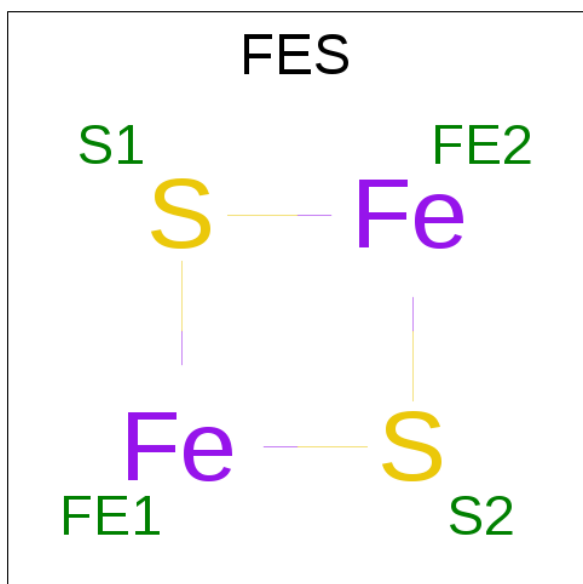
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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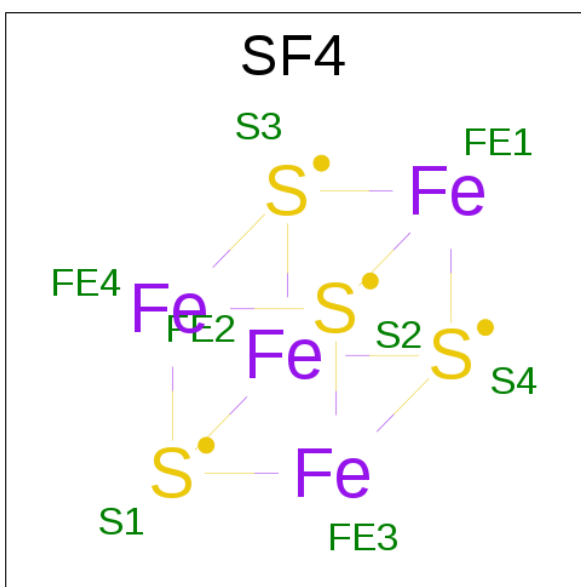
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



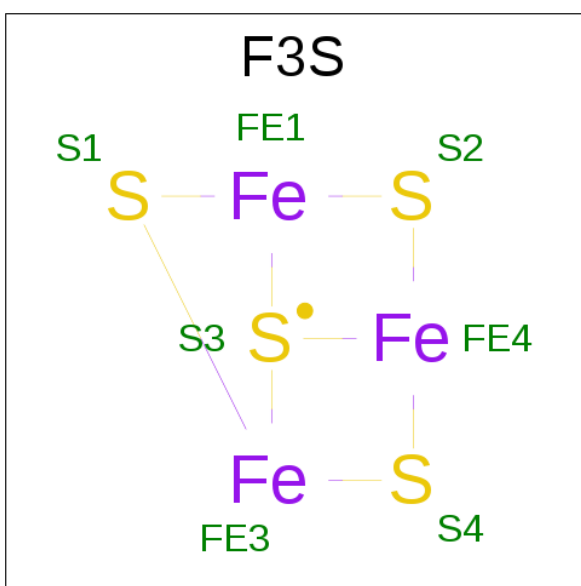
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



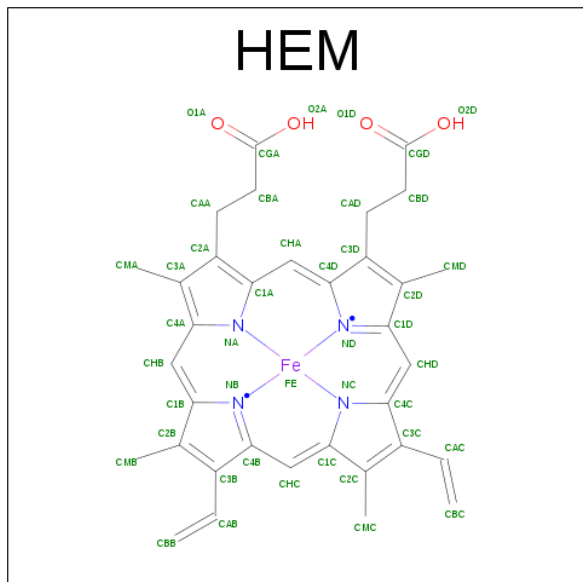
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



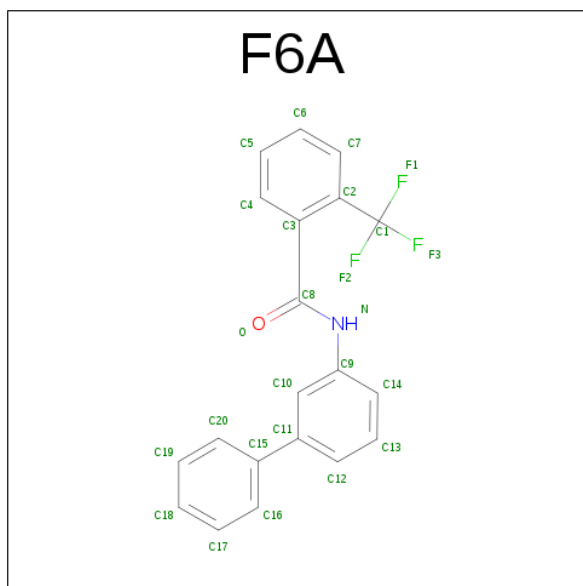
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- 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	
			43	34	1	4	4	0
10	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

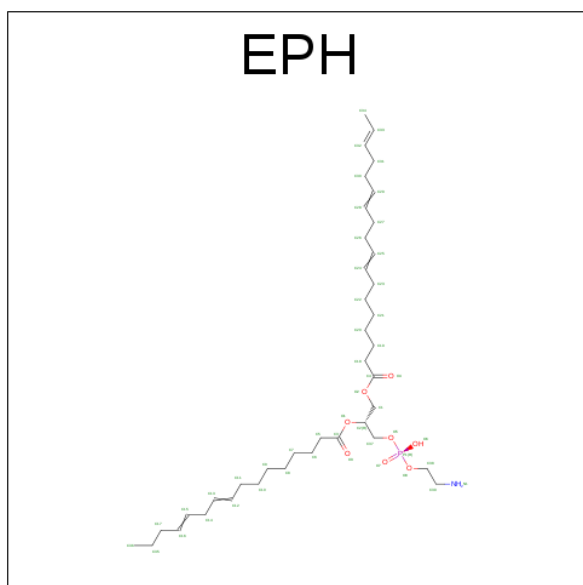
- Molecule 11 is N-biphenyl-3-yl-2-(trifluoromethyl)benzamide (three-letter code: F6A) (formula:  $C_{20}H_{14}F_3NO$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	0	0
			25	20	3	1	1		
11	G	1	Total	C	F	N	O	0	0
			25	20	3	1	1		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: C<sub>39</sub>H<sub>68</sub>NO<sub>8</sub>P).

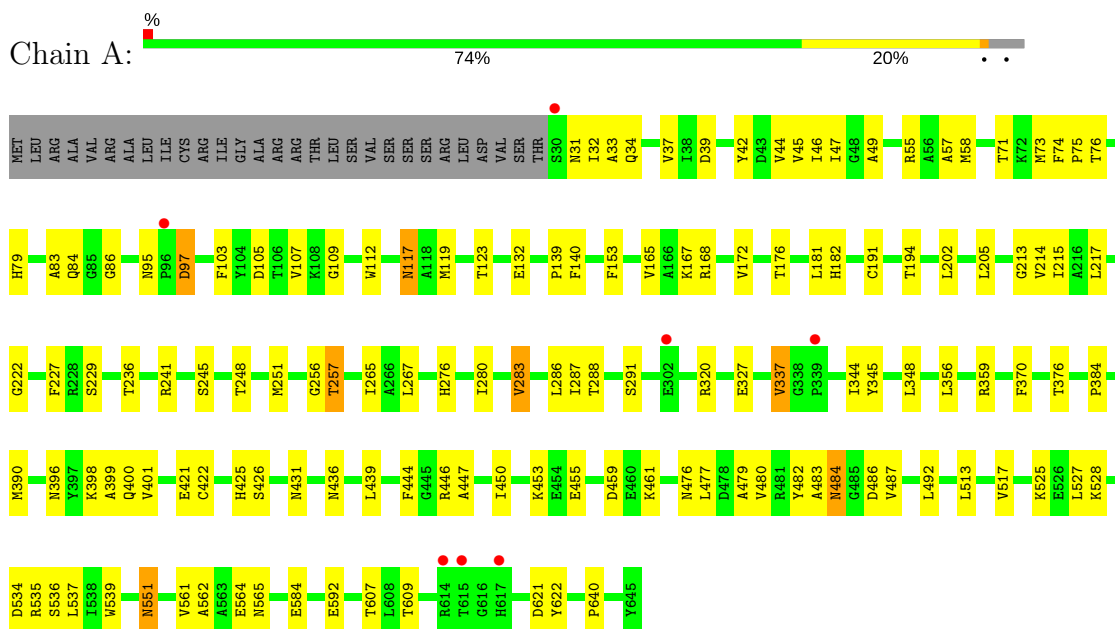


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

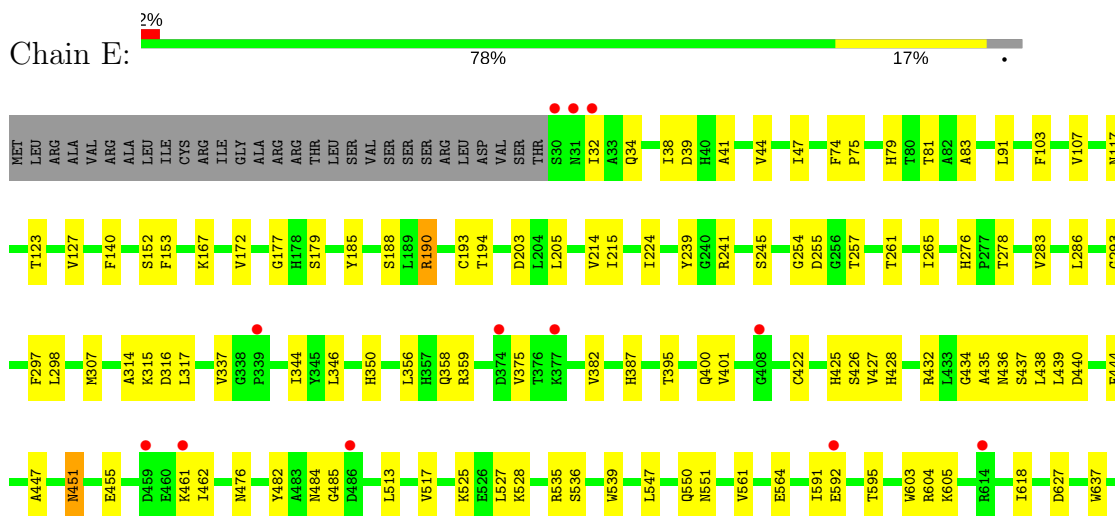
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Succinate dehydrogenase flavoprotein



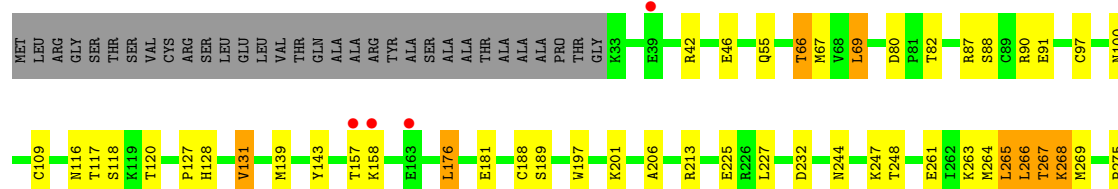
#### • Molecule 1: Succinate dehydrogenase flavoprotein





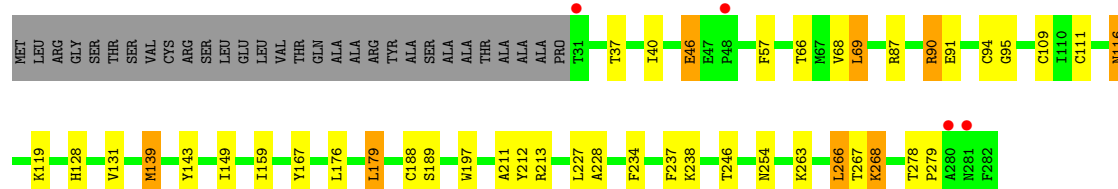
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B: 2% 71% 15% 11%



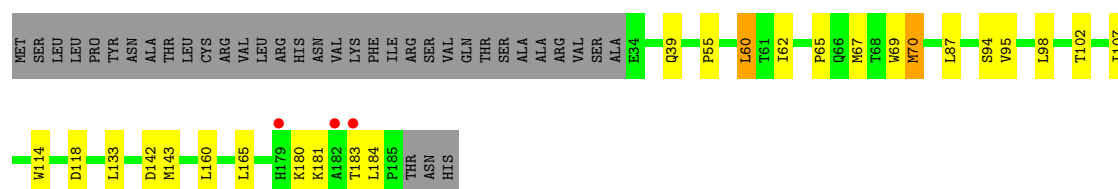
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F: 74% 13% 11%



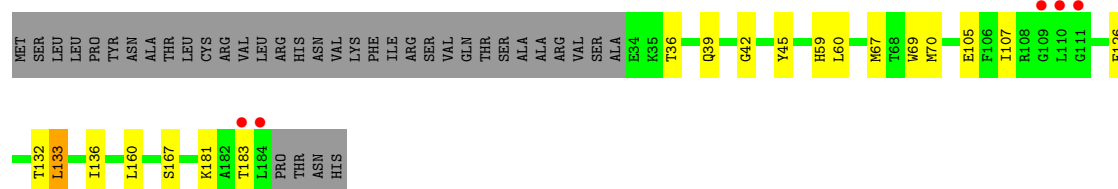
- Molecule 3: Cytochrome b-large subunit

Chain C: 2% 68% 12% 19%

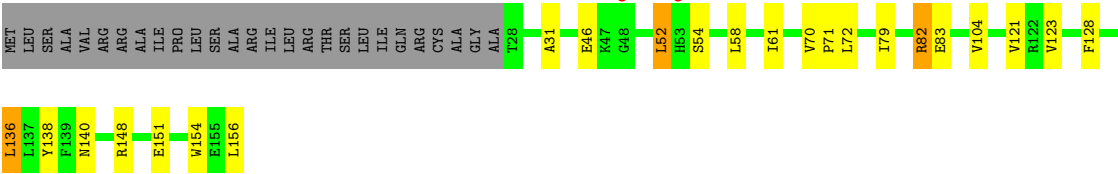


- Molecule 3: Cytochrome b-large subunit

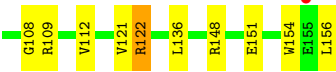
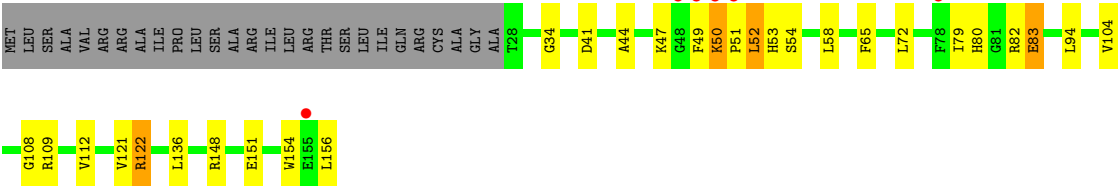
Chain G: 3% 70% 10% 20%



- 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, $\alpha$ , $\beta$ , $\gamma$	123.65Å 126.43Å 220.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-3.40) 94.9 (20.00-3.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 3.36Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.178 , 0.245 0.180 , 0.241	Depositor DCC
$R_{free}$ test set	2333 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MLI, F6A, F3S, FES, EPH, 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	0.39	0/4889	0.61	0/6605
1	E	0.40	0/4889	0.62	0/6605
2	B	0.44	0/2029	0.63	0/2739
2	F	0.43	0/2038	0.62	0/2751
3	C	0.39	0/1248	0.59	0/1699
3	G	0.38	0/1240	0.56	0/1687
4	D	0.43	0/1030	0.59	0/1406
4	H	0.38	0/1030	0.56	0/1406
All	All	0.40	0/18393	0.60	0/24898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4787	0	4722	76	0
1	E	4787	0	4722	64	0
2	B	1985	0	2001	39	0
2	F	1994	0	2007	24	0
3	C	1210	0	1258	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1203	0	1251	12	0
4	D	998	0	985	12	0
4	H	998	0	985	17	0
5	A	7	0	2	0	0
5	E	7	0	2	1	0
6	A	53	0	31	6	0
6	E	53	0	31	12	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	4	0
10	G	43	0	30	5	0
11	C	25	0	14	2	0
11	G	25	0	14	3	0
12	D	44	0	53	1	0
All	All	18300	0	18138	248	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 7.

All (248) 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)
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.68	1.09
2:B:267:THR:O	2:B:268:LYS:HB2	1.48	1.08
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.70	1.06
2:B:265:LEU:HD23	2:B:265:LEU:H	1.19	1.05
1:A:79:HIS:CE1	6:A:702:FAD:HM82	1.94	1.03
1:A:484:ASN:C	1:A:484:ASN:HD22	1.62	1.01
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.25	0.99
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.35	0.89
2:B:265:LEU:HD23	2:B:265:LEU:N	1.85	0.87
2:B:265:LEU:N	2:B:265:LEU:CD2	2.38	0.86
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.59	0.81
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.63	0.81
1:E:307:MET:HB2	1:E:316:ASP:OD2	1.81	0.79
1:A:484:ASN:ND2	1:A:484:ASN:C	2.36	0.75
4:H:49:PHE:CZ	4:H:52:LEU:HD23	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:ARG:NH1	6:E:702:FAD:H1'2	2.03	0.73
1:E:79:HIS:CE1	6:E:702:FAD:HM82	2.22	0.73
2:B:263:LYS:O	2:B:267:THR:HG23	1.89	0.73
3:C:60:LEU:HD22	11:C:202:F6A:H12	1.71	0.72
1:E:432:ARG:HH12	6:E:702:FAD:H1'2	1.56	0.69
2:B:267:THR:O	2:B:268:LYS:CB	2.30	0.69
1:A:79:HIS:NE2	6:A:702:FAD:HM81	2.05	0.69
2:B:227:LEU:HD22	2:B:266:LEU:CD1	2.22	0.69
2:B:261:GLU:O	2:B:265:LEU:HD23	1.93	0.68
2:B:267:THR:OG1	2:B:269:MET:HG2	1.92	0.68
3:G:60:LEU:HD22	11:G:202:F6A:H12	1.75	0.68
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.77	0.67
2:F:116:ASN:C	2:F:116:ASN:HD22	1.97	0.67
2:F:167:TYR:HB3	2:F:278:THR:HG22	1.77	0.66
2:F:228:ALA:O	4:H:52:LEU:HD22	1.95	0.66
4:H:108:GLY:O	4:H:122:ARG:NH2	2.28	0.66
10:C:201:HEM:HHA	10:C:201:HEM:HBD1	1.78	0.66
1:A:484:ASN:O	1:A:484:ASN:ND2	2.30	0.65
2:B:267:THR:OG1	2:B:269:MET:CG	2.45	0.65
2:B:263:LYS:NZ	3:C:142:ASP:OD1	2.27	0.64
1:A:32:ILE:HG23	1:A:482:TYR:CD1	2.32	0.64
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.46	0.62
1:E:103:PHE:HA	1:E:123:THR:HG21	1.80	0.62
1:A:492:LEU:HD21	1:A:527:LEU:HD12	1.82	0.62
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.81	0.62
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.82	0.61
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.81	0.61
2:B:261:GLU:O	2:B:265:LEU:CD2	2.48	0.61
2:B:232:ASP:HB3	4:D:52:LEU:HD13	1.82	0.61
1:E:432:ARG:NH2	6:E:702:FAD:N1	2.49	0.59
1:A:109:GLY:O	1:A:431:ASN:HB3	2.02	0.59
3:G:133:LEU:O	3:G:136:ILE:HG13	2.01	0.59
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.38	0.59
2:F:40:ILE:HD12	2:F:57:PHE:CD1	2.38	0.59
1:A:117:ASN:HD22	1:A:117:ASN:N	2.01	0.58
4:H:50:LYS:N	4:H:51:PRO:HD3	2.18	0.58
1:E:278:THR:HG22	1:E:382:VAL:HG21	1.86	0.58
1:A:42:TYR:O	1:A:229:SER:HA	2.04	0.58
4:H:51:PRO:C	4:H:52:LEU:HG	2.23	0.57
2:F:263:LYS:O	2:F:267:THR:HG23	2.04	0.57
1:A:37:VAL:O	4:D:31:ALA:HB1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:NH1	1:A:132:GLU:OE2	2.32	0.57
1:A:117:ASN:HD22	1:A:117:ASN:H	1.52	0.56
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.88	0.56
4:H:50:LYS:H	4:H:51:PRO:HD3	1.69	0.56
1:A:565:ASN:ND2	1:A:622:TYR:OH	2.39	0.56
3:C:60:LEU:HD22	11:C:202:F6A:C12	2.35	0.56
1:A:425:HIS:N	1:A:426:SER:HA	2.19	0.56
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.56
1:A:217:LEU:HD22	1:A:477:LEU:HD11	1.87	0.56
1:E:190:ARG:HG3	1:E:190:ARG:O	2.05	0.55
10:C:201:HEM:HHD	10:C:201:HEM:HBC2	1.89	0.55
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.06	0.55
3:G:60:LEU:HD22	11:G:202:F6A:C12	2.35	0.55
1:E:432:ARG:HH12	6:E:702:FAD:C1'	2.20	0.55
1:A:139:PRO:HB3	2:B:176:LEU:HD23	1.88	0.55
1:E:451:ASN:N	1:E:451:ASN:HD22	2.04	0.55
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.41	0.55
1:E:314:ALA:O	1:E:315:LYS:HB2	2.06	0.55
3:C:180:LYS:O	3:C:184:LEU:HB2	2.08	0.54
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.90	0.54
1:E:41:ALA:HB1	1:E:462:ILE:HD13	1.90	0.53
1:E:603:TRP:HA	1:E:605:LYS:HE3	1.90	0.53
2:B:264:MET:O	2:B:268:LYS:N	2.37	0.53
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.91	0.53
4:H:50:LYS:N	4:H:51:PRO:CD	2.72	0.53
3:C:70:MET:HA	3:C:70:MET:HE3	1.91	0.53
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.90	0.53
2:F:149:ILE:HD12	2:F:211:ALA:HA	1.90	0.53
2:F:267:THR:O	2:F:268:LYS:HB2	2.08	0.53
1:E:432:ARG:NH2	5:E:701:MLI:O6	2.42	0.53
1:A:551:ASN:N	1:A:551:ASN:HD22	2.06	0.52
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.90	0.52
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.91	0.52
2:B:188:CYS:SG	2:B:206:ALA:HB2	2.50	0.52
3:G:107:ILE:HD11	4:H:156:LEU:CD1	2.35	0.52
4:D:82:ARG:NH2	4:D:140:ASN:O	2.42	0.52
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.93	0.51
1:E:438:LEU:HG	6:E:702:FAD:C2	2.39	0.51
1:E:276:HIS:CE1	1:E:286:LEU:HD11	2.46	0.51
1:E:425:HIS:HB2	1:E:427:VAL:HG13	1.92	0.51
4:H:83:GLU:CD	4:H:83:GLU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LYS:O	2:B:264:MET:C	2.49	0.51
1:A:95:ASN:HD21	1:A:167:LYS:HB2	1.75	0.50
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.75	0.50
1:E:517:VAL:HG13	1:E:561:VAL:HG12	1.92	0.50
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.44	0.50
2:B:128:HIS:O	2:B:128:HIS:ND1	2.42	0.50
1:E:47:ILE:HD11	1:E:214:VAL:CG2	2.41	0.50
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.47	0.49
1:A:621:ASP:OD1	1:A:622:TYR:N	2.44	0.49
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.93	0.49
1:E:427:VAL:HG11	1:E:444:PHE:CE1	2.47	0.49
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.93	0.49
1:E:91:LEU:HD23	1:E:127:VAL:HG13	1.94	0.49
1:E:297:PHE:CE2	1:E:350:HIS:CE1	3.00	0.49
1:E:185:TYR:O	1:E:188:SER:OG	2.27	0.49
1:A:476:ASN:O	1:A:480:VAL:HG23	2.12	0.49
1:A:33:ALA:HB2	1:A:482:TYR:HE1	1.78	0.49
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.94	0.49
1:A:280:ILE:HD11	1:A:287:ILE:HD11	1.95	0.48
1:E:513:LEU:O	1:E:517:VAL:HG23	2.13	0.48
2:B:263:LYS:O	2:B:266:LEU:N	2.47	0.48
1:A:479:ALA:O	1:A:483:ALA:HB2	2.13	0.48
1:E:190:ARG:CG	1:E:190:ARG:O	2.61	0.48
2:B:197:TRP:HH2	3:C:60:LEU:HD21	1.79	0.48
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.94	0.48
3:C:107:ILE:HD11	4:D:156:LEU:HD11	1.95	0.48
3:C:94:SER:HB3	4:D:138:TYR:CD1	2.49	0.48
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.95	0.48
1:A:83:ALA:HA	6:A:702:FAD:C6	2.44	0.48
1:A:58:MET:HA	1:A:191:CYS:SG	2.54	0.48
1:E:286:LEU:HD22	6:E:702:FAD:C6	2.43	0.48
1:A:265:ILE:HD13	1:A:401:VAL:HG11	1.95	0.48
1:A:76:THR:HG23	1:A:182:HIS:NE2	2.29	0.48
1:E:434:GLY:O	1:E:435:ALA:HB3	2.14	0.47
2:F:94:CYS:SG	2:F:95:GLY:N	2.87	0.47
1:A:49:ALA:HB1	1:A:75:PRO:HB3	1.96	0.47
2:B:188:CYS:SG	2:B:189:SER:N	2.86	0.47
10:G:201:HEM:HH2	10:G:201:HEM:HBC2	1.95	0.47
1:A:398:LYS:O	1:A:399:ALA:HB3	2.14	0.47
1:A:276:HIS:O	1:A:384:PRO:HA	2.14	0.47
1:E:79:HIS:NE2	6:E:702:FAD:HM81	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:HG22	1:A:267:LEU:HD22	1.97	0.47
1:A:356:LEU:HD23	1:A:376:THR:HG22	1.95	0.47
1:A:103:PHE:HA	1:A:123:THR:HG21	1.97	0.47
1:E:536:SER:HB2	2:F:46:GLU:OE1	2.16	0.46
1:E:627:ASP:O	1:E:637:TRP:HB2	2.15	0.46
2:F:188:CYS:SG	2:F:189:SER:N	2.89	0.46
1:A:222:GLY:O	1:A:537:LEU:HD13	2.14	0.46
4:D:70:VAL:N	4:D:71:PRO:HD2	2.31	0.46
1:E:32:ILE:HG13	1:E:32:ILE:O	2.14	0.46
1:E:432:ARG:CZ	1:E:437:SER:HB2	2.46	0.46
1:A:107:VAL:HG22	1:A:119:MET:HE3	1.98	0.46
1:A:344:ILE:HG22	1:A:345:TYR:N	2.32	0.45
2:F:90:ARG:HD2	2:F:90:ARG:H	1.82	0.45
1:A:517:VAL:HG13	1:A:561:VAL:HG12	1.98	0.45
1:A:97:ASP:OD2	1:A:168:ARG:NH1	2.50	0.45
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.99	0.45
4:D:104:VAL:HG13	4:D:121:VAL:HG12	1.99	0.45
3:C:107:ILE:HD11	4:D:156:LEU:CD1	2.47	0.45
2:B:66:THR:HG23	2:B:67:MET:HG2	1.99	0.45
2:B:264:MET:CE	3:C:143:MET:HB3	2.47	0.45
1:A:534:ASP:OD2	1:A:536:SER:OG	2.29	0.45
3:G:69:TRP:CZ2	11:G:202:F6A:C18	3.00	0.45
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.47	0.44
1:E:551:ASN:N	1:E:551:ASN:HD22	2.15	0.44
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.99	0.44
4:H:49:PHE:HZ	4:H:52:LEU:HD23	1.79	0.44
1:A:241:ARG:NH2	1:A:248:THR:O	2.51	0.44
1:A:75:PRO:O	1:A:181:LEU:HD21	2.18	0.44
1:A:446:ARG:HD3	1:A:450:ILE:HD11	1.98	0.44
3:G:126:PHE:HA	3:G:167:SER:OG	2.17	0.44
1:A:396:ASN:HD21	1:A:400:GLN:HB2	1.81	0.44
1:E:255:ASP:OD1	1:E:255:ASP:N	2.50	0.44
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.53	0.44
3:G:42:GLY:O	3:G:45:TYR:HB3	2.18	0.44
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.53	0.44
2:F:69:LEU:HD12	2:F:109:CYS:HB3	1.99	0.43
1:A:337:VAL:HG11	1:A:345:TYR:CD1	2.54	0.43
1:E:215:ILE:HD11	1:E:224:ILE:CG2	2.48	0.43
1:E:395:THR:HA	1:E:400:GLN:O	2.19	0.43
1:E:591:ILE:N	1:E:591:ILE:HD12	2.34	0.43
2:F:246:THR:OG1	2:F:254:ASN:OD1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:LEU:HD23	1:E:375:VAL:HG23	2.01	0.43
1:A:45:VAL:HG23	1:A:229:SER:HB3	2.01	0.43
2:B:267:THR:HG1	2:B:269:MET:H	1.63	0.43
3:C:98:LEU:HD12	3:C:102:THR:OG1	2.19	0.43
2:B:264:MET:HE1	3:C:143:MET:HB3	2.01	0.43
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.33	0.43
3:G:132:THR:HG23	10:G:201:HEM:CAB	2.49	0.43
4:H:109:ARG:HB2	4:H:112:VAL:HG12	1.99	0.43
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.89	0.43
1:E:307:MET:CB	1:E:316:ASP:OD2	2.58	0.43
1:E:103:PHE:O	1:E:107:VAL:HG23	2.19	0.43
1:E:152:SER:O	1:E:293:GLY:HA3	2.18	0.43
1:A:32:ILE:CG1	1:A:32:ILE:O	2.66	0.42
2:B:264:MET:HB2	2:B:265:LEU:CD2	2.49	0.42
1:E:140:PHE:HA	1:E:172:VAL:HG22	2.00	0.42
2:F:179:LEU:HD21	2:F:212:TYR:CD2	2.54	0.42
1:A:283:VAL:HG21	1:A:370:PHE:HB3	2.01	0.42
2:B:97:CYS:O	2:B:97:CYS:SG	2.77	0.42
2:F:128:HIS:ND1	2:F:128:HIS:O	2.52	0.42
2:F:68:VAL:HG23	2:F:111:CYS:O	2.20	0.42
1:E:32:ILE:HG23	1:E:482:TYR:CD1	2.55	0.42
2:F:237:PHE:CZ	2:F:266:LEU:HD23	2.55	0.42
1:A:46:ILE:HD12	1:A:57:ALA:HB2	2.01	0.42
3:C:95:VAL:O	3:C:95:VAL:HG12	2.19	0.42
1:A:286:LEU:HD22	6:A:702:FAD:HM73	2.01	0.42
1:A:33:ALA:HB2	1:A:482:TYR:CE1	2.53	0.42
2:F:116:ASN:ND2	2:F:116:ASN:C	2.69	0.42
2:B:266:LEU:HA	2:B:266:LEU:HD12	1.82	0.42
4:D:151:GLU:HG2	12:D:201:EPH:O6	2.20	0.42
1:E:47:ILE:HD11	1:E:214:VAL:HG21	2.01	0.42
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.50	0.42
2:B:127:PRO:HG3	3:C:62:ILE:HD11	2.01	0.41
2:F:237:PHE:CE1	2:F:266:LEU:HD23	2.55	0.41
4:H:41:ASP:HB3	4:H:44:ALA:HB3	2.02	0.41
1:A:86:GLY:HA2	1:A:176:THR:HG21	2.01	0.41
1:A:73:MET:SD	1:A:251:MET:HG3	2.60	0.41
1:E:276:HIS:HB2	1:E:387:HIS:HB2	2.01	0.41
1:E:278:THR:HG21	1:E:346:LEU:HD22	2.03	0.41
1:A:213:GLY:HA3	1:A:227:PHE:O	2.20	0.41
2:B:157:THR:O	2:B:158:LYS:C	2.58	0.41
4:D:136:LEU:HA	4:D:136:LEU:HD12	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.02	0.41
2:F:197:TRP:HH2	3:G:60:LEU:HD21	1.86	0.41
2:B:80:ASP:OD2	2:B:82:THR:OG1	2.24	0.41
1:A:327:GLU:OE2	1:A:384:PRO:HD3	2.20	0.41
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.55	0.41
4:D:52:LEU:HG	4:D:52:LEU:H	1.27	0.41
2:B:264:MET:O	2:B:265:LEU:C	2.57	0.41
3:C:95:VAL:CG1	3:C:95:VAL:O	2.69	0.41
4:H:80:HIS:ND1	4:H:151:GLU:OE1	2.53	0.41
1:A:337:VAL:HG21	1:A:345:TYR:CD2	2.56	0.41
2:B:69:LEU:HB2	2:B:109:CYS:HA	2.03	0.41
1:A:47:ILE:HD11	1:A:214:VAL:HG22	2.02	0.41
10:C:201:HEM:CBD	10:C:201:HEM:HHA	2.49	0.41
1:E:603:TRP:O	1:E:605:LYS:N	2.54	0.41
4:H:65:PHE:CE2	4:H:94:LEU:HD23	2.55	0.41
1:E:74:PHE:HA	1:E:75:PRO:HD3	1.96	0.41
1:E:432:ARG:NH2	6:E:702:FAD:C2	2.85	0.40
3:G:36:THR:OG1	3:G:39:GLN:HG3	2.22	0.40
1:A:202:LEU:HB2	1:A:215:ILE:HG23	2.03	0.40
1:A:291:SER:HB2	1:A:348:LEU:HD21	2.02	0.40
1:A:74:PHE:CD1	2:B:143:TYR:CE2	3.09	0.40
2:F:167:TYR:CD1	2:F:279:PRO:HD2	2.56	0.40
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.57	0.40
3:G:132:THR:HG23	10:G:201:HEM:CBB	2.51	0.40
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.22	0.40
1:A:84:GLN:OE1	1:A:288:THR:HB	2.21	0.40
3:C:87:LEU:HD22	4:D:128:PHE:CD1	2.57	0.40
1:E:286:LEU:HB2	6:E:702:FAD:HM73	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/645 (95%)	566 (92%)	46 (8%)	2 (0%)	44	79
1	E	614/645 (95%)	577 (94%)	35 (6%)	2 (0%)	44	79
2	B	248/282 (88%)	228 (92%)	17 (7%)	3 (1%)	15	54
2	F	250/282 (89%)	229 (92%)	21 (8%)	0	100	100
3	C	150/188 (80%)	145 (97%)	5 (3%)	0	100	100
3	G	149/188 (79%)	140 (94%)	9 (6%)	0	100	100
4	D	127/156 (81%)	124 (98%)	3 (2%)	0	100	100
4	H	127/156 (81%)	119 (94%)	8 (6%)	0	100	100
All	All	2279/2542 (90%)	2128 (93%)	144 (6%)	7 (0%)	44	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	ASN
1	E	604	ARG
2	B	268	LYS
1	A	31	ASN
1	A	421	GLU
2	B	88	SER
1	E	485	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	502/527 (95%)	467 (93%)	35 (7%)	18	55
1	E	502/527 (95%)	463 (92%)	39 (8%)	15	49
2	B	220/242 (91%)	198 (90%)	22 (10%)	9	36
2	F	220/242 (91%)	203 (92%)	17 (8%)	15	49
3	C	126/158 (80%)	116 (92%)	10 (8%)	14	48
3	G	125/158 (79%)	117 (94%)	8 (6%)	20	58
4	D	98/119 (82%)	85 (87%)	13 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	98/119 (82%)	84 (86%)	14 (14%)	4	20
All	All	1891/2092 (90%)	1733 (92%)	158 (8%)	13	45

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	39	ASP
1	A	44	VAL
1	A	71	THR
1	A	97	ASP
1	A	117	ASN
1	A	153	PHE
1	A	165	VAL
1	A	194	THR
1	A	205	LEU
1	A	245	SER
1	A	257	THR
1	A	283	VAL
1	A	320	ARG
1	A	337	VAL
1	A	359	ARG
1	A	390	MET
1	A	422	CYS
1	A	436	ASN
1	A	439	LEU
1	A	453	LYS
1	A	455	GLU
1	A	459	ASP
1	A	461	LYS
1	A	484	ASN
1	A	486	ASP
1	A	487	VAL
1	A	525	LYS
1	A	528	LYS
1	A	535	ARG
1	A	539	TRP
1	A	551	ASN
1	A	584	GLU
1	A	592	GLU
1	A	609	THR
2	B	66	THR

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Mol	Chain	Res	Type
2	B	69	LEU
2	B	87	ARG
2	B	90	ARG
2	B	91	GLU
2	B	100	ASN
2	B	117	THR
2	B	118	SER
2	B	120	THR
2	B	131	VAL
2	B	139	MET
2	B	176	LEU
2	B	181	GLU
2	B	213	ARG
2	B	225	GLU
2	B	244	ASN
2	B	247	LYS
2	B	248	THR
2	B	265	LEU
2	B	266	LEU
2	B	267	THR
2	B	275	PRO
3	C	60	LEU
3	C	67	MET
3	C	70	MET
3	C	114	TRP
3	C	118	ASP
3	C	133	LEU
3	C	160	LEU
3	C	165	LEU
3	C	181	LYS
3	C	183	THR
4	D	46	GLU
4	D	52	LEU
4	D	54	SER
4	D	58	LEU
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	82	ARG
4	D	83	GLU
4	D	123	VAL
4	D	136	LEU

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Mol	Chain	Res	Type
4	D	148	ARG
4	D	154	TRP
1	E	34	GLN
1	E	39	ASP
1	E	44	VAL
1	E	81	THR
1	E	117	ASN
1	E	153	PHE
1	E	167	LYS
1	E	179	SER
1	E	190	ARG
1	E	193	CYS
1	E	194	THR
1	E	203	ASP
1	E	205	LEU
1	E	241	ARG
1	E	245	SER
1	E	257	THR
1	E	261	THR
1	E	283	VAL
1	E	298	LEU
1	E	337	VAL
1	E	344	ILE
1	E	358	GLN
1	E	359	ARG
1	E	422	CYS
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	451	ASN
1	E	455	GLU
1	E	461	LYS
1	E	484	ASN
1	E	525	LYS
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	539	TRP
1	E	547	LEU
1	E	592	GLU
1	E	595	THR
2	F	37	THR

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Mol	Chain	Res	Type
2	F	46	GLU
2	F	66	THR
2	F	69	LEU
2	F	87	ARG
2	F	90	ARG
2	F	91	GLU
2	F	116	ASN
2	F	119	LYS
2	F	131	VAL
2	F	139	MET
2	F	159	ILE
2	F	176	LEU
2	F	179	LEU
2	F	213	ARG
2	F	266	LEU
2	F	268	LYS
3	G	59	HIS
3	G	67	MET
3	G	70	MET
3	G	105	GLU
3	G	133	LEU
3	G	160	LEU
3	G	181	LYS
3	G	183	THR
4	H	47	LYS
4	H	50	LYS
4	H	52	LEU
4	H	53	HIS
4	H	54	SER
4	H	58	LEU
4	H	72	LEU
4	H	79	ILE
4	H	82	ARG
4	H	83	GLU
4	H	122	ARG
4	H	136	LEU
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	95	ASN
1	A	102	HIS
1	A	117	ASN
1	A	120	HIS
1	A	156	GLN
1	A	178	HIS
1	A	436	ASN
1	A	451	ASN
1	A	484	ASN
1	A	497	GLN
1	A	503	HIS
1	A	551	ASN
1	A	565	ASN
1	A	573	HIS
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	116	ASN
2	B	154	GLN
2	B	165	GLN
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	355	GLN
1	E	358	GLN
1	E	436	ASN
1	E	484	ASN
1	E	497	GLN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
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 ⓘ

15 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	-	51,58,58	1.37	8 (15%)	54,89,89	2.24	13 (24%)
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	28,50,50	0.82	1 (3%)	17,82,82	1.59	2 (11%)
11	F6A	C	202	-	27,27,27	1.26	1 (3%)	38,38,38	0.82	0
12	EPH	D	201	-	43,43,48	1.10	2 (4%)	45,48,53	1.07	3 (6%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	-	51,58,58	1.37	6 (11%)	54,89,89	2.30	12 (22%)
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	28,50,50	0.88	1 (3%)	17,82,82	1.71	3 (17%)
11	F6A	G	202	-	27,27,27	1.12	1 (3%)	38,38,38	0.89	1 (2%)

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	-	-	0/28/50/50	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	F6A	C	202	-	-	0/18/18/18	0/3/3/3
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	-	-	0/28/50/50	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	-	2/6/54/54	0/0/8/8
11	F6A	G	202	-	-	0/18/18/18	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	C3B-C2B	-2.93	1.36	1.40
6	A	702	FAD	C6-C5X	-2.31	1.38	1.41
6	A	702	FAD	C2-N3	-2.21	1.33	1.38
10	C	201	HEM	C3B-C2B	-2.21	1.37	1.40
6	A	702	FAD	C2B-C1B	-2.19	1.50	1.53
6	E	702	FAD	C9A-N10	2.11	1.41	1.38
6	E	702	FAD	C8-C7	2.50	1.47	1.41
6	A	702	FAD	C8-C7	2.52	1.47	1.41
6	E	702	FAD	C5A-C4A	2.57	1.46	1.40
6	A	702	FAD	C5A-C4A	2.81	1.46	1.40
6	A	702	FAD	C9A-C5X	3.19	1.49	1.42
6	E	702	FAD	C9A-C5X	3.46	1.49	1.42
6	A	702	FAD	C4-C4X	3.66	1.48	1.41
6	E	702	FAD	C4-C4X	3.71	1.48	1.41
6	A	702	FAD	C4X-C10	4.14	1.48	1.41
6	E	702	FAD	C4X-C10	4.38	1.48	1.41
12	D	201	EPH	O2-C4	4.46	1.46	1.33
12	D	201	EPH	O1-C3	4.46	1.47	1.34
11	G	202	F6A	C3-C2	5.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	202	F6A	C3-C2	5.94	1.50	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	N3A-C2A-N1A	-7.93	121.95	128.86
6	E	702	FAD	N3A-C2A-N1A	-7.32	122.49	128.86
6	E	702	FAD	C4-C4X-C10	-4.02	116.71	119.96
6	E	702	FAD	C4X-C4-N3	-3.81	118.06	123.48
6	A	702	FAD	C4-C4X-C10	-3.77	116.91	119.96
6	A	702	FAD	C4X-C4-N3	-3.75	118.15	123.48
6	A	702	FAD	C1B-N9A-C4A	-3.41	120.75	126.64
6	E	702	FAD	C4A-C5A-N7A	-3.20	106.31	109.41
6	A	702	FAD	C4A-C5A-N7A	-3.10	106.42	109.41
6	A	702	FAD	C4'-C3'-C2'	-2.94	107.09	113.41
10	C	201	HEM	CAD-C3D-C2D	-2.87	120.81	129.00
10	G	201	HEM	CAD-C3D-C2D	-2.78	121.07	129.00
6	E	702	FAD	O2'-C2'-C3'	-2.61	102.62	109.09
12	D	201	EPH	O2-C4-O4	-2.56	117.20	123.55
6	A	702	FAD	O2'-C2'-C3'	-2.21	103.61	109.09
10	G	201	HEM	CAA-CBA-CGA	-2.19	108.92	112.66
11	G	202	F6A	F1-C1-C2	-2.14	108.83	112.69
6	A	702	FAD	O2A-PA-O1A	2.04	122.84	112.28
6	E	702	FAD	C2A-N1A-C6A	2.07	122.40	118.77
6	E	702	FAD	C1'-C2'-C3'	2.34	116.50	109.82
6	A	702	FAD	C2A-N1A-C6A	2.59	123.30	118.77
6	E	702	FAD	C5X-C9A-N10	3.04	119.92	117.66
6	E	702	FAD	C4-C4X-N5	3.10	122.08	118.68
6	E	702	FAD	C4X-N5-C5X	3.12	120.06	116.76
12	D	201	EPH	O2-C4-C18	3.18	121.16	111.90
6	A	702	FAD	C4X-N5-C5X	3.26	120.21	116.76
6	A	702	FAD	C4-C4X-N5	3.27	122.26	118.68
12	D	201	EPH	O1-C3-C5	3.97	119.79	111.55
6	A	702	FAD	C1'-N10-C9A	4.53	122.50	118.35
10	C	201	HEM	CBD-CAD-C3D	4.61	121.25	112.47
10	G	201	HEM	CBD-CAD-C3D	4.98	121.97	112.47
6	E	702	FAD	C1'-N10-C9A	6.77	124.55	118.35
6	A	702	FAD	C4-N3-C2	7.61	121.81	115.16
6	E	702	FAD	C4-N3-C2	8.13	122.27	115.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	FAD	6	0
10	C	201	HEM	4	0
11	C	202	F6A	2	0
12	D	201	EPH	1	0
5	E	701	MLI	1	0
6	E	702	FAD	12	0
10	G	201	HEM	5	0
11	G	202	F6A	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	616/645 (95%)	-0.37	7 (1%) 80 76	44, 75, 107, 145	0
1	E	616/645 (95%)	-0.31	13 (2%) 64 60	46, 77, 114, 140	0
2	B	250/282 (88%)	-0.38	5 (2%) 65 61	42, 68, 100, 122	0
2	F	252/282 (89%)	-0.40	4 (1%) 72 67	47, 65, 99, 131	0
3	C	152/188 (80%)	-0.40	3 (1%) 65 61	51, 78, 116, 148	0
3	G	151/188 (80%)	-0.17	5 (3%) 47 43	52, 82, 142, 155	0
4	D	129/156 (82%)	-0.37	2 (1%) 72 67	57, 81, 115, 143	0
4	H	129/156 (82%)	-0.27	6 (4%) 32 30	55, 84, 130, 171	0
All	All	2295/2542 (90%)	-0.34	45 (1%) 65 61	42, 76, 115, 171	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	31	ASN	4.3
4	H	51	PRO	3.5
3	G	184	LEU	3.3
4	D	48	GLY	3.3
3	G	111	GLY	3.2
2	F	31	THR	3.1
1	E	30	SER	3.1
3	C	183	THR	3.0
1	A	30	SER	2.9
1	E	486	ASP	2.8
4	H	78	PHE	2.7
2	B	158	LYS	2.7
4	H	49	PHE	2.7
1	E	32	ILE	2.7
2	F	280	ALA	2.6
2	B	281	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	339	PRO	2.6
1	E	374	ASP	2.5
1	E	592	GLU	2.5
4	D	53	HIS	2.4
3	G	183	THR	2.4
1	A	614	ARG	2.4
2	F	281	ASN	2.4
1	E	459	ASP	2.4
2	F	48	PRO	2.4
3	C	179	HIS	2.4
2	B	39	GLU	2.4
1	E	408	GLY	2.4
1	A	96	PRO	2.3
1	E	377	LYS	2.3
1	E	644	SER	2.3
3	G	109	GLY	2.2
1	E	339	PRO	2.2
4	H	48	GLY	2.2
1	A	302	GLU	2.2
2	B	163	GLU	2.2
1	A	615	THR	2.1
4	H	50	LYS	2.1
4	H	155	GLU	2.1
1	A	617	HIS	2.1
1	E	461	LYS	2.1
3	C	182	ALA	2.1
3	G	110	LEU	2.1
2	B	157	THR	2.0
1	E	614	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	F6A	C	202	25/25	0.84	0.33	3.62	92,97,138,138	0
5	MLI	E	701	7/7	0.95	0.23	1.99	71,74,77,79	0
5	MLI	A	701	7/7	0.93	0.21	1.82	68,72,80,85	0
10	HEM	C	201	43/43	0.97	0.20	1.60	78,87,96,107	0
12	EPH	D	201	44/49	0.92	0.22	1.34	75,100,118,123	0
10	HEM	G	201	43/43	0.97	0.18	0.93	69,90,101,106	0
11	F6A	G	202	25/25	0.95	0.22	0.63	67,80,98,100	0
6	FAD	E	702	53/53	0.97	0.16	0.03	46,52,58,59	0
9	F3S	F	303	7/7	0.99	0.14	-0.60	49,60,62,67	0
9	F3S	B	303	7/7	0.99	0.15	-0.65	43,52,58,60	0
6	FAD	A	702	53/53	0.98	0.13	-0.90	42,46,56,57	0
7	FES	B	301	4/4	0.98	0.11	-1.16	51,55,55,56	0
7	FES	F	301	4/4	0.98	0.12	-1.46	46,46,49,50	0
8	SF4	B	302	8/8	1.00	0.10	-1.52	39,42,46,47	0
8	SF4	F	302	8/8	1.00	0.11	-1.58	35,37,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.