



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:49 am BST

PDB ID : 4YT0  
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with 2-methyl-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 : 3.66 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

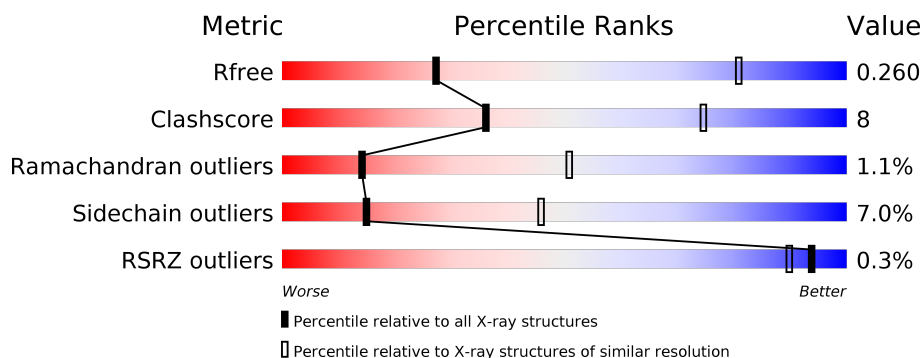
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.66 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))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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 respectively. 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: 75%;"></div> <div style="width: 19%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> </div>
1	E	645	<div> <div style="width: 75%;"></div> <div style="width: 20%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> </div>
2	B	282	<div> <div style="width: 65%;"></div> <div style="width: 21%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> </div>
2	F	282	<div> <div style="width: 61%;"></div> <div style="width: 25%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> </div>
3	C	188	<div> <div style="width: 63%;"></div> <div style="width: 17%;"></div> <div style="width: 19%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> </div>
3	G	188	<div> <div style="width: 2%;"></div> <div style="width: 66%;"></div> <div style="width: 12%;"></div> <div style="width: 20%;"></div> <div style="width: 0%;"></div> </div>

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Mol	Chain	Length	Quality of chain
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
5	MLI	E	701	-	-	X	-
8	SF4	B	302	-	-	X	-
8	SF4	F	302	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18236 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			

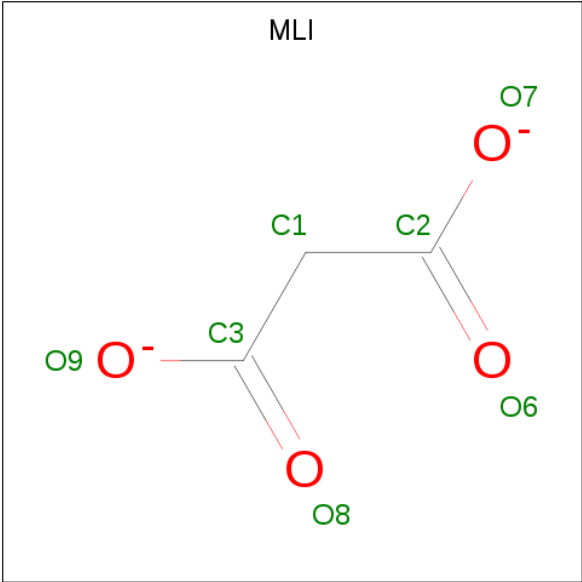
- Molecule 3 is a protein called Cytochrome b-large subunit.

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	150	Total	C	N	O	S	0	0	0
			1195	798	201	190	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>).



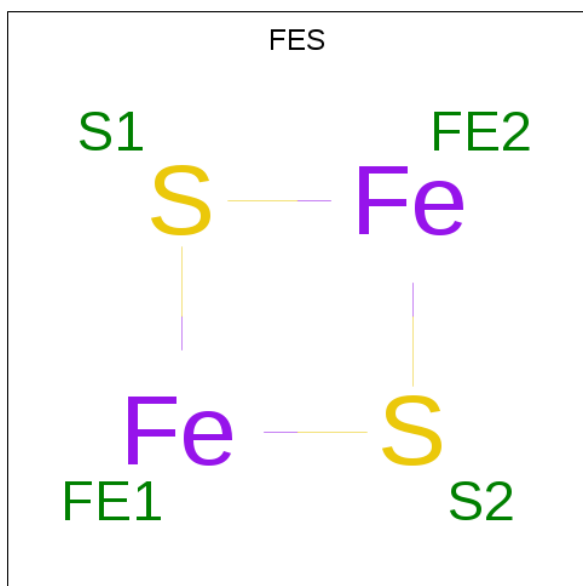
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			53	27	9	15		

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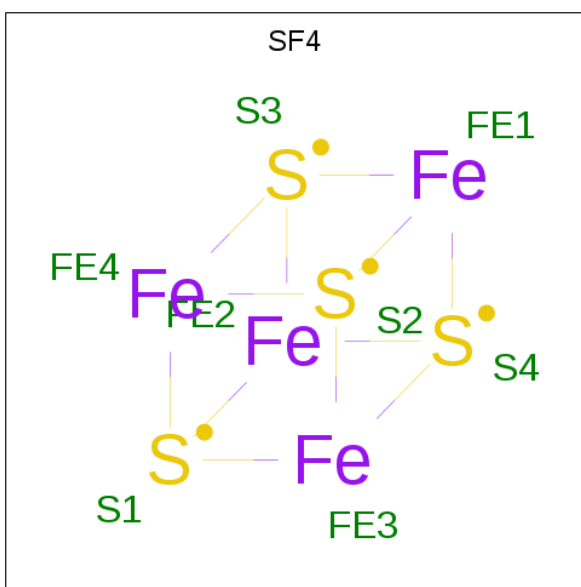
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



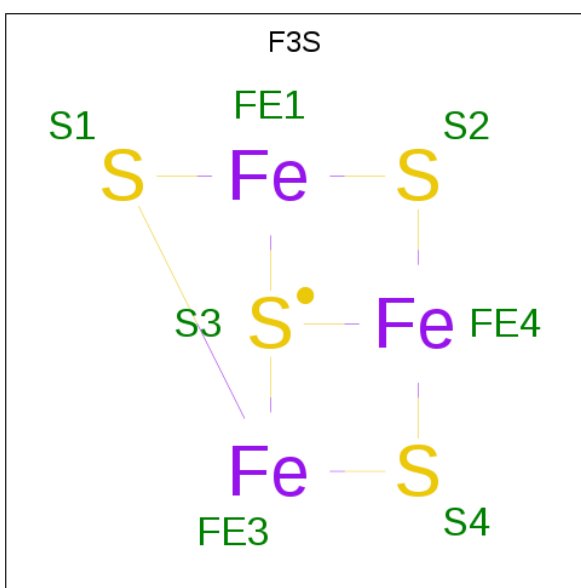
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



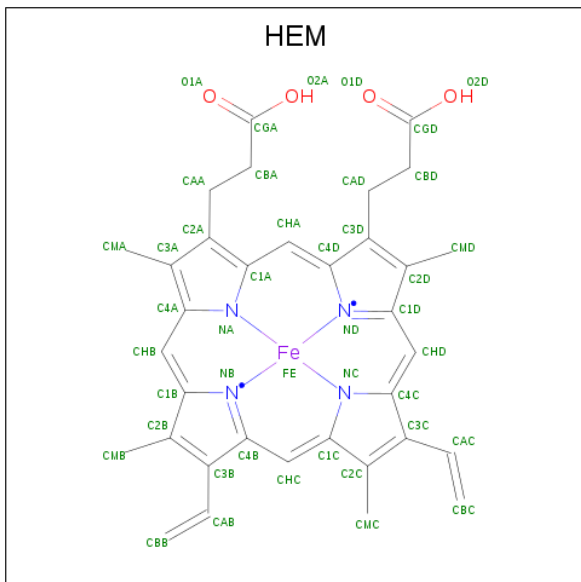
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



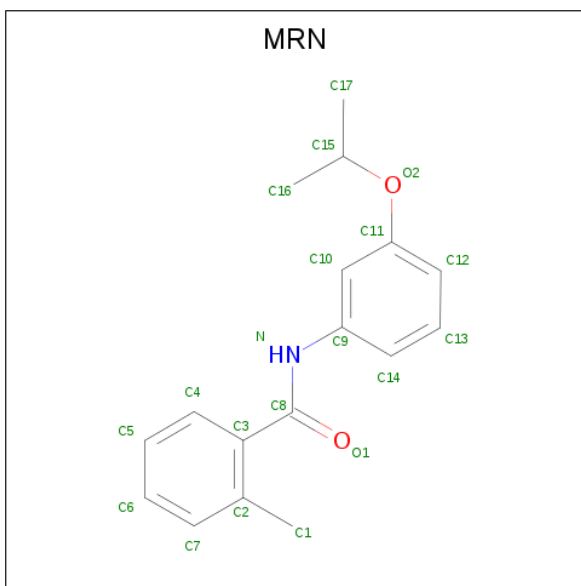
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- 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	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-methyl-N-[3-(1-methylethoxy)phenyl]benzamide (three-letter code: MRN) (formula:  $C_{17}H_{19}NO_2$ ).



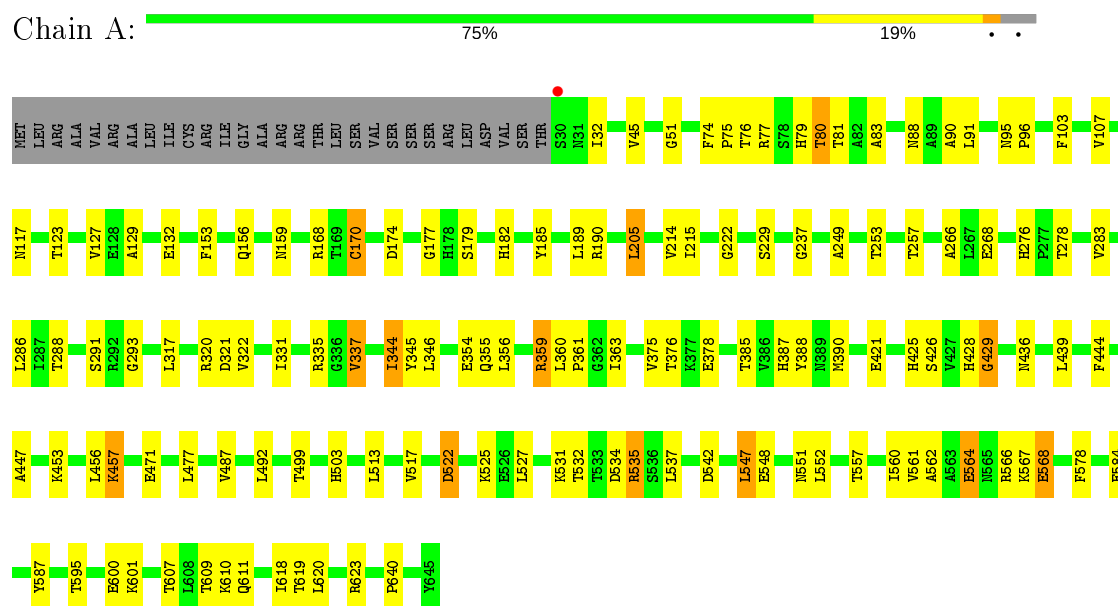


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			20	17	1	2		
11	G	1	Total	C	N	O	0	0
			20	17	1	2		

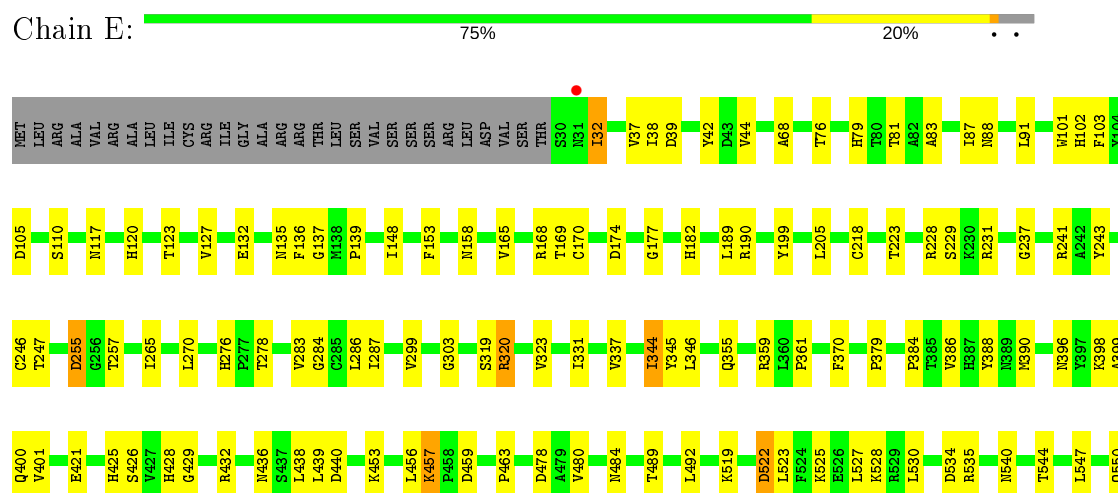
### 3 Residue-property plots

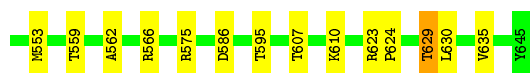
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

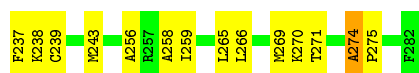
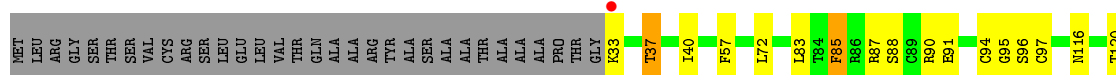


#### • Molecule 1: Succinate dehydrogenase flavoprotein

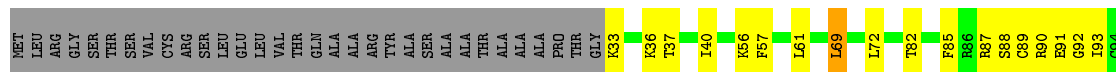




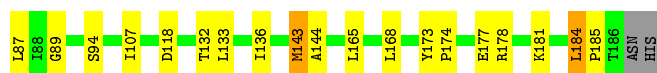
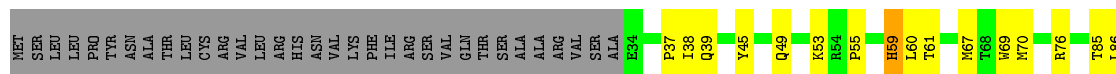
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



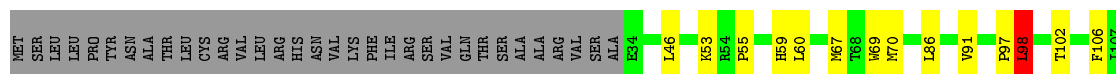
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Cytochrome b-large subunit

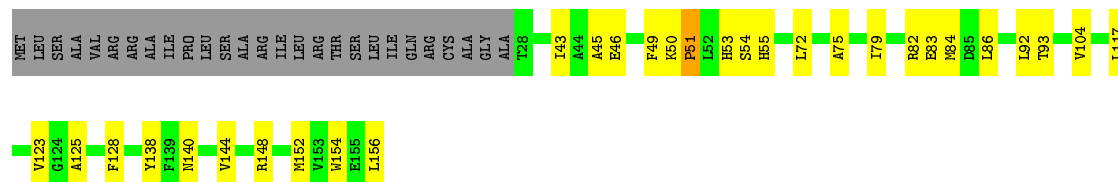


- Molecule 3: Cytochrome b-large subunit



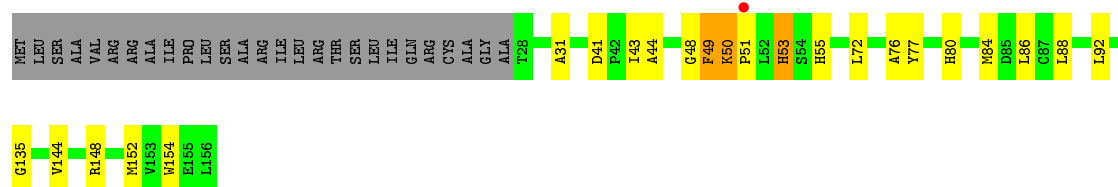
- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D: 



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

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.80Å 123.39Å 219.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.66 19.94 – 3.66	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-3.66) 89.2 (19.94-3.66)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.193 , 0.262 0.196 , 0.260	Depositor DCC
$R_{free}$ test set	1644 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 25.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.058 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, MRN, 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	0.34	0/4889	0.56	0/6605
1	E	0.34	0/4889	0.57	0/6605
2	B	0.35	0/2029	0.56	0/2739
2	F	0.35	0/2029	0.54	0/2739
3	C	0.36	0/1255	0.56	0/1709
3	G	0.35	0/1232	0.54	0/1676
4	D	0.38	0/1030	0.54	0/1406
4	H	0.35	0/1030	0.53	0/1406
All	All	0.35	0/18383	0.56	0/24885

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	4720	75	0
1	E	4787	0	4720	81	0
2	B	1985	0	2002	45	0
2	F	1985	0	2003	44	0
3	C	1217	0	1265	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1195	0	1240	14	0
4	D	998	0	985	17	0
4	H	998	0	985	14	0
5	A	7	0	2	0	0
5	E	7	0	2	2	0
6	A	53	0	31	8	0
6	E	53	0	31	8	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	2	0
8	F	8	0	0	3	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	4	0
11	C	20	0	19	1	0
11	G	20	0	19	2	0
All	All	18236	0	18084	290	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 8.

All (290) 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	1.75	1.02
2:B:182:CYS:HG	8:B:302:SF4:FE3	0.79	1.00
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.10	0.86
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.44	0.80
2:F:185:CYS:HG	8:F:302:SF4:FE1	0.93	0.80
2:F:185:CYS:SG	8:F:302:SF4:FE1	1.74	0.79
3:C:86:LEU:HD11	4:D:92:LEU:HD23	1.66	0.78
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.98	0.78
1:E:101:TRP:CD2	1:E:158:ASN:O	2.39	0.75
1:E:91:LEU:HD12	1:E:170:CYS:SG	2.25	0.75
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.68	0.75
1:E:103:PHE:HA	1:E:123:THR:HG21	1.70	0.73
1:E:566:ARG:O	1:E:575:ARG:NH2	2.20	0.73
2:F:195:TYR:O	2:F:199:ALA:HB2	1.88	0.72
3:C:132:THR:HG22	10:C:201:HEM:CBB	2.20	0.72
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.50	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.73	0.71
2:B:274:ALA:HB1	2:B:275:PRO:CD	2.22	0.69
2:B:188:CYS:SG	2:B:206:ALA:HB2	2.32	0.69
1:A:103:PHE:HA	1:A:123:THR:HG21	1.75	0.69
1:E:91:LEU:HD23	1:E:127:VAL:HG13	1.75	0.69
2:B:212:TYR:HA	2:B:215:ILE:HD12	1.75	0.68
2:B:182:CYS:SG	8:B:302:SF4:FE3	1.85	0.67
1:A:79:HIS:NE2	6:A:702:FAD:HM81	2.10	0.67
1:E:190:ARG:HA	4:H:43:ILE:HD11	1.77	0.66
2:F:139:MET:O	2:F:141:LEU:N	2.30	0.65
2:B:94:CYS:SG	2:B:96:SER:OG	2.50	0.64
1:A:425:HIS:N	1:A:426:SER:HA	2.13	0.64
1:A:253:THR:HG21	1:A:548:GLU:HB3	1.80	0.62
2:B:139:MET:O	2:B:141:LEU:N	2.32	0.62
2:B:159:ILE:HD11	2:B:164:LYS:HE2	1.82	0.62
1:A:499:THR:O	1:A:503:HIS:ND1	2.32	0.61
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.81	0.61
1:E:425:HIS:N	1:E:426:SER:HA	2.14	0.61
2:B:274:ALA:HB1	2:B:275:PRO:HD2	1.80	0.61
3:G:168:LEU:O	3:G:172:VAL:HG12	2.00	0.61
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.81	0.61
10:C:201:HEM:HHA	10:C:201:HEM:HBD1	1.83	0.61
2:B:185:CYS:SG	2:B:187:CYS:N	2.67	0.60
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.36	0.60
1:A:190:ARG:HA	4:D:43:ILE:HD11	1.83	0.60
2:B:227:LEU:HD22	2:B:266:LEU:CD1	2.32	0.60
2:B:95:GLY:HA2	2:B:183:ILE:HD12	1.82	0.60
1:A:83:ALA:HA	6:A:702:FAD:C6	2.30	0.60
1:E:101:TRP:CE3	1:E:158:ASN:O	2.55	0.60
3:C:94:SER:HA	4:D:138:TYR:CE1	2.37	0.59
1:A:268:GLU:OE2	1:A:623:ARG:NH1	2.35	0.59
1:E:32:ILE:HG23	1:E:478:ASP:OD1	2.03	0.59
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.86	0.58
2:B:185:CYS:SG	2:B:186:ALA:N	2.76	0.58
2:F:212:TYR:HB2	2:F:262:ILE:HD11	1.86	0.57
1:A:532:THR:O	1:A:535:ARG:NH2	2.37	0.57
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.85	0.57
2:F:69:LEU:HD12	2:F:109:CYS:HB3	1.86	0.57
4:D:50:LYS:N	4:D:51:PRO:CD	2.68	0.57
1:E:522:ASP:O	1:E:525:LYS:HG2	2.05	0.57
2:B:37:THR:HG23	2:B:120:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.87	0.56
1:A:91:LEU:HD23	1:A:127:VAL:HG13	1.88	0.56
1:E:38:ILE:HD12	1:E:223:THR:HB	1.87	0.56
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.41	0.56
2:B:243:MET:HE1	2:B:256:ALA:HB1	1.87	0.56
10:G:201:HEM:HHD	10:G:201:HEM:HBC2	1.87	0.56
2:F:264:MET:SD	3:G:143:MET:HA	2.45	0.56
3:C:87:LEU:HD22	4:D:128:PHE:CE1	2.40	0.56
1:A:492:LEU:HD21	1:A:527:LEU:HD12	1.87	0.56
1:A:561:VAL:HG21	1:A:618:ILE:HG21	1.86	0.55
1:E:534:ASP:HA	2:F:82:THR:HG22	1.88	0.55
1:A:88:ASN:HD21	1:A:156:GLN:HE22	1.54	0.55
1:E:331:ILE:HD11	1:E:344:ILE:HG23	1.88	0.55
2:F:128:HIS:CE1	2:F:196:TRP:O	2.59	0.55
1:A:288:THR:O	1:A:291:SER:OG	2.23	0.54
4:D:82:ARG:NH2	4:D:140:ASN:O	2.39	0.54
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.43	0.54
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.89	0.54
1:E:480:VAL:HG21	1:E:550:GLN:OE1	2.08	0.54
2:F:239:CYS:SG	2:F:259:ILE:HG21	2.48	0.54
1:A:456:LEU:HD23	1:A:457:LYS:N	2.23	0.54
1:E:101:TRP:CG	1:E:158:ASN:O	2.61	0.54
2:F:72:LEU:HB3	2:F:85:PHE:CE1	2.43	0.53
1:E:283:VAL:HG21	1:E:370:PHE:CD1	2.44	0.53
2:F:159:ILE:HD11	2:F:164:LYS:CE	2.39	0.53
2:B:150:GLN:NE2	4:D:46:GLU:OE1	2.41	0.53
1:E:79:HIS:NE2	6:E:702:FAD:C8	2.71	0.53
1:E:629:THR:HG21	1:E:635:VAL:O	2.09	0.53
3:C:173:TYR:HB3	3:C:174:PRO:HD3	1.91	0.52
4:D:144:VAL:HG11	4:D:152:MET:SD	2.50	0.52
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.91	0.52
3:G:172:VAL:HG13	3:G:172:VAL:O	2.08	0.52
2:B:179:LEU:HD23	2:B:213:ARG:HA	1.90	0.52
2:F:40:ILE:HD12	2:F:57:PHE:CD1	2.45	0.52
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.91	0.52
3:C:69:TRP:CH2	11:C:202:MRN:H17A	2.45	0.52
2:F:176:LEU:HD21	2:F:217:ASP:OD2	2.09	0.52
3:C:86:LEU:CD1	4:D:92:LEU:HD23	2.37	0.52
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.45	0.52
4:H:50:LYS:N	4:H:51:PRO:CD	2.73	0.52
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:CG	1:E:68:ALA:HB2	2.45	0.51
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.90	0.51
1:A:331:ILE:HD11	1:A:344:ILE:HG23	1.93	0.51
2:F:115:GLN:HA	2:F:115:GLN:HE21	1.75	0.51
1:A:356:LEU:HD23	1:A:375:VAL:HG23	1.92	0.51
2:B:243:MET:CE	2:B:256:ALA:HB1	2.41	0.51
2:F:181:GLU:HB2	2:F:253:LEU:HD21	1.93	0.51
2:F:182:CYS:SG	2:F:184:LEU:HD12	2.51	0.51
1:E:286:LEU:HD22	6:E:702:FAD:H6	1.93	0.51
2:F:242:ILE:O	2:F:243:MET:HB2	2.09	0.51
3:C:107:ILE:CD1	4:D:156:LEU:HD13	2.39	0.51
1:E:319:SER:O	1:E:323:VAL:HG23	2.11	0.51
10:C:201:HEM:HHO	10:C:201:HEM:HBC2	1.92	0.51
1:A:288:THR:HG22	1:A:363:ILE:HG21	1.92	0.50
1:E:247:THR:HG22	1:E:284:GLY:O	2.12	0.50
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.93	0.50
4:H:76:ALA:HB1	4:H:88:LEU:HD11	1.94	0.50
1:E:102:HIS:ND1	1:E:123:THR:HG22	2.27	0.50
1:A:551:ASN:N	1:A:551:ASN:HD22	2.09	0.49
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.42	0.49
1:E:489:THR:HG22	1:E:530:LEU:HD11	1.94	0.49
1:E:189:LEU:HD13	2:F:147:ALA:HA	1.94	0.49
1:E:456:LEU:HD23	1:E:457:LYS:N	2.27	0.49
1:A:79:HIS:O	1:A:80:THR:C	2.49	0.49
2:B:85:PHE:N	2:B:85:PHE:CD2	2.81	0.49
3:C:181:LYS:HA	3:C:184:LEU:HD13	1.95	0.49
2:B:270:LYS:O	2:B:271:THR:HG23	2.12	0.49
1:E:199:TYR:CE2	1:E:218:CYS:HB2	2.46	0.49
1:E:139:PRO:HB3	2:F:176:LEU:HD23	1.95	0.49
1:E:492:LEU:HD21	1:E:527:LEU:HD12	1.95	0.49
1:A:253:THR:HG22	1:A:552:LEU:HD11	1.94	0.49
1:A:288:THR:HG23	1:A:291:SER:H	1.78	0.49
3:G:69:TRP:CZ2	11:G:202:MRN:H17A	2.48	0.48
1:A:129:ALA:O	1:A:132:GLU:HB2	2.12	0.48
2:B:235:SER:OG	3:C:39:GLN:NE2	2.47	0.48
4:H:144:VAL:HG11	4:H:152:MET:SD	2.54	0.48
1:A:356:LEU:HD22	1:A:376:THR:HG22	1.95	0.48
2:B:72:LEU:HB3	2:B:85:PHE:CE1	2.48	0.48
1:A:286:LEU:HD13	1:A:387:HIS:CE1	2.49	0.48
2:F:220:ASP:O	2:F:272:LYS:NZ	2.44	0.48
1:E:42:TYR:CD2	1:E:68:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASP:OD1	1:A:322:VAL:N	2.47	0.48
2:B:40:ILE:HD12	2:B:57:PHE:CD1	2.48	0.48
1:E:237:GLY:HA2	1:E:421:GLU:HB3	1.95	0.48
3:G:91:VAL:HG22	4:H:135:GLY:HA3	1.96	0.48
3:C:38:ILE:HG23	3:C:39:GLN:HG3	1.95	0.47
4:D:104:VAL:HG21	4:D:125:ALA:HB2	1.95	0.47
2:B:239:CYS:SG	2:B:259:ILE:HG21	2.54	0.47
1:E:255:ASP:OD1	1:E:255:ASP:N	2.47	0.47
3:G:132:THR:HG23	10:G:201:HEM:CAB	2.44	0.47
1:A:74:PHE:HB3	1:A:77:ARG:HG2	1.95	0.47
3:C:132:THR:HG22	10:C:201:HEM:CAB	2.44	0.47
3:C:85:THR:O	3:C:89:GLY:N	2.41	0.47
1:A:79:HIS:O	1:A:81:THR:N	2.48	0.47
1:A:95:ASN:HB2	1:A:96:PRO:HD2	1.96	0.47
2:B:85:PHE:HD2	2:B:85:PHE:N	2.12	0.47
1:E:398:LYS:O	1:E:399:ALA:HB3	2.14	0.47
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.15	0.47
1:A:487:VAL:O	1:A:531:LYS:N	2.47	0.47
1:E:79:HIS:CE1	6:E:702:FAD:HM82	2.47	0.47
4:D:50:LYS:N	4:D:51:PRO:HD2	2.30	0.47
1:E:623:ARG:HG3	1:E:624:PRO:HD2	1.96	0.47
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.96	0.46
2:F:159:ILE:HD11	2:F:164:LYS:HE2	1.96	0.46
3:G:86:LEU:CD1	4:H:92:LEU:HD23	2.45	0.46
2:B:150:GLN:HA	2:B:152:TRP:CZ3	2.50	0.46
2:F:160:ASN:HB3	2:F:163:GLU:HG2	1.97	0.46
2:B:139:MET:HB3	2:B:143:TYR:CE2	2.50	0.46
1:E:519:LYS:O	1:E:523:LEU:HD13	2.15	0.46
1:E:540:ASN:O	1:E:544:THR:HG23	2.15	0.46
1:A:103:PHE:O	1:A:107:VAL:HG23	2.15	0.46
4:H:41:ASP:HB3	4:H:44:ALA:HB3	1.98	0.46
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.98	0.46
2:B:185:CYS:O	2:B:186:ALA:HB3	2.16	0.46
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.98	0.46
2:F:234:PHE:O	2:F:235:SER:C	2.54	0.46
1:A:237:GLY:HA2	1:A:421:GLU:HB3	1.98	0.46
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.51	0.46
2:F:131:VAL:HG22	3:G:55:PRO:HG2	1.97	0.46
2:B:188:CYS:SG	2:B:189:SER:N	2.89	0.45
1:E:345:TYR:CE1	1:E:379:PRO:HG2	2.52	0.45
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:HIS:O	1:A:429:GLY:C	2.53	0.45
1:E:286:LEU:HD22	6:E:702:FAD:C6	2.47	0.45
2:B:95:GLY:CA	2:B:183:ILE:HD12	2.45	0.45
1:E:286:LEU:HD21	5:E:701:MLI:C3	2.46	0.45
1:E:132:GLU:O	1:E:136:PHE:N	2.49	0.45
1:E:270:LEU:O	1:E:559:THR:HG23	2.15	0.45
2:F:200:ASP:HB3	3:G:46:LEU:HD11	1.97	0.45
1:E:44:VAL:HG23	1:E:231:ARG:HB2	1.98	0.45
2:F:146:TYR:HA	2:F:207:VAL:HG13	1.98	0.45
2:F:146:TYR:O	2:F:149:ILE:HG12	2.17	0.45
2:B:237:PHE:O	2:B:239:CYS:N	2.50	0.45
2:F:95:GLY:CA	2:F:183:ILE:HD12	2.47	0.45
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.98	0.44
1:E:299:VAL:HG12	1:E:303:GLY:HA2	1.99	0.44
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.98	0.44
2:B:212:TYR:CD2	2:B:258:ALA:HB1	2.52	0.44
1:E:276:HIS:O	1:E:384:PRO:HA	2.17	0.44
1:E:37:VAL:HB	4:H:31:ALA:HB2	1.99	0.44
1:A:534:ASP:HB3	1:A:542:ASP:HB3	1.99	0.44
2:B:128:HIS:CE1	2:B:196:TRP:O	2.70	0.44
1:A:276:HIS:N	1:A:385:THR:O	2.50	0.44
1:E:88:ASN:ND2	1:E:169:THR:OG1	2.50	0.44
3:G:173:TYR:HB3	3:G:174:PRO:HD3	1.99	0.44
3:C:37:PRO:CB	4:D:45:ALA:HB1	2.48	0.44
1:E:388:TYR:CD2	1:E:432:ARG:HD2	2.53	0.44
1:E:527:LEU:HD11	1:E:553:MET:HG3	1.98	0.44
2:B:97:CYS:O	2:B:97:CYS:SG	2.75	0.43
1:E:190:ARG:CA	4:H:43:ILE:HD11	2.46	0.43
4:H:76:ALA:CB	4:H:88:LEU:HD11	2.47	0.43
1:A:249:ALA:HB1	2:B:88:SER:O	2.18	0.43
1:E:278:THR:HG21	1:E:346:LEU:HD22	2.00	0.43
2:F:243:MET:CE	2:F:256:ALA:HB1	2.48	0.43
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.53	0.43
1:E:137:GLY:HA2	2:F:153:LEU:HD22	2.00	0.43
1:A:185:TYR:CZ	1:A:189:LEU:HD21	2.54	0.43
2:F:100:ASN:HD21	2:F:103:GLY:H	1.66	0.43
2:F:159:ILE:HD11	2:F:164:LYS:HE3	2.00	0.43
1:E:110:SER:HB2	1:E:429:GLY:HA3	1.99	0.43
1:E:83:ALA:HB1	6:E:702:FAD:C4X	2.49	0.43
1:E:286:LEU:HB2	6:E:702:FAD:HM73	2.01	0.43
1:A:286:LEU:HB2	6:A:702:FAD:HM73	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:HG21	1:A:346:LEU:HD13	2.01	0.43
1:A:359:ARG:O	1:A:360:LEU:HD23	2.19	0.43
2:B:146:TYR:HA	2:B:207:VAL:HG13	2.00	0.43
2:B:265:LEU:HD23	2:B:271:THR:HA	2.00	0.43
1:A:566:ARG:NH1	1:A:568:GLU:OE2	2.49	0.42
1:E:76:THR:HG23	1:E:182:HIS:NE2	2.34	0.42
1:E:345:TYR:CD1	1:E:379:PRO:HG2	2.54	0.42
2:F:92:GLY:HA2	2:F:109:CYS:SG	2.59	0.42
4:H:77:TYR:O	4:H:80:HIS:NE2	2.51	0.42
1:A:45:VAL:HG23	1:A:229:SER:HB3	2.02	0.42
1:A:557:THR:OG1	1:A:611:GLN:NE2	2.53	0.42
1:E:287:ILE:HG21	1:E:346:LEU:HD23	2.00	0.42
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.17	0.42
3:G:69:TRP:CE2	11:G:202:MRN:H17A	2.55	0.42
1:A:90:ALA:HA	1:A:168:ARG:HG2	2.00	0.42
1:A:32:ILE:HG13	1:A:32:ILE:O	2.19	0.42
1:E:396:ASN:HD21	1:E:400:GLN:HB2	1.84	0.42
1:A:331:ILE:HD11	1:A:344:ILE:CG2	2.49	0.42
1:A:600:GLU:N	1:A:600:GLU:OE2	2.53	0.42
1:E:105:ASP:OD2	1:E:168:ARG:NH2	2.53	0.42
2:F:227:LEU:HD22	2:F:266:LEU:CD1	2.49	0.42
1:A:293:GLY:HA2	1:A:317:LEU:HD11	2.02	0.42
1:E:135:ASN:ND2	2:F:161:LEU:O	2.53	0.42
2:F:276:LEU:HB3	2:F:277:PRO:HD2	2.02	0.42
3:G:59:HIS:CD2	3:G:59:HIS:N	2.88	0.42
1:E:91:LEU:CD1	1:E:170:CYS:SG	3.02	0.42
1:E:428:HIS:HB3	1:E:432:ARG:HA	2.02	0.42
1:E:87:ILE:HD12	1:E:438:LEU:HB3	2.01	0.42
2:B:159:ILE:HD11	2:B:164:LYS:CE	2.50	0.41
3:C:178:ARG:HA	3:C:181:LYS:HD3	2.01	0.41
1:A:522:ASP:O	1:A:525:LYS:HG2	2.20	0.41
1:A:609:THR:HG22	1:A:620:LEU:CD2	2.49	0.41
2:B:94:CYS:SG	2:B:95:GLY:N	2.94	0.41
3:C:45:TYR:CE2	3:C:49:GLN:HG3	2.55	0.41
2:B:201:LYS:HA	3:C:39:GLN:HG2	2.02	0.41
1:E:241:ARG:HD2	1:E:246:CYS:SG	2.61	0.41
2:F:185:CYS:SG	8:F:302:SF4:S3	3.18	0.41
3:G:97:PRO:O	3:G:98:LEU:C	2.59	0.41
1:A:76:THR:HG23	1:A:182:HIS:NE2	2.36	0.41
4:D:50:LYS:O	4:D:51:PRO:C	2.59	0.41
1:E:228:ARG:NH1	1:E:463:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:LYS:HB2	2:F:61:LEU:HD11	2.03	0.41
1:A:388:TYR:CE1	1:A:421:GLU:HG3	2.56	0.41
4:D:53:HIS:O	4:D:55:HIS:N	2.54	0.41
1:A:517:VAL:HG22	1:A:560:ILE:HG23	2.03	0.41
1:E:148:ILE:HG21	1:E:170:CYS:HB3	2.02	0.41
1:A:91:LEU:HD12	1:A:170:CYS:SG	2.61	0.41
1:A:286:LEU:CB	6:A:702:FAD:HM73	2.51	0.41
3:C:76:ARG:HE	10:C:201:HEM:CGD	2.34	0.41
1:A:214:VAL:HG12	1:A:215:ILE:N	2.36	0.41
1:A:74:PHE:CD1	1:A:75:PRO:HD2	2.56	0.41
1:E:91:LEU:HD23	1:E:127:VAL:CG1	2.44	0.41
1:A:567:LYS:HB3	1:A:578:PHE:CD1	2.56	0.41
2:B:139:MET:HB3	2:B:143:TYR:CD2	2.56	0.41
2:B:196:TRP:CZ3	3:C:59:HIS:HB2	2.56	0.41
4:H:48:GLY:O	4:H:49:PHE:C	2.59	0.41
2:B:234:PHE:O	2:B:235:SER:C	2.58	0.40
4:D:75:ALA:O	4:D:79:ILE:HG12	2.22	0.40
1:A:205:LEU:HD11	1:A:215:ILE:HB	2.02	0.40
2:B:191:SER:O	2:B:193:PRO:HD3	2.21	0.40
3:C:143:MET:O	3:C:144:ALA:HB3	2.21	0.40
1:E:32:ILE:HG13	1:E:32:ILE:O	2.22	0.40
1:E:120:HIS:HD2	1:E:630:LEU:HB2	1.85	0.40
4:H:53:HIS:O	4:H:55:HIS:N	2.54	0.40
1:A:587:TYR:CE1	1:A:640:PRO:HB2	2.56	0.40
2:F:154:GLN:HE21	2:F:222:SER:CB	2.35	0.40
1:A:477:LEU:HD12	1:A:547:LEU:HD21	2.04	0.40
1:E:42:TYR:O	1:E:229:SER:HA	2.22	0.40
2:F:95:GLY:HA2	2:F:183:ILE:HD12	2.04	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%)	568 (92%)	43 (7%)	3 (0%)	29	66
1	E	614/645 (95%)	563 (92%)	51 (8%)	0	100	100
2	B	248/282 (88%)	215 (87%)	28 (11%)	5 (2%)	7	39
2	F	248/282 (88%)	219 (88%)	22 (9%)	7 (3%)	5	33
3	C	151/188 (80%)	139 (92%)	11 (7%)	1 (1%)	22	59
3	G	148/188 (79%)	134 (90%)	11 (7%)	3 (2%)	7	39
4	D	127/156 (81%)	119 (94%)	5 (4%)	3 (2%)	6	35
4	H	127/156 (81%)	114 (90%)	11 (9%)	2 (2%)	9	43
All	All	2277/2542 (90%)	2071 (91%)	182 (8%)	24 (1%)	14	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	THR
2	B	140	ASN
2	F	140	ASN
2	F	243	MET
4	D	54	SER
2	F	88	SER
4	H	49	PHE
2	B	238	LYS
4	D	49	PHE
2	F	158	LYS
2	F	235	SER
2	B	83	LEU
2	B	137	PRO
2	B	274	ALA
3	C	185	PRO
2	F	89	CYS
3	G	98	LEU
3	G	173	TYR
4	H	50	LYS
1	A	51	GLY
2	F	275	PRO
1	A	429	GLY
4	D	51	PRO
3	G	172	VAL

### 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%)	471 (94%)	31 (6%)	18	50
1	E	502/527 (95%)	472 (94%)	30 (6%)	19	51
2	B	220/242 (91%)	206 (94%)	14 (6%)	17	49
2	F	220/242 (91%)	204 (93%)	16 (7%)	14	44
3	C	127/158 (80%)	113 (89%)	14 (11%)	6	29
3	G	124/158 (78%)	111 (90%)	13 (10%)	7	30
4	D	98/119 (82%)	89 (91%)	9 (9%)	9	36
4	H	98/119 (82%)	92 (94%)	6 (6%)	18	50
All	All	1891/2092 (90%)	1758 (93%)	133 (7%)	15	46

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	153	PHE
1	A	159	ASN
1	A	170	CYS
1	A	179	SER
1	A	205	LEU
1	A	257	THR
1	A	283	VAL
1	A	320	ARG
1	A	335	ARG
1	A	337	VAL
1	A	344	ILE
1	A	354	GLU
1	A	355	GLN
1	A	359	ARG
1	A	378	GLU
1	A	390	MET
1	A	436	ASN
1	A	439	LEU

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Mol	Chain	Res	Type
1	A	453	LYS
1	A	457	LYS
1	A	471	GLU
1	A	522	ASP
1	A	535	ARG
1	A	547	LEU
1	A	564	GLU
1	A	568	GLU
1	A	584	GLU
1	A	595	THR
1	A	601	LYS
1	A	619	THR
2	B	33	LYS
2	B	37	THR
2	B	85	PHE
2	B	87	ARG
2	B	90	ARG
2	B	91	GLU
2	B	116	ASN
2	B	131	VAL
2	B	132	ILE
2	B	139	MET
2	B	156	LYS
2	B	176	LEU
2	B	213	ARG
2	B	269	MET
3	C	53	LYS
3	C	59	HIS
3	C	60	LEU
3	C	61	THR
3	C	67	MET
3	C	70	MET
3	C	118	ASP
3	C	133	LEU
3	C	136	ILE
3	C	143	MET
3	C	165	LEU
3	C	168	LEU
3	C	177	GLU
3	C	184	LEU
4	D	72	LEU
4	D	83	GLU

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Mol	Chain	Res	Type
4	D	84	MET
4	D	86	LEU
4	D	93	THR
4	D	117	LEU
4	D	123	VAL
4	D	148	ARG
4	D	154	TRP
1	E	32	ILE
1	E	39	ASP
1	E	81	THR
1	E	117	ASN
1	E	153	PHE
1	E	165	VAL
1	E	205	LEU
1	E	255	ASP
1	E	257	THR
1	E	320	ARG
1	E	337	VAL
1	E	344	ILE
1	E	355	GLN
1	E	359	ARG
1	E	390	MET
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	457	LYS
1	E	459	ASP
1	E	484	ASN
1	E	522	ASP
1	E	528	LYS
1	E	535	ARG
1	E	547	LEU
1	E	586	ASP
1	E	595	THR
1	E	610	LYS
1	E	629	THR
2	F	33	LYS
2	F	37	THR
2	F	56	LYS
2	F	69	LEU
2	F	87	ARG

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Mol	Chain	Res	Type
2	F	90	ARG
2	F	91	GLU
2	F	93	ILE
2	F	115	GLN
2	F	116	ASN
2	F	131	VAL
2	F	156	LYS
2	F	200	ASP
2	F	213	ARG
2	F	216	ILE
2	F	248	THR
3	G	53	LYS
3	G	60	LEU
3	G	67	MET
3	G	70	MET
3	G	98	LEU
3	G	102	THR
3	G	106	PHE
3	G	108	ARG
3	G	110	LEU
3	G	118	ASP
3	G	133	LEU
3	G	160	LEU
3	G	179	HIS
4	H	53	HIS
4	H	72	LEU
4	H	84	MET
4	H	86	LEU
4	H	148	ARG
4	H	154	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	358	GLN
1	A	428	HIS
1	A	436	ASN
1	A	476	ASN
1	A	497	GLN

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Mol	Chain	Res	Type
1	A	551	ASN
1	A	565	ASN
1	A	617	HIS
2	B	55	GLN
2	B	105	ASN
2	B	115	GLN
2	B	116	ASN
2	B	145	GLN
2	B	150	GLN
2	B	165	GLN
4	D	105	ASN
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	252	ASN
1	E	347	GLN
1	E	358	GLN
1	E	436	ASN
1	E	451	ASN
1	E	497	GLN
1	E	551	ASN
1	E	565	ASN
1	E	594	GLN
2	F	55	GLN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	145	GLN
3	G	66	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 ⓘ

14 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
8	SF4	F	302	2	0,12,12	0.00	-	-		
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	-		
10	HEM	C	201	3,4	27,50,50	1.01	2 (7%)	17,82,82	1.76	2 (11%)
9	F3S	B	303	2	0,9,9	0.00	-	-		
6	FAD	E	702	-	51,58,58	1.91	7 (13%)	60,89,89	2.14	15 (25%)
10	HEM	G	201	3,4	27,50,50	1.01	2 (7%)	17,82,82	1.58	2 (11%)
11	MRN	C	202	-	21,21,21	1.99	3 (14%)	28,28,28	1.10	2 (7%)
7	FES	F	301	2	0,4,4	0.00	-	-		
11	MRN	G	202	-	21,21,21	2.00	3 (14%)	28,28,28	1.39	3 (10%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
7	FES	B	301	2	0,4,4	0.00	-	-		
8	SF4	B	302	2	0,12,12	0.00	-	-		
6	FAD	A	702	-	51,58,58	1.83	5 (9%)	60,89,89	2.02	11 (18%)

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
8	SF4	F	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/0/4/4	-
9	F3S	F	303	2	-	-	0/3/3/3
10	HEM	C	201	3,4	-	2/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	F3S	B	303	2	-	-	0/3/3/3
6	FAD	E	702	-	-	8/30/50/50	0/6/6/6
10	HEM	G	201	3,4	-	3/6/54/54	-
11	MRN	C	202	-	-	6/12/12/12	0/2/2/2
7	FES	F	301	2	-	-	0/1/1/1
11	MRN	G	202	-	-	6/12/12/12	0/2/2/2
5	MLI	E	701	-	-	0/0/4/4	-
7	FES	B	301	2	-	-	0/1/1/1
8	SF4	B	302	2	-	-	0/6/5/5
6	FAD	A	702	-	-	7/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C4X-C10	9.80	1.48	1.38
6	A	702	FAD	C4X-C10	9.69	1.48	1.38
11	C	202	MRN	C3-C8	-5.91	1.38	1.50
11	G	202	MRN	C3-C8	-5.40	1.39	1.50
11	C	202	MRN	C1-C2	-5.15	1.40	1.51
11	G	202	MRN	C1-C2	-5.02	1.41	1.51
11	G	202	MRN	C9-N	-4.95	1.31	1.41
6	E	702	FAD	C4-C4X	4.36	1.48	1.41
11	C	202	MRN	C9-N	-4.07	1.33	1.41
6	E	702	FAD	C8-C7	3.94	1.50	1.40
6	A	702	FAD	C4-C4X	3.89	1.48	1.41
6	A	702	FAD	C9A-C5X	3.56	1.49	1.42
6	E	702	FAD	C9A-C5X	3.47	1.49	1.42
10	G	201	HEM	C4D-C3D	3.02	1.49	1.42
6	A	702	FAD	C8-C7	2.97	1.48	1.40
10	G	201	HEM	C3B-C2B	-2.73	1.36	1.40
10	C	201	HEM	C4D-C3D	2.60	1.48	1.42
10	C	201	HEM	C3B-C2B	-2.53	1.36	1.40
6	E	702	FAD	C10-N1	2.30	1.36	1.33
6	A	702	FAD	C5A-C4A	2.29	1.47	1.40
6	E	702	FAD	C5A-C4A	2.17	1.46	1.40
6	E	702	FAD	C9A-N10	2.15	1.41	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	C4-N3-C2	8.48	122.30	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	C4-N3-C2	8.40	122.23	115.14
6	E	702	FAD	C4-C4X-C10	-6.29	115.79	119.95
6	A	702	FAD	C1'-N10-C9A	5.63	122.72	118.29
10	C	201	HEM	CBD-CAD-C3D	5.47	122.55	112.48
11	G	202	MRN	C9-N-C8	-4.99	113.61	126.58
10	G	201	HEM	CBD-CAD-C3D	4.81	121.34	112.48
6	E	702	FAD	C1'-N10-C9A	4.61	121.92	118.29
11	C	202	MRN	C9-N-C8	-4.61	114.61	126.58
6	A	702	FAD	C4X-C4-N3	-4.30	117.56	123.43
6	E	702	FAD	N3A-C2A-N1A	-3.81	122.73	128.68
6	E	702	FAD	C4X-N5-C5X	3.79	120.56	116.77
6	A	702	FAD	N3A-C2A-N1A	-3.75	122.82	128.68
6	E	702	FAD	C4-C4X-N5	3.72	122.85	118.60
11	G	202	MRN	C2-C3-C8	3.68	123.32	120.56
6	A	702	FAD	C4X-N5-C5X	3.57	120.34	116.77
6	A	702	FAD	C9A-N10-C10	-3.55	117.25	121.91
6	E	702	FAD	C4X-C4-N3	-3.13	119.14	123.43
6	A	702	FAD	C4-C4X-C10	-2.97	117.98	119.95
6	A	702	FAD	C4A-C5A-N7A	-2.82	106.46	109.40
6	E	702	FAD	C4'-C3'-C2'	-2.80	107.54	113.36
6	E	702	FAD	C1'-C2'-C3'	2.77	117.54	109.79
10	G	201	HEM	CAD-C3D-C2D	-2.72	119.43	127.25
6	E	702	FAD	C4A-C5A-N7A	-2.71	106.57	109.40
6	E	702	FAD	P-O3P-PA	-2.61	123.88	132.83
11	G	202	MRN	C11-O2-C15	-2.48	116.20	119.37
6	E	702	FAD	C9A-N10-C10	-2.42	118.74	121.91
6	E	702	FAD	O2'-C2'-C3'	-2.40	103.25	109.10
6	A	702	FAD	C1'-C2'-C3'	2.39	116.47	109.79
6	A	702	FAD	C5X-C9A-N10	2.36	119.42	117.72
6	E	702	FAD	C8M-C8-C7	2.22	125.29	120.74
10	C	201	HEM	CAD-C3D-C2D	-2.19	120.95	127.25
6	A	702	FAD	C2A-N1A-C6A	2.17	122.46	118.75
11	C	202	MRN	C11-O2-C15	-2.09	116.70	119.37
6	E	702	FAD	C2A-N1A-C6A	2.05	122.26	118.75

There are no chirality outliers.

All (32) 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
6	E	702	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
6	E	702	FAD	N10-C1'-C2'-C3'
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
6	A	702	FAD	N10-C1'-C2'-O2'
11	G	202	MRN	C10-C9-N-C8
11	G	202	MRN	C14-C9-N-C8
11	C	202	MRN	C16-C15-O2-C11
11	C	202	MRN	C17-C15-O2-C11
11	C	202	MRN	C10-C9-N-C8
6	A	702	FAD	PA-O3P-P-O5'
6	E	702	FAD	C5'-O5'-P-O3P
11	C	202	MRN	C14-C9-N-C8
6	A	702	FAD	N10-C1'-C2'-C3'
6	E	702	FAD	O2'-C2'-C3'-O3'
11	G	202	MRN	C16-C15-O2-C11
11	G	202	MRN	C17-C15-O2-C11
6	A	702	FAD	O2'-C2'-C3'-O3'
6	E	702	FAD	P-O3P-PA-O1A
6	E	702	FAD	P-O3P-PA-O2A
11	G	202	MRN	C10-C11-O2-C15
10	G	201	HEM	C2A-CAA-CBA-CGA
11	G	202	MRN	C12-C11-O2-C15
11	C	202	MRN	C10-C11-O2-C15
6	A	702	FAD	O4B-C4B-C5B-O5B
6	A	702	FAD	O2'-C2'-C3'-C4'
6	E	702	FAD	O4B-C4B-C5B-O5B
6	E	702	FAD	C1'-C2'-C3'-O3'
6	A	702	FAD	C1'-C2'-C3'-O3'
11	C	202	MRN	C12-C11-O2-C15

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	302	SF4	3	0
10	C	201	HEM	6	0
6	E	702	FAD	8	0
10	G	201	HEM	4	0
11	C	202	MRN	1	0
11	G	202	MRN	2	0
5	E	701	MLI	2	0
8	B	302	SF4	2	0

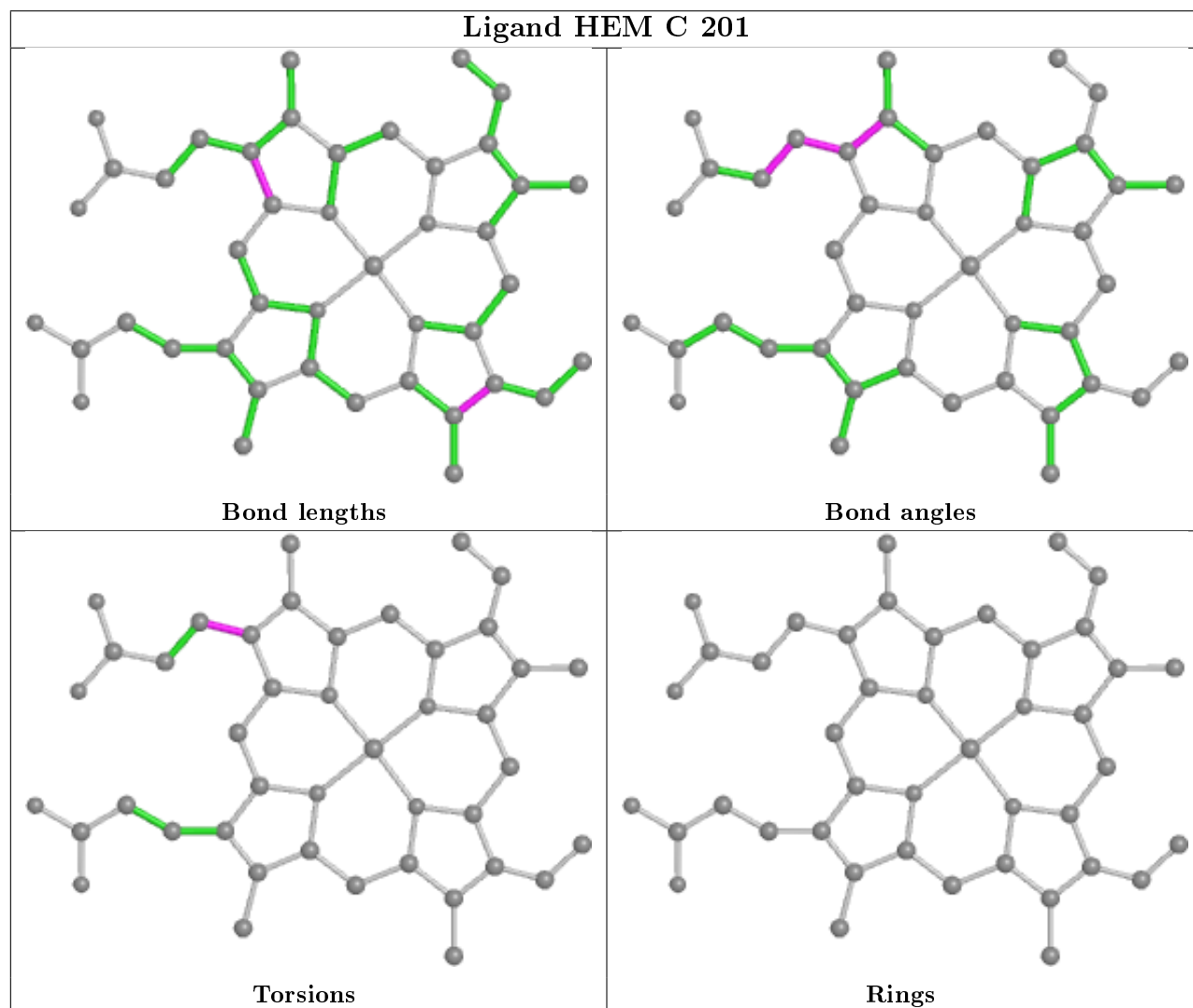
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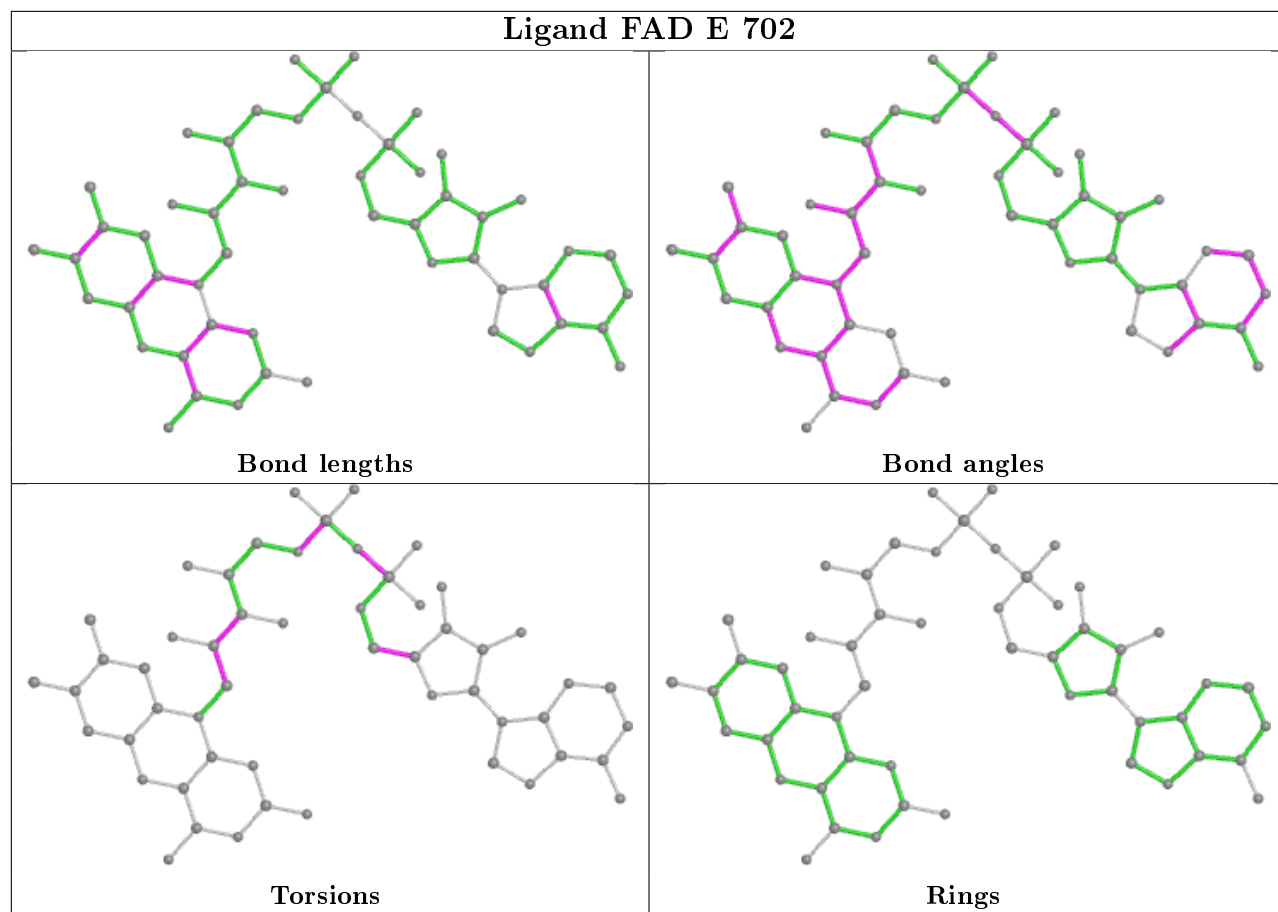


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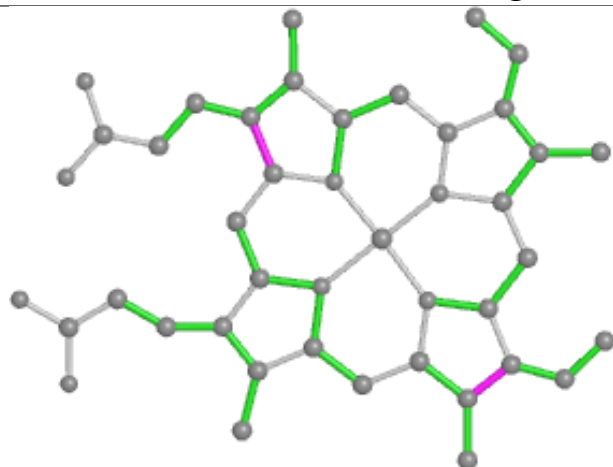
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	FAD	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

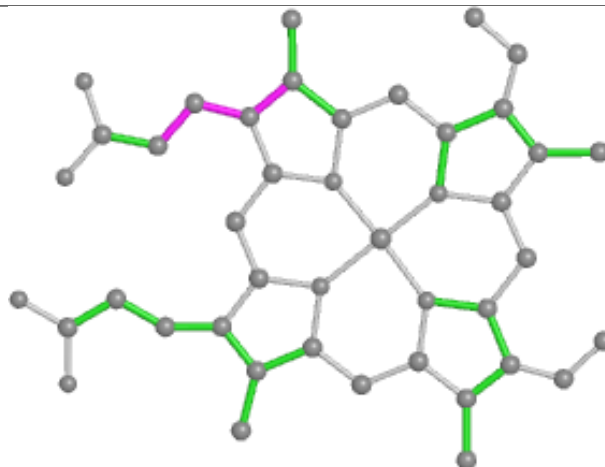




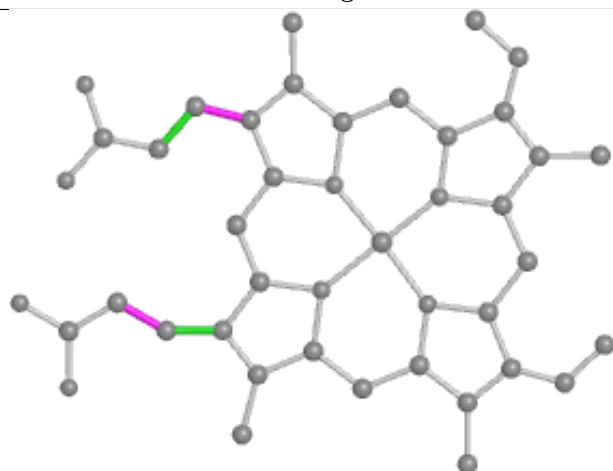
## Ligand HEM G 201



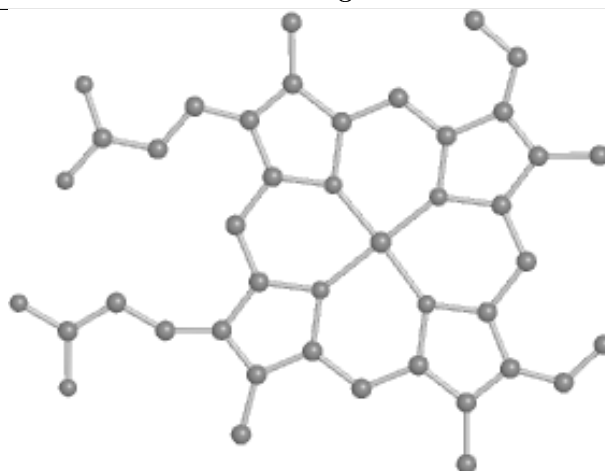
Bond lengths



Bond angles

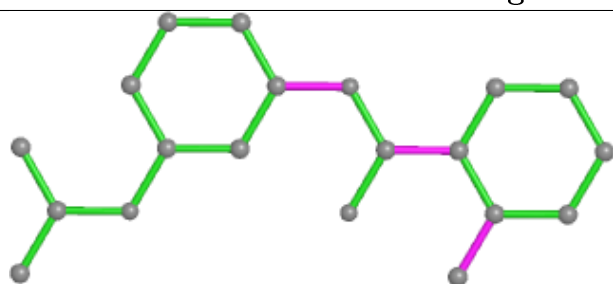


Torsions

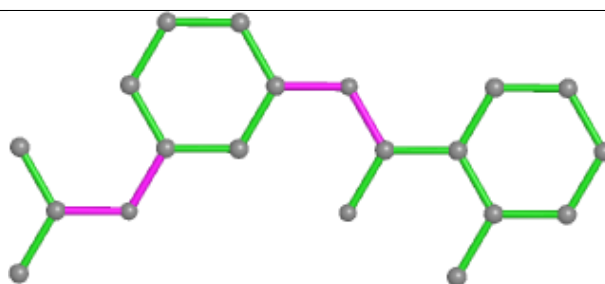


Rings

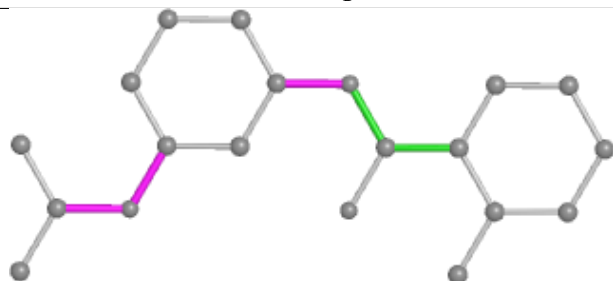
## Ligand MRN C 202



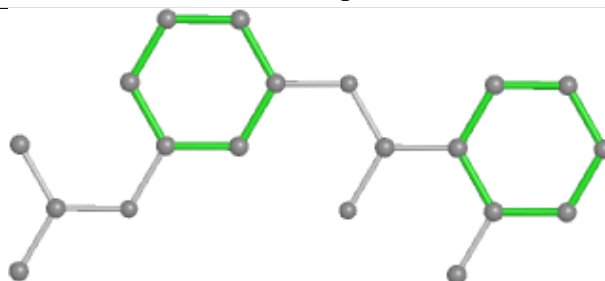
Bond lengths



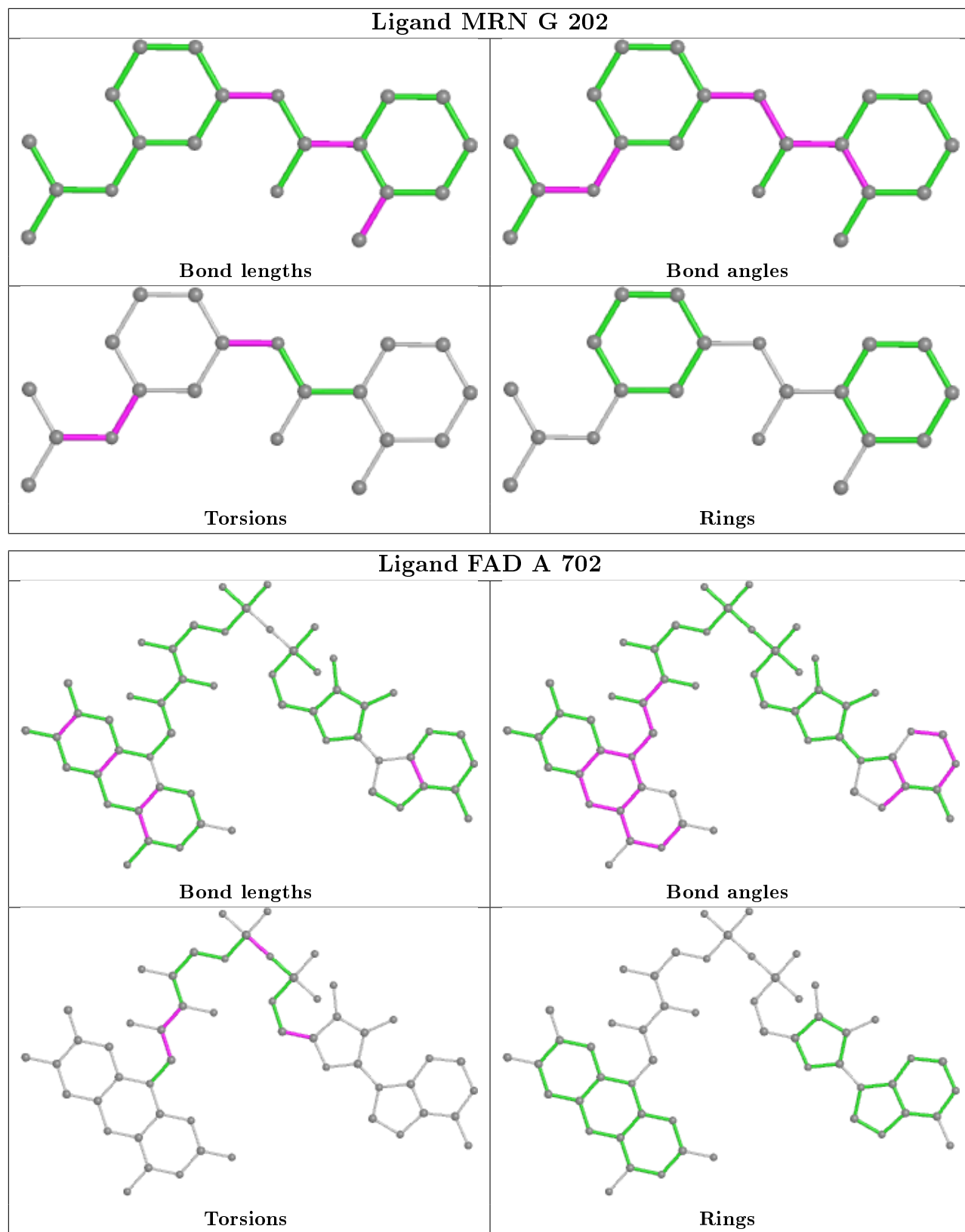
Bond angles



Torsions



Rings



## 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, 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%)	-0.68	1 (0%) 95 92	29, 50, 76, 96	1 (0%)
1	E	616/645 (95%)	-0.64	1 (0%) 95 92	30, 59, 85, 119	1 (0%)
2	B	250/282 (88%)	-0.64	1 (0%) 92 88	30, 53, 87, 115	0
2	F	250/282 (88%)	-0.70	0 100 100	30, 51, 75, 100	0
3	C	153/188 (81%)	-0.54	0 100 100	44, 61, 106, 126	0
3	G	150/188 (79%)	-0.43	4 (2%) 54 40	42, 67, 133, 161	0
4	D	129/156 (82%)	-0.58	0 100 100	44, 64, 90, 125	0
4	H	129/156 (82%)	-0.44	1 (0%) 86 77	45, 70, 112, 135	0
All	All	2293/2542 (90%)	-0.62	8 (0%) 94 90	29, 57, 91, 161	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	LYS	3.3
3	G	114	TRP	3.3
1	E	31	ASN	2.9
4	H	51	PRO	2.2
3	G	182	ALA	2.1
3	G	183	THR	2.1
3	G	181	LYS	2.0
1	A	30	SER	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 ⓘ

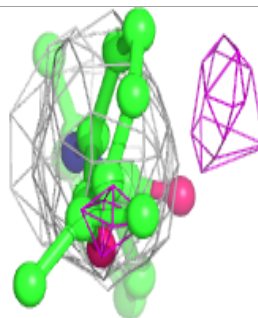
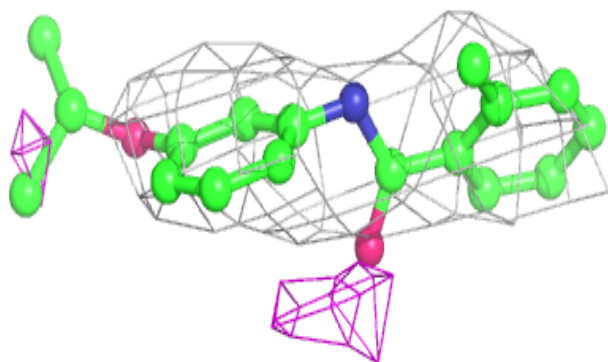
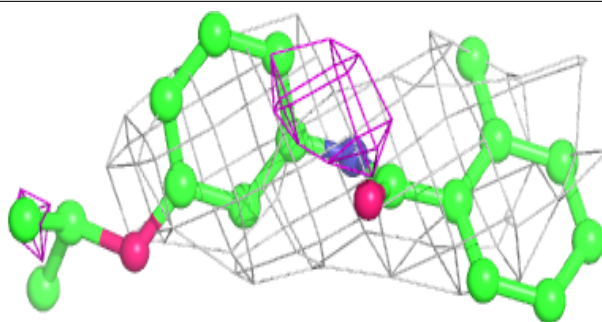
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	MRN	G	202	20/20	0.88	0.33	83,90,127,129	0
11	MRN	C	202	20/20	0.91	0.32	62,68,83,83	0
10	HEM	C	201	43/43	0.94	0.22	66,72,76,78	0
10	HEM	G	201	43/43	0.95	0.20	69,75,77,78	0
6	FAD	E	702	53/53	0.96	0.15	33,35,39,40	0
5	MLI	E	701	7/7	0.97	0.12	48,49,50,51	0
6	FAD	A	702	53/53	0.97	0.13	24,26,29,30	0
5	MLI	A	701	7/7	0.98	0.12	41,43,46,46	0
9	F3S	F	303	7/7	0.99	0.12	38,41,45,47	0
7	FES	B	301	4/4	0.99	0.09	22,22,23,23	0
9	F3S	B	303	7/7	0.99	0.13	39,41,45,46	0
8	SF4	F	302	8/8	1.00	0.10	28,28,29,29	0
8	SF4	B	302	8/8	1.00	0.10	26,27,27,28	0
7	FES	F	301	4/4	1.00	0.07	29,29,30,31	0

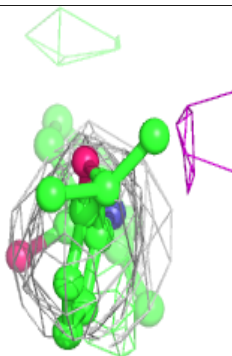
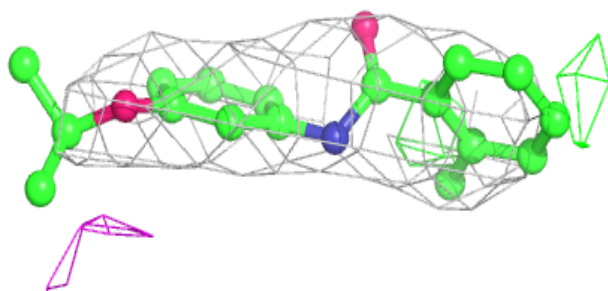
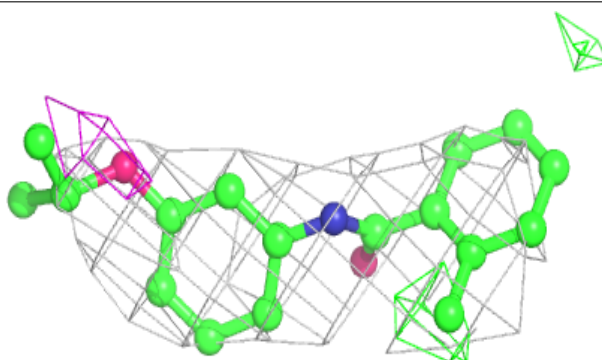
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around MRN G 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MRN C 202:**

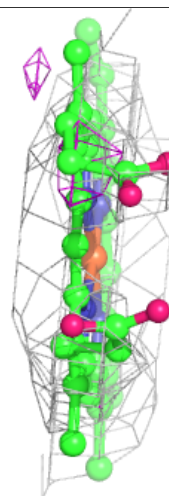
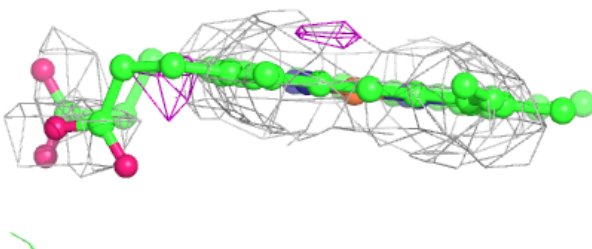
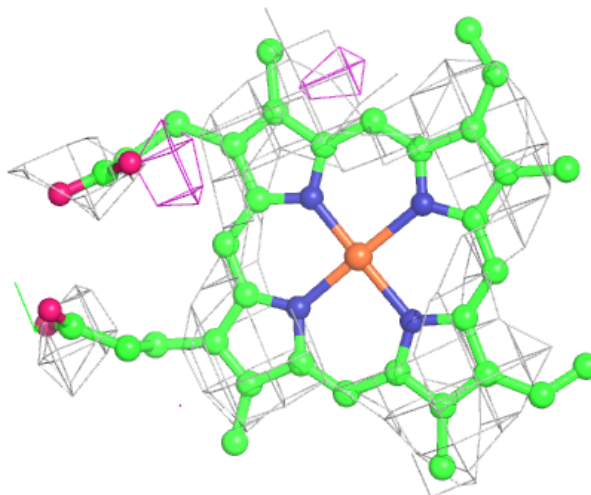
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





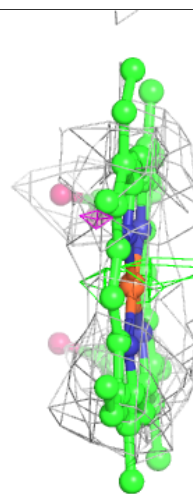
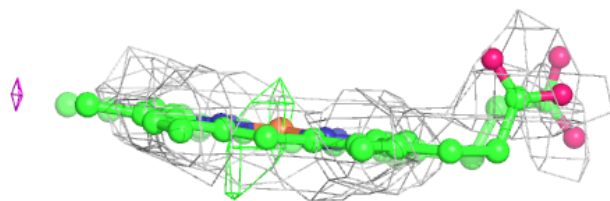
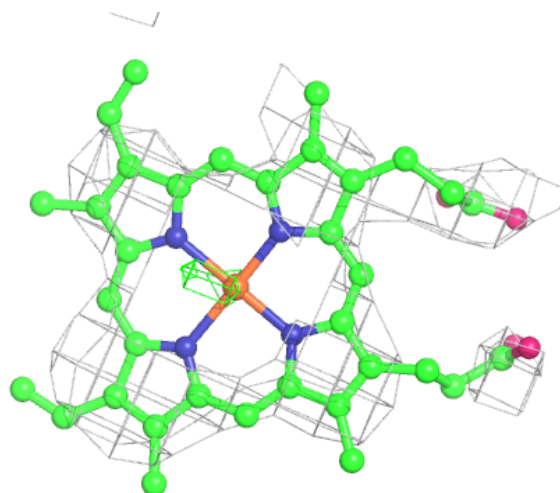
**Electron density around HEM C 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



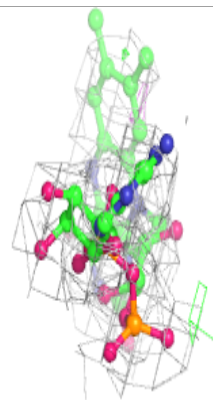
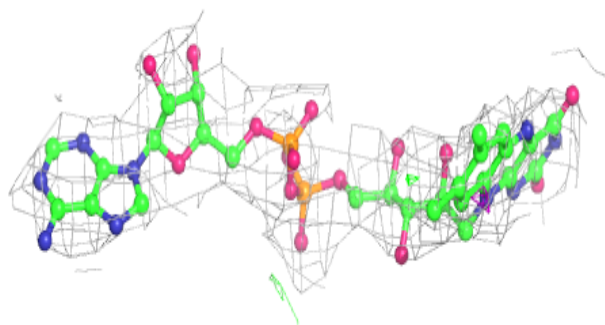
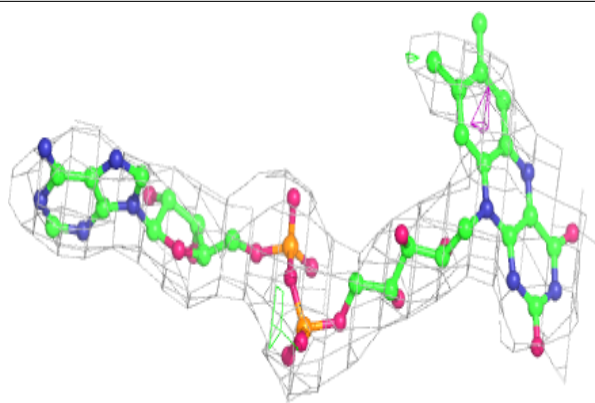
**Electron density around HEM G 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

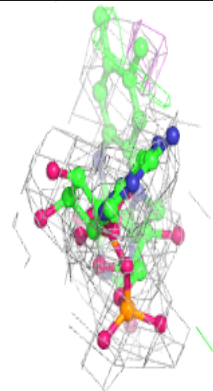
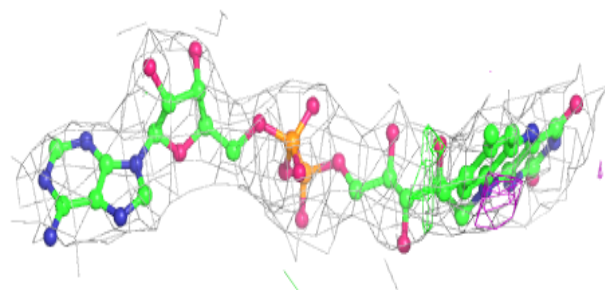
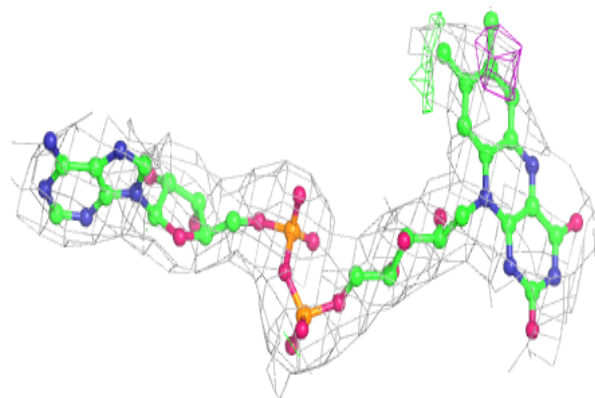


**Electron density around FAD E 702:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD A 702:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.