



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:04 am BST

PDB ID : 4YTN
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with N-[3-(pentafluorophenoxy)phenyl]-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 : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

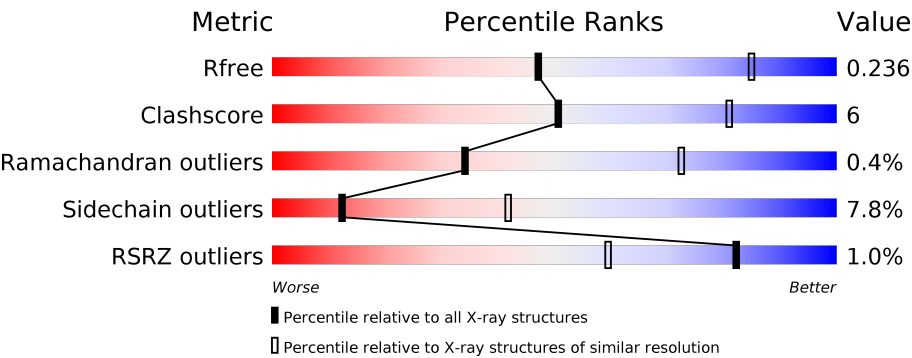
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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></div><div>76%19%••</div></div>
1	E	645	<div><div></div><div>78%17%••</div></div>
2	B	282	<div><div>2%</div><div>74%12%•11%</div></div>
2	F	282	<div><div></div><div>76%10%•11%</div></div>
3	C	188	<div><div>2%</div><div>66%13%•19%</div></div>
3	G	188	<div><div>4%</div><div>66%14%•19%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	156	<div> <div>%</div> <div> </div> <div>66% 15% 17%</div> </div>
4	H	156	<div> <div>3%</div> <div> </div> <div>65% 17% 17%</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	FD8	C	202	-	-	-	X
11	FD8	F	304	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18320 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Succinate dehydrogenase flavoprotein.

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

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

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

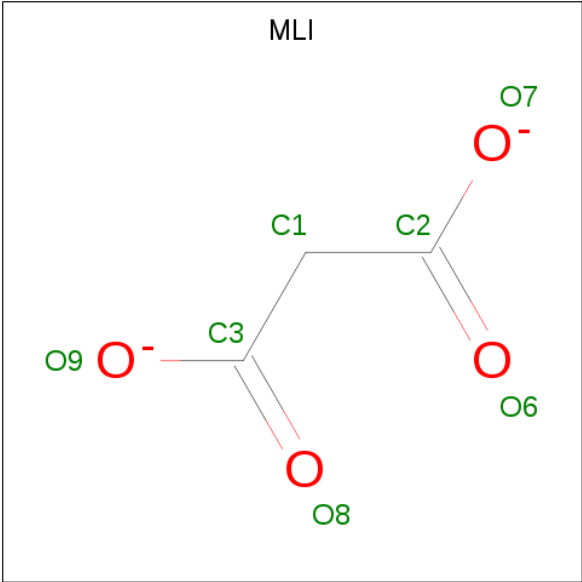
- Molecule 3 is a protein called Cytochrome b-large subunit.

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

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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	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: $C_{27}H_{33}N_9O_{15}P_2$).



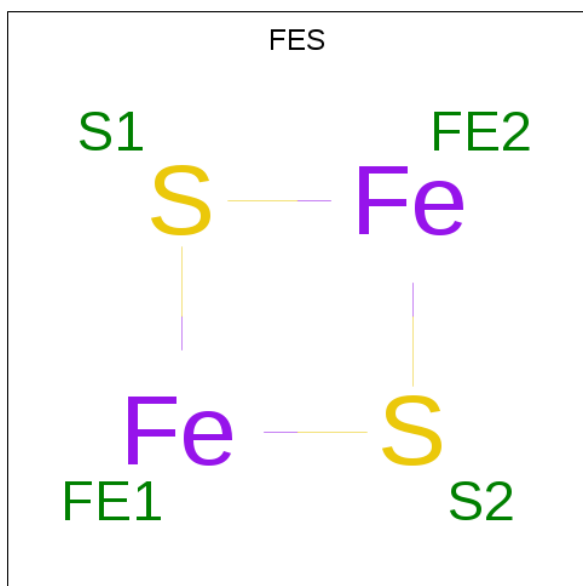
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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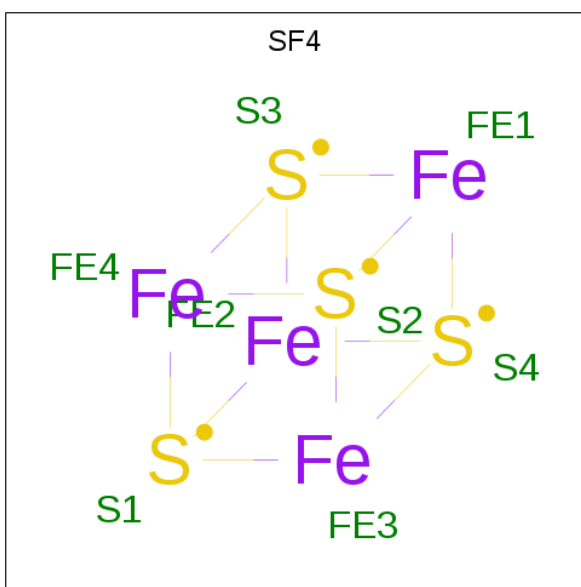
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



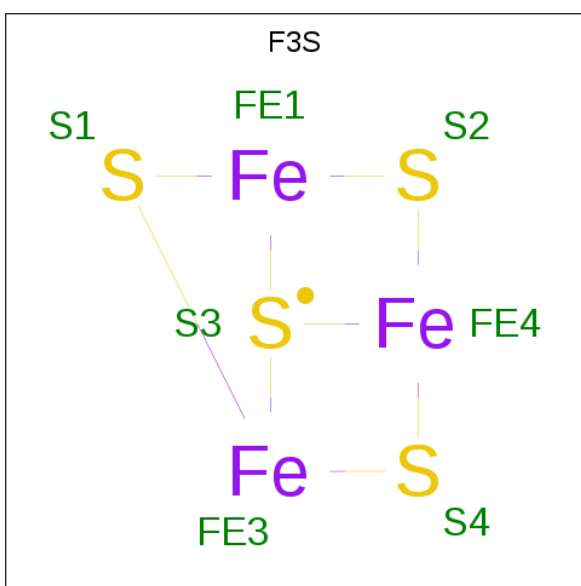
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

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



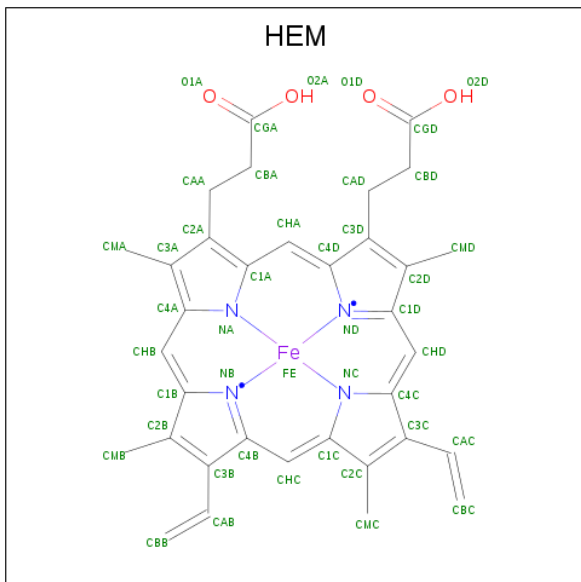
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



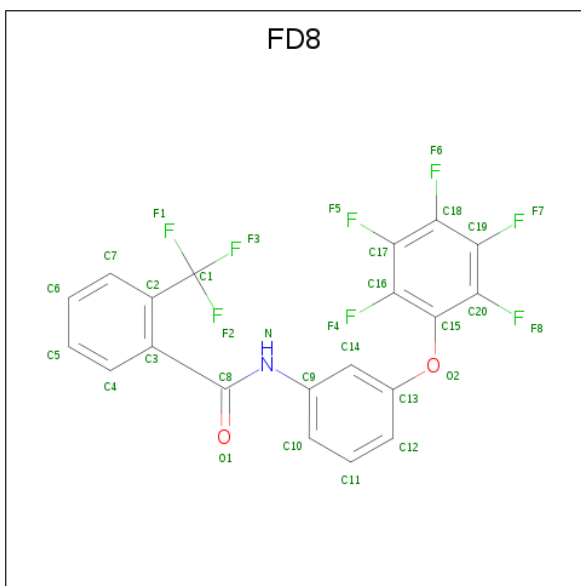
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

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



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

- Molecule 11 is N-[3-(pentafluorophenoxy)phenyl]-2-(trifluoromethyl)benzamide (three-letter code: FD8) (formula: $C_{20}H_9F_8NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	0	0
			31	20	8	1	2		
11	F	1	Total	C	F	N	O	0	0
			31	20	8	1	2		

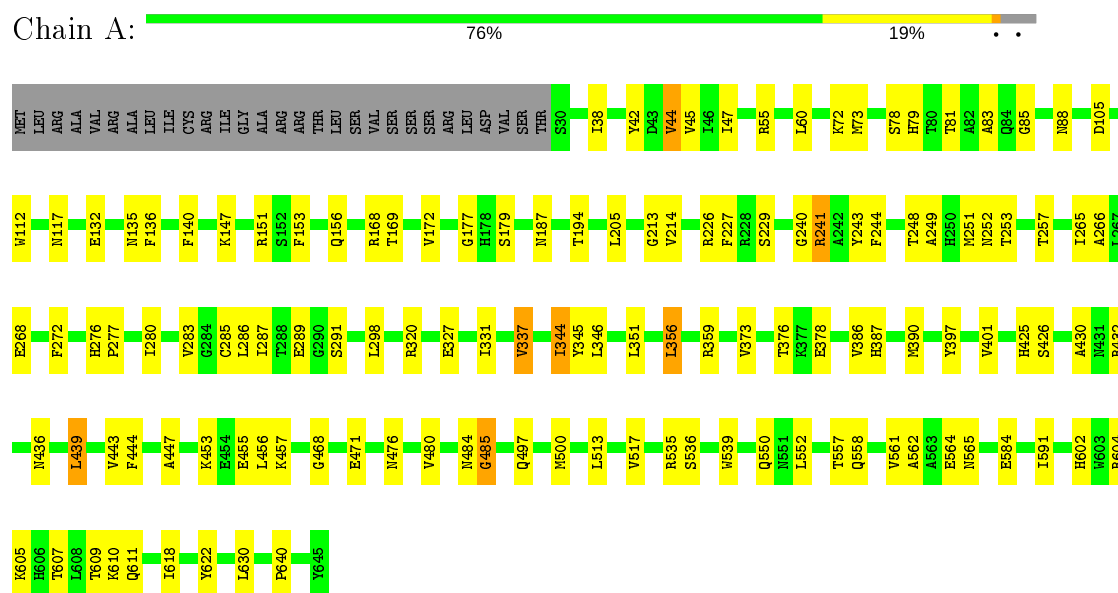
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	17	Total	O	0	0
			17	17		
12	B	4	Total	O	0	0
			4	4		
12	C	4	Total	O	0	0
			4	4		
12	D	2	Total	O	0	0
			2	2		
12	E	12	Total	O	0	0
			12	12		
12	H	1	Total	O	0	0
			1	1		

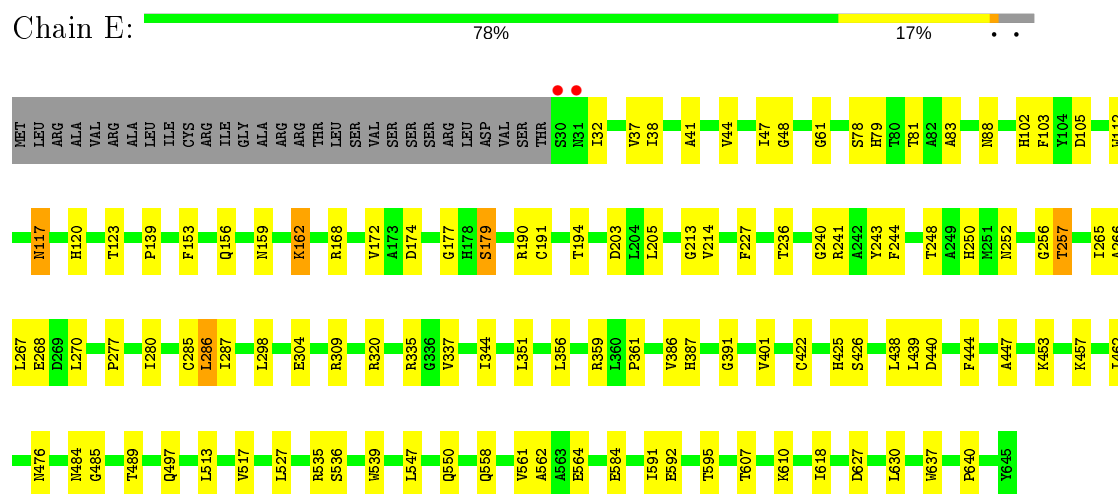
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

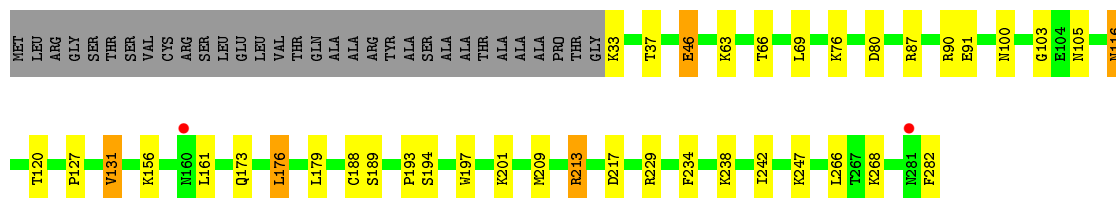
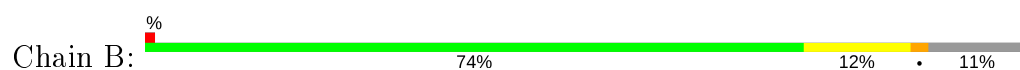
- Molecule 1: Succinate dehydrogenase flavoprotein



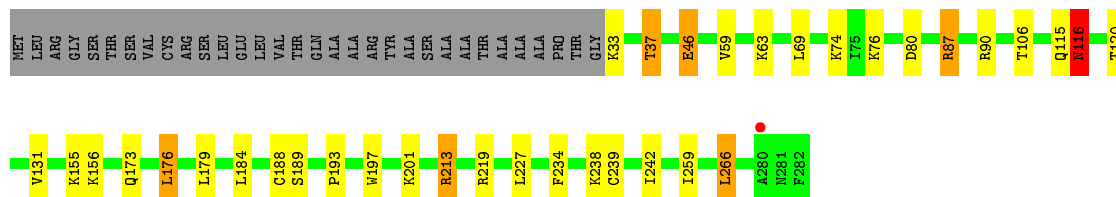
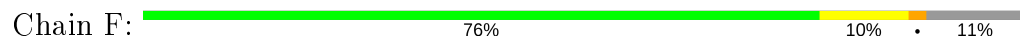
- Molecule 1: Succinate dehydrogenase flavoprotein



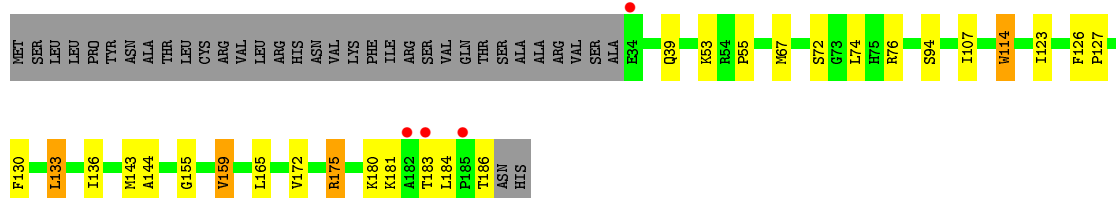
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



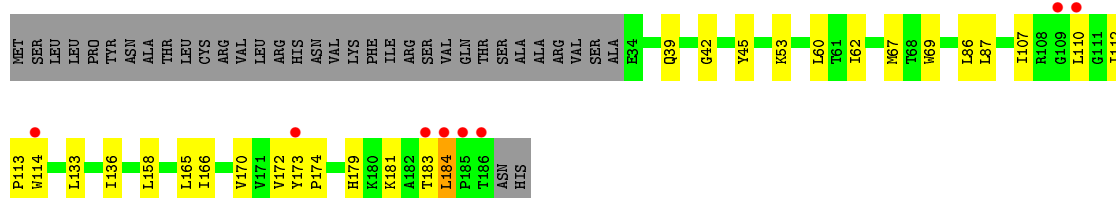
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Cytochrome b-large subunit



- Molecule 3: Cytochrome b-large subunit

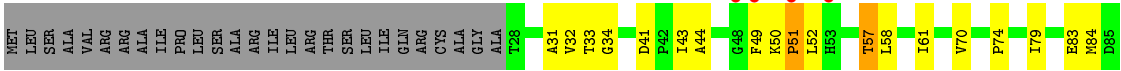


- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.61Å 125.48Å 219.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-3.00) 93.9 (19.99-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.190 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	3264 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18320	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, F3S, FES, FD8, 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	0.35	0/4889	0.60	0/6605
1	E	0.36	0/4889	0.60	0/6605
2	B	0.38	0/2029	0.59	0/2739
2	F	0.36	0/2029	0.56	0/2739
3	C	0.34	0/1255	0.52	0/1709
3	G	0.36	0/1255	0.53	0/1709
4	D	0.37	0/1030	0.53	0/1406
4	H	0.35	0/1030	0.51	0/1406
All	All	0.36	0/18406	0.58	0/24918

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	76	0
1	E	4787	0	4720	59	0
2	B	1985	0	2001	18	0
2	F	1985	0	2001	17	0
3	C	1217	0	1265	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1217	0	1265	12	0
4	D	998	0	985	14	0
4	H	998	0	985	15	0
5	A	7	0	2	1	0
5	E	7	0	2	1	0
6	A	53	0	31	11	0
6	E	53	0	31	5	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	2	0
10	G	43	0	30	3	0
11	C	31	0	9	2	0
11	F	31	0	9	1	0
12	A	17	0	0	0	0
12	B	4	0	0	1	0
12	C	4	0	0	0	0
12	D	2	0	0	0	0
12	E	12	0	0	0	0
12	H	1	0	0	0	0
All	All	18320	0	18086	207	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 6.

All (207) 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	1.49	1.27
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.53	0.90
1:A:79:HIS:NE2	6:A:702:FAD:HM81	1.87	0.89
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.12	0.84
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.40	0.84
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.40	0.83
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.28	0.80
1:A:135:ASN:ND2	2:B:161:LEU:O	2.21	0.73
1:A:425:HIS:N	1:A:426:SER:HA	2.05	0.72
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.74	0.68
1:A:79:HIS:CE1	6:A:702:FAD:C8M	2.77	0.68
1:A:78:SER:O	1:A:81:THR:HG22	1.95	0.67
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.77	0.67
2:F:116:ASN:C	2:F:116:ASN:HD22	1.99	0.65
4:D:104:VAL:HG13	4:D:121:VAL:HG12	1.81	0.63
1:A:47:ILE:HD11	1:A:214:VAL:HG21	1.81	0.63
1:A:265:ILE:HD13	1:A:401:VAL:HG11	1.80	0.62
1:E:277:PRO:CD	1:E:320:ARG:HG3	2.30	0.62
1:E:425:HIS:N	1:E:426:SER:HA	2.14	0.62
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.29	0.62
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.81	0.61
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.83	0.61
2:B:179:LEU:HD23	2:B:213:ARG:HA	1.83	0.60
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.50	0.59
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.85	0.59
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.38	0.58
1:A:484:ASN:O	1:A:485:GLY:O	2.22	0.57
1:E:61:GLY:HA3	1:E:191:CYS:HB2	1.86	0.57
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.87	0.57
1:A:83:ALA:HA	6:A:702:FAD:C6	2.35	0.56
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.87	0.55
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.88	0.55
1:E:277:PRO:HD3	1:E:320:ARG:HG3	1.88	0.55
1:A:240:GLY:HA3	1:A:248:THR:HG21	1.88	0.55
3:C:74:LEU:HD23	3:C:130:PHE:CE1	2.41	0.55
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.19	0.54
1:E:240:GLY:HA3	1:E:248:THR:HG21	1.89	0.54
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.89	0.54
3:C:107:ILE:HD11	4:D:156:LEU:CD1	2.33	0.54
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.43	0.54
1:E:103:PHE:HA	1:E:123:THR:HG21	1.90	0.54
2:F:37:THR:HG23	2:F:120:THR:HG22	1.90	0.53
1:A:291:SER:OG	1:A:346:LEU:HD21	2.09	0.53
4:H:41:ASP:OD2	4:H:44:ALA:HB2	2.08	0.53
1:E:102:HIS:ND1	1:E:123:THR:HG22	2.23	0.53
3:C:126:PHE:HB3	3:C:127:PRO:HD3	1.91	0.52
3:C:114:TRP:HB2	3:C:175:ARG:NH1	2.25	0.52
10:C:201:HEM:HHD	10:C:201:HEM:HBC2	1.91	0.52
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.91	0.52
3:C:76:ARG:NH1	11:C:202:FD8:F2	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.92	0.52
1:A:42:TYR:O	1:A:229:SER:HA	2.10	0.52
2:F:155:LYS:NZ	2:F:219:ARG:O	2.43	0.52
1:E:267:LEU:HD12	1:E:270:LEU:HD11	1.92	0.52
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.44	0.52
1:A:476:ASN:O	1:A:480:VAL:HG23	2.10	0.52
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.91	0.52
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.92	0.52
1:E:244:PHE:HA	1:E:497:GLN:HB3	1.92	0.52
1:E:286:LEU:HD13	1:E:387:HIS:CE1	2.45	0.52
1:E:47:ILE:HD11	1:E:214:VAL:CG2	2.40	0.52
1:E:78:SER:O	1:E:81:THR:HG22	2.09	0.52
4:D:59:PHE:O	4:D:63:ARG:HG2	2.11	0.51
1:E:47:ILE:HD11	1:E:214:VAL:HG21	1.92	0.51
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.93	0.51
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.24	0.51
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.91	0.51
1:E:213:GLY:HA3	1:E:227:PHE:O	2.11	0.50
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.46	0.50
1:E:37:VAL:HB	4:H:31:ALA:HB2	1.93	0.50
10:G:201:HEM:HH1	10:G:201:HEM:HBC2	1.93	0.50
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.92	0.50
1:E:536:SER:HB2	2:F:46:GLU:OE1	2.11	0.50
2:B:76:LYS:HA	2:B:80:ASP:O	2.12	0.50
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.94	0.49
1:E:190:ARG:HG3	4:H:43:ILE:HD11	1.95	0.49
1:E:117:ASN:HD22	1:E:117:ASN:N	2.11	0.49
3:C:72:SER:OG	11:C:202:FD8:H6	2.13	0.49
1:A:327:GLU:OE2	1:A:344:ILE:HD11	2.13	0.49
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.94	0.49
1:A:565:ASN:ND2	1:A:622:TYR:OH	2.46	0.48
1:E:41:ALA:HB1	1:E:462:ILE:HD13	1.96	0.48
4:H:50:LYS:N	4:H:51:PRO:CD	2.76	0.48
1:A:286:LEU:HD22	6:A:702:FAD:HM73	1.95	0.48
1:E:266:ALA:HB2	1:E:610:LYS:HG2	1.94	0.48
4:H:57:THR:O	4:H:61:ILE:HG23	2.12	0.48
2:F:239:CYS:SG	2:F:259:ILE:HG21	2.53	0.48
2:B:193:PRO:HD2	2:B:242:ILE:HD13	1.94	0.48
1:E:476:ASN:ND2	1:E:550:GLN:HE22	2.11	0.48
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.96	0.48
3:G:184:LEU:HD23	3:G:184:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ASP:OD2	1:E:168:ARG:NH2	2.47	0.47
1:A:55:ARG:NH1	1:A:132:GLU:OE2	2.43	0.47
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.48	0.47
1:A:286:LEU:HG	1:A:287:ILE:N	2.30	0.47
1:E:280:ILE:HD11	1:E:287:ILE:HD11	1.97	0.47
2:B:197:TRP:O	4:D:109:ARG:HD3	2.15	0.47
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.96	0.47
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.50	0.47
1:A:373:VAL:HG13	1:A:378:GLU:HB2	1.96	0.46
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.45	0.46
1:A:280:ILE:HD11	1:A:287:ILE:HD11	1.96	0.46
3:C:133:LEU:HB3	3:C:159:VAL:HG22	1.96	0.46
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.51	0.46
2:F:116:ASN:ND2	2:F:116:ASN:C	2.66	0.46
2:B:209:MET:HE2	12:B:403:HOH:O	2.14	0.46
2:B:100:ASN:HD21	2:B:103:GLY:CA	2.29	0.46
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.98	0.45
1:A:591:ILE:H	1:A:591:ILE:HD12	1.81	0.45
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.51	0.45
1:A:272:PHE:CD2	1:A:430:ALA:HA	2.51	0.45
3:G:86:LEU:CD1	4:H:92:LEU:HD23	2.47	0.45
1:A:280:ILE:HD12	1:A:285:CYS:HB2	1.97	0.45
1:A:356:LEU:HD23	1:A:376:THR:HG22	1.99	0.45
1:E:48:GLY:HA2	6:E:702:FAD:H1B	1.99	0.45
1:A:517:VAL:HG13	1:A:561:VAL:HG12	1.98	0.45
4:D:50:LYS:N	4:D:51:PRO:HD2	2.32	0.45
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.17	0.45
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.99	0.45
1:A:253:THR:HA	1:A:552:LEU:HD21	1.98	0.45
2:B:116:ASN:C	2:B:116:ASN:HD22	2.21	0.45
3:C:184:LEU:HD23	3:C:184:LEU:N	2.31	0.45
1:E:117:ASN:H	1:E:117:ASN:HD22	1.64	0.44
11:F:304:FD8:H11	3:G:60:LEU:HD22	1.99	0.44
1:A:331:ILE:HD11	1:A:344:ILE:HG23	1.99	0.44
1:E:591:ILE:H	1:E:591:ILE:HD12	1.82	0.44
1:E:558:GLN:HA	1:E:618:ILE:HD13	1.98	0.44
1:A:468:GLY:O	1:A:471:GLU:HB2	2.17	0.44
1:A:88:ASN:ND2	1:A:169:THR:OG1	2.51	0.44
3:G:107:ILE:HD11	4:H:156:LEU:CD1	2.44	0.44
2:B:188:CYS:SG	2:B:189:SER:N	2.90	0.44
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH2	1:A:248:THR:O	2.51	0.44
1:A:286:LEU:CB	6:A:702:FAD:HM73	2.48	0.44
2:B:194:SER:OG	2:B:238:LYS:O	2.31	0.44
1:E:517:VAL:HG13	1:E:561:VAL:HG12	1.98	0.44
1:E:79:HIS:CD2	6:E:702:FAD:HM82	2.40	0.44
2:B:176:LEU:HD21	2:B:217:ASP:OD2	2.17	0.44
3:G:42:GLY:O	3:G:45:TYR:HB3	2.18	0.44
1:A:147:LYS:HG2	2:B:282:PHE:CE1	2.54	0.43
2:F:193:PRO:HD2	2:F:242:ILE:HD13	1.99	0.43
3:G:166:ILE:O	3:G:170:VAL:HG23	2.19	0.43
1:A:277:PRO:CD	1:A:320:ARG:HG3	2.49	0.43
4:D:50:LYS:N	4:D:51:PRO:CD	2.82	0.43
2:F:197:TRP:O	4:H:109:ARG:HD3	2.18	0.43
1:A:289:GLU:OE2	1:A:320:ARG:HD2	2.18	0.43
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.16	0.43
1:A:425:HIS:H	1:A:426:SER:HA	1.83	0.43
1:A:276:HIS:HB2	1:A:387:HIS:CB	2.48	0.43
1:A:79:HIS:HE1	6:A:702:FAD:HM82	1.77	0.43
1:E:280:ILE:HD12	1:E:285:CYS:HB2	2.00	0.43
1:E:438:LEU:HG	6:E:702:FAD:C2	2.49	0.43
3:C:180:LYS:O	3:C:184:LEU:HB3	2.19	0.43
1:A:73:MET:SD	1:A:251:MET:HG3	2.59	0.42
3:C:184:LEU:HD12	3:C:186:THR:CG2	2.49	0.42
1:E:304:GLU:OE2	1:E:309:ARG:HD3	2.18	0.42
2:B:234:PHE:CD1	2:B:238:LYS:HG3	2.54	0.42
1:E:159:ASN:O	1:E:162:LYS:HG2	2.19	0.42
1:E:250:HIS:HB3	2:F:87:ARG:NH1	2.34	0.42
4:D:72:LEU:HD21	4:D:88:LEU:HD23	2.01	0.42
1:A:244:PHE:HA	1:A:497:GLN:HB3	2.01	0.42
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.32	0.42
1:E:172:VAL:HG21	1:E:179:SER:HB3	2.01	0.42
2:F:227:LEU:HD22	2:F:266:LEU:HD13	2.01	0.42
2:F:59:VAL:HG13	2:F:74:LYS:HD3	2.01	0.42
1:A:249:ALA:HB3	1:A:252:ASN:ND2	2.35	0.42
1:A:268:GLU:HA	1:A:607:THR:O	2.19	0.42
1:E:120:HIS:HD2	1:E:630:LEU:H	1.66	0.42
1:A:72:LYS:HD3	6:A:702:FAD:C5A	2.50	0.42
2:B:131:VAL:HG22	3:C:55:PRO:HG2	2.02	0.42
2:B:229:ARG:NH1	4:D:46:GLU:OE1	2.53	0.42
1:E:102:HIS:CE1	1:E:123:THR:HG22	2.55	0.42
1:E:513:LEU:HD13	1:E:564:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:70:VAL:O	4:H:74:PRO:HD2	2.20	0.42
1:E:257:THR:HG22	1:E:267:LEU:HD22	2.01	0.41
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.51	0.41
1:A:47:ILE:HD11	1:A:214:VAL:HG22	2.02	0.41
3:C:143:MET:O	3:C:144:ALA:HB3	2.21	0.41
1:A:136:PHE:HB3	1:A:187:ASN:ND2	2.35	0.41
3:C:155:GLY:O	3:C:159:VAL:HB	2.20	0.41
3:C:94:SER:HA	4:D:138:TYR:CE1	2.56	0.41
1:E:172:VAL:HG21	1:E:179:SER:CB	2.51	0.41
3:G:173:TYR:HB3	3:G:174:PRO:HD3	2.01	0.41
1:A:213:GLY:HA3	1:A:227:PHE:O	2.20	0.41
2:F:76:LYS:HA	2:F:80:ASP:O	2.20	0.41
1:A:471:GLU:OE2	4:D:28:THR:HA	2.21	0.41
1:A:38:ILE:CG2	4:D:34:GLY:HA3	2.51	0.41
1:A:602:HIS:O	1:A:605:LYS:HE2	2.21	0.41
1:A:38:ILE:HG23	4:D:34:GLY:HA3	2.02	0.41
1:E:476:ASN:HD21	1:E:550:GLN:NE2	2.18	0.41
3:G:62:ILE:HD12	3:G:62:ILE:C	2.41	0.41
1:E:268:GLU:HA	1:E:607:THR:O	2.21	0.40
4:H:50:LYS:N	4:H:51:PRO:HD2	2.36	0.40
3:C:123:ILE:O	3:C:127:PRO:CD	2.69	0.40
1:E:627:ASP:HB3	1:E:637:TRP:CE3	2.55	0.40
2:F:188:CYS:SG	2:F:189:SER:N	2.94	0.40
1:A:558:GLN:HA	1:A:618:ILE:HD13	2.03	0.40
4:D:65:PHE:CE2	4:D:94:LEU:HD23	2.57	0.40
1:E:88:ASN:ND2	1:E:156:GLN:HE22	2.19	0.40
1:E:139:PRO:HB3	2:F:176:LEU:HD23	2.02	0.40
1:A:439:LEU:HD22	1:A:443:VAL:HG23	2.03	0.40
1:A:557:THR:OG1	1:A:611:GLN:NE2	2.50	0.40
1:A:397:TYR:CD1	1:A:630:LEU:HD21	2.56	0.40
1:A:85:GLY:O	1:A:151:ARG:NH2	2.53	0.40
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.54	0.40
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/645 (95%)	585 (95%)	27 (4%)	2 (0%)	41	76
1	E	614/645 (95%)	583 (95%)	29 (5%)	2 (0%)	41	76
2	B	248/282 (88%)	229 (92%)	19 (8%)	0	100	100
2	F	248/282 (88%)	235 (95%)	12 (5%)	1 (0%)	34	72
3	C	151/188 (80%)	146 (97%)	5 (3%)	0	100	100
3	G	151/188 (80%)	148 (98%)	2 (1%)	1 (1%)	22	60
4	D	127/156 (81%)	122 (96%)	4 (3%)	1 (1%)	19	57
4	H	127/156 (81%)	118 (93%)	7 (6%)	2 (2%)	9	40
All	All	2280/2542 (90%)	2166 (95%)	105 (5%)	9 (0%)	34	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY
3	G	113	PRO
4	D	51	PRO
1	E	485	GLY
1	A	604	ARG
2	F	116	ASN
4	H	51	PRO
4	H	49	PHE
1	E	391	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%)	473 (94%)	29 (6%)	20	55
1	E	502/527 (95%)	468 (93%)	34 (7%)	16	48
2	B	220/242 (91%)	201 (91%)	19 (9%)	10	37
2	F	220/242 (91%)	203 (92%)	17 (8%)	13	42
3	C	127/158 (80%)	116 (91%)	11 (9%)	10	37
3	G	127/158 (80%)	112 (88%)	15 (12%)	5	22
4	D	98/119 (82%)	86 (88%)	12 (12%)	5	21
4	H	98/119 (82%)	87 (89%)	11 (11%)	6	24
All	All	1894/2092 (90%)	1746 (92%)	148 (8%)	12	42

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	117	ASN
1	A	153	PHE
1	A	179	SER
1	A	194	THR
1	A	205	LEU
1	A	226	ARG
1	A	241	ARG
1	A	257	THR
1	A	283	VAL
1	A	298	LEU
1	A	337	VAL
1	A	344	ILE
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	390	MET
1	A	432	ARG
1	A	436	ASN
1	A	439	LEU
1	A	453	LYS
1	A	455	GLU
1	A	456	LEU
1	A	457	LYS
1	A	500	MET

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Mol	Chain	Res	Type
1	A	535	ARG
1	A	539	TRP
1	A	584	GLU
1	A	609	THR
2	B	33	LYS
2	B	37	THR
2	B	46	GLU
2	B	63	LYS
2	B	66	THR
2	B	69	LEU
2	B	87	ARG
2	B	90	ARG
2	B	91	GLU
2	B	116	ASN
2	B	120	THR
2	B	131	VAL
2	B	156	LYS
2	B	173	GLN
2	B	176	LEU
2	B	213	ARG
2	B	247	LYS
2	B	266	LEU
2	B	268	LYS
3	C	53	LYS
3	C	67	MET
3	C	114	TRP
3	C	133	LEU
3	C	136	ILE
3	C	159	VAL
3	C	165	LEU
3	C	172	VAL
3	C	175	ARG
3	C	181	LYS
3	C	183	THR
4	D	46	GLU
4	D	50	LYS
4	D	52	LEU
4	D	58	LEU
4	D	61	ILE
4	D	79	ILE
4	D	84	MET
4	D	86	LEU

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Mol	Chain	Res	Type
4	D	92	LEU
4	D	136	LEU
4	D	148	ARG
4	D	154	TRP
1	E	32	ILE
1	E	44	VAL
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	179	SER
1	E	194	THR
1	E	203	ASP
1	E	205	LEU
1	E	241	ARG
1	E	252	ASN
1	E	257	THR
1	E	286	LEU
1	E	298	LEU
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE
1	E	351	LEU
1	E	356	LEU
1	E	359	ARG
1	E	422	CYS
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	457	LYS
1	E	484	ASN
1	E	489	THR
1	E	527	LEU
1	E	535	ARG
1	E	539	TRP
1	E	547	LEU
1	E	584	GLU
1	E	592	GLU
1	E	595	THR
2	F	33	LYS
2	F	37	THR
2	F	46	GLU
2	F	63	LYS

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Mol	Chain	Res	Type
2	F	69	LEU
2	F	87	ARG
2	F	90	ARG
2	F	106	THR
2	F	115	GLN
2	F	116	ASN
2	F	131	VAL
2	F	156	LYS
2	F	173	GLN
2	F	176	LEU
2	F	184	LEU
2	F	213	ARG
2	F	266	LEU
3	G	53	LYS
3	G	67	MET
3	G	69	TRP
3	G	110	LEU
3	G	112	ILE
3	G	114	TRP
3	G	133	LEU
3	G	136	ILE
3	G	158	LEU
3	G	165	LEU
3	G	172	VAL
3	G	179	HIS
3	G	181	LYS
3	G	183	THR
3	G	184	LEU
4	H	32	VAL
4	H	33	THR
4	H	52	LEU
4	H	57	THR
4	H	58	LEU
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	117	LEU
4	H	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	252	ASN
1	A	349	HIS
1	A	355	GLN
1	A	436	ASN
1	A	451	ASN
1	A	476	ASN
1	A	484	ASN
1	A	497	GLN
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	145	GLN
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	349	HIS
1	E	355	GLN
1	E	389	ASN
1	E	436	ASN
1	E	451	ASN
1	E	484	ASN
1	E	497	GLN
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
2	F	231	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
7	FES	F	301	2	0,4,4	0.00	-	-		
11	FD8	C	202	-	33,33,33	1.88	6 (18%)	49,49,49	1.40	6 (12%)
9	F3S	B	303	2	0,9,9	0.00	-	-		
6	FAD	A	702	-	51,58,58	1.66	7 (13%)	60,89,89	2.15	14 (23%)
8	SF4	B	302	2	0,12,12	0.00	-	-		
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	-		
10	HEM	G	201	3,4	27,50,50	0.94	2 (7%)	17,82,82	1.68	2 (11%)
6	FAD	E	702	-	51,58,58	1.81	6 (11%)	60,89,89	2.28	19 (31%)
10	HEM	C	201	3,4	27,50,50	0.86	1 (3%)	17,82,82	1.36	3 (17%)
8	SF4	F	302	2	0,12,12	0.00	-	-		
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
7	FES	B	301	2	0,4,4	0.00	-	-		
11	FD8	F	304	-	33,33,33	1.88	7 (21%)	49,49,49	1.34	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	F	301	2	-	-	0/1/1/1
11	FD8	C	202	-	-	12/18/18/18	0/3/3/3
9	F3S	B	303	2	-	-	0/3/3/3
6	FAD	A	702	-	-	6/30/50/50	0/6/6/6
8	SF4	B	302	2	-	-	0/6/5/5
5	MLI	E	701	-	-	0/0/4/4	-
9	F3S	F	303	2	-	-	0/3/3/3
11	FD8	F	304	-	-	2/18/18/18	0/3/3/3
10	HEM	G	201	3,4	-	2/6/54/54	-
6	FAD	E	702	-	-	9/30/50/50	0/6/6/6
10	HEM	C	201	3,4	-	0/6/54/54	-
8	SF4	F	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/0/4/4	-
7	FES	B	301	2	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C4X-C10	9.10	1.47	1.38
6	A	702	FAD	C4X-C10	8.18	1.47	1.38
11	C	202	FD8	F7-C19	4.83	1.42	1.35
11	F	304	FD8	F4-C16	-4.64	1.27	1.35
11	C	202	FD8	C3-C8	-4.24	1.41	1.50
11	C	202	FD8	F6-C18	4.12	1.41	1.35
11	F	304	FD8	C3-C8	-4.07	1.41	1.50
6	E	702	FAD	C4-C4X	3.94	1.48	1.41
11	C	202	FD8	C1-C2	-3.90	1.42	1.50
11	F	304	FD8	F8-C20	3.86	1.41	1.35
6	E	702	FAD	C8-C7	3.54	1.49	1.40
6	E	702	FAD	C9A-C5X	3.49	1.49	1.42
11	F	304	FD8	F6-C18	3.45	1.40	1.35
6	A	702	FAD	C9A-C5X	3.44	1.49	1.42
11	C	202	FD8	C9-N	-3.41	1.34	1.41
11	F	304	FD8	C9-N	-3.33	1.34	1.41
11	F	304	FD8	F7-C19	3.14	1.39	1.35
6	A	702	FAD	C4-C4X	3.07	1.46	1.41
11	C	202	FD8	F5-C17	2.96	1.39	1.35
6	A	702	FAD	C9A-N10	2.92	1.42	1.38
11	F	304	FD8	C1-C2	-2.78	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	FAD	C8-C7	2.70	1.47	1.40
10	G	201	HEM	C4D-C3D	2.67	1.48	1.42
10	C	201	HEM	C3B-C2B	-2.57	1.36	1.40
10	G	201	HEM	C3B-C2B	-2.54	1.36	1.40
6	E	702	FAD	C9A-N10	2.30	1.41	1.38
6	E	702	FAD	C5A-C4A	2.19	1.46	1.40
6	A	702	FAD	C6-C5X	-2.12	1.38	1.41
6	A	702	FAD	C5A-C4A	2.05	1.46	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	C4-N3-C2	8.44	122.27	115.14
6	A	702	FAD	C4-N3-C2	7.36	121.35	115.14
6	A	702	FAD	C1'-N10-C9A	7.24	123.99	118.29
6	E	702	FAD	C1'-N10-C9A	6.57	123.47	118.29
6	E	702	FAD	C4-C4X-C10	-6.45	115.68	119.95
11	F	304	FD8	C13-O2-C15	6.25	128.53	118.48
10	G	201	HEM	CBD-CAD-C3D	5.54	122.68	112.48
11	C	202	FD8	C2-C3-C8	4.38	129.36	122.80
6	E	702	FAD	N3A-C2A-N1A	-4.36	121.87	128.68
6	A	702	FAD	N3A-C2A-N1A	-4.17	122.16	128.68
6	A	702	FAD	C8M-C8-C7	-4.16	112.20	120.74
6	A	702	FAD	C4X-N5-C5X	4.16	120.93	116.77
6	E	702	FAD	C4-C4X-N5	4.08	123.26	118.60
6	E	702	FAD	C4X-N5-C5X	3.99	120.75	116.77
6	A	702	FAD	C4X-C4-N3	-3.98	117.99	123.43
11	C	202	FD8	C1-C2-C3	3.95	127.43	121.97
6	A	702	FAD	C6-C5X-N5	-3.80	114.87	119.05
11	C	202	FD8	C13-O2-C15	3.58	124.24	118.48
6	E	702	FAD	C4X-C4-N3	-3.38	118.81	123.43
6	A	702	FAD	C4A-C5A-N7A	-3.00	106.27	109.40
6	E	702	FAD	C9A-N10-C10	-2.92	118.08	121.91
6	E	702	FAD	C4A-C5A-N7A	-2.87	106.41	109.40
6	E	702	FAD	C1'-C2'-C3'	2.77	117.52	109.79
6	A	702	FAD	C6-C5X-C9A	2.72	122.61	119.05
6	E	702	FAD	C5X-C9A-N10	2.62	119.61	117.72
6	A	702	FAD	C4'-C3'-C2'	-2.62	107.92	113.36
6	A	702	FAD	C2A-N1A-C6A	2.53	123.08	118.75
11	C	202	FD8	C4-C3-C8	-2.44	111.91	118.43
6	E	702	FAD	C1B-N9A-C4A	-2.41	122.40	126.64
10	C	201	HEM	CMA-C3A-C4A	-2.41	124.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	201	HEM	CAD-CBD-CGD	2.40	116.70	112.67
6	E	702	FAD	C8M-C8-C9	-2.37	114.67	120.34
6	A	702	FAD	O2'-C2'-C3'	-2.34	103.41	109.10
6	E	702	FAD	O2'-C2'-C3'	-2.31	103.49	109.10
11	F	304	FD8	C1-C2-C3	2.28	125.11	121.97
10	G	201	HEM	CAD-C3D-C2D	-2.25	120.78	127.25
6	A	702	FAD	C9A-N10-C10	-2.24	118.98	121.91
6	E	702	FAD	O2P-P-O1P	2.19	123.06	112.24
6	E	702	FAD	O3'-C3'-C2'	2.18	114.08	108.81
11	C	202	FD8	C7-C2-C1	-2.15	113.83	118.12
10	C	201	HEM	CBD-CAD-C3D	-2.14	108.54	112.48
11	C	202	FD8	C20-C15-C16	2.12	120.91	116.86
6	E	702	FAD	C4'-C3'-C2'	-2.11	108.98	113.36
6	A	702	FAD	C1'-C2'-C3'	2.10	115.65	109.79
6	E	702	FAD	C2A-N1A-C6A	2.09	122.32	118.75
6	E	702	FAD	C8M-C8-C7	2.06	124.95	120.74

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	O4'-C4'-C5'-O5'
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
6	E	702	FAD	O4'-C4'-C5'-O5'
11	F	304	FD8	C16-C15-O2-C13
11	C	202	FD8	C10-C9-N-C8
11	C	202	FD8	F3-C1-C2-C3
11	C	202	FD8	C14-C9-N-C8
11	C	202	FD8	F1-C1-C2-C3
11	C	202	FD8	F2-C1-C2-C3
11	F	304	FD8	C20-C15-O2-C13
6	E	702	FAD	PA-O3P-P-O5'
11	C	202	FD8	F3-C1-C2-C7
6	E	702	FAD	P-O3P-PA-O2A
11	C	202	FD8	F1-C1-C2-C7
11	C	202	FD8	F2-C1-C2-C7
11	C	202	FD8	C4-C3-C8-O1

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Mol	Chain	Res	Type	Atoms
6	A	702	FAD	PA-O3P-P-O5'
11	C	202	FD8	C20-C15-O2-C13
6	A	702	FAD	O4B-C4B-C5B-O5B
6	E	702	FAD	C5B-O5B-PA-O3P
6	E	702	FAD	O4B-C4B-C5B-O5B
6	A	702	FAD	P-O3P-PA-O1A
11	C	202	FD8	C16-C15-O2-C13
6	E	702	FAD	C5B-O5B-PA-O1A
11	C	202	FD8	C4-C3-C8-N
6	E	702	FAD	C1'-C2'-C3'-O3'

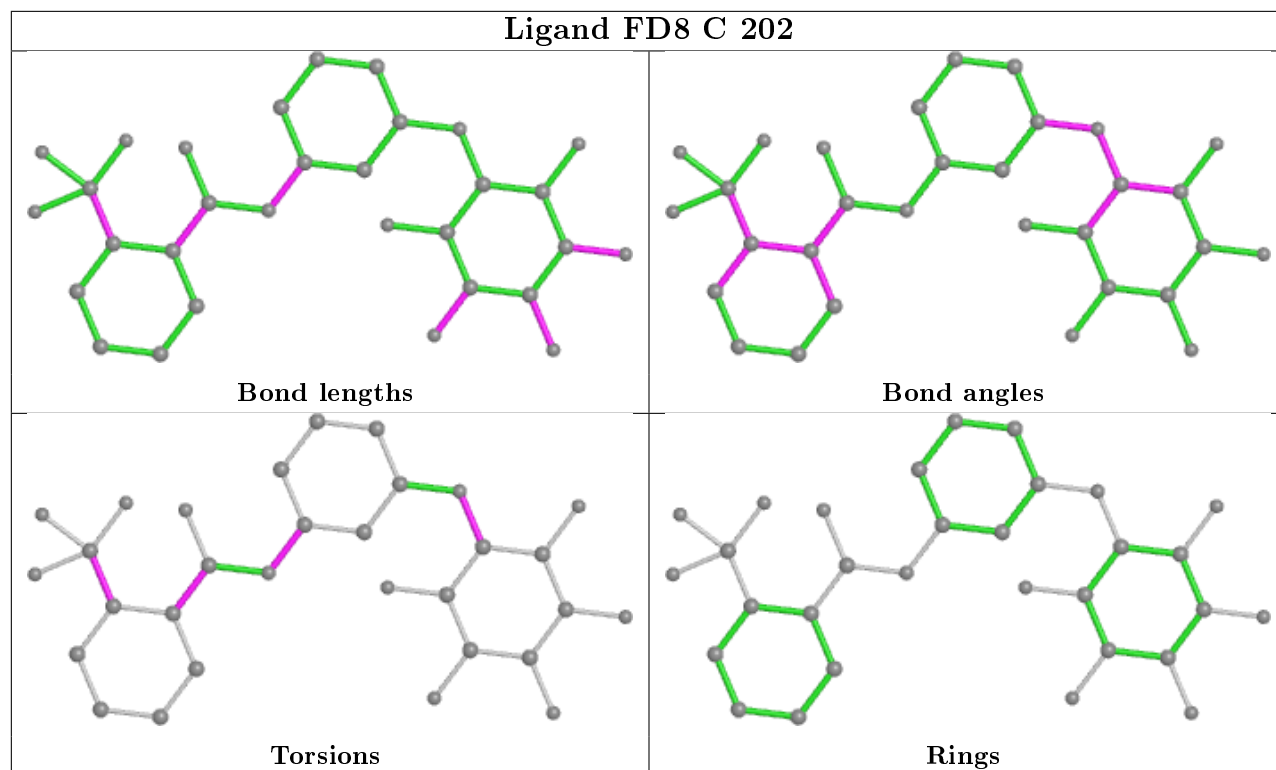
There are no ring outliers.

8 monomers are involved in 26 short contacts:

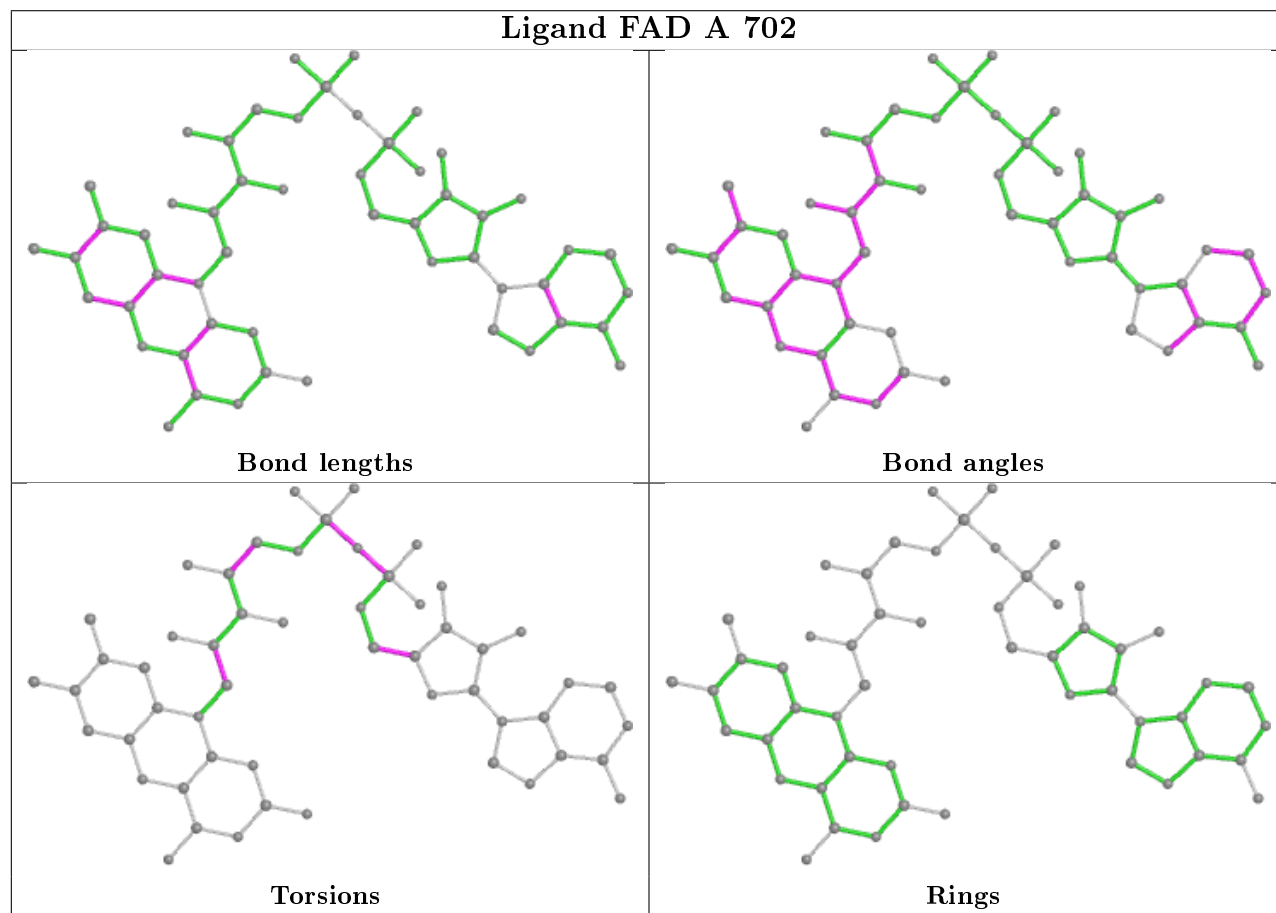
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	202	FD8	2	0
6	A	702	FAD	11	0
5	E	701	MLI	1	0
10	G	201	HEM	3	0
6	E	702	FAD	5	0
10	C	201	HEM	2	0
5	A	701	MLI	1	0
11	F	304	FD8	1	0

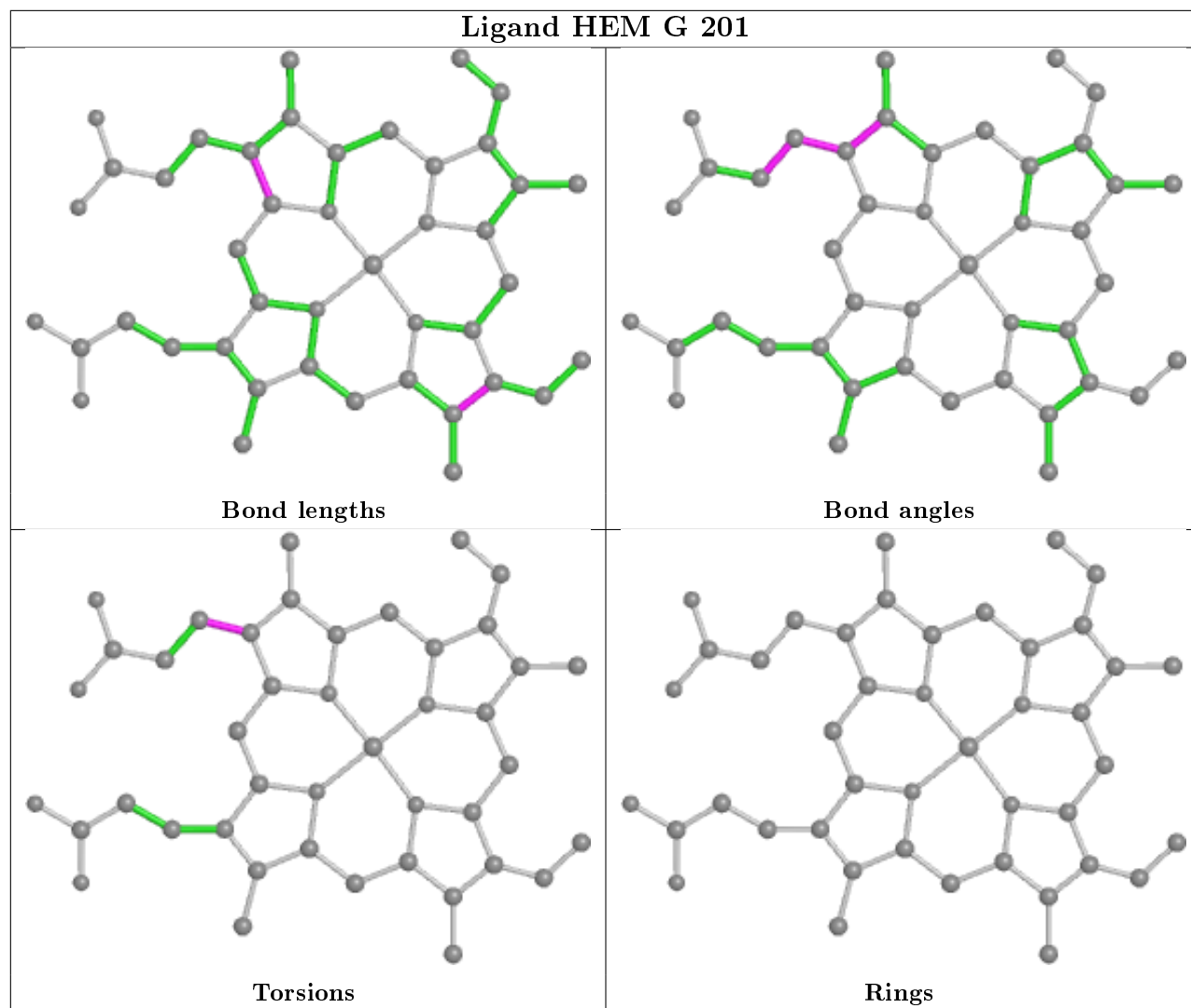
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

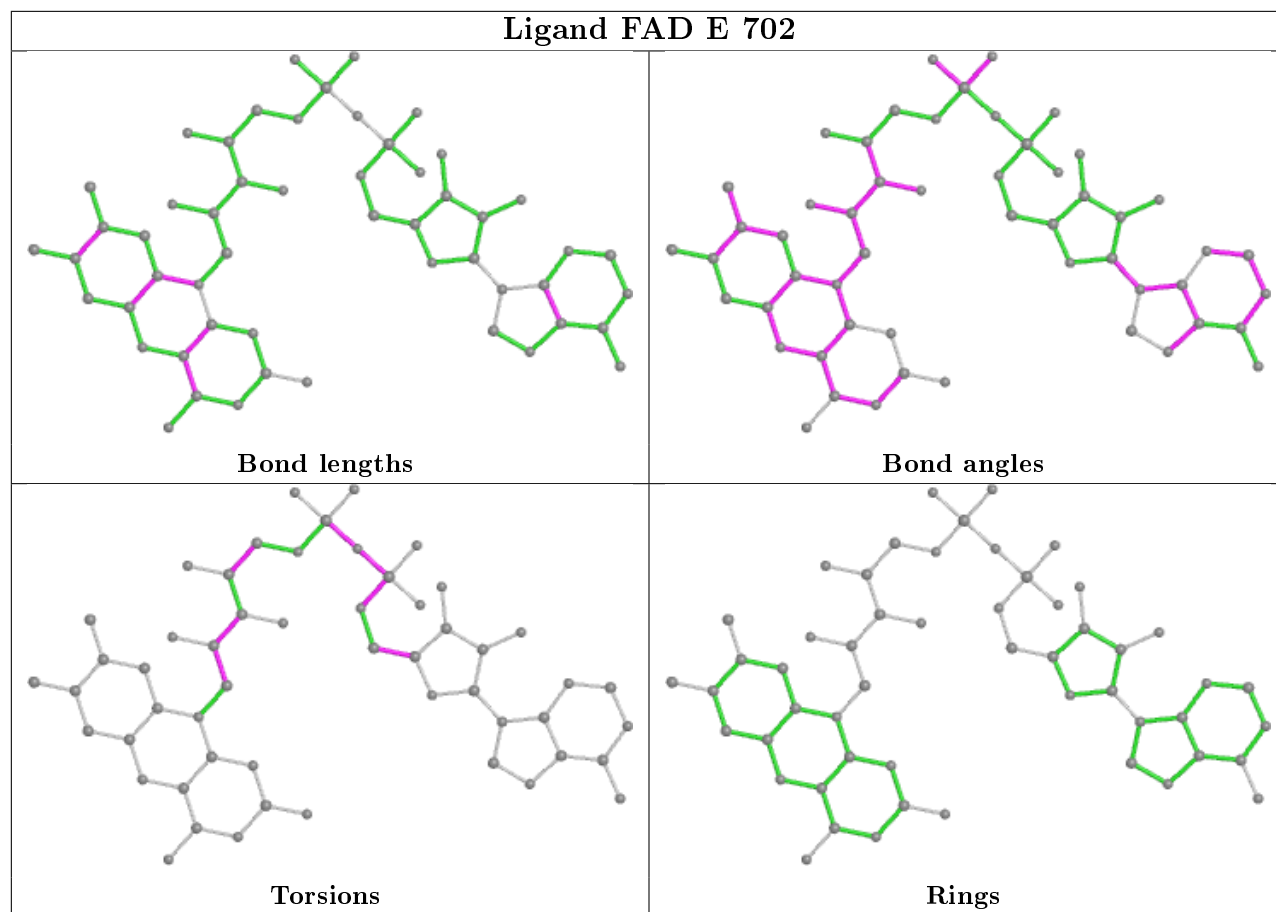
Ligand FD8 C 202

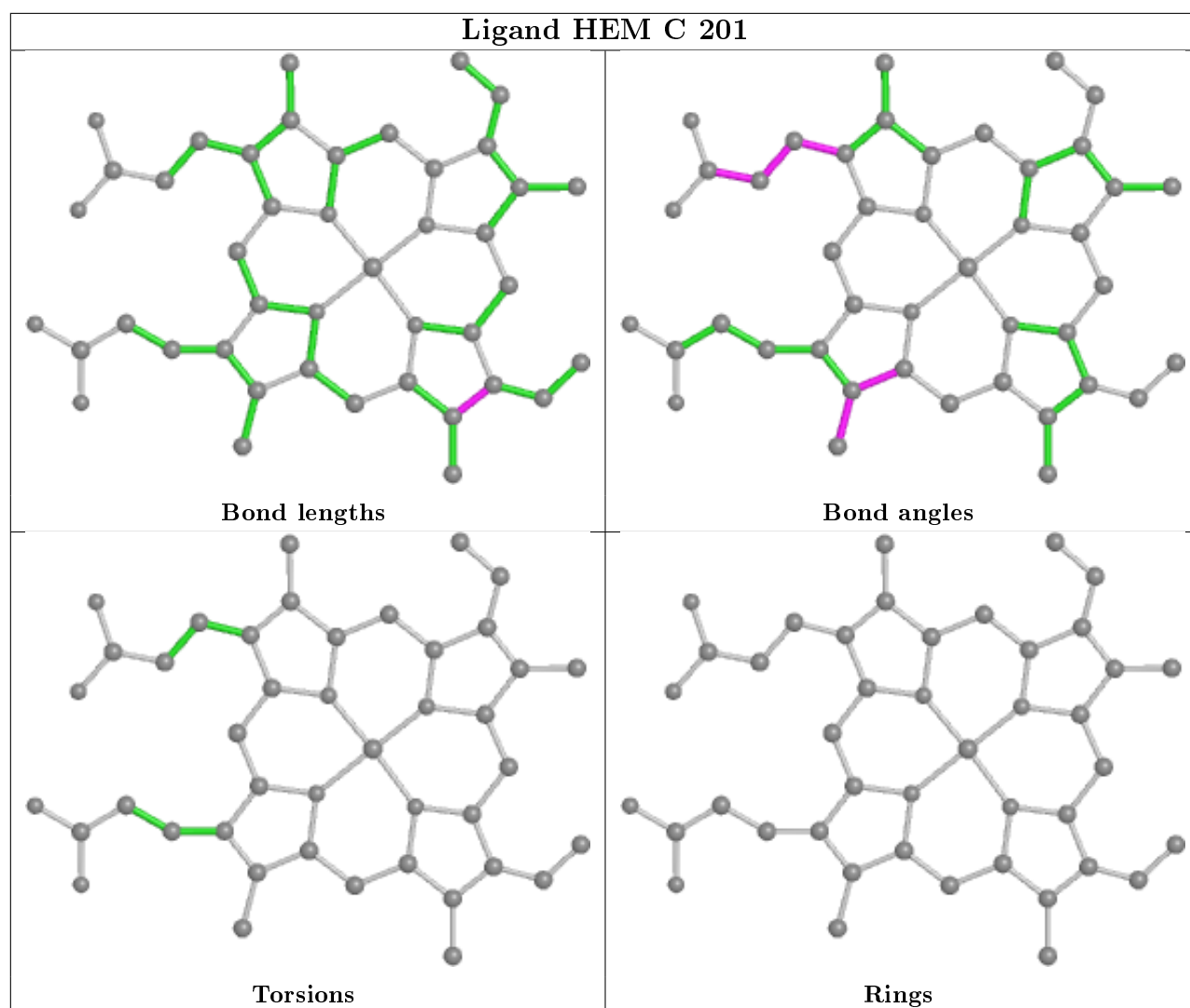


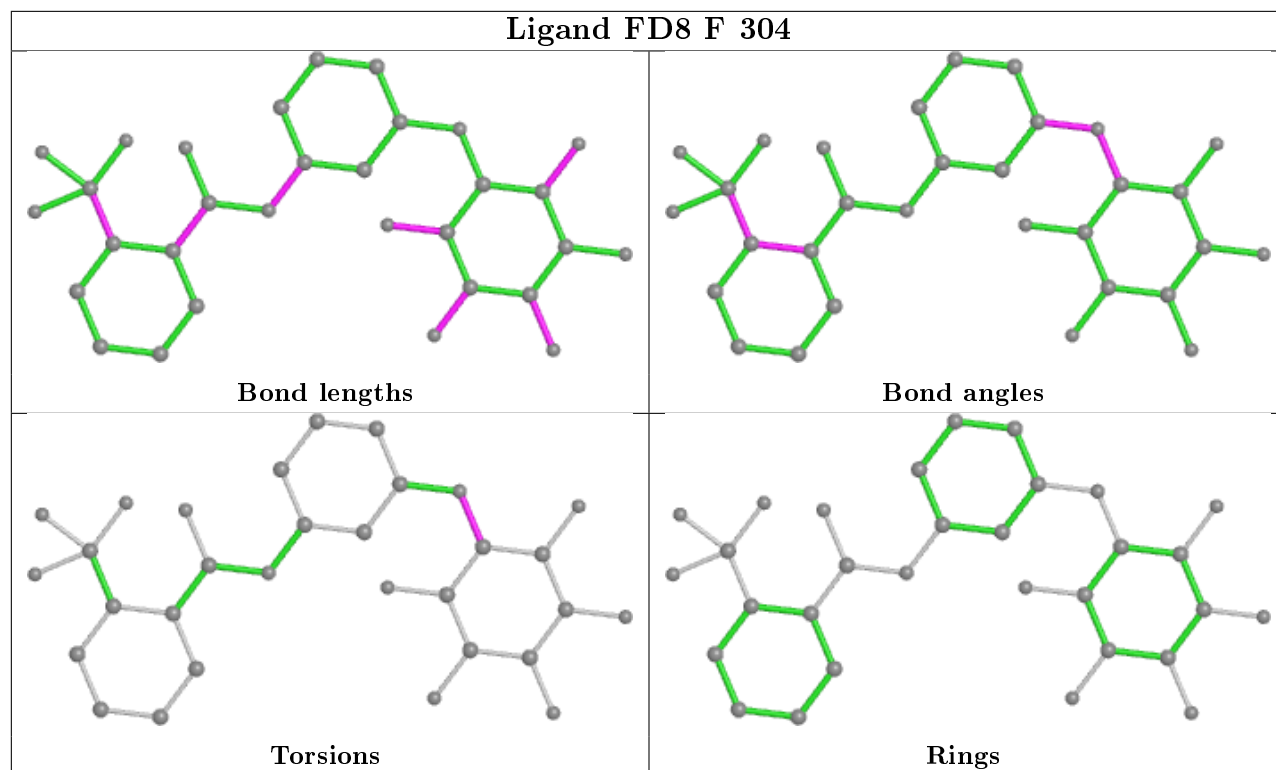
Ligand FAD A 702











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	616/645 (95%)	-0.57	0 100 100	34, 55, 81, 115	0
1	E	616/645 (95%)	-0.56	2 (0%) 94 84	38, 59, 85, 120	0
2	B	250/282 (88%)	-0.58	2 (0%) 86 65	39, 55, 81, 100	0
2	F	250/282 (88%)	-0.61	1 (0%) 92 79	39, 57, 82, 106	0
3	C	153/188 (81%)	-0.45	4 (2%) 56 27	40, 64, 106, 173	0
3	G	153/188 (81%)	-0.12	8 (5%) 27 10	51, 75, 142, 177	0
4	D	129/156 (82%)	-0.48	1 (0%) 86 65	54, 67, 106, 144	0
4	H	129/156 (82%)	-0.29	4 (3%) 49 21	56, 73, 123, 157	0
All	All	2296/2542 (90%)	-0.51	22 (0%) 82 59	34, 60, 98, 177	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	185	PRO	7.1
3	C	185	PRO	4.8
1	E	31	ASN	3.7
3	C	182	ALA	3.4
3	G	186	THR	3.4
3	G	184	LEU	3.1
1	E	30	SER	3.0
3	G	114	TRP	2.9
4	H	49	PHE	2.9
4	H	51	PRO	2.8
4	D	52	LEU	2.7
2	F	280	ALA	2.5
3	C	183	THR	2.5
3	G	173	TYR	2.4
2	B	281	ASN	2.4
3	C	34	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	H	48	GLY	2.3
3	G	183	THR	2.2
4	H	53	HIS	2.1
2	B	160	ASN	2.1
3	G	109	GLY	2.1
3	G	110	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

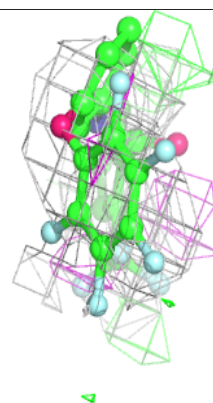
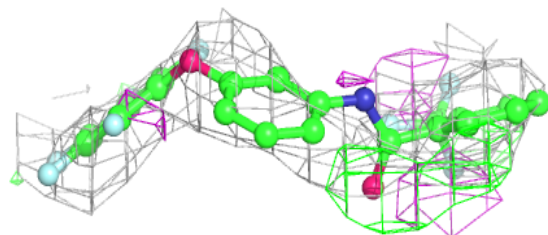
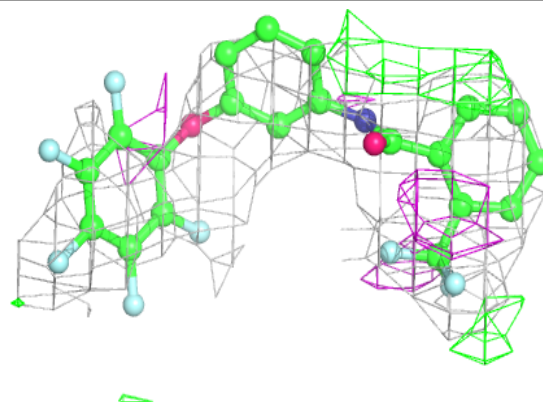
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	FD8	C	202	31/31	0.65	0.45	115,139,146,147	0
11	FD8	F	304	31/31	0.76	0.40	99,126,143,144	0
10	HEM	G	201	43/43	0.96	0.18	62,80,87,89	0
10	HEM	C	201	43/43	0.97	0.17	56,67,72,81	0
6	FAD	E	702	53/53	0.97	0.13	38,48,55,60	0
6	FAD	A	702	53/53	0.98	0.13	35,38,44,45	0
5	MLI	A	701	7/7	0.98	0.11	50,51,52,52	0
5	MLI	E	701	7/7	0.98	0.10	49,51,52,56	0
8	SF4	B	302	8/8	0.99	0.10	36,38,42,42	0
9	F3S	B	303	7/7	0.99	0.14	45,51,53,54	0
8	SF4	F	302	8/8	0.99	0.11	38,43,47,49	0
9	F3S	F	303	7/7	0.99	0.12	45,51,56,57	0
7	FES	B	301	4/4	0.99	0.09	33,36,36,41	0
7	FES	F	301	4/4	0.99	0.11	42,45,45,47	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.

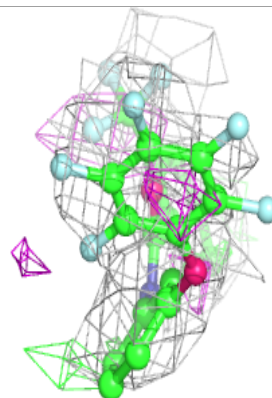
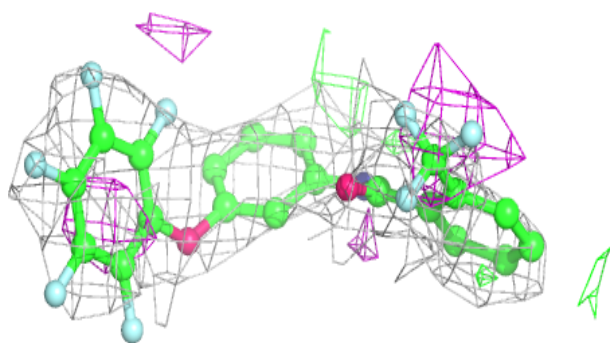
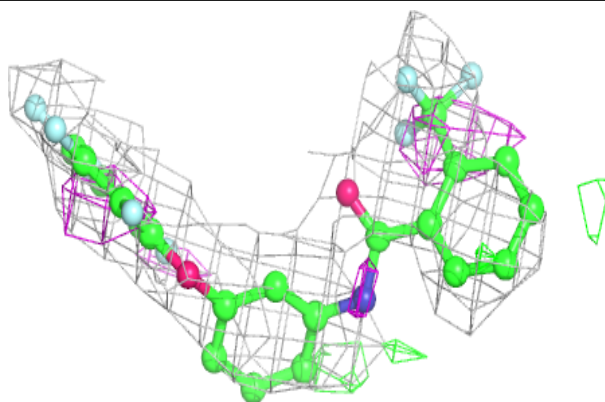
Electron density around FD8 C 202:

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



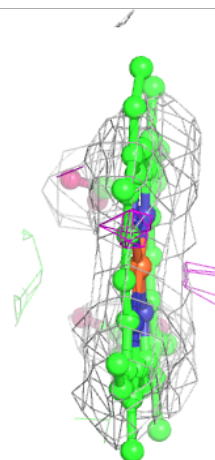
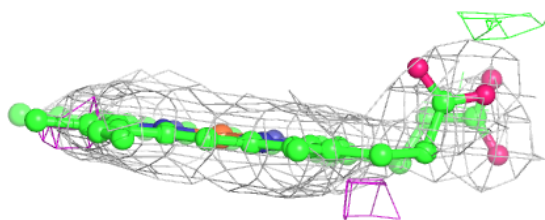
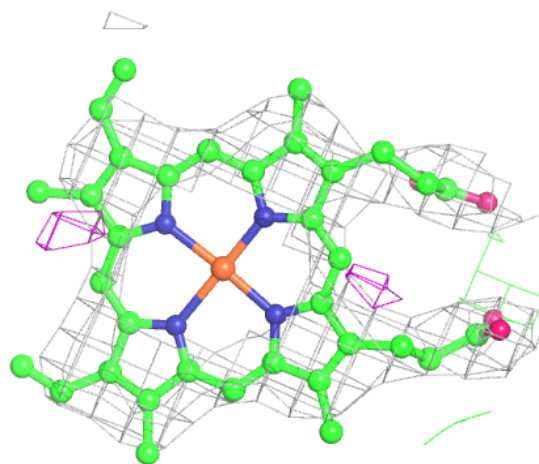
Electron density around FD8 F 304:

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



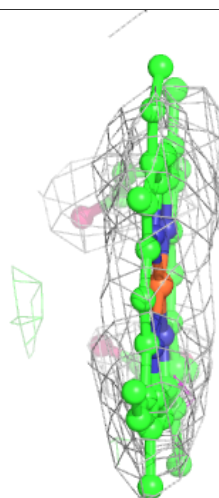
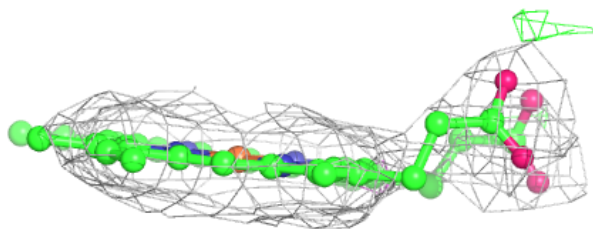
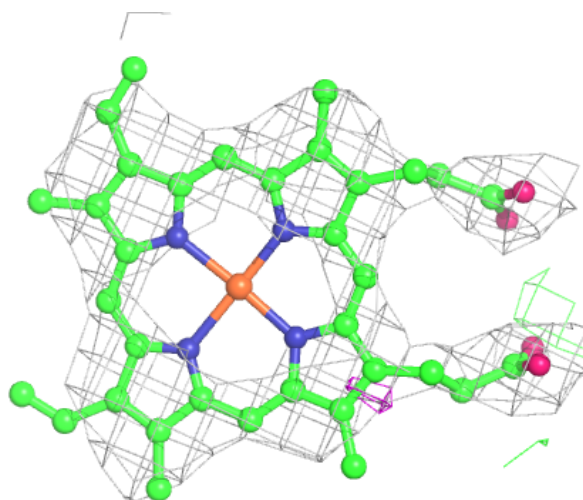
Electron density around HEM G 201:

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



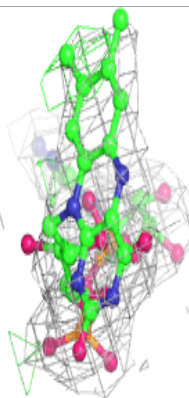
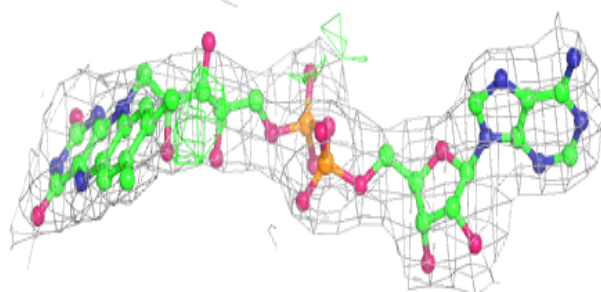
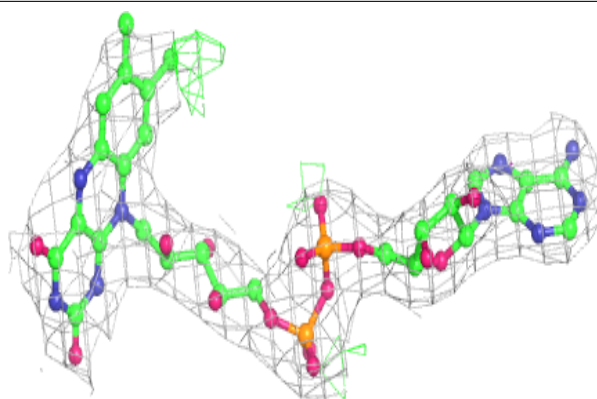
Electron density around HEM C 201:

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

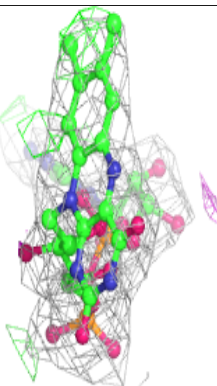
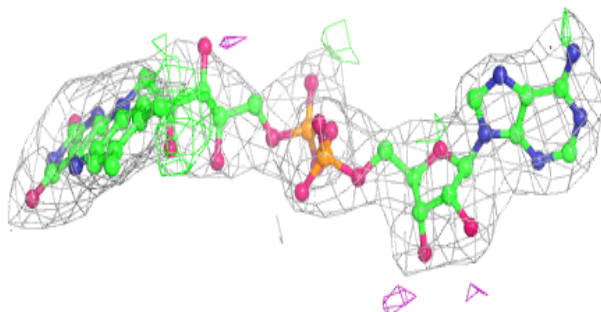
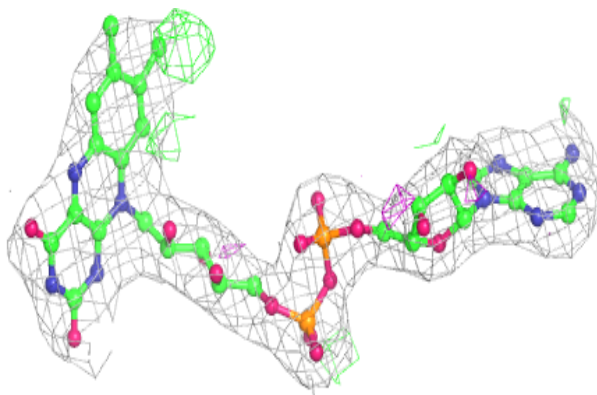


Electron density around FAD E 702:

$2mF_o - DF_c$ (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 [i](#)

There are no such residues in this entry.