Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:33 AM JST

PDB ID	:	4YSX / pdb_00004ysx
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with the specific inhibitor NN23
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	:	2.25 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

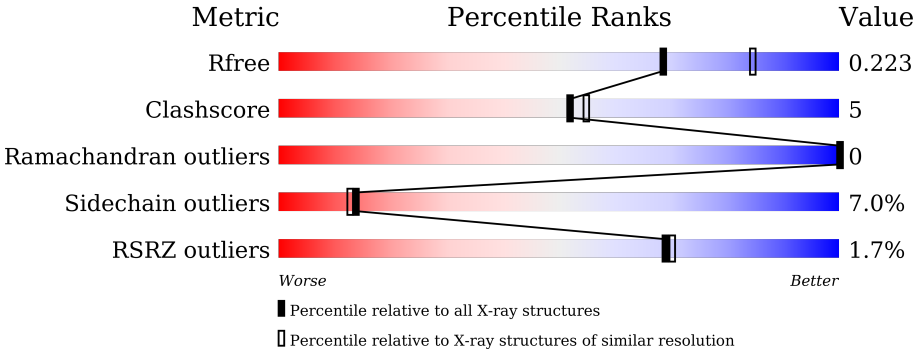
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 of 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 <=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	.% 78% 16% • •
1	E	645	.% 80% 13% • •
2	B	282	78% 8% • 11%
2	F	282	.% 79% 9% • 11%
3	C	188	3% 72% 8% • 19%

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Mol	Chain	Length	Quality of chain
3	G	188	3% 72% 10% • 18%
4	D	156	4% 69% 12% • 17%
4	H	156	5% 69% 12% • 17%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 19103 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
			Total	C	N	O	S			
1	A	616	4787	3004	855	900	28	0	0	0
1	E	616	4787	3004	855	900	28	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	250	1985	1263	338	361	23	0	0	0
2	F	252	1994	1268	340	363	23	0	0	0

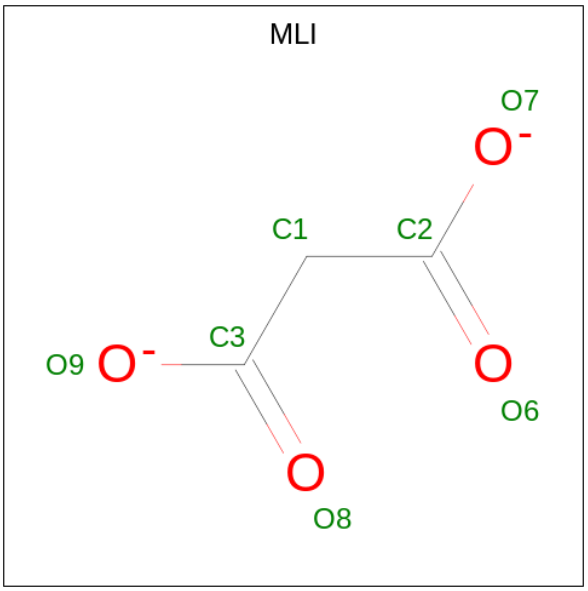
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	153	1217	813	204	194	6	0	0	0
3	G	155	1236	823	209	198	6	0	0	0

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

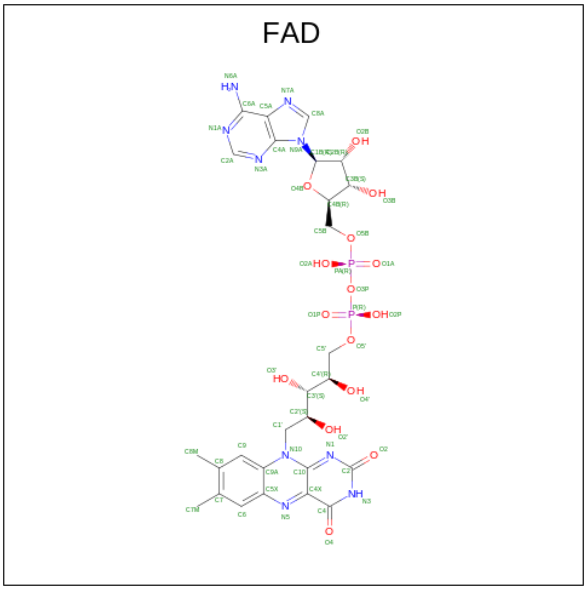
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	129	998	659	165	169	5	0	0	0
4	H	129	998	659	165	169	5	0	0	0

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



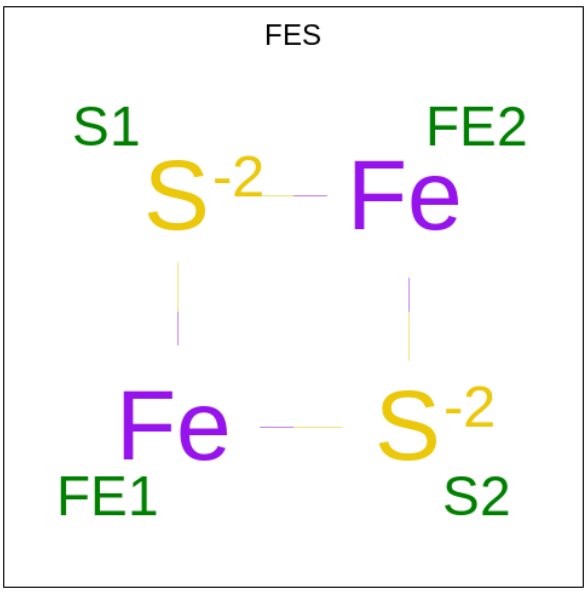
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	3	4		0	0
			Total	C	O			
5	E	1	7	3	4		0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



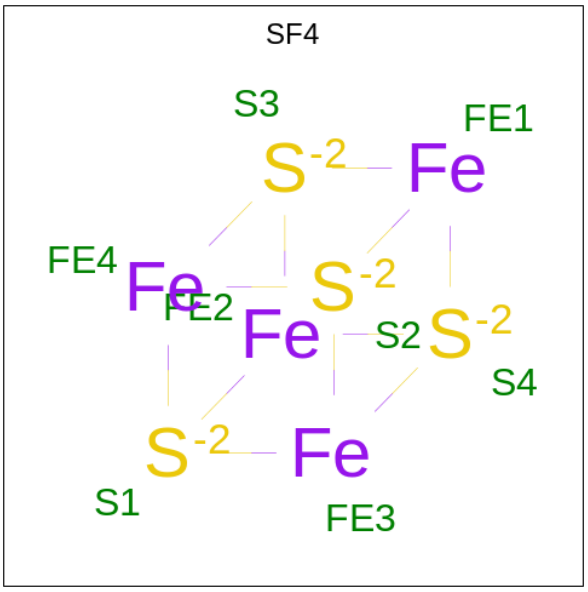
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
6	E	1	53	27	9	15	2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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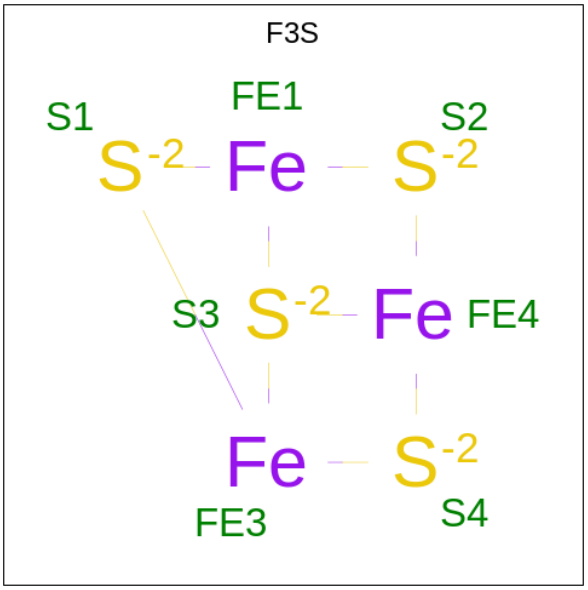
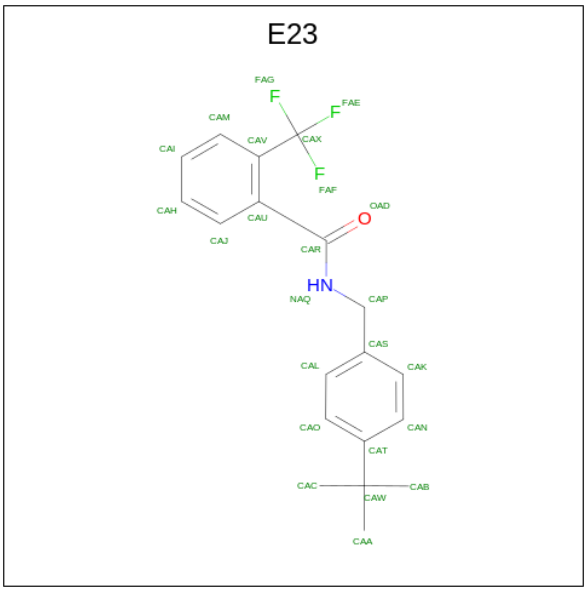
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	F	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



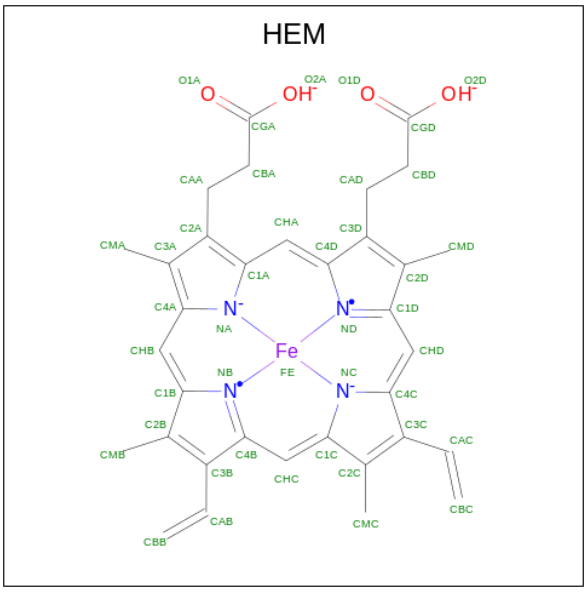
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0
9	F	1	7	3	4	0	0

- Molecule 10 is N-(4-tert-butylbenzyl)-2-(trifluoromethyl)benzamide (CCD ID: E23) (formula: $C_{19}H_{20}F_3NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
10	B	1	24	19	3	1	1	0	0
			Total	C	F	N	O		
10	G	1	24	19	3	1	1	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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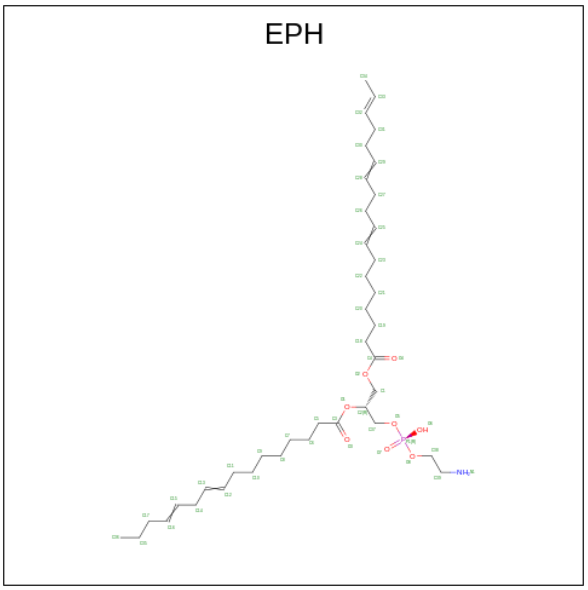
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
11	G	1	43	34	1	4	4	0	0

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



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	186	186	186	0	0
			Total	O		
13	B	104	104	104	0	0
			Total	O		
13	C	33	33	33	0	0
			Total	O		
13	D	27	27	27	0	0
			Total	O		
13	E	207	207	207	0	0
			Total	O		
13	F	111	111	111	0	0

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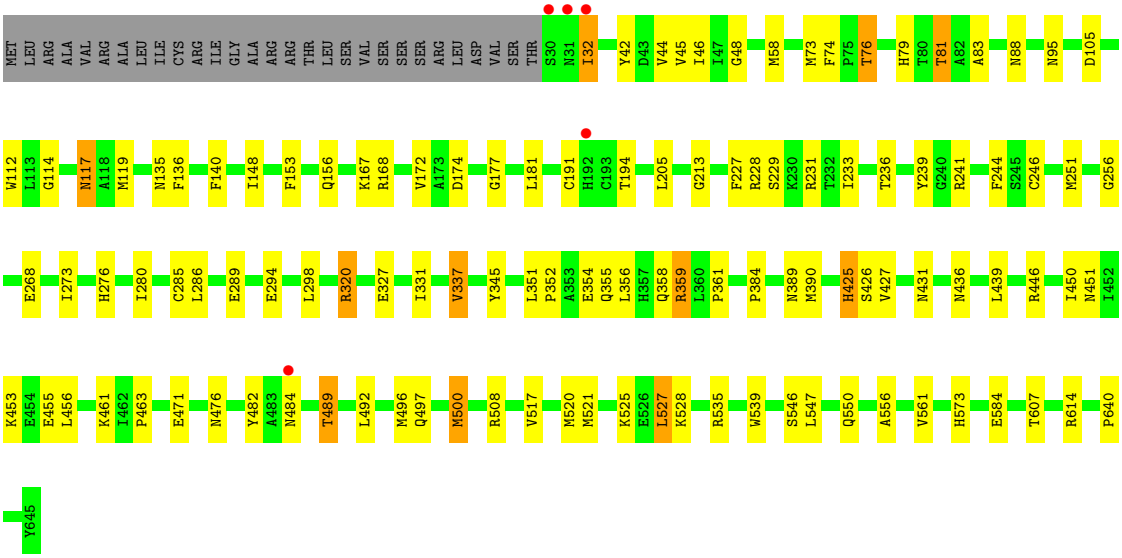
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	G	36	36	36	0	0
			Total	O		
13	H	17	17	17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

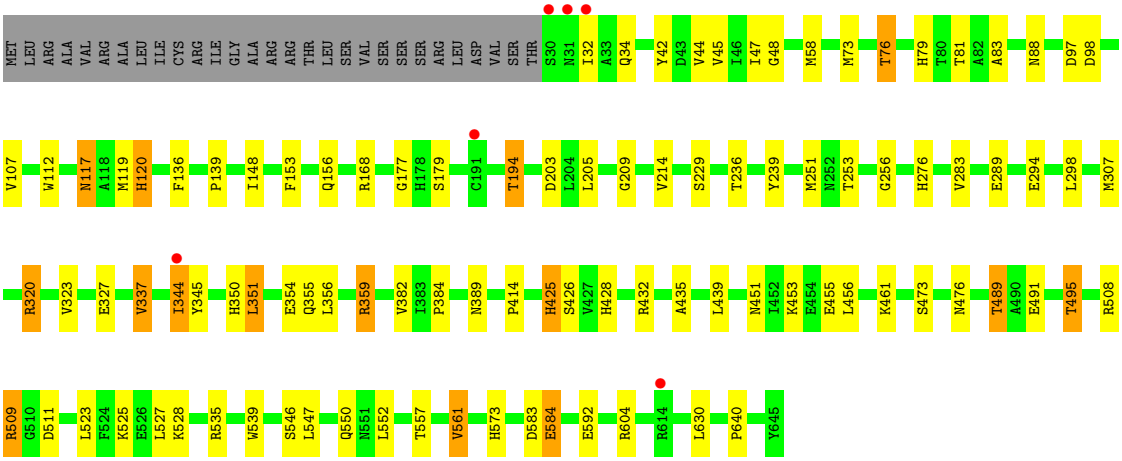
• Molecule 1: Succinate dehydrogenase flavoprotein

Chain A:



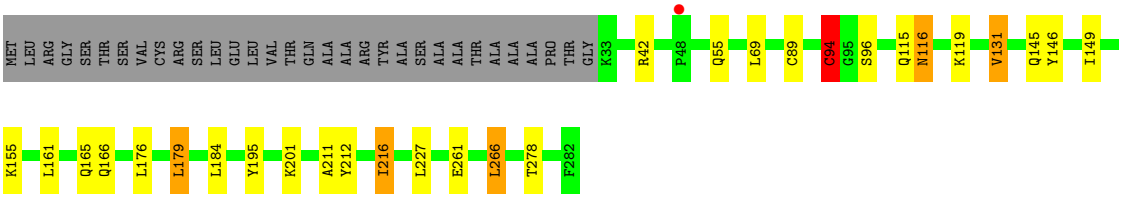
• Molecule 1: Succinate dehydrogenase flavoprotein

Chain E:



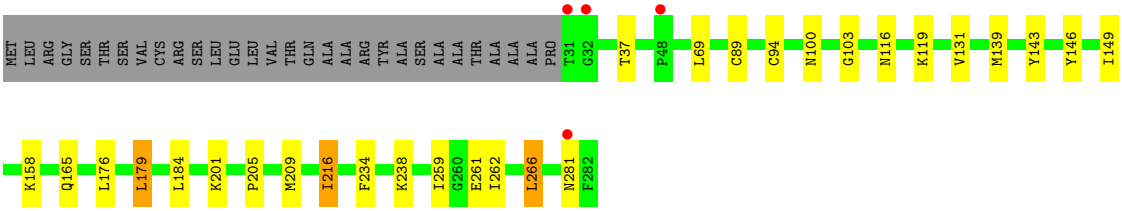
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



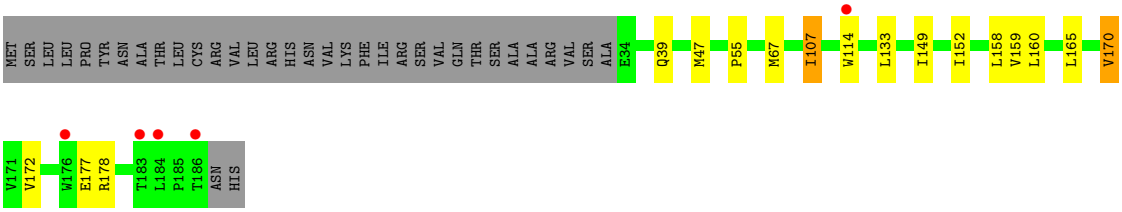
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



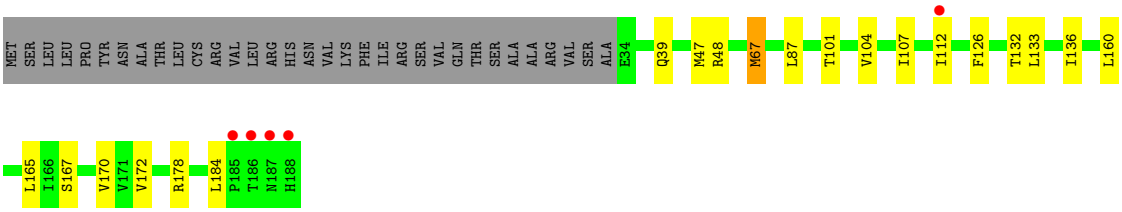
• Molecule 3: Cytochrome b-large subunit

Chain C:



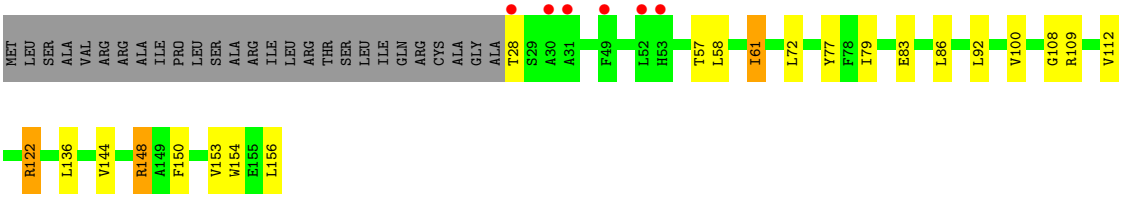
• Molecule 3: Cytochrome b-large subunit

Chain G:



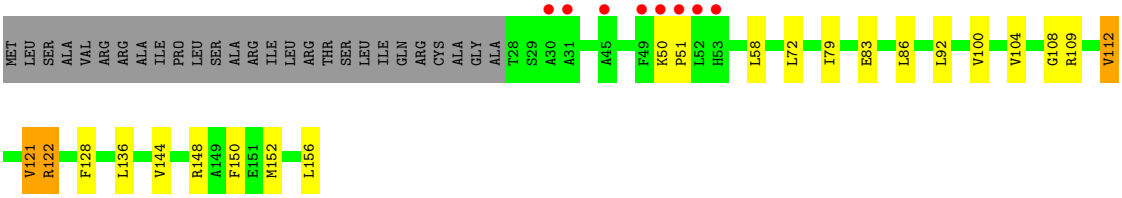
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.20Å 127.91Å 220.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.25) 96.2 (20.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.221 0.185 , 0.223	Depositor DCC
R_{free} test set	8058 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19103	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, MLI, E23, FES, F3S, EPH, SF4, HEM

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	0.60	0/4889	0.84	2/6605 (0.0%)
1	E	0.62	0/4889	0.86	1/6605 (0.0%)
2	B	0.63	0/2029	0.84	2/2739 (0.1%)
2	F	0.64	1/2038 (0.0%)	0.81	3/2751 (0.1%)
3	C	0.57	0/1255	0.82	0/1709
3	G	0.59	0/1275	0.81	0/1735
4	D	0.61	0/1030	0.81	0/1406
4	H	0.60	0/1030	0.86	0/1406
All	All	0.61	1/18435 (0.0%)	0.84	8/24956 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	CYS	C-N	-6.45	1.23	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	425	HIS	N-CA-C	6.16	118.07	111.36
2	F	94	CYS	N-CA-C	6.15	118.07	111.36
1	A	425	HIS	N-CA-C	6.05	117.96	111.36
2	B	94	CYS	N-CA-C	5.71	117.58	111.36
2	B	211	ALA	N-CA-C	-5.55	105.31	111.36
2	F	89	CYS	CA-C-N	-5.31	113.78	122.54
2	F	89	CYS	C-N-CA	-5.31	113.78	122.54
1	A	273	ILE	CB-CA-C	-5.22	103.83	110.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4787	0	4722	64	0
1	E	4787	0	4720	57	0
2	B	1985	0	2001	16	0
2	F	1994	0	2006	12	0
3	C	1217	0	1265	8	0
3	G	1236	0	1278	12	0
4	D	998	0	985	11	0
4	H	998	0	985	13	0
5	A	7	0	2	0	0
5	E	7	0	2	1	0
6	A	53	0	31	7	0
6	E	53	0	31	7	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	B	24	0	20	0	0
10	G	24	0	20	0	0
11	C	43	0	30	5	0
11	G	43	0	30	5	0
12	D	44	0	53	2	0
12	H	44	0	53	1	0
13	A	186	0	0	4	0
13	B	104	0	0	2	0
13	C	33	0	0	0	0
13	D	27	0	0	1	0
13	E	207	0	0	3	0
13	F	111	0	0	3	0
13	G	36	0	0	1	0
13	H	17	0	0	1	0
All	All	19103	0	18234	186	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 5.

All (186) 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:A:79:HIS:NE2	6:A:702:FAD:HM82	1.17	1.41
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.10	1.41
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.07	1.16
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.12	1.13
1:A:79:HIS:CD2	6:A:702:FAD:HM82	1.98	0.99
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.19	0.91
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.23	0.86
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.58	0.85
1:A:76:THR:HG23	13:B:415:HOH:O	1.84	0.77
4:D:144:VAL:HB	4:D:148:ARG:HG2	1.67	0.77
1:E:79:HIS:CE1	6:E:702:FAD:HM82	2.16	0.74
1:E:79:HIS:CD2	6:E:702:FAD:HM82	2.18	0.69
3:G:107:ILE:HD11	4:H:156:LEU:CD1	2.24	0.68
11:G:201:HEM:HBD1	11:G:201:HEM:HHA	1.78	0.66
1:E:289:GLU:OE2	1:E:320:ARG:HD2	1.95	0.65
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.22	0.65
1:E:76:THR:HG23	13:F:409:HOH:O	1.96	0.64
2:B:89:CYS:HB3	2:B:94:CYS:HB3	1.77	0.64
1:A:135:ASN:ND2	2:B:161:LEU:O	2.31	0.64
1:A:289:GLU:OE2	1:A:320:ARG:HD2	1.98	0.64
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.78	0.63
4:D:108:GLY:O	4:D:122:ARG:NH2	2.32	0.63
1:E:489:THR:HG21	1:E:546:SER:OG	1.99	0.63
1:E:337:VAL:HG21	1:E:345:TYR:CE2	2.35	0.61
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.83	0.61
11:C:201:HEM:HBD1	11:C:201:HEM:HHA	1.83	0.61
11:G:201:HEM:HBB2	11:G:201:HEM:HHC	1.83	0.60
5:E:701:MLI:H12	6:E:702:FAD:N5	2.17	0.59
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.83	0.59
4:H:108:GLY:O	4:H:122:ARG:NH2	2.35	0.59
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.50	0.59
1:A:425:HIS:N	1:A:426:SER:HA	2.17	0.57
1:E:97:ASP:OD1	1:E:168:ARG:CG	2.53	0.57
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.57
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.86	0.57
1:E:76:THR:CG2	13:F:409:HOH:O	2.53	0.56
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.40	0.56
1:E:327:GLU:OE2	1:E:344:ILE:HD11	2.06	0.56
11:G:201:HEM:HBD2	13:H:303:HOH:O	2.05	0.55
1:E:491:GLU:O	1:E:495:THR:HG23	2.06	0.55
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:VAL:HG22	1:E:119:MET:HE3	1.90	0.54
1:E:83:ALA:HA	6:E:702:FAD:C6	2.38	0.54
1:E:327:GLU:OE2	1:E:344:ILE:CD1	2.56	0.53
1:E:476:ASN:HD21	1:E:550:GLN:NE2	1.98	0.53
11:C:201:HEM:HBB2	11:C:201:HEM:HHC	1.90	0.53
1:E:239:TYR:H	1:E:389:ASN:ND2	2.07	0.53
3:G:132:THR:HG23	11:G:201:HEM:CAB	2.39	0.53
4:H:104:VAL:HG13	4:H:121:VAL:CG1	2.38	0.53
1:A:42:TYR:O	1:A:229:SER:HA	2.09	0.52
1:A:489:THR:HG21	1:A:546:SER:OG	2.10	0.52
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.93	0.51
1:E:42:TYR:O	1:E:229:SER:HA	2.11	0.51
3:G:178:ARG:NH2	4:H:156:LEU:OXT	2.44	0.51
2:F:116:ASN:C	2:F:116:ASN:HD22	2.18	0.50
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.46	0.50
1:E:350:HIS:CD2	1:E:351:LEU:HD13	2.46	0.50
1:A:191:CYS:HB3	13:A:907:HOH:O	2.12	0.50
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.08	0.50
2:B:155:LYS:HD2	2:B:166:GLN:NE2	2.27	0.50
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.93	0.50
11:C:201:HEM:HBD2	13:D:310:HOH:O	2.11	0.50
1:E:194:THR:HG23	13:E:954:HOH:O	2.11	0.50
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.93	0.49
11:G:201:HEM:HBC2	11:G:201:HEM:HHD	1.94	0.49
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.77	0.49
2:B:116:ASN:HD22	2:B:116:ASN:C	2.20	0.48
1:A:492:LEU:HD21	1:A:527:LEU:HD12	1.94	0.48
1:A:500:MET:HE1	1:A:556:ALA:O	2.13	0.48
1:E:209:GLY:O	1:E:414:PRO:HD2	2.13	0.48
1:E:294:GLU:CD	1:E:359:ARG:HG2	2.37	0.48
2:F:209:MET:HE2	13:F:479:HOH:O	2.13	0.48
4:D:109:ARG:HB2	4:D:112:VAL:HG12	1.94	0.48
2:B:179:LEU:HD23	2:B:216:ILE:HD11	1.95	0.48
1:A:117:ASN:HD22	1:A:117:ASN:N	2.11	0.48
3:C:170:VAL:HG22	4:D:77:TYR:CE1	2.49	0.47
11:C:201:HEM:HBC2	11:C:201:HEM:HHD	1.96	0.47
1:A:241:ARG:HD2	1:A:246:CYS:SG	2.53	0.47
1:E:32:ILE:O	1:E:32:ILE:HG13	2.14	0.47
3:G:126:PHE:HA	3:G:167:SER:OG	2.14	0.47
1:A:228:ARG:HD2	1:A:463:PRO:O	2.15	0.47
3:G:67:MET:HA	3:G:67:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:THR:CG2	13:B:415:HOH:O	2.53	0.47
1:A:148:ILE:H	2:B:165:GLN:HE22	1.63	0.47
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.14	0.47
1:E:489:THR:HG23	13:E:875:HOH:O	2.14	0.47
1:E:584:GLU:OE2	1:E:604:ARG:HD3	2.15	0.47
1:A:294:GLU:OE1	1:A:359:ARG:HG2	2.15	0.46
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.98	0.46
4:H:150:PHE:HB3	12:H:201:EPH:H2	1.95	0.46
4:D:77:TYR:CD1	12:D:201:EPH:H11	2.49	0.46
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.98	0.46
1:E:451:ASN:O	1:E:455:GLU:HG3	2.15	0.46
1:A:32:ILE:HD11	1:A:482:TYR:CZ	2.50	0.46
1:E:344:ILE:CD1	1:E:382:VAL:HG23	2.45	0.46
1:E:120:HIS:HD2	1:E:630:LEU:H	1.65	0.45
2:F:179:LEU:CD2	2:F:216:ILE:HD11	2.47	0.45
3:C:158:LEU:C	3:C:158:LEU:HD23	2.42	0.45
1:A:58:MET:HE1	1:A:136:PHE:CE2	2.52	0.45
1:A:239:TYR:H	1:A:389:ASN:ND2	2.13	0.45
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.98	0.45
1:E:509:ARG:HD2	1:E:511:ASP:OD2	2.16	0.45
2:B:146:TYR:O	2:B:149:ILE:HG12	2.16	0.45
4:D:153:VAL:HG23	4:D:154:TRP:HE3	1.82	0.44
1:E:557:THR:O	1:E:561:VAL:HG13	2.17	0.44
3:G:48:ARG:NH2	13:G:301:HOH:O	2.35	0.44
1:A:81:THR:HB	1:A:181:LEU:HD23	1.99	0.44
1:A:425:HIS:HB2	1:A:427:VAL:HG13	1.99	0.44
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.52	0.44
1:A:73:MET:SD	1:A:251:MET:HG3	2.58	0.44
4:H:50:LYS:N	4:H:51:PRO:CD	2.80	0.44
1:A:117:ASN:HD22	1:A:117:ASN:H	1.65	0.44
1:A:451:ASN:O	1:A:455:GLU:HG3	2.17	0.44
1:A:517:VAL:O	1:A:521:MET:HG2	2.18	0.44
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.99	0.44
1:A:48:GLY:HA2	6:A:702:FAD:H1B	2.00	0.43
1:A:88:ASN:HD21	1:A:156:GLN:HE22	1.66	0.43
1:A:508:ARG:HH11	1:A:573:HIS:HD2	1.64	0.43
1:E:47:ILE:HD11	1:E:214:VAL:HG21	2.00	0.43
2:F:205:PRO:HA	2:F:259:ILE:HD11	2.00	0.43
1:A:148:ILE:H	2:B:165:GLN:NE2	2.17	0.43
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.00	0.43
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:104:VAL:HG21	4:H:152:MET:HE2	2.00	0.43
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.30	0.43
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.51	0.43
1:E:203:ASP:OD2	1:E:473:SER:OG	2.29	0.43
1:A:174:ASP:HB2	1:A:361:PRO:HD2	2.01	0.43
1:E:253:THR:HA	1:E:552:LEU:HD21	2.01	0.43
4:H:109:ARG:HB2	4:H:112:VAL:HG13	2.00	0.43
1:E:432:ARG:HH21	1:E:435:ALA:H	1.66	0.43
1:A:276:HIS:O	1:A:384:PRO:HA	2.19	0.43
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.54	0.43
3:C:47:MET:HA	3:C:47:MET:HE2	2.01	0.42
1:E:117:ASN:HD22	1:E:117:ASN:N	2.17	0.42
1:A:280:ILE:HD12	1:A:285:CYS:HB2	2.01	0.42
1:A:268:GLU:HA	1:A:607:THR:O	2.20	0.42
3:C:178:ARG:NH2	4:D:156:LEU:OXT	2.48	0.42
1:E:58:MET:HE1	1:E:136:PHE:CE2	2.53	0.42
1:A:359:ARG:NH2	13:A:810:HOH:O	2.52	0.42
1:A:431:ASN:ND2	13:A:812:HOH:O	2.53	0.42
1:A:471:GLU:OE2	4:D:28:THR:HA	2.20	0.42
2:B:155:LYS:HD2	2:B:166:GLN:HE21	1.85	0.42
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.20	0.42
3:G:101:THR:HA	4:H:152:MET:HE1	2.02	0.42
1:A:231:ARG:NH2	13:A:809:HOH:O	2.52	0.42
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.55	0.42
1:A:83:ALA:HA	6:A:702:FAD:C6	2.50	0.42
1:E:307:MET:HE2	1:E:323:VAL:HG22	2.01	0.42
1:A:337:VAL:HG21	1:A:345:TYR:CD2	2.55	0.41
1:E:88:ASN:ND2	1:E:156:GLN:HE22	2.18	0.41
1:E:476:ASN:ND2	1:E:550:GLN:HE22	2.00	0.41
2:F:146:TYR:O	2:F:149:ILE:HG12	2.19	0.41
1:A:213:GLY:HA3	1:A:227:PHE:O	2.20	0.41
1:A:244:PHE:HA	1:A:497:GLN:HB3	2.02	0.41
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.51	0.41
1:A:352:PRO:HD2	1:A:355:GLN:HE21	1.85	0.41
2:B:145:GLN:NE2	2:B:195:TYR:OH	2.53	0.41
1:E:45:VAL:HG23	1:E:229:SER:HB3	2.01	0.41
1:E:148:ILE:H	2:F:165:GLN:HE22	1.68	0.41
3:G:47:MET:HA	3:G:47:MET:HE2	2.03	0.41
2:B:131:VAL:HG22	3:C:55:PRO:HG2	2.02	0.41
1:E:355:GLN:O	1:E:359:ARG:HB2	2.21	0.41
1:E:583:ASP:OD1	1:E:604:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CE2	1:A:76:THR:HB	2.56	0.41
4:H:144:VAL:HB	4:H:148:ARG:HG2	2.03	0.41
1:A:114:GLY:C	1:A:119:MET:HE2	2.45	0.41
11:C:201:HEM:HHA	11:C:201:HEM:CBD	2.48	0.41
1:E:337:VAL:HG21	1:E:345:TYR:CD2	2.55	0.41
1:A:79:HIS:CD2	6:A:702:FAD:C8M	2.88	0.41
1:A:327:GLU:O	1:A:331:ILE:HG12	2.21	0.41
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.20	0.41
4:D:57:THR:O	4:D:61:ILE:HG23	2.20	0.41
1:E:97:ASP:OD2	1:E:98:ASP:N	2.50	0.41
1:A:446:ARG:HD3	1:A:450:ILE:HD11	2.02	0.40
1:E:73:MET:SD	1:E:251:MET:HG3	2.61	0.40
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.56	0.40
1:A:95:ASN:HD21	1:A:167:LYS:HB2	1.85	0.40
2:B:94:CYS:SG	2:B:96:SER:HB2	2.61	0.40
3:C:149:ILE:HA	3:C:152:ILE:HD12	2.03	0.40
1:E:139:PRO:HD2	1:E:179:SER:OG	2.21	0.40
1:E:276:HIS:O	1:E:384:PRO:HA	2.20	0.40
1:A:354:GLU:O	1:A:358:GLN:HB2	2.20	0.40
1:A:496:MET:HG3	1:A:520:MET:HE1	2.04	0.40
1:A:46:ILE:HG12	1:A:233:ILE:HD12	2.03	0.40
1:E:359:ARG:NH2	13:E:814:HOH:O	2.55	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%)	594 (97%)	20 (3%)	0	100	100
1	E	614/645 (95%)	599 (98%)	15 (2%)	0	100	100
2	B	248/282 (88%)	239 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	250/282 (89%)	243 (97%)	7 (3%)	0	100	100
3	C	151/188 (80%)	147 (97%)	4 (3%)	0	100	100
3	G	153/188 (81%)	151 (99%)	2 (1%)	0	100	100
4	D	127/156 (81%)	125 (98%)	2 (2%)	0	100	100
4	H	127/156 (81%)	122 (96%)	5 (4%)	0	100	100
All	All	2284/2542 (90%)	2220 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	470 (94%)	32 (6%)	16	15
1	E	502/527 (95%)	467 (93%)	35 (7%)	14	13
2	B	220/242 (91%)	208 (94%)	12 (6%)	19	20
2	F	220/242 (91%)	208 (94%)	12 (6%)	19	20
3	C	127/158 (80%)	117 (92%)	10 (8%)	11	9
3	G	129/158 (82%)	120 (93%)	9 (7%)	14	13
4	D	98/119 (82%)	87 (89%)	11 (11%)	6	4
4	H	98/119 (82%)	87 (89%)	11 (11%)	6	4
All	All	1896/2092 (91%)	1764 (93%)	132 (7%)	14	13

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	44	VAL
1	A	76	THR
1	A	81	THR
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	153	PHE
1	A	194	THR
1	A	205	LEU
1	A	298	LEU
1	A	320	ARG
1	A	337	VAL
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	390	MET
1	A	436	ASN
1	A	439	LEU
1	A	453	LYS
1	A	456	LEU
1	A	461	LYS
1	A	484	ASN
1	A	489	THR
1	A	500	MET
1	A	525	LYS
1	A	527	LEU
1	A	528	LYS
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	561	VAL
1	A	584	GLU
1	A	614	ARG
2	B	69	LEU
2	B	94	CYS
2	B	115	GLN
2	B	116	ASN
2	B	119	LYS
2	B	131	VAL
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	216	ILE
2	B	266	LEU
2	B	278	THR
3	C	67	MET
3	C	107	ILE
3	C	114	TRP

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Mol	Chain	Res	Type
3	C	133	LEU
3	C	159	VAL
3	C	160	LEU
3	C	165	LEU
3	C	170	VAL
3	C	172	VAL
3	C	177	GLU
4	D	58	LEU
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	83	GLU
4	D	86	LEU
4	D	92	LEU
4	D	100	VAL
4	D	122	ARG
4	D	136	LEU
4	D	148	ARG
1	E	34	GLN
1	E	44	VAL
1	E	76	THR
1	E	81	THR
1	E	117	ASN
1	E	120	HIS
1	E	153	PHE
1	E	194	THR
1	E	205	LEU
1	E	283	VAL
1	E	298	LEU
1	E	320	ARG
1	E	337	VAL
1	E	344	ILE
1	E	351	LEU
1	E	354	GLU
1	E	356	LEU
1	E	359	ARG
1	E	439	LEU
1	E	453	LYS
1	E	456	LEU
1	E	461	LYS
1	E	489	THR
1	E	495	THR

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Mol	Chain	Res	Type
1	E	509	ARG
1	E	523	LEU
1	E	525	LYS
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	539	TRP
1	E	547	LEU
1	E	561	VAL
1	E	584	GLU
1	E	592	GLU
2	F	37	THR
2	F	69	LEU
2	F	119	LYS
2	F	131	VAL
2	F	158	LYS
2	F	176	LEU
2	F	179	LEU
2	F	184	LEU
2	F	216	ILE
2	F	261	GLU
2	F	266	LEU
2	F	281	ASN
3	G	67	MET
3	G	112	ILE
3	G	133	LEU
3	G	136	ILE
3	G	160	LEU
3	G	165	LEU
3	G	170	VAL
3	G	172	VAL
3	G	184	LEU
4	H	58	LEU
4	H	72	LEU
4	H	79	ILE
4	H	83	GLU
4	H	86	LEU
4	H	92	LEU
4	H	100	VAL
4	H	112	VAL
4	H	121	VAL
4	H	122	ARG

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Mol	Chain	Res	Type
4	H	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	95	ASN
1	A	117	ASN
1	A	355	GLN
1	A	389	ASN
1	A	436	ASN
1	A	451	ASN
1	A	497	GLN
1	A	550	GLN
1	A	551	ASN
1	A	558	GLN
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
2	B	166	GLN
4	D	55	HIS
4	D	140	ASN
1	E	34	GLN
1	E	88	ASN
1	E	95	ASN
1	E	117	ASN
1	E	120	HIS
1	E	135	ASN
1	E	252	ASN
1	E	355	GLN
1	E	389	ASN
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	497	GLN
1	E	503	HIS

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Mol	Chain	Res	Type
1	E	551	ASN
1	E	558	GLN
1	E	573	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	116	ASN
2	F	140	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
3	G	66	GLN
3	G	187	ASN
4	H	55	HIS
4	H	140	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	HEM	G	201	4,3	50,50,50	1.52	6 (12%)	66,82,82	2.29	22 (33%)
8	SF4	B	302	2	0,12,12	-	-	-		
5	MLI	E	701	-	6,6,6	1.07	0	7,7,7	1.41	1 (14%)
6	FAD	E	702	-	56,58,58	1.38	9 (16%)	81,89,89	1.78	22 (27%)
6	FAD	A	702	-	56,58,58	1.44	11 (19%)	81,89,89	1.79	21 (25%)
5	MLI	A	701	-	6,6,6	1.03	0	7,7,7	1.07	0
7	FES	B	301	2	0,4,4	-	-	-		
9	F3S	B	303	2	0,9,9	-	-	-		
8	SF4	F	302	2	0,12,12	-	-	-		
9	F3S	F	303	2	0,9,9	-	-	-		
11	HEM	C	201	4,3	50,50,50	1.57	8 (16%)	66,82,82	2.18	21 (31%)
12	EPH	D	201	-	43,43,48	1.13	2 (4%)	45,48,53	1.18	4 (8%)
10	E23	B	304	-	25,25,25	0.48	0	37,37,37	1.09	3 (8%)
10	E23	G	202	-	25,25,25	0.40	0	37,37,37	0.97	4 (10%)
12	EPH	H	201	-	43,43,48	1.17	2 (4%)	45,48,53	1.18	4 (8%)
7	FES	F	301	2	0,4,4	-	-	-		

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
11	HEM	G	201	4,3	-	5/14/54/54	-
8	SF4	B	302	2	-	-	0/6/5/5
5	MLI	E	701	-	-	2/4/4/4	-
6	FAD	E	702	-	-	6/34/50/50	0/6/6/6
6	FAD	A	702	-	-	6/34/50/50	0/6/6/6
5	MLI	A	701	-	-	0/4/4/4	-
11	HEM	C	201	4,3	-	5/14/54/54	-
7	FES	B	301	2	-	-	0/1/1/1
12	EPH	D	201	-	-	28/47/47/52	-
8	SF4	F	302	2	-	-	0/6/5/5
9	F3S	B	303	2	-	-	0/3/3/3
9	F3S	F	303	2	-	-	0/3/3/3
10	E23	B	304	-	-	6/21/21/21	0/2/2/2
10	E23	G	202	-	-	0/21/21/21	0/2/2/2
12	EPH	H	201	-	-	22/47/47/52	-
7	FES	F	301	2	-	-	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	201	EPH	O2-C4	4.99	1.47	1.33
11	G	201	HEM	FE-NB	4.97	2.10	1.94
11	C	201	HEM	FE-NB	4.91	2.10	1.94
12	D	201	EPH	O2-C4	4.63	1.46	1.33
12	H	201	EPH	O1-C3	4.61	1.47	1.34
12	D	201	EPH	O1-C3	4.61	1.47	1.34
6	A	702	FAD	C9A-C5X	4.33	1.48	1.41
6	E	702	FAD	C5A-C4A	4.17	1.46	1.39
6	E	702	FAD	C9A-C5X	4.12	1.48	1.41
11	G	201	HEM	FE-NC	4.07	2.08	1.95
6	A	702	FAD	C5A-C4A	3.97	1.46	1.39
11	C	201	HEM	FE-NC	3.65	2.07	1.95
11	G	201	HEM	C1B-NB	-3.65	1.34	1.40
11	C	201	HEM	C1B-NB	-3.61	1.34	1.40
11	C	201	HEM	C1C-C2C	-3.00	1.39	1.45
6	E	702	FAD	C8A-N7A	2.90	1.37	1.31
11	G	201	HEM	C4B-NB	-2.84	1.32	1.38
6	A	702	FAD	C8A-N7A	2.83	1.36	1.31
11	C	201	HEM	C4B-NB	-2.70	1.33	1.38
11	C	201	HEM	C3B-C4B	2.67	1.50	1.44
6	A	702	FAD	C8-C7	2.64	1.47	1.40
6	A	702	FAD	C1'-C2'	2.60	1.56	1.52
6	A	702	FAD	C4-N3	-2.59	1.34	1.38
11	C	201	HEM	C4D-ND	-2.54	1.35	1.40
6	E	702	FAD	C5A-C6A	2.52	1.48	1.41
6	A	702	FAD	C5A-C6A	2.43	1.47	1.41
6	E	702	FAD	C8-C7	2.41	1.46	1.40
6	A	702	FAD	C5X-N5	-2.37	1.34	1.39
6	E	702	FAD	C5A-N7A	-2.36	1.34	1.39
11	G	201	HEM	C1C-C2C	-2.33	1.40	1.45
11	G	201	HEM	C4D-ND	-2.29	1.36	1.40
6	A	702	FAD	C2-N3	-2.23	1.33	1.39
6	A	702	FAD	C5A-N7A	-2.23	1.34	1.39
6	E	702	FAD	C4A-N9A	-2.17	1.32	1.37
6	E	702	FAD	C4-N3	-2.15	1.34	1.38
11	C	201	HEM	C1D-ND	-2.14	1.34	1.38
6	A	702	FAD	C4A-N9A	-2.07	1.33	1.37
6	E	702	FAD	C2-N3	-2.05	1.34	1.39

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	201	HEM	CAD-C3D-C4D	6.28	135.63	124.66
11	C	201	HEM	CAD-C3D-C4D	5.65	134.53	124.66
6	E	702	FAD	C5A-C4A-N3A	-5.50	119.57	126.75
6	A	702	FAD	C5A-C4A-N3A	-5.44	119.66	126.75
11	G	201	HEM	O2D-CGD-CBD	5.27	130.96	114.03
11	G	201	HEM	C1B-NB-C4B	5.27	110.51	105.07
11	G	201	HEM	CHD-C1D-ND	4.92	129.77	124.42
11	C	201	HEM	C1B-NB-C4B	4.86	110.10	105.07
11	G	201	HEM	CAD-C3D-C2D	-4.81	118.92	127.88
11	C	201	HEM	O2D-CGD-CBD	4.63	128.91	114.03
11	C	201	HEM	CHD-C1D-ND	4.48	129.28	124.42
6	A	702	FAD	N3A-C2A-N1A	-4.36	121.78	128.60
12	H	201	EPH	O1-C3-C5	4.28	120.72	111.50
11	C	201	HEM	CAD-C3D-C2D	-4.26	119.94	127.88
12	D	201	EPH	O1-C3-C5	4.18	120.51	111.50
6	A	702	FAD	C2A-N3A-C4A	4.16	121.58	111.75
11	C	201	HEM	C4C-NC-C1C	4.14	109.40	105.35
11	G	201	HEM	CAD-CBD-CGD	4.11	122.45	113.60
6	A	702	FAD	N3A-C4A-N9A	3.93	133.55	127.08
12	H	201	EPH	O2-C4-C18	3.91	124.19	111.91
11	G	201	HEM	C4C-NC-C1C	3.81	109.08	105.35
6	E	702	FAD	N3A-C4A-N9A	3.78	133.32	127.08
6	E	702	FAD	N3A-C2A-N1A	-3.78	122.70	128.60
12	D	201	EPH	O2-C4-C18	3.76	123.71	111.91
6	E	702	FAD	C2A-N3A-C4A	3.75	120.61	111.75
11	C	201	HEM	CAD-CBD-CGD	3.71	121.58	113.60
11	C	201	HEM	CAC-C3C-C4C	3.51	133.37	124.90
11	G	201	HEM	CHA-C4D-ND	3.47	128.65	124.37
11	G	201	HEM	CAC-C3C-C4C	3.43	133.18	124.90
6	A	702	FAD	C4A-C5A-N7A	-3.37	106.52	110.62
6	E	702	FAD	C4A-C5A-N7A	-3.36	106.52	110.62
11	G	201	HEM	O1D-CGD-CBD	-3.32	112.40	123.08
6	E	702	FAD	O2-C2-N1	-3.28	116.39	121.83
6	E	702	FAD	C4X-C10-N1	-3.26	117.17	124.73
11	C	201	HEM	CHA-C4D-ND	3.26	128.39	124.37
11	C	201	HEM	CBD-CAD-C3D	3.25	121.65	112.63
11	G	201	HEM	CBD-CAD-C3D	3.19	121.48	112.63
11	G	201	HEM	CHB-C1B-NB	3.17	128.29	124.37
11	C	201	HEM	CHD-C1D-C2D	-3.12	120.10	124.98
11	G	201	HEM	CHD-C1D-C2D	-3.11	120.12	124.98
6	A	702	FAD	O2-C2-N1	-3.10	116.70	121.83
6	A	702	FAD	O4-C4-C4X	-3.06	118.48	126.60
6	A	702	FAD	C6A-C5A-N7A	3.04	137.69	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	201	HEM	CHC-C4B-NB	3.04	127.72	124.42
10	B	304	E23	FAE-CAX-CAV	-3.01	107.45	112.70
6	E	702	FAD	C10-N1-C2	2.96	122.83	116.90
11	G	201	HEM	CMD-C2D-C1D	2.96	129.54	125.04
11	C	201	HEM	O2D-CGD-O1D	-2.93	115.99	123.30
11	C	201	HEM	CHC-C1C-NC	2.92	127.59	124.44
11	G	201	HEM	CAC-C3C-C2C	-2.90	119.05	128.60
11	C	201	HEM	CHB-C1B-NB	2.89	127.94	124.37
12	D	201	EPH	O2-C4-O4	-2.89	116.31	123.59
11	C	201	HEM	CMD-C2D-C1D	2.88	129.42	125.04
10	B	304	E23	FAF-CAX-CAV	-2.87	107.70	112.70
6	E	702	FAD	O4-C4-C4X	-2.82	119.13	126.60
6	A	702	FAD	C4A-N9A-C8A	2.82	108.78	105.73
6	A	702	FAD	C5A-N7A-C8A	2.79	107.47	103.51
11	C	201	HEM	CMB-C2B-C1B	2.74	129.21	125.04
6	E	702	FAD	C4X-C10-N10	2.71	120.45	116.48
6	A	702	FAD	C10-N1-C2	2.68	122.27	116.90
11	G	201	HEM	O2D-CGD-O1D	-2.67	116.63	123.30
6	A	702	FAD	C4-C4X-N5	2.67	122.03	118.23
6	E	702	FAD	C6A-C5A-N7A	2.64	136.93	132.02
12	H	201	EPH	O2-C4-O4	-2.62	116.97	123.59
6	A	702	FAD	C4X-C10-N1	-2.60	118.69	124.73
11	C	201	HEM	CAB-C3B-C2B	-2.60	120.04	128.60
12	D	201	EPH	O1-C3-O3	-2.60	117.43	123.70
11	C	201	HEM	CAC-C3C-C2C	-2.59	120.07	128.60
6	E	702	FAD	C5A-N7A-C8A	2.57	107.16	103.51
6	E	702	FAD	C2A-N1A-C6A	2.56	123.16	118.77
10	B	304	E23	CAP-NAQ-CAR	2.55	127.84	121.81
6	A	702	FAD	N9A-C8A-N7A	-2.54	110.44	113.91
11	G	201	HEM	CHC-C1C-NC	2.52	127.17	124.44
5	E	701	MLI	O7-C2-C1	2.52	122.59	114.54
11	C	201	HEM	O1D-CGD-CBD	-2.49	115.07	123.08
6	A	702	FAD	O4B-C1B-N9A	2.49	112.96	108.06
11	G	201	HEM	CMB-C2B-C1B	2.45	128.78	125.04
11	G	201	HEM	CHA-C4D-C3D	-2.45	120.72	125.33
6	A	702	FAD	O2'-C2'-C3'	-2.44	103.17	109.10
11	C	201	HEM	CHA-C4D-C3D	-2.43	120.77	125.33
6	A	702	FAD	C1'-C2'-C3'	2.40	116.50	109.79
11	G	201	HEM	CAB-C3B-C2B	-2.39	120.73	128.60
6	E	702	FAD	C1'-C2'-C3'	2.38	116.44	109.79
6	E	702	FAD	O4B-C1B-N9A	2.35	112.70	108.06
6	E	702	FAD	C4-C4X-N5	2.33	121.55	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	702	FAD	C4A-N9A-C8A	2.30	108.22	105.73
10	G	202	E23	CAS-CAP-NAQ	-2.30	108.12	113.05
10	G	202	E23	FAG-CAX-CAV	-2.29	108.72	112.70
6	E	702	FAD	C9A-N10-C10	-2.26	117.25	120.77
6	A	702	FAD	C2A-N1A-C6A	2.25	122.64	118.77
10	G	202	E23	FAF-CAX-CAV	-2.22	108.83	112.70
11	C	201	HEM	CHC-C4B-NB	2.21	126.82	124.42
6	E	702	FAD	C5X-N5-C4X	2.20	121.73	118.07
6	A	702	FAD	C4X-C4-N3	2.20	118.78	113.19
10	G	202	E23	CAP-NAQ-CAR	2.19	126.99	121.81
6	E	702	FAD	N9A-C8A-N7A	-2.14	110.98	113.91
6	A	702	FAD	C4X-C10-N10	2.12	119.57	116.48
6	E	702	FAD	C4-N3-C2	-2.11	121.74	125.64
12	H	201	EPH	C1-O2-C4	2.11	124.93	117.12
11	G	201	HEM	CHD-C4C-C3C	2.11	128.86	125.26
6	E	702	FAD	C10-C4X-N5	-2.03	120.55	124.86
6	A	702	FAD	C8M-C8-C9	-2.02	115.76	119.49

There are no chirality outliers.

All (80) 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	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
11	C	201	HEM	C2D-C3D-CAD-CBD
11	C	201	HEM	C4D-C3D-CAD-CBD
11	G	201	HEM	C2D-C3D-CAD-CBD
11	G	201	HEM	C4D-C3D-CAD-CBD
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	C28-C29-C30-C31
12	D	201	EPH	O8-C38-C39-N1
12	H	201	EPH	C25-C26-C27-C28
12	H	201	EPH	C13-C14-C15-C16
12	H	201	EPH	O4-C4-O2-C1
12	H	201	EPH	C18-C4-O2-C1
12	D	201	EPH	O4-C4-O2-C1
12	H	201	EPH	C5-C3-O1-C2
12	D	201	EPH	C18-C4-O2-C1
12	H	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	H	201	EPH	C4-C18-C19-C20
12	D	201	EPH	C2-C1-O2-C4
12	D	201	EPH	C37-O5-P1-O8
12	H	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C11-C10-C9-C8
12	D	201	EPH	C9-C10-C11-C12
12	H	201	EPH	C11-C10-C9-C8
12	H	201	EPH	O2-C1-C2-C37
12	H	201	EPH	C7-C8-C9-C10
12	H	201	EPH	C18-C19-C20-C21
12	D	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C7-C8-C9-C10
12	D	201	EPH	C5-C3-O1-C2
12	D	201	EPH	O2-C1-C2-C37
12	D	201	EPH	C21-C22-C23-C24
12	H	201	EPH	C9-C10-C11-C12
11	G	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	C19-C20-C21-C22
6	A	702	FAD	P-O3P-PA-O1A
11	C	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	C12-C13-C14-C15
6	A	702	FAD	O4B-C4B-C5B-O5B
6	E	702	FAD	PA-O3P-P-O5'
12	H	201	EPH	C28-C29-C30-C31
12	H	201	EPH	O1-C2-C37-O5
11	C	201	HEM	C4B-C3B-CAB-CBB
11	C	201	HEM	C4C-C3C-CAC-CBC
11	G	201	HEM	C4B-C3B-CAB-CBB
11	G	201	HEM	C4C-C3C-CAC-CBC
12	H	201	EPH	O2-C1-C2-O1
6	E	702	FAD	P-O3P-PA-O1A
12	H	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C37-O5-P1-O6
12	D	201	EPH	C37-O5-P1-O7
12	H	201	EPH	C1-C2-C37-O5
12	D	201	EPH	C39-C38-O8-P1
12	H	201	EPH	C39-C38-O8-P1
12	D	201	EPH	O1-C2-C37-O5
12	D	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C1-C2-O1-C3
12	D	201	EPH	C38-O8-P1-O5
6	A	702	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	E	702	FAD	P-O3P-PA-O2A
12	D	201	EPH	C10-C11-C12-C13
12	H	201	EPH	C12-C13-C14-C15
5	E	701	MLI	C2-C1-C3-O9
12	D	201	EPH	O2-C1-C2-O1
5	E	701	MLI	C2-C1-C3-O8
12	H	201	EPH	C37-C2-O1-C3
12	D	201	EPH	C1-C2-C37-O5
10	B	304	E23	CAN-CAT-CAW-CAC
10	B	304	E23	CAO-CAT-CAW-CAC
6	A	702	FAD	C3B-C4B-C5B-O5B
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	C37-O5-P1-O7
6	E	702	FAD	O4B-C4B-C5B-O5B
10	B	304	E23	CAO-CAT-CAW-CAA
10	B	304	E23	CAN-CAT-CAW-CAA
10	B	304	E23	CAO-CAT-CAW-CAB
10	B	304	E23	CAN-CAT-CAW-CAB

There are no ring outliers.

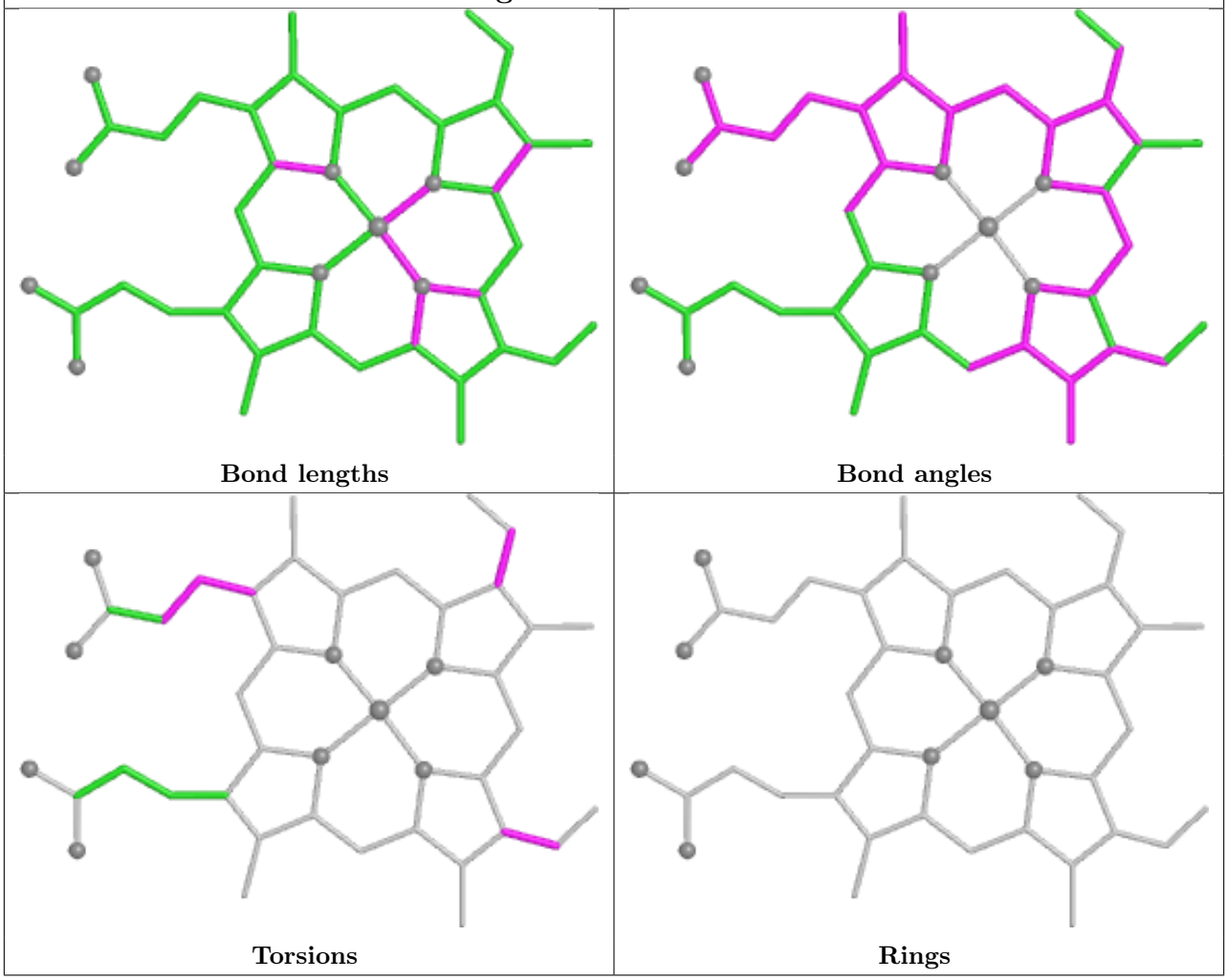
7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	201	HEM	5	0
5	E	701	MLI	1	0
6	E	702	FAD	7	0
6	A	702	FAD	7	0
11	C	201	HEM	5	0
12	D	201	EPH	2	0
12	H	201	EPH	1	0

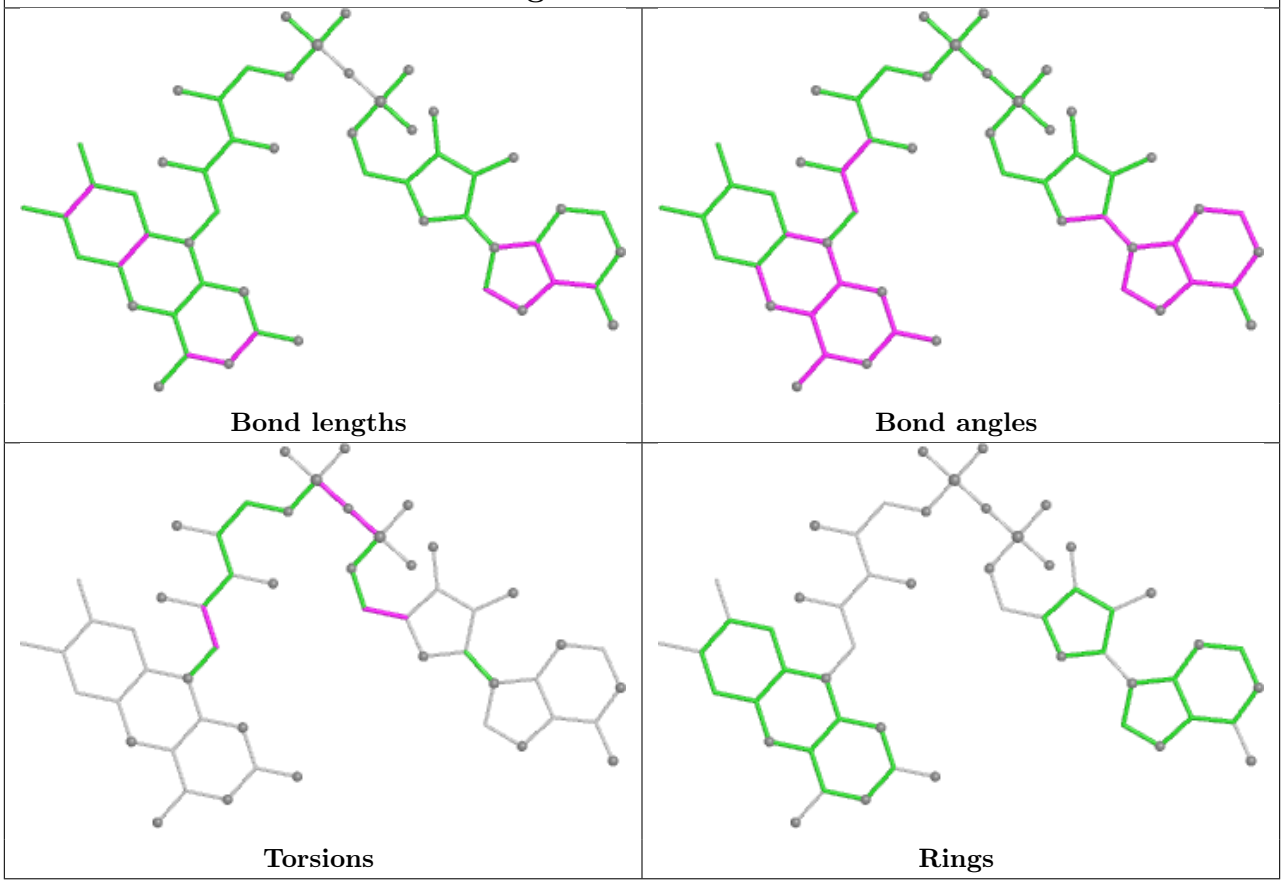
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

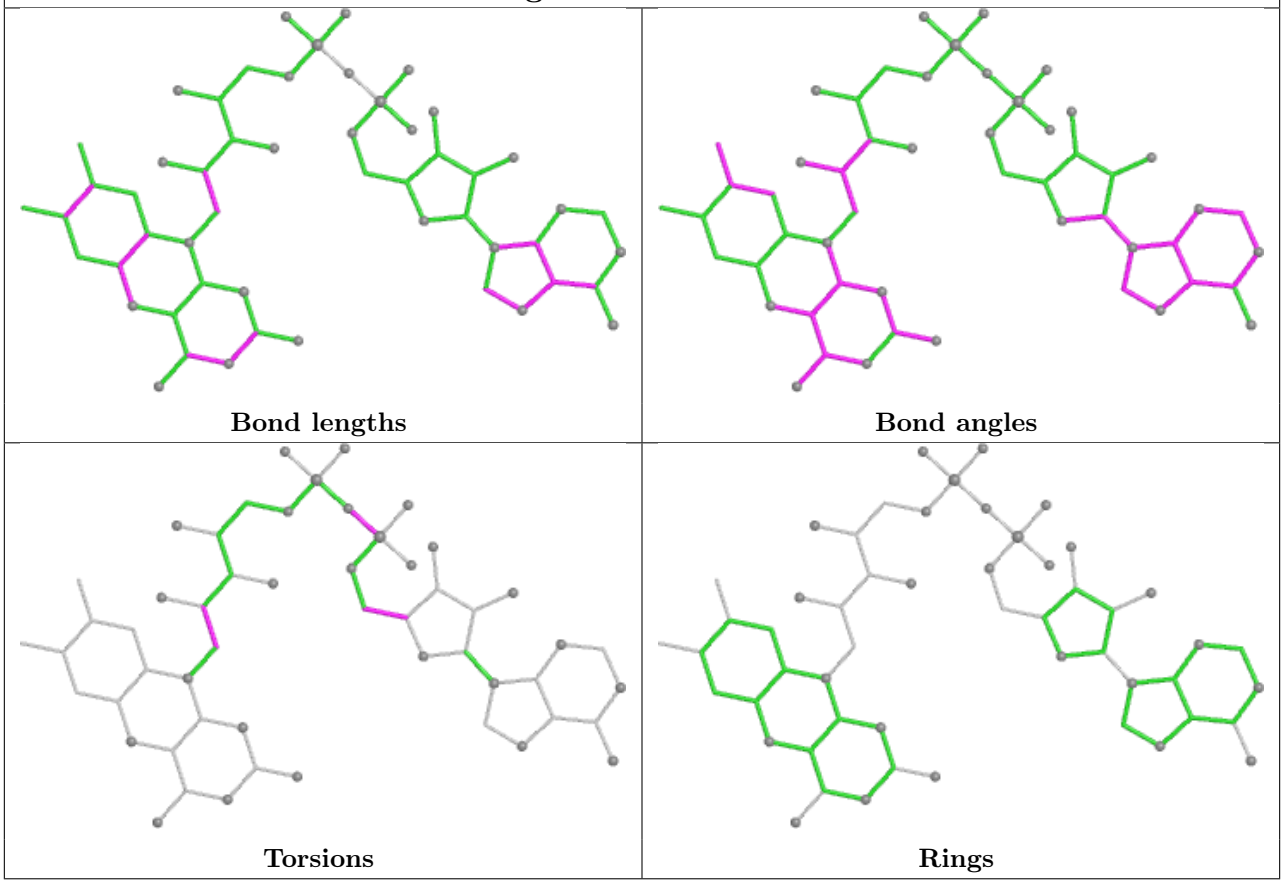
Ligand HEM G 201



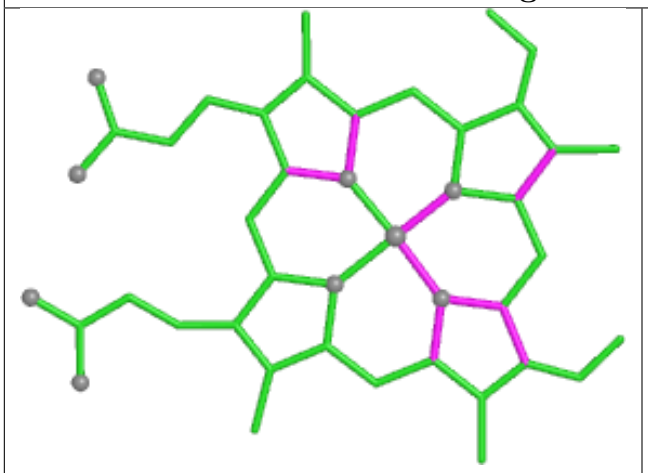
Ligand FAD E 702



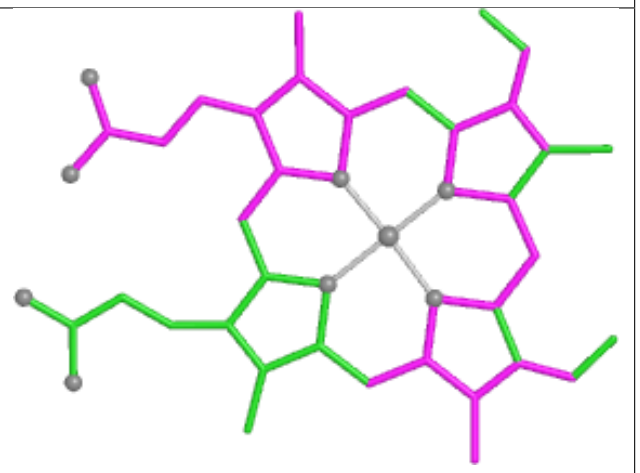
Ligand FAD A 702



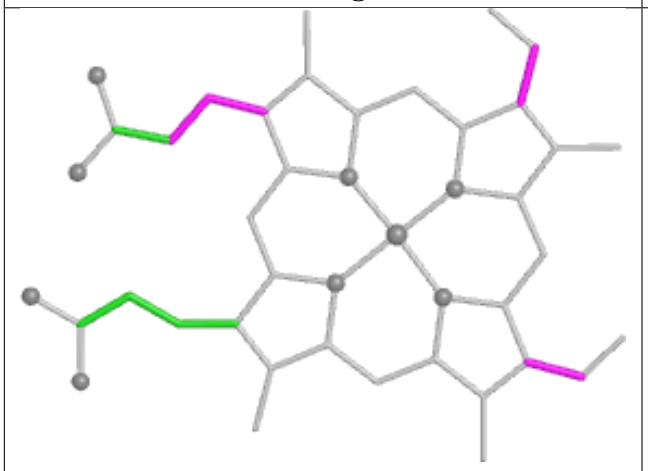
Ligand HEM C 201



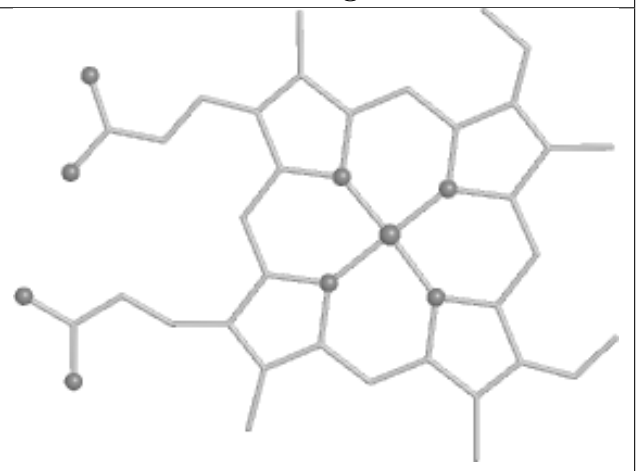
Bond lengths



Bond angles

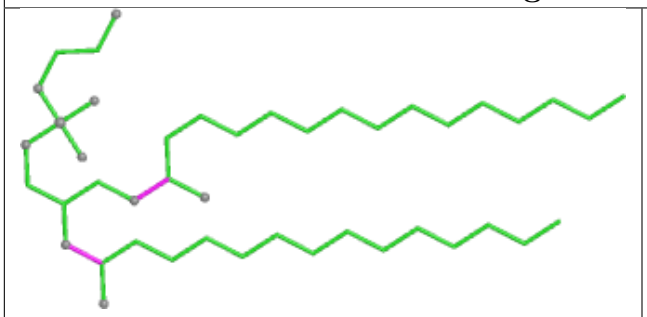


Torsions

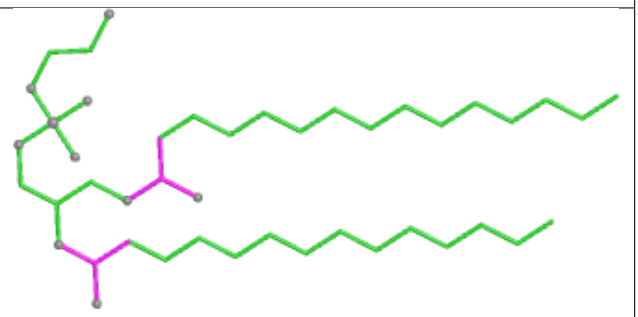


Rings

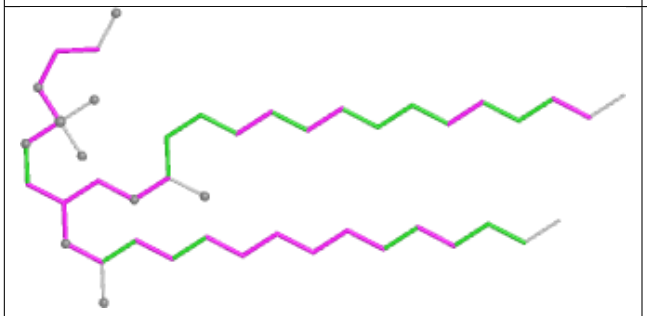
Ligand EPH D 201



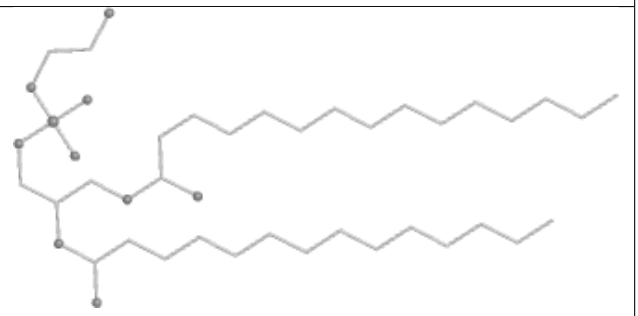
Bond lengths



Bond angles

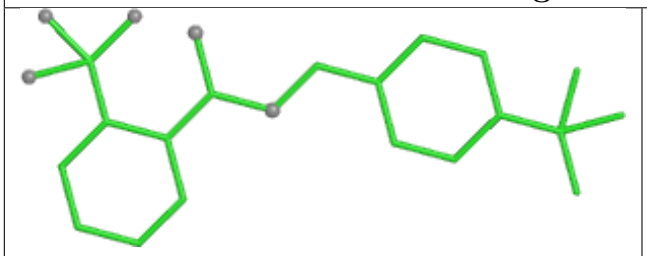


Torsions

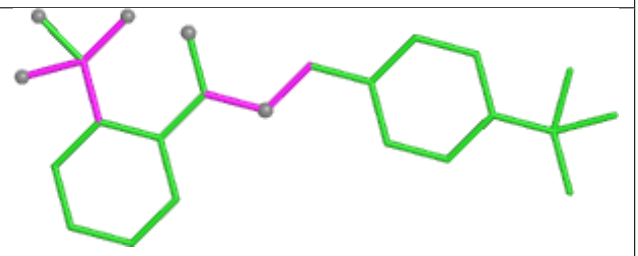


Rings

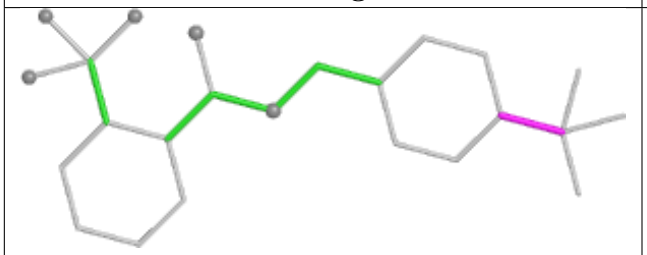
Ligand E23 B 304



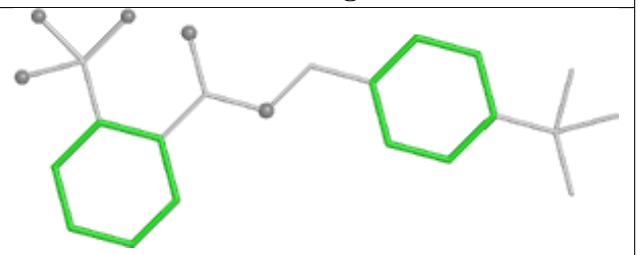
Bond lengths



Bond angles

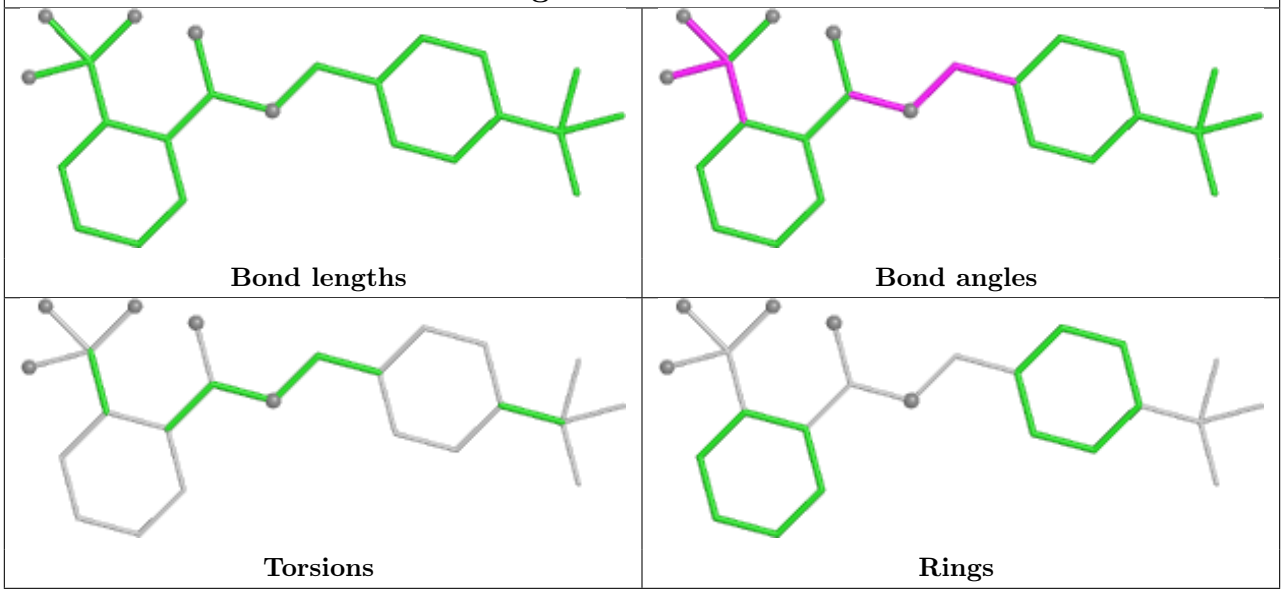


Torsions

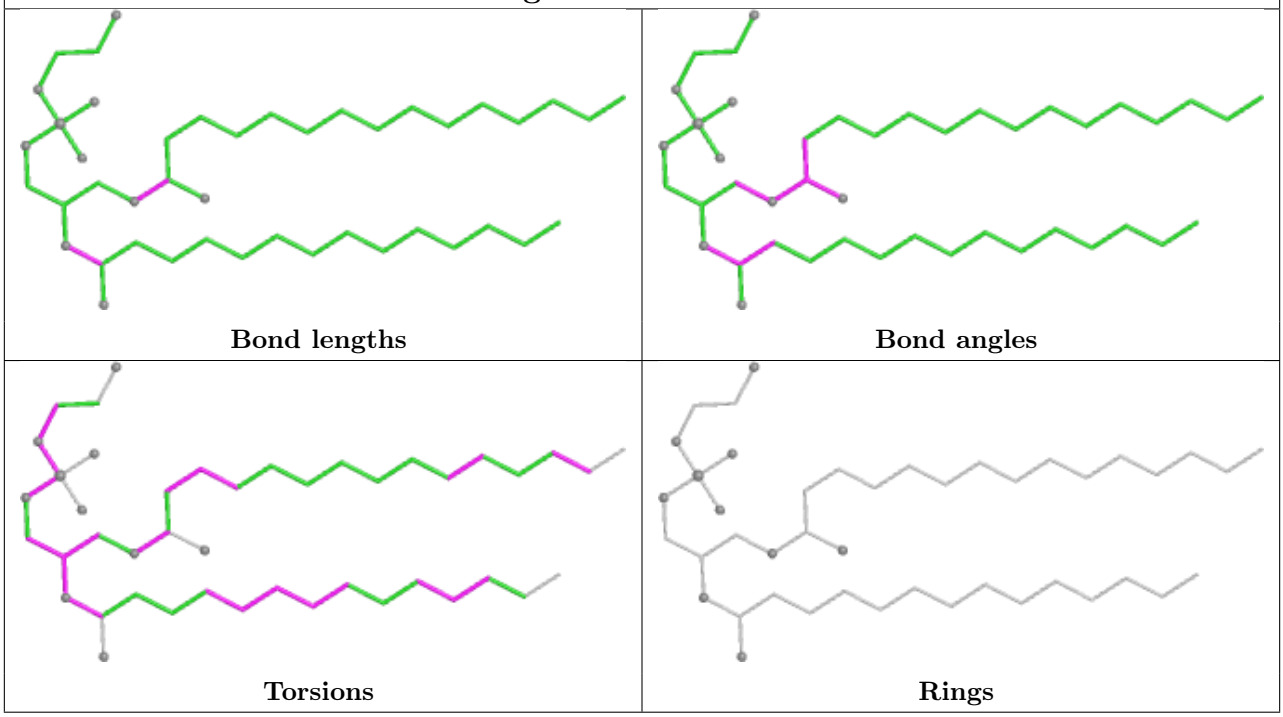


Rings

Ligand E23 G 202



Ligand EPH H 201



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.25	5 (0%)	82	84	32, 46, 70, 100	0
1	E	616/645 (95%)	-0.32	6 (0%)	79	81	31, 43, 64, 123	0
2	B	250/282 (88%)	-0.38	1 (0%)	88	89	32, 41, 64, 87	0
2	F	252/282 (89%)	-0.31	4 (1%)	70	71	33, 41, 68, 98	0
3	C	153/188 (81%)	0.10	5 (3%)	49	49	35, 50, 88, 127	0
3	G	155/188 (82%)	0.12	5 (3%)	50	50	38, 51, 88, 129	0
4	D	129/156 (82%)	0.14	6 (4%)	36	35	40, 51, 91, 116	0
4	H	129/156 (82%)	0.32	8 (6%)	26	24	42, 53, 110, 151	0
All	All	2300/2542 (90%)	-0.19	40 (1%)	69	70	31, 46, 76, 151	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	30	ALA	7.1
4	D	30	ALA	6.1
4	H	51	PRO	5.9
2	F	31	THR	5.6
1	E	32	ILE	5.5
4	H	49	PHE	5.5
3	G	185	PRO	5.1
3	G	186	THR	5.0
4	H	52	LEU	4.4
3	C	186	THR	4.4
3	G	188	HIS	3.7
1	A	30	SER	3.7
4	D	49	PHE	3.3
3	G	187	ASN	3.3
1	E	30	SER	3.3
2	F	32	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	53	HIS	2.9
1	A	32	ILE	2.9
4	H	50	LYS	2.8
4	D	52	LEU	2.8
1	A	192	HIS	2.6
3	C	184	LEU	2.5
4	H	53	HIS	2.5
4	D	28	THR	2.5
1	A	31	ASN	2.5
2	F	48	PRO	2.5
3	C	183	THR	2.4
1	E	344	ILE	2.3
2	B	48	PRO	2.3
3	C	176	TRP	2.3
4	H	45	ALA	2.3
1	A	484	ASN	2.2
4	D	31	ALA	2.2
3	G	112	ILE	2.2
4	H	31	ALA	2.2
1	E	614	ARG	2.2
1	E	31	ASN	2.2
3	C	114	TRP	2.1
1	E	191	CYS	2.0
2	F	281	ASN	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 oligosaccharides in this entry.

6.4 Ligands (i)

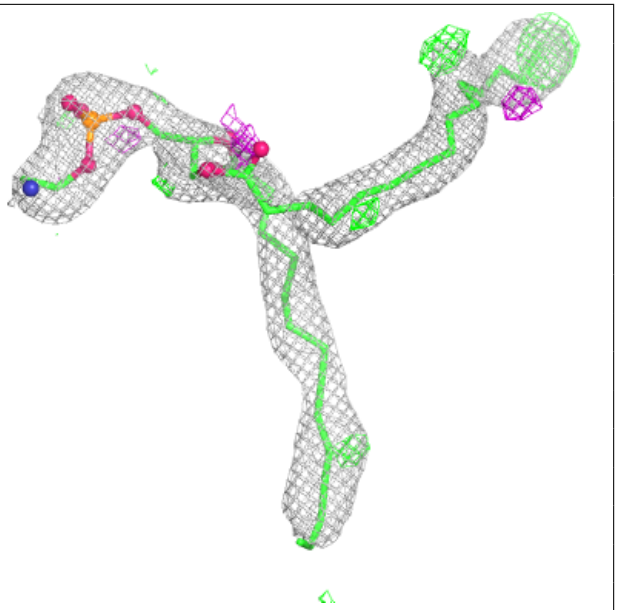
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

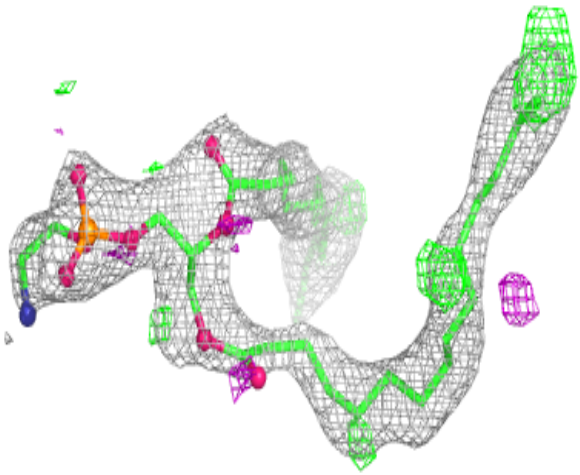
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	EPH	H	201	44/49	0.83	0.18	61,76,84,97	0
12	EPH	D	201	44/49	0.86	0.15	57,68,73,87	0
5	MLI	E	701	7/7	0.95	0.07	37,39,42,45	0
10	E23	G	202	24/24	0.95	0.07	36,42,60,61	0
10	E23	B	304	24/24	0.96	0.07	36,40,58,59	0
6	FAD	A	702	53/53	0.97	0.06	31,35,39,40	0
11	HEM	C	201	43/43	0.97	0.09	43,47,52,56	0
11	HEM	G	201	43/43	0.97	0.09	43,45,54,59	0
6	FAD	E	702	53/53	0.97	0.06	30,34,40,45	0
5	MLI	A	701	7/7	0.97	0.07	40,41,45,46	0
8	SF4	B	302	8/8	0.98	0.04	34,35,36,36	0
8	SF4	F	302	8/8	0.98	0.04	35,36,37,37	0
9	F3S	F	303	7/7	0.98	0.04	35,35,37,37	0
7	FES	F	301	4/4	0.99	0.03	32,32,33,34	0
9	F3S	B	303	7/7	0.99	0.03	35,36,38,38	0
7	FES	B	301	4/4	0.99	0.03	33,33,34,34	0

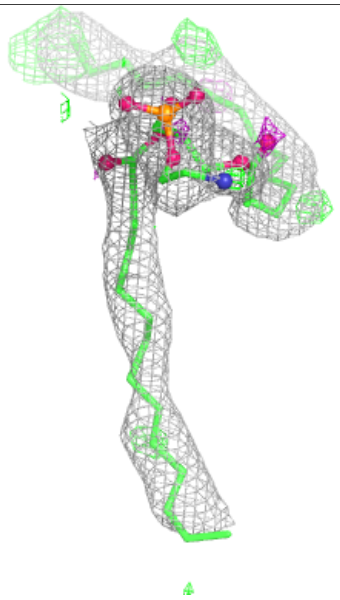
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EPH H 201:

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

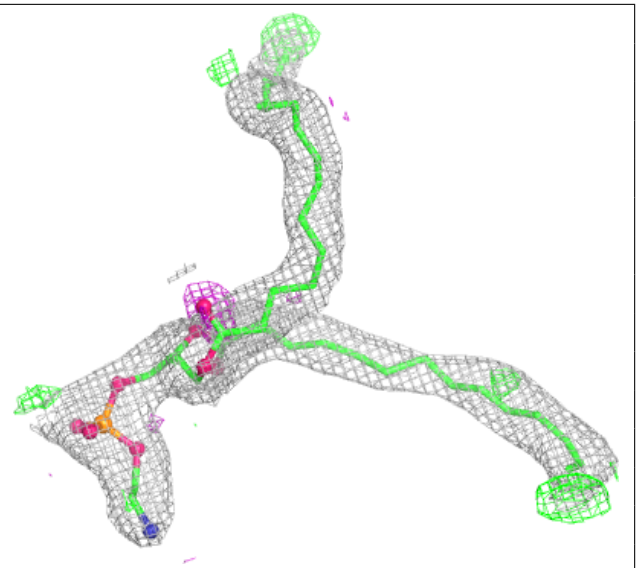


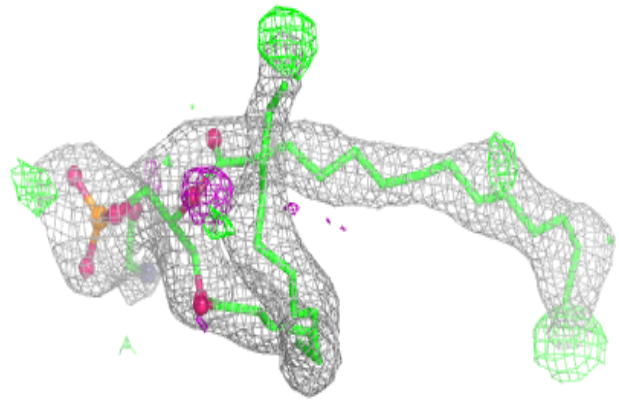


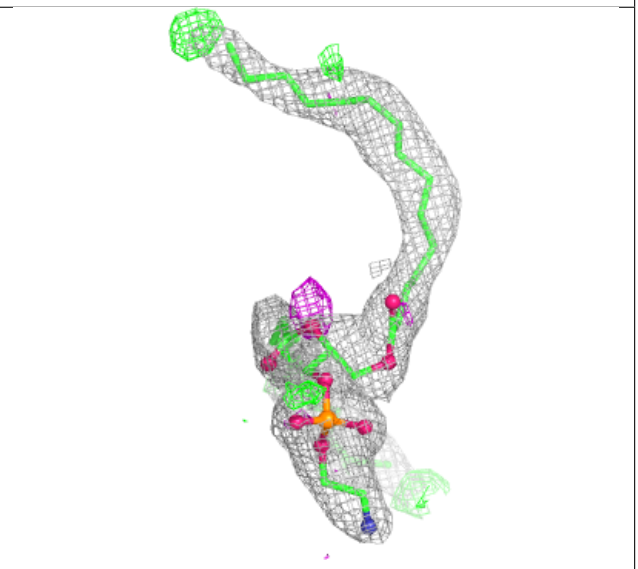


Electron density around EPH D 201:

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

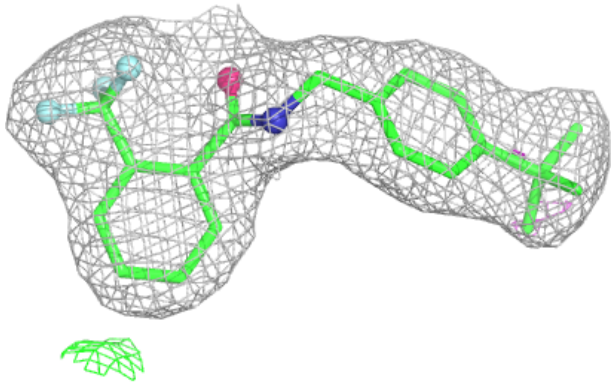


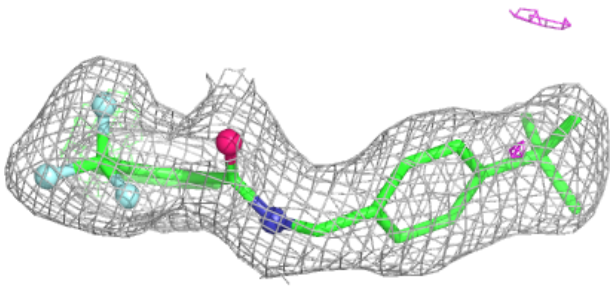


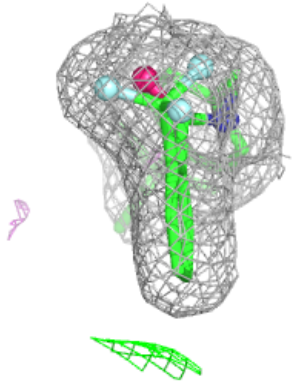


Electron density around E23 G 202:

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

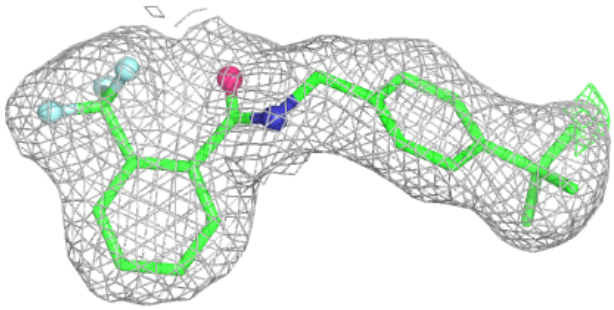


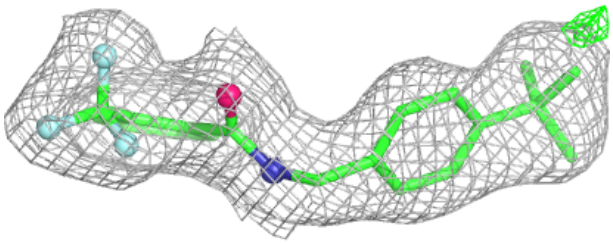


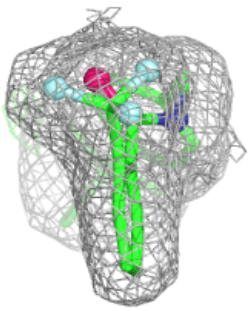


Electron density around E23 B 304:

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

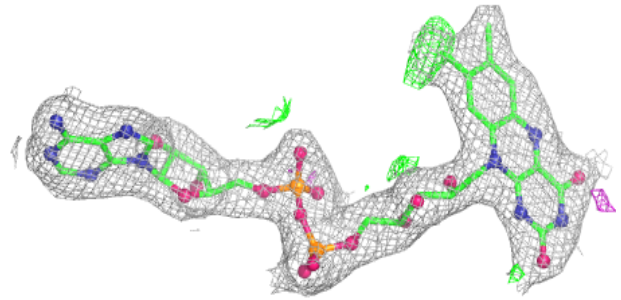


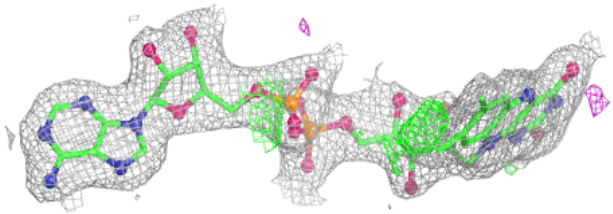


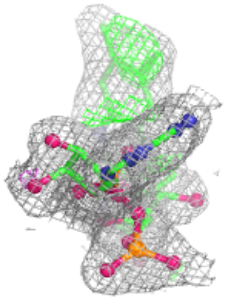


Electron density around FAD A 702:

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

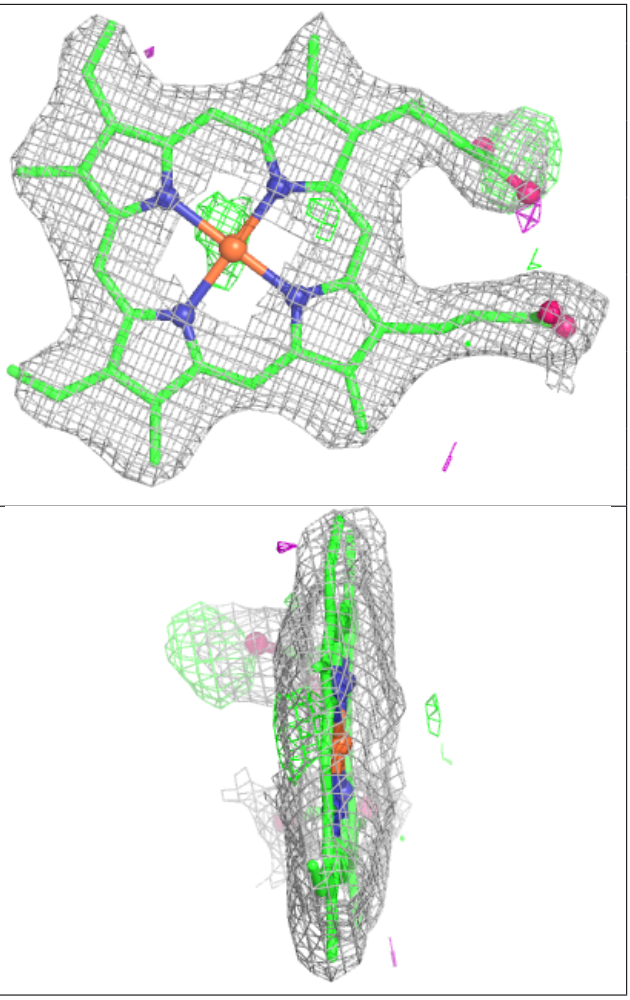






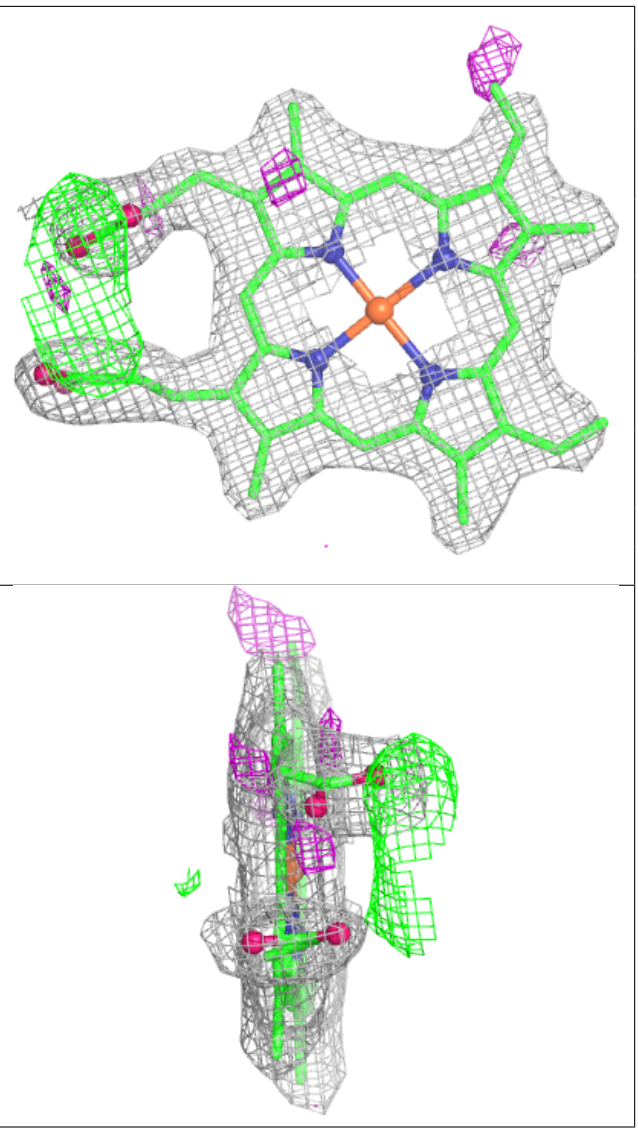
Electron density around HEM C 201:

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



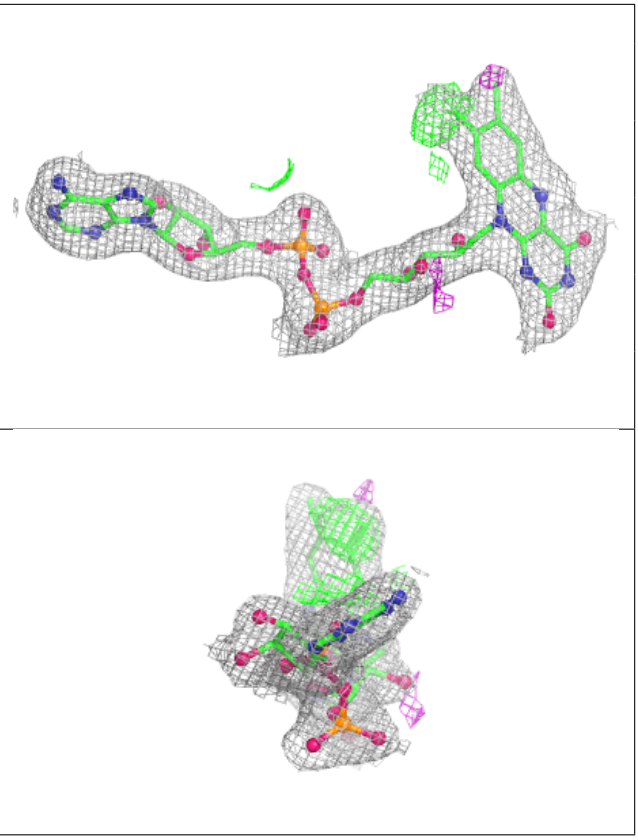
Electron density around HEM G 201:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.