Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:25 AM JST

PDB ID	:	4YTM / pdb_00004ytm
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with N-biphenyl-3-yl-2-(trifluoromethyl)benzamide
Authors	:	Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on	:	2015-03-18
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

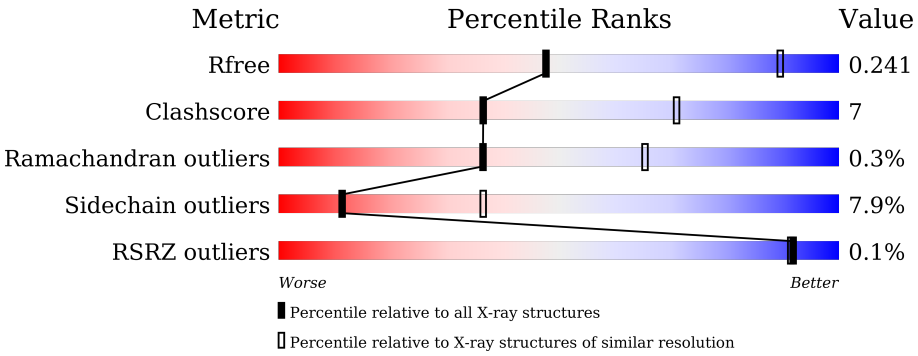
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 3.40 Å.

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



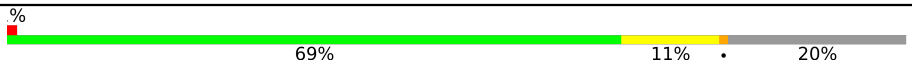
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	74% 20% • •
1	E	645	77% 18% • •
2	B	282	71% 15% • 11%
2	F	282	73% 13% • 11%
3	C	188	68% 12% • 19%

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

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Succinate dehydrogenase flavoprotein.

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

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

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

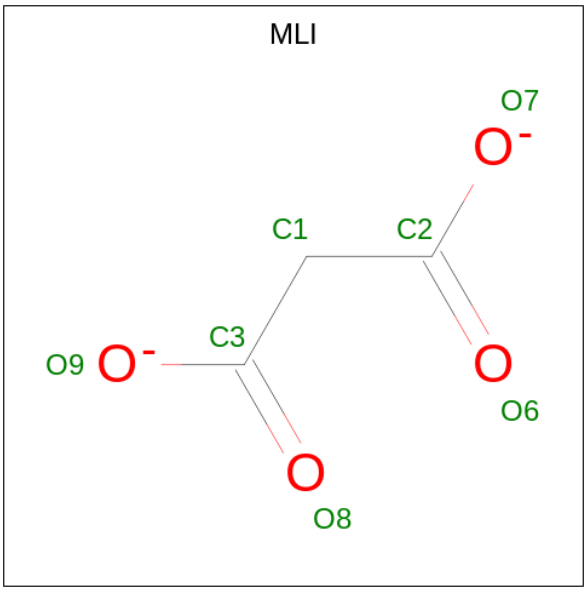
- Molecule 3 is a protein called Cytochrome b-large subunit.

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

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

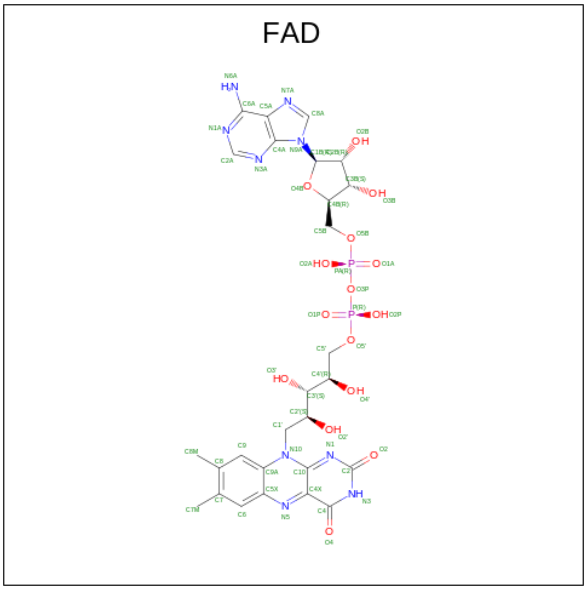
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

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



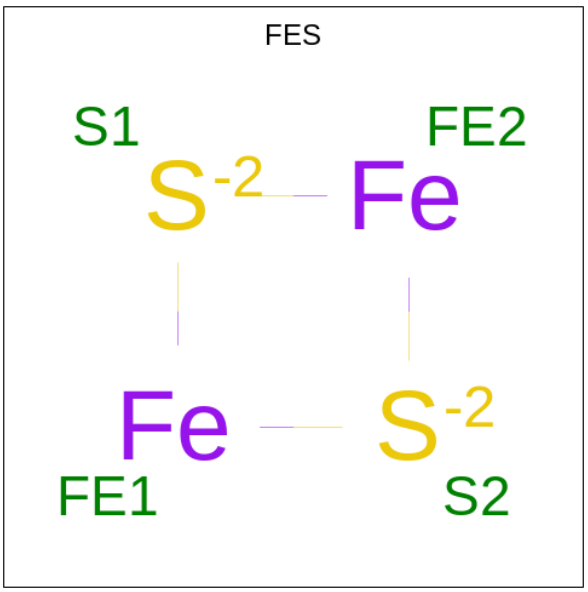
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

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



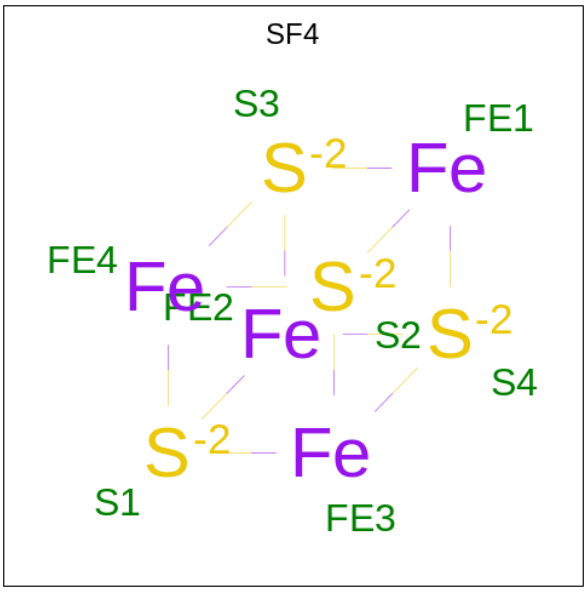
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

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



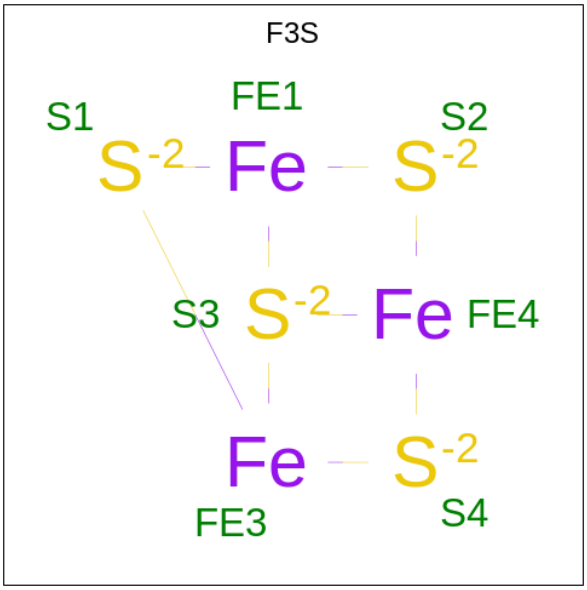
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 8 4 4	0	0

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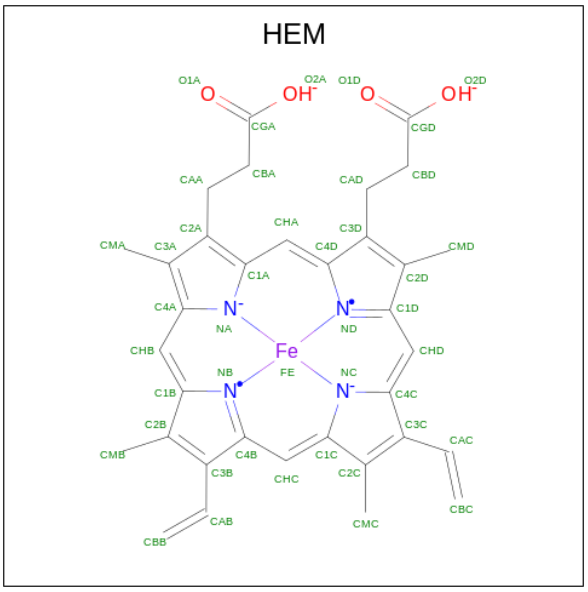
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Fe S 8 4 4	0	0

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



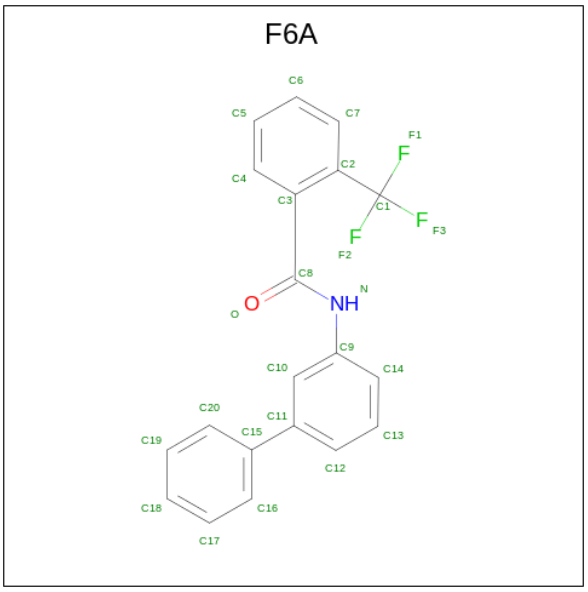
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0
9	F	1	Total Fe S 7 3 4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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-biphenyl-3-yl-2-(trifluoromethyl)benzamide (CCD ID: F6A) (formula: $C_{20}H_{14}F_3NO$).



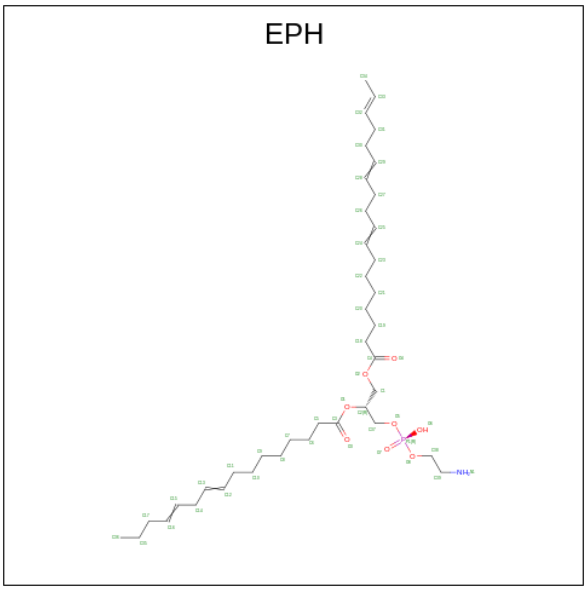
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	0	0
			25	20	3	1	1		

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

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



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

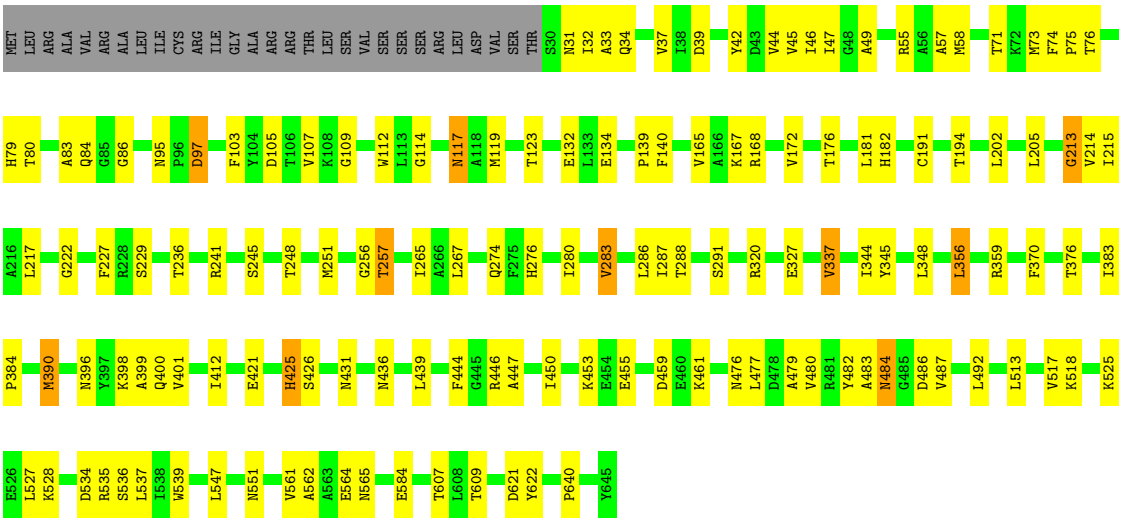
3 Residue-property plots (i)

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

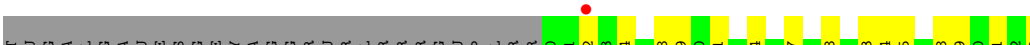
Chain A:





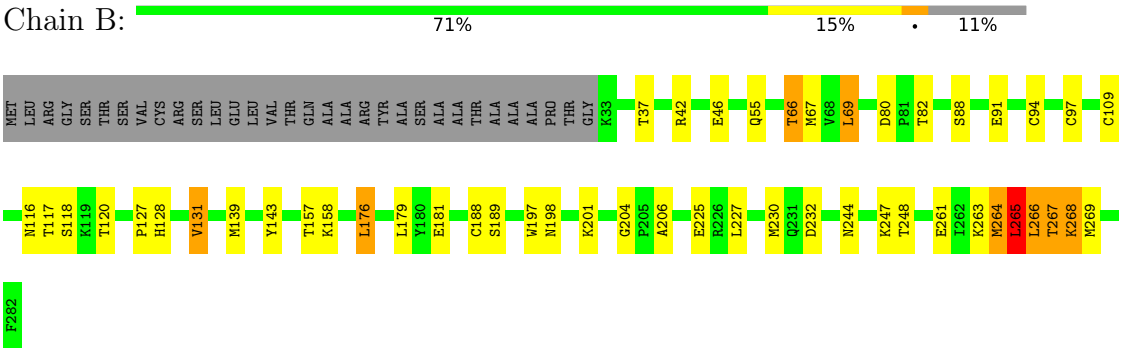
• Molecule 1: Succinate dehydrogenase flavoprotein

Chain E:



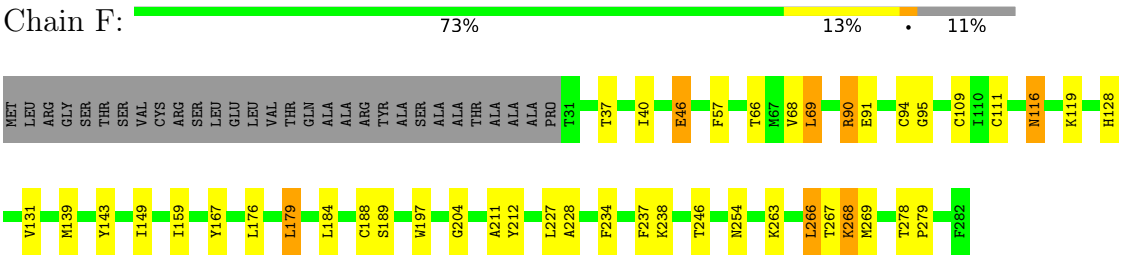
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



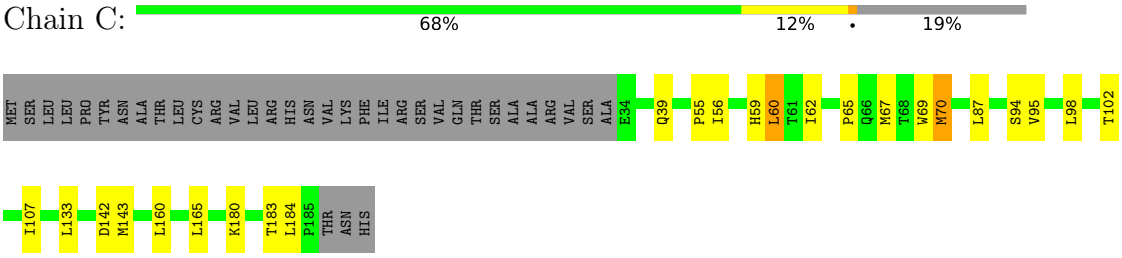
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



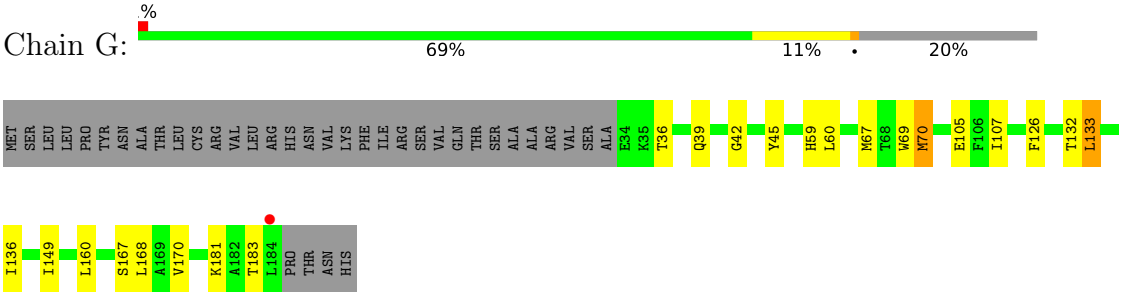
• Molecule 3: Cytochrome b-large subunit

Chain C:



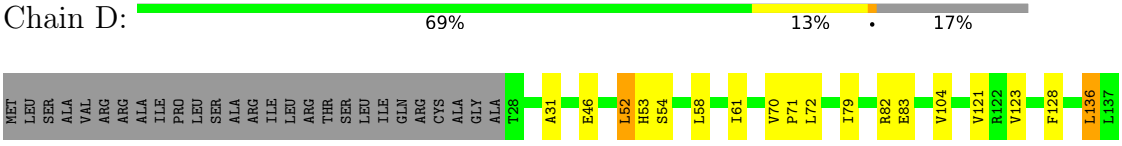
• Molecule 3: Cytochrome b-large subunit

Chain G:



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

Chain D:

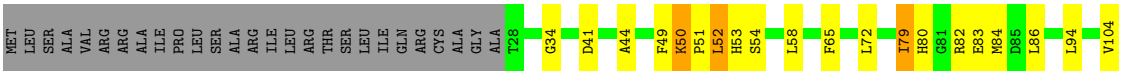




• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

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	123.65Å 126.43Å 220.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-3.40) 94.4 (20.00-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.36Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.178 , 0.245 0.180 , 0.241	Depositor DCC
R_{free} test set	2333 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	76.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18300	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

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

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, FES, EPH, HEM, FAD, MLI, F6A

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	0.56	0/4889	0.85	2/6605 (0.0%)
1	E	0.58	0/4889	0.84	1/6605 (0.0%)
2	B	0.63	0/2029	0.90	6/2739 (0.2%)
2	F	0.60	0/2038	0.86	3/2751 (0.1%)
3	C	0.56	0/1248	0.84	0/1699
3	G	0.55	0/1240	0.84	1/1687 (0.1%)
4	D	0.66	0/1030	0.85	0/1406
4	H	0.54	0/1030	0.84	0/1406
All	All	0.58	0/18393	0.85	13/24898 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	264	MET	N-CA-C	-8.06	102.50	111.28
2	B	204	GLY	CA-C-N	7.96	127.52	119.24
2	B	204	GLY	C-N-CA	7.96	127.52	119.24
2	B	94	CYS	N-CA-C	7.20	119.20	111.36
1	A	425	HIS	N-CA-C	6.67	118.56	111.28
2	B	265	LEU	N-CA-C	-6.11	104.62	111.28
1	E	425	HIS	N-CA-C	6.08	119.90	112.23
2	F	269	MET	N-CA-C	-6.08	104.97	112.38
2	F	204	GLY	CA-C-N	6.05	125.53	119.24
2	F	204	GLY	C-N-CA	6.05	125.53	119.24
1	A	213	GLY	N-CA-C	5.48	117.57	110.45
3	G	149	ILE	CB-CA-C	-5.47	108.55	114.35
2	B	198	ASN	N-CA-C	5.03	116.90	110.61

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	78	0
1	E	4787	0	4722	69	0
2	B	1985	0	2001	40	0
2	F	1994	0	2007	23	0
3	C	1210	0	1258	20	0
3	G	1203	0	1251	15	0
4	D	998	0	985	14	0
4	H	998	0	985	18	0
5	A	7	0	2	0	0
5	E	7	0	2	1	0
6	A	53	0	31	4	0
6	E	53	0	31	12	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	4	0
10	G	43	0	30	5	0
11	C	25	0	14	2	0
11	G	25	0	14	3	0
12	D	44	0	53	1	0
All	All	18300	0	18138	261	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (261) 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	1.43	1.34
2:B:267:THR:O	2:B:268:LYS:HB2	1.48	1.08
1:A:484:ASN:HD22	1:A:484:ASN:C	1.62	1.06
1:A:79:HIS:CE1	6:A:702:FAD:HM82	1.91	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LEU:HD23	2:B:265:LEU:H	1.19	1.05
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.25	0.99
1:E:79:HIS:NE2	6:E:702:FAD:HM83	1.84	0.91
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.35	0.89
2:B:265:LEU:HD23	2:B:265:LEU:N	1.85	0.87
2:B:265:LEU:N	2:B:265:LEU:CD2	2.38	0.86
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.59	0.81
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.63	0.81
1:A:484:ASN:C	1:A:484:ASN:ND2	2.36	0.79
3:C:69:TRP:CZ3	3:C:70:MET:HE3	2.17	0.79
1:E:307:MET:HB2	1:E:316:ASP:OD2	1.81	0.79
1:A:274:GLN:HB2	1:A:390:MET:HE1	1.66	0.77
4:H:49:PHE:CZ	4:H:52:LEU:HD23	2.22	0.73
1:E:432:ARG:NH1	6:E:702:FAD:H1'2	2.03	0.73
2:B:263:LYS:O	2:B:267:THR:HG23	1.89	0.73
3:C:60:LEU:HD22	11:C:202:F6A:H12	1.71	0.72
2:F:116:ASN:C	2:F:116:ASN:HD22	1.97	0.71
1:E:432:ARG:HH12	6:E:702:FAD:H1'2	1.56	0.69
2:B:267:THR:O	2:B:268:LYS:CB	2.30	0.69
2:B:227:LEU:HD22	2:B:266:LEU:CD1	2.22	0.69
2:B:261:GLU:O	2:B:265:LEU:HD23	1.93	0.68
2:B:267:THR:OG1	2:B:269:MET:HG2	1.92	0.68
3:G:60:LEU:HD22	11:G:202:F6A:H12	1.75	0.68
1:E:79:HIS:NE2	6:E:702:FAD:HM81	2.09	0.67
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.77	0.67
2:F:167:TYR:HB3	2:F:278:THR:HG22	1.77	0.66
2:F:228:ALA:O	4:H:52:LEU:HD22	1.95	0.66
2:B:263:LYS:NZ	3:C:142:ASP:OD1	2.27	0.66
4:H:108:GLY:O	4:H:122:ARG:NH2	2.28	0.66
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.78	0.66
1:A:484:ASN:ND2	1:A:484:ASN:O	2.30	0.65
2:B:267:THR:OG1	2:B:269:MET:CG	2.45	0.65
1:A:32:ILE:HG23	1:A:482:TYR:CD1	2.32	0.64
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.46	0.62
4:H:51:PRO:C	4:H:52:LEU:HG	2.23	0.62
1:E:103:PHE:HA	1:E:123:THR:HG21	1.80	0.62
1:A:492:LEU:HD21	1:A:527:LEU:HD12	1.82	0.62
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.81	0.62
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.82	0.61
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.81	0.61
2:B:261:GLU:O	2:B:265:LEU:CD2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:ASP:HB3	4:D:52:LEU:HD13	1.82	0.61
2:B:264:MET:HE1	3:C:143:MET:HB3	1.84	0.60
1:E:432:ARG:NH2	6:E:702:FAD:N1	2.49	0.59
1:A:109:GLY:O	1:A:431:ASN:HB3	2.02	0.59
3:G:133:LEU:O	3:G:136:ILE:HG13	2.01	0.59
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.38	0.59
2:F:40:ILE:HD12	2:F:57:PHE:CD1	2.38	0.59
1:A:117:ASN:N	1:A:117:ASN:HD22	2.01	0.58
4:H:50:LYS:N	4:H:51:PRO:HD3	2.18	0.58
1:E:278:THR:HG22	1:E:382:VAL:HG21	1.86	0.58
1:A:42:TYR:O	1:A:229:SER:HA	2.04	0.58
2:F:263:LYS:O	2:F:267:THR:HG23	2.04	0.57
1:A:37:VAL:O	4:D:31:ALA:HB1	2.04	0.57
1:A:55:ARG:NH1	1:A:132:GLU:OE2	2.32	0.57
1:A:117:ASN:HD22	1:A:117:ASN:H	1.52	0.56
4:H:50:LYS:H	4:H:51:PRO:HD3	1.69	0.56
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.88	0.56
1:A:565:ASN:ND2	1:A:622:TYR:OH	2.39	0.56
3:C:60:LEU:HD22	11:C:202:F6A:C12	2.35	0.56
1:A:425:HIS:N	1:A:426:SER:HA	2.19	0.56
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.56
1:A:217:LEU:HD22	1:A:477:LEU:HD11	1.87	0.56
1:E:190:ARG:O	1:E:190:ARG:HG3	2.05	0.55
2:B:263:LYS:O	2:B:264:MET:C	2.49	0.55
10:C:201:HEM:HBC2	10:C:201:HEM:HHD	1.89	0.55
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.06	0.55
3:G:60:LEU:HD22	11:G:202:F6A:C12	2.35	0.55
3:G:69:TRP:CZ3	3:G:70:MET:HE3	2.41	0.55
1:E:432:ARG:HH12	6:E:702:FAD:C1'	2.20	0.55
1:A:139:PRO:HB3	2:B:176:LEU:HD23	1.88	0.55
4:H:83:GLU:CD	4:H:83:GLU:H	2.14	0.55
1:E:451:ASN:HD22	1:E:451:ASN:N	2.04	0.55
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.41	0.55
1:E:314:ALA:O	1:E:315:LYS:HB2	2.06	0.55
3:C:180:LYS:O	3:C:184:LEU:HB2	2.08	0.54
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.90	0.54
1:E:58:MET:HE3	1:E:187:ASN:HB3	1.89	0.54
2:B:269:MET:CE	3:C:143:MET:HE3	2.38	0.53
1:E:41:ALA:HB1	1:E:462:ILE:HD13	1.90	0.53
1:E:603:TRP:HA	1:E:605:LYS:HE3	1.90	0.53
2:B:264:MET:O	2:B:268:LYS:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:201:HEM:HHC	10:C:201:HEM:HBB2	1.91	0.53
4:H:50:LYS:N	4:H:51:PRO:CD	2.72	0.53
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.90	0.53
2:F:149:ILE:HD12	2:F:211:ALA:HA	1.90	0.53
2:F:267:THR:O	2:F:268:LYS:HB2	2.08	0.53
1:E:432:ARG:NH2	5:E:701:MLI:O6	2.42	0.53
2:B:80:ASP:OD2	2:B:82:THR:OG1	2.24	0.52
1:A:551:ASN:HD22	1:A:551:ASN:N	2.06	0.52
10:G:201:HEM:HHC	10:G:201:HEM:HBB2	1.90	0.52
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.91	0.52
2:B:188:CYS:SG	2:B:206:ALA:HB2	2.50	0.52
3:G:107:ILE:HD11	4:H:156:LEU:CD1	2.35	0.52
4:D:82:ARG:NH2	4:D:140:ASN:O	2.42	0.52
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.93	0.51
1:E:438:LEU:HG	6:E:702:FAD:C2	2.39	0.51
1:E:276:HIS:CE1	1:E:286:LEU:HD11	2.46	0.51
1:E:425:HIS:HB2	1:E:427:VAL:HG13	1.92	0.51
1:A:95:ASN:HD21	1:A:167:LYS:HB2	1.75	0.50
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.75	0.50
1:E:517:VAL:HG13	1:E:561:VAL:HG12	1.92	0.50
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.44	0.50
2:B:128:HIS:O	2:B:128:HIS:ND1	2.42	0.50
1:E:47:ILE:HD11	1:E:214:VAL:CG2	2.41	0.50
1:E:307:MET:HE2	1:E:323:VAL:HG22	1.94	0.50
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.47	0.49
1:A:621:ASP:OD1	1:A:622:TYR:N	2.44	0.49
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.93	0.49
1:E:427:VAL:HG11	1:E:444:PHE:CE1	2.47	0.49
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.93	0.49
1:E:91:LEU:HD23	1:E:127:VAL:HG13	1.94	0.49
1:E:297:PHE:CE2	1:E:350:HIS:CE1	3.00	0.49
1:E:185:TYR:O	1:E:188:SER:OG	2.27	0.49
1:A:33:ALA:HB2	1:A:482:TYR:HE1	1.78	0.49
1:A:476:ASN:O	1:A:480:VAL:HG23	2.12	0.49
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.94	0.49
1:A:280:ILE:HD11	1:A:287:ILE:HD11	1.95	0.48
1:E:513:LEU:O	1:E:517:VAL:HG23	2.13	0.48
1:A:114:GLY:C	1:A:119:MET:HE2	2.39	0.48
2:B:263:LYS:O	2:B:266:LEU:N	2.47	0.48
1:A:479:ALA:O	1:A:483:ALA:HB2	2.13	0.48
2:B:197:TRP:HH2	3:C:60:LEU:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.94	0.48
3:C:94:SER:HB3	4:D:138:TYR:CD1	2.49	0.48
3:C:107:ILE:HD11	4:D:156:LEU:HD11	1.95	0.48
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.95	0.48
1:A:83:ALA:HA	6:A:702:FAD:C6	2.44	0.48
1:A:58:MET:HA	1:A:191:CYS:SG	2.54	0.48
1:E:286:LEU:HD22	6:E:702:FAD:C6	2.43	0.48
1:A:76:THR:HG23	1:A:182:HIS:NE2	2.29	0.48
1:A:265:ILE:HD13	1:A:401:VAL:HG11	1.95	0.48
1:E:434:GLY:O	1:E:435:ALA:HB3	2.14	0.47
2:F:94:CYS:SG	2:F:95:GLY:N	2.87	0.47
1:A:49:ALA:HB1	1:A:75:PRO:HB3	1.96	0.47
2:B:188:CYS:SG	2:B:189:SER:N	2.86	0.47
10:G:201:HEM:HHD	10:G:201:HEM:HBC2	1.95	0.47
1:A:398:LYS:O	1:A:399:ALA:HB3	2.14	0.47
1:A:276:HIS:O	1:A:384:PRO:HA	2.14	0.47
1:A:257:THR:HG22	1:A:267:LEU:HD22	1.97	0.47
1:A:356:LEU:HD23	1:A:376:THR:HG22	1.95	0.47
1:A:103:PHE:HA	1:A:123:THR:HG21	1.97	0.47
1:E:190:ARG:O	1:E:190:ARG:CG	2.61	0.47
1:E:536:SER:HB2	2:F:46:GLU:OE1	2.16	0.46
1:E:627:ASP:O	1:E:637:TRP:HB2	2.15	0.46
2:F:188:CYS:SG	2:F:189:SER:N	2.89	0.46
1:A:222:GLY:O	1:A:537:LEU:HD13	2.14	0.46
2:B:157:THR:O	2:B:158:LYS:C	2.58	0.46
4:D:70:VAL:N	4:D:71:PRO:HD2	2.31	0.46
1:E:32:ILE:HG13	1:E:32:ILE:O	2.14	0.46
1:E:432:ARG:CZ	1:E:437:SER:HB2	2.46	0.46
2:B:264:MET:O	2:B:265:LEU:C	2.57	0.46
1:A:344:ILE:HG22	1:A:345:TYR:N	2.32	0.45
2:F:90:ARG:H	2:F:90:ARG:HD2	1.82	0.45
1:A:517:VAL:HG13	1:A:561:VAL:HG12	1.98	0.45
1:A:97:ASP:OD2	1:A:168:ARG:NH1	2.50	0.45
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.99	0.45
4:D:104:VAL:HG13	4:D:121:VAL:HG12	1.99	0.45
3:C:107:ILE:HD11	4:D:156:LEU:CD1	2.47	0.45
3:G:69:TRP:CH2	3:G:70:MET:HE3	2.52	0.45
2:B:66:THR:HG23	2:B:67:MET:HG2	1.99	0.45
1:A:534:ASP:OD2	1:A:536:SER:OG	2.29	0.45
1:E:73:MET:HE3	1:E:78:SER:HA	1.99	0.45
3:G:69:TRP:CZ2	11:G:202:F6A:C18	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.47	0.44
1:E:551:ASN:N	1:E:551:ASN:HD22	2.15	0.44
1:E:191:CYS:O	1:E:192:HIS:C	2.59	0.44
1:E:79:HIS:CE1	6:E:702:FAD:HM81	2.52	0.44
1:E:79:HIS:CD2	6:E:702:FAD:HM83	2.50	0.44
1:A:79:HIS:O	1:A:80:THR:C	2.60	0.44
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.99	0.44
4:H:49:PHE:HZ	4:H:52:LEU:HD23	1.79	0.44
4:H:79:ILE:HD11	4:H:84:MET:HE3	1.98	0.44
1:A:241:ARG:NH2	1:A:248:THR:O	2.51	0.44
1:A:75:PRO:O	1:A:181:LEU:HD21	2.18	0.44
1:A:446:ARG:HD3	1:A:450:ILE:HD11	1.98	0.44
3:G:126:PHE:HA	3:G:167:SER:OG	2.17	0.44
1:A:396:ASN:HD21	1:A:400:GLN:HB2	1.81	0.44
1:E:255:ASP:OD1	1:E:255:ASP:N	2.50	0.44
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.53	0.44
3:G:42:GLY:O	3:G:45:TYR:HB3	2.18	0.44
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.53	0.44
1:E:390:MET:HE3	1:E:431:ASN:HA	2.00	0.43
2:F:69:LEU:HD12	2:F:109:CYS:HB3	1.99	0.43
1:A:337:VAL:HG11	1:A:345:TYR:CD1	2.54	0.43
1:E:215:ILE:HD11	1:E:224:ILE:CG2	2.48	0.43
1:E:395:THR:HA	1:E:400:GLN:O	2.19	0.43
1:E:591:ILE:N	1:E:591:ILE:HD12	2.34	0.43
2:F:246:THR:OG1	2:F:254:ASN:OD1	2.33	0.43
1:E:356:LEU:HD23	1:E:375:VAL:HG23	2.01	0.43
1:A:45:VAL:HG23	1:A:229:SER:HB3	2.01	0.43
2:B:267:THR:HG1	2:B:269:MET:H	1.63	0.43
3:C:98:LEU:HD12	3:C:102:THR:OG1	2.19	0.43
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.33	0.43
3:G:132:THR:HG23	10:G:201:HEM:CAB	2.49	0.43
4:H:109:ARG:HB2	4:H:112:VAL:HG12	1.99	0.43
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.89	0.43
1:E:307:MET:CB	1:E:316:ASP:OD2	2.58	0.43
1:E:103:PHE:O	1:E:107:VAL:HG23	2.19	0.43
1:E:152:SER:O	1:E:293:GLY:HA3	2.18	0.43
1:A:32:ILE:CG1	1:A:32:ILE:O	2.66	0.42
2:B:264:MET:HB2	2:B:265:LEU:CD2	2.49	0.42
1:E:140:PHE:HA	1:E:172:VAL:HG22	2.00	0.42
2:F:179:LEU:HD21	2:F:212:TYR:CD2	2.54	0.42
1:A:283:VAL:HG21	1:A:370:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:CYS:O	2:B:97:CYS:SG	2.77	0.42
4:D:138:TYR:CD1	4:D:138:TYR:C	2.98	0.42
2:F:128:HIS:O	2:F:128:HIS:ND1	2.52	0.42
2:F:68:VAL:HG23	2:F:111:CYS:O	2.20	0.42
1:E:32:ILE:HG23	1:E:482:TYR:CD1	2.55	0.42
2:F:237:PHE:CZ	2:F:266:LEU:HD23	2.55	0.42
1:A:46:ILE:HD12	1:A:57:ALA:HB2	2.01	0.42
3:C:95:VAL:O	3:C:95:VAL:HG12	2.19	0.42
1:A:33:ALA:HB2	1:A:482:TYR:CE1	2.53	0.42
1:A:107:VAL:HG13	1:A:119:MET:HE1	2.02	0.42
2:B:266:LEU:HD12	2:B:266:LEU:HA	1.82	0.42
4:D:151:GLU:HG2	12:D:201:EPH:O6	2.20	0.42
1:E:47:ILE:HD11	1:E:214:VAL:HG21	2.01	0.42
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.50	0.42
2:B:127:PRO:HG3	3:C:62:ILE:HD11	2.01	0.41
2:F:237:PHE:CE1	2:F:266:LEU:HD23	2.55	0.41
4:H:41:ASP:HB3	4:H:44:ALA:HB3	2.02	0.41
1:A:73:MET:SD	1:A:251:MET:HG3	2.60	0.41
1:A:86:GLY:HA2	1:A:176:THR:HG21	2.01	0.41
1:E:276:HIS:HB2	1:E:387:HIS:HB2	2.01	0.41
1:E:278:THR:HG21	1:E:346:LEU:HD22	2.03	0.41
1:A:213:GLY:HA3	1:A:227:PHE:O	2.20	0.41
4:D:136:LEU:HD12	4:D:136:LEU:HA	1.93	0.41
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.02	0.41
2:F:197:TRP:HH2	3:G:60:LEU:HD21	1.86	0.41
1:A:327:GLU:OE2	1:A:384:PRO:HD3	2.20	0.41
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.55	0.41
4:D:52:LEU:H	4:D:52:LEU:HG	1.27	0.41
3:G:168:LEU:C	3:G:170:VAL:H	2.29	0.41
2:B:264:MET:CE	3:C:143:MET:HB3	2.47	0.41
3:C:95:VAL:O	3:C:95:VAL:CG1	2.69	0.41
4:H:80:HIS:ND1	4:H:151:GLU:OE1	2.53	0.41
1:A:337:VAL:HG21	1:A:345:TYR:CD2	2.56	0.41
1:A:47:ILE:HD11	1:A:214:VAL:HG22	2.02	0.41
2:B:69:LEU:HB2	2:B:109:CYS:HA	2.03	0.41
10:C:201:HEM:HHA	10:C:201:HEM:CBD	2.49	0.41
1:E:603:TRP:O	1:E:605:LYS:N	2.54	0.41
4:H:65:PHE:CE2	4:H:94:LEU:HD23	2.55	0.41
1:E:74:PHE:HA	1:E:75:PRO:HD3	1.96	0.41
1:A:134:GLU:C	1:A:134:GLU:CD	2.89	0.40
1:E:432:ARG:NH2	6:E:702:FAD:C2	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:36:THR:OG1	3:G:39:GLN:HG3	2.22	0.40
1:A:74:PHE:CD1	2:B:143:TYR:CE2	3.09	0.40
1:A:202:LEU:HB2	1:A:215:ILE:HG23	2.03	0.40
1:A:291:SER:HB2	1:A:348:LEU:HD21	2.02	0.40
4:D:52:LEU:O	4:D:53:HIS:C	2.63	0.40
2:F:167:TYR:CD1	2:F:279:PRO:HD2	2.56	0.40
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.57	0.40
3:G:132:THR:HG23	10:G:201:HEM:CBB	2.51	0.40
1:A:84:GLN:OE1	1:A:288:THR:HB	2.21	0.40
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.22	0.40
3:C:87:LEU:HD22	4:D:128:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/645 (95%)	566 (92%)	46 (8%)	2 (0%)	36	65
1	E	614/645 (95%)	577 (94%)	35 (6%)	2 (0%)	36	65
2	B	248/282 (88%)	228 (92%)	17 (7%)	3 (1%)	10	35
2	F	250/282 (89%)	229 (92%)	21 (8%)	0	100	100
3	C	150/188 (80%)	145 (97%)	5 (3%)	0	100	100
3	G	149/188 (79%)	140 (94%)	9 (6%)	0	100	100
4	D	127/156 (81%)	124 (98%)	3 (2%)	0	100	100
4	H	127/156 (81%)	119 (94%)	8 (6%)	0	100	100
All	All	2279/2542 (90%)	2128 (93%)	144 (6%)	7 (0%)	36	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	ASN
1	E	604	ARG
2	B	268	LYS
1	A	31	ASN
1	A	421	GLU
2	B	88	SER
1	E	485	GLY

5.3.2 Protein sidechains (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%)	466 (93%)	36 (7%)	13 39
1	E	502/527 (95%)	463 (92%)	39 (8%)	11 37
2	B	220/242 (91%)	200 (91%)	20 (9%)	9 30
2	F	220/242 (91%)	205 (93%)	15 (7%)	14 40
3	C	126/158 (80%)	117 (93%)	9 (7%)	13 39
3	G	125/158 (79%)	117 (94%)	8 (6%)	16 42
4	D	98/119 (82%)	88 (90%)	10 (10%)	7 25
4	H	98/119 (82%)	86 (88%)	12 (12%)	5 19
All	All	1891/2092 (90%)	1742 (92%)	149 (8%)	11 36

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	39	ASP
1	A	44	VAL
1	A	71	THR
1	A	97	ASP
1	A	117	ASN
1	A	165	VAL
1	A	194	THR
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	245	SER
1	A	257	THR
1	A	283	VAL
1	A	320	ARG
1	A	337	VAL
1	A	356	LEU
1	A	359	ARG
1	A	383	ILE
1	A	390	MET
1	A	412	ILE
1	A	436	ASN
1	A	439	LEU
1	A	453	LYS
1	A	455	GLU
1	A	459	ASP
1	A	461	LYS
1	A	484	ASN
1	A	486	ASP
1	A	487	VAL
1	A	518	LYS
1	A	525	LYS
1	A	528	LYS
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	584	GLU
1	A	609	THR
2	B	37	THR
2	B	66	THR
2	B	69	LEU
2	B	91	GLU
2	B	117	THR
2	B	118	SER
2	B	120	THR
2	B	131	VAL
2	B	139	MET
2	B	176	LEU
2	B	179	LEU
2	B	181	GLU
2	B	225	GLU
2	B	230	MET
2	B	244	ASN

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Mol	Chain	Res	Type
2	B	247	LYS
2	B	248	THR
2	B	265	LEU
2	B	266	LEU
2	B	267	THR
3	C	56	ILE
3	C	59	HIS
3	C	60	LEU
3	C	67	MET
3	C	70	MET
3	C	133	LEU
3	C	160	LEU
3	C	165	LEU
3	C	183	THR
4	D	46	GLU
4	D	52	LEU
4	D	54	SER
4	D	58	LEU
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	83	GLU
4	D	123	VAL
4	D	136	LEU
1	E	34	GLN
1	E	39	ASP
1	E	44	VAL
1	E	81	THR
1	E	117	ASN
1	E	179	SER
1	E	190	ARG
1	E	193	CYS
1	E	194	THR
1	E	205	LEU
1	E	241	ARG
1	E	245	SER
1	E	255	ASP
1	E	257	THR
1	E	261	THR
1	E	283	VAL
1	E	298	LEU
1	E	320	ARG

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Mol	Chain	Res	Type
1	E	337	VAL
1	E	344	ILE
1	E	356	LEU
1	E	358	GLN
1	E	359	ARG
1	E	422	CYS
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	461	LYS
1	E	484	ASN
1	E	525	LYS
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	539	TRP
1	E	547	LEU
1	E	561	VAL
1	E	592	GLU
1	E	595	THR
1	E	596	LYS
2	F	37	THR
2	F	46	GLU
2	F	66	THR
2	F	69	LEU
2	F	90	ARG
2	F	91	GLU
2	F	116	ASN
2	F	119	LYS
2	F	131	VAL
2	F	159	ILE
2	F	176	LEU
2	F	179	LEU
2	F	184	LEU
2	F	266	LEU
2	F	268	LYS
3	G	59	HIS
3	G	67	MET
3	G	70	MET
3	G	105	GLU
3	G	133	LEU
3	G	160	LEU

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Mol	Chain	Res	Type
3	G	181	LYS
3	G	183	THR
4	H	50	LYS
4	H	52	LEU
4	H	53	HIS
4	H	54	SER
4	H	58	LEU
4	H	72	LEU
4	H	79	ILE
4	H	82	ARG
4	H	86	LEU
4	H	122	ARG
4	H	123	VAL
4	H	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	95	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	156	GLN
1	A	178	HIS
1	A	347	GLN
1	A	431	ASN
1	A	436	ASN
1	A	476	ASN
1	A	484	ASN
1	A	497	GLN
1	A	550	GLN
1	A	551	ASN
1	A	565	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	160	ASN
2	B	165	GLN
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN

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Mol	Chain	Res	Type
1	E	355	GLN
1	E	358	GLN
1	E	431	ASN
1	E	436	ASN
1	E	484	ASN
1	E	497	GLN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
1	E	558	GLN
1	E	611	GLN
2	F	55	GLN
2	F	105	ASN
2	F	112	ASN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
2	F	210	GLN
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)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MLI	E	701	-	6,6,6	1.18	0	7,7,7	1.33	1 (14%)
9	F3S	B	303	2	0,9,9	-	-	-		
7	FES	B	301	2	0,4,4	-	-	-		
8	SF4	F	302	2	0,12,12	-	-	-		
10	HEM	C	201	3,4	50,50,50	1.56	7 (14%)	66,82,82	1.88	18 (27%)
6	FAD	A	702	-	56,58,58	1.47	10 (17%)	81,89,89	1.84	25 (30%)
8	SF4	B	302	2	0,12,12	-	-	-		
11	F6A	G	202	-	27,27,27	1.07	1 (3%)	38,38,38	0.90	1 (2%)
6	FAD	E	702	-	56,58,58	1.44	10 (17%)	81,89,89	1.83	23 (28%)
10	HEM	G	201	3,4	50,50,50	1.60	7 (14%)	66,82,82	1.90	19 (28%)
12	EPH	D	201	-	43,43,48	1.11	2 (4%)	45,48,53	1.01	4 (8%)
11	F6A	C	202	-	27,27,27	1.21	1 (3%)	38,38,38	0.82	0
9	F3S	F	303	2	0,9,9	-	-	-		
7	FES	F	301	2	0,4,4	-	-	-		
5	MLI	A	701	-	6,6,6	1.28	0	7,7,7	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	E	701	-	-	0/4/4/4	-
10	HEM	C	201	3,4	-	5/14/54/54	-
11	F6A	G	202	-	-	0/18/18/18	0/3/3/3
7	FES	B	301	2	-	-	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
6	FAD	A	702	-	-	6/34/50/50	0/6/6/6
8	SF4	B	302	2	-	-	0/6/5/5
9	F3S	B	303	2	-	-	0/3/3/3
6	FAD	E	702	-	-	6/34/50/50	0/6/6/6
10	HEM	G	201	3,4	-	8/14/54/54	-
12	EPH	D	201	-	-	27/47/47/52	-
11	F6A	C	202	-	-	2/18/18/18	0/3/3/3
9	F3S	F	303	2	-	-	0/3/3/3
7	FES	F	301	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	A	701	-	-	0/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	202	F6A	C3-C2	5.69	1.50	1.40
10	G	201	HEM	FE-NB	5.66	2.12	1.94
10	C	201	HEM	FE-NB	5.27	2.11	1.94
6	E	702	FAD	C9A-C5X	5.08	1.49	1.41
11	G	202	F6A	C3-C2	4.89	1.48	1.40
6	A	702	FAD	C9A-C5X	4.74	1.49	1.41
12	D	201	EPH	O1-C3	4.59	1.47	1.34
12	D	201	EPH	O2-C4	4.49	1.46	1.33
6	A	702	FAD	C5A-C4A	4.20	1.46	1.39
10	G	201	HEM	FE-NC	4.10	2.09	1.95
6	E	702	FAD	C5A-C4A	3.90	1.46	1.39
10	C	201	HEM	FE-NC	3.85	2.08	1.95
10	C	201	HEM	C1B-NB	-3.27	1.34	1.40
10	G	201	HEM	C1B-NB	-3.18	1.34	1.40
6	A	702	FAD	C4-N3	-3.12	1.33	1.38
10	G	201	HEM	C3B-C4B	2.95	1.50	1.44
10	C	201	HEM	C3B-C4B	2.94	1.50	1.44
6	A	702	FAD	C5A-C6A	2.83	1.48	1.41
6	A	702	FAD	C8A-N7A	2.64	1.36	1.31
6	E	702	FAD	C8A-N7A	2.62	1.36	1.31
6	A	702	FAD	C8-C7	2.58	1.47	1.40
6	E	702	FAD	C8-C7	2.56	1.47	1.40
6	E	702	FAD	C5A-C6A	2.54	1.48	1.41
6	A	702	FAD	C4A-N9A	-2.49	1.32	1.37
6	E	702	FAD	C4A-N9A	-2.46	1.32	1.37
10	G	201	HEM	C4D-ND	-2.44	1.36	1.40
6	E	702	FAD	C4-N3	-2.39	1.34	1.38
6	A	702	FAD	C5X-N5	-2.34	1.34	1.39
10	C	201	HEM	C1C-C2C	-2.31	1.40	1.45
6	E	702	FAD	C5X-N5	-2.28	1.35	1.39
6	A	702	FAD	C2-N3	-2.25	1.33	1.39
10	C	201	HEM	C4D-ND	-2.23	1.36	1.40
6	E	702	FAD	C5A-N7A	-2.21	1.34	1.39
6	E	702	FAD	C4X-N5	2.20	1.35	1.30
10	G	201	HEM	C1D-ND	-2.17	1.34	1.38
10	G	201	HEM	C1C-C2C	-2.15	1.41	1.45
10	C	201	HEM	C4B-NB	-2.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	FAD	C4X-N5	2.02	1.34	1.30

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	201	HEM	CAD-C3D-C4D	5.63	134.50	124.66
10	C	201	HEM	CAD-C3D-C4D	5.63	134.50	124.66
6	E	702	FAD	C5A-C4A-N3A	-5.60	119.45	126.75
6	A	702	FAD	C5A-C4A-N3A	-4.67	120.66	126.75
10	C	201	HEM	C1B-NB-C4B	4.40	109.62	105.07
10	C	201	HEM	C4C-NC-C1C	4.31	109.57	105.35
10	G	201	HEM	C4C-NC-C1C	4.26	109.52	105.35
6	A	702	FAD	N3A-C2A-N1A	-4.25	121.95	128.60
6	E	702	FAD	C2A-N3A-C4A	4.12	121.47	111.75
6	A	702	FAD	C2A-N3A-C4A	3.92	121.02	111.75
6	E	702	FAD	N3A-C2A-N1A	-3.91	122.49	128.60
6	E	702	FAD	N3A-C4A-N9A	3.88	133.47	127.08
12	D	201	EPH	O1-C3-C5	3.85	119.79	111.50
10	C	201	HEM	CAD-C3D-C2D	-3.79	120.81	127.88
10	G	201	HEM	CHD-C1D-ND	3.78	128.52	124.42
6	A	702	FAD	C4A-N9A-C8A	3.73	109.77	105.73
10	G	201	HEM	C1B-NB-C4B	3.66	108.85	105.07
10	G	201	HEM	CAD-C3D-C2D	-3.65	121.07	127.88
10	C	201	HEM	CHD-C1D-ND	3.65	128.38	124.42
10	G	201	HEM	CAC-C3C-C4C	3.56	133.50	124.90
6	A	702	FAD	N3A-C4A-N9A	3.56	132.95	127.08
6	E	702	FAD	C4A-C5A-N7A	-3.53	106.31	110.62
6	A	702	FAD	C4A-C5A-N7A	-3.45	106.42	110.62
6	A	702	FAD	C6A-C5A-N7A	3.37	138.31	132.02
10	G	201	HEM	CBD-CAD-C3D	3.36	121.97	112.63
6	E	702	FAD	O2-C2-N1	-3.31	116.34	121.83
10	G	201	HEM	CHB-C1B-NB	3.28	128.42	124.37
6	A	702	FAD	O4B-C1B-N9A	3.24	114.44	108.06
6	E	702	FAD	O4B-C1B-N9A	3.22	114.41	108.06
10	C	201	HEM	CAC-C3C-C4C	3.21	132.65	124.90
10	C	201	HEM	CHB-C1B-NB	3.18	128.30	124.37
10	C	201	HEM	CBD-CAD-C3D	3.11	121.25	112.63
6	A	702	FAD	C4'-C3'-C2'	-3.02	107.09	113.36
6	A	702	FAD	N9A-C8A-N7A	-2.99	109.82	113.91
12	D	201	EPH	O2-C4-C18	2.95	121.16	111.91
6	A	702	FAD	C5A-N7A-C8A	2.88	107.60	103.51
6	A	702	FAD	C4X-C10-N1	-2.84	118.13	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	702	FAD	C4X-C10-N10	2.84	120.64	116.48
6	A	702	FAD	C4-C4X-N5	2.83	122.26	118.23
6	E	702	FAD	C5A-N7A-C8A	2.75	107.42	103.51
6	E	702	FAD	C4A-N9A-C8A	2.74	108.70	105.73
10	C	201	HEM	CMD-C2D-C1D	2.74	129.21	125.04
6	A	702	FAD	P-O3P-PA	-2.73	123.44	132.83
10	G	201	HEM	CMD-C2D-C1D	2.72	129.18	125.04
6	E	702	FAD	C4-C4X-N5	2.71	122.08	118.23
6	A	702	FAD	O2-C2-N1	-2.68	117.39	121.83
6	E	702	FAD	C4X-C10-N1	-2.66	118.55	124.73
6	E	702	FAD	O2'-C2'-C3'	-2.66	102.62	109.10
10	C	201	HEM	CHD-C1D-C2D	-2.65	120.84	124.98
6	A	702	FAD	C4X-C10-N10	2.64	120.34	116.48
6	A	702	FAD	C2A-N1A-C6A	2.64	123.30	118.77
10	C	201	HEM	O2D-CGD-CBD	2.62	122.44	114.03
6	E	702	FAD	C6A-C5A-N7A	2.58	136.82	132.02
10	C	201	HEM	CHC-C1C-NC	2.57	127.22	124.44
10	G	201	HEM	CAC-C3C-C2C	-2.55	120.20	128.60
12	D	201	EPH	O2-C4-O4	-2.53	117.20	123.59
6	E	702	FAD	N9A-C8A-N7A	-2.50	110.50	113.91
6	E	702	FAD	C9A-N10-C10	-2.49	116.89	120.77
10	C	201	HEM	CAC-C3C-C2C	-2.46	120.52	128.60
6	A	702	FAD	C4A-N9A-C1B	-2.45	120.75	126.59
10	G	201	HEM	CHA-C4D-ND	2.44	127.38	124.37
6	E	702	FAD	C1'-N10-C9A	2.42	124.55	120.51
6	E	702	FAD	C1'-C2'-C3'	2.40	116.50	109.79
10	C	201	HEM	O2D-CGD-O1D	-2.39	117.34	123.30
10	G	201	HEM	O2D-CGD-CBD	2.37	121.66	114.03
6	E	702	FAD	O4-C4-C4X	-2.37	120.31	126.60
10	C	201	HEM	CHA-C4D-ND	2.35	127.27	124.37
6	A	702	FAD	N3-C2-N1	2.33	123.96	119.38
6	E	702	FAD	C10-N1-C2	2.32	121.55	116.90
10	G	201	HEM	CHD-C1D-C2D	-2.30	121.38	124.98
10	C	201	HEM	CHA-C4D-C3D	-2.29	121.03	125.33
6	A	702	FAD	O2'-C2'-C3'	-2.26	103.61	109.10
6	A	702	FAD	C9-C8-C7	2.25	122.89	119.67
10	G	201	HEM	CAB-C3B-C2B	-2.23	121.25	128.60
11	G	202	F6A	F1-C1-C2	-2.22	108.83	112.70
5	E	701	MLI	O7-C2-C1	2.20	121.58	114.54
10	G	201	HEM	CHA-C4D-C3D	-2.19	121.21	125.33
10	G	201	HEM	CAA-CBA-CGA	-2.18	108.92	113.60
6	E	702	FAD	P-O3P-PA	-2.17	125.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	702	FAD	O2A-PA-O1A	2.14	122.84	112.24
6	E	702	FAD	C2A-N1A-C6A	2.12	122.40	118.77
10	G	201	HEM	CHB-C1B-C2B	-2.10	120.89	126.73
10	G	201	HEM	CHC-C1C-NC	2.08	126.69	124.44
12	D	201	EPH	O1-C3-O3	-2.07	118.69	123.70
6	A	702	FAD	C4-N3-C2	-2.07	121.81	125.64
6	A	702	FAD	C10-N1-C2	2.07	121.03	116.90
10	G	201	HEM	C4B-C3B-C2B	-2.06	105.48	107.11
6	E	702	FAD	C9-C8-C7	2.03	122.58	119.67
10	C	201	HEM	C4B-C3B-C2B	-2.02	105.51	107.11
10	C	201	HEM	CAB-C3B-C2B	-2.02	121.96	128.60
6	A	702	FAD	C9A-N10-C10	-2.00	117.64	120.77

There are no chirality outliers.

All (54) 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	PA-O3P-P-O5'
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
10	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	O8-C38-C39-N1
12	D	201	EPH	O4-C4-O2-C1
12	D	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C18-C4-O2-C1
12	D	201	EPH	C5-C3-O1-C2
12	D	201	EPH	C4-C18-C19-C20
12	D	201	EPH	C3-C5-C6-C7
12	D	201	EPH	C11-C10-C9-C8
10	C	201	HEM	C4C-C3C-CAC-CBC
10	G	201	HEM	C4C-C3C-CAC-CBC
12	D	201	EPH	C9-C10-C11-C12
10	G	201	HEM	C2A-CAA-CBA-CGA
12	D	201	EPH	C7-C8-C9-C10
10	C	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	O2-C1-C2-C37

Continued on next page...

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C12-C13-C14-C15
12	D	201	EPH	C13-C14-C15-C16
10	G	201	HEM	C3D-CAD-CBD-CGD
6	E	702	FAD	PA-O3P-P-O5'
12	D	201	EPH	C28-C29-C30-C31
12	D	201	EPH	C5-C6-C7-C8
12	D	201	EPH	O1-C2-C37-O5
10	C	201	HEM	C4B-C3B-CAB-CBB
10	G	201	HEM	C4B-C3B-CAB-CBB
12	D	201	EPH	O2-C1-C2-O1
6	A	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	P-O3P-PA-O1A
12	D	201	EPH	C2-C1-O2-C4
12	D	201	EPH	C1-C2-C37-O5
12	D	201	EPH	C38-O8-P1-O5
6	A	702	FAD	P-O3P-PA-O1A
12	D	201	EPH	C1-C2-O1-C3
6	E	702	FAD	P-O3P-PA-O2A
6	A	702	FAD	O4B-C4B-C5B-O5B
12	D	201	EPH	C10-C11-C12-C13
12	D	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C24-C25-C26-C27
10	G	201	HEM	CAA-CBA-CGA-O2A
6	E	702	FAD	O4B-C4B-C5B-O5B
11	C	202	F6A	C10-C9-N-C8
12	D	201	EPH	C38-O8-P1-O7
12	D	201	EPH	C18-C19-C20-C21
10	G	201	HEM	CAA-CBA-CGA-O1A
11	C	202	F6A	C14-C9-N-C8

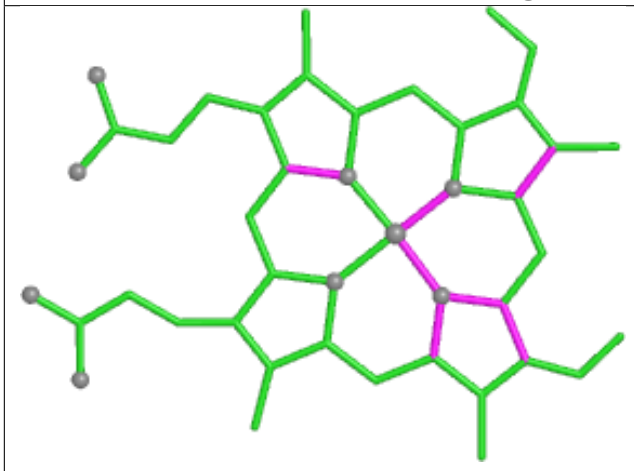
There are no ring outliers.

8 monomers are involved in 32 short contacts:

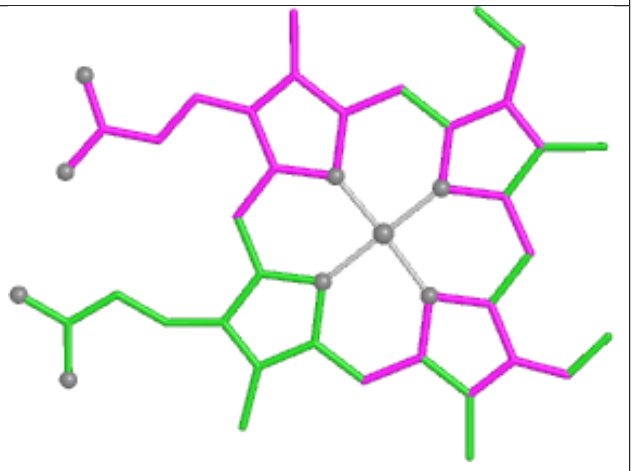
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	701	MLI	1	0
10	C	201	HEM	4	0
6	A	702	FAD	4	0
11	G	202	F6A	3	0
6	E	702	FAD	12	0
10	G	201	HEM	5	0
12	D	201	EPH	1	0
11	C	202	F6A	2	0

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.

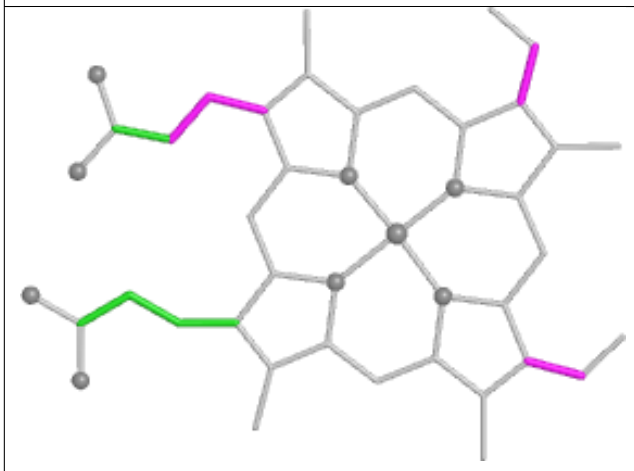
Ligand HEM C 201



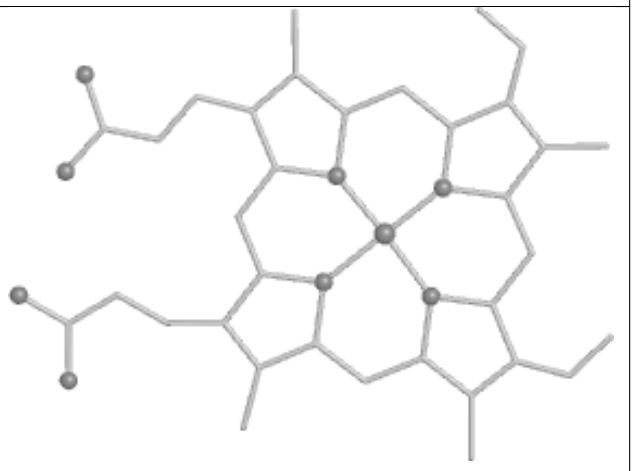
Bond lengths



Bond angles

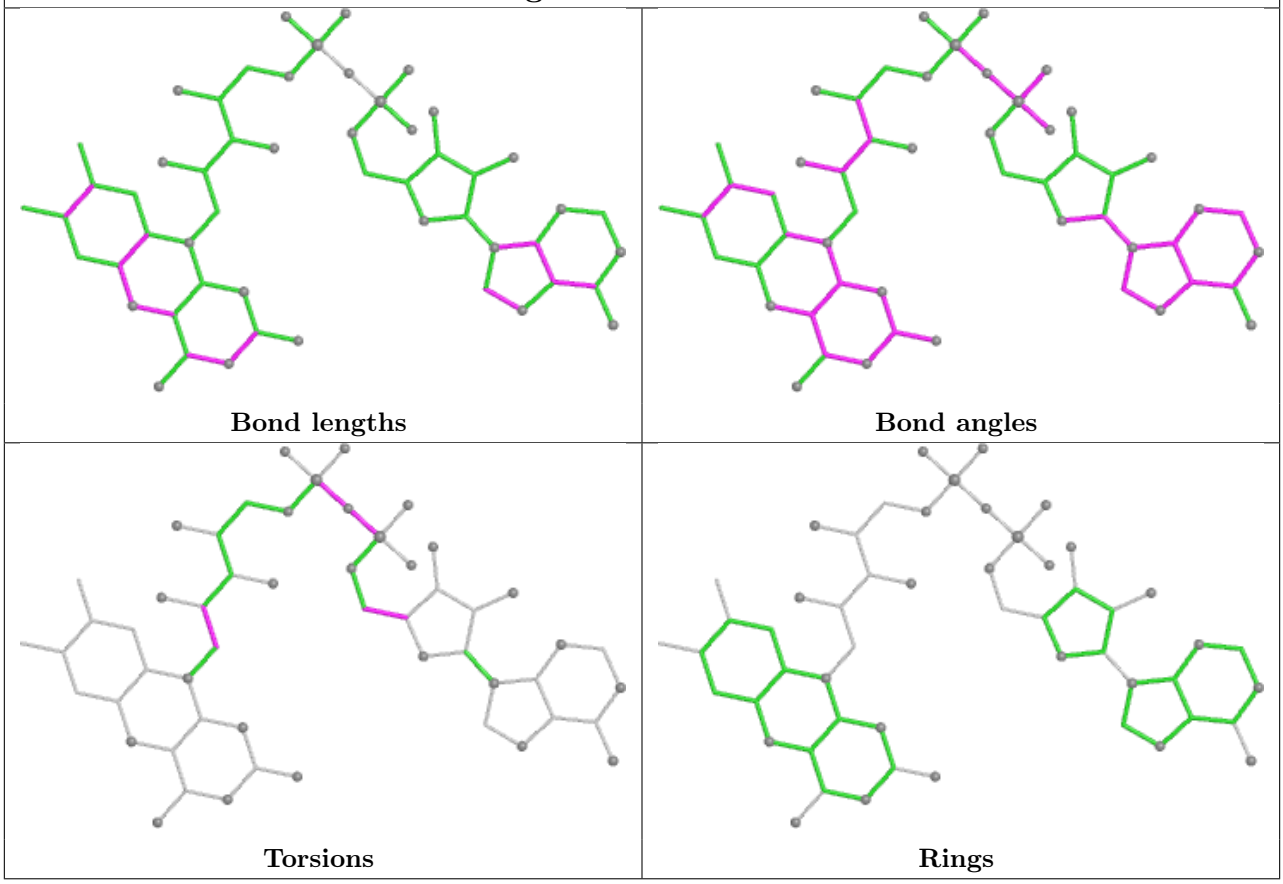


Torsions

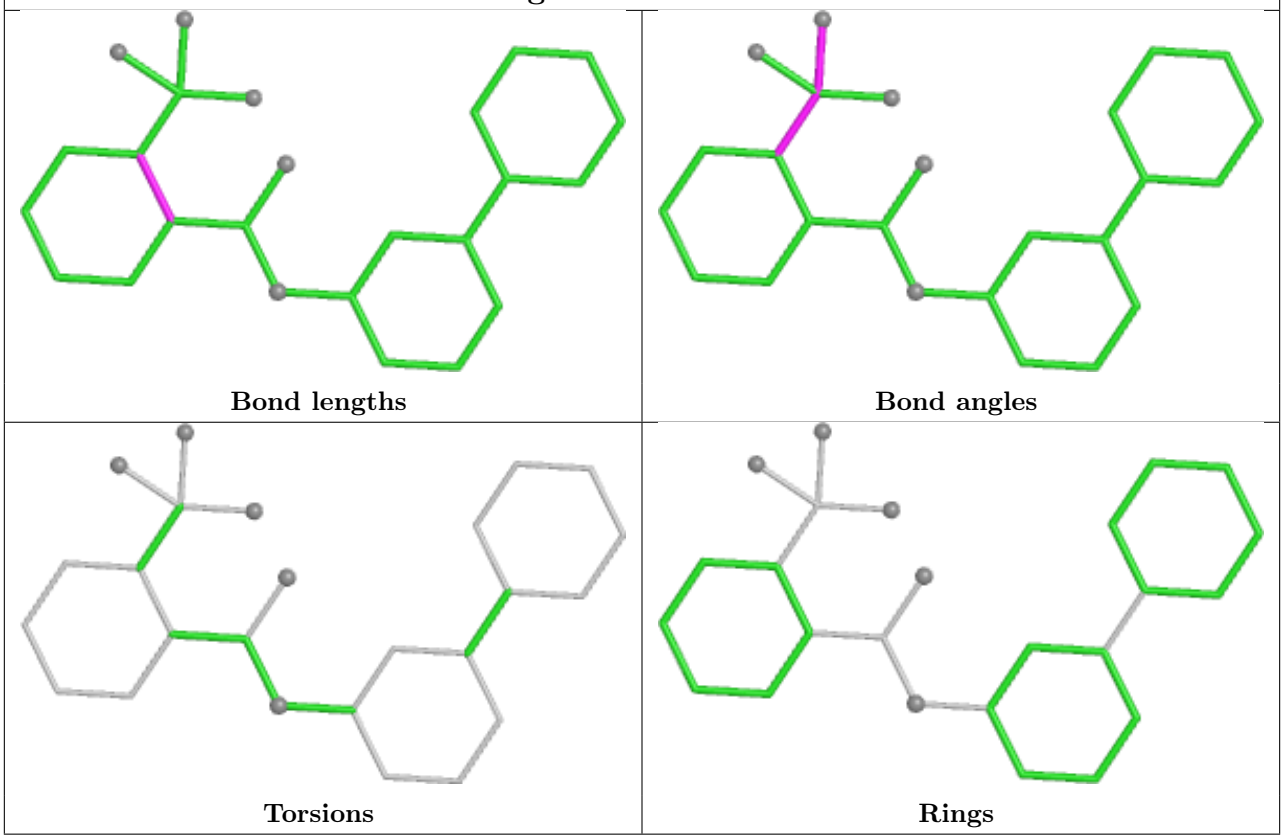


Rings

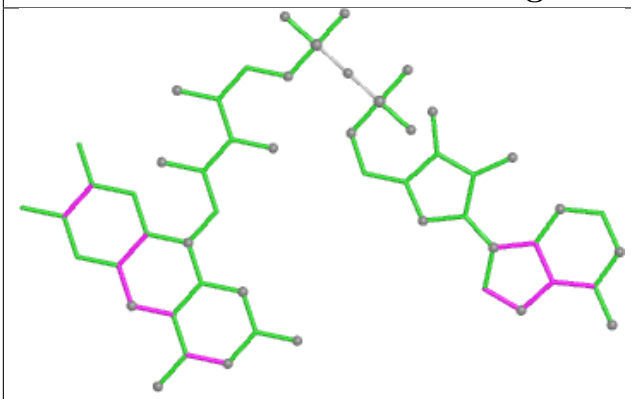
Ligand FAD A 702



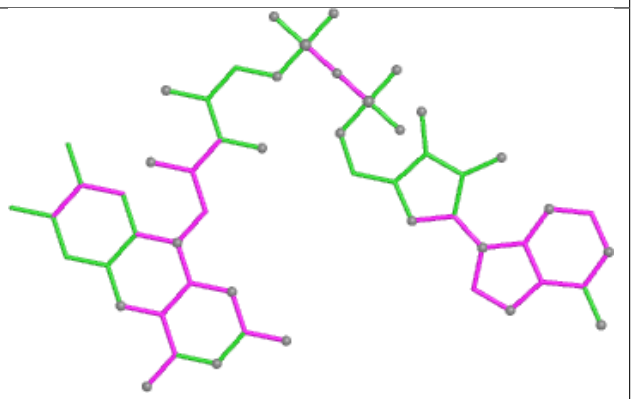
Ligand F6A G 202



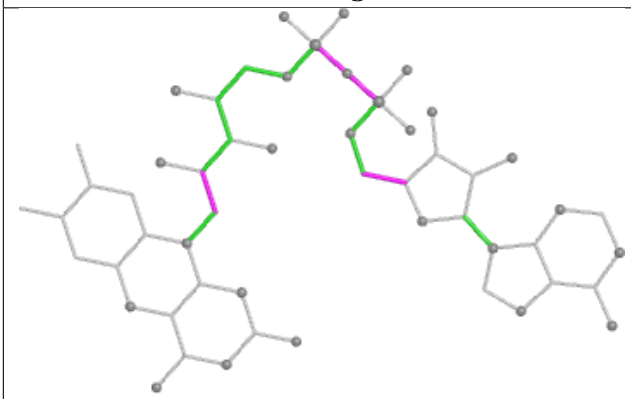
Ligand FAD E 702



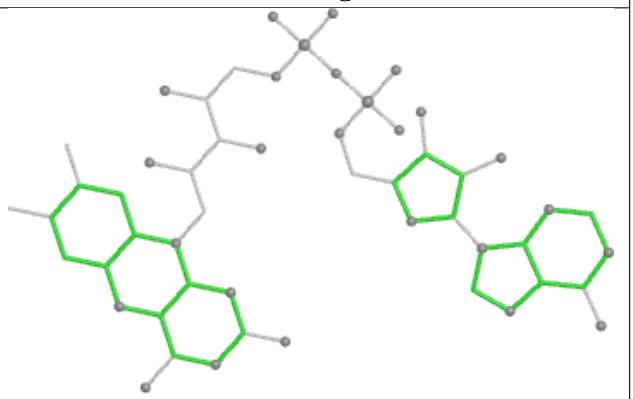
Bond lengths



Bond angles

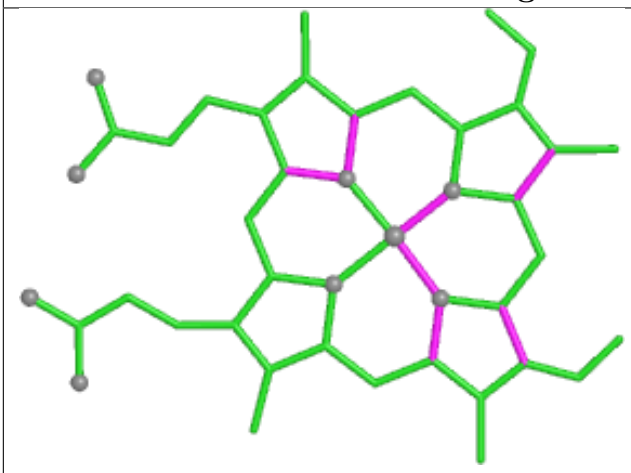


Torsions

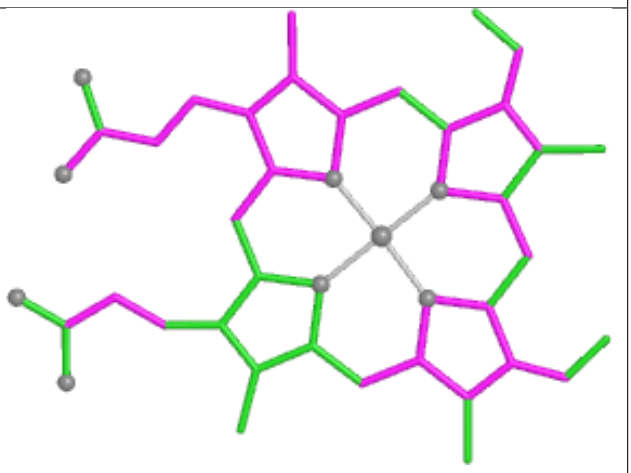


Rings

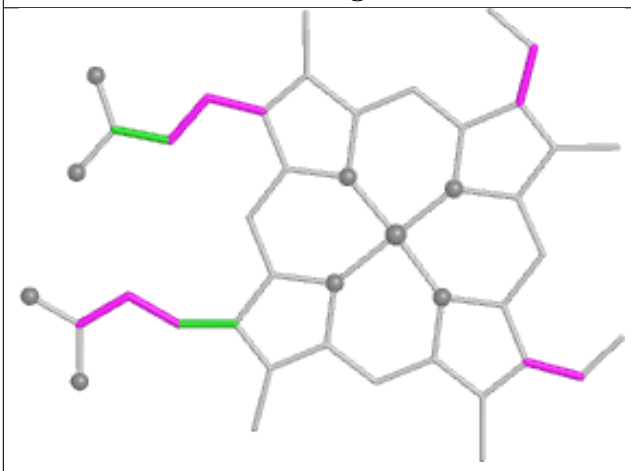
Ligand HEM G 201



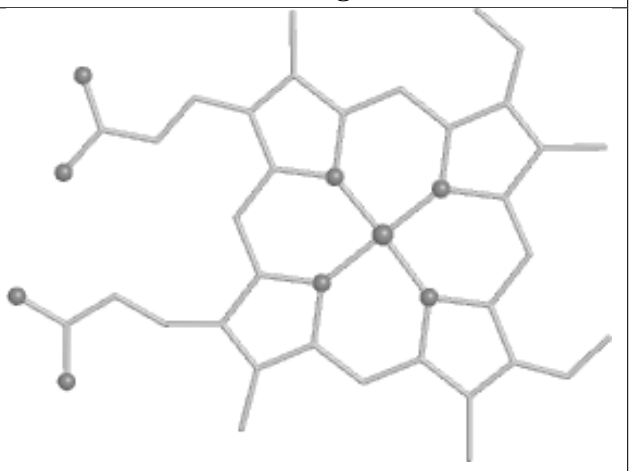
Bond lengths



Bond angles

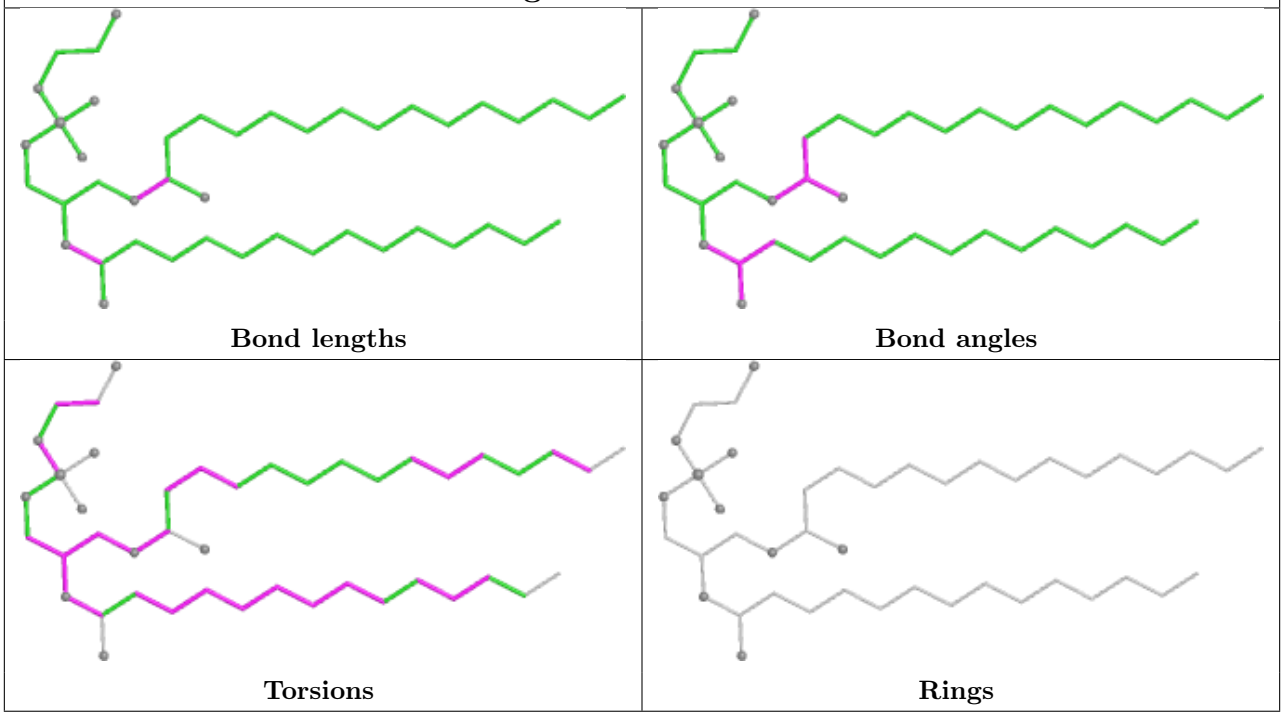


Torsions

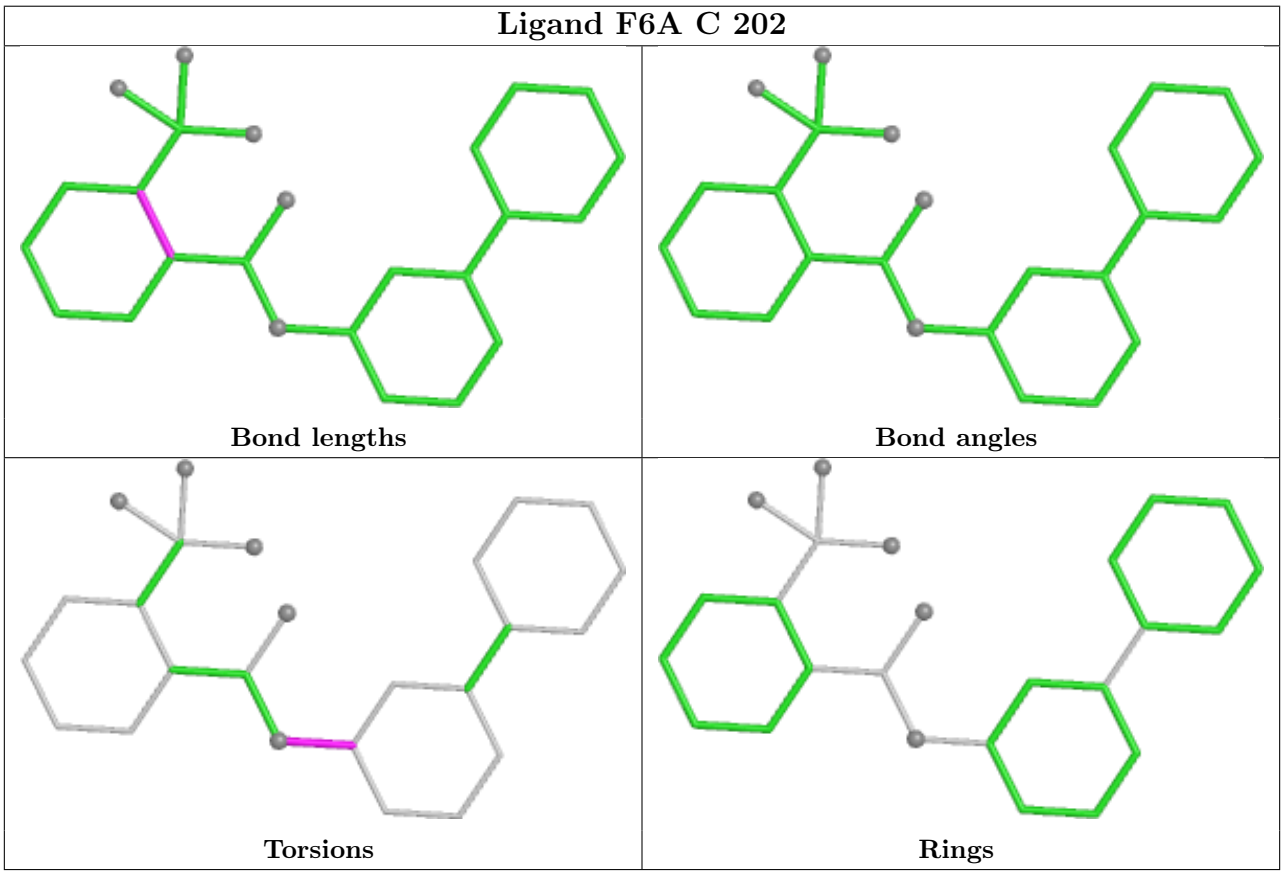


Rings

Ligand EPH D 201



Ligand F6A C 202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.49	0 100 100	44, 75, 107, 145	0
1	E	616/645 (95%)	-0.45	1 (0%) 91 87	46, 77, 114, 140	0
2	B	250/282 (88%)	-0.49	0 100 100	42, 68, 100, 122	0
2	F	252/282 (89%)	-0.50	0 100 100	47, 65, 99, 131	0
3	C	152/188 (80%)	-0.43	0 100 100	51, 78, 116, 148	0
3	G	151/188 (80%)	-0.38	1 (0%) 84 73	52, 82, 142, 155	0
4	D	129/156 (82%)	-0.46	0 100 100	57, 81, 115, 143	0
4	H	129/156 (82%)	-0.43	0 100 100	55, 84, 130, 171	0
All	All	2295/2542 (90%)	-0.46	2 (0%) 92 91	42, 76, 115, 171	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	32	ILE	2.3
3	G	184	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

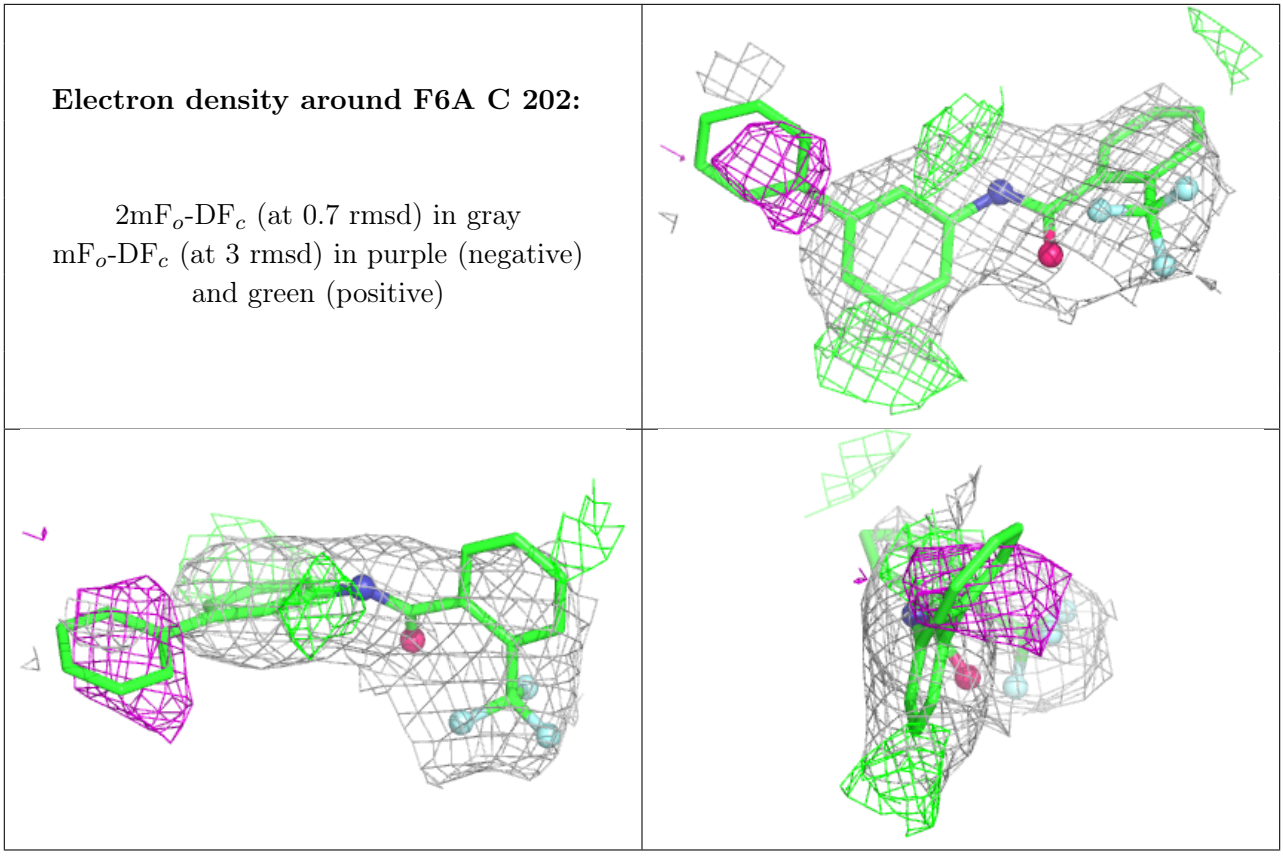
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	F6A	C	202	25/25	0.89	0.17	92,97,138,138	0
12	EPH	D	201	44/49	0.91	0.14	75,100,118,123	0
5	MLI	A	701	7/7	0.93	0.14	68,72,80,85	0
11	F6A	G	202	25/25	0.94	0.10	67,80,98,100	0
5	MLI	E	701	7/7	0.94	0.15	71,74,77,79	0
6	FAD	E	702	53/53	0.95	0.07	46,52,58,59	0
10	HEM	G	201	43/43	0.97	0.11	69,90,101,106	0
6	FAD	A	702	53/53	0.97	0.06	42,46,56,57	0
7	FES	F	301	4/4	0.98	0.05	46,46,49,50	0
10	HEM	C	201	43/43	0.98	0.10	78,87,96,107	0
7	FES	B	301	4/4	0.99	0.04	51,55,55,56	0
8	SF4	B	302	8/8	0.99	0.03	39,42,46,47	0
8	SF4	F	302	8/8	0.99	0.03	35,37,41,42	0
9	F3S	B	303	7/7	0.99	0.04	43,52,58,60	0
9	F3S	F	303	7/7	0.99	0.05	49,60,62,67	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.

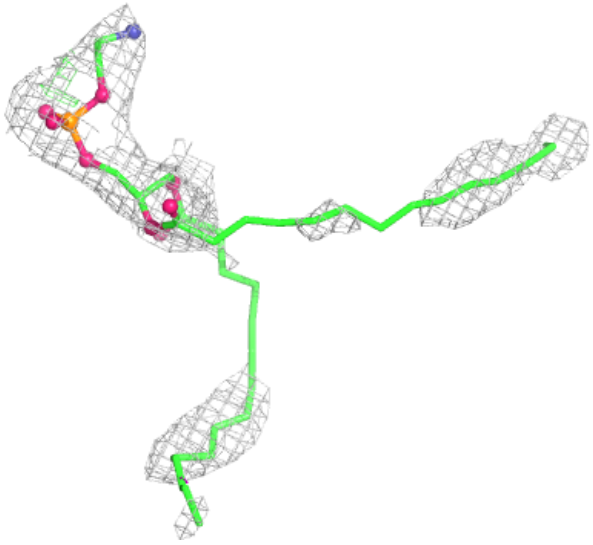
Electron density around F6A C 202:

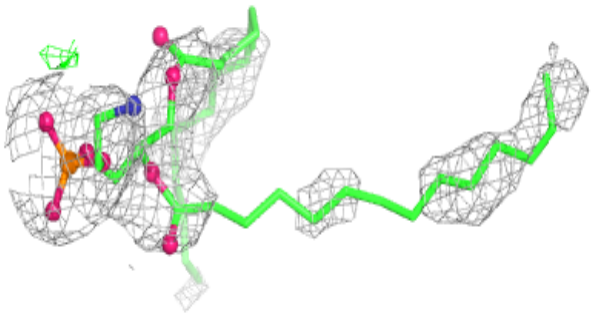
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

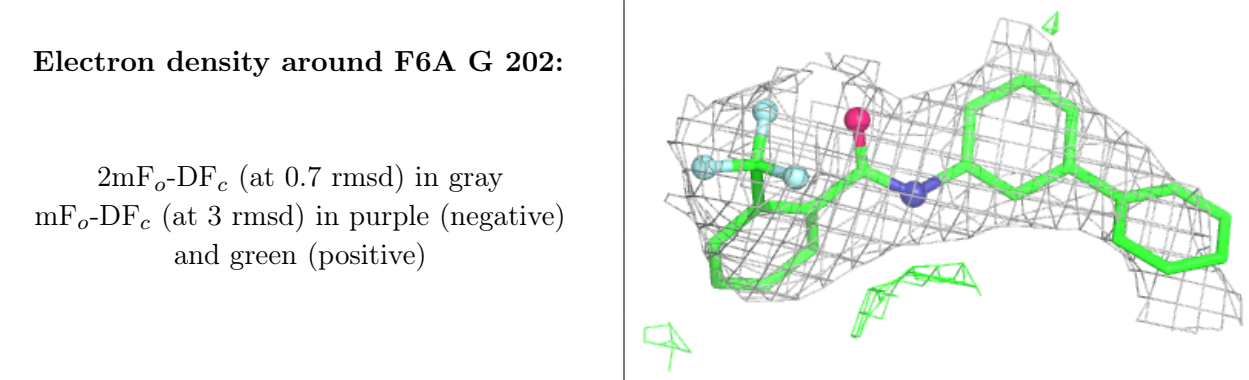






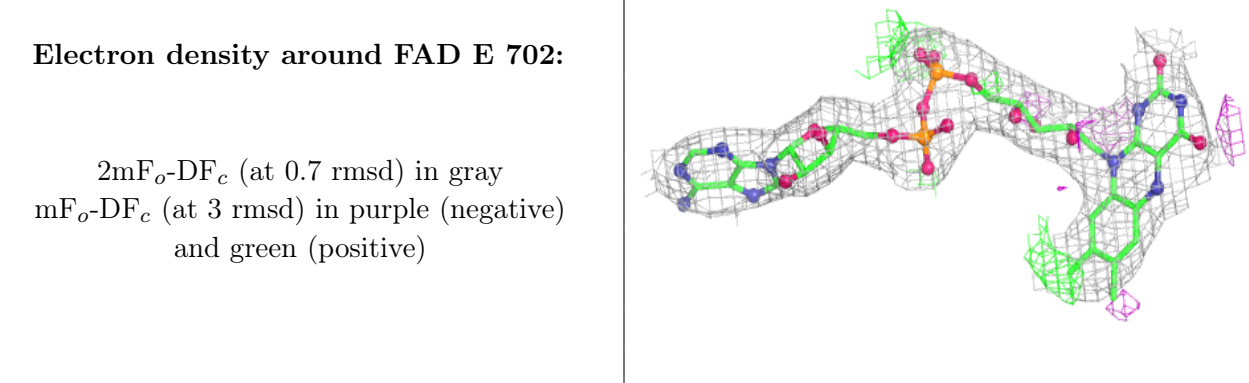
Electron density around F6A G 202:

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



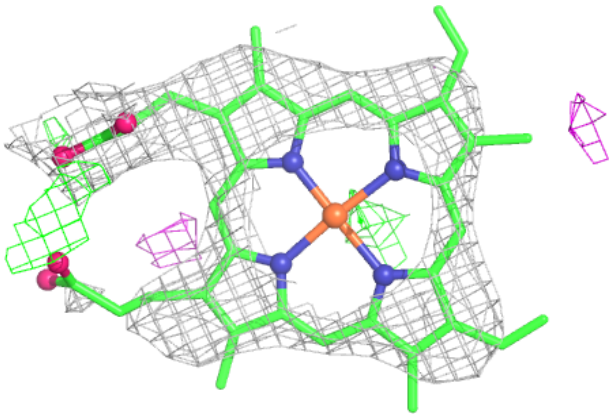
Electron density around FAD E 702:

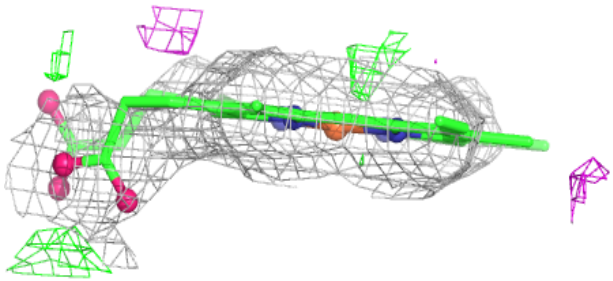
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

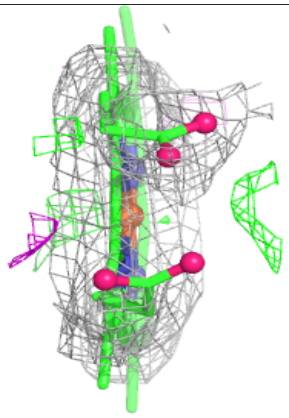


Electron density around HEM G 201:

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

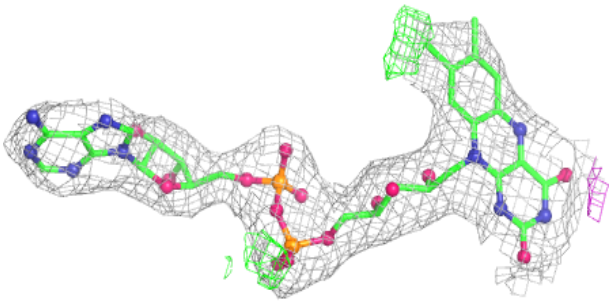


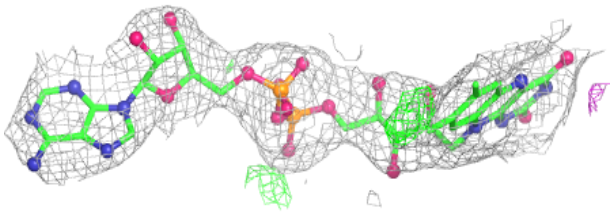


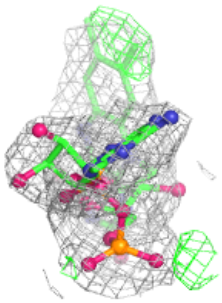


Electron density around FAD A 702:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

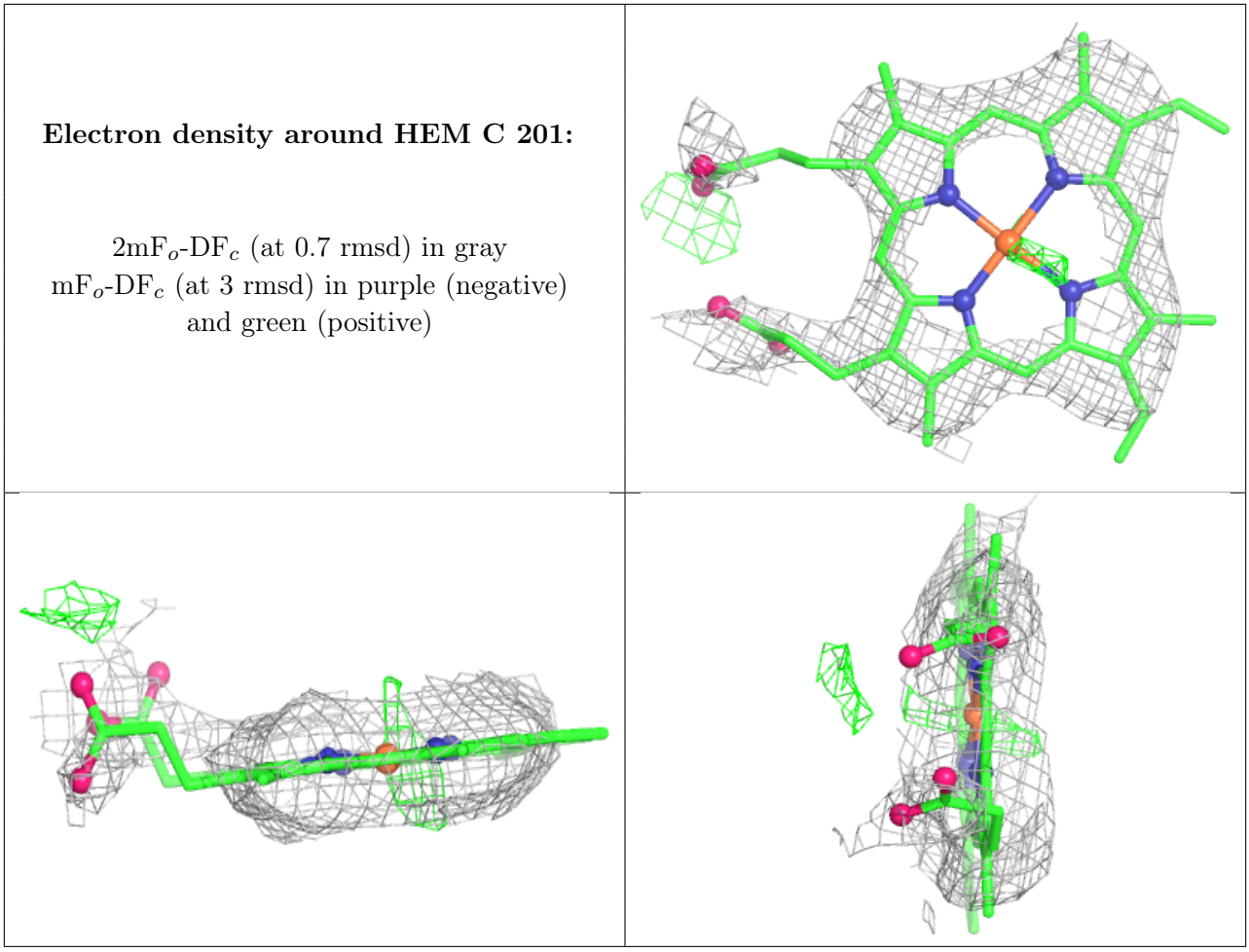






Electron density around HEM C 201:

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



6.5 Other polymers

There are no such residues in this entry.