Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 10:59 AM JST

PDB ID	:	5C2T
Title	:	Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from Ascaris suum with rhodoquinone-2
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	:	2015-06-16
Resolution	:	2.75 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:

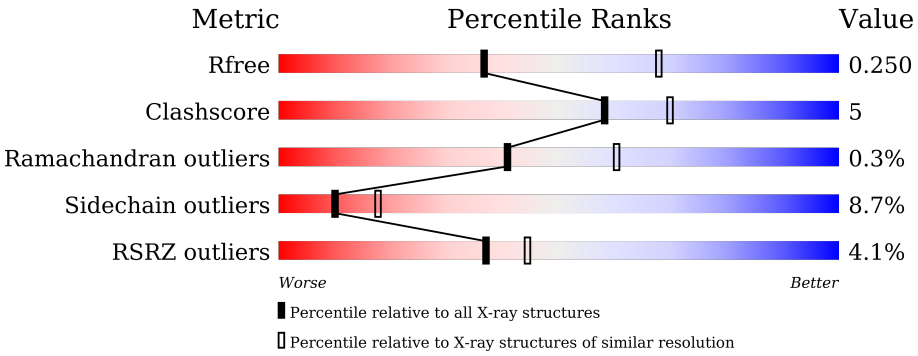
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	2% 78% 17% • •
1	E	645	3% 77% 17% • •
2	B	282	4% 76% 12% • 11%
2	F	282	4% 76% 11% • 11%
3	C	188	3% 69% 11% • 19%

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Mol	Chain	Length	Quality of chain
3	G	188	11% 68% 13% 19%
4	D	156	2% 65% 16% 17%
4	H	156	6% 69% 13% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	4YP	G	202	-	-	-	X
12	EPH	H	201	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18467 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 [ubiquinone] flavoprotein subunit, mitochondrial.

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

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

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

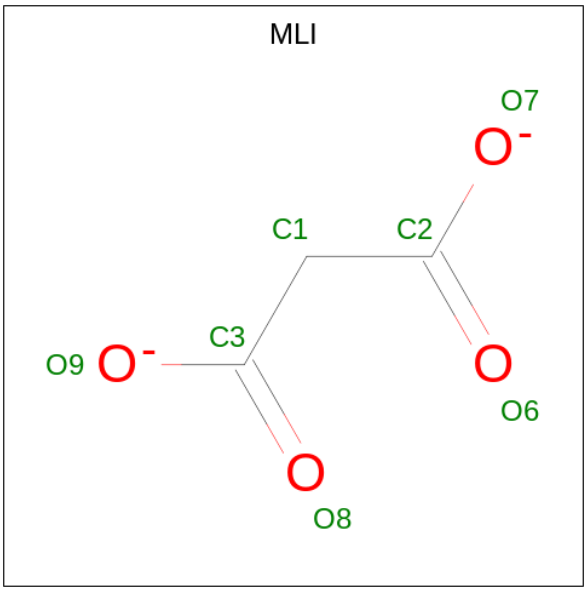
- Molecule 3 is a protein called Cytochrome b-large subunit.

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

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

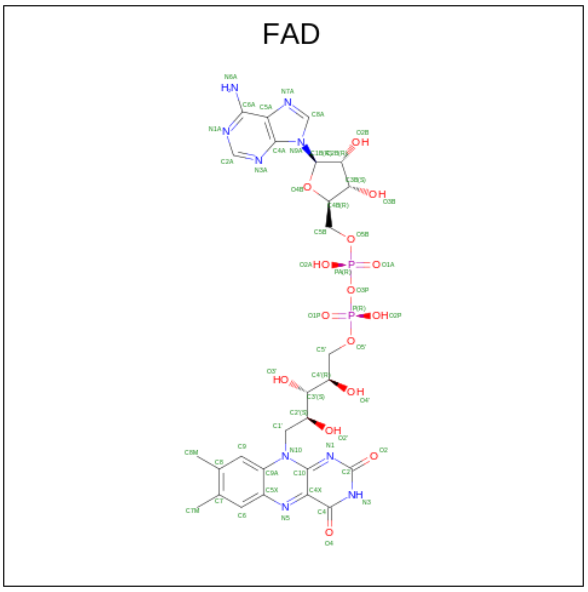
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	1	0
			1009	665	169	170	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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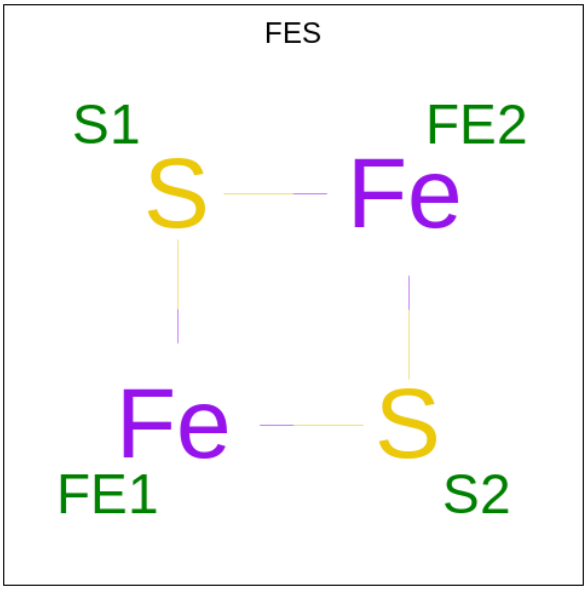
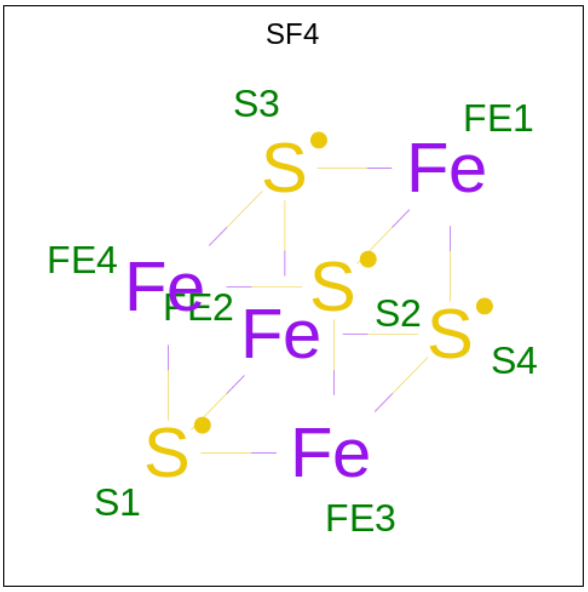
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



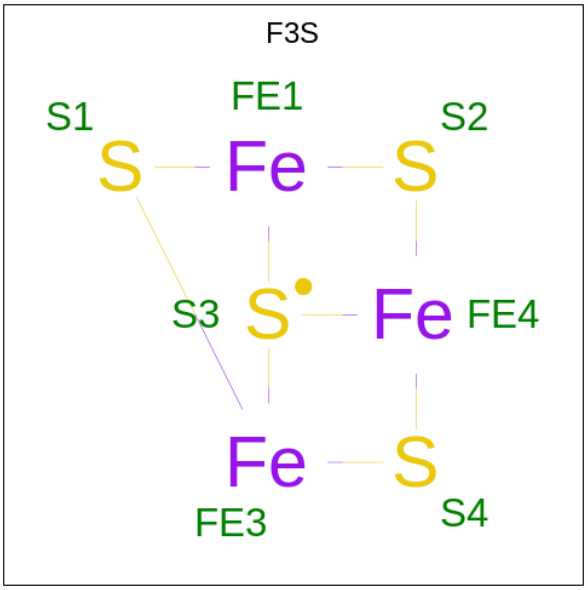
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Fe	S		0	0
			4	2	2			
7	F	1	Total	Fe	S		0	0
			4	2	2			

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



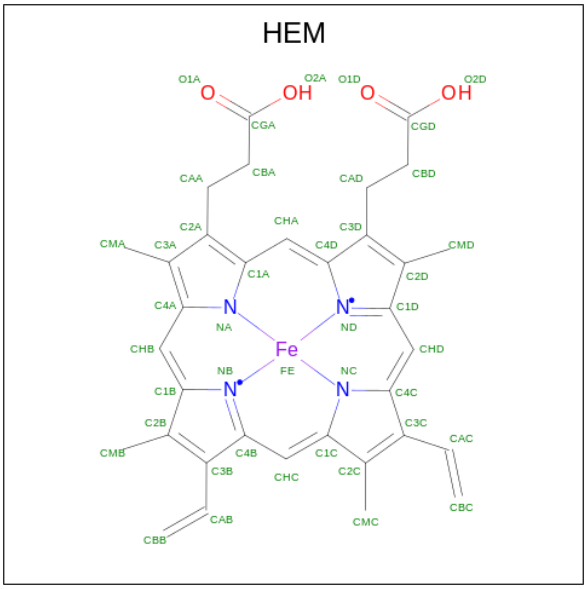
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 8 4 4	0	0
8	F	1	Total Fe S 8 4 4	0	0

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



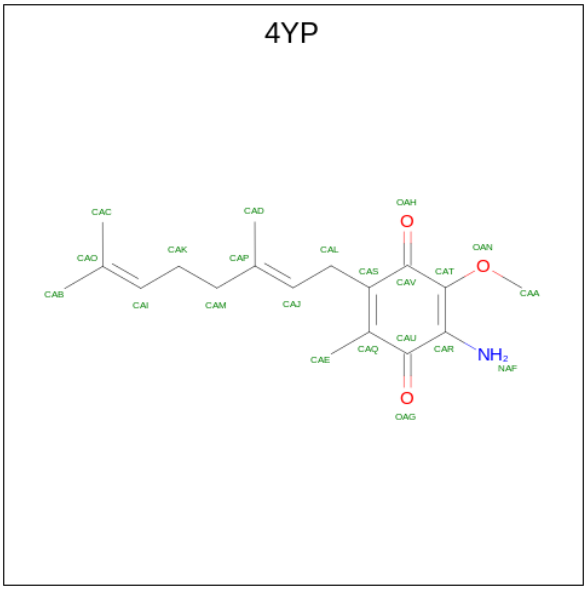
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0
9	F	1	Total Fe S 7 3 4	0	0

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



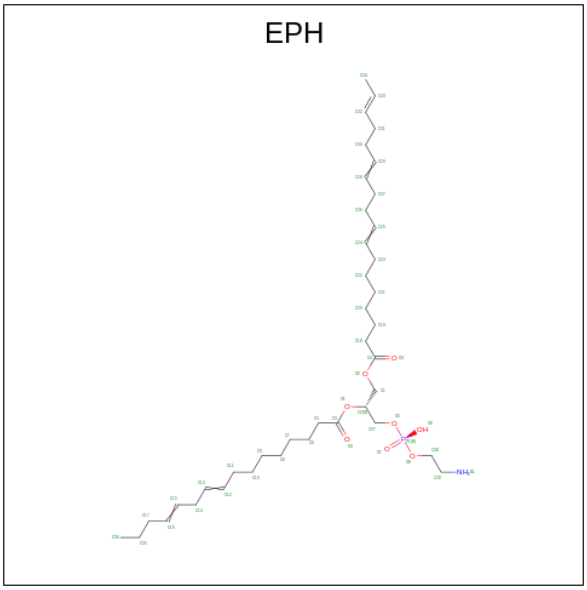
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 2-amino-5-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-3-methoxy-6-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: 4YP) (formula: $C_{18}H_{25}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C N O 22 18 1 3	0	0
11	G	1	Total C N O 22 18 1 3	0	0

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



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	54	Total O 54 54	0	0
13	B	13	Total O 13 13	0	0
13	C	6	Total O 6 6	0	0
13	D	7	Total O 7 7	0	0
13	E	10	Total O 10 10	0	0

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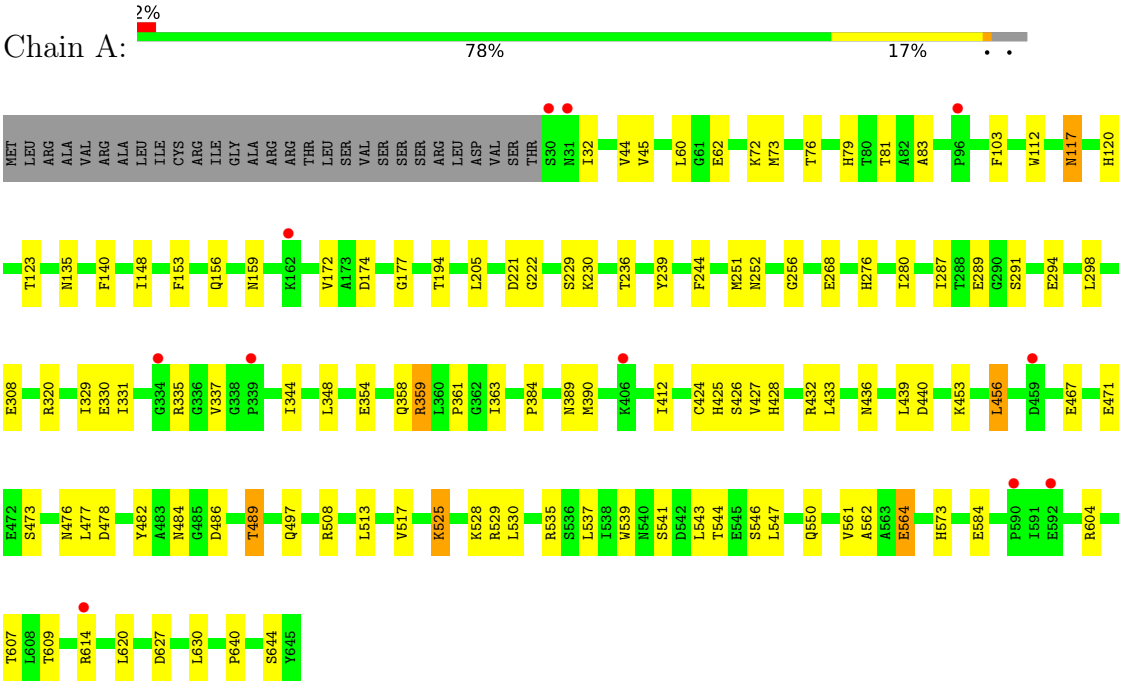
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	F	10	Total O 10 10	0	0
13	G	4	Total O 4 4	0	0
13	H	2	Total O 2 2	0	0

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.

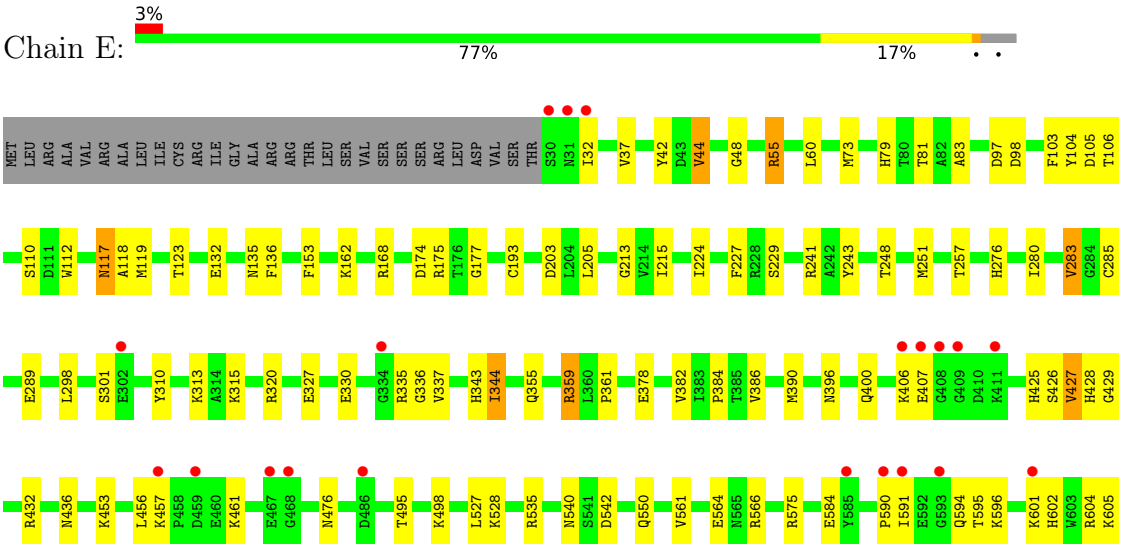
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

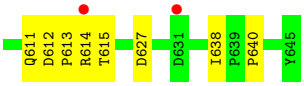
Chain A:



• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

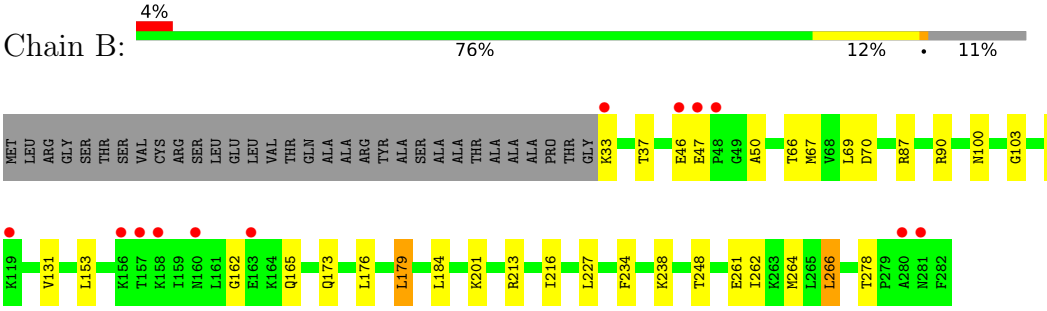
Chain E:





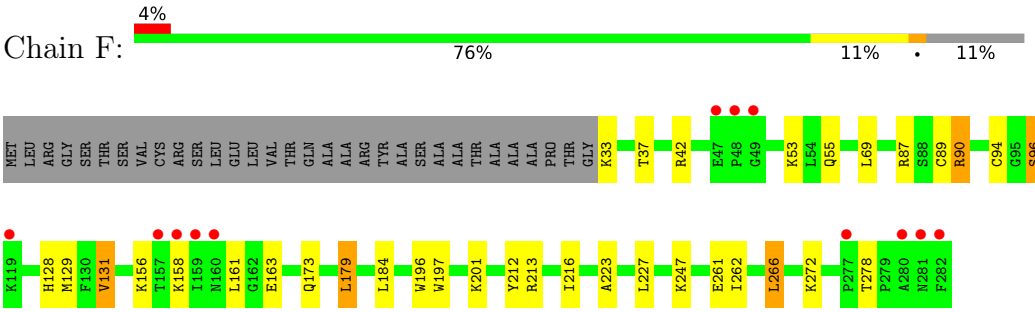
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



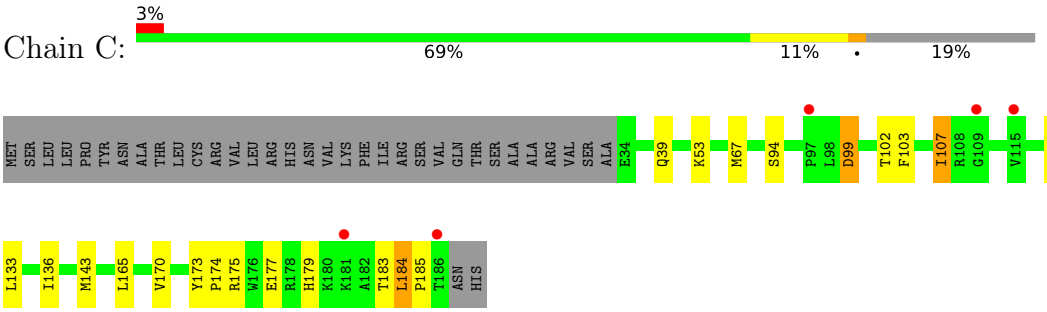
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F:



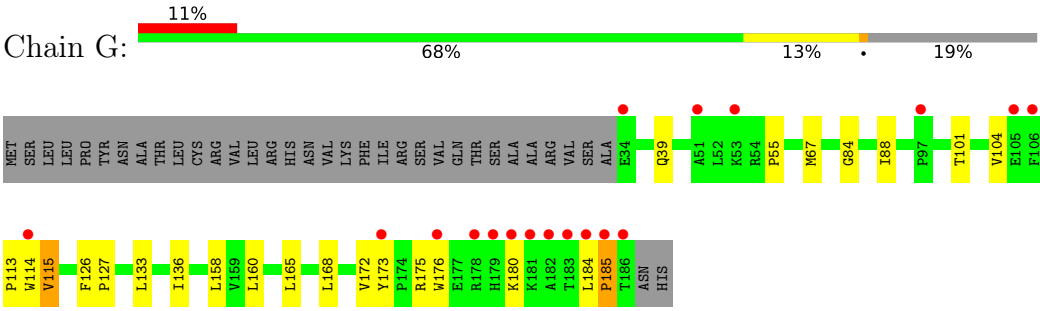
• Molecule 3: Cytochrome b-large subunit

Chain C:



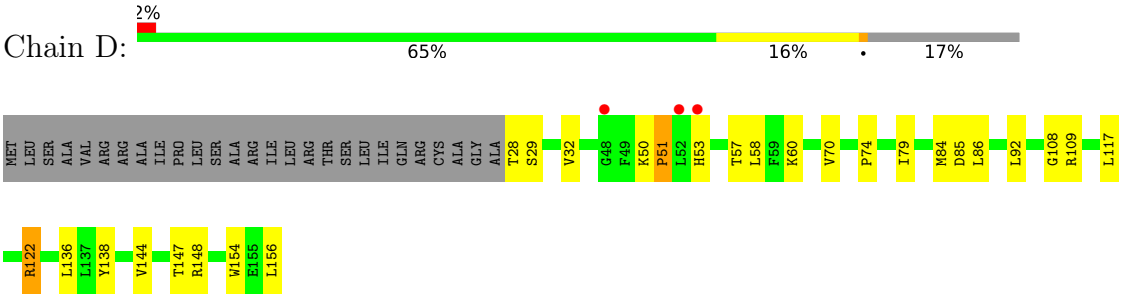
• Molecule 3: Cytochrome b-large subunit

Chain G:



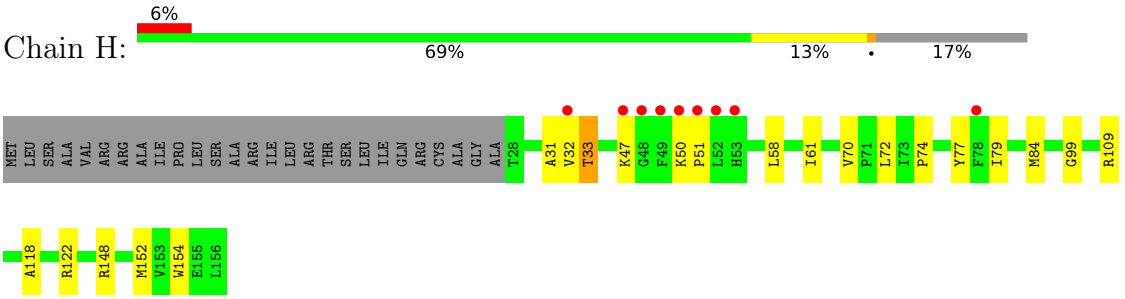
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

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	122.81Å 123.63Å 219.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 19.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.75) 94.3 (19.98-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.252 0.199 , 0.250	Depositor DCC
R_{free} test set	4112 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18467	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

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

[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: EPH, SF4, FAD, MLI, HEM, 4YP, F3S, FES

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	0.42	0/4889	0.65	0/6605
1	E	0.38	0/4889	0.62	0/6605
2	B	0.41	0/2029	0.62	0/2739
2	F	0.41	0/2029	0.61	0/2739
3	C	0.38	0/1255	0.58	0/1709
3	G	0.39	0/1255	0.57	0/1709
4	D	0.40	0/1041	0.57	0/1420
4	H	0.38	0/1030	0.52	0/1406
All	All	0.40	0/18417	0.62	0/24932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	61	0
1	E	4787	0	4722	56	0
2	B	1985	0	2001	13	0
2	F	1985	0	2001	18	0
3	C	1217	0	1265	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1217	0	1265	10	0
4	D	1009	0	997	9	0
4	H	998	0	985	10	0
5	A	7	0	2	1	0
5	E	7	0	2	1	0
6	A	53	0	31	8	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	C	43	0	30	3	0
10	G	43	0	30	4	0
11	C	22	0	25	0	0
11	G	22	0	25	2	0
12	D	44	0	53	0	0
12	H	44	0	53	2	0
13	A	54	0	0	0	0
13	B	13	0	0	0	0
13	C	6	0	0	0	0
13	D	7	0	0	0	0
13	E	10	0	0	0	0
13	F	10	0	0	0	0
13	G	4	0	0	0	0
13	H	2	0	0	0	0
All	All	18467	0	18240	177	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 (177) 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	1.37	1.36
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.57	1.15
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.11	1.12
1:E:79:HIS:CE1	6:E:702:FAD:HM82	1.95	1.01
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.22	1.01
2:F:94:CYS:SG	2:F:96:SER:OG	2.22	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LEU:HD11	1:A:543:LEU:HD21	1.53	0.89
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.15	0.82
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.38	0.72
4:D:108:GLY:O	4:D:122[A]:ARG:NH2	2.23	0.71
1:E:117:ASN:HD22	1:E:118:ALA:H	1.41	0.69
1:E:604:ARG:NH2	1:E:627:ASP:OD1	2.26	0.69
1:E:289:GLU:OE2	1:E:320:ARG:HD2	1.93	0.68
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.75	0.67
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.77	0.66
1:A:289:GLU:OE2	1:A:320:ARG:HD2	1.96	0.66
3:G:180:LYS:HG2	3:G:184:LEU:HD13	1.79	0.64
1:E:79:HIS:NE2	6:E:702:FAD:HM81	2.12	0.64
1:A:477:LEU:CD1	1:A:543:LEU:HD21	2.28	0.63
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.81	0.63
2:F:197:TRP:NE1	11:G:202:4YP:OAH	2.29	0.62
1:A:425:HIS:N	1:A:426:SER:HA	2.15	0.62
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.81	0.62
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.82	0.61
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.82	0.61
1:A:103:PHE:HA	1:A:123:THR:HG21	1.82	0.60
1:E:327:GLU:OE2	1:E:344:ILE:HD11	2.02	0.60
1:A:489:THR:HG21	1:A:546:SER:OG	2.01	0.60
1:A:79:HIS:NE2	6:A:702:FAD:HM81	2.13	0.59
2:B:262:ILE:HG22	2:B:266:LEU:HD22	1.84	0.59
1:E:117:ASN:HD22	1:E:118:ALA:N	2.00	0.58
1:A:72:LYS:HD3	6:A:702:FAD:C5A	2.32	0.58
1:E:590:PRO:O	1:E:594:GLN:OE1	2.21	0.58
1:E:566:ARG:O	1:E:575:ARG:NH2	2.37	0.58
1:A:471:GLU:OE2	4:D:28:THR:HA	2.04	0.57
3:G:172:VAL:O	3:G:172:VAL:HG13	2.05	0.56
1:A:83:ALA:HA	6:A:702:FAD:C6	2.34	0.56
10:C:201:HEM:HBC2	10:C:201:HEM:HHD	1.87	0.56
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.86	0.56
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.56
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.87	0.56
4:D:50:LYS:N	4:D:51:PRO:CD	2.68	0.56
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.86	0.56
1:E:301:SER:HB3	1:E:336:GLY:O	2.06	0.56
3:G:184:LEU:HB2	3:G:185:PRO:CD	2.36	0.55
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.88	0.55
4:H:77:TYR:HA	12:H:201:EPH:H11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.37	0.55
1:A:525:LYS:O	1:A:528:LYS:HE2	2.07	0.55
1:A:148:ILE:H	2:B:165:GLN:HE22	1.55	0.55
4:H:77:TYR:HA	12:H:201:EPH:C1	2.37	0.55
1:A:73:MET:SD	1:A:251:MET:HG3	2.46	0.54
1:A:117:ASN:HD22	1:A:117:ASN:N	2.05	0.54
1:A:604:ARG:NH2	1:A:627:ASP:OD2	2.39	0.54
10:G:201:HEM:HAD1	4:H:99:GLY:CA	2.37	0.54
3:C:179:HIS:O	3:C:183:THR:HG22	2.07	0.54
2:F:42:ARG:HG3	2:F:55:GLN:HE21	1.72	0.53
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.89	0.53
4:D:144:VAL:HB	4:D:148:ARG:HG2	1.90	0.53
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.21	0.53
1:E:83:ALA:HA	6:E:702:FAD:C6	2.39	0.53
1:A:291:SER:HB2	1:A:348:LEU:HD21	1.89	0.53
4:H:50:LYS:N	4:H:51:PRO:CD	2.72	0.53
1:E:213:GLY:HA3	1:E:227:PHE:O	2.09	0.52
3:G:114:TRP:CD1	3:G:115:VAL:HG13	2.44	0.52
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.91	0.52
2:B:67:MET:O	2:B:70:ASP:HB2	2.09	0.52
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.91	0.52
1:A:489:THR:HG22	1:A:530:LEU:HD11	1.91	0.52
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.90	0.52
1:A:508:ARG:HH11	1:A:573:HIS:HD2	1.57	0.52
1:A:609:THR:HG22	1:A:620:LEU:HD23	1.92	0.51
1:A:135:ASN:O	2:B:153:LEU:HD23	2.10	0.51
1:A:276:HIS:O	1:A:384:PRO:HA	2.10	0.51
2:B:47:GLU:HB3	2:B:50:ALA:HB2	1.91	0.51
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.93	0.50
2:F:131:VAL:HG22	3:G:55:PRO:HG2	1.94	0.50
1:A:156:GLN:HG3	1:A:433:LEU:HD21	1.94	0.50
4:D:70:VAL:O	4:D:74:PRO:HD2	2.12	0.50
1:E:105:ASP:OD2	1:E:168:ARG:NH2	2.45	0.50
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.93	0.50
1:A:239:TYR:H	1:A:389:ASN:ND2	2.10	0.49
1:E:355:GLN:O	1:E:359:ARG:HB2	2.13	0.49
1:A:32:ILE:HG23	1:A:482:TYR:CD1	2.48	0.48
1:A:120:HIS:HD2	1:A:630:LEU:H	1.61	0.48
1:E:276:HIS:O	1:E:384:PRO:HA	2.12	0.48
1:E:612:ASP:HB3	1:E:615:THR:OG1	2.12	0.48
1:E:104:TYR:HA	1:E:638:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:LEU:C	3:C:184:LEU:HD12	2.33	0.48
4:D:85:ASP:OD2	4:D:147:THR:HG23	2.13	0.48
1:E:215:ILE:HD11	1:E:224:ILE:HG21	1.94	0.48
1:E:55:ARG:NH1	1:E:132:GLU:OE2	2.47	0.48
1:E:396:ASN:HD21	1:E:400:GLN:HB2	1.79	0.48
1:A:32:ILE:HG22	1:A:478:ASP:OD1	2.13	0.47
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.14	0.47
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.95	0.47
1:A:244:PHE:HA	1:A:497:GLN:HB3	1.97	0.47
1:E:110:SER:HB2	1:E:429:GLY:HA3	1.97	0.47
2:B:234:PHE:CD1	2:B:238:LYS:HG3	2.49	0.47
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.27	0.47
1:E:106:THR:HG22	1:E:119:MET:SD	2.54	0.47
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.98	0.46
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.51	0.46
2:F:197:TRP:O	4:H:109:ARG:HD3	2.14	0.46
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.97	0.46
3:C:126:PHE:HB3	3:C:127:PRO:HD3	1.96	0.46
4:D:50:LYS:N	4:D:51:PRO:HD2	2.30	0.46
1:E:44:VAL:HG11	1:E:60:LEU:HD13	1.97	0.46
3:C:173:TYR:HB3	3:C:174:PRO:HD3	1.98	0.46
1:E:73:MET:SD	1:E:251:MET:HG3	2.56	0.46
1:A:230:LYS:HE2	1:A:456:LEU:HD11	1.98	0.45
1:E:42:TYR:O	1:E:229:SER:HA	2.16	0.45
1:A:354:GLU:O	1:A:358:GLN:HB2	2.16	0.45
1:E:280:ILE:HD12	1:E:285:CYS:HB2	1.99	0.45
1:E:602:HIS:O	1:E:605:LYS:HE2	2.16	0.45
1:A:117:ASN:HD22	1:A:117:ASN:H	1.64	0.45
1:A:174:ASP:OD2	1:A:363:ILE:N	2.44	0.45
1:E:136:PHE:CE1	2:F:161:LEU:HD11	2.52	0.45
1:A:427:VAL:HG23	1:A:428:HIS:CE1	2.51	0.45
1:A:477:LEU:HD12	1:A:543:LEU:HD11	1.97	0.45
1:A:424:CYS:SG	1:A:426:SER:HB2	2.56	0.44
3:G:84:GLY:O	3:G:88:ILE:HG12	2.17	0.44
1:E:310:TYR:OH	1:E:330:GLU:OE1	2.36	0.44
1:A:135:ASN:ND2	2:B:162:GLY:H	2.15	0.44
1:A:280:ILE:HD11	1:A:287:ILE:HD11	2.00	0.44
1:E:103:PHE:HA	1:E:123:THR:HG21	2.00	0.44
2:B:100:ASN:HD21	2:B:103:GLY:HA2	1.82	0.44
11:G:202:4YP:H15	11:G:202:4YP:H20	2.00	0.44
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:104:VAL:HG21	4:H:152:MET:HE3	1.99	0.44
10:G:201:HEM:HBC2	10:G:201:HEM:HHD	2.00	0.44
1:A:513:LEU:O	1:A:517:VAL:HG23	2.18	0.43
1:E:135:ASN:ND2	2:F:161:LEU:O	2.48	0.43
1:E:283:VAL:O	2:F:90:ARG:NH1	2.51	0.43
4:H:32:VAL:HG22	4:H:33:THR:N	2.33	0.43
2:F:89:CYS:HB3	2:F:94:CYS:HB3	2.00	0.43
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.18	0.43
2:F:223:ALA:HB2	2:F:272:LYS:HD2	2.00	0.43
2:B:264:MET:SD	3:C:143:MET:HA	2.59	0.43
1:E:215:ILE:HD11	1:E:224:ILE:CG2	2.48	0.43
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.66	0.43
1:A:486:ASP:OD1	1:A:529:ARG:NH2	2.47	0.43
2:F:116:ASN:C	2:F:116:ASN:HD22	2.21	0.43
1:E:611:GLN:O	1:E:613:PRO:HD3	2.19	0.42
1:E:119:MET:O	1:E:123:THR:OG1	2.25	0.42
1:E:83:ALA:HA	6:E:702:FAD:C5X	2.48	0.42
1:E:427:VAL:HG23	1:E:428:HIS:CD2	2.54	0.42
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.34	0.42
1:E:540:ASN:OD1	1:E:542:ASP:HB3	2.19	0.42
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.55	0.42
1:E:97:ASP:OD2	1:E:98:ASP:N	2.53	0.42
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.55	0.42
1:E:344:ILE:CD1	1:E:382:VAL:HG23	2.50	0.41
4:H:118:ALA:HB1	4:H:122:ARG:HH21	1.85	0.41
3:C:103:PHE:O	3:C:107:ILE:HG23	2.20	0.41
1:E:456:LEU:HD23	1:E:457:LYS:N	2.35	0.41
1:A:268:GLU:HA	1:A:607:THR:O	2.21	0.41
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.41	0.41
3:G:126:PHE:HB3	3:G:127:PRO:HD3	2.02	0.41
2:B:179:LEU:HD23	2:B:216:ILE:HD11	2.03	0.41
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.51	0.41
1:E:241:ARG:NH2	1:E:248:THR:O	2.54	0.41
1:E:343:HIS:HB2	1:E:382:VAL:O	2.20	0.41
1:A:135:ASN:HD22	2:B:162:GLY:H	1.69	0.41
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.56	0.41
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.02	0.41
1:A:513:LEU:HD13	1:A:564:GLU:HA	2.03	0.41
3:C:99:ASP:OD1	3:C:102:THR:HG23	2.20	0.40
1:A:83:ALA:HA	6:A:702:FAD:N5	2.36	0.40
2:F:116:ASN:HD22	2:F:118:SER:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:OD2	1:A:221:ASP:C	2.60	0.40
1:A:329:ILE:O	1:A:330:GLU:C	2.59	0.40
1:A:541:SER:HA	1:A:544:THR:OG1	2.22	0.40
3:C:94:SER:HA	4:D:138:TYR:CE1	2.57	0.40
3:G:184:LEU:HB2	3:G:185:PRO:HD2	2.04	0.40
1:E:37:VAL:HB	4:H:31:ALA:CB	2.51	0.40
4:H:70:VAL:O	4:H:74:PRO:HD2	2.21	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%)	583 (95%)	31 (5%)	0	100	100
1	E	614/645 (95%)	570 (93%)	44 (7%)	0	100	100
2	B	248/282 (88%)	238 (96%)	9 (4%)	1 (0%)	34	53
2	F	248/282 (88%)	237 (96%)	10 (4%)	1 (0%)	34	53
3	C	151/188 (80%)	148 (98%)	2 (1%)	1 (1%)	22	39
3	G	151/188 (80%)	138 (91%)	10 (7%)	3 (2%)	7	13
4	D	128/156 (82%)	119 (93%)	8 (6%)	1 (1%)	19	34
4	H	127/156 (81%)	118 (93%)	9 (7%)	0	100	100
All	All	2281/2542 (90%)	2151 (94%)	123 (5%)	7 (0%)	41	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	ASN
3	C	185	PRO
4	D	51	PRO

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Mol	Chain	Res	Type
3	G	113	PRO
2	F	163	GLU
3	G	173	TYR
3	G	185	PRO

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%)	465 (93%)	37 (7%)	13 24
1	E	502/527 (95%)	461 (92%)	41 (8%)	11 20
2	B	220/242 (91%)	200 (91%)	20 (9%)	9 16
2	F	220/242 (91%)	201 (91%)	19 (9%)	10 18
3	C	127/158 (80%)	116 (91%)	11 (9%)	10 18
3	G	127/158 (80%)	115 (91%)	12 (9%)	8 15
4	D	99/119 (83%)	83 (84%)	16 (16%)	2 3
4	H	98/119 (82%)	89 (91%)	9 (9%)	9 16
All	All	1895/2092 (91%)	1730 (91%)	165 (9%)	10 18

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	76	THR
1	A	81	THR
1	A	117	ASN
1	A	153	PHE
1	A	159	ASN
1	A	194	THR
1	A	205	LEU
1	A	252	ASN
1	A	298	LEU
1	A	308	GLU

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Mol	Chain	Res	Type
1	A	331	ILE
1	A	335	ARG
1	A	337	VAL
1	A	344	ILE
1	A	359	ARG
1	A	390	MET
1	A	412	ILE
1	A	432	ARG
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP
1	A	453	LYS
1	A	456	LEU
1	A	467	GLU
1	A	473	SER
1	A	484	ASN
1	A	489	THR
1	A	525	LYS
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	561	VAL
1	A	564	GLU
1	A	584	GLU
1	A	614	ARG
1	A	644	SER
2	B	33	LYS
2	B	37	THR
2	B	46	GLU
2	B	66	THR
2	B	69	LEU
2	B	87	ARG
2	B	90	ARG
2	B	115	GLN
2	B	116	ASN
2	B	118	SER
2	B	131	VAL
2	B	173	GLN
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	213	ARG

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Mol	Chain	Res	Type
2	B	248	THR
2	B	261	GLU
2	B	266	LEU
2	B	278	THR
3	C	53	LYS
3	C	67	MET
3	C	99	ASP
3	C	107	ILE
3	C	133	LEU
3	C	136	ILE
3	C	165	LEU
3	C	170	VAL
3	C	175	ARG
3	C	177	GLU
3	C	184	LEU
4	D	29	SER
4	D	32	VAL
4	D	53	HIS
4	D	57	THR
4	D	58	LEU
4	D	60	LYS
4	D	79	ILE
4	D	84	MET
4	D	86	LEU
4	D	92	LEU
4	D	109	ARG
4	D	117	LEU
4	D	122[A]	ARG
4	D	122[B]	ARG
4	D	136	LEU
4	D	154	TRP
1	E	32	ILE
1	E	44	VAL
1	E	55	ARG
1	E	81	THR
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	175	ARG
1	E	193	CYS
1	E	203	ASP
1	E	205	LEU

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Mol	Chain	Res	Type
1	E	257	THR
1	E	283	VAL
1	E	298	LEU
1	E	313	LYS
1	E	315	LYS
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE
1	E	359	ARG
1	E	378	GLU
1	E	390	MET
1	E	406	LYS
1	E	407	GLU
1	E	427	VAL
1	E	436	ASN
1	E	453	LYS
1	E	461	LYS
1	E	495	THR
1	E	498	LYS
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	561	VAL
1	E	564	GLU
1	E	584	GLU
1	E	591	ILE
1	E	595	THR
1	E	596	LYS
1	E	601	LYS
1	E	614	ARG
2	F	33	LYS
2	F	37	THR
2	F	53	LYS
2	F	69	LEU
2	F	87	ARG
2	F	90	ARG
2	F	96	SER
2	F	116	ASN
2	F	129	MET
2	F	131	VAL
2	F	156	LYS
2	F	158	LYS

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Mol	Chain	Res	Type
2	F	173	GLN
2	F	179	LEU
2	F	184	LEU
2	F	213	ARG
2	F	247	LYS
2	F	266	LEU
2	F	278	THR
3	G	67	MET
3	G	101	THR
3	G	112	ILE
3	G	115	VAL
3	G	133	LEU
3	G	136	ILE
3	G	158	LEU
3	G	160	LEU
3	G	165	LEU
3	G	168	LEU
3	G	175	ARG
3	G	176	TRP
4	H	33	THR
4	H	47	LYS
4	H	58	LEU
4	H	61	ILE
4	H	72	LEU
4	H	79	ILE
4	H	84	MET
4	H	148	ARG
4	H	154	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	135	ASN
1	A	159	ASN
1	A	182	HIS
1	A	355	GLN
1	A	389	ASN
1	A	436	ASN
1	A	451	ASN

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Mol	Chain	Res	Type
1	A	476	ASN
1	A	484	ASN
1	A	497	GLN
1	A	551	ASN
1	A	573	HIS
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	115	GLN
2	B	116	ASN
2	B	145	GLN
2	B	154	GLN
2	B	165	GLN
4	D	105	ASN
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	156	GLN
1	E	252	ASN
1	E	355	GLN
1	E	357	HIS
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	497	GLN
1	E	551	ASN
1	E	573	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
3	G	59	HIS
3	G	66	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 monosaccharides 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	$\#\|Z\| > 2$
10	HEM	G	201	3,4	41,50,50	1.39	5 (12%)	45,82,82	2.13	15 (33%)
10	HEM	C	201	3,4	41,50,50	1.39	7 (17%)	45,82,82	1.97	15 (33%)
12	EPH	H	201	-	43,43,48	1.08	2 (4%)	45,48,53	1.22	4 (8%)
9	F3S	F	303	2	0,9,9	-	-	-		
8	SF4	B	302	2	0,12,12	-	-	-		
11	4YP	G	202	-	22,22,22	3.45	8 (36%)	24,30,30	1.23	1 (4%)
7	FES	B	301	2	0,4,4	-	-	-		
5	MLI	E	701	-	6,6,6	1.05	0	7,7,7	0.93	0
9	F3S	B	303	2	0,9,9	-	-	-		
6	FAD	A	702	-	53,58,58	1.30	6 (11%)	68,89,89	1.66	13 (19%)
12	EPH	D	201	-	43,43,48	1.09	2 (4%)	45,48,53	1.02	4 (8%)
7	FES	F	301	2	0,4,4	-	-	-		
11	4YP	C	202	-	22,22,22	3.34	8 (36%)	24,30,30	1.57	8 (33%)
8	SF4	F	302	2	0,12,12	-	-	-		
5	MLI	A	701	-	6,6,6	1.12	0	7,7,7	1.24	0
6	FAD	E	702	-	53,58,58	1.25	6 (11%)	68,89,89	1.47	11 (16%)

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
10	HEM	G	201	3,4	-	4/12/54/54	-
10	HEM	C	201	3,4	-	1/12/54/54	-
12	EPH	H	201	-	-	27/47/47/52	-
9	F3S	F	303	2	-	-	0/3/3/3
8	SF4	B	302	2	-	-	0/6/5/5
11	4YP	G	202	-	-	2/13/37/37	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
5	MLI	E	701	-	-	0/4/4/4	-
9	F3S	B	303	2	-	-	0/3/3/3
6	FAD	A	702	-	-	10/30/50/50	0/6/6/6
12	EPH	D	201	-	-	22/47/47/52	-
7	FES	F	301	2	-	-	0/1/1/1
11	4YP	C	202	-	-	3/13/37/37	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/4/4/4	-
6	FAD	E	702	-	-	7/30/50/50	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	202	4YP	CAJ-CAP	9.40	1.55	1.33
11	C	202	4YP	CAJ-CAP	9.08	1.54	1.33
11	G	202	4YP	CAI-CAO	8.28	1.56	1.32
11	C	202	4YP	CAI-CAO	7.82	1.54	1.32
11	C	202	4YP	CAE-CAQ	-5.52	1.39	1.50
11	G	202	4YP	CAE-CAQ	-5.51	1.39	1.50
11	G	202	4YP	CAL-CAS	-4.73	1.43	1.51
12	H	201	EPH	O2-C4	4.58	1.46	1.33
12	D	201	EPH	O2-C4	4.53	1.46	1.33
12	D	201	EPH	O1-C3	4.51	1.47	1.34
12	H	201	EPH	O1-C3	4.42	1.46	1.34
6	E	702	FAD	C9A-C5X	4.37	1.48	1.41
6	A	702	FAD	C9A-C5X	4.35	1.48	1.41
11	C	202	4YP	CAL-CAS	-4.30	1.44	1.51
10	G	201	HEM	C1B-NB	-4.17	1.33	1.40
11	C	202	4YP	CAL-CAJ	3.81	1.56	1.50
10	C	201	HEM	C1B-NB	-3.62	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	202	4YP	CAS-CAQ	3.60	1.41	1.35
11	G	202	4YP	CAS-CAV	3.21	1.55	1.46
6	A	702	FAD	C8-C7	3.05	1.48	1.40
11	C	202	4YP	CAS-CAV	3.04	1.55	1.46
11	G	202	4YP	CAL-CAJ	3.03	1.55	1.50
11	C	202	4YP	CAS-CAQ	2.95	1.40	1.35
6	A	702	FAD	C5X-N5	-2.95	1.33	1.39
10	C	201	HEM	C3B-C4B	2.83	1.50	1.44
10	C	201	HEM	FE-NB	2.75	2.10	1.96
10	C	201	HEM	C4D-ND	-2.73	1.35	1.40
10	G	201	HEM	C3B-C4B	2.62	1.50	1.44
6	E	702	FAD	C8-C7	2.48	1.47	1.40
10	G	201	HEM	C4B-NB	-2.46	1.33	1.38
10	G	201	HEM	FE-NB	2.44	2.08	1.96
6	E	702	FAD	C8M-C8	-2.30	1.46	1.51
10	C	201	HEM	C4B-NB	-2.27	1.34	1.38
11	C	202	4YP	CAM-CAP	2.26	1.56	1.51
6	E	702	FAD	C4X-N5	2.22	1.35	1.30
11	G	202	4YP	CAQ-CAU	2.19	1.55	1.47
10	C	201	HEM	CHB-C1B	2.18	1.40	1.35
6	E	702	FAD	C1'-C2'	2.17	1.55	1.52
6	A	702	FAD	C8M-C8	-2.17	1.46	1.51
6	A	702	FAD	O4-C4	2.12	1.27	1.23
6	A	702	FAD	C2B-C1B	-2.06	1.50	1.53
6	E	702	FAD	C4-N3	-2.05	1.35	1.38
10	C	201	HEM	C1A-CHA	-2.03	1.35	1.41
10	G	201	HEM	C4D-C3D	2.01	1.48	1.45

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	201	HEM	CAD-C3D-C4D	5.62	134.47	124.66
12	H	201	EPH	O1-C3-C5	5.49	123.33	111.50
6	A	702	FAD	O2-C2-N1	-5.35	112.96	121.83
10	G	201	HEM	C1B-NB-C4B	4.82	110.05	105.07
10	C	201	HEM	C1B-NB-C4B	4.74	109.97	105.07
10	C	201	HEM	CHA-C4D-ND	4.59	130.05	124.38
10	G	201	HEM	CHD-C1D-ND	4.51	129.34	124.43
6	E	702	FAD	N3A-C2A-N1A	-4.24	122.05	128.68
10	C	201	HEM	CHA-C4D-C3D	-4.04	117.75	125.33
12	D	201	EPH	O1-C3-C5	3.80	119.70	111.50
10	G	201	HEM	CAD-C3D-C2D	-3.54	121.28	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	702	FAD	O4-C4-C4X	-3.52	117.25	126.60
10	G	201	HEM	CBD-CAD-C3D	3.50	122.34	112.63
10	G	201	HEM	CHD-C1D-C2D	-3.36	119.73	124.98
6	A	702	FAD	N3A-C2A-N1A	-3.35	123.45	128.68
6	A	702	FAD	O4-C4-N3	3.28	126.40	120.12
12	D	201	EPH	O2-C4-C18	3.19	121.92	111.91
10	C	201	HEM	CHD-C1D-ND	3.10	127.80	124.43
12	H	201	EPH	O2-C4-C18	2.99	121.29	111.91
10	C	201	HEM	CMD-C2D-C1D	2.94	129.52	125.04
6	E	702	FAD	C1'-C2'-C3'	2.94	118.00	109.79
6	A	702	FAD	O2-C2-N3	2.93	124.35	118.65
11	C	202	4YP	CAE-CAQ-CAS	-2.93	119.62	124.40
6	E	702	FAD	O4-C4-C4X	-2.92	118.85	126.60
6	A	702	FAD	C9-C8-C7	2.88	123.80	119.67
6	E	702	FAD	O2-C2-N1	-2.88	117.06	121.83
6	E	702	FAD	C9-C8-C7	2.86	123.77	119.67
10	C	201	HEM	CBD-CAD-C3D	-2.80	104.84	112.63
12	H	201	EPH	O1-C3-O3	-2.75	117.06	123.70
11	C	202	4YP	CAS-CAQ-CAU	2.74	121.35	119.18
10	C	201	HEM	CHB-C1B-NB	2.72	127.74	124.38
10	G	201	HEM	C4B-CHC-C1C	2.70	126.13	122.56
11	C	202	4YP	CAL-CAS-CAV	2.68	121.71	118.48
10	G	201	HEM	CHB-C1B-NB	2.65	127.66	124.38
6	A	702	FAD	C4A-C5A-N7A	-2.61	106.68	109.40
11	C	202	4YP	CAU-CAR-NAF	2.57	120.85	114.38
10	G	201	HEM	CHA-C4D-ND	2.55	127.53	124.38
11	C	202	4YP	CAD-CAP-CAM	2.53	119.53	115.27
12	D	201	EPH	O2-C4-O4	-2.52	117.24	123.59
10	G	201	HEM	CHA-C4D-C3D	-2.46	120.72	125.33
6	A	702	FAD	C4X-C10-N1	-2.41	119.13	124.73
6	A	702	FAD	C10-N1-C2	2.41	121.72	116.90
6	E	702	FAD	C4A-C5A-N7A	-2.40	106.90	109.40
10	G	201	HEM	CHC-C4B-NB	2.38	127.02	124.43
10	C	201	HEM	CHD-C1D-C2D	-2.36	121.29	124.98
10	C	201	HEM	C4B-CHC-C1C	2.35	125.66	122.56
6	E	702	FAD	C4X-C10-N1	-2.34	119.31	124.73
10	C	201	HEM	CAB-C3B-C2B	-2.33	120.93	128.60
10	G	201	HEM	O2D-CGD-CBD	2.33	121.50	114.03
11	G	202	4YP	CAD-CAP-CAJ	-2.32	117.74	123.68
6	A	702	FAD	C1'-C2'-C3'	2.31	116.24	109.79
11	C	202	4YP	CAQ-CAS-CAV	-2.31	117.41	119.58
10	C	201	HEM	C3C-C4C-NC	-2.30	106.60	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	201	HEM	CAD-CBD-CGD	2.30	118.55	113.60
10	G	201	HEM	CMA-C3A-C4A	-2.27	124.97	128.46
6	A	702	FAD	C4X-C10-N10	2.23	119.75	116.48
6	E	702	FAD	C5X-C9A-N10	2.21	120.24	117.95
6	E	702	FAD	O2'-C2'-C3'	-2.21	103.72	109.10
10	C	201	HEM	CMB-C2B-C1B	2.21	128.41	125.04
10	C	201	HEM	O2D-CGD-O1D	-2.19	117.84	123.30
10	C	201	HEM	C4B-C3B-C2B	-2.13	105.42	107.11
10	G	201	HEM	CAB-C3B-C2B	-2.12	121.62	128.60
6	A	702	FAD	C8M-C8-C9	-2.10	115.61	119.49
12	D	201	EPH	O1-C3-O3	-2.08	118.68	123.70
10	G	201	HEM	C4B-C3B-C2B	-2.08	105.47	107.11
11	C	202	4YP	CAK-CAI-CAO	-2.06	120.69	127.75
6	A	702	FAD	P-O3P-PA	-2.05	125.80	132.83
12	H	201	EPH	O2-C4-O4	-2.04	118.44	123.59
11	C	202	4YP	CAC-CAO-CAB	2.01	119.05	114.60
6	E	702	FAD	N3-C2-N1	2.00	123.32	119.38
6	E	702	FAD	C4X-C10-N10	2.00	119.41	116.48

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	C3'-C4'-C5'-O5'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	A	702	FAD	C5'-O5'-P-O1P
6	A	702	FAD	C5'-O5'-P-O2P
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
6	E	702	FAD	PA-O3P-P-O5'
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
11	C	202	4YP	CAI-CAK-CAM-CAP
11	C	202	4YP	CAJ-CAL-CAS-CAV
11	C	202	4YP	CAJ-CAL-CAS-CAQ
11	G	202	4YP	CAI-CAK-CAM-CAP
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C5-C3-O1-C2
12	D	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C38-O8-P1-O7

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Mol	Chain	Res	Type	Atoms
12	H	201	EPH	C25-C26-C27-C28
12	H	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C38-O8-P1-O5
12	H	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O8-C38-C39-N1
12	D	201	EPH	O4-C4-O2-C1
12	D	201	EPH	C18-C4-O2-C1
12	H	201	EPH	C18-C4-O2-C1
12	H	201	EPH	O4-C4-O2-C1
12	H	201	EPH	C5-C3-O1-C2
12	H	201	EPH	C37-O5-P1-O8
12	H	201	EPH	O3-C3-O1-C2
12	H	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C7-C8-C9-C10
12	H	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C5-C6-C7-C8
12	D	201	EPH	C7-C8-C9-C10
12	D	201	EPH	C6-C7-C8-C9
12	D	201	EPH	O2-C1-C2-C37
12	H	201	EPH	C20-C21-C22-C23
12	H	201	EPH	C2-C1-O2-C4
12	D	201	EPH	C19-C20-C21-C22
12	D	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C12-C13-C14-C15
12	H	201	EPH	C13-C14-C15-C16
12	H	201	EPH	O1-C3-C5-C6
6	A	702	FAD	PA-O3P-P-O5'
12	D	201	EPH	C25-C26-C27-C28
12	H	201	EPH	O2-C1-C2-C37
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	C5'-O5'-P-O3P
6	E	702	FAD	P-O3P-PA-O1A
12	D	201	EPH	C37-O5-P1-O8
12	H	201	EPH	O2-C1-C2-O1
11	G	202	4YP	CAJ-CAL-CAS-CAV
12	D	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C9-C10-C11-C12
6	A	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C22-C23-C24-C25
12	D	201	EPH	O8-C38-C39-N1
6	A	702	FAD	O4B-C4B-C5B-O5B
12	D	201	EPH	C1-C2-O1-C3
12	D	201	EPH	C13-C14-C15-C16
12	H	201	EPH	C10-C11-C12-C13
12	D	201	EPH	C24-C25-C26-C27
12	H	201	EPH	O3-C3-C5-C6
6	E	702	FAD	C5'-O5'-P-O3P
6	E	702	FAD	O4B-C4B-C5B-O5B
6	A	702	FAD	P-O3P-PA-O1A
12	H	201	EPH	C18-C19-C20-C21
12	D	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C19-C20-C21-C22
10	G	201	HEM	CAD-CBD-CGD-O2D

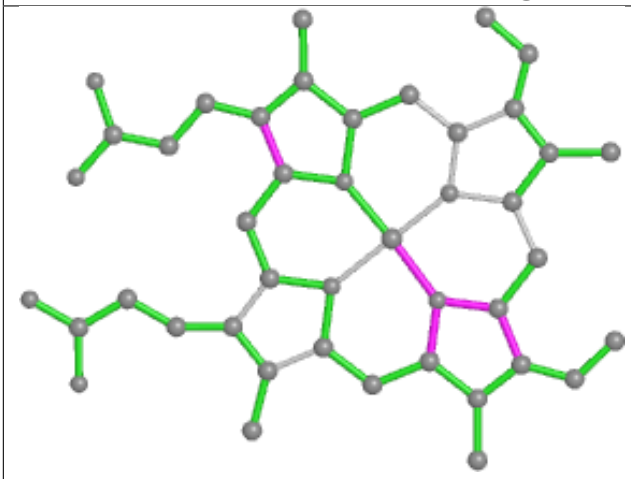
There are no ring outliers.

8 monomers are involved in 28 short contacts:

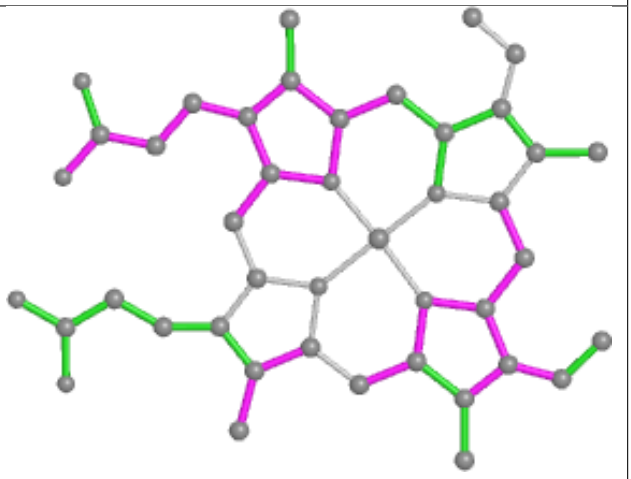
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	201	HEM	4	0
10	C	201	HEM	3	0
12	H	201	EPH	2	0
11	G	202	4YP	2	0
5	E	701	MLI	1	0
6	A	702	FAD	8	0
5	A	701	MLI	1	0
6	E	702	FAD	7	0

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.

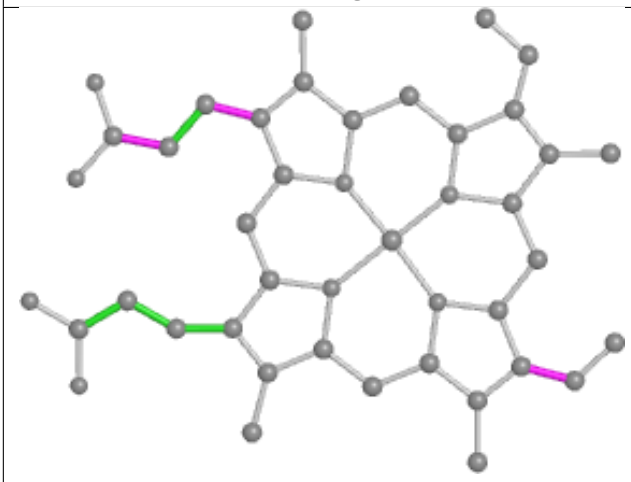
Ligand HEM G 201



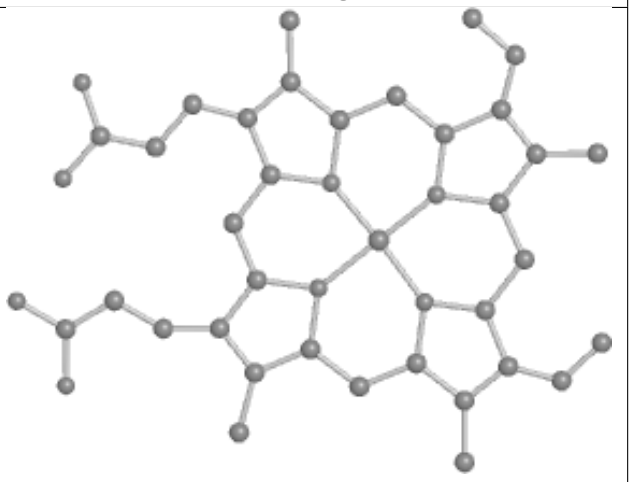
Bond lengths



Bond angles

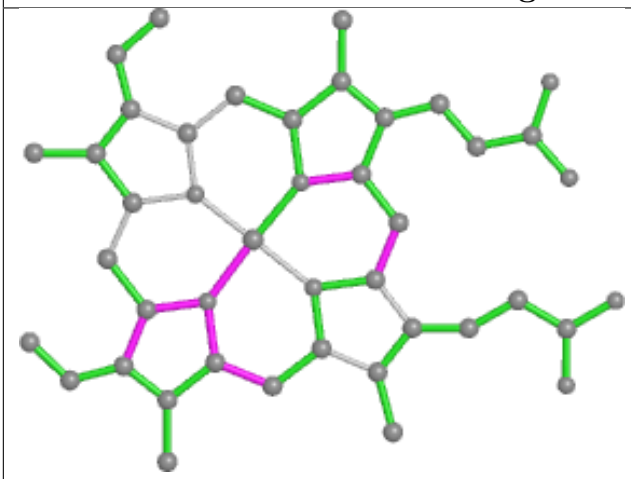


Torsions

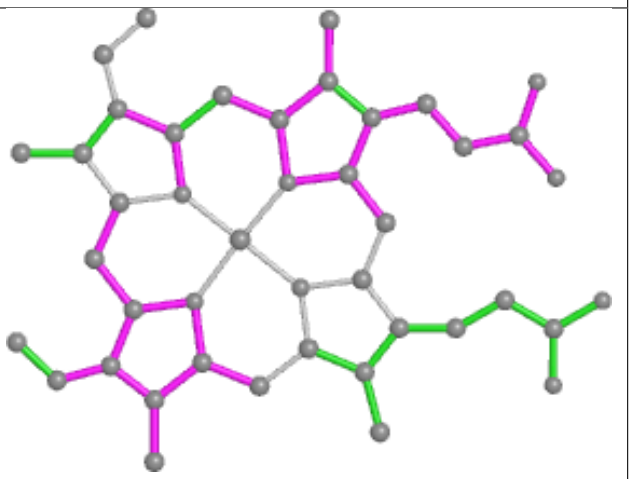


Rings

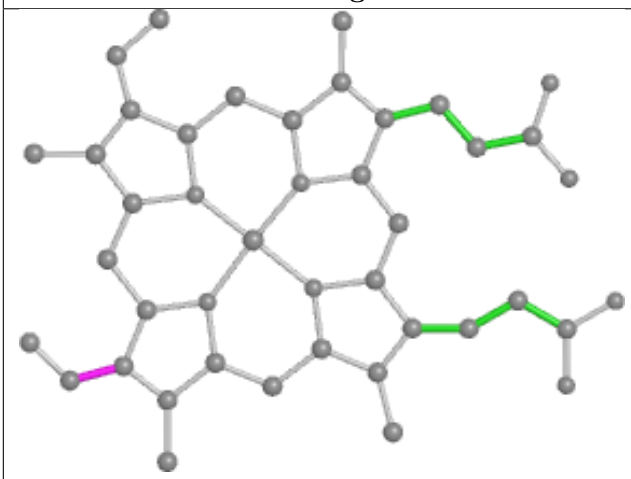
Ligand HEM C 201



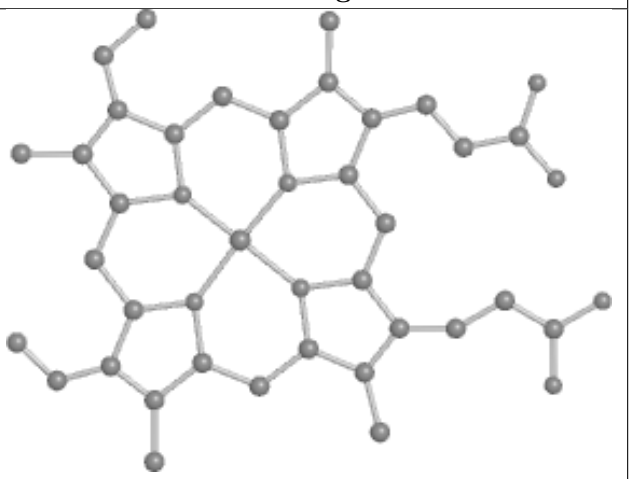
Bond lengths



Bond angles

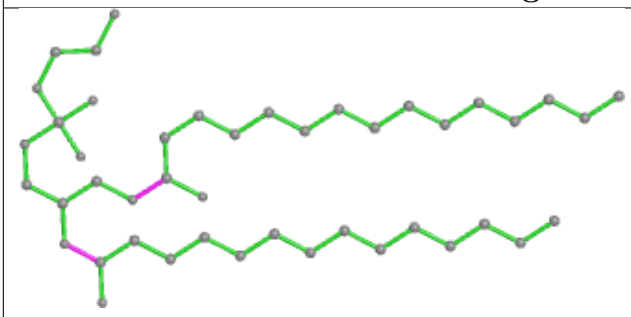


Torsions

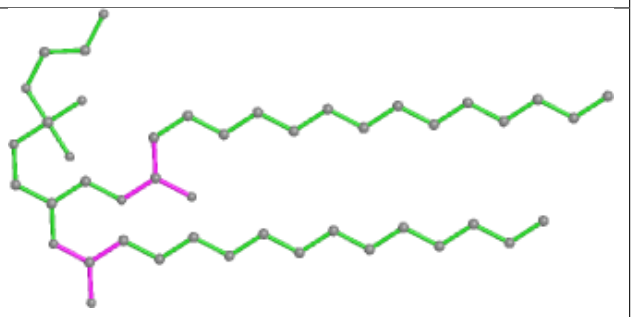


Rings

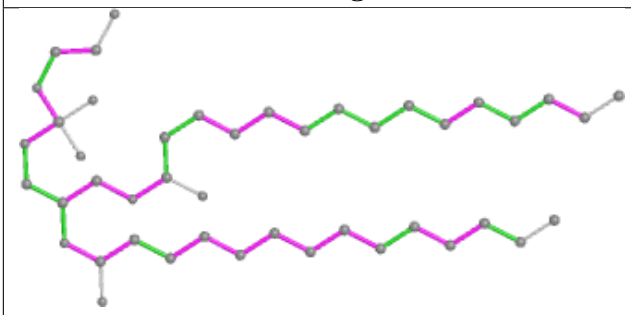
Ligand EPH H 201



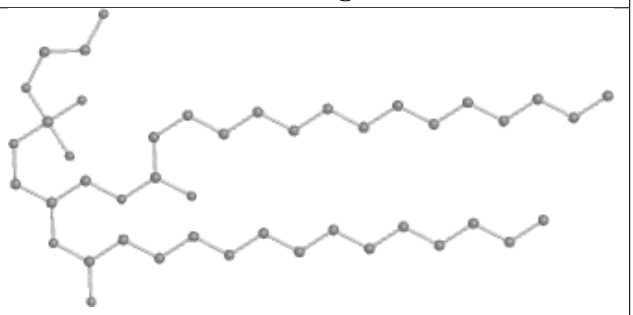
Bond lengths



Bond angles

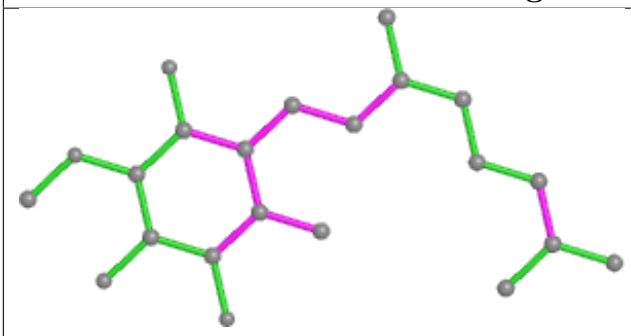


Torsions



Rings

Ligand 4YP G 202



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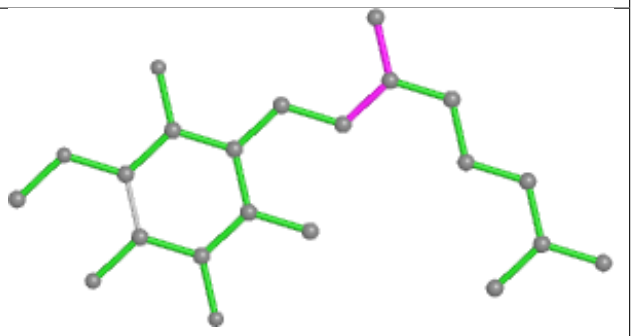
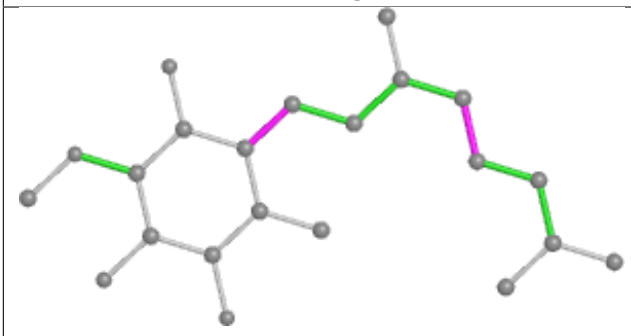
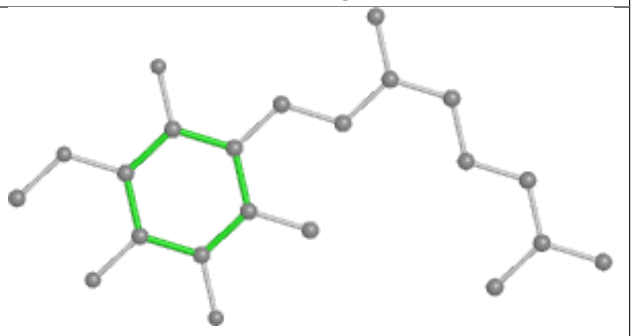


Bond angles

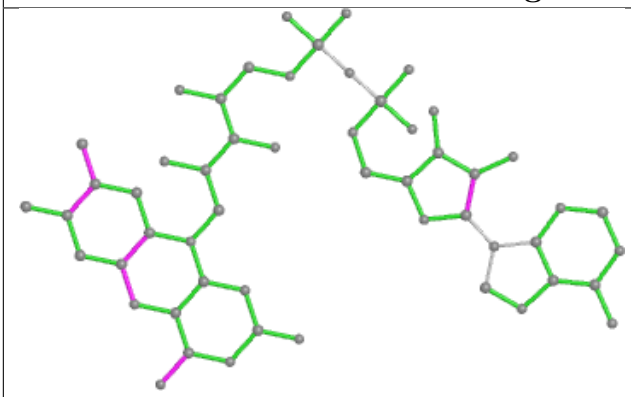


Torsions

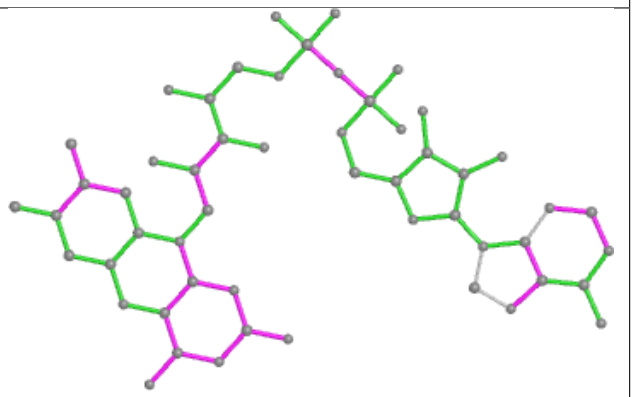


Rings

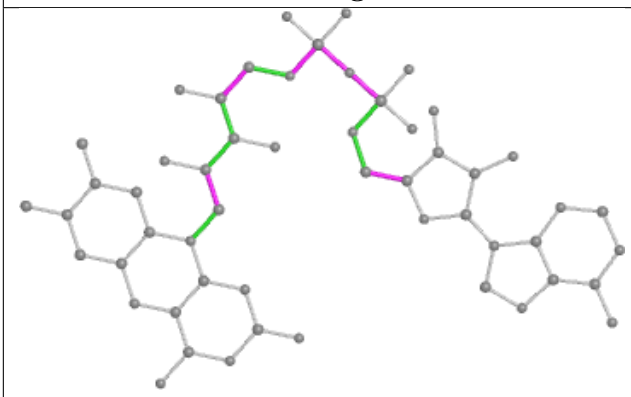
Ligand FAD A 702



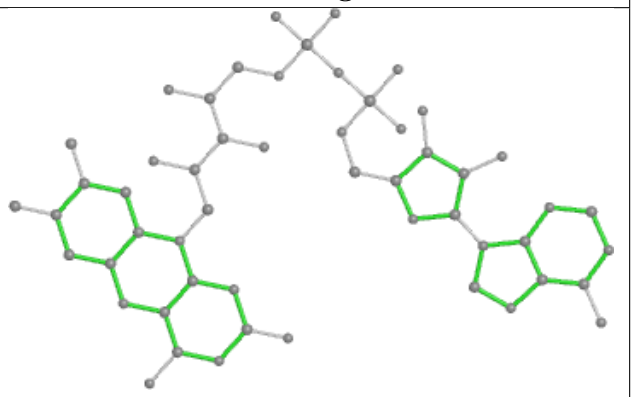
Bond lengths



Bond angles

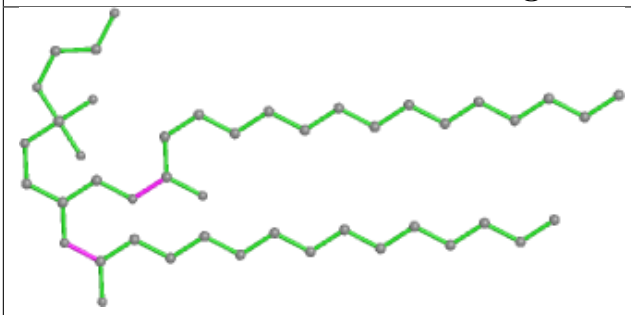


Torsions

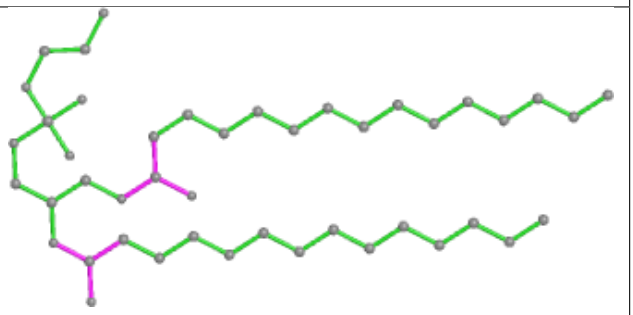


Rings

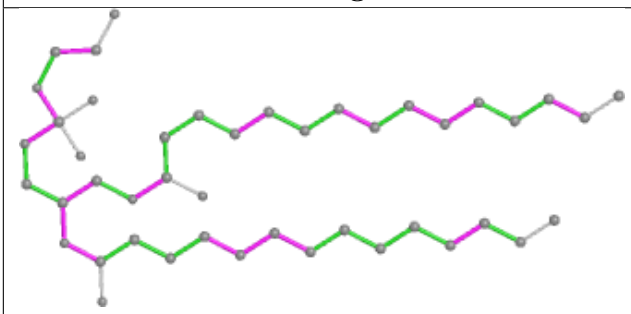
Ligand EPH D 201



Bond lengths



Bond angles



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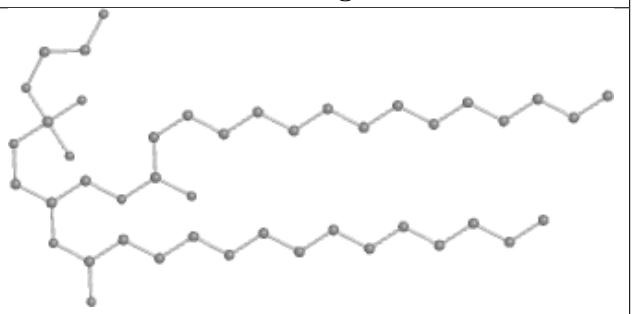
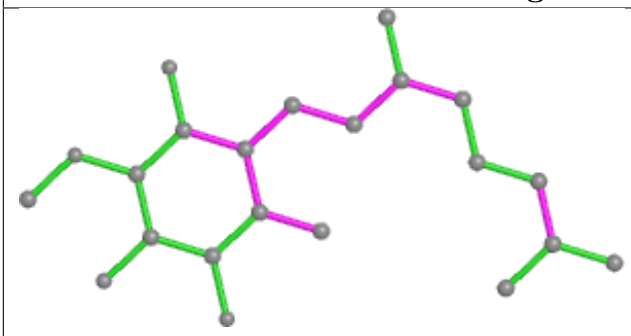
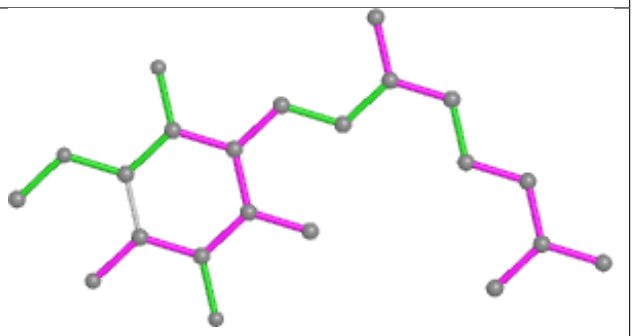


Rings

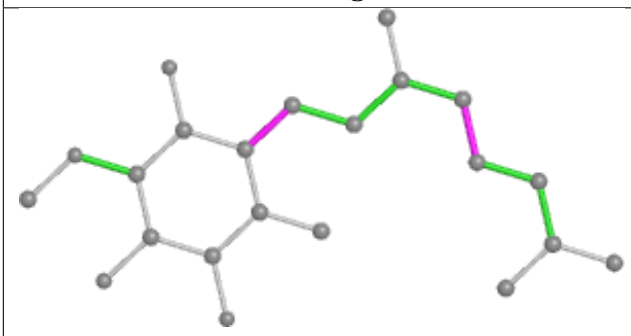
Ligand 4YP C 202



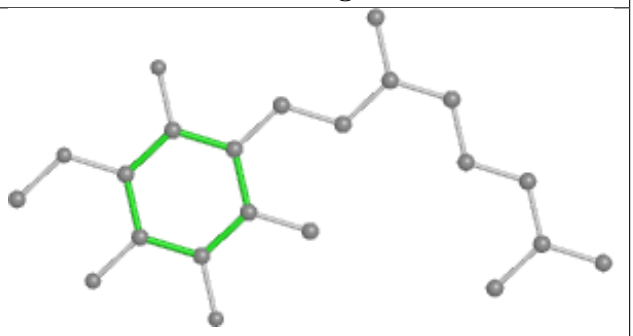
Bond lengths



Bond angles

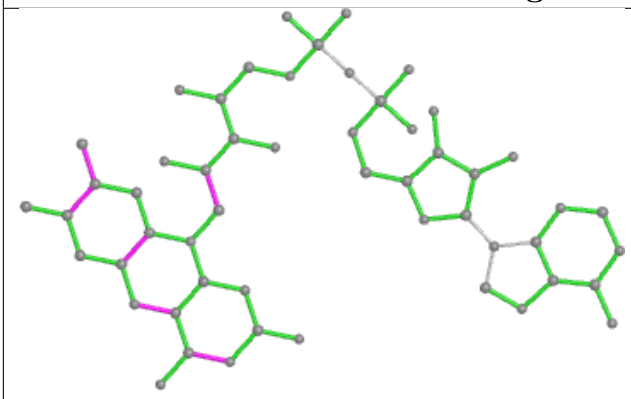


Torsions

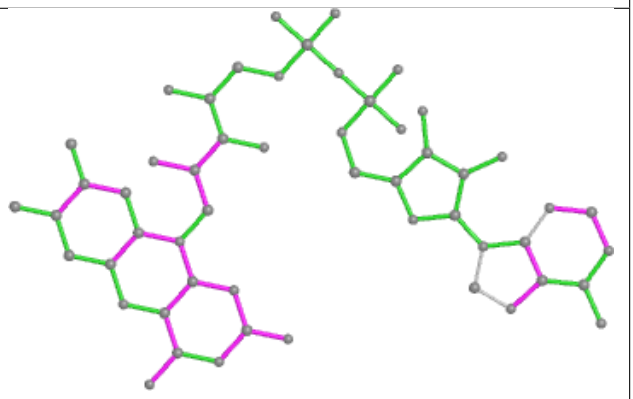


Rings

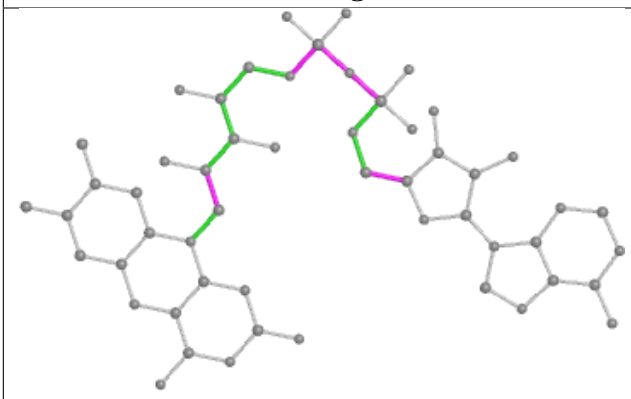
Ligand FAD E 702



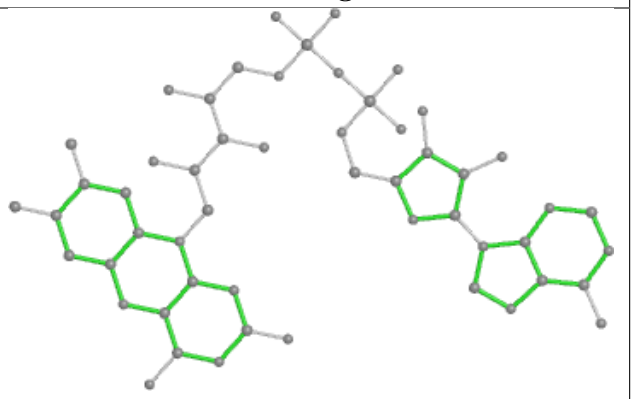
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	-0.32	11 (1%) 68 76	22, 37, 62, 87	0
1	E	616/645 (95%)	-0.02	22 (3%) 42 51	27, 53, 85, 116	0
2	B	250/282 (88%)	-0.26	12 (4%) 30 36	24, 37, 70, 97	0
2	F	250/282 (88%)	-0.21	12 (4%) 30 36	24, 43, 73, 93	0
3	C	153/188 (81%)	-0.09	5 (3%) 46 54	28, 55, 84, 112	0
3	G	153/188 (81%)	0.55	20 (13%) 3 4	33, 60, 134, 191	0
4	D	129/156 (82%)	-0.20	3 (2%) 60 69	35, 50, 72, 97	0
4	H	129/156 (82%)	0.08	9 (6%) 16 19	35, 59, 99, 130	0
All	All	2296/2542 (90%)	-0.12	94 (4%) 37 44	22, 47, 85, 191	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	184	LEU	11.5
3	G	186	THR	11.3
3	G	185	PRO	10.5
3	G	180	LYS	9.4
3	G	183	THR	7.9
4	H	49	PHE	6.1
3	G	114	TRP	5.5
3	G	176	TRP	5.2
3	G	178	ARG	5.0
1	E	30	SER	4.9
3	G	182	ALA	4.8
3	G	173	TYR	4.8
1	E	31	ASN	4.8
4	H	51	PRO	4.6
1	E	408	GLY	4.6
4	D	48	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	48	PRO	4.5
3	G	181	LYS	4.4
2	F	280	ALA	4.4
3	G	179	HIS	4.2
4	H	50	LYS	4.1
1	E	486	ASP	3.9
4	H	52	LEU	3.9
3	G	97	PRO	3.8
1	E	32	ILE	3.8
4	D	52	LEU	3.6
1	E	591	ILE	3.5
3	C	186	THR	3.5
2	B	33	LYS	3.4
2	B	281	ASN	3.4
2	F	48	PRO	3.4
2	F	157	THR	3.3
3	C	115	VAL	3.3
1	E	593	GLY	3.3
1	E	459	ASP	3.2
2	F	49	GLY	3.2
2	F	282	PHE	3.1
1	E	601	LYS	3.0
1	E	409	GLY	2.9
1	E	406	LYS	2.9
4	H	47	LYS	2.9
3	G	105	GLU	2.9
2	F	158	LYS	2.9
1	A	31	ASN	2.8
4	H	78	PHE	2.8
1	A	30	SER	2.8
4	D	53	HIS	2.8
2	F	47	GLU	2.8
2	F	281	ASN	2.7
3	G	51	ALA	2.7
2	B	157	THR	2.7
1	A	339	PRO	2.6
3	C	97	PRO	2.6
3	G	34	GLU	2.6
1	A	614	ARG	2.6
2	B	156	LYS	2.6
3	G	109	GLY	2.6
1	A	590	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	LYS	2.5
2	B	280	ALA	2.5
3	G	112	ILE	2.5
1	E	590	PRO	2.5
3	C	181	LYS	2.5
1	E	614	ARG	2.5
1	A	459	ASP	2.5
1	A	334	GLY	2.5
1	E	411	LYS	2.4
2	F	277	PRO	2.4
3	G	106	PHE	2.3
1	A	592	GLU	2.3
1	E	467	GLU	2.3
1	A	96	PRO	2.3
1	E	334	GLY	2.2
2	B	119	LYS	2.2
2	B	158	LYS	2.2
2	F	159	ILE	2.2
1	E	302	GLU	2.2
2	B	47	GLU	2.2
2	F	160	ASN	2.2
2	B	46	GLU	2.2
1	E	468	GLY	2.2
2	B	160	ASN	2.1
1	E	407	GLU	2.1
1	A	406	LYS	2.1
3	G	53	LYS	2.1
4	H	32	VAL	2.1
4	H	53	HIS	2.1
4	H	48	GLY	2.1
2	B	163	GLU	2.1
1	E	585	TYR	2.1
1	E	631	ASP	2.1
3	C	109	GLY	2.1
2	F	119	LYS	2.0
1	E	457	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

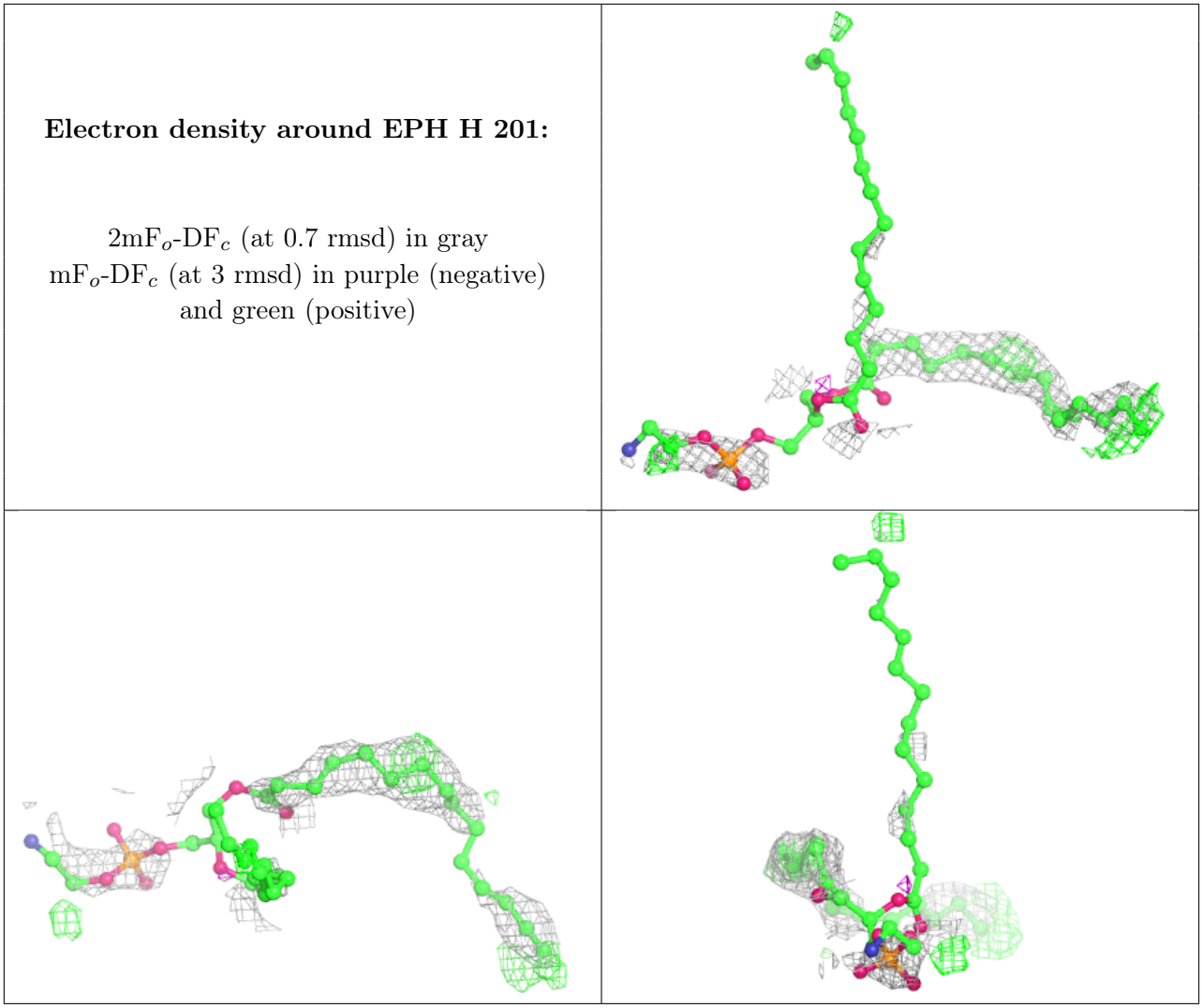
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
12	EPH	H	201	44/49	0.53	0.54	56,76,102,105	44
11	4YP	G	202	22/22	0.63	0.42	49,58,65,65	22
11	4YP	C	202	22/22	0.69	0.36	55,57,59,61	22
12	EPH	D	201	44/49	0.76	0.36	42,63,74,77	44
6	FAD	E	702	53/53	0.96	0.14	28,32,40,43	0
10	HEM	C	201	43/43	0.97	0.15	39,53,59,69	0
10	HEM	G	201	43/43	0.97	0.17	51,59,68,73	0
5	MLI	A	701	7/7	0.97	0.12	36,37,38,38	0
6	FAD	A	702	53/53	0.98	0.11	18,22,27,27	0
5	MLI	E	701	7/7	0.98	0.12	37,38,39,40	0
7	FES	B	301	4/4	0.98	0.09	22,24,26,31	0
8	SF4	B	302	8/8	0.98	0.10	24,27,28,30	0
8	SF4	F	302	8/8	0.98	0.11	28,29,32,33	0
9	F3S	F	303	7/7	0.98	0.12	32,36,38,41	0
9	F3S	B	303	7/7	0.99	0.13	31,35,37,37	0
7	FES	F	301	4/4	0.99	0.08	28,30,30,36	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.

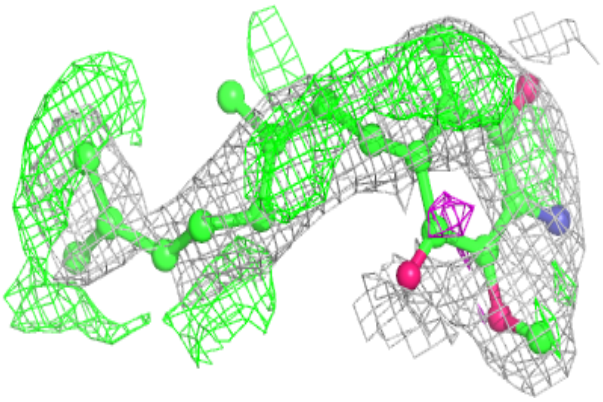
Electron density around EPH H 201:

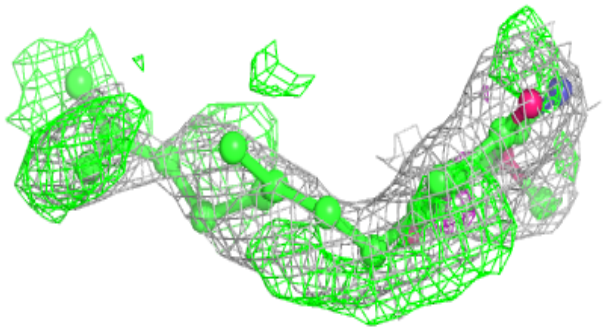
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

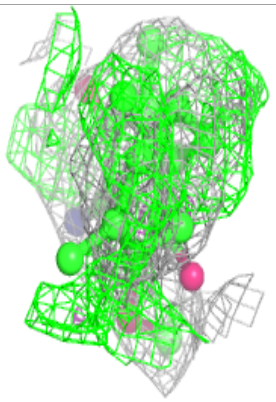


Electron density around 4YP G 202:

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

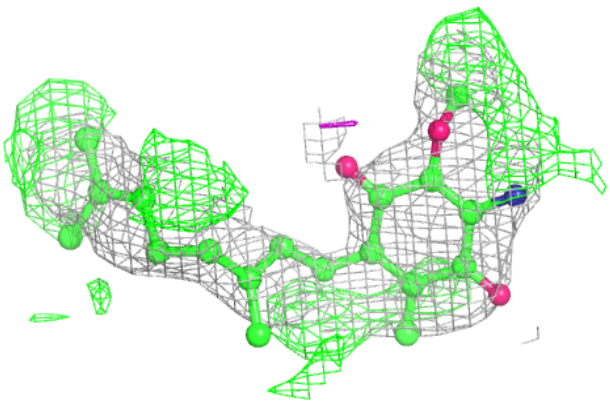


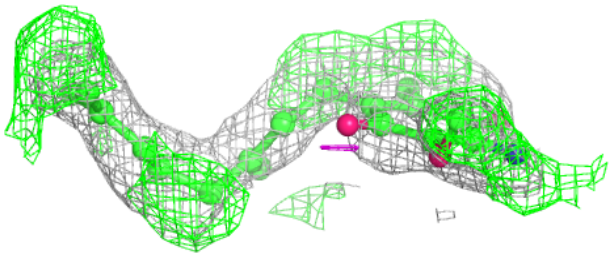




Electron density around 4YP C 202:

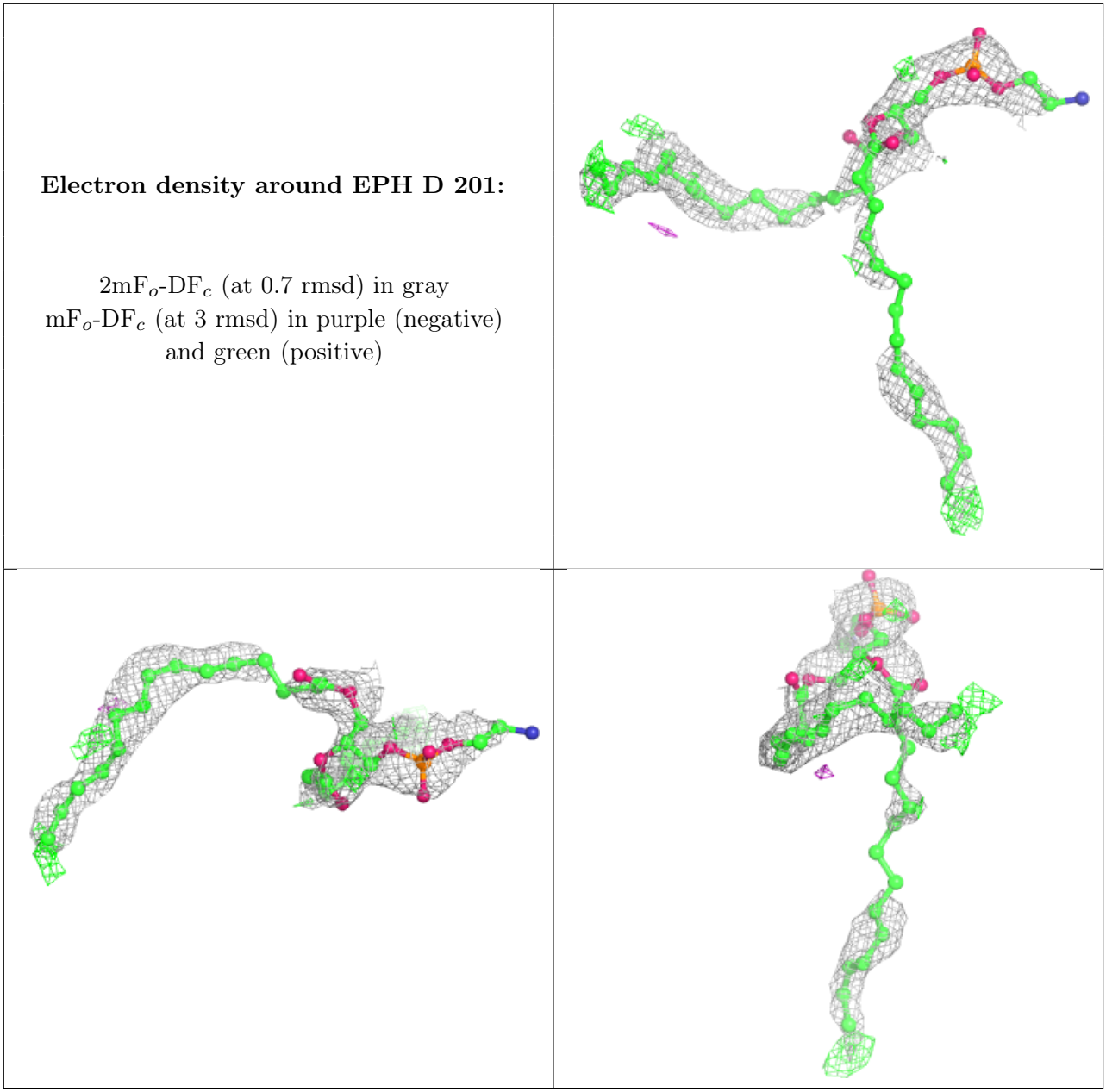
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





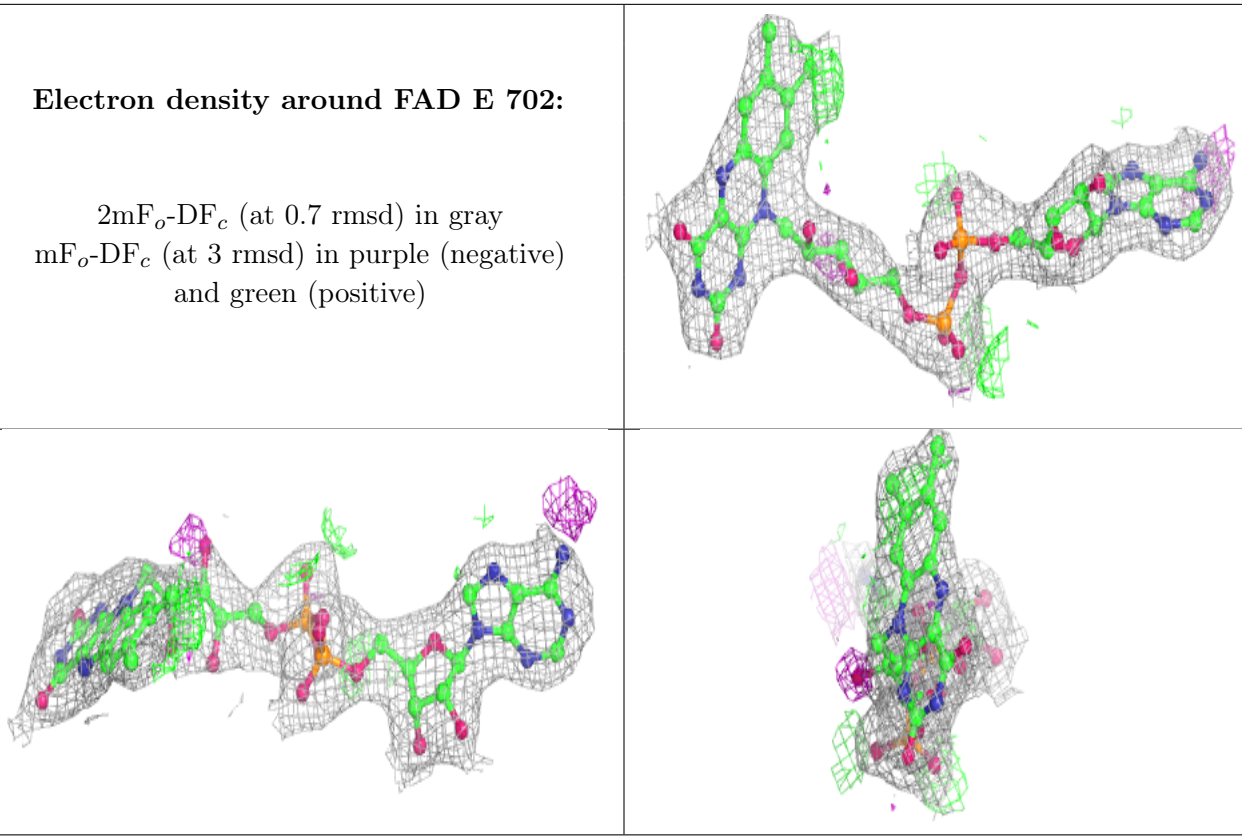
Electron density around EPH D 201:

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



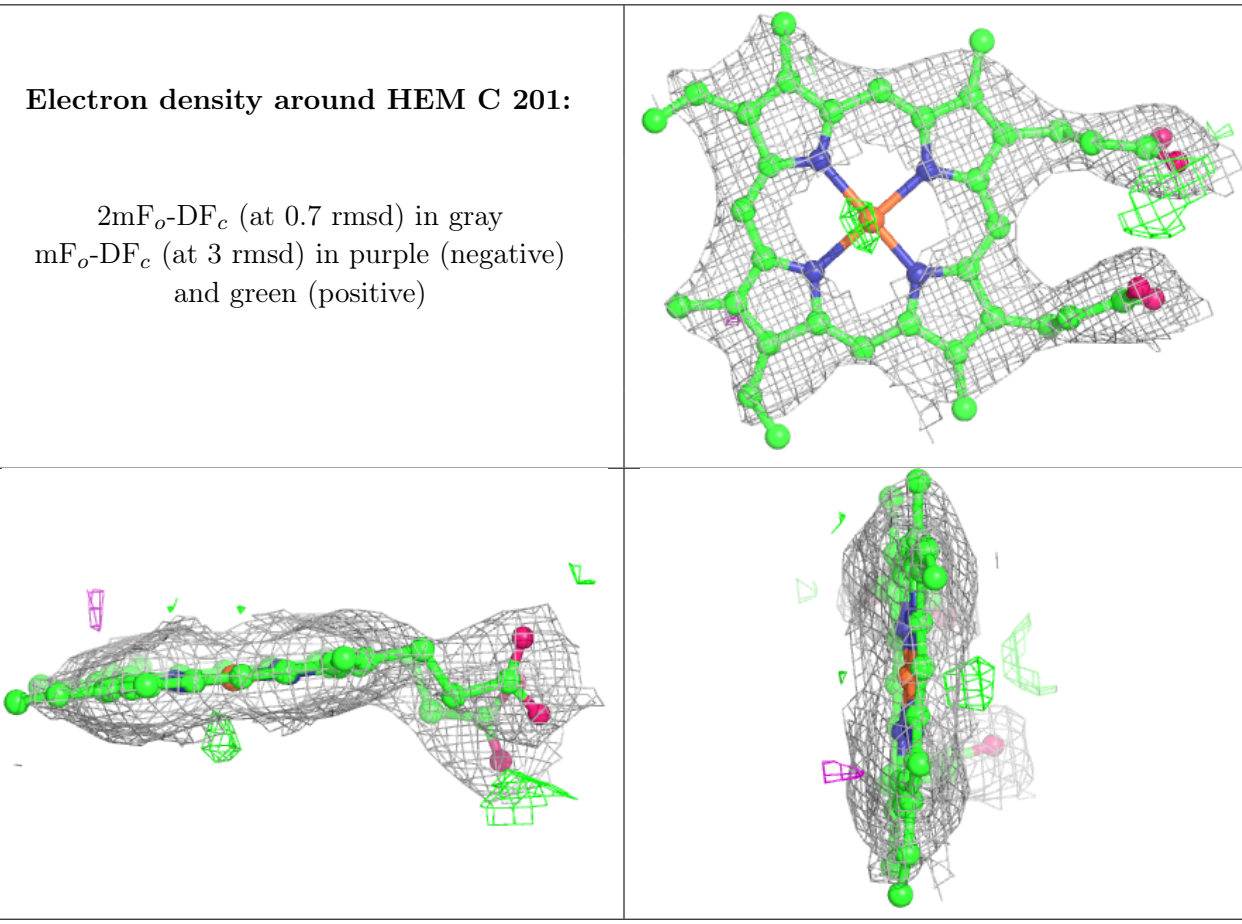
Electron density around FAD E 702:

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



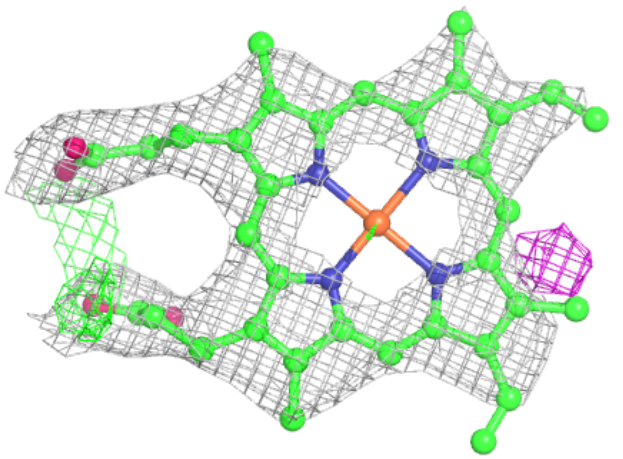
Electron density around HEM C 201:

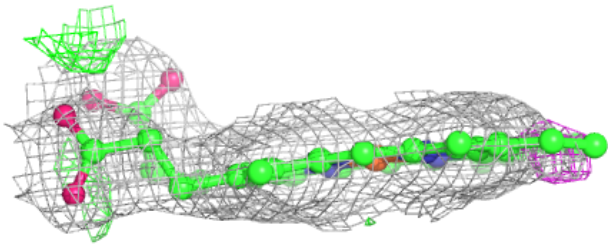
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

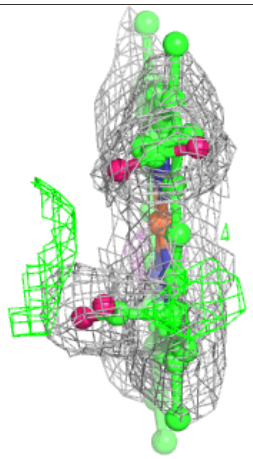


Electron density around HEM G 201:

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

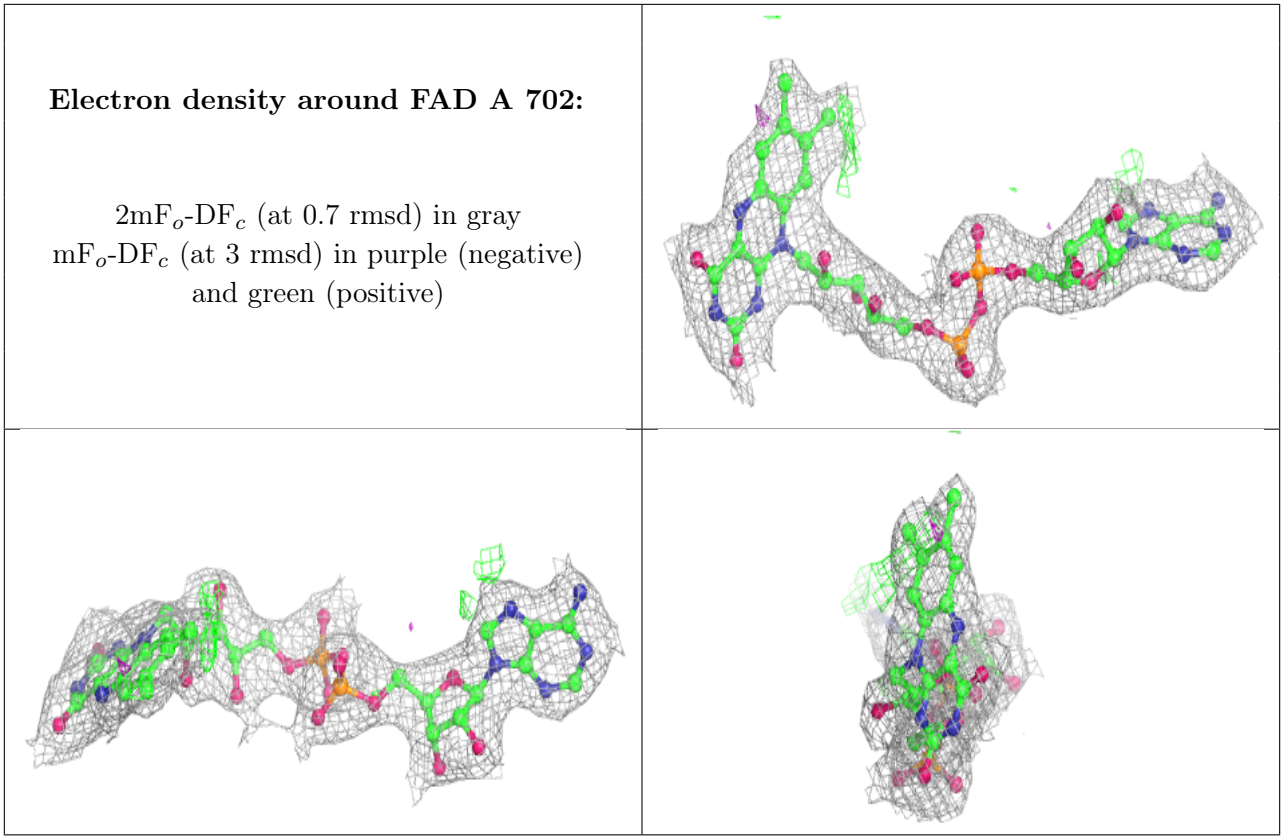






Electron density around FAD A 702:

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



6.5 Other polymers (i)

There are no such residues in this entry.