



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:17 am BST

PDB ID : 3VR8
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum*
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on : 2012-04-07
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

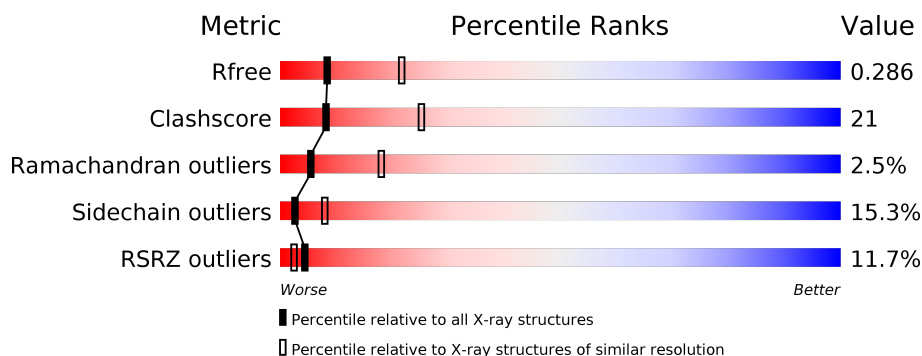
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	
1	E	645	
2	B	282	
2	F	282	
3	C	188	
3	G	188	

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Mol	Chain	Length	Quality of chain
4	D	156	
4	H	156	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	A	701	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18232 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			
1	E	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			
2	F	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			

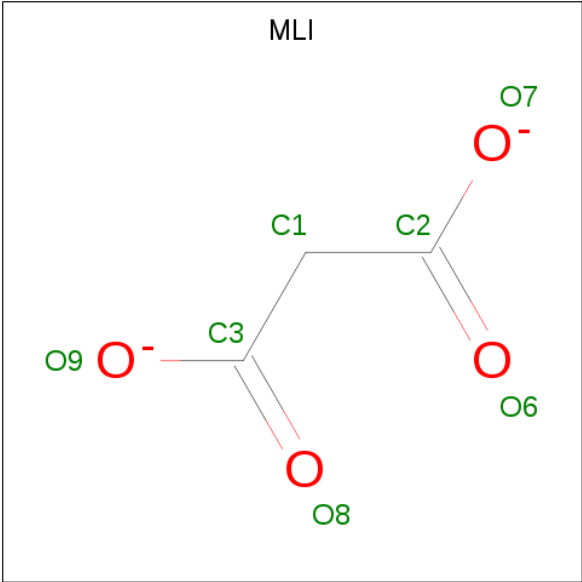
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	150	Total	C	N	O	S	0	0	0
			1195	798	201	190	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

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



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

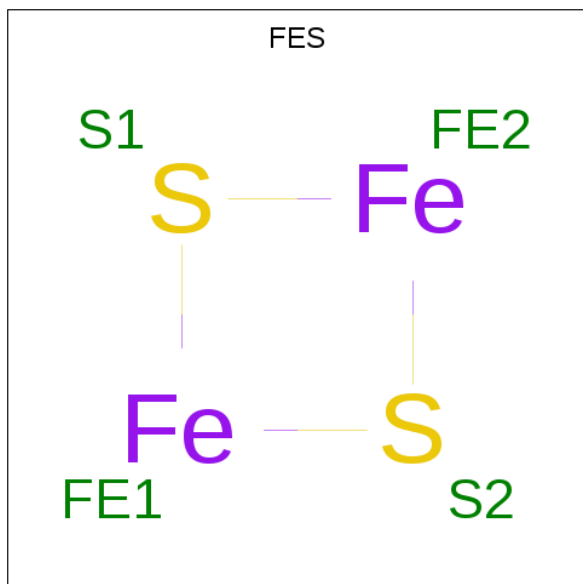
- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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



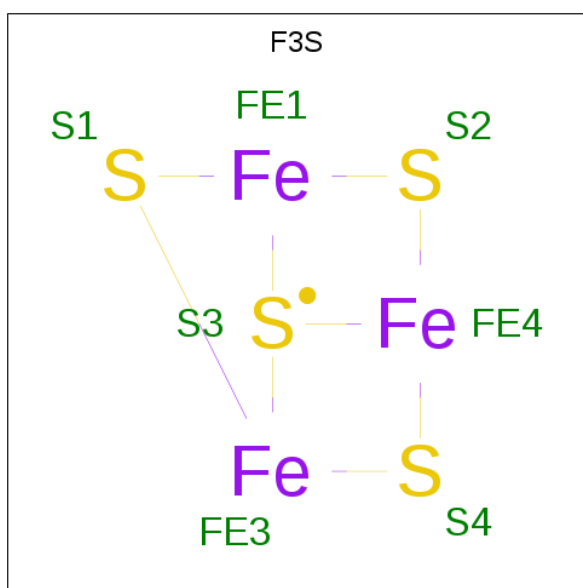
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

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



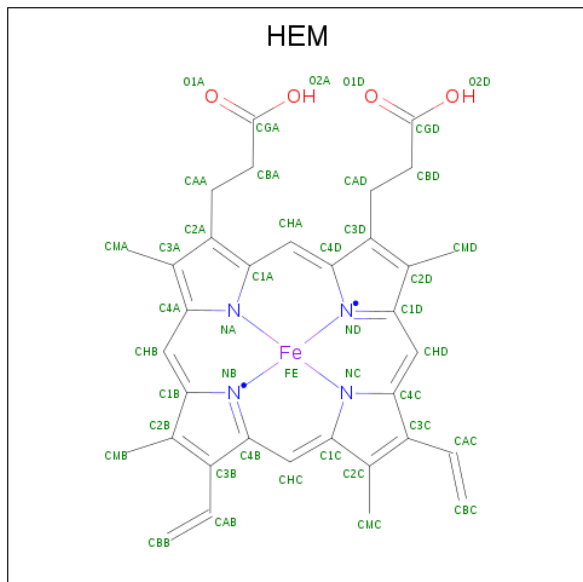
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



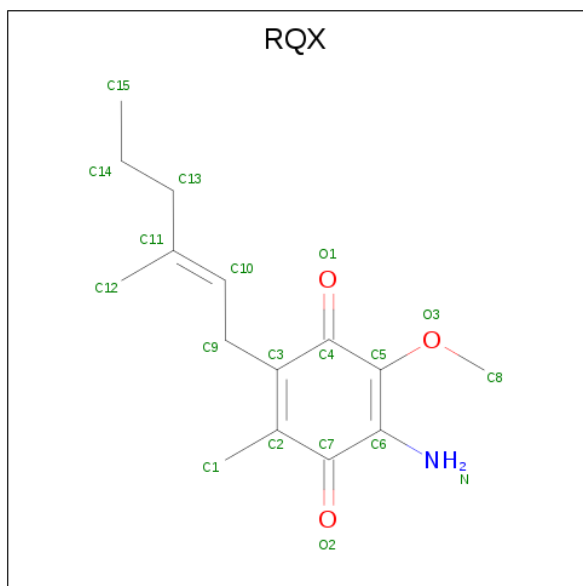
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

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



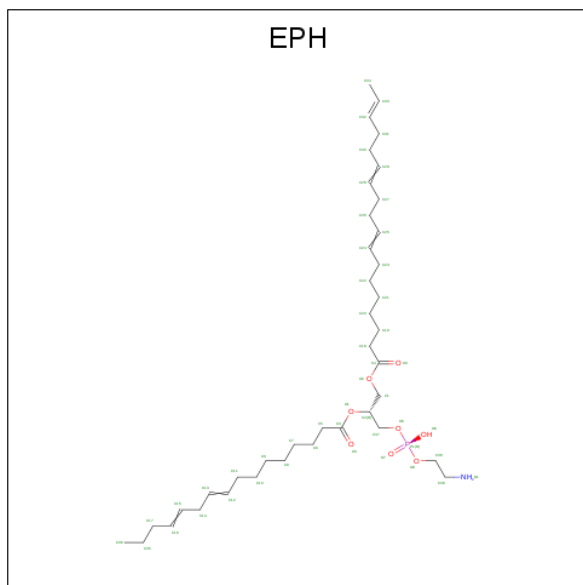
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 2-amino-3-methoxy-6-methyl-5-[(2E)-3-methylhex-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (three-letter code: RQX) (formula: $C_{15}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			19	15	1	3		
11	G	1	Total	C	N	O	0	0
			19	15	1	3		

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

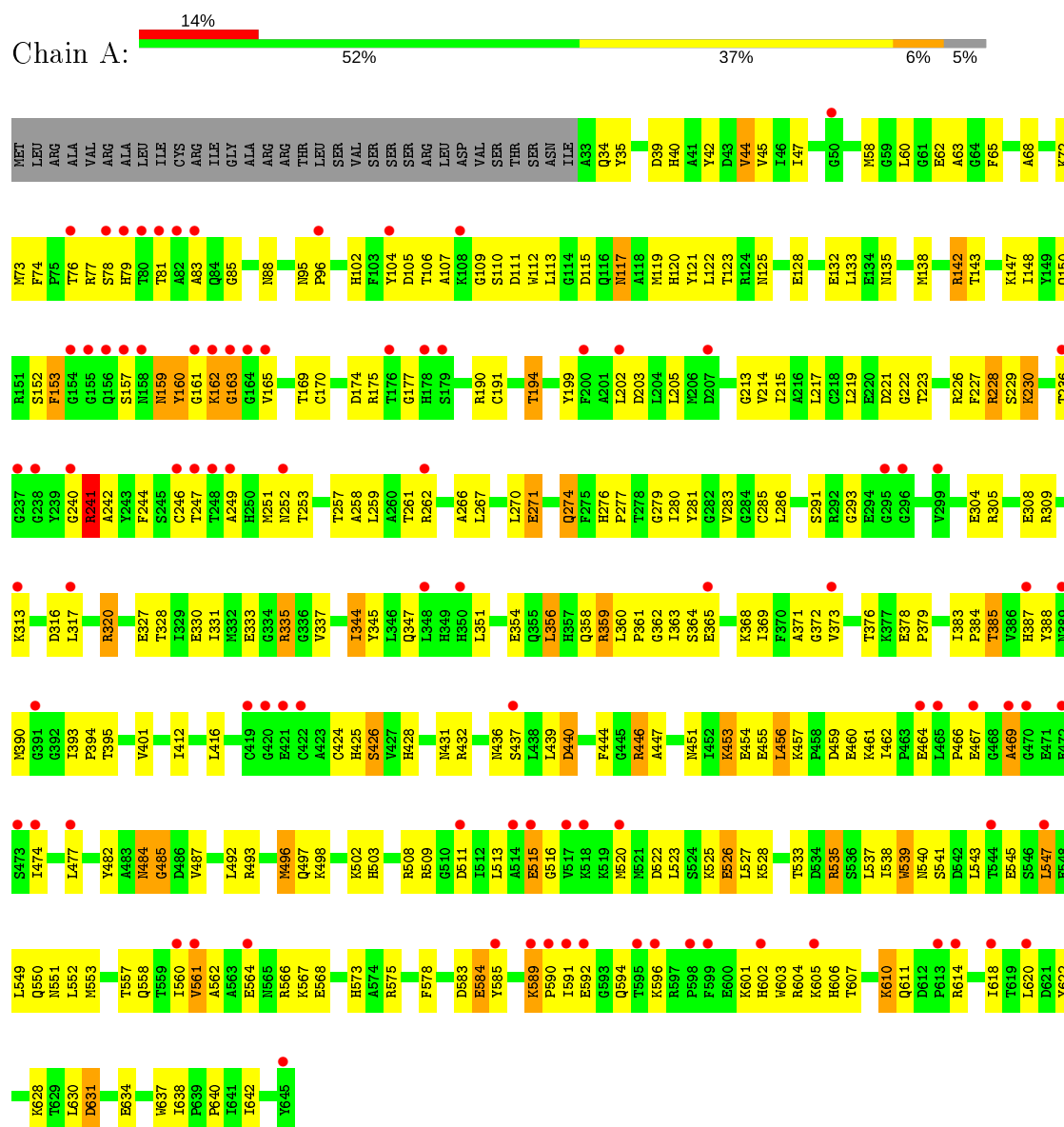


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

3 Residue-property plots

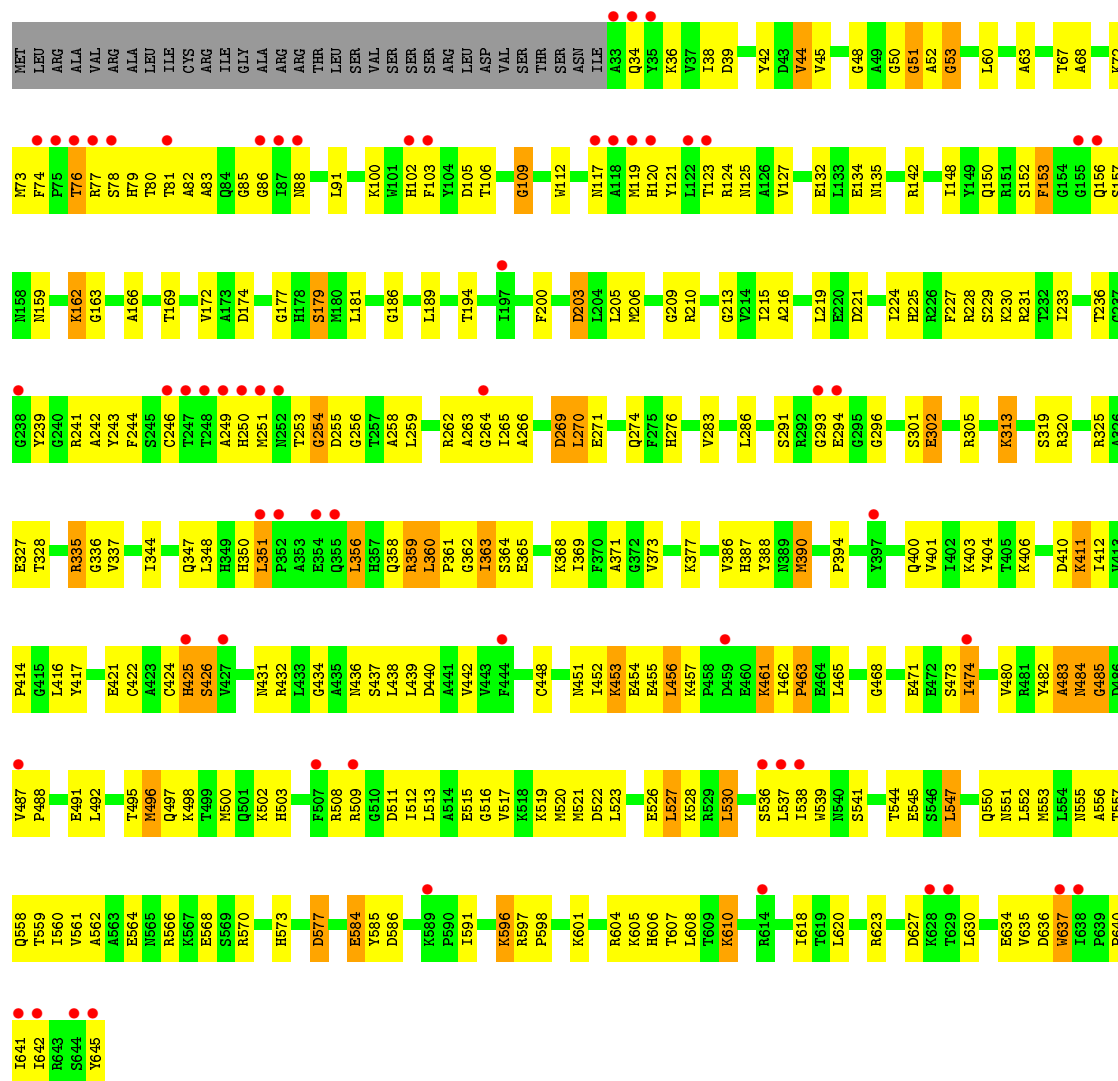
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flavoprotein subunit of complex II

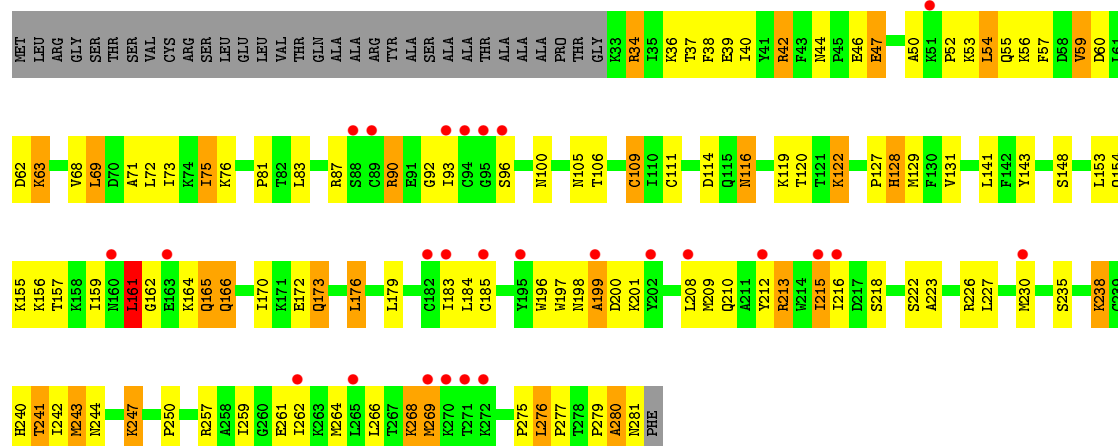


• Molecule 1: Flavoprotein subunit of complex II

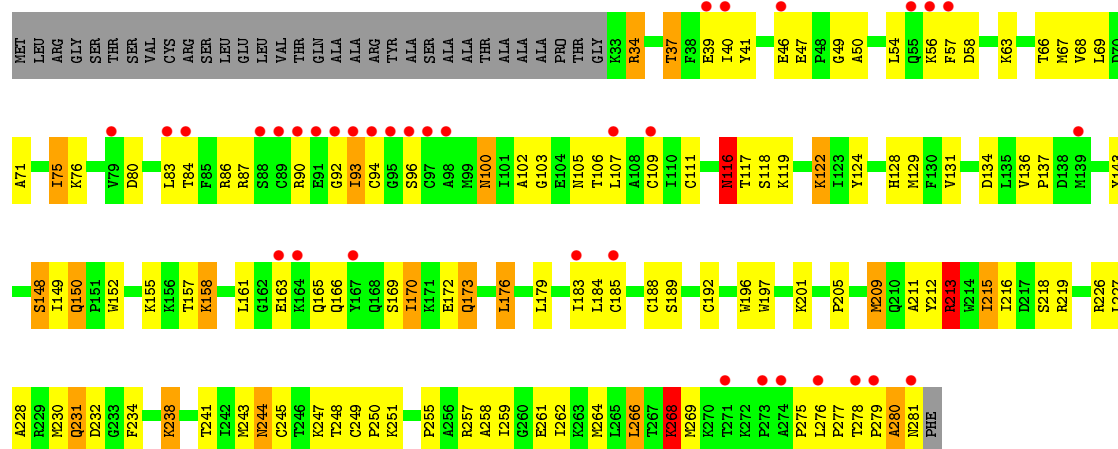
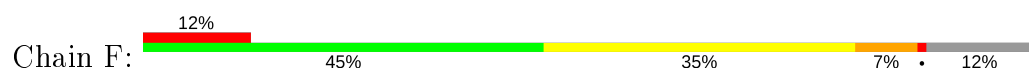




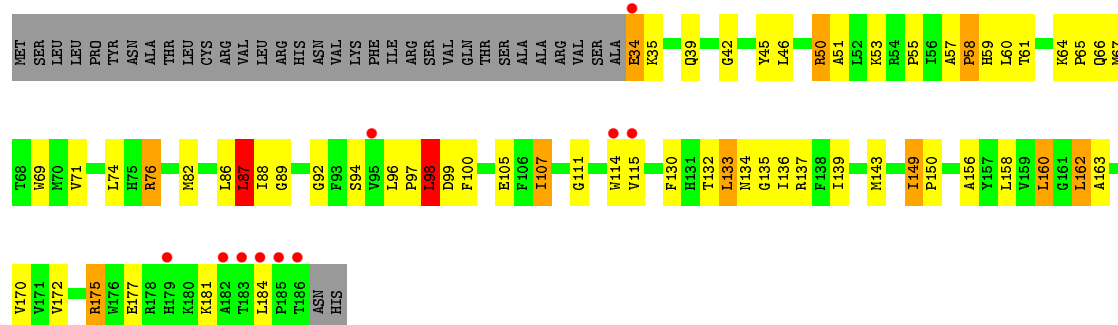
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase



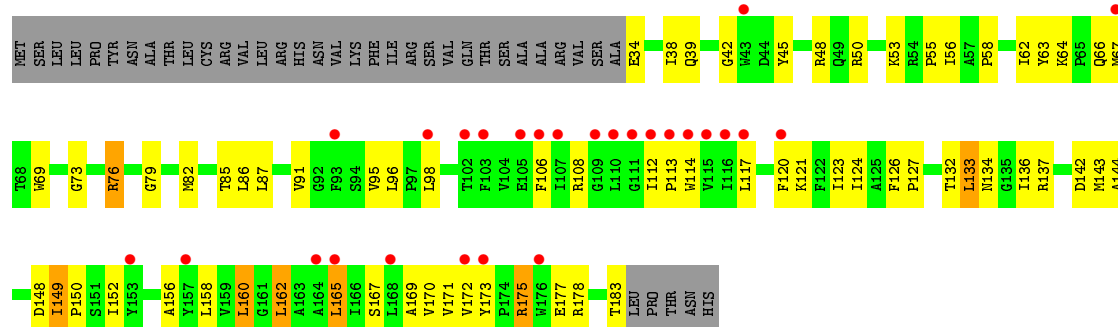
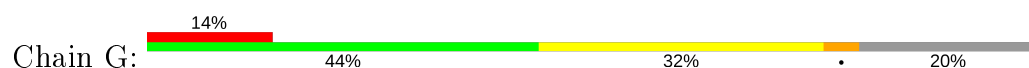
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase



• Molecule 3: Cytochrome b-large subunit

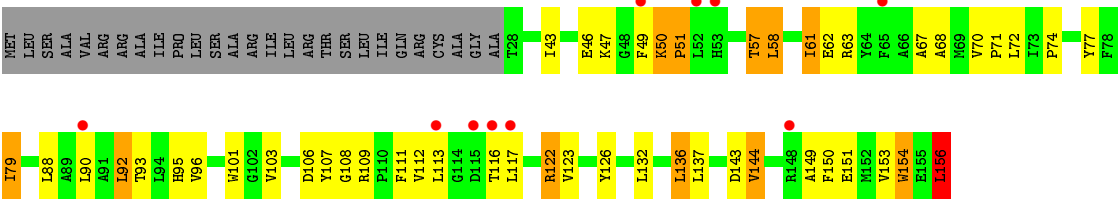


• Molecule 3: Cytochrome b-large subunit

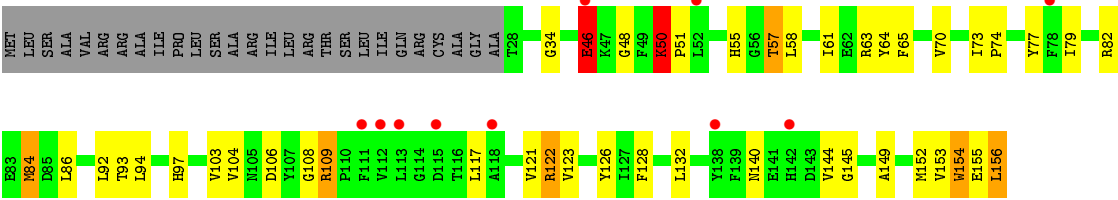


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 129.09Å 221.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.81 48.56 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.81) 92.0 (48.56-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.297 0.223 , 0.286	Depositor DCC
R_{free} test set	4025 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/4859	0.75	1/6564 (0.0%)
1	E	0.64	0/4859	0.77	1/6564 (0.0%)
2	B	0.68	0/2016	0.81	0/2723
2	F	0.74	0/2016	0.81	0/2723
3	C	0.65	0/1255	0.78	1/1709 (0.1%)
3	G	0.63	0/1232	0.68	0/1676
4	D	0.66	0/1026	0.74	1/1402 (0.1%)
4	H	0.63	0/1026	0.74	1/1402 (0.1%)
All	All	0.65	0/18289	0.77	5/24763 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	98	LEU	CA-CB-CG	7.37	132.24	115.30
1	E	351	LEU	CA-CB-CG	6.39	130.00	115.30
4	D	156	LEU	CA-CB-CG	5.49	127.92	115.30
4	H	156	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	142	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	HIS	Peptide

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	4758	0	4692	203	0
1	E	4758	0	4692	207	0
2	B	1973	0	1993	93	0
2	F	1973	0	1992	107	0
3	C	1217	0	1265	53	0
3	G	1195	0	1240	70	0
4	D	994	0	977	43	0
4	H	994	0	977	37	0
5	A	7	0	2	2	0
5	E	7	0	2	0	0
6	A	53	0	31	7	0
6	E	53	0	31	10	0
7	B	4	0	0	1	0
7	F	4	0	0	0	0
8	B	8	0	0	1	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	15	0
10	G	43	0	30	9	0
11	C	19	0	21	8	0
11	G	19	0	21	6	0
12	D	44	0	53	6	0
12	H	44	0	53	8	0
All	All	18232	0	18102	764	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 21.

The worst 5 of 764 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	1.00	1.31
1:E:79:HIS:NE2	6:E:702:FAD:HM82	0.88	1.20
1:A:446:ARG:HH11	1:A:446:ARG:HG3	1.07	1.18
2:F:34:ARG:HH21	2:F:34:ARG:HG2	1.14	1.12
1:E:79:HIS:CD2	6:E:702:FAD:HM82	1.85	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/645 (95%)	531 (87%)	68 (11%)	12 (2%)	7	23
1	E	611/645 (95%)	540 (88%)	56 (9%)	15 (2%)	5	18
2	B	247/282 (88%)	214 (87%)	26 (10%)	7 (3%)	5	15
2	F	247/282 (88%)	206 (83%)	33 (13%)	8 (3%)	4	13
3	C	151/188 (80%)	127 (84%)	18 (12%)	6 (4%)	3	9
3	G	148/188 (79%)	127 (86%)	18 (12%)	3 (2%)	7	23
4	D	127/156 (81%)	109 (86%)	16 (13%)	2 (2%)	9	29
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	4	13
All	All	2269/2542 (89%)	1959 (86%)	253 (11%)	57 (2%)	5	18

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	TYR
1	A	163	GLY
1	A	372	GLY
1	A	485	GLY
2	B	161	LEU

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	498/526 (95%)	425 (85%)	73 (15%)	3	9
1	E	498/526 (95%)	437 (88%)	61 (12%)	5	14
2	B	219/242 (90%)	173 (79%)	46 (21%)	1	3
2	F	219/242 (90%)	179 (82%)	40 (18%)	1	5
3	C	127/158 (80%)	107 (84%)	20 (16%)	2	7
3	G	124/158 (78%)	108 (87%)	16 (13%)	4	12
4	D	96/119 (81%)	79 (82%)	17 (18%)	2	5
4	H	96/119 (81%)	82 (85%)	14 (15%)	3	9
All	All	1877/2090 (90%)	1590 (85%)	287 (15%)	2	8

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	99	ASP
1	E	76	THR
3	G	133	LEU
3	C	149	ILE
4	D	90	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	240	HIS
1	E	120	HIS
2	F	165	GLN
2	B	244	ASN
1	E	88	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 carbohydrates 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$
9	F3S	F	303	2	0,9,9	0.00	-	-		
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
8	SF4	F	302	2	0,12,12	0.00	-	-		
6	FAD	E	702	1	51,58,58	1.59	7 (13%)	60,89,89	2.13	14 (23%)
10	HEM	G	201	3,4	27,50,50	2.18	6 (22%)	17,82,82	1.58	3 (17%)
8	SF4	B	302	2	0,12,12	0.00	-	-		
6	FAD	A	702	1	51,58,58	1.39	6 (11%)	60,89,89	2.03	13 (21%)
10	HEM	C	201	3,4	27,50,50	2.25	8 (29%)	17,82,82	1.92	5 (29%)
7	FES	B	301	2	0,4,4	0.00	-	-		
7	FES	F	301	2	0,4,4	0.00	-	-		
11	RQX	C	202	-	19,19,19	2.23	3 (15%)	20,26,26	2.38	5 (25%)
9	F3S	B	303	2	0,9,9	0.00	-	-		
11	RQX	G	202	-	19,19,19	2.51	2 (10%)	20,26,26	2.00	4 (20%)
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
12	EPH	D	201	-	43,43,48	1.88	8 (18%)	45,48,53	2.40	5 (11%)
12	EPH	H	201	-	43,43,48	1.87	9 (20%)	45,48,53	2.34	5 (11%)

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
9	F3S	F	303	2	-	-	0/3/3/3
6	FAD	A	702	1	-	12/30/50/50	0/6/6/6
8	SF4	F	302	2	-	-	0/6/5/5
6	FAD	E	702	1	-	12/30/50/50	0/6/6/6
10	HEM	G	201	3,4	-	5/6/54/54	-
12	EPH	D	201	-	-	29/47/47/52	-
5	MLI	E	701	-	-	0/0/4/4	-
10	HEM	C	201	3,4	-	5/6/54/54	-
7	FES	B	301	2	-	-	0/1/1/1
7	FES	F	301	2	-	-	0/1/1/1
11	RQX	C	202	-	-	7/10/34/34	0/1/1/1
9	F3S	B	303	2	-	-	0/3/3/3
11	RQX	G	202	-	-	6/10/34/34	0/1/1/1
5	MLI	A	701	-	-	0/0/4/4	-
8	SF4	B	302	2	-	-	0/6/5/5
12	EPH	H	201	-	-	24/47/47/52	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	202	RQX	C3-C2	7.98	1.49	1.35
12	D	201	EPH	C29-C28	6.95	1.72	1.31
12	H	201	EPH	C29-C28	6.78	1.71	1.31
11	C	202	RQX	C3-C2	6.62	1.47	1.35
11	G	202	RQX	C6-C5	5.85	1.50	1.39

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C27-C26-C25	12.29	145.13	112.92
12	D	201	EPH	C27-C26-C25	11.70	143.60	112.92
6	E	702	FAD	C4-N3-C2	7.22	121.24	115.14
11	C	202	RQX	C9-C3-C4	6.88	126.75	118.48
12	D	201	EPH	C2-O1-C3	6.10	132.81	117.79

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

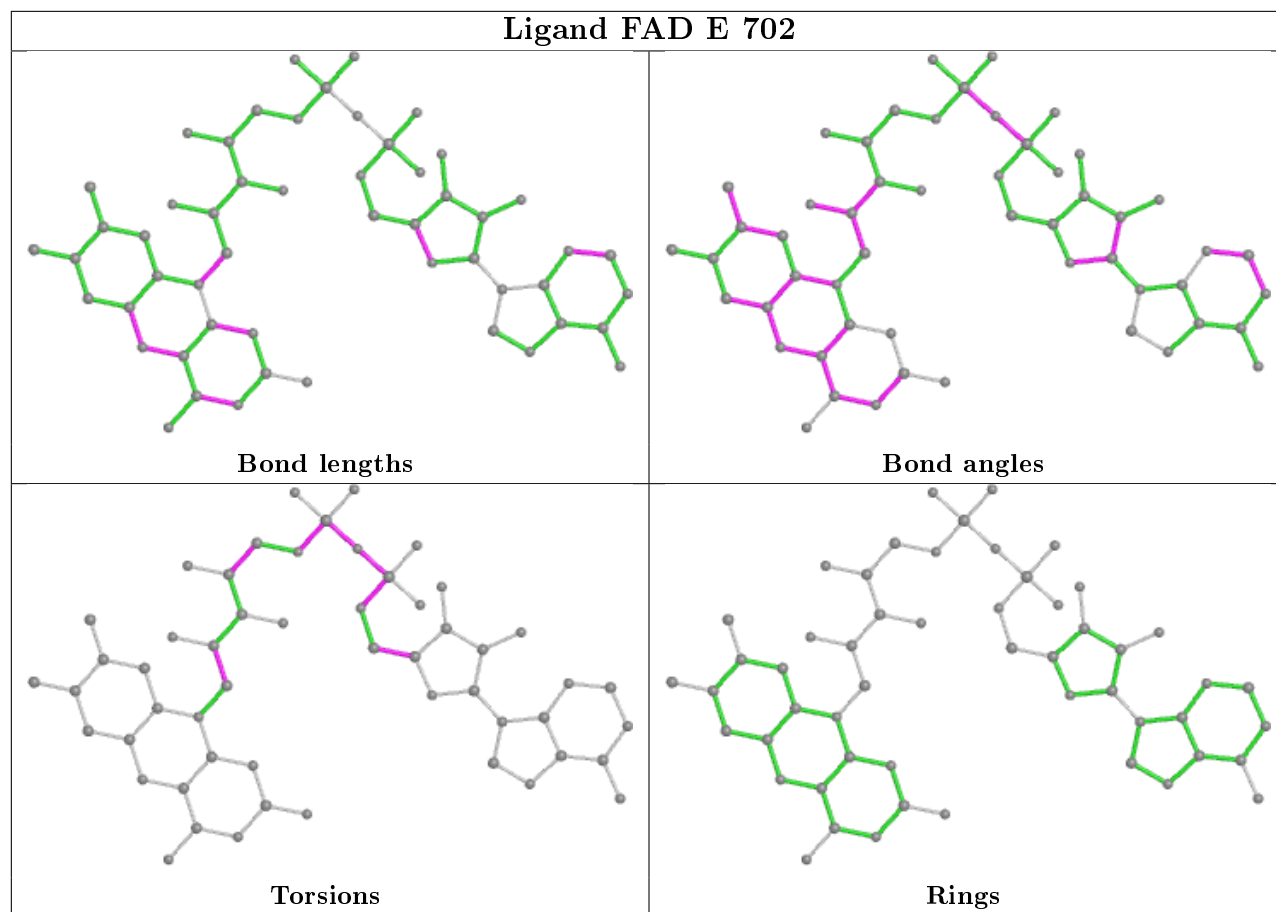
Mol	Chain	Res	Type	Atoms
6	E	702	FAD	C3'-C4'-C5'-O5'
6	E	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	C5'-O5'-P-O2P
10	G	201	HEM	C1A-C2A-CAA-CBA
10	G	201	HEM	C3A-C2A-CAA-CBA

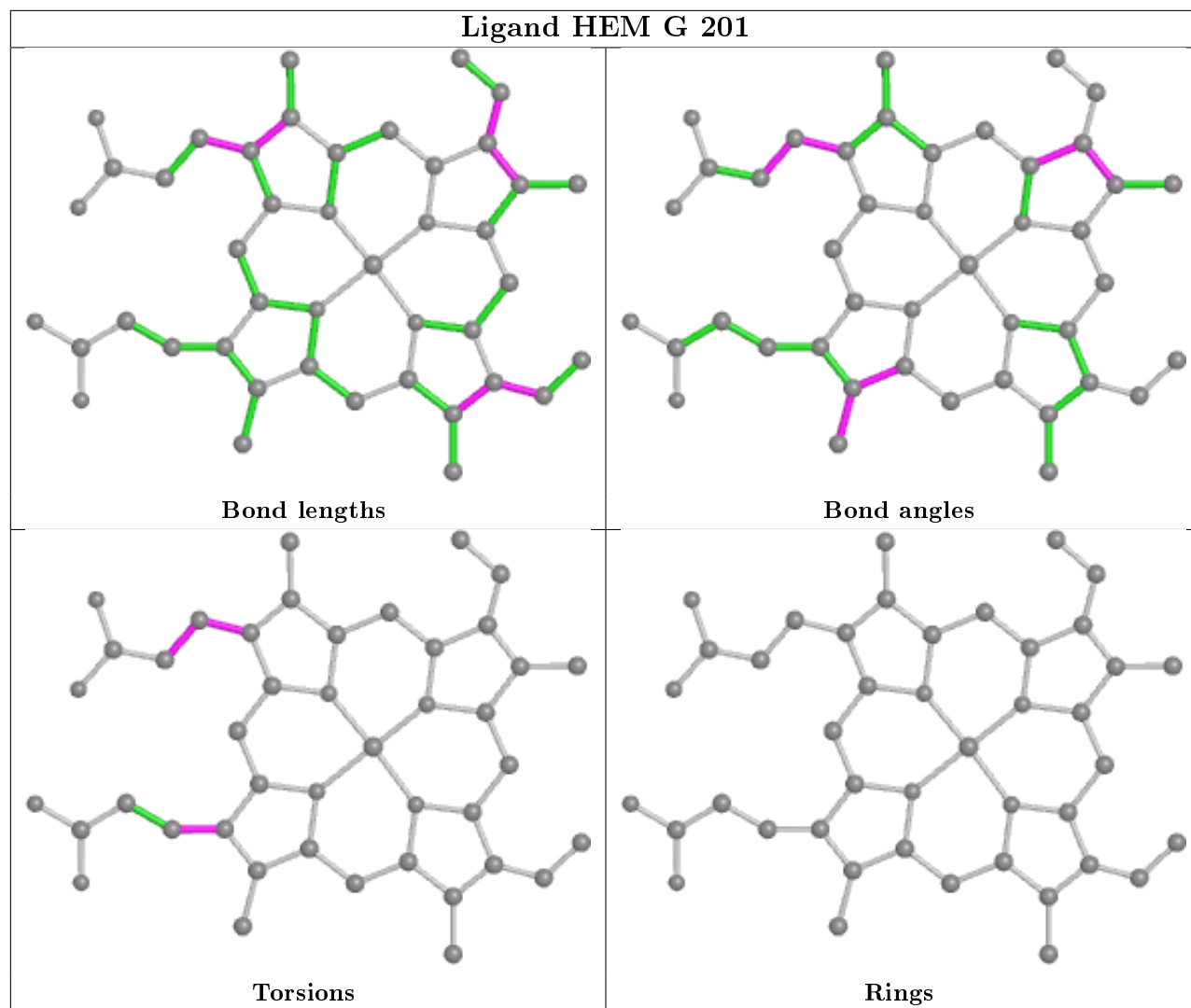
There are no ring outliers.

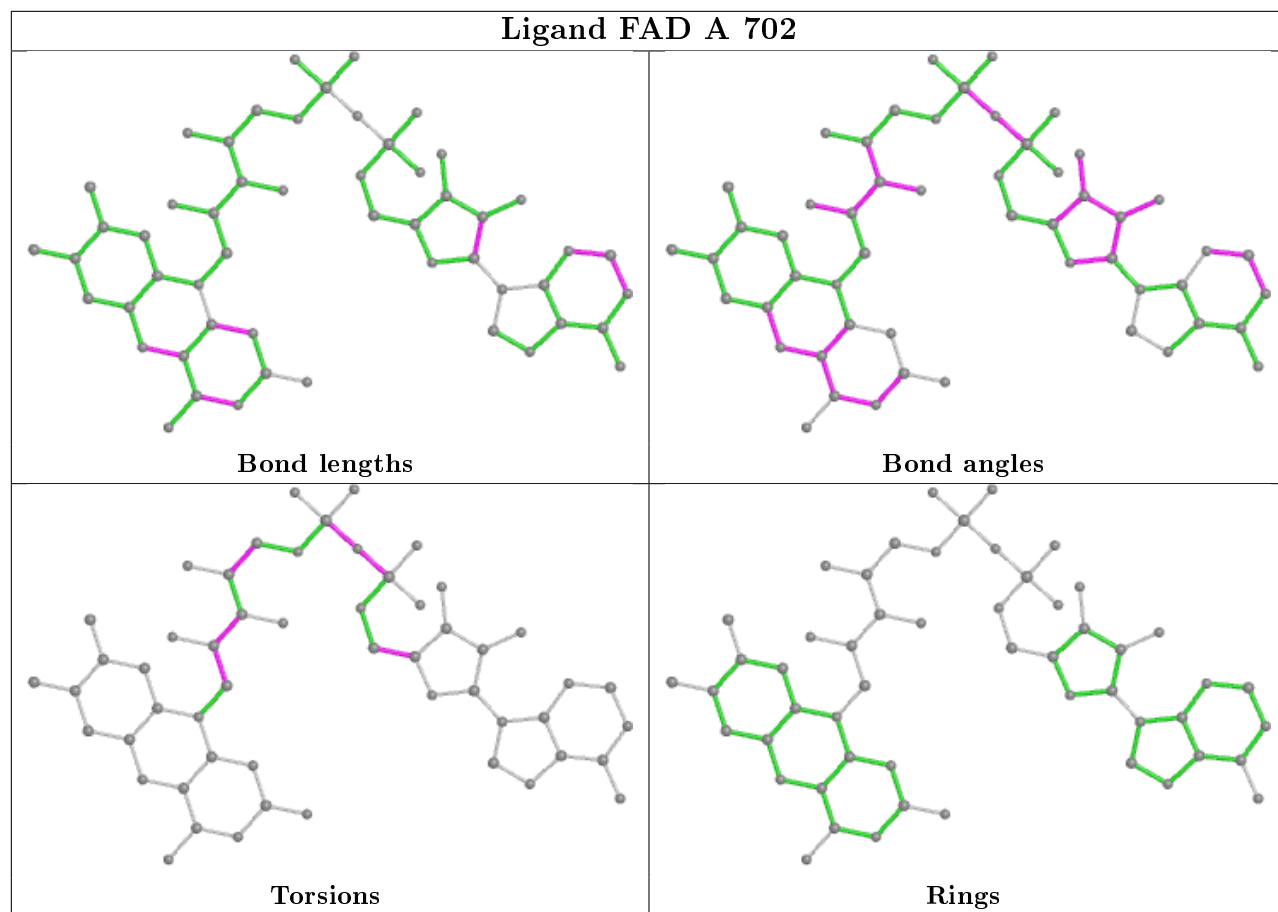
11 monomers are involved in 73 short contacts:

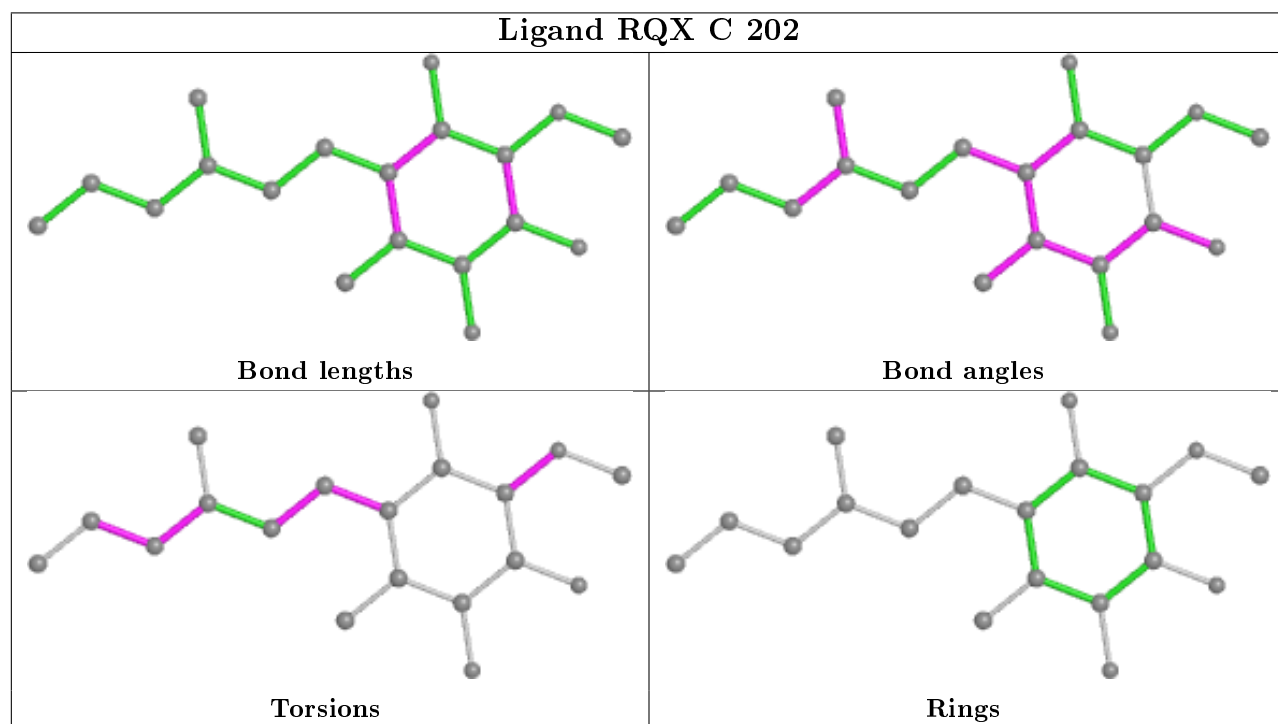
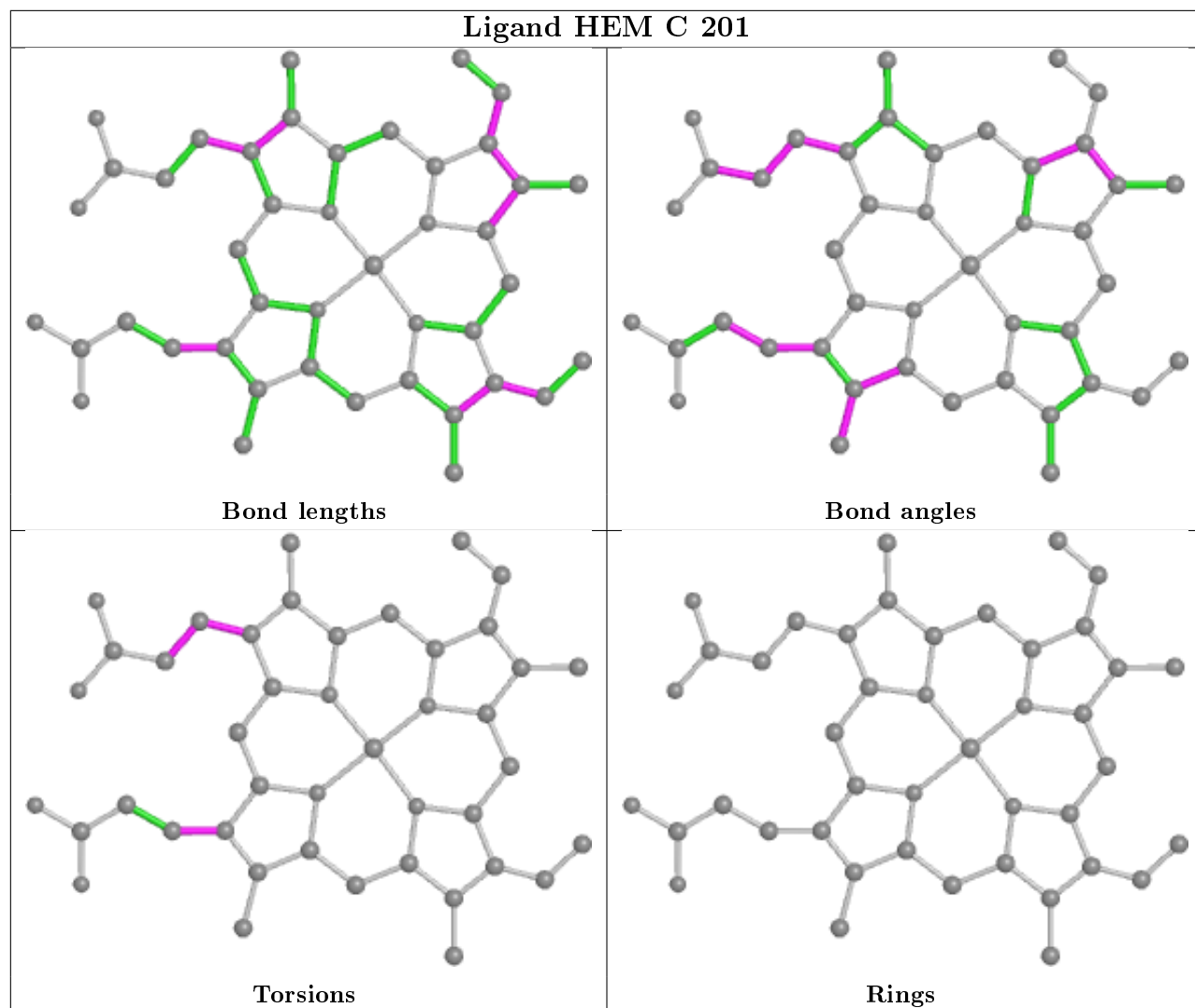
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	702	FAD	10	0
10	G	201	HEM	9	0
8	B	302	SF4	1	0
6	A	702	FAD	7	0
10	C	201	HEM	15	0
7	B	301	FES	1	0
11	C	202	RQX	8	0
11	G	202	RQX	6	0
5	A	701	MLI	2	0
12	D	201	EPH	6	0
12	H	201	EPH	8	0

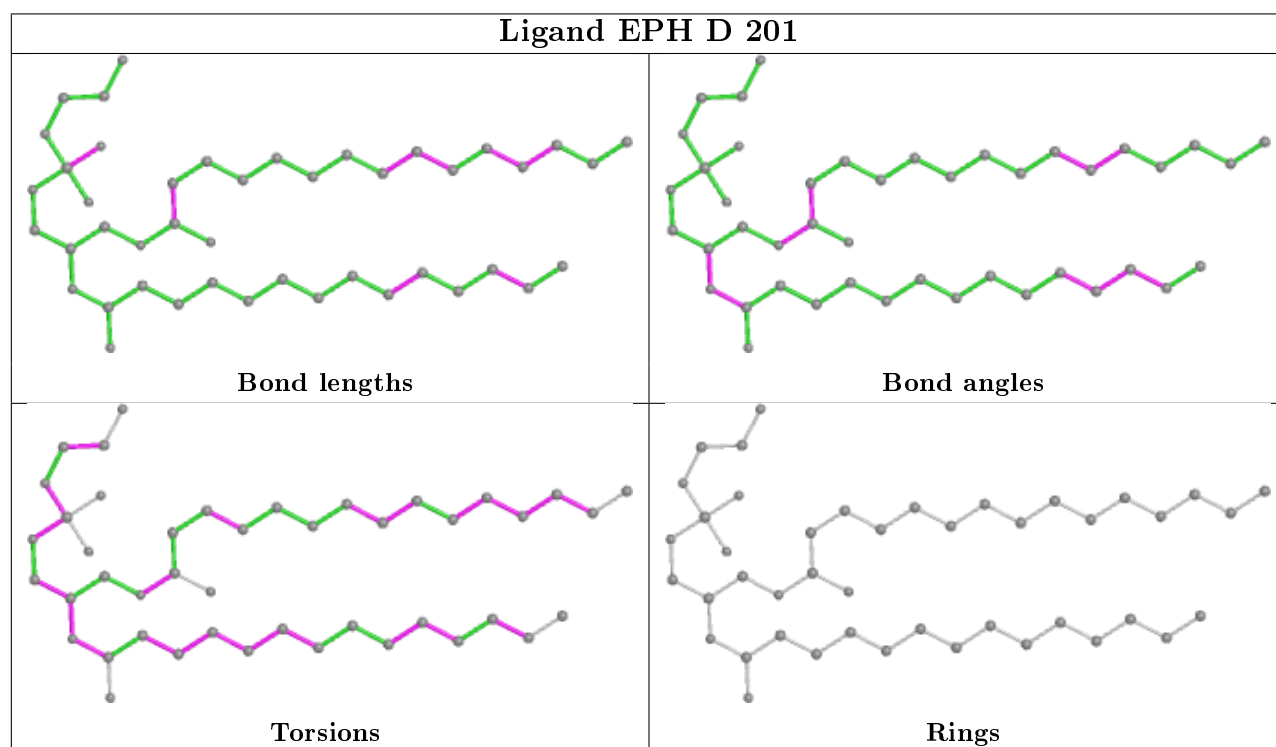
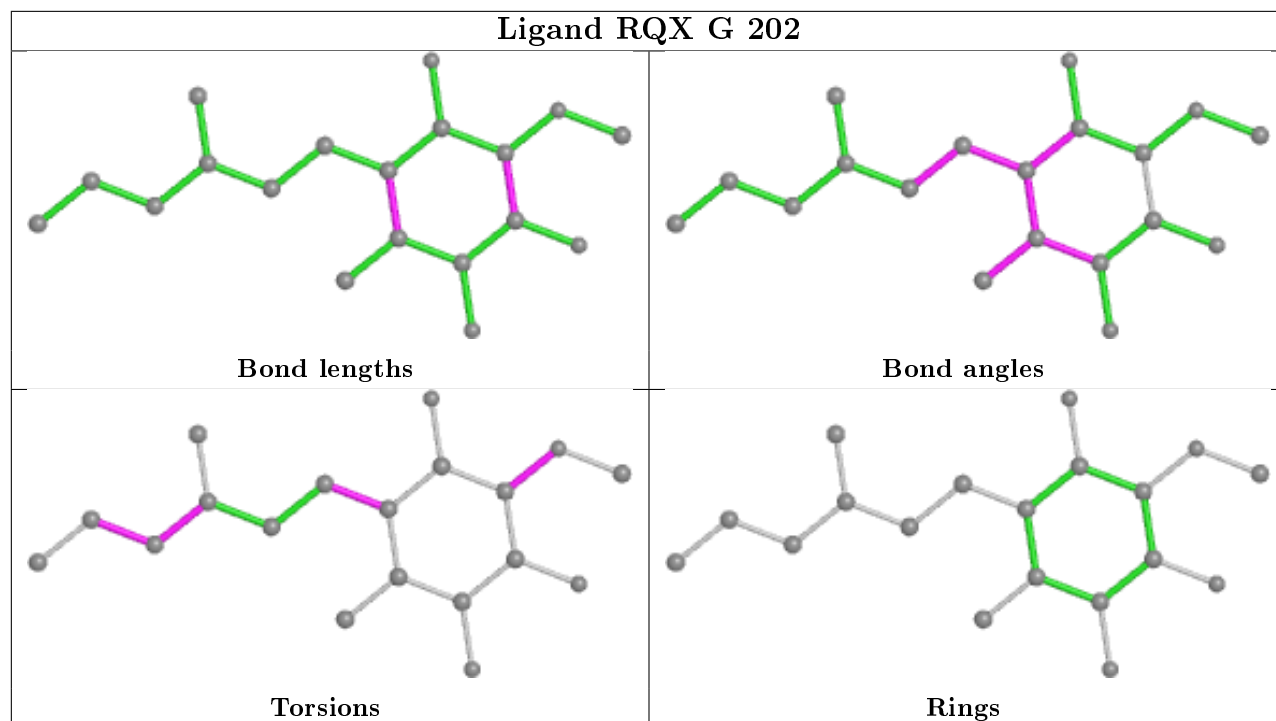
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

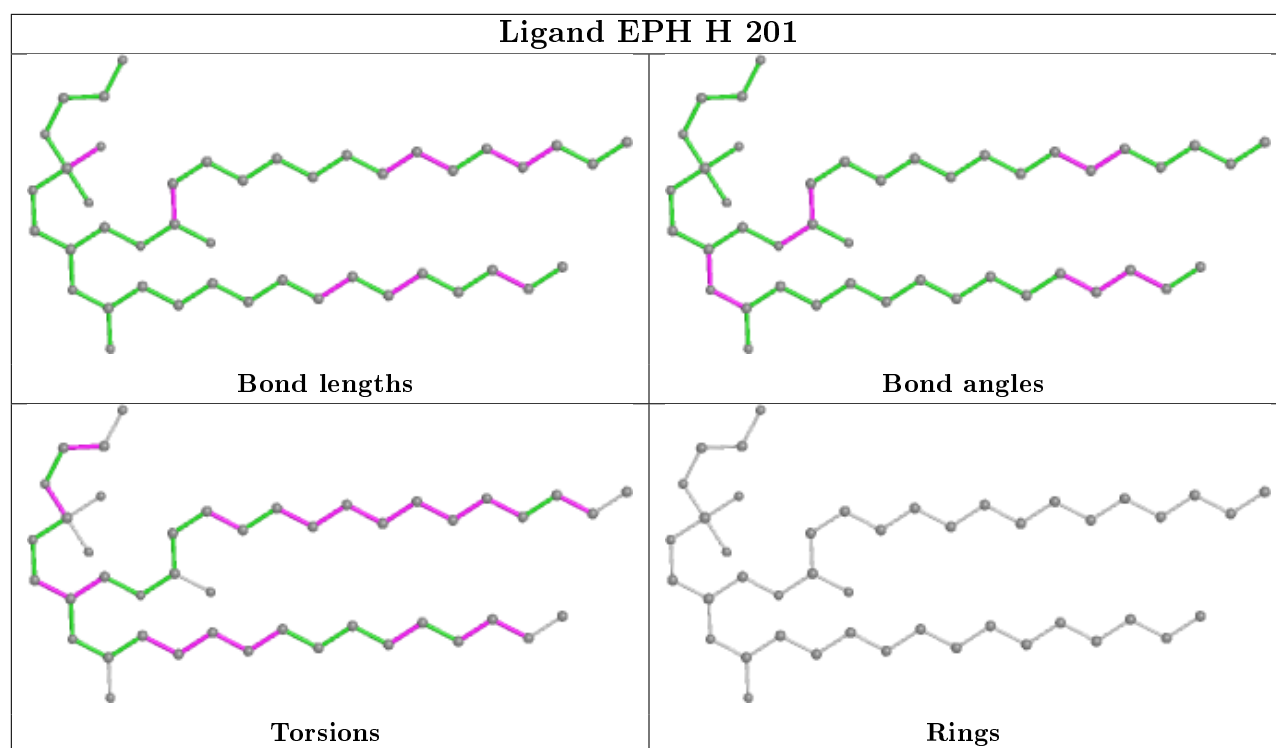












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/645 (95%)	0.42	90 (14%) 2 1	71, 96, 118, 136	0
1	E	613/645 (95%)	0.21	60 (9%) 7 4	70, 90, 113, 126	0
2	B	249/282 (88%)	0.15	26 (10%) 6 3	72, 89, 117, 137	0
2	F	249/282 (88%)	0.44	35 (14%) 2 1	67, 86, 109, 120	0
3	C	153/188 (81%)	0.19	10 (6%) 18 11	78, 97, 142, 162	0
3	G	150/188 (79%)	0.60	27 (18%) 1 1	77, 100, 151, 156	0
4	D	129/156 (82%)	0.18	10 (7%) 13 7	89, 101, 129, 142	0
4	H	129/156 (82%)	0.17	10 (7%) 13 7	86, 103, 133, 146	0
All	All	2285/2542 (89%)	0.30	268 (11%) 4 2	67, 94, 124, 162	0

The worst 5 of 268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	9.6
4	D	49	PHE	7.2
3	G	115	VAL	6.3
3	G	112	ILE	6.2
3	C	183	THR	6.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

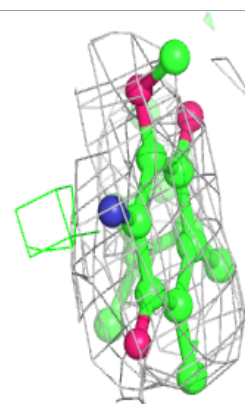
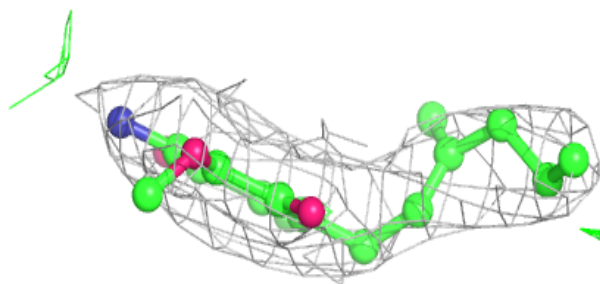
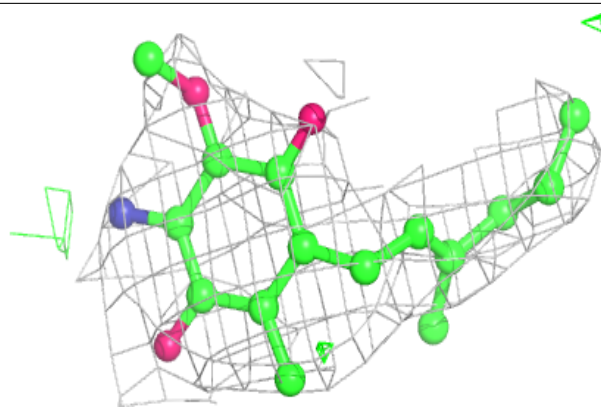
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	RQX	C	202	19/19	0.79	0.29	113,116,119,119	0
11	RQX	G	202	19/19	0.80	0.35	120,125,127,127	0
12	EPH	H	201	44/49	0.80	0.34	97,113,134,135	0
12	EPH	D	201	44/49	0.88	0.24	94,102,121,122	0
5	MLI	A	701	7/7	0.91	0.32	102,103,106,106	0
6	FAD	A	702	53/53	0.92	0.40	77,83,87,89	0
5	MLI	E	701	7/7	0.95	0.21	92,93,93,93	0
6	FAD	E	702	53/53	0.96	0.26	63,79,88,89	0
10	HEM	C	201	43/43	0.97	0.20	89,93,96,98	0
10	HEM	G	201	43/43	0.98	0.19	92,97,103,106	0
9	F3S	B	303	7/7	0.98	0.15	83,85,86,87	0
8	SF4	F	302	8/8	0.99	0.22	57,61,64,65	0
7	FES	F	301	4/4	0.99	0.29	60,66,68,75	0
8	SF4	B	302	8/8	0.99	0.20	63,66,68,70	0
9	F3S	F	303	7/7	0.99	0.18	82,83,84,87	0
7	FES	B	301	4/4	1.00	0.27	70,70,72,78	0

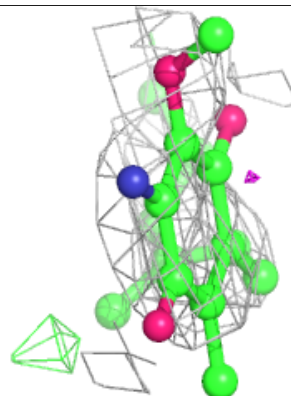
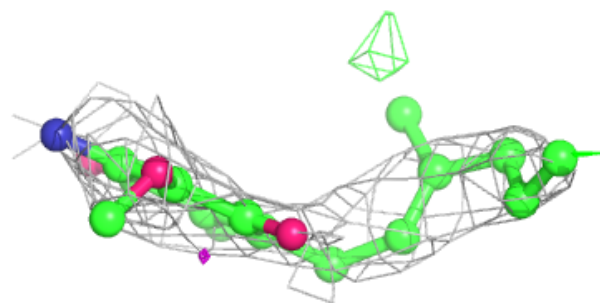
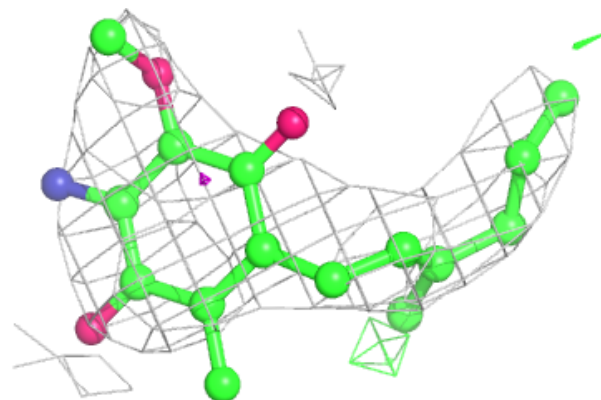
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RQX 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)

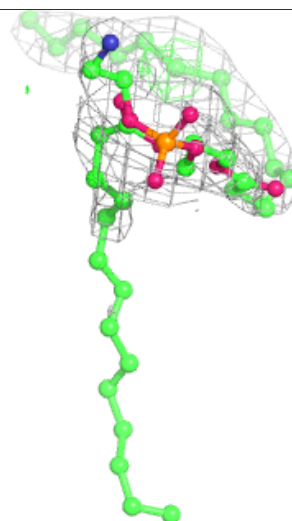
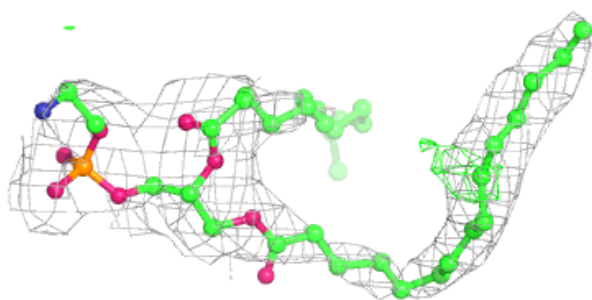
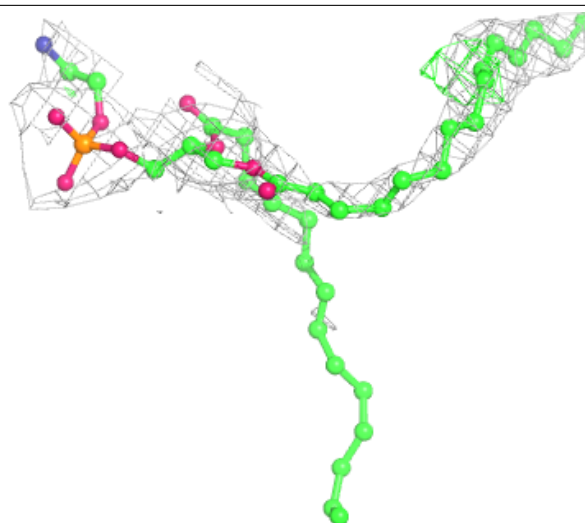
**Electron density around RQX G 202:**

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



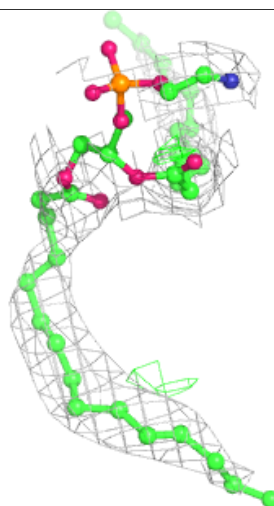
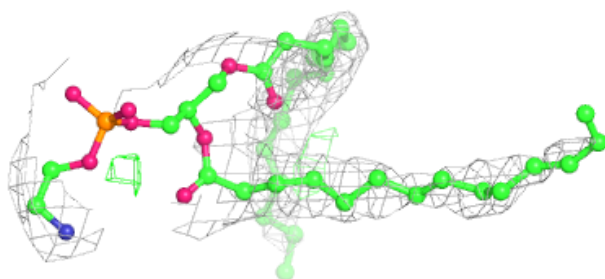
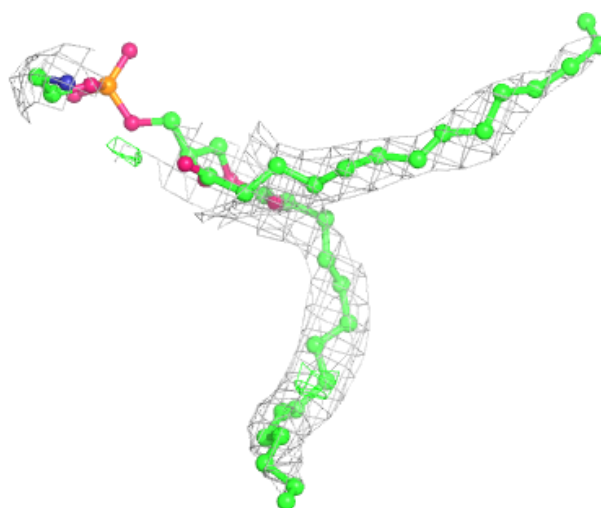
Electron density around EPH H 201:

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



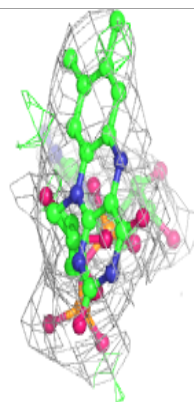
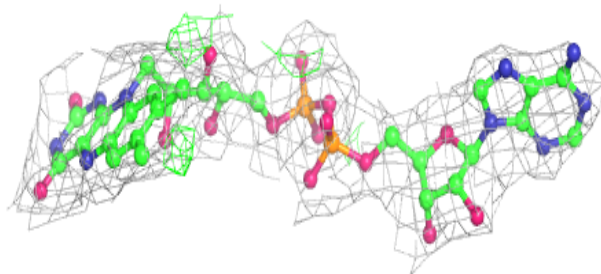
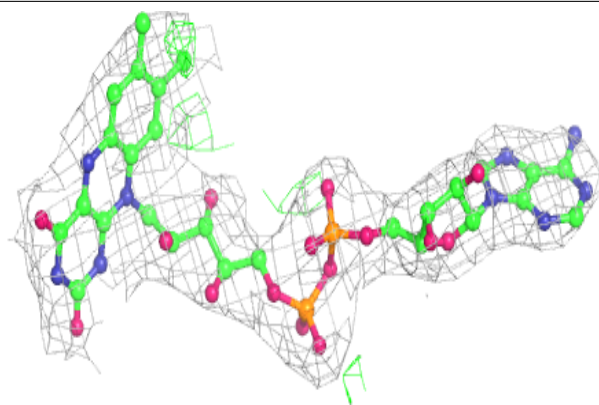
Electron density around EPH D 201:

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

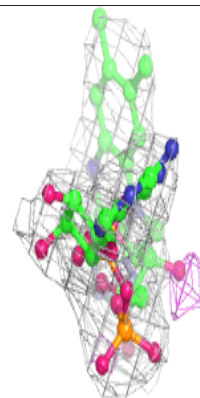
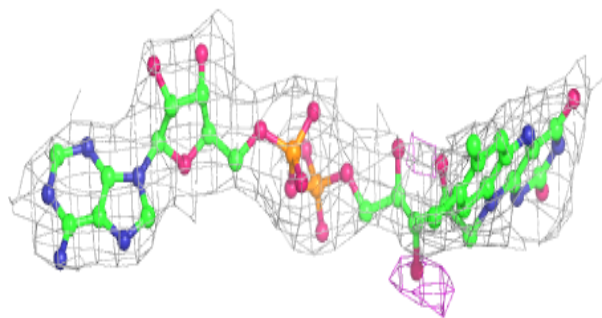
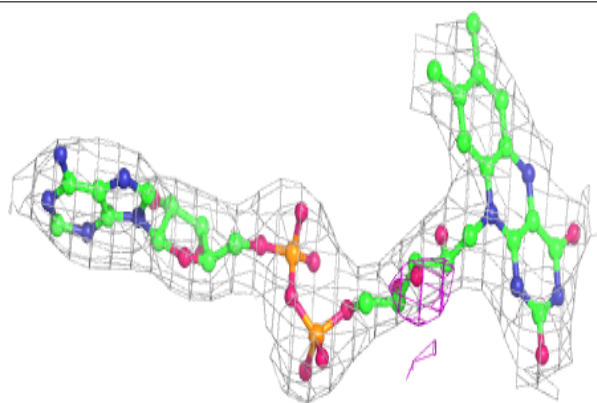


Electron density around FAD A 702:

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

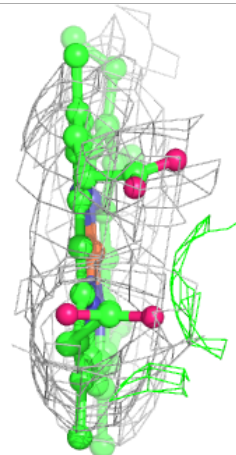
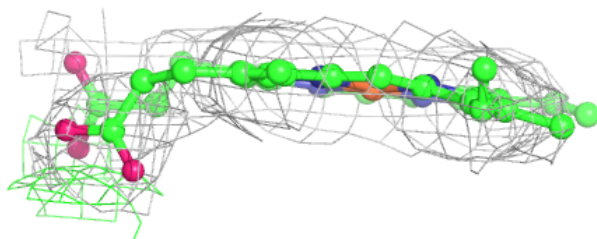
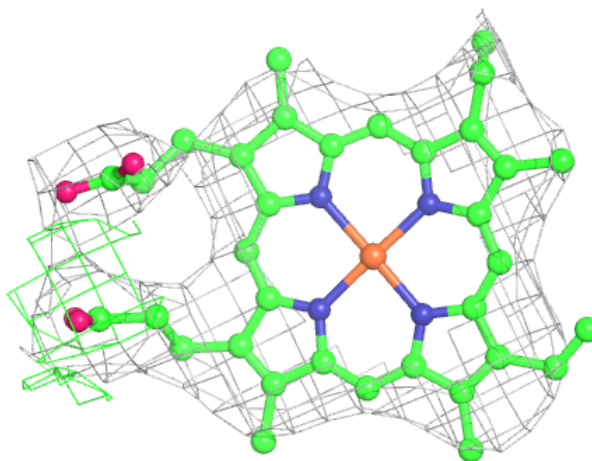
**Electron density around FAD E 702:**

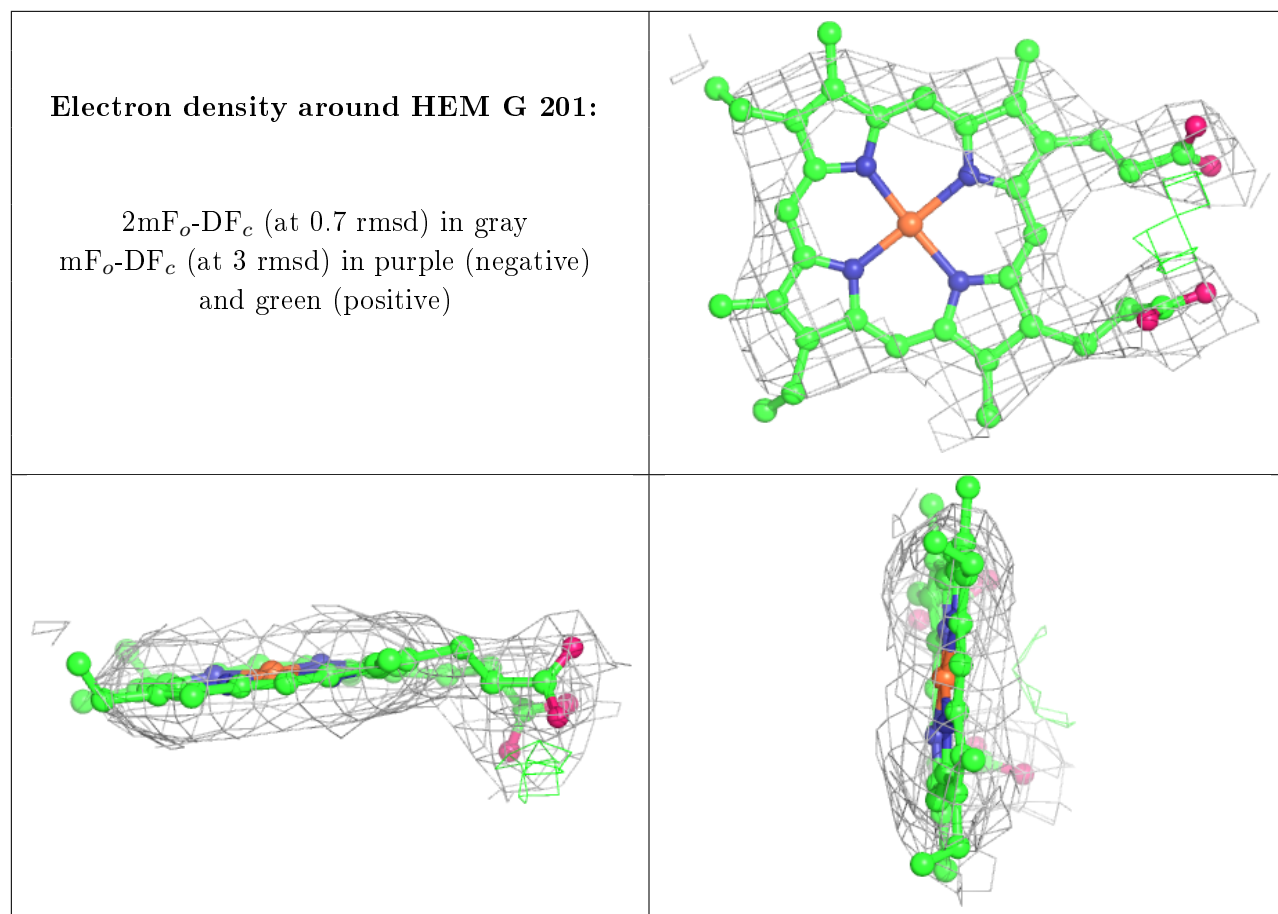
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.