



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 06:06 PM EDT

PDB ID : 3VR8 / pdb_00003vr8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

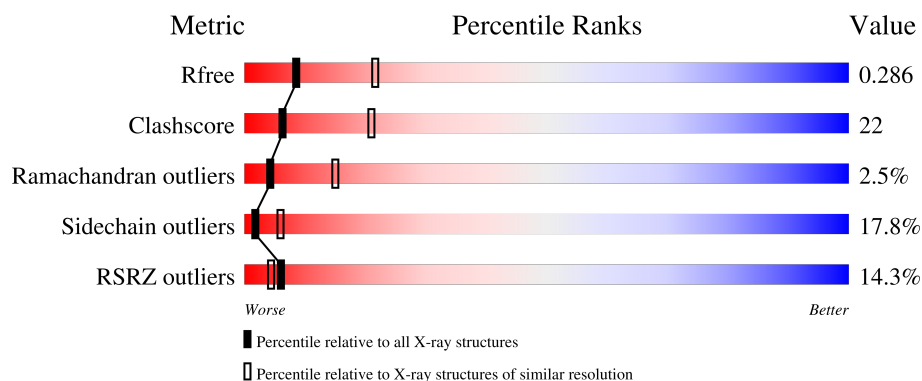
1 Overall quality at a glance ⓘ

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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 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 $\leq 5\%$. 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	12% 49% 38% 7% 5%
1	E	645	14% 46% 41% 8% 5%
2	B	282	15% 45% 33% 9% 12%
2	F	282	11% 42% 36% 9% 12%

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Mol	Chain	Length	Quality of chain
3	C	188	
3	G	188	
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			

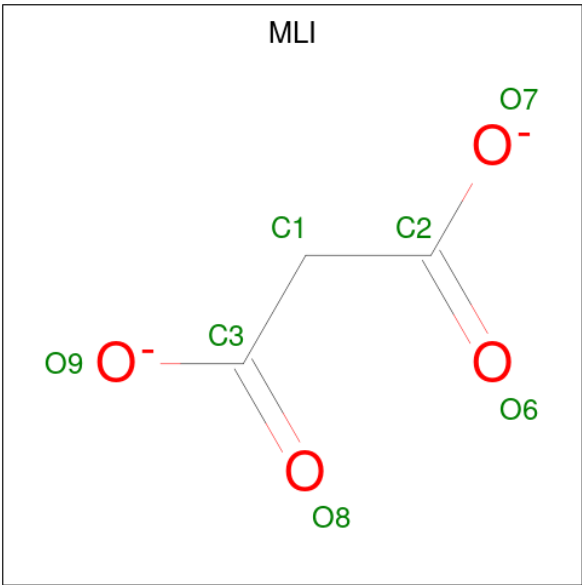
- Molecule 3 is a protein called Cytochrome b-large subunit.

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.

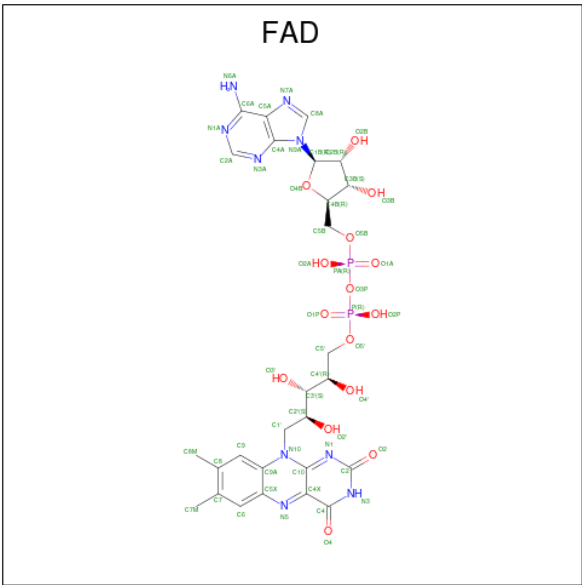
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



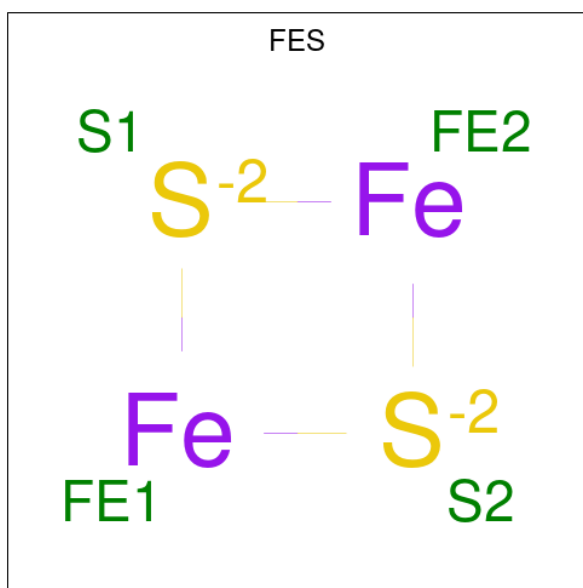
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

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



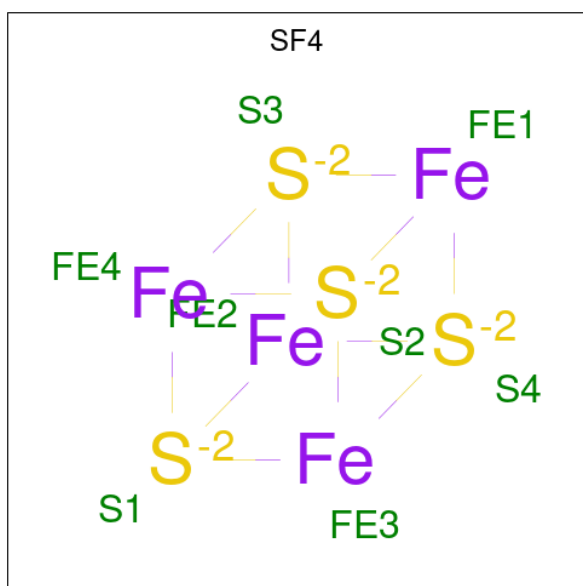
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
6	E	1	Total	C	N	O	P	0
			53	27	9	15	2	

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



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

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



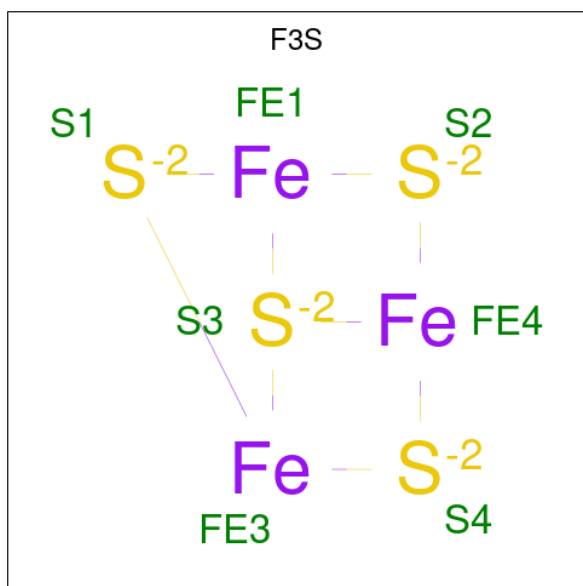
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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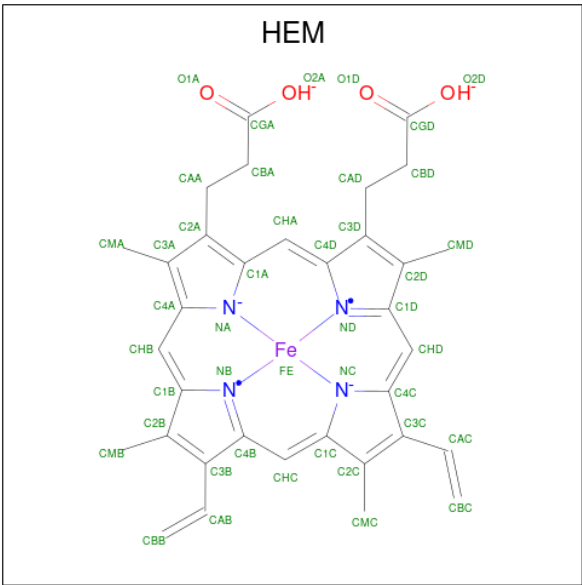
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



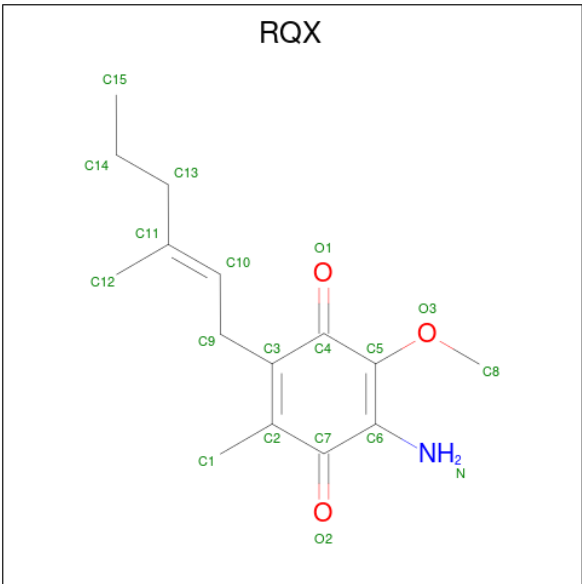
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 11 is 2-amino-3-methoxy-6-methyl-5-[(2E)-3-methylhex-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: RQX) (formula: C₁₅H₂₁NO₃).



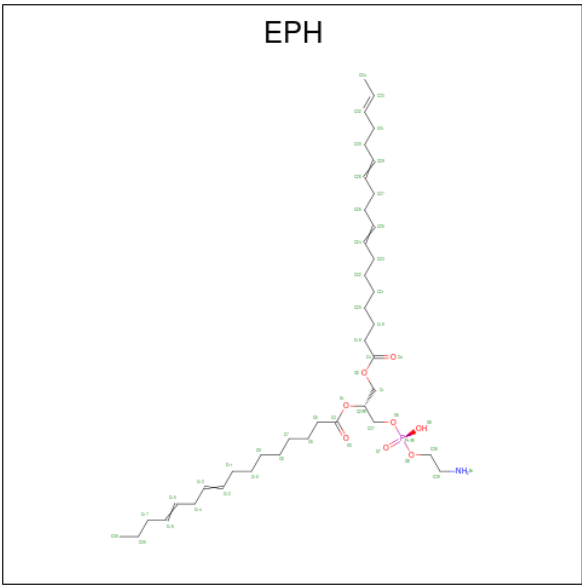
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			19	15	1	3		

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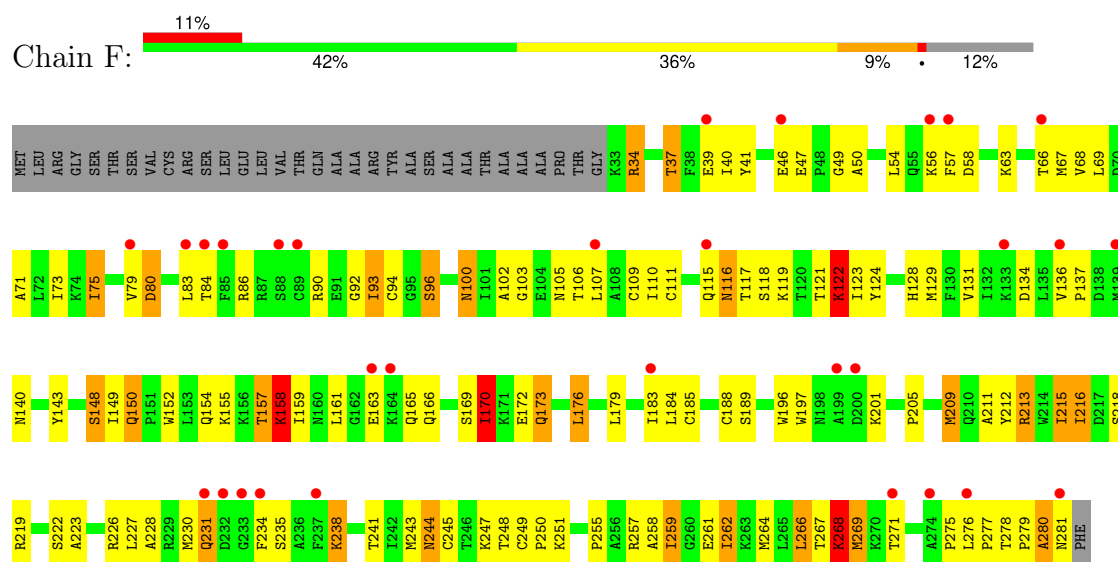
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	G	1	Total	C	N	O	0	0
			19	15	1	3		

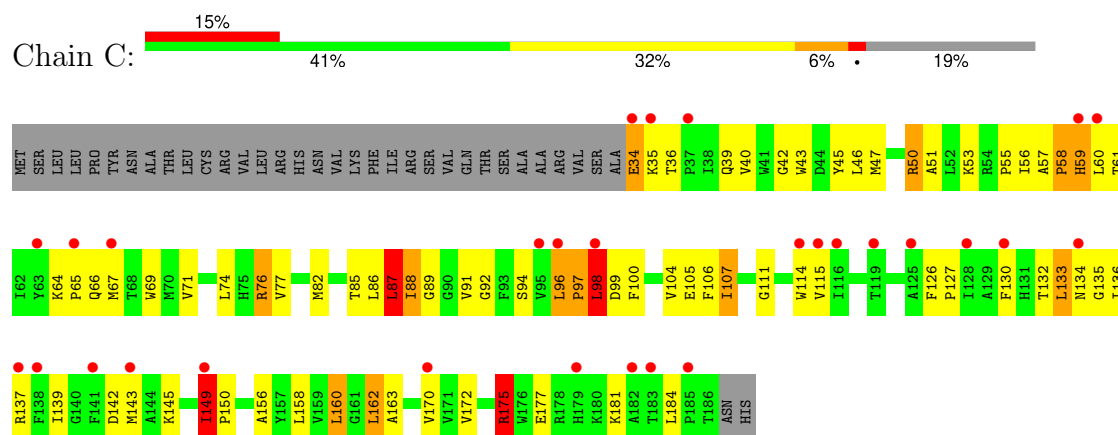
- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).



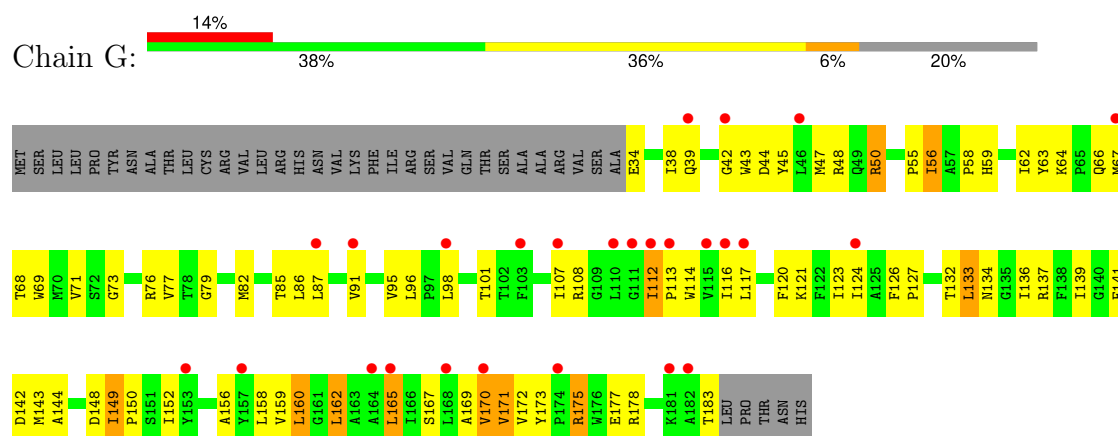
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		



• Molecule 3: Cytochrome b-large subunit

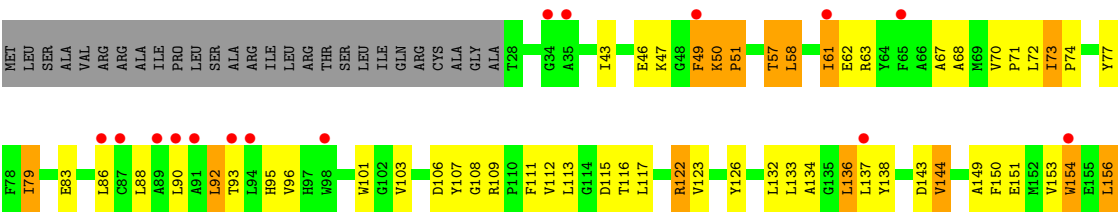


• Molecule 3: Cytochrome b-large subunit

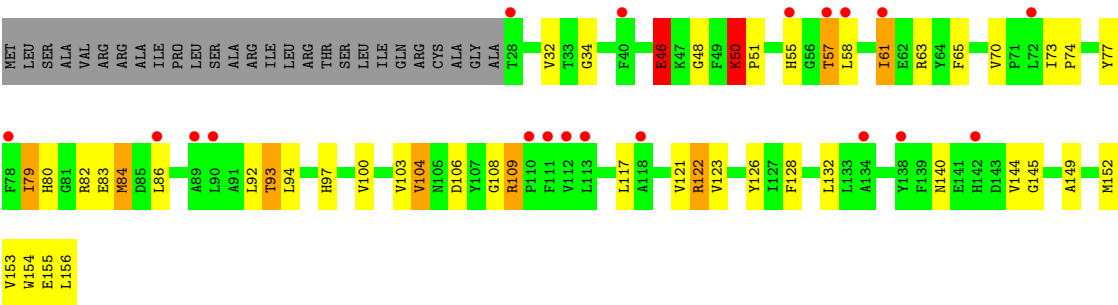


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





• 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) 92.1 (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)	0.27 , 32.1	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: MLI, FAD, SF4, RQX, F3S, FES, HEM, EPH

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	0.79	1/4859 (0.0%)	1.09	12/6564 (0.2%)
1	E	0.80	1/4859 (0.0%)	1.11	17/6564 (0.3%)
2	B	0.87	0/2016	1.13	8/2723 (0.3%)
2	F	0.93	3/2016 (0.1%)	1.12	9/2723 (0.3%)
3	C	0.83	1/1255 (0.1%)	1.14	5/1709 (0.3%)
3	G	0.80	0/1232	1.01	0/1676
4	D	0.85	0/1026	1.11	2/1402 (0.1%)
4	H	0.80	0/1026	1.04	1/1402 (0.1%)
All	All	0.83	6/18289 (0.0%)	1.10	54/24763 (0.2%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	267	THR	CA-C	8.87	1.56	1.52
2	F	271	THR	CA-CB	5.72	1.60	1.53
1	A	412	ILE	CA-CB	5.67	1.59	1.54
1	E	194	THR	CA-CB	5.08	1.60	1.53
2	F	170	ILE	CA-CB	5.03	1.61	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	ASN	N-CA-C	8.27	121.33	111.33
2	F	269	MET	N-CA-C	7.66	120.46	110.43
1	A	373	VAL	N-CA-C	7.49	119.37	108.58
1	E	142	ARG	N-CA-C	7.49	121.80	109.06
1	A	425	HIS	N-CA-C	-7.29	104.36	113.18

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	210	0
1	E	4758	0	4692	220	0
2	B	1973	0	1993	96	0
2	F	1973	0	1992	108	0
3	C	1217	0	1265	59	0
3	G	1195	0	1240	76	0
4	D	994	0	977	46	0
4	H	994	0	977	38	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	1	0
9	F	7	0	0	0	0
10	C	43	0	30	17	0
10	G	43	0	30	9	0
11	C	19	0	21	8	0
11	G	19	0	21	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	44	0	53	6	0
12	H	44	0	53	8	0
All	All	18232	0	18102	803	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 22.

The worst 5 of 803 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:HIS:NE2	6:E:702:FAD:HM81	1.16	1.41
1:A:79:HIS:NE2	6:A:702:FAD:C8M	1.84	1.38
1:E:79:HIS:NE2	6:E:702:FAD:C8M	1.84	1.37
1:A:79:HIS:NE2	6:A:702:FAD:HM82	0.90	1.21
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.07	1.18

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	611/645 (95%)	531 (87%)	68 (11%)	12 (2%)	6	19
1	E	611/645 (95%)	540 (88%)	56 (9%)	15 (2%)	4	15
2	B	247/282 (88%)	214 (87%)	26 (10%)	7 (3%)	4	13
2	F	247/282 (88%)	206 (83%)	33 (13%)	8 (3%)	3	10
3	C	151/188 (80%)	127 (84%)	18 (12%)	6 (4%)	2	7
3	G	148/188 (79%)	127 (86%)	18 (12%)	3 (2%)	6	19
4	D	127/156 (81%)	109 (86%)	16 (13%)	2 (2%)	7	24
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2269/2542 (89%)	1959 (86%)	253 (11%)	57 (2%)	4	15

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 ⓘ

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%)	419 (84%)	79 (16%)	2	8
1	E	498/526 (95%)	423 (85%)	75 (15%)	3	9
2	B	219/242 (90%)	173 (79%)	46 (21%)	1	3
2	F	219/242 (90%)	176 (80%)	43 (20%)	1	4
3	C	127/158 (80%)	98 (77%)	29 (23%)	1	3
3	G	124/158 (78%)	99 (80%)	25 (20%)	1	4
4	D	96/119 (81%)	76 (79%)	20 (21%)	1	4
4	H	96/119 (81%)	79 (82%)	17 (18%)	2	6
All	All	1877/2090 (90%)	1543 (82%)	334 (18%)	2	6

5 of 334 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	515	GLU
2	F	259	ILE
1	E	584	GLU
2	F	117	THR
3	G	91	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	573	HIS
4	H	140	ASN
2	F	100	ASN
2	F	165	GLN
2	B	100	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	EPH	H	201	-	43,43,48	1.91	9 (20%)	46,48,53	2.42	5 (10%)
12	EPH	D	201	-	43,43,48	1.91	9 (20%)	46,48,53	2.48	6 (13%)
5	MLI	A	701	-	6,6,6	4.70	2 (33%)	7,7,7	1.32	0
11	RQX	C	202	-	19,19,19	2.18	3 (15%)	19,26,26	2.83	6 (31%)
7	FES	B	301	2	0,4,4	-	-	-		
9	F3S	F	303	2	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEM	C	201	4,3	50,50,50	1.86	10 (20%)	67,82,82	1.41	6 (8%)
6	FAD	E	702	-	58,58,58	1.25	6 (10%)	85,89,89	1.87	22 (25%)
9	F3S	B	303	2	0,9,9	-	-	-	-	-
8	SF4	B	302	2	0,12,12	-	-	-	-	-
10	HEM	G	201	4,3	50,50,50	1.87	9 (18%)	67,82,82	1.40	7 (10%)
11	RQX	G	202	-	19,19,19	2.47	2 (10%)	19,26,26	2.33	5 (26%)
8	SF4	F	302	2	0,12,12	-	-	-	-	-
7	FES	F	301	2	0,4,4	-	-	-	-	-
5	MLI	E	701	-	6,6,6	4.57	1 (16%)	7,7,7	1.70	1 (14%)
6	FAD	A	702	-	58,58,58	1.24	7 (12%)	85,89,89	1.92	25 (29%)

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
12	EPH	H	201	-	-	24/47/47/52	-
12	EPH	D	201	-	-	28/47/47/52	-
5	MLI	A	701	-	-	2/4/4/4	-
11	RQX	C	202	-	-	6/10/34/34	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
9	F3S	F	303	2	-	-	0/3/3/3
10	HEM	C	201	4,3	-	8/14/54/54	-
6	FAD	E	702	-	-	12/34/50/50	0/6/6/6
9	F3S	B	303	2	-	-	0/3/3/3
8	SF4	B	302	2	-	-	0/6/5/5
10	HEM	G	201	4,3	-	12/14/54/54	-
11	RQX	G	202	-	-	6/10/34/34	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
7	FES	F	301	2	-	-	0/1/1/1
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	A	702	-	-	11/34/50/50	0/6/6/6

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	MLI	C1-C2	-10.97	1.34	1.51
5	E	701	MLI	C1-C2	-10.75	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	202	RQX	C3-C2	8.13	1.49	1.35
10	G	201	HEM	C3D-C2D	7.65	1.53	1.36
10	C	201	HEM	C3D-C2D	7.61	1.53	1.36

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C27-C26-C25	12.90	145.13	112.73
12	D	201	EPH	C27-C26-C25	12.29	143.60	112.73
11	C	202	RQX	C9-C3-C4	7.09	126.75	118.52
12	D	201	EPH	C2-O1-C3	6.27	132.81	117.80
11	C	202	RQX	C9-C3-C2	-6.25	114.17	124.89

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	C1'-C2'-C3'-O3'
6	A	702	FAD	C1'-C2'-C3'-C4'
6	A	702	FAD	O2'-C2'-C3'-O3'

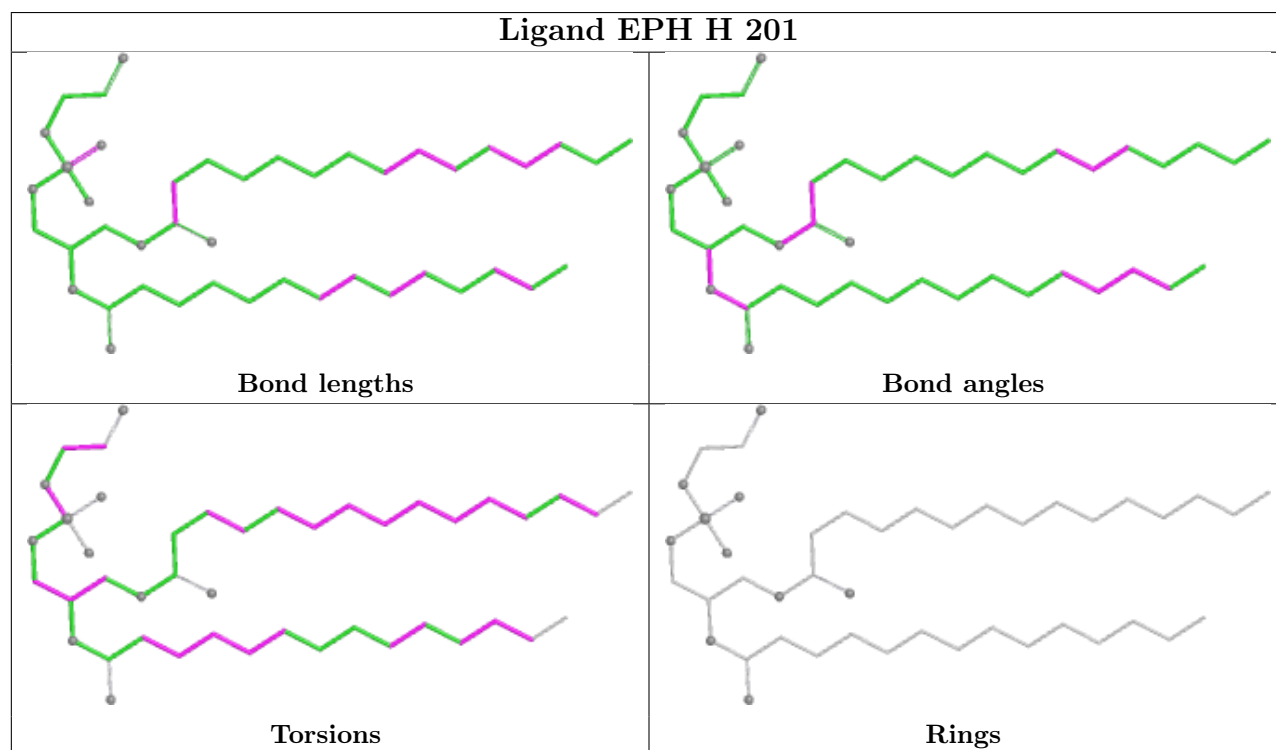
There are no ring outliers.

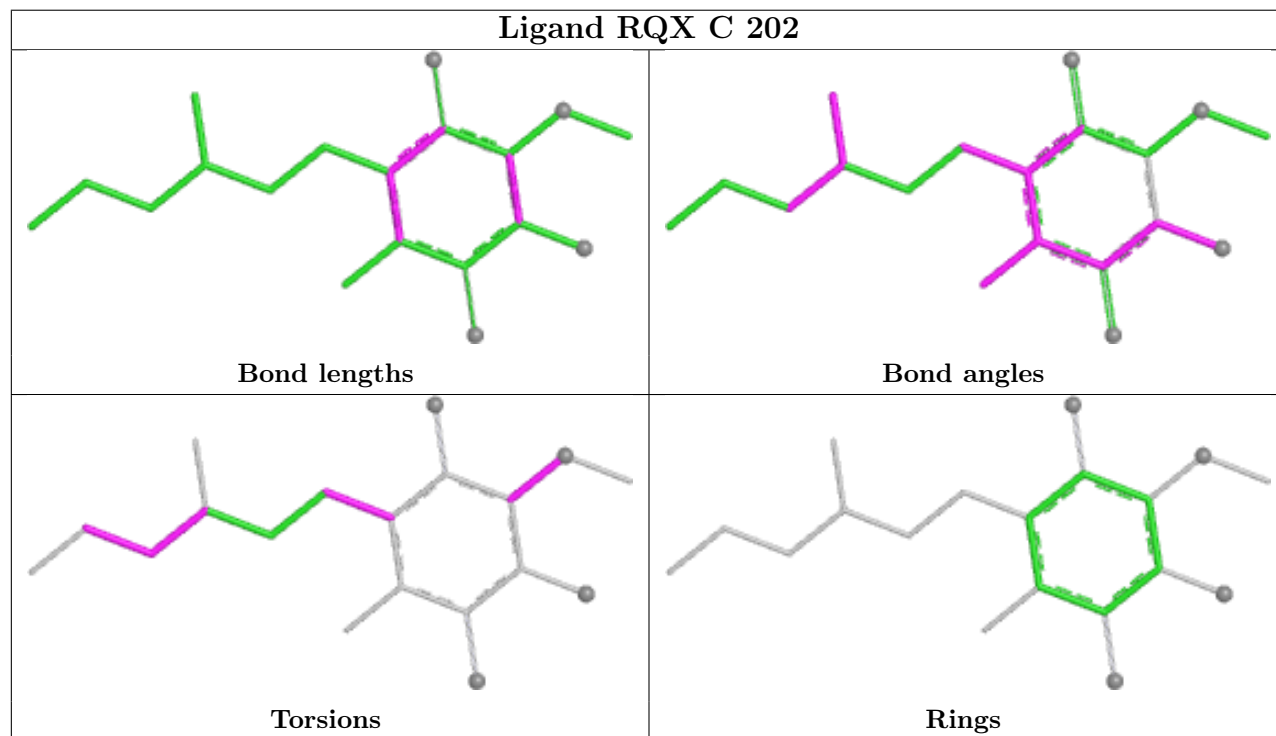
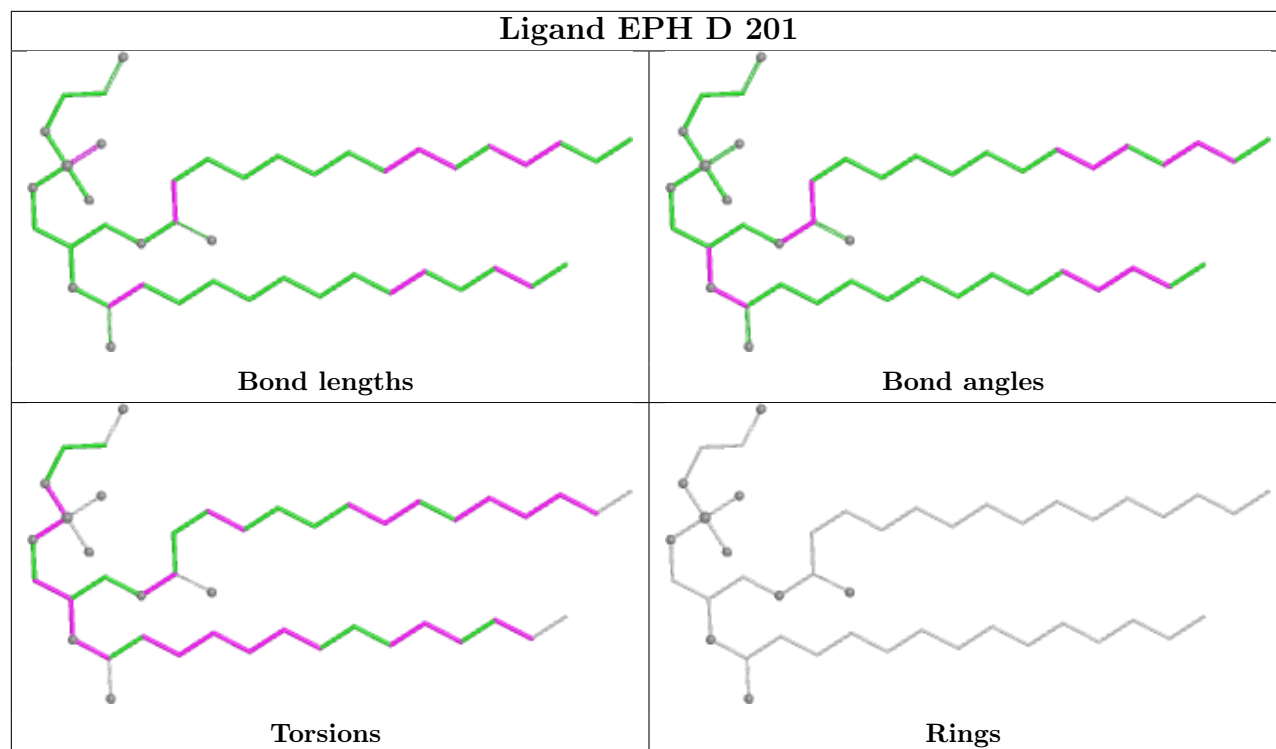
12 monomers are involved in 77 short contacts:

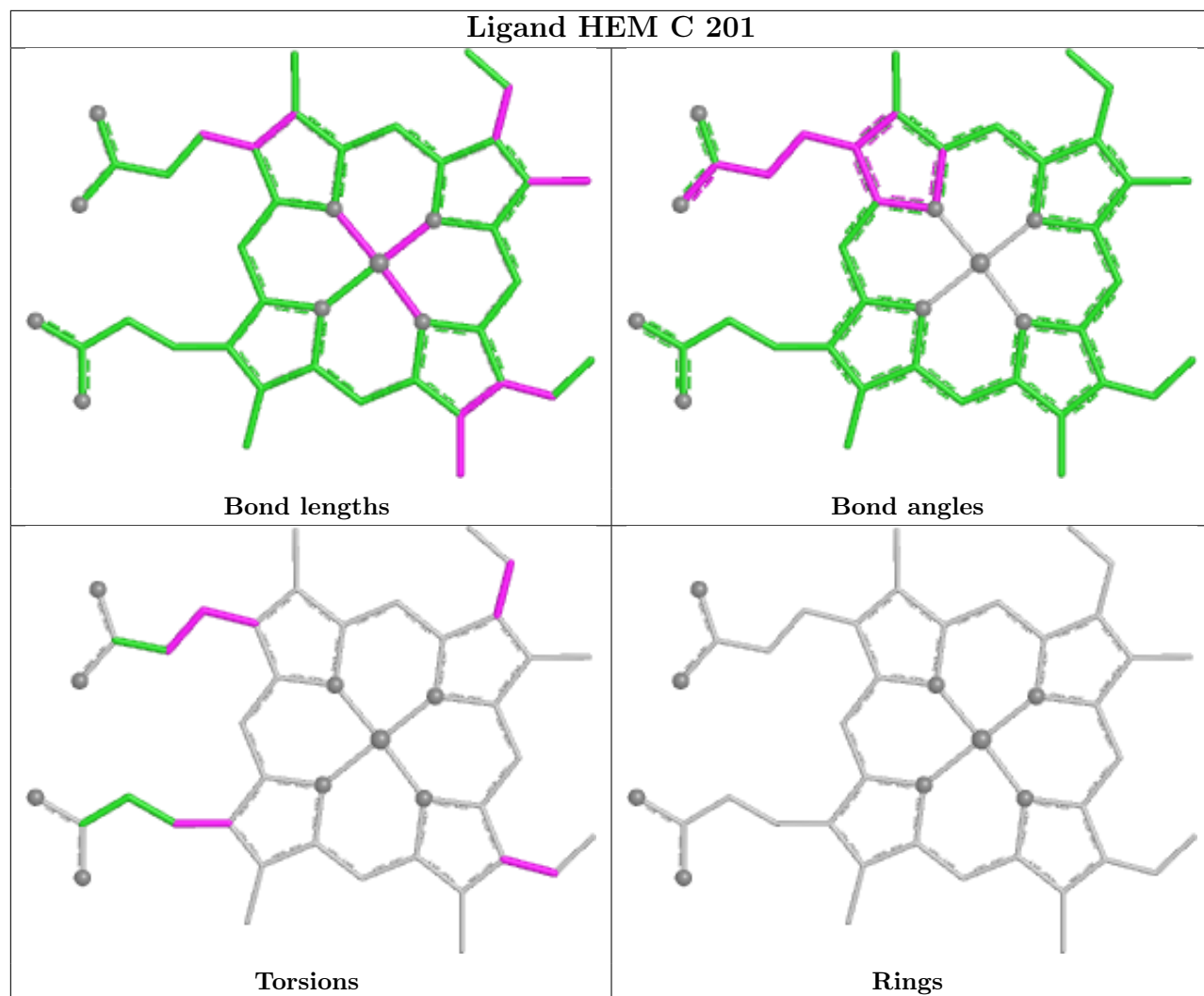
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	201	EPH	8	0
12	D	201	EPH	6	0
5	A	701	MLI	2	0
11	C	202	RQX	8	0
7	B	301	FES	1	0
10	C	201	HEM	17	0
6	E	702	FAD	10	0
9	B	303	F3S	1	0
8	B	302	SF4	1	0
10	G	201	HEM	9	0
11	G	202	RQX	7	0
6	A	702	FAD	7	0

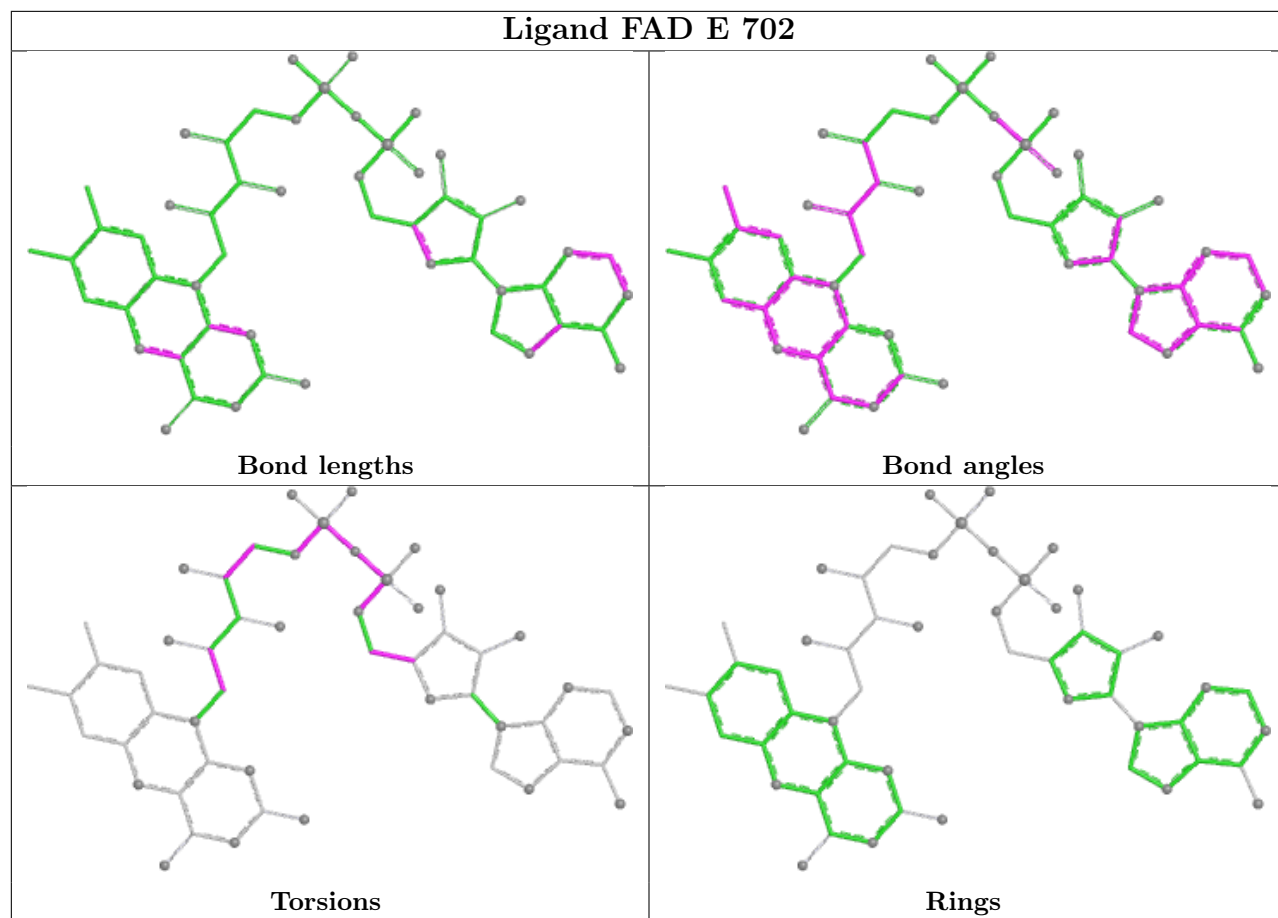
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

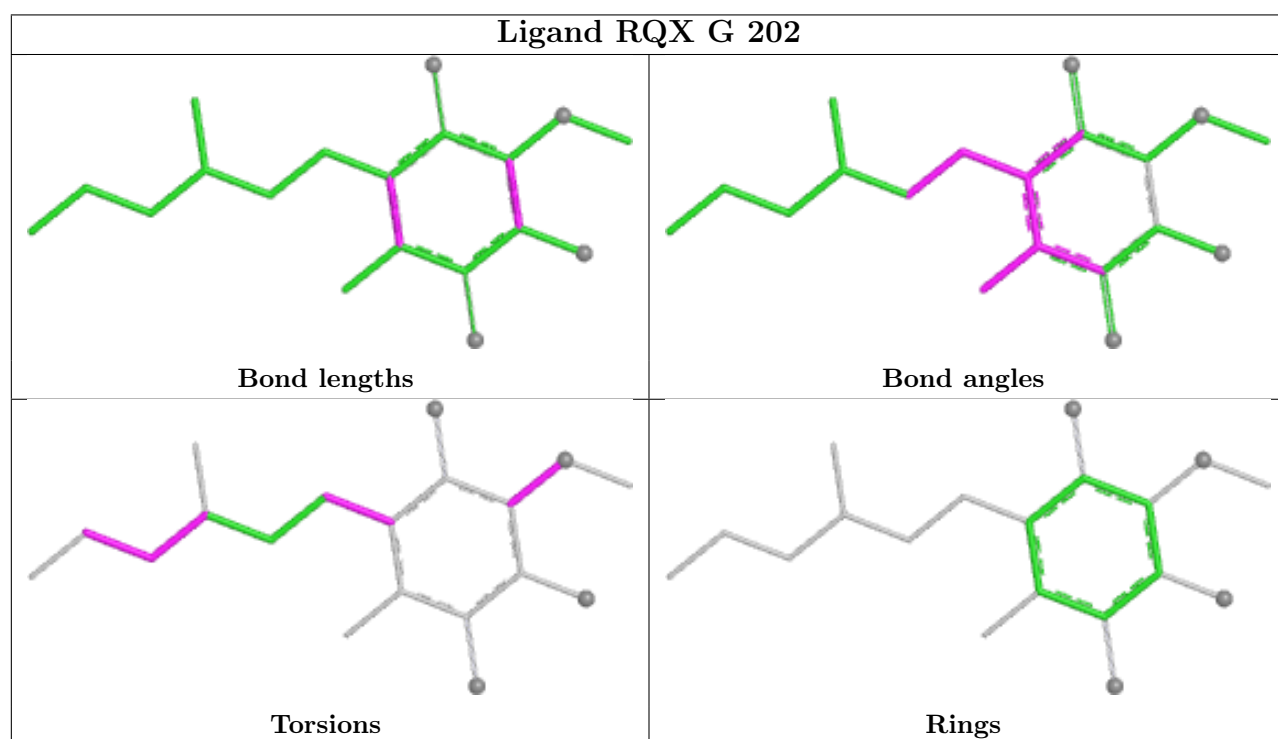
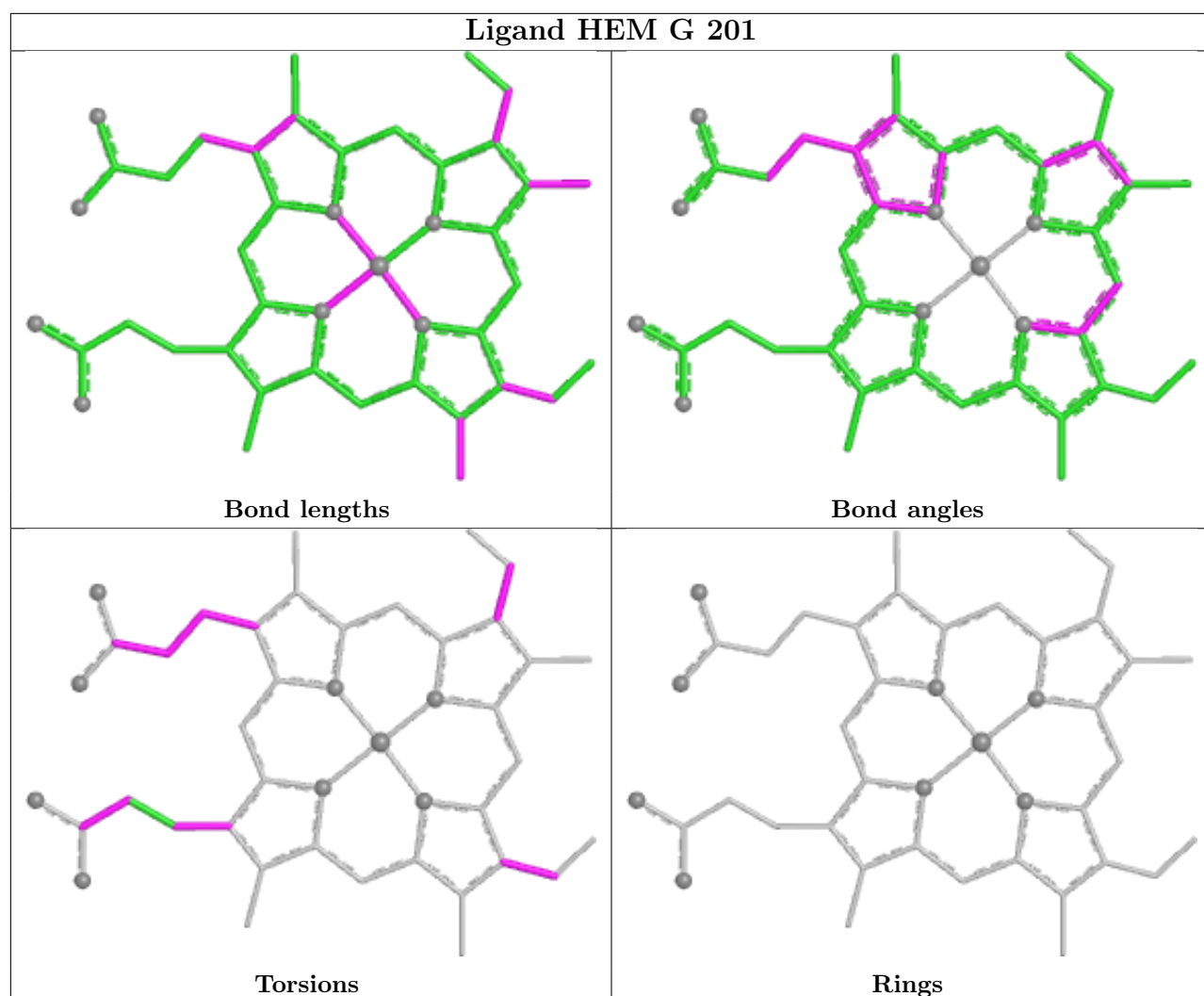
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

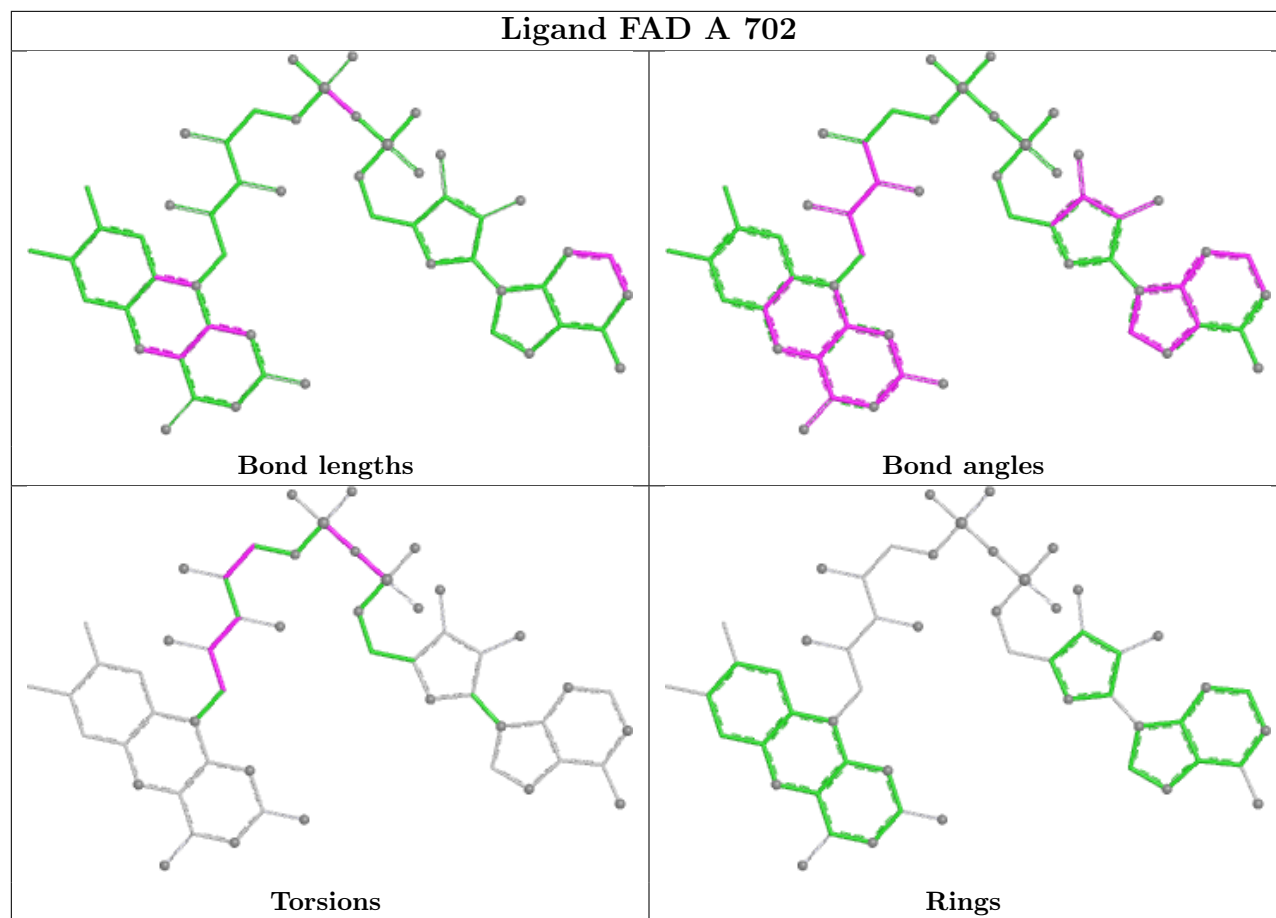












5.7 Other polymers [i](#)

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%)	0.57	76 (12%) 8 6	71, 96, 118, 136	0
1	E	613/645 (95%)	0.64	90 (14%) 6 4	70, 90, 112, 126	0
2	B	249/282 (88%)	0.67	42 (16%) 4 3	72, 89, 117, 137	0
2	F	249/282 (88%)	0.46	30 (12%) 9 6	67, 86, 109, 120	0
3	C	153/188 (81%)	0.86	29 (18%) 3 2	78, 97, 142, 162	0
3	G	150/188 (79%)	0.79	26 (17%) 4 3	77, 100, 151, 156	0
4	D	129/156 (82%)	0.69	15 (11%) 9 7	89, 101, 129, 142	0
4	H	129/156 (82%)	0.62	19 (14%) 6 4	86, 103, 133, 146	0
All	All	2285/2542 (89%)	0.63	327 (14%) 6 4	67, 94, 124, 162	0

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	8.3
4	D	90	LEU	8.0
1	E	86	GLY	7.9
1	E	103	PHE	7.8
1	E	444	PHE	7.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

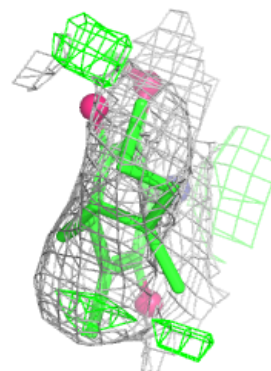
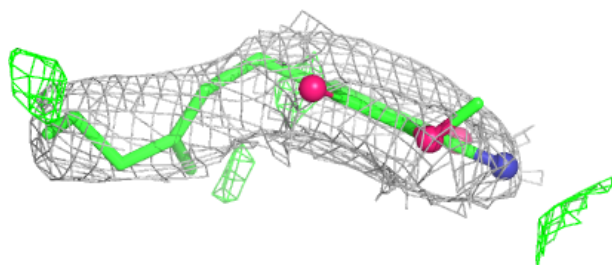
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.75	0.27	113,116,119,119	0
11	RQX	G	202	19/19	0.80	0.24	120,125,127,127	0
12	EPH	H	201	44/49	0.89	0.20	97,113,134,135	0
5	MLI	A	701	7/7	0.92	0.09	102,103,106,106	0
12	EPH	D	201	44/49	0.93	0.16	94,102,121,122	0
6	FAD	A	702	53/53	0.93	0.11	77,83,87,89	0
10	HEM	C	201	43/43	0.95	0.12	89,93,96,98	0
6	FAD	E	702	53/53	0.96	0.08	63,79,88,89	0
5	MLI	E	701	7/7	0.96	0.06	92,93,93,93	0
9	F3S	B	303	7/7	0.98	0.05	83,85,86,87	0
10	HEM	G	201	43/43	0.98	0.08	92,97,103,106	0
7	FES	F	301	4/4	0.99	0.07	60,66,68,75	0
9	F3S	F	303	7/7	0.99	0.04	82,83,84,87	0
8	SF4	F	302	8/8	1.00	0.04	57,61,64,65	0
7	FES	B	301	4/4	1.00	0.05	70,70,72,78	0
8	SF4	B	302	8/8	1.00	0.03	63,66,68,70	0

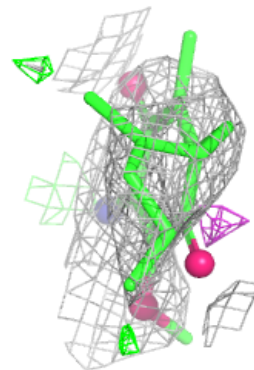
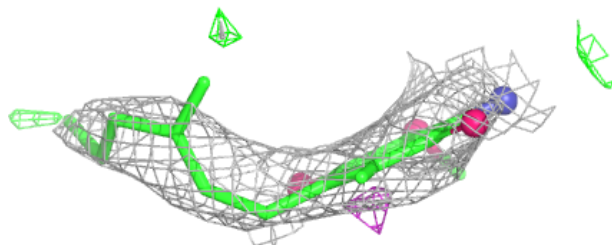
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

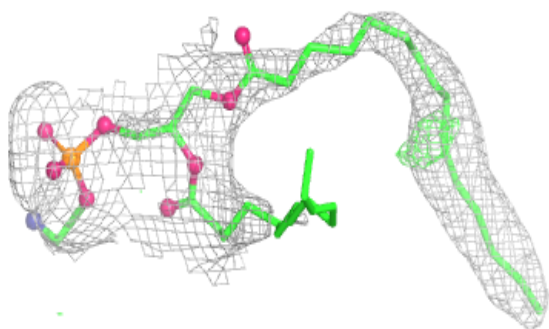
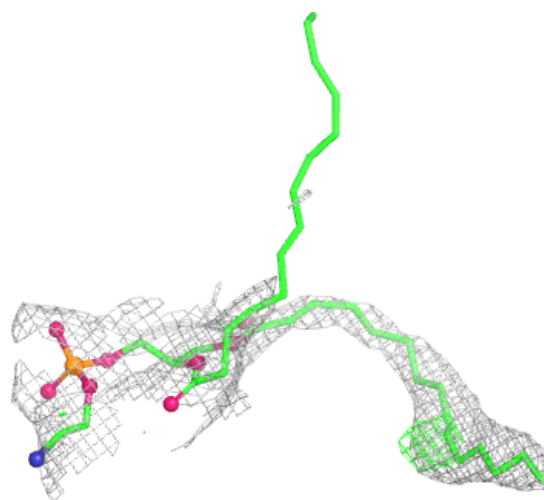
**Electron density around RQX G 202:**

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



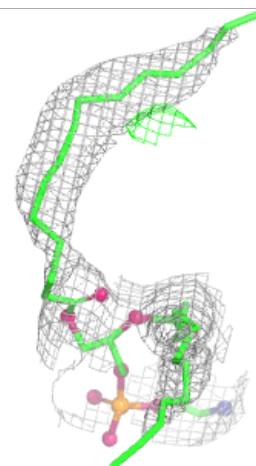
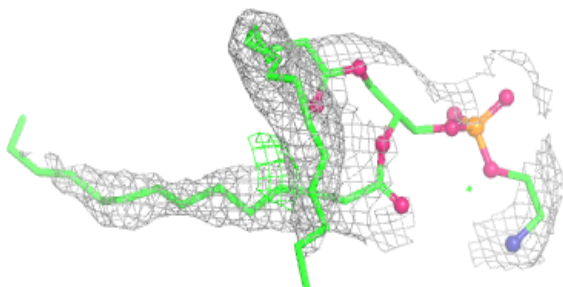
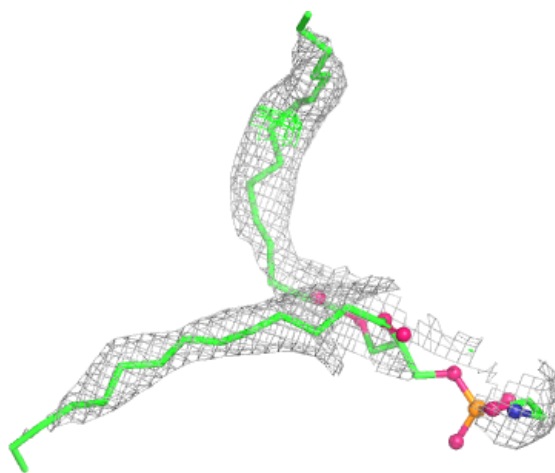
Electron density around EPH H 201:

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



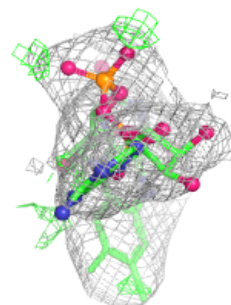
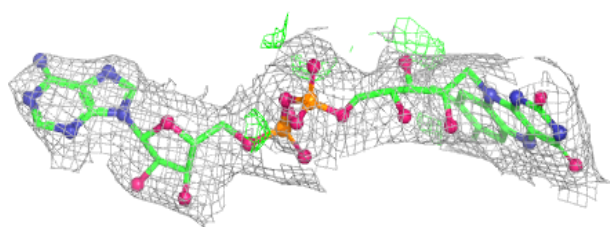
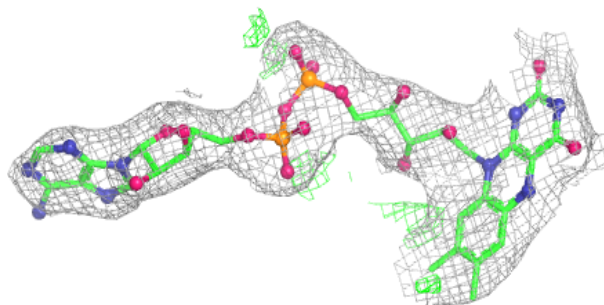
Electron density around EPH D 201:

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



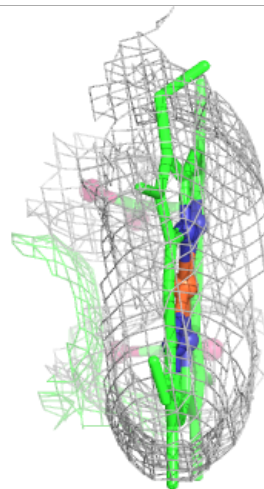
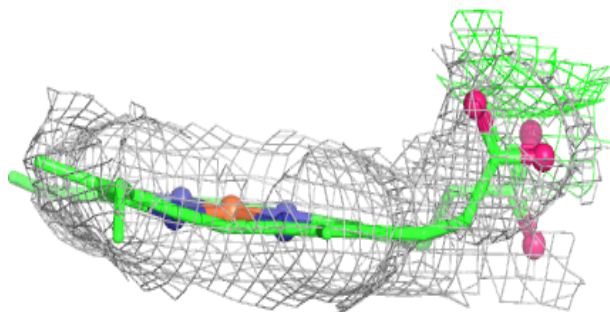
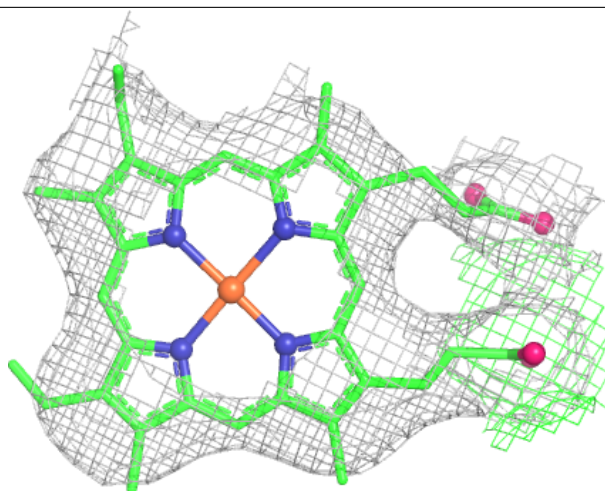
Electron density around FAD A 702:

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



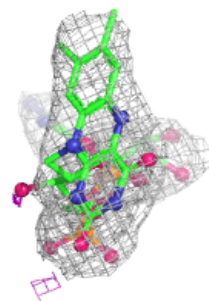
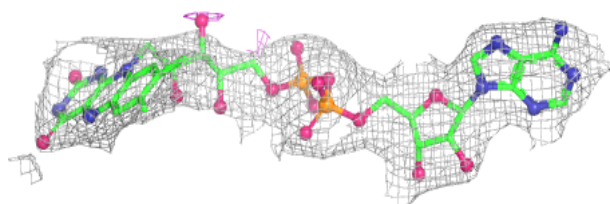
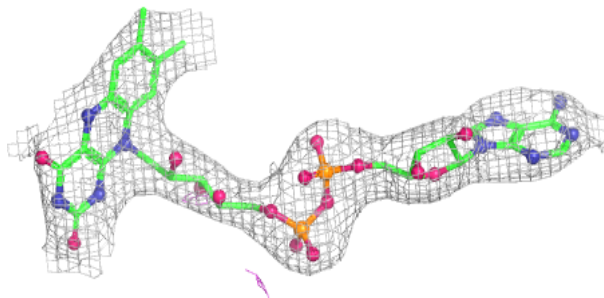
Electron density around HEM C 201:

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

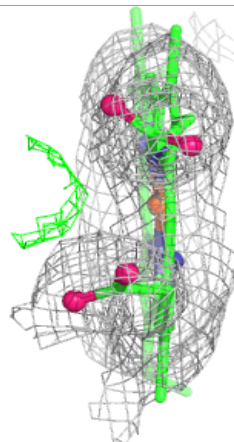
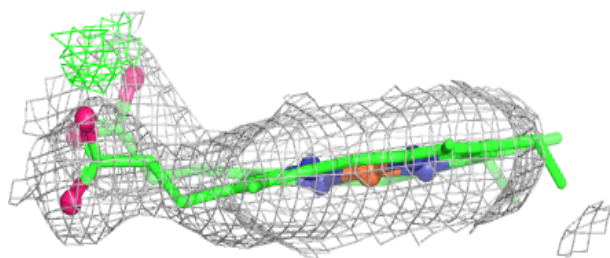
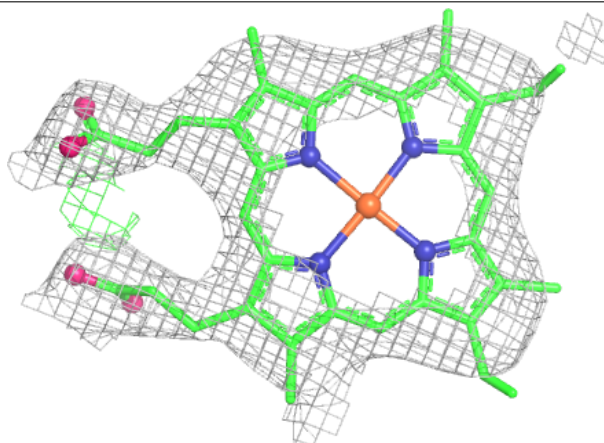


Electron density around FAD E 702:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.