WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 06:29 PM EDT

PDB ID	:	6MYR
Title	:	Avian mitochondrial complex II with thiapronil bound
Authors	:	Huang, L.-S.; Luemmen, P.; Berry, E.A.
Deposited on	:	2018-11-02
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36.2
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)	:	2.36.2

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 2.15 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.
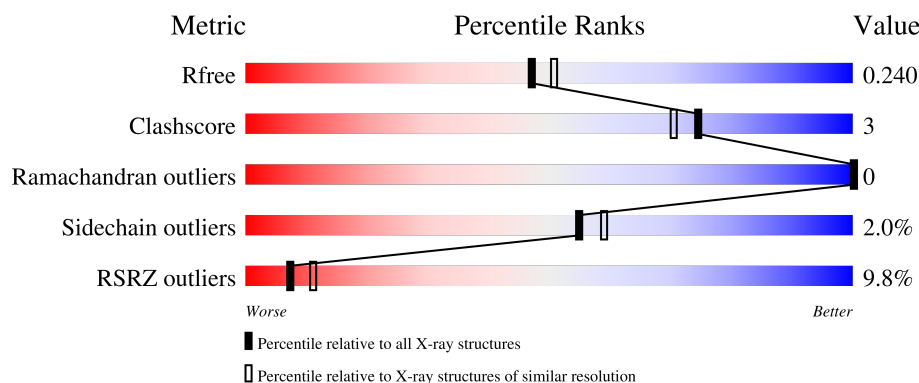
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	621	11% / 90% / 9% ·
2	B	252	8% / 88% / 6% · 5%
3	C	140	7% / 94% / 6% ·
4	D	103	5% / 90% / 9% ·

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
6	OAA	A	1002	-	-	X	-
8	PEG	A	1004	-	-	-	X
9	UNL	A	1014	-	-	-	X
9	UNL	C	208	-	-	-	X
9	UNL	D	1006	-	-	-	X
9	UNL	D	1012	-	-	-	X

2 Entry composition ⓘ

There are 18 unique types of molecules in this entry. The entry contains 9126 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	611	Total	C	N	O	S	0	2	0
			4734	2962	847	896	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			1928	1219	326	361	22			

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b, large subunit.

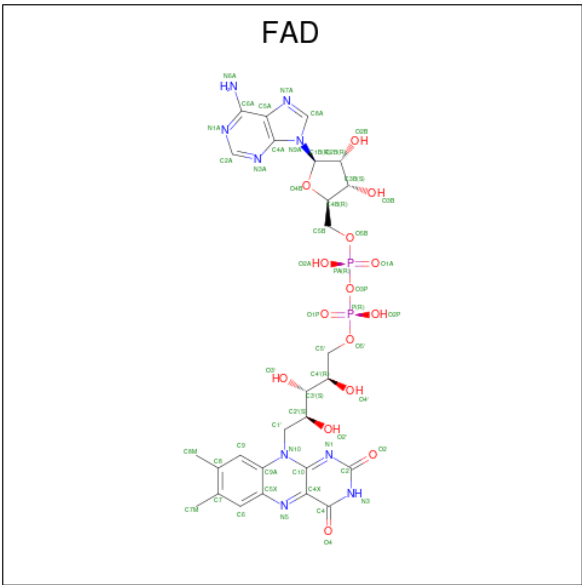| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1075	706	178	186	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	ALA	SER	conflict	UNP D0VWW3
C	140	MET	GLU	conflict	UNP D0VWW3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			771	508	122	138	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).

OAA
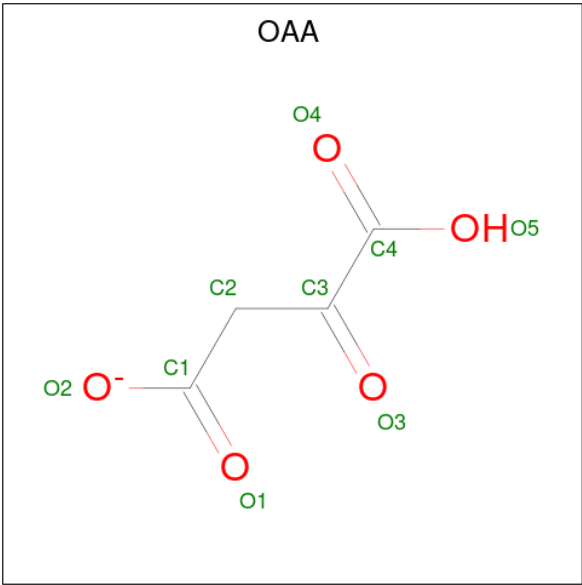
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total K		0	0
			1 1			

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
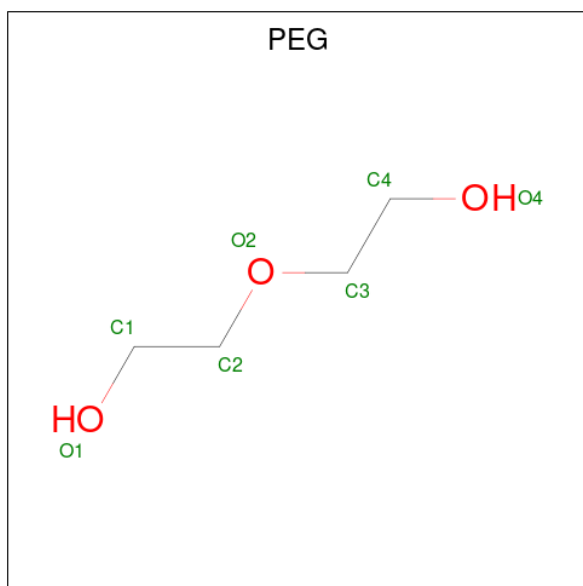
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 9 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	15	Total	C	N	O	P	S	0	0
			53	20	10	19	1	3		
9	B	12	Total	C	N	O	S		0	0
			53	21	11	19	2			
9	C	5	Total	C	O				0	0
			13	6	7					
9	D	11	Total	C	N	O			0	0
			65	36	3	26				

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

FES

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

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

SF4
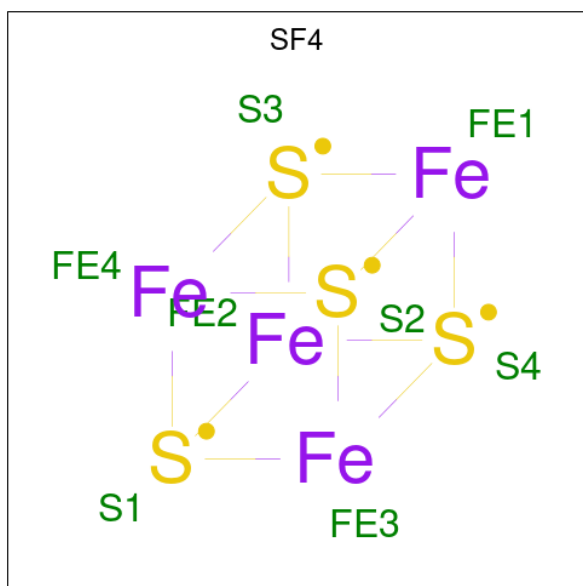
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

F3S
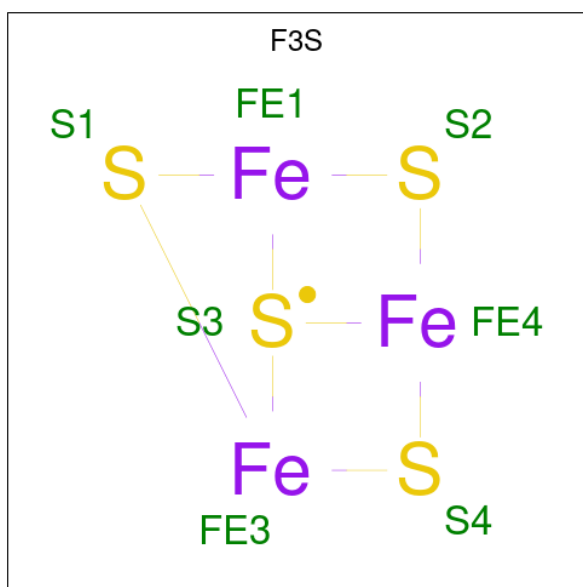
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is thiapronil (three-letter code: K7G) (formula: $C_{18}H_{11}ClN_2OS$) (labeled as "Ligand of Interest" by depositor).
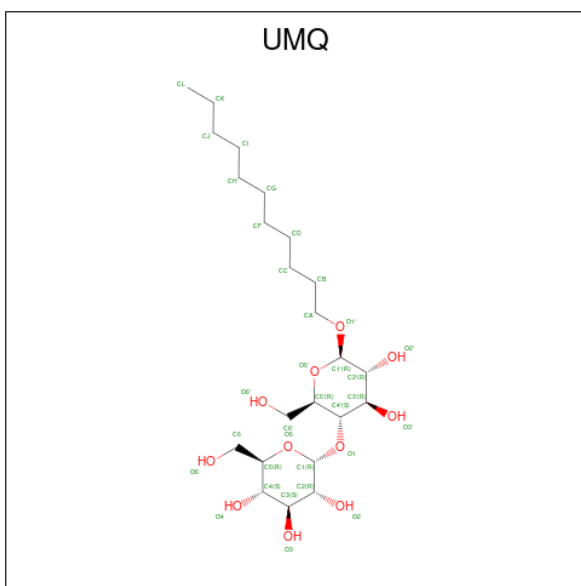

K7G
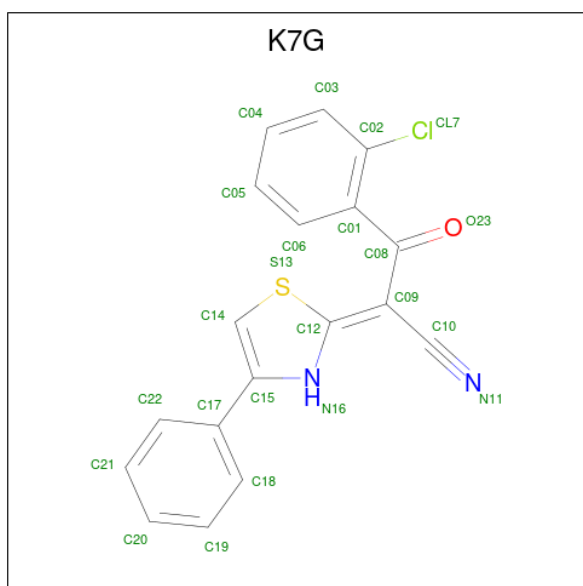
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	C	1	Total	C	Cl	N	O	S	0	0
			23	18	1	2	1	1		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
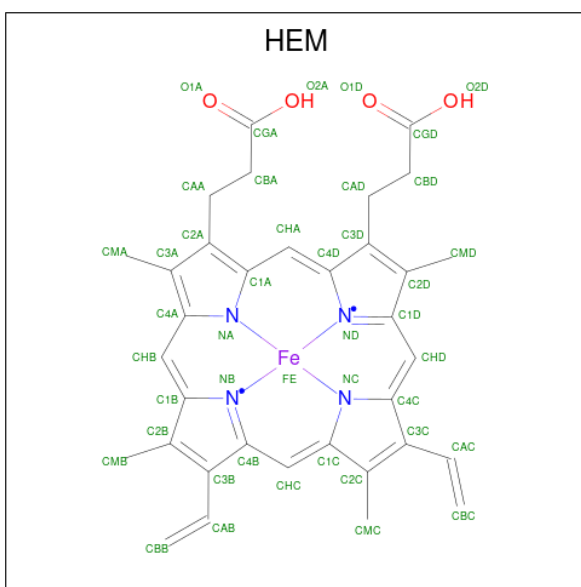
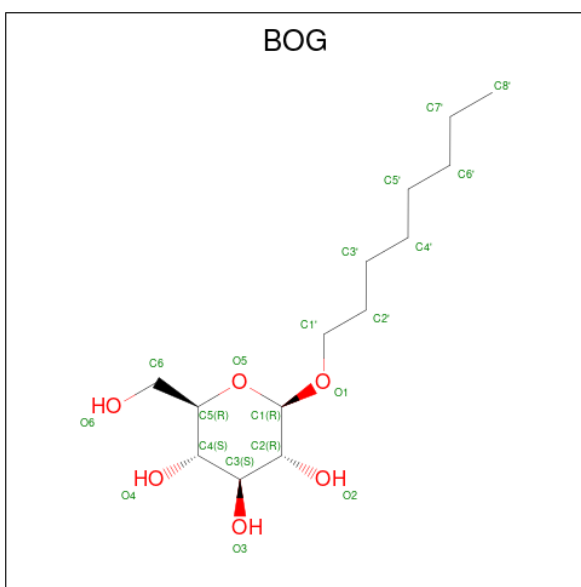| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	C	1	41	32	1	4	4	0	0

- Molecule 15 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).

UMQ

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	C	1	34	23	11	0	0

- Molecule 16 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).

BOG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 17 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).

3PE
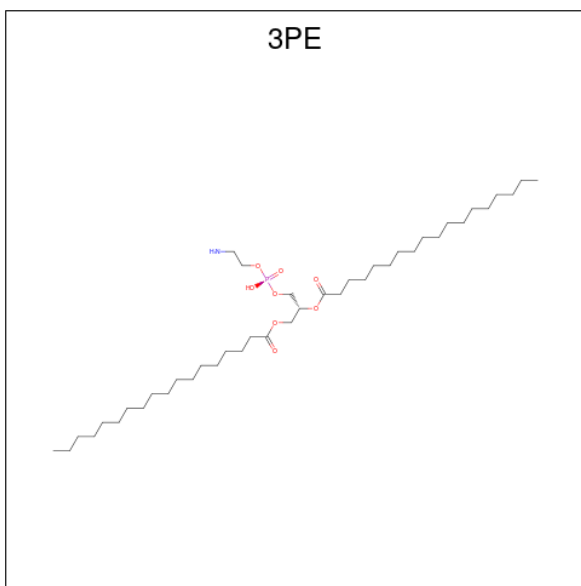
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	73	Total 73	O 73	0	0
18	B	82	Total 82	O 82	0	0
18	C	23	Total 23	O 23	0	0
18	D	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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.
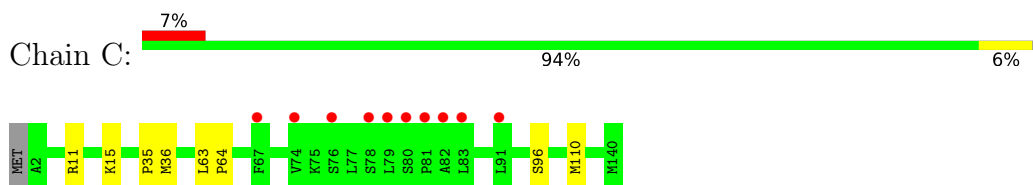
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
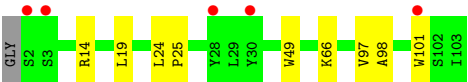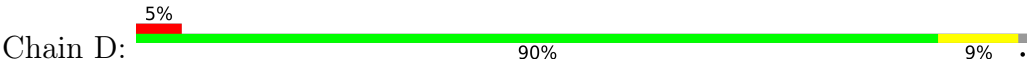
Chain A:
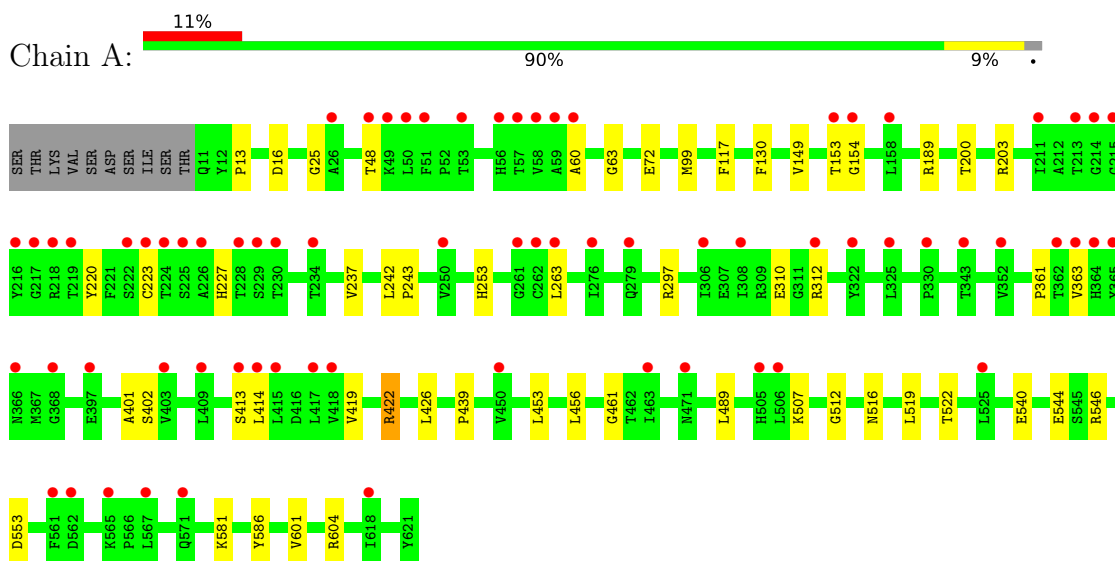
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:
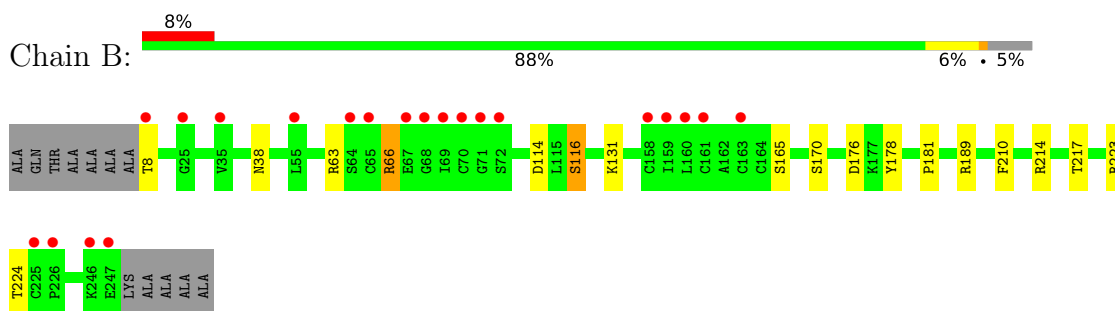
- Molecule 3: Succinate dehydrogenase cytochrome b, large subunit

Chain C:

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

Chain D:

5%

90%

9%

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.36Å 84.62Å 293.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.15 47.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.7 (47.93-2.15) 75.9 (47.93-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.14Å)	Xtriage
Refinement program	PHENIX dev_3150	Depositor
R, R_{free}	0.218 , 0.238 0.220 , 0.240	Depositor DCC
R_{free} test set	2652 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.0	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FAD, OAA, K, SF4, BOG, PEG, FES, HEM, K7G, UNL, 3PE, F3S, UMQ

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	0.28	0/4835	0.48	0/6545
2	B	0.30	0/1970	0.48	0/2656
3	C	0.30	0/1104	0.45	0/1500
4	D	0.28	0/794	0.42	0/1089
All	All	0.29	0/8703	0.47	0/11790

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	4734	0	4620	38	0
2	B	1928	0	1921	10	0
3	C	1075	0	1115	4	0
4	D	771	0	763	4	0
5	A	53	0	29	5	0
6	A	9	0	2	6	0
7	A	1	0	0	0	0
8	A	5	0	5	1	0
9	A	53	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	53	0	0	0	0
9	C	13	0	0	0	0
9	D	65	0	0	2	0
10	B	4	0	0	0	0
11	B	8	0	0	0	0
12	B	7	0	0	0	0
13	C	23	0	0	0	0
14	C	41	0	24	0	0
15	C	34	0	44	1	0
16	D	20	0	28	0	0
17	D	40	0	54	2	0
18	A	73	0	0	2	0
18	B	82	0	0	1	0
18	C	23	0	0	1	0
18	D	11	0	0	0	0
All	All	9126	0	8605	56	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 3.

The worst 5 of 56 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:297:ARG:HH22	6:A:1002:OAA:C2	1.78	0.95
1:A:297:ARG:HH22	6:A:1002:OAA:C1	1.94	0.79
1:A:297:ARG:NH2	6:A:1002:OAA:H22	2.00	0.76
1:A:297:ARG:HH22	6:A:1002:OAA:H22	1.49	0.75
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.70	0.74

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	611/621 (98%)	588 (96%)	23 (4%)	0	100	100
2	B	238/252 (94%)	233 (98%)	5 (2%)	0	100	100
3	C	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
4	D	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
All	All	1086/1116 (97%)	1056 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	497/506 (98%)	492 (99%)	5 (1%)	76	81
2	B	216/219 (99%)	209 (97%)	7 (3%)	39	38
3	C	117/118 (99%)	114 (97%)	3 (3%)	46	47
4	D	78/79 (99%)	74 (95%)	4 (5%)	24	20
All	All	908/922 (98%)	889 (98%)	19 (2%)	55	57

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	96	SER
4	D	66	LYS
4	D	101	TRP
4	D	19	LEU
2	B	170	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 1 is monoatomic and 43 are unknown - leaving 11 for Mogul analysis.

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	#$|Z| > 2$
16	BOG	D	1001	-	20,20,20	0.58	1 (5%)	25,25,25	0.82	1 (4%)
8	PEG	A	1004	-	4,4,6	0.45	0	3,3,5	0.26	0
10	FES	B	1001	2	0,4,4	-	-	-		
5	FAD	A	1001	1	53,58,58	0.82	1 (1%)	68,89,89	1.31	10 (14%)
14	HEM	C	201	4,3	40,48,50	1.31	3 (7%)	46,80,82	1.48	9 (19%)
13	K7G	C	202	-	24,25,25	2.18	8 (33%)	24,34,34	2.71	3 (12%)
15	UMQ	C	203	-	35,35,35	0.49	0	46,46,46	0.81	0
12	F3S	B	1003	2	0,9,9	-	-	-		
17	3PE	D	201	-	39,39,50	1.07	2 (5%)	42,44,55	1.06	3 (7%)
6	OAA	A	1002	-	8,8,8	2.58	4 (50%)	9,10,10	1.54	2 (22%)
11	SF4	B	1002	2	0,12,12	-	-	-		

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
14	HEM	C	201	4,3	-	5/10/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	A	1004	-	-	2/2/2/4	-
5	FAD	A	1001	1	-	6/30/50/50	0/6/6/6
15	UMQ	C	203	-	-	3/20/60/60	0/2/2/2
13	K7G	C	202	-	-	3/17/18/18	0/3/3/3
10	FES	B	1001	2	-	-	0/1/1/1
11	SF4	B	1002	2	-	-	0/6/5/5
12	F3S	B	1003	2	-	-	0/3/3/3
17	3PE	D	201	-	-	18/43/43/54	-
6	OAA	A	1002	-	-	3/8/8/8	-
16	BOG	D	1001	-	-	3/11/31/31	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	OAA	O3-C3	5.30	1.33	1.23
13	C	202	K7G	C10-C09	4.94	1.53	1.43
17	D	201	3PE	O31-C31	4.42	1.46	1.33
13	C	202	K7G	C12-S13	-4.29	1.68	1.73
13	C	202	K7G	C09-C12	-4.26	1.32	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	202	K7G	C14-S13-C12	12.23	98.66	90.27
5	A	1001	FAD	C4-N3-C2	-4.17	117.94	125.64
17	D	201	3PE	O21-C21-C22	3.65	119.38	111.50
5	A	1001	FAD	C4X-C4-N3	3.52	122.13	113.19
14	C	201	HEM	C4D-ND-C1D	3.07	108.24	105.07

There are no chirality outliers.
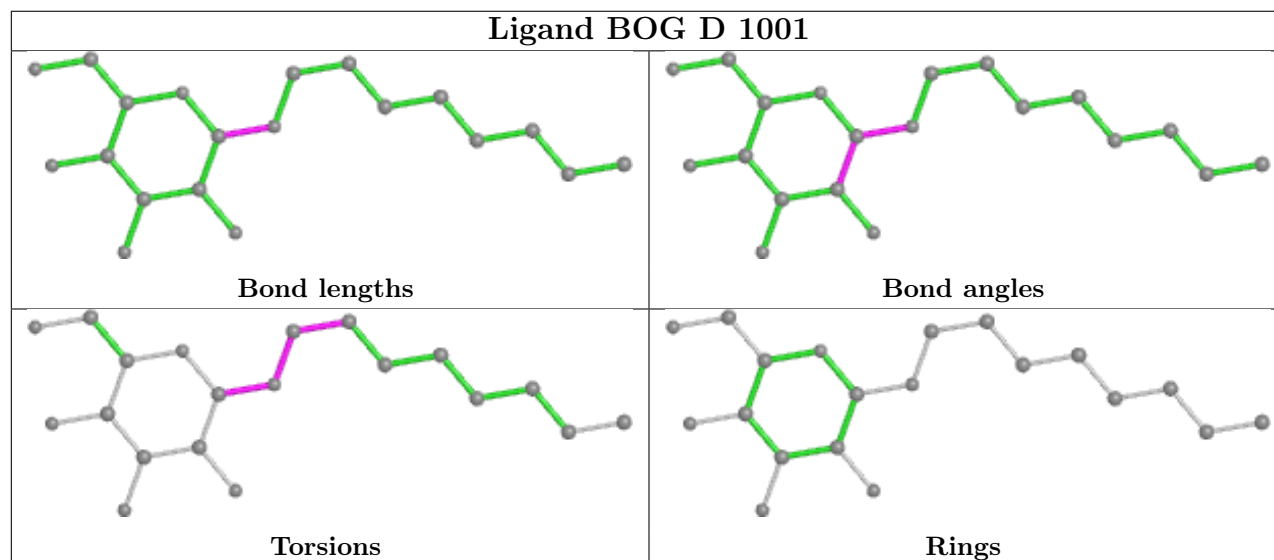
5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
5	A	1001	FAD	PA-O3P-P-O5'
6	A	1002	OAA	O3-C3-C4-O4
6	A	1002	OAA	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1004	PEG	1	0
5	A	1001	FAD	5	0
15	C	203	UMQ	1	0
17	D	201	3PE	2	0
6	A	1002	OAA	6	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.
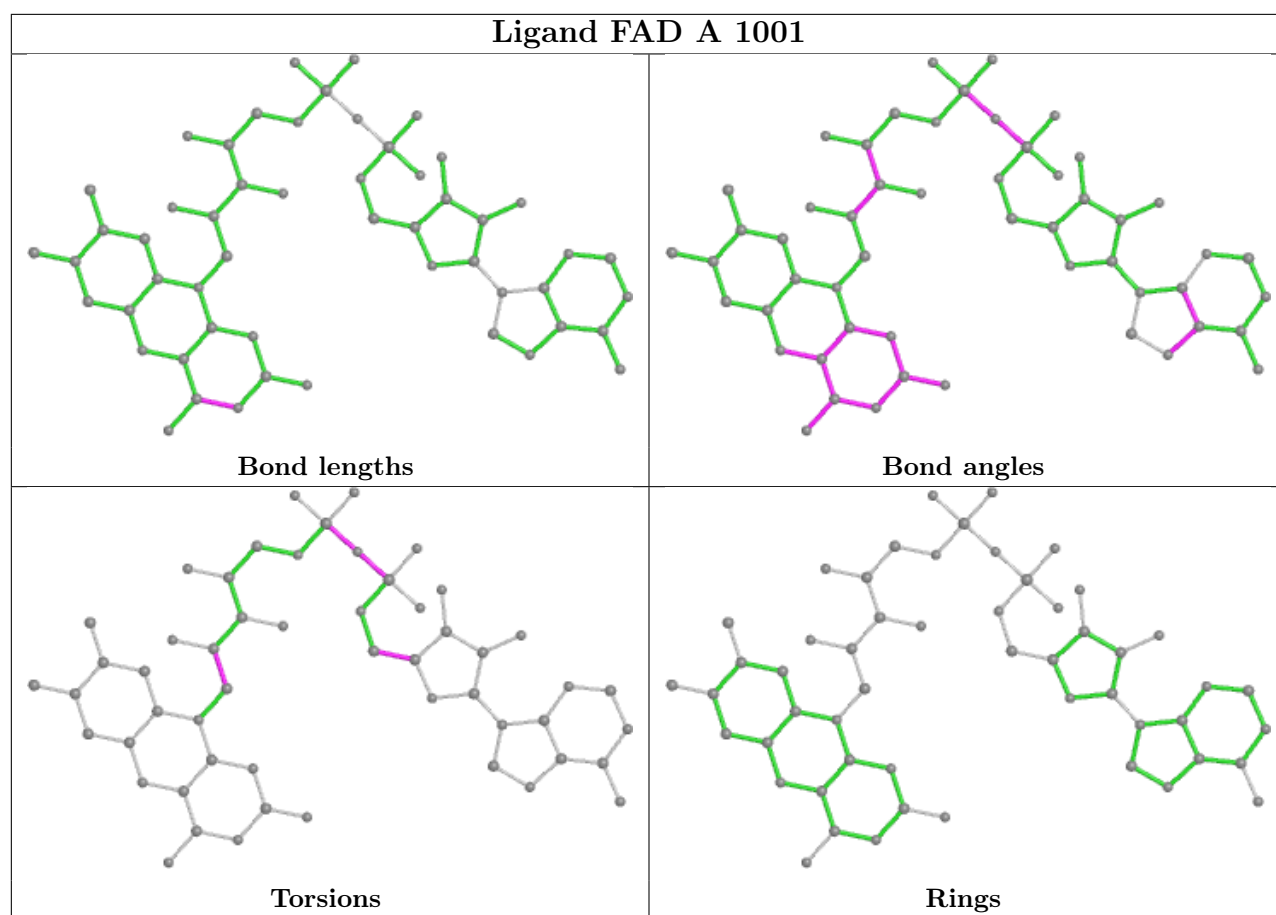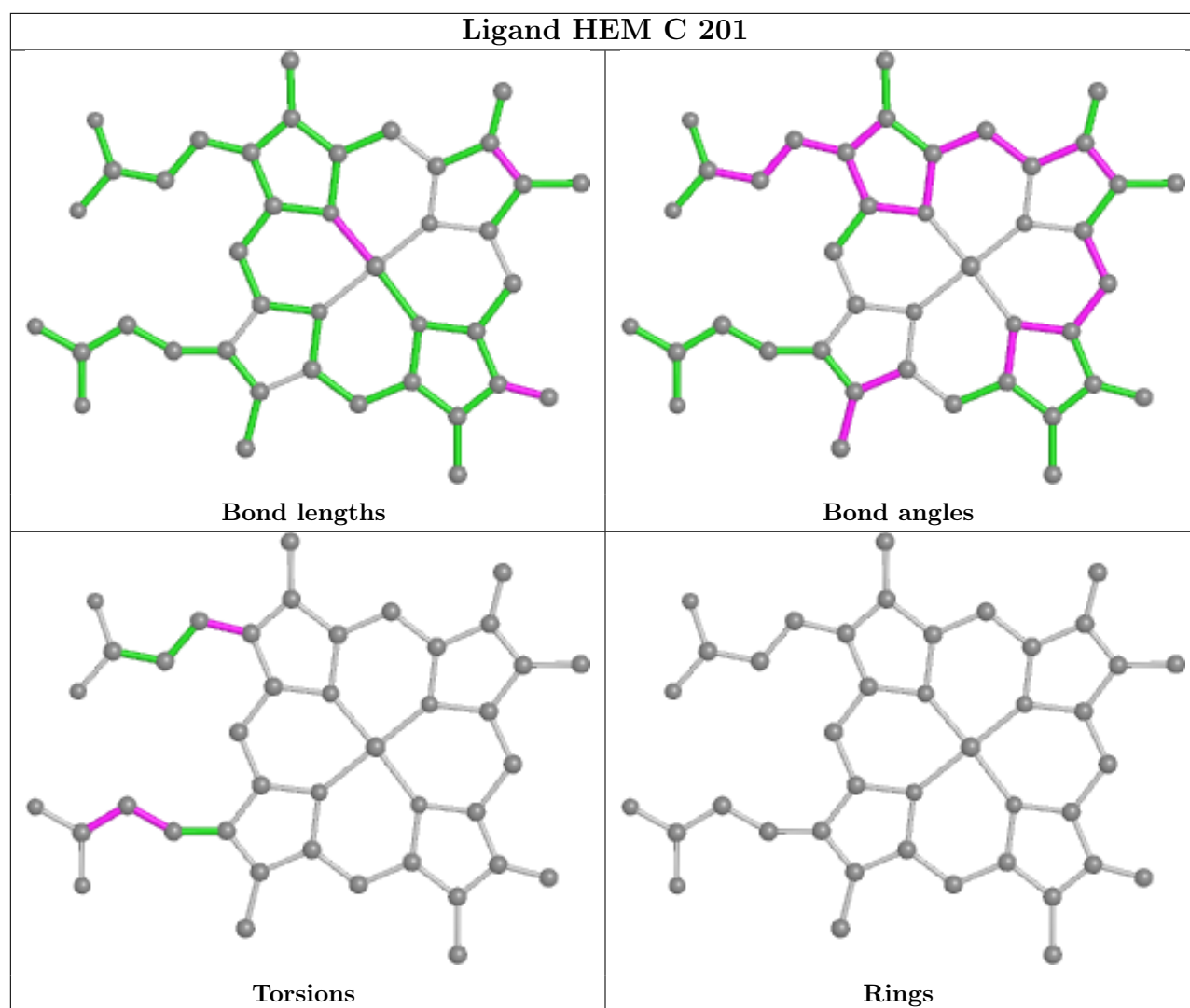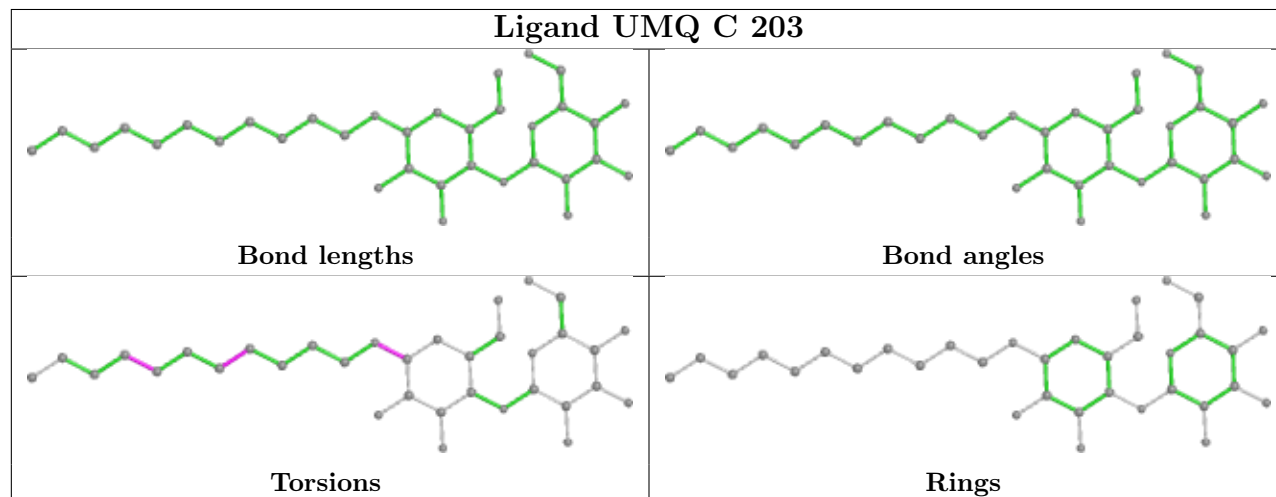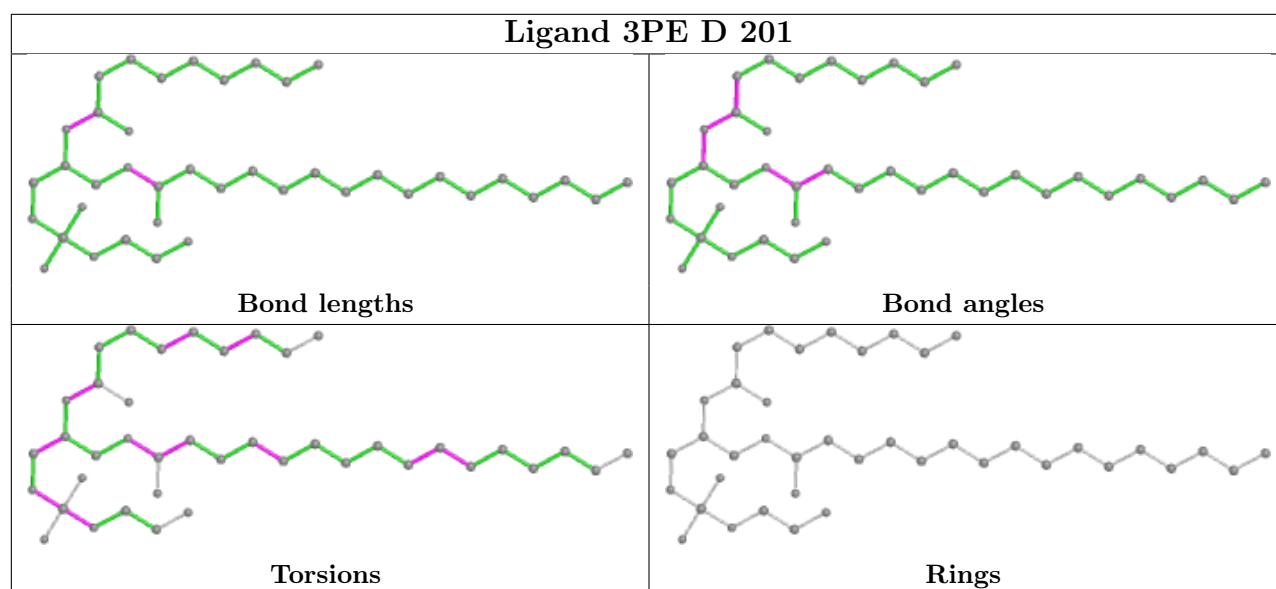

Ligand BOG D 1001

Bond lengths   Bond angles

Torsions   Rings

Ligand FAD A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand K7G C 202

Bond lengths

Bond angles

Torsions

Rings

Ligand UMQ C 203

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE D 201

Bond lengths

Bond angles

Torsions

Rings
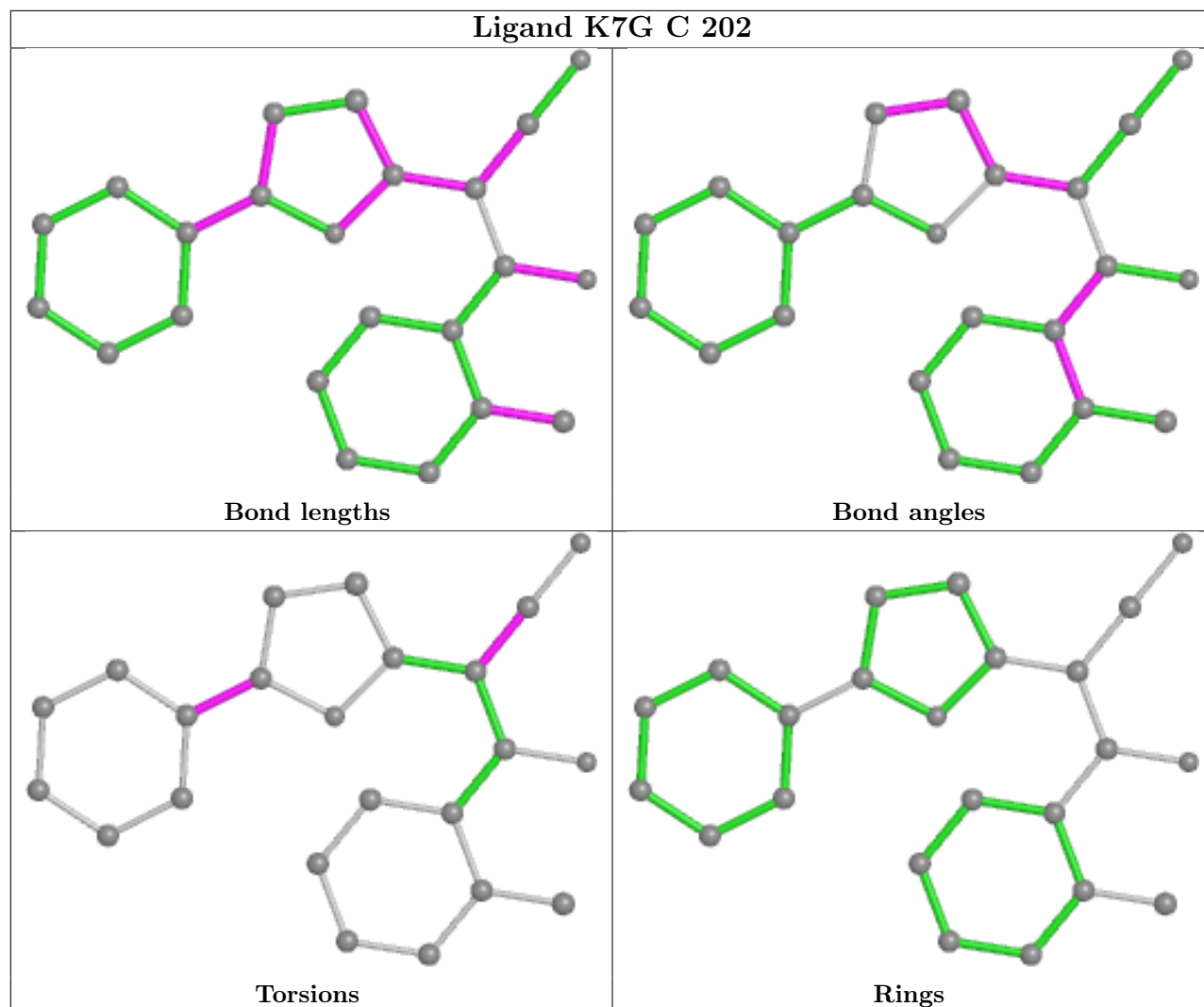
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	611/621 (98%)	0.81	71 (11%)	4	6	45, 71, 104, 122	0
2	B	240/252 (95%)	0.57	21 (8%)	10	14	43, 57, 100, 129	0
3	C	139/140 (99%)	0.39	10 (7%)	15	21	51, 65, 99, 106	0
4	D	102/103 (99%)	0.13	5 (4%)	29	38	49, 65, 83, 103	0
All	All	1092/1116 (97%)	0.64	107 (9%)	7	11	43, 67, 102, 129	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	567	LEU	5.6
1	A	223	CYS	5.1
4	D	2	SER	4.8
1	A	226	ALA	4.7
3	C	79	LEU	4.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å²)	Q<0.9
9	UNL	A	1007	1/-	0.28	0.23	85,85,85,85	0
9	UNL	D	1012	1/-	0.56	0.48	88,88,88,88	0
9	UNL	C	206	2/-	0.60	0.30	77,77,77,78	0
9	UNL	A	1017	1/-	0.63	0.34	66,66,66,66	1
9	UNL	A	1006	15/-	0.64	0.32	112,113,137,138	0
9	UNL	C	207	4/-	0.66	0.24	81,83,85,86	0
9	UNL	A	1014	1/-	0.66	0.45	55,55,55,55	0
9	UNL	B	1013	6/-	0.68	0.33	81,84,85,86	0
9	UNL	A	1013	3/-	0.68	0.32	62,62,64,64	3
9	UNL	D	1007	5/-	0.69	0.29	84,89,93,95	0
9	UNL	D	1006	3/-	0.70	0.49	49,49,51,53	3
17	3PE	D	201	40/51	0.70	0.35	75,87,130,131	0
9	UNL	D	1010	11/-	0.71	0.21	86,93,98,98	0
9	UNL	B	1014	1/-	0.71	0.25	59,59,59,59	0
9	UNL	D	1005	9/-	0.71	0.34	102,106,108,109	0
8	PEG	A	1004	5/7	0.73	0.43	63,66,68,69	5
9	UNL	B	1008	3/-	0.74	0.37	67,67,68,70	0
9	UNL	D	1008	7/-	0.75	0.39	93,97,104,107	0
9	UNL	A	1012	3/-	0.76	0.34	54,54,61,65	3
9	UNL	A	1010	4/-	0.76	0.14	88,89,90,92	0
9	UNL	C	208	1/-	0.78	1.07	53,53,53,53	1
9	UNL	A	1018	1/-	0.79	0.29	75,75,75,75	1
9	UNL	B	1005	15/-	0.80	0.32	82,100,125,127	0
9	UNL	D	1003	10/-	0.80	0.13	83,90,97,97	0
9	UNL	A	1016	1/-	0.80	0.17	67,67,67,67	0
9	UNL	B	1010	7/-	0.81	0.52	75,78,80,81	0
9	UNL	B	1011	3/-	0.82	0.21	80,80,81,81	0
9	UNL	D	1011	5/-	0.82	0.17	65,70,72,73	0
9	UNL	B	1004	4/-	0.83	0.26	97,98,99,99	0
16	BOG	D	1001	20/20	0.83	0.27	72,83,95,98	0
9	UNL	D	1009	9/-	0.83	0.10	73,84,99,101	0
9	UNL	A	1019	1/-	0.84	0.41	67,67,67,67	0
9	UNL	B	1006	4/-	0.86	0.17	57,63,68,77	0
9	UNL	A	1008	5/-	0.86	0.17	72,81,82,83	0
9	UNL	B	1007	3/-	0.88	0.20	73,73,75,79	0
9	UNL	B	1009	3/-	0.88	0.10	74,74,76,77	0
9	UNL	A	1009	4/-	0.89	0.13	73,76,79,84	0
9	UNL	C	205	3/-	0.89	0.37	74,74,77,80	0
6	OAA	A	1002	9/9	0.90	0.18	59,64,65,66	0
9	UNL	D	1004	4/-	0.90	0.50	85,87,88,89	0
9	UNL	A	1015	1/-	0.90	0.70	60,60,60,60	0
9	UNL	B	1015	1/-	0.91	0.19	44,44,44,44	0
15	UMQ	C	203	34/34	0.91	0.19	67,85,105,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UNL	D	1013	1/-	0.92	0.35	99,99,99,99	0
9	UNL	A	1011	5/-	0.92	0.12	119,120,121,122	0
9	UNL	B	1012	3/-	0.93	0.57	62,62,62,65	3
5	FAD	A	1001	53/53	0.94	0.28	46,53,59,61	0
9	UNL	A	1005	7/-	0.95	0.19	74,79,81,83	0
14	HEM	C	201	41/43	0.96	0.13	50,55,66,69	0
9	UNL	C	204	3/-	0.96	0.22	61,61,64,64	0
7	K	A	1003	1/1	0.96	0.12	70,70,70,70	0
11	SF4	B	1002	8/8	0.96	0.18	44,47,52,54	0
12	F3S	B	1003	7/7	0.97	0.18	44,49,52,56	0
13	K7G	C	202	23/23	0.97	0.11	50,54,60,63	0
10	FES	B	1001	4/4	0.97	0.20	55,55,55,56	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 3PE D 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
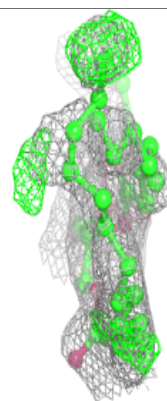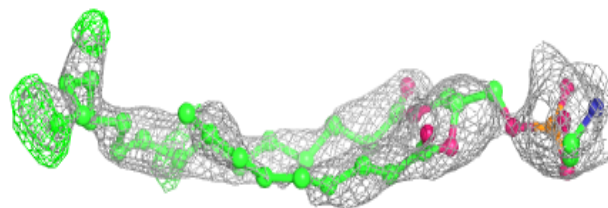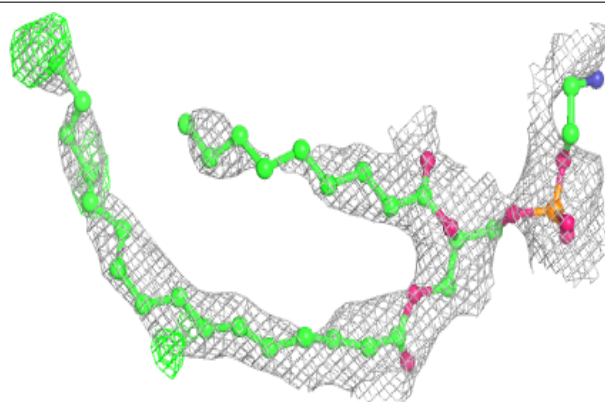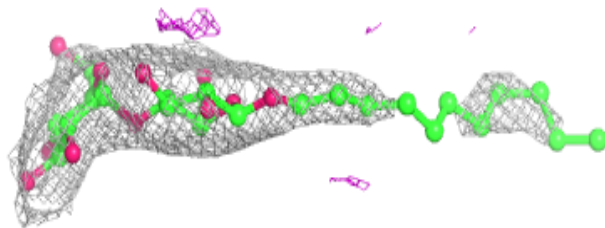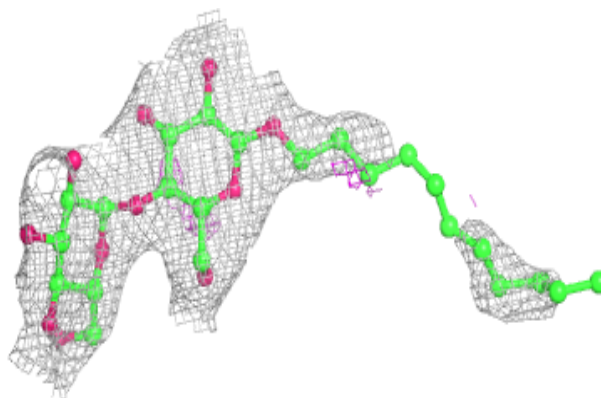
Electron density around BOG D 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
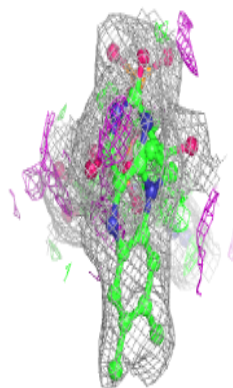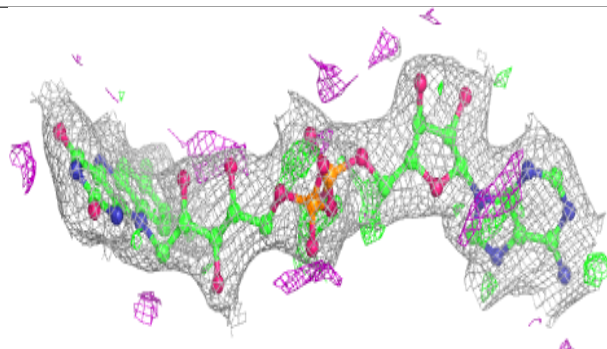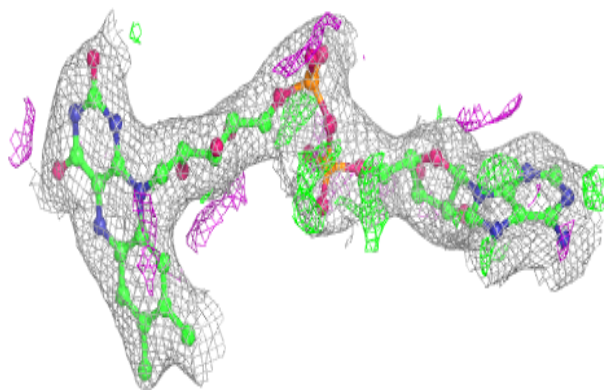and green (positive)
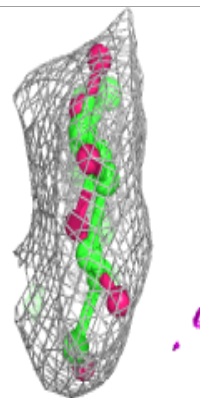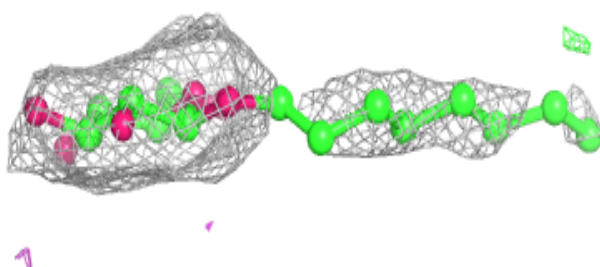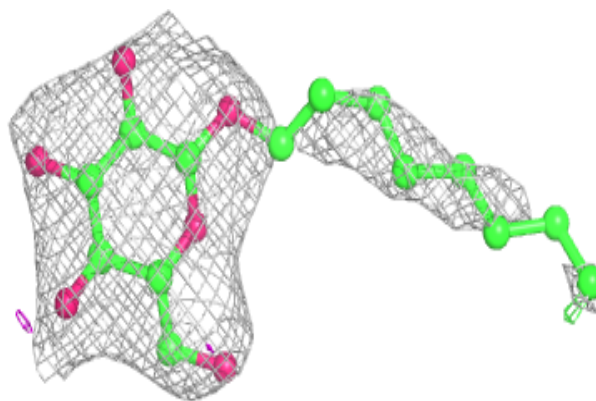
Electron density around UMQ C 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
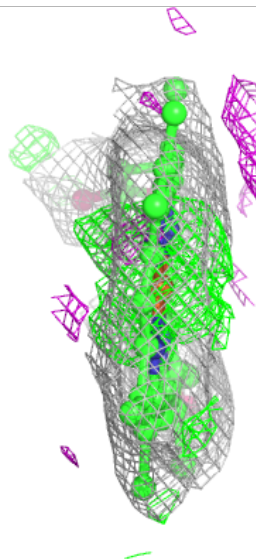mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
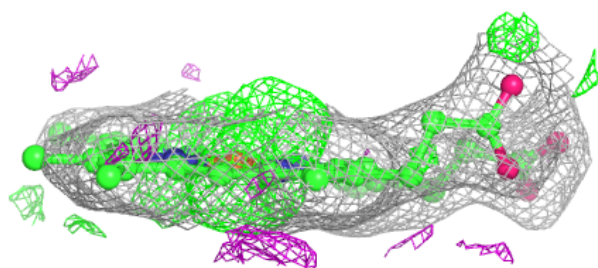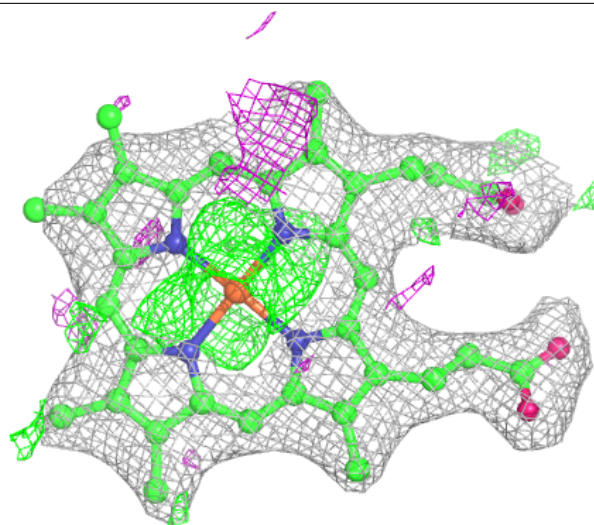
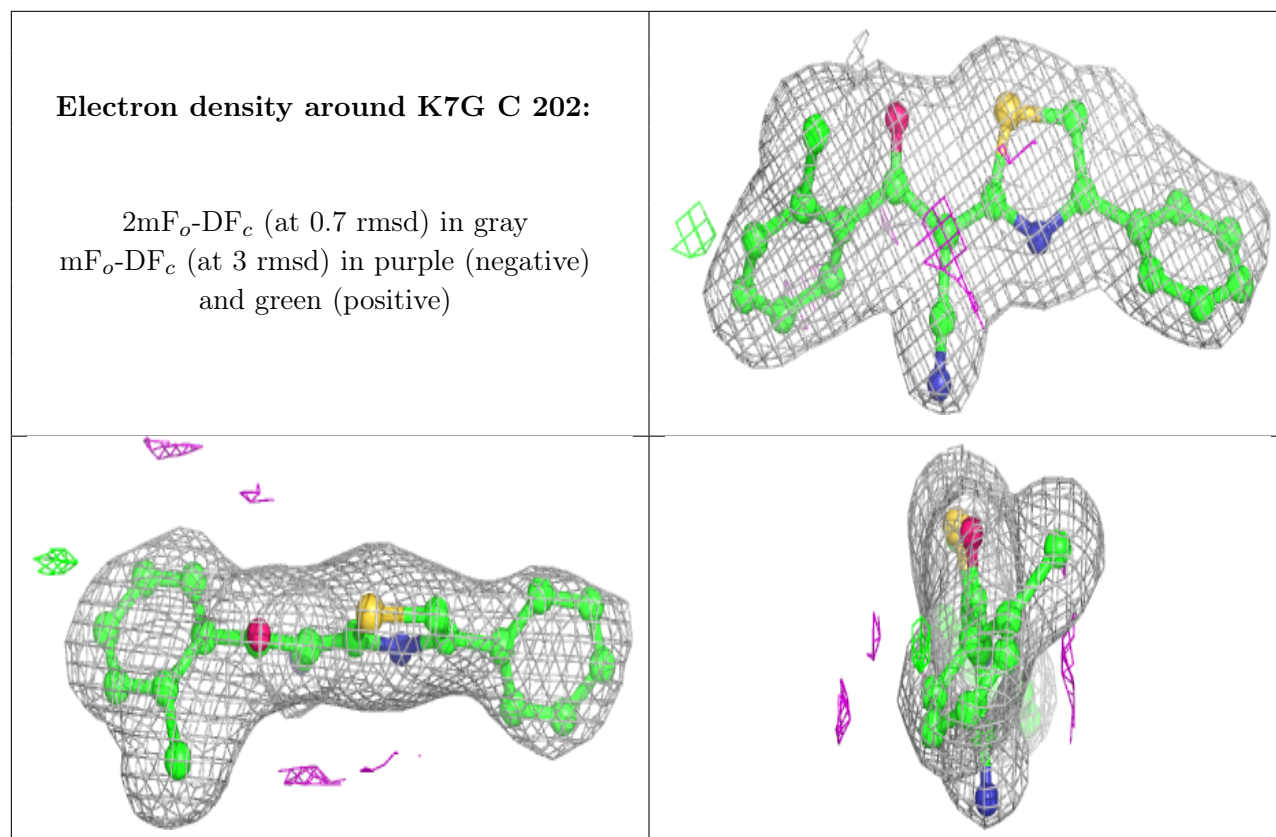**Electron density around FAD A 1001:**

$2mF_o$-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:

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

Electron density around K7G 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.