



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2021 – 02:06 PM EDT

PDB ID : 6MYO
Title : Avian mitochondrial complex II with flutolanyl bound
Authors : Berry, E.A.; Huang, L.-S.
Deposited on : 2018-11-02
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.22
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) : 2.22

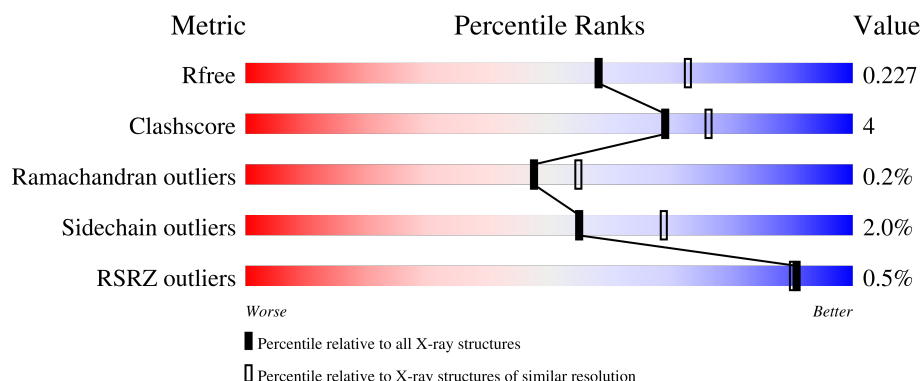
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	621	
2	B	252	
3	C	140	
4	D	103	

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
10	UNL	A	1017	-	-	-	X
10	UNL	A	1018	-	-	-	X
10	UNL	B	1008	-	-	X	-
10	UNL	D	211	-	-	-	X
6	OAA	A	1002	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 9321 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	612	Total	C	N	O	S	0	2	0
			4740	2966	846	899	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
			1076	707	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.

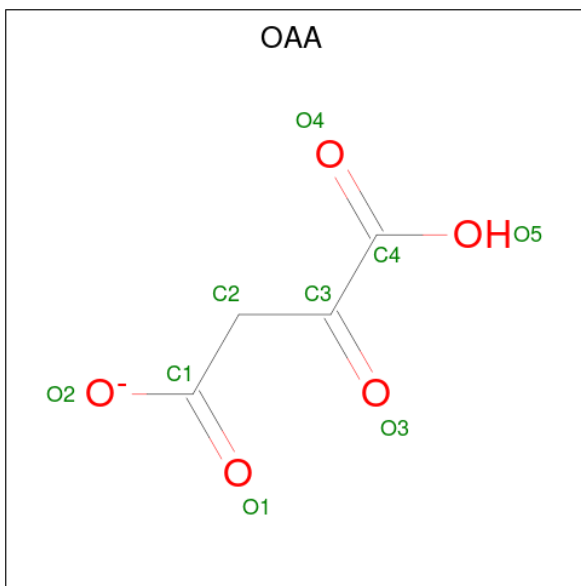
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			771	508	122	138	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: $C_4H_3O_5$).



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

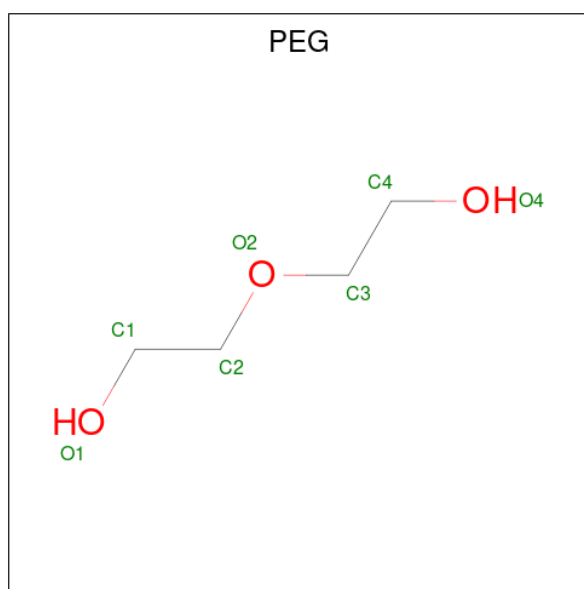
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mn 1 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

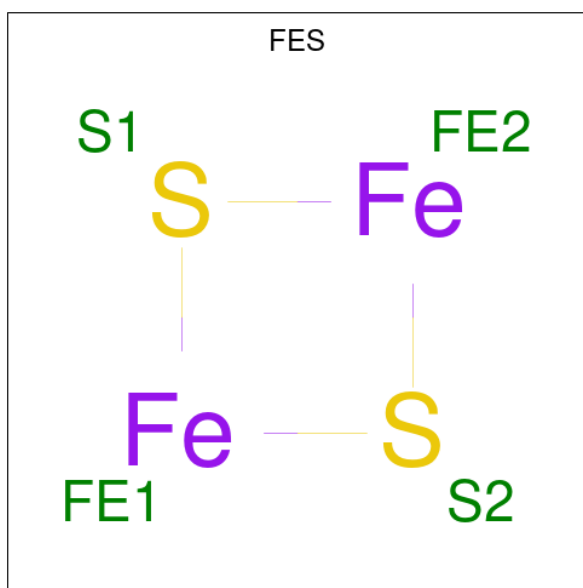


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 5 3 2	0	0

- Molecule 10 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

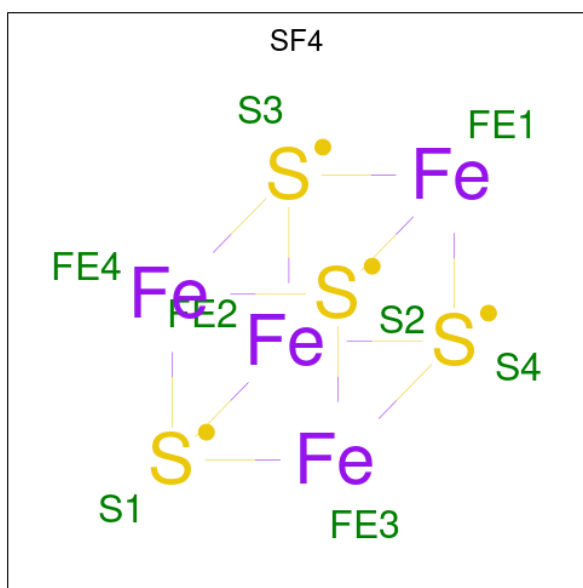
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	20	Total C N O S 54 19 8 25 2	0	0
10	B	10	Total C N O S 21 2 12 6 1	0	0
10	C	5	Total C O 20 12 8	0	0
10	D	14	Total C N O 57 31 2 24	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



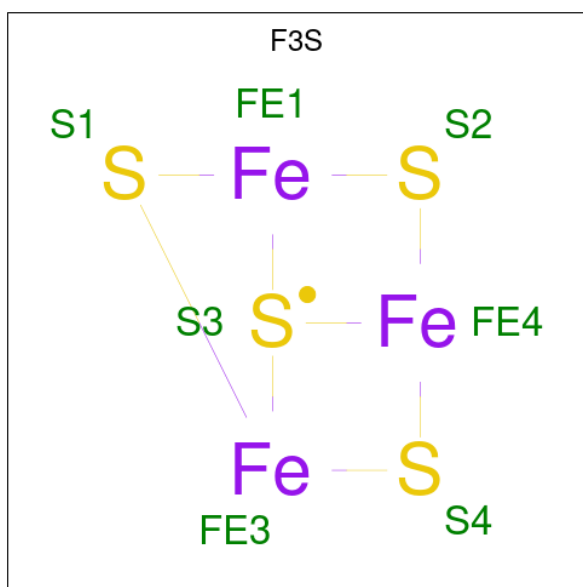
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



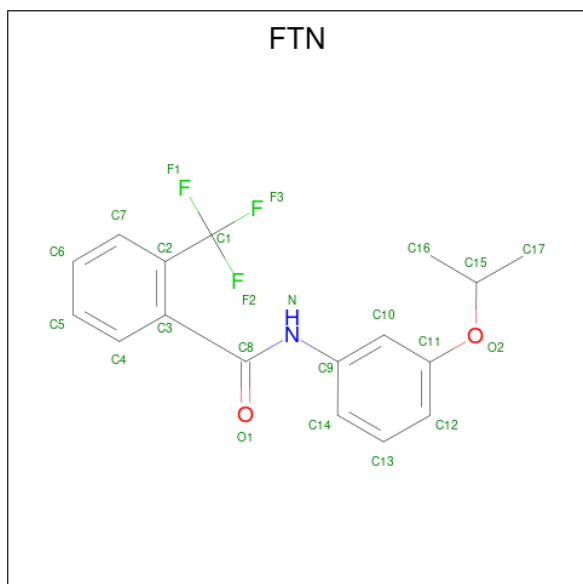
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 13 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



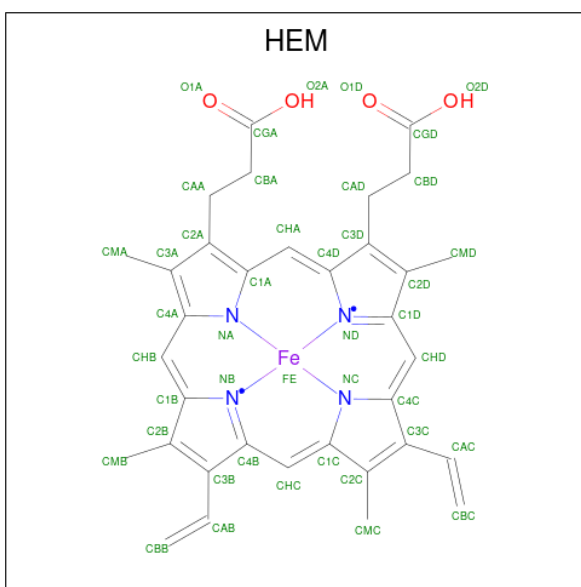
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 14 is N-[3-(1-methylethoxy)phenyl]-2-(trifluoromethyl)benzamide (three-letter code: FTN) (formula: $C_{17}H_{16}F_3NO_2$).



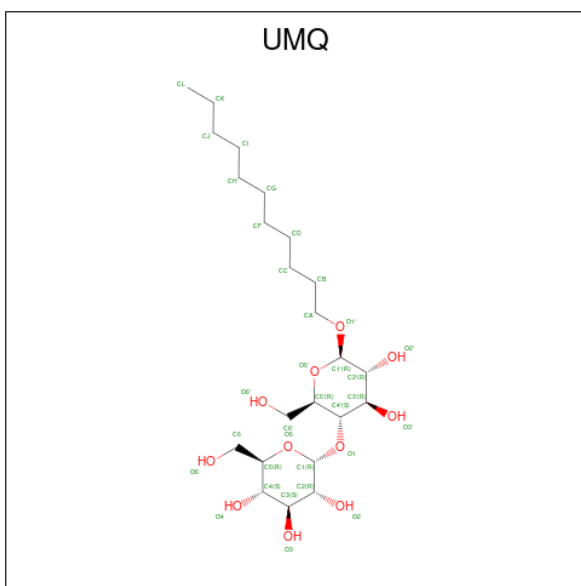
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	F	N	O	
			23	17	3	1	2	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



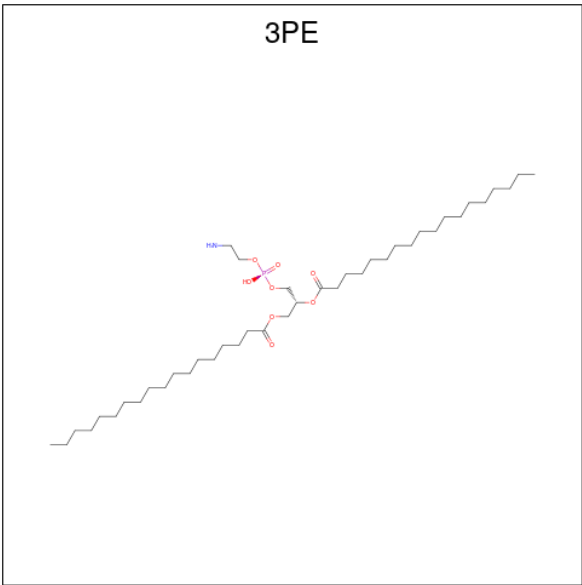
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

- Molecule 16 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	0	0
			42	32	1	8	1		

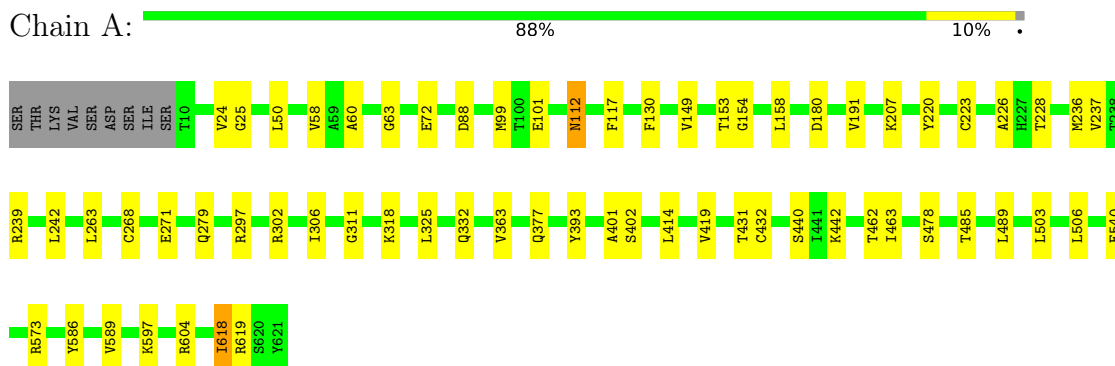
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	214	Total	O	0	0
			214	214		
18	B	131	Total	O	0	0
			131	131		
18	C	46	Total	O	0	0
			46	46		
18	D	35	Total	O	0	0
			35	35		

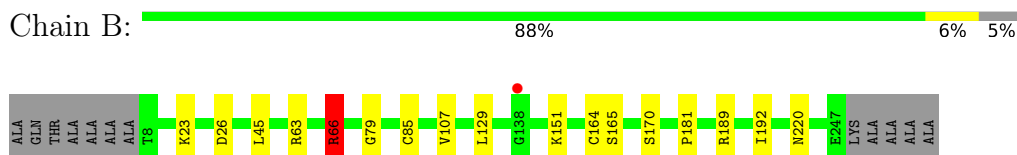
3 Residue-property plots

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.

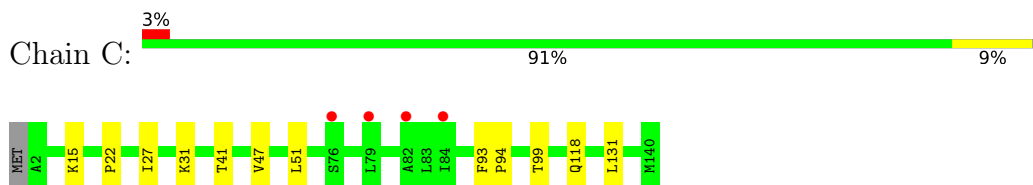
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



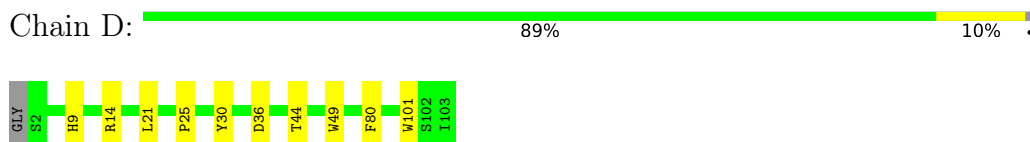
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Succinate dehydrogenase cytochrome b, large subunit



- 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	69.64Å 83.78Å 289.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.20 80.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (47.64-2.20) 86.2 (80.48-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.20Å)	Xtriage
Refinement program	PHENIX (DEV_3150: ???)	Depositor
R, R_{free}	0.189 , 0.227 0.190 , 0.227	Depositor DCC
R_{free} test set	2349 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9321	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, K, FAD, MLZ, UMQ, F3S, SF4, FES, PEG, 3PE, FTN, HEM, UNL, MN

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	0.39	0/4841	0.56	0/6554
2	B	0.41	0/1970	0.56	0/2656
3	C	0.37	0/1094	0.52	0/1486
4	D	0.40	0/794	0.53	0/1089
All	All	0.39	0/8699	0.55	0/11785

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4740	0	4625	44	0
2	B	1928	0	1921	9	0
3	C	1076	0	1116	8	0
4	D	771	0	763	5	0
5	A	53	0	29	6	0
6	A	9	0	2	5	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	5	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	54	0	0	2	0
10	B	21	0	0	2	0
10	C	20	0	0	1	0
10	D	57	0	0	3	0
11	B	4	0	0	0	0
12	B	8	0	0	0	0
13	B	7	0	0	0	0
14	C	23	0	16	1	0
15	C	41	0	24	1	0
16	C	34	0	44	1	0
17	D	42	0	61	0	0
18	A	214	0	0	5	0
18	B	131	0	0	0	0
18	C	46	0	0	0	0
18	D	35	0	0	1	0
All	All	9321	0	8606	65	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 4.

All (65) 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	1.63	1.11
1:A:297:ARG:NH2	6:A:1002:OAA:H22	1.65	1.11
1:A:297:ARG:HH22	6:A:1002:OAA:H22	0.88	1.04
3:C:118:GLN:OE1	10:C:1007:UNL:O	2.05	0.74
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.70	0.73
1:A:401:ALA:N	1:A:402:SER:HA	2.05	0.70
4:D:36:ASP:OD2	10:D:213:UNL:O	2.20	0.60
3:C:99:THR:HG23	15:C:201:HEM:HMC3	1.85	0.59
10:D:214:UNL:O	10:D:215:UNL:O	2.23	0.57
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.85	0.56
1:A:604:ARG:NH1	18:A:1107:HOH:O	2.39	0.55
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.90	0.53
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.90	0.53
2:B:23:LYS:HB2	2:B:26:ASP:HB2	1.90	0.53
1:A:442[B]:LYS:N	18:A:1109:HOH:O	2.40	0.53
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.91	0.52
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.43	0.52
1:A:442[A]:LYS:N	18:A:1109:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG13	1:A:242:LEU:HB2	1.92	0.51
2:B:107:VAL:HB	3:C:22:PRO:HG2	1.93	0.50
4:D:21:LEU:O	4:D:25:PRO:HD2	2.12	0.50
1:A:377:GLN:HG2	1:A:393:TYR:CE2	2.46	0.49
1:A:88:ASP:OD2	10:A:1023:UNL:O	2.30	0.48
4:D:49:TRP:HE1	10:D:202:UNL:C5	2.26	0.48
9:A:1005:PEG:H32	18:A:1238:HOH:O	2.14	0.47
3:C:27:ILE:HG22	14:C:202:FTN:H12	1.96	0.47
1:A:239:ARG:HG2	1:A:589:VAL:HG11	1.96	0.47
4:D:9:HIS:HE1	18:D:305:HOH:O	1.98	0.47
1:A:586:TYR:CE1	1:A:597:LYS:HD2	2.51	0.46
1:A:297:ARG:HH12	6:A:1002:OAA:C1	2.30	0.45
2:B:165:SER:HA	2:B:181:PRO:HD2	1.99	0.45
1:A:489:LEU:HD13	1:A:540:GLU:HA	1.98	0.45
1:A:271:GLU:HB3	1:A:332:GLN:NE2	2.32	0.45
2:B:164:CYS:SG	2:B:165:SER:N	2.91	0.44
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.47	0.44
1:A:302:ARG:O	1:A:306:ILE:HG13	2.18	0.44
1:A:573:ARG:NH1	18:A:1106:HOH:O	2.50	0.44
1:A:263:LEU:HD22	5:A:1001:FAD:C6	2.47	0.44
1:A:318:LYS:HE3	1:A:318:LYS:HB3	1.71	0.43
1:A:431:THR:HG22	1:A:432:CYS:SG	2.58	0.43
1:A:101:GLU:OE2	10:A:1025:UNL:O	2.36	0.43
1:A:297:ARG:HH22	6:A:1002:OAA:C3	2.24	0.43
2:B:151:LYS:HB3	2:B:192:ILE:HD12	2.00	0.43
2:B:45:LEU:HD22	2:B:85:CYS:HB3	2.00	0.43
1:A:63:GLY:HA2	1:A:153:THR:HG21	1.99	0.43
5:A:1001:FAD:H1'1	5:A:1001:FAD:H9	1.71	0.43
3:C:47:VAL:O	3:C:51:LEU:HG	2.19	0.42
1:A:268:CYS:HB3	1:A:325:LEU:HD21	2.02	0.42
1:A:271:GLU:HB3	1:A:332:GLN:HE21	1.84	0.42
1:A:618:ILE:HG12	1:A:619:ARG:N	2.35	0.42
3:C:41:THR:HG21	16:C:1002:UMQ:HL2	2.02	0.42
1:A:226:ALA:HB2	10:B:1008:UNL:N1	2.34	0.41
2:B:79:GLY:HA3	3:C:31:LYS:HB3	2.02	0.41
1:A:58:VAL:HB	1:A:158:LEU:HD23	2.02	0.41
1:A:503:LEU:HD22	1:A:506:LEU:HD11	2.01	0.41
1:A:462:THR:HG22	1:A:463:ILE:HG13	2.02	0.41
1:A:223:CYS:O	2:B:66:ARG:NH2	2.53	0.41
1:A:112:ASN:O	2:B:129:LEU:HD23	2.21	0.41
1:A:180:ASP:HA	1:A:236:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ALA:HB2	10:B:1008:UNL:N2	2.36	0.41
1:A:24:VAL:HG21	1:A:191:VAL:HG11	2.03	0.41
1:A:99:MET:HA	1:A:419:VAL:HG11	2.03	0.40
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.51	0.40
3:C:93:PHE:HB3	3:C:94:PRO:HD3	2.04	0.40
1:A:414:LEU:HG	5:A:1001:FAD:C2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	612/621 (99%)	587 (96%)	24 (4%)	1 (0%)	47	55
2	B	238/252 (94%)	228 (96%)	9 (4%)	1 (0%)	34	37
3	C	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
4	D	100/103 (97%)	98 (98%)	2 (2%)	0	100	100
All	All	1086/1116 (97%)	1047 (96%)	37 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
1	A	311	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/506 (98%)	489 (98%)	9 (2%)	59	72
2	B	216/219 (99%)	211 (98%)	5 (2%)	50	63
3	C	116/117 (99%)	115 (99%)	1 (1%)	78	88
4	D	78/79 (99%)	75 (96%)	3 (4%)	33	42
All	All	908/921 (99%)	890 (98%)	18 (2%)	55	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	112	ASN
1	A	130	PHE
1	A	207	LYS
1	A	279	GLN
1	A	440	SER
1	A	478	SER
1	A	485	THR
1	A	618	ILE
2	B	63	ARG
2	B	66	ARG
2	B	170	SER
2	B	189	ARG
2	B	220	ASN
3	C	131	LEU
4	D	14	ARG
4	D	30	TYR
4	D	101	TRP

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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	MLZ	C	15	3	8,9,10	0.68	0	4,9,11	1.60	1 (25%)

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
3	MLZ	C	15	3	-	1/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	MLZ	CM-NZ-CE	2.83	120.14	111.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	15	MLZ	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 61 ligands modelled in this entry, 2 are monoatomic and 49 are unknown - leaving 10 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	$\# Z > 2$
6	OAA	A	1002	-	2,8,8	0.76	0	2,10,10	3.11	1 (50%)
16	UMQ	C	1002	-	35,35,35	0.58	0	46,46,46	1.16	4 (8%)
14	FTN	C	202	-	24,24,24	1.61	3 (12%)	34,34,34	1.10	1 (2%)
15	HEM	C	201	4,3	26,48,50	1.45	4 (15%)	21,80,82	1.55	6 (28%)
17	3PE	D	201	-	41,41,50	1.11	2 (4%)	44,46,55	1.16	2 (4%)
9	PEG	A	1005	-	4,4,6	0.52	0	3,3,5	0.30	0
11	FES	B	1001	2	0,4,4	0.00	-	-	-	-
5	FAD	A	1001	1	51,58,58	0.81	1 (1%)	60,89,89	1.36	6 (10%)
12	SF4	B	1002	2	0,12,12	0.00	-	-	-	-
13	F3S	B	1003	2	0,9,9	0.00	-	-	-	-

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
6	OAA	A	1002	-	-	0/2/8/8	-
16	UMQ	C	1002	-	-	7/20/60/60	0/2/2/2
14	FTN	C	202	-	-	4/18/18/18	0/2/2/2
15	HEM	C	201	4,3	-	2/6/50/54	-
17	3PE	D	201	-	-	22/45/45/54	-
9	PEG	A	1005	-	-	0/2/2/4	-
5	FAD	A	1001	1	-	5/30/50/50	0/6/6/6
11	FES	B	1001	2	-	-	0/1/1/1
12	SF4	B	1002	2	-	-	0/6/5/5
13	F3S	B	1003	2	-	-	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	202	FTN	C8-N	4.85	1.48	1.35
17	D	201	3PE	O21-C21	4.77	1.47	1.34
17	D	201	3PE	O31-C31	4.32	1.46	1.33
14	C	202	FTN	C9-N	3.71	1.49	1.41
5	A	1001	FAD	C4X-C10	2.70	1.41	1.38
14	C	202	FTN	O2-C15	-2.39	1.39	1.45
15	C	201	HEM	C3B-C2B	-2.29	1.33	1.41
15	C	201	HEM	C3C-C2C	-2.18	1.34	1.41
15	C	201	HEM	CAA-C2A	2.03	1.55	1.52
15	C	201	HEM	C4D-C3D	2.02	1.47	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	3PE	O21-C21-C22	4.95	122.18	111.50
5	A	1001	FAD	C4-C4X-C10	-4.49	116.98	119.95
6	A	1002	OAA	C1-C2-C3	3.94	122.52	115.51
5	A	1001	FAD	C4-N3-C2	3.80	118.35	115.14
5	A	1001	FAD	C1'-N10-C10	3.58	121.62	118.41
14	C	202	FTN	C11-O2-C15	3.48	123.82	119.37
15	C	201	HEM	C4B-C3B-C2B	2.83	109.55	106.92
16	C	1002	UMQ	O5'-C5'-C6'	2.76	113.29	106.44
5	A	1001	FAD	C4-C4X-N5	2.75	121.74	118.60
5	A	1001	FAD	C4X-N5-C5X	2.58	119.35	116.77
16	C	1002	UMQ	O5-C5-C4	2.56	114.34	109.69
15	C	201	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
15	C	201	HEM	CBA-CAA-C2A	-2.41	108.04	112.49
15	C	201	HEM	C1C-C2C-C3C	2.35	108.47	106.85
15	C	201	HEM	C1D-C2D-C3D	2.21	108.54	107.00
5	A	1001	FAD	O5'-C5'-C4'	-2.20	103.49	109.36
17	D	201	3PE	C3-C2-C1	-2.19	106.61	111.79
15	C	201	HEM	C4A-C3A-C2A	2.19	108.52	107.00
16	C	1002	UMQ	C1'-O5'-C5'	-2.15	109.46	113.69
16	C	1002	UMQ	C6-C5-C4	-2.02	108.28	113.00

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	PA-O3P-P-O5'

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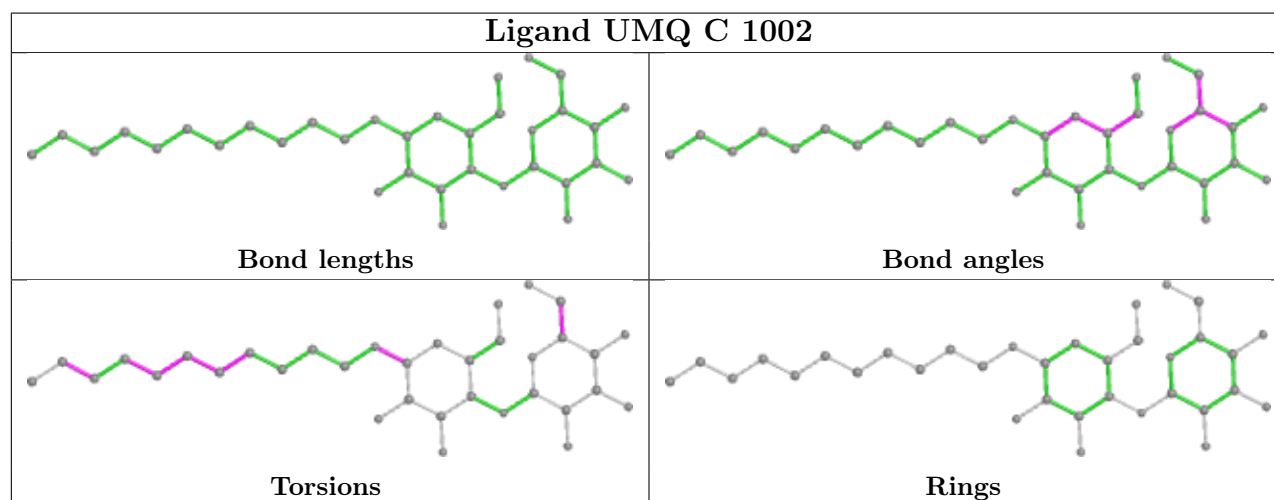
Mol	Chain	Res	Type	Atoms
15	C	201	HEM	C2D-C3D-CAD-CBD
15	C	201	HEM	C4D-C3D-CAD-CBD
16	C	1002	UMQ	O5'-C1'-O1'-CA
17	D	201	3PE	O13-C11-C12-N
17	D	201	3PE	C22-C21-O21-C2
14	C	202	FTN	C16-C15-O2-C11
17	D	201	3PE	O22-C21-O21-C2
17	D	201	3PE	C3E-C3F-C3G-C3H
17	D	201	3PE	C31-C32-C33-C34
17	D	201	3PE	C22-C23-C24-C25
17	D	201	3PE	C36-C37-C38-C39
16	C	1002	UMQ	CG-CH-CI-CJ
14	C	202	FTN	C17-C15-O2-C11
16	C	1002	UMQ	O5-C5-C6-O6
17	D	201	3PE	C38-C39-C3A-C3B
17	D	201	3PE	C3C-C3D-C3E-C3F
16	C	1002	UMQ	CF-CG-CH-CI
16	C	1002	UMQ	CC-CD-CF-CG
17	D	201	3PE	C26-C27-C28-C29
17	D	201	3PE	C11-O13-P-O11
17	D	201	3PE	C3D-C3E-C3F-C3G
5	A	1001	FAD	P-O3P-PA-O2A
17	D	201	3PE	C32-C31-O31-C3
17	D	201	3PE	O32-C31-O31-C3
17	D	201	3PE	C39-C3A-C3B-C3C
17	D	201	3PE	C24-C25-C26-C27
16	C	1002	UMQ	CI-CJ-CK-CL
17	D	201	3PE	O21-C2-C3-O31
17	D	201	3PE	C32-C33-C34-C35
17	D	201	3PE	O21-C21-C22-C23
14	C	202	FTN	C10-C11-O2-C15
5	A	1001	FAD	O4B-C4B-C5B-O5B
5	A	1001	FAD	P-O3P-PA-O1A
16	C	1002	UMQ	CD-CF-CG-CH
17	D	201	3PE	O22-C21-C22-C23
17	D	201	3PE	C11-O13-P-O14
14	C	202	FTN	C12-C11-O2-C15
17	D	201	3PE	O31-C31-C32-C33

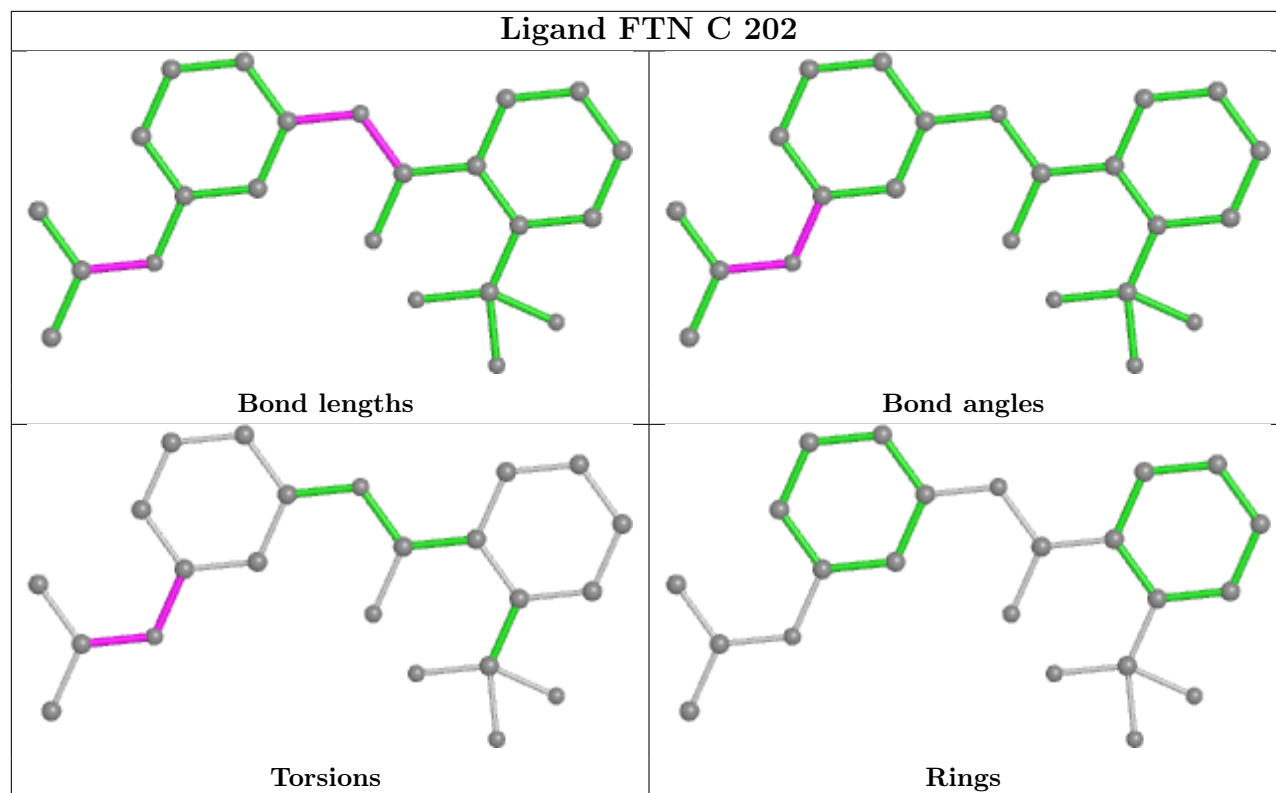
There are no ring outliers.

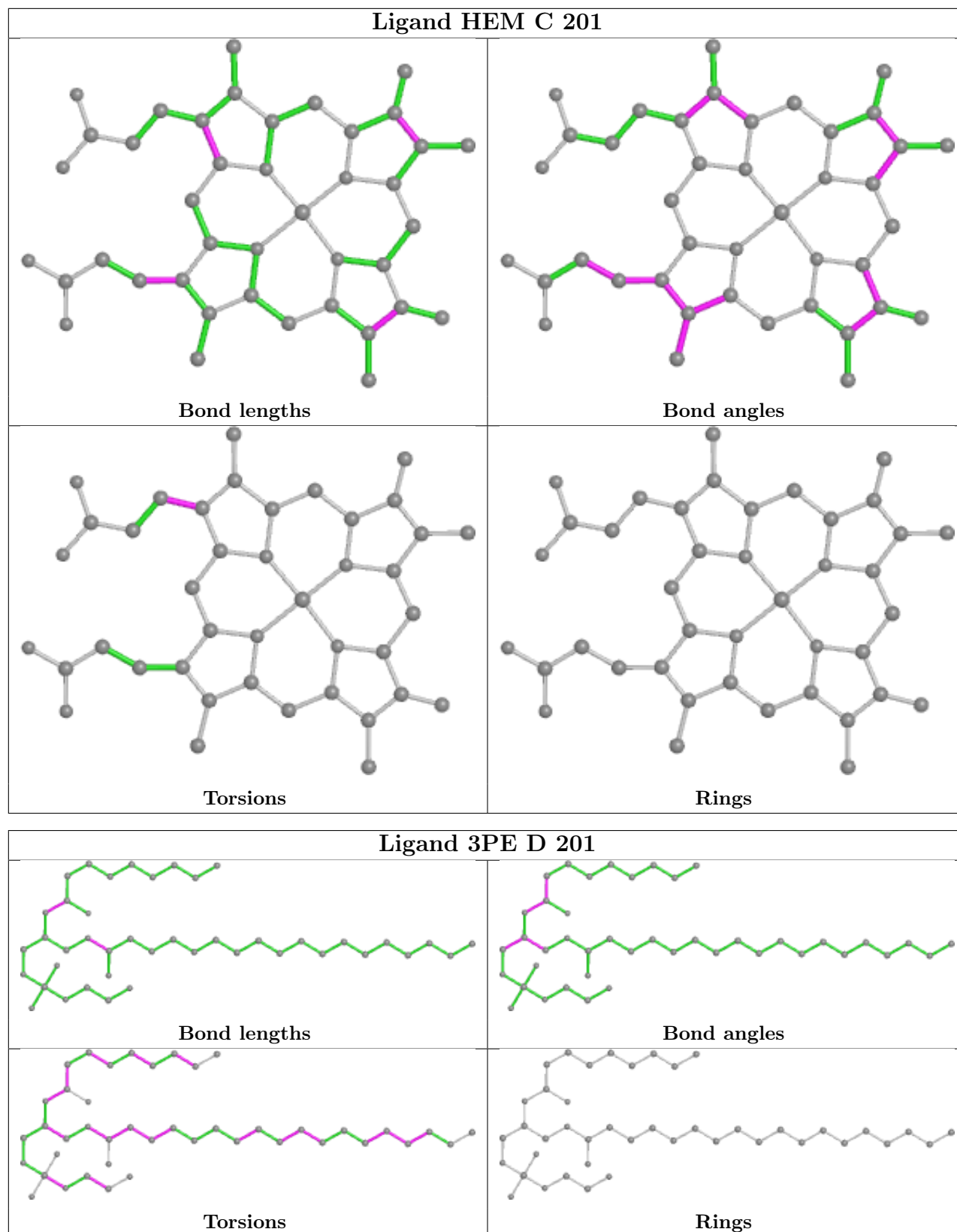
6 monomers are involved in 15 short contacts:

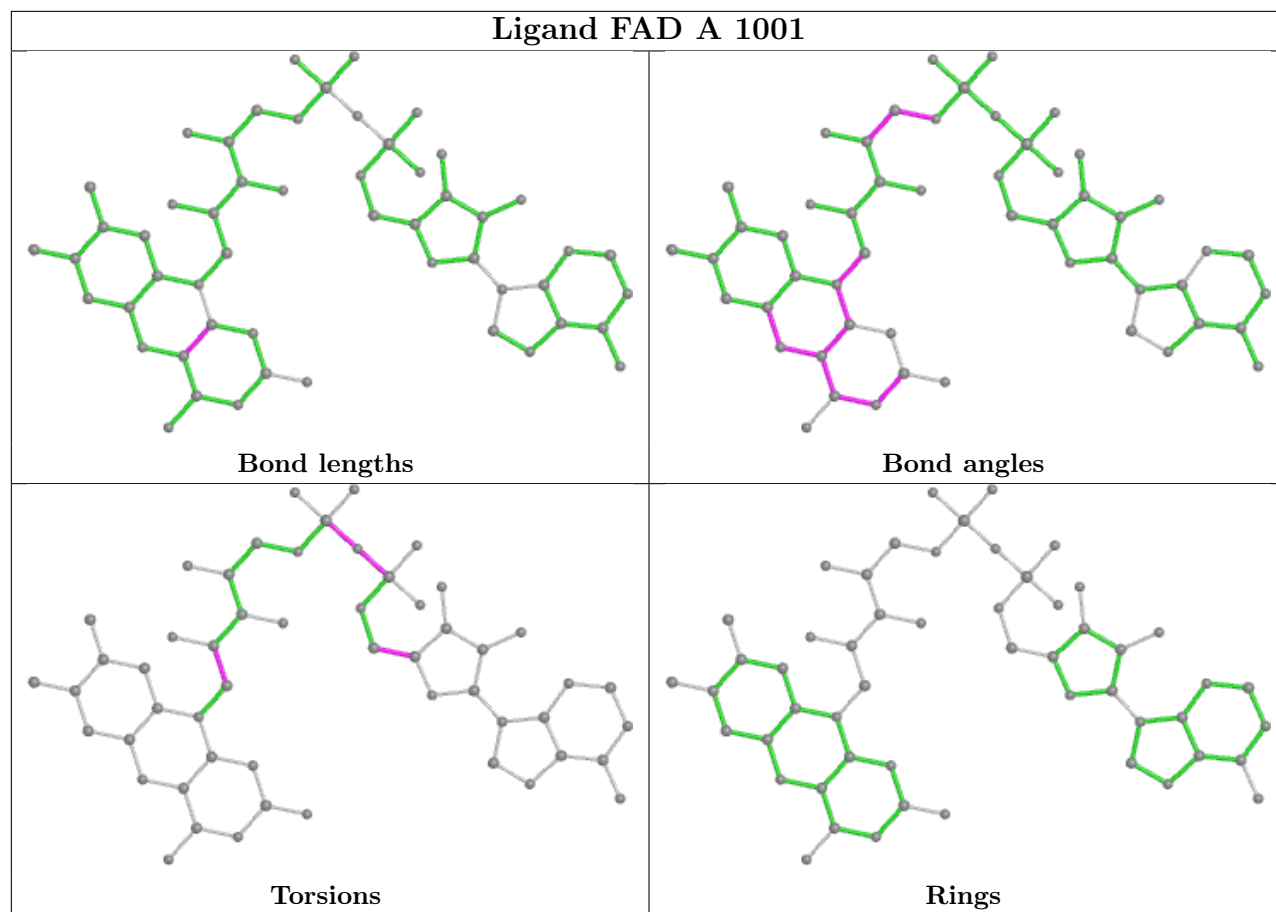
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	OAA	5	0
16	C	1002	UMQ	1	0
14	C	202	FTN	1	0
15	C	201	HEM	1	0
9	A	1005	PEG	1	0
5	A	1001	FAD	6	0

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 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	612/621 (98%)	-0.26	0 100 100	37, 57, 82, 108	1 (0%)
2	B	240/252 (95%)	-0.27	1 (0%) 92 91	36, 48, 81, 104	0
3	C	138/140 (98%)	-0.01	4 (2%) 51 49	40, 52, 83, 96	0
4	D	102/103 (99%)	-0.08	0 100 100	41, 52, 73, 99	0
All	All	1092/1116 (97%)	-0.22	5 (0%) 91 90	36, 54, 81, 108	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	138	GLY	3.2
3	C	82	ALA	2.4
3	C	84	ILE	2.3
3	C	79	LEU	2.0
3	C	76	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	MLZ	C	15	10/11	0.93	0.14	52,60,66,66	0

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
10	UNL	D	210	1/-	0.11	0.16	73,73,73,73	0
10	UNL	D	211	1/-	0.24	0.72	68,68,68,68	0
10	UNL	D	204	1/-	0.31	0.20	70,70,70,70	0
10	UNL	A	1024	1/-	0.41	0.30	86,86,86,86	0
10	UNL	A	1018	3/-	0.66	0.49	66,66,67,70	0
10	UNL	D	207	12/-	0.68	0.39	78,89,97,98	0
10	UNL	B	1014	1/-	0.68	0.25	57,57,57,57	0
10	UNL	D	206	7/-	0.68	0.35	74,83,89,92	0
10	UNL	B	1007	3/-	0.72	0.27	62,62,66,74	0
10	UNL	A	1017	2/-	0.76	0.45	74,74,74,77	0
10	UNL	B	1008	3/-	0.78	0.19	36,36,46,64	0
10	UNL	D	208	10/-	0.78	0.21	76,92,101,103	0
10	UNL	A	1021	1/-	0.79	0.19	75,75,75,75	0
10	UNL	D	209	10/-	0.80	0.26	55,67,79,83	10
10	UNL	D	215	1/-	0.80	0.32	63,63,63,63	0
10	UNL	A	1020	1/-	0.81	0.48	81,81,81,81	0
10	UNL	B	1012	1/-	0.82	0.20	61,61,61,61	0
10	UNL	B	1013	1/-	0.82	0.41	46,46,46,46	1
10	UNL	B	1006	3/-	0.82	0.18	63,63,65,67	0
10	UNL	D	202	7/-	0.82	0.19	68,77,82,86	0
17	3PE	D	201	42/51	0.82	0.39	55,76,121,127	0
10	UNL	C	1006	1/-	0.83	0.14	65,65,65,65	0
10	UNL	A	1025	1/-	0.84	0.14	50,50,50,50	0
10	UNL	A	1022	1/-	0.84	0.13	56,56,56,56	0
9	PEG	A	1005	5/7	0.84	0.38	59,72,81,81	0
10	UNL	D	205	1/-	0.85	0.60	59,59,59,59	0
10	UNL	A	1007	4/-	0.85	0.12	75,75,76,77	0
10	UNL	A	1015	3/-	0.85	0.20	51,51,62,71	0
10	UNL	C	1007	1/-	0.86	0.16	43,43,43,43	1
10	UNL	C	1005	12/-	0.87	0.30	53,80,82,83	0
10	UNL	D	214	1/-	0.87	0.37	59,59,59,59	0
10	UNL	A	1014	3/-	0.88	0.27	46,46,50,59	0
10	UNL	A	1013	2/-	0.89	0.11	67,67,67,69	0
10	UNL	A	1009	4/-	0.90	0.19	70,74,75,76	0
10	UNL	A	1019	1/-	0.91	0.16	64,64,64,64	0
10	UNL	A	1008	4/-	0.91	0.15	79,81,86,93	0
10	UNL	A	1016	3/-	0.91	0.17	57,57,63,65	3

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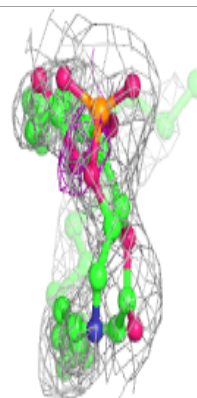
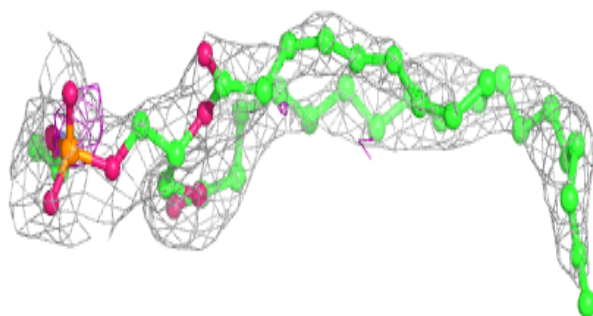
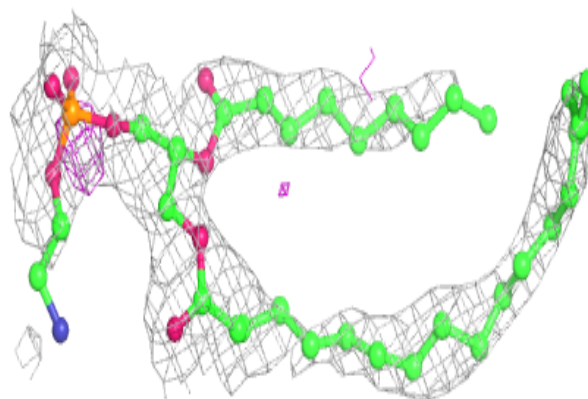
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	UNL	A	1006	7/-	0.92	0.14	42,62,64,69	7
6	OAA	A	1002	9/9	0.92	0.10	46,53,62,62	0
16	UMQ	C	1002	34/34	0.92	0.20	45,65,88,93	0
10	UNL	A	1012	4/-	0.92	0.12	54,56,71,74	0
10	UNL	A	1023	1/-	0.93	0.32	55,55,55,55	0
10	UNL	C	1003	3/-	0.93	0.09	59,59,63,64	0
10	UNL	B	1011	1/-	0.93	0.12	50,50,50,50	0
10	UNL	A	1011	4/-	0.94	0.08	59,62,65,79	0
10	UNL	B	1009	3/-	0.95	0.09	63,63,65,68	0
10	UNL	A	1010	4/-	0.95	0.11	67,69,69,70	0
12	SF4	B	1002	8/8	0.95	0.18	39,43,45,47	0
10	UNL	C	1004	3/-	0.95	0.42	59,59,62,70	0
10	UNL	D	212	1/-	0.95	0.27	58,58,58,58	0
11	FES	B	1001	4/4	0.96	0.20	45,45,50,54	0
10	UNL	D	203	3/-	0.96	0.15	43,43,51,54	0
14	FTN	C	202	23/23	0.96	0.14	37,46,68,73	0
15	HEM	C	201	41/43	0.96	0.14	40,47,55,57	0
10	UNL	B	1005	4/-	0.96	0.17	51,53,62,70	0
10	UNL	B	1010	1/-	0.96	0.17	51,51,51,51	0
10	UNL	D	213	1/-	0.97	0.09	56,56,56,56	0
13	F3S	B	1003	7/7	0.97	0.20	32,40,47,48	0
8	MN	A	1004	1/1	0.97	0.10	79,79,79,79	1
5	FAD	A	1001	53/53	0.98	0.12	36,45,52,56	0
7	K	A	1003	1/1	0.98	0.12	51,51,51,51	0

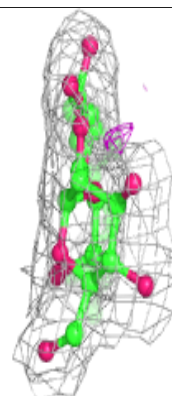
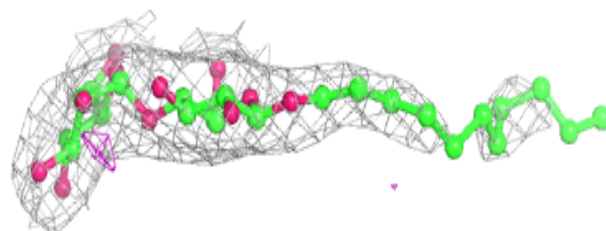
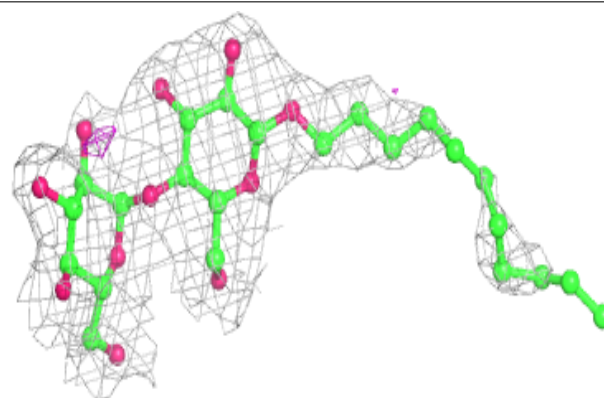
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3PE D 201:

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

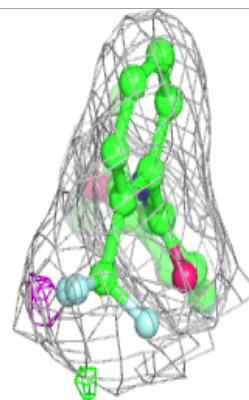
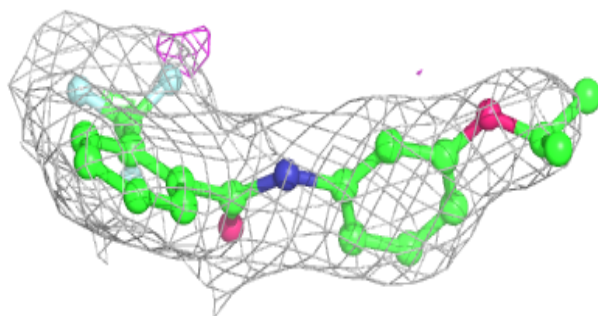
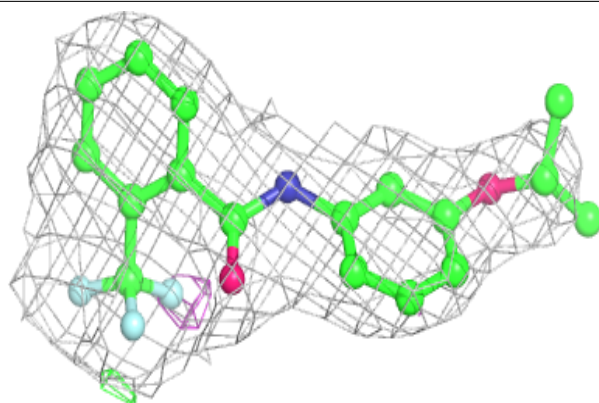
**Electron density around UMQ C 1002:**

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



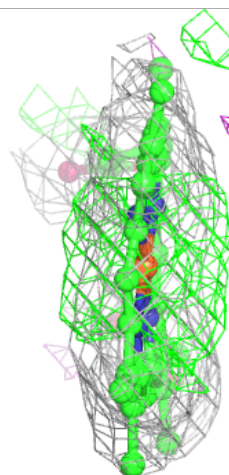
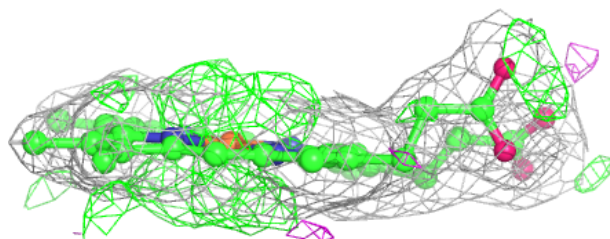
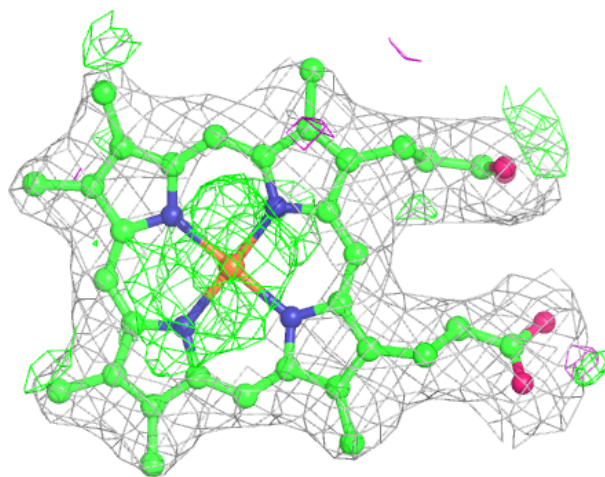
Electron density around FTN C 202:

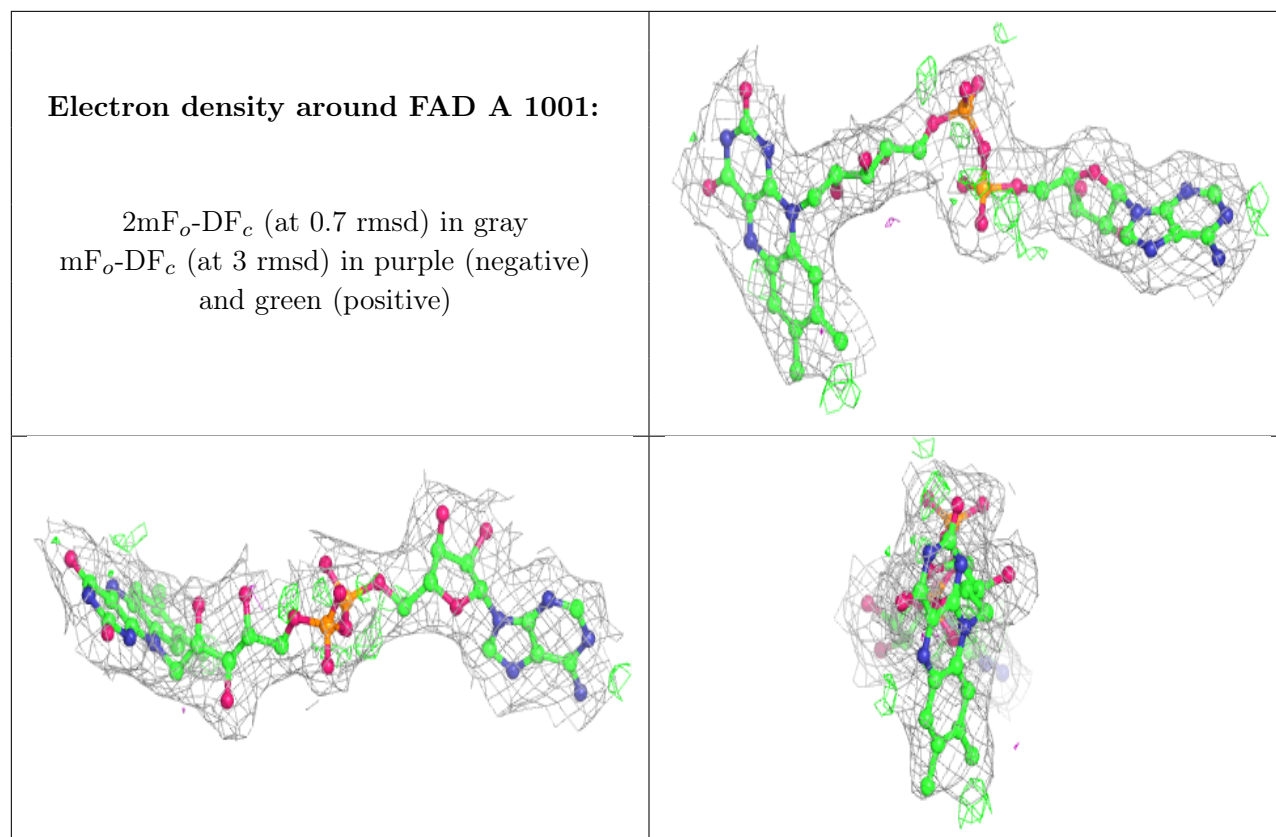
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.