Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 08:10 PM EDT

PDB ID	:	6MYU
Title	:	Avian mitochondrial complex II crystallized in the presence of HQNO
Authors	:	Berry, E.A.; Huang, L.-S.
Deposited on	:	2018-11-02
Resolution	:	1.97 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 (i) 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 (i)) were used in the production of this report:

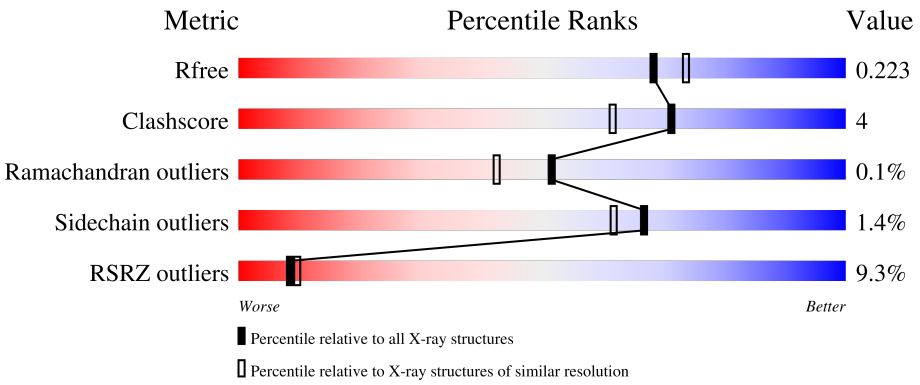
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	10% 90% 8% •
2	B	252	9% 89% 6% 5%
3	C	140	7% 92% 6% ••
4	D	103	6% 89% 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	UNL	A	1011	-	-	-	X
8	UNL	A	1012	-	-	-	X
8	UNL	A	1020	-	-	X	-
8	UNL	A	1026	-	-	-	X
8	UNL	A	1031[A]	-	-	-	X
8	UNL	A	1031[B]	-	-	-	X
8	UNL	B	1009	-	-	-	X
8	UNL	C	205	-	-	-	X
8	UNL	C	220	-	-	-	X
8	UNL	D	207	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 9421 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
			Total	C	N	O	S			
1	A	611	4723	2956	843	895	29	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	139	1076	707	178	186	5	0	0	0

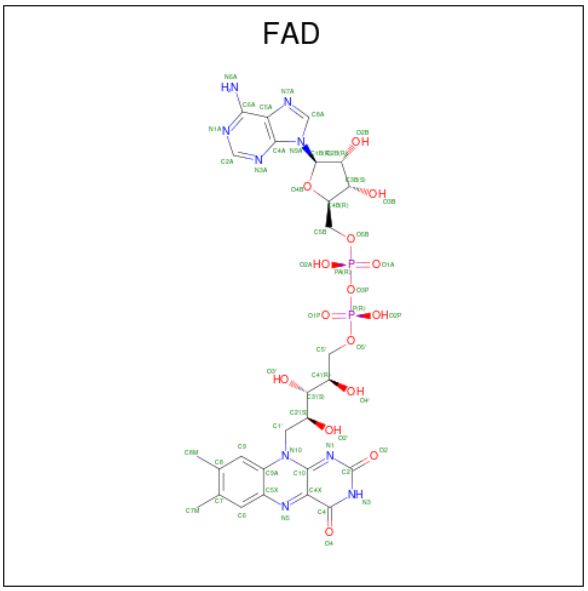
There are 2 discrepancies between the modelled and reference sequences:

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.

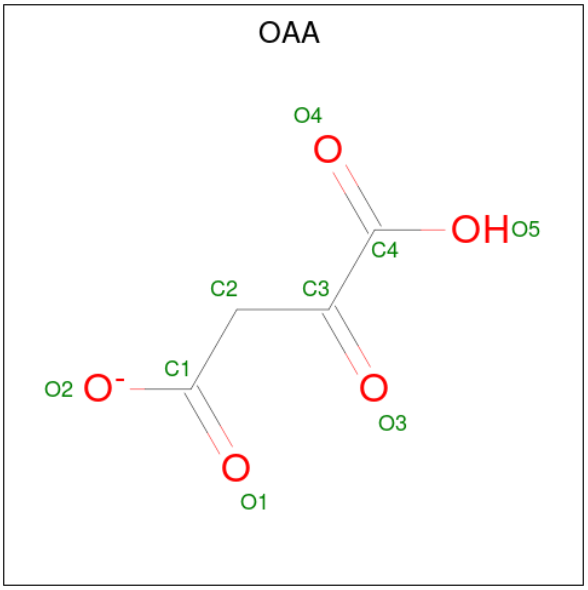
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	771	508	122	138	3	0	0	0

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



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

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



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

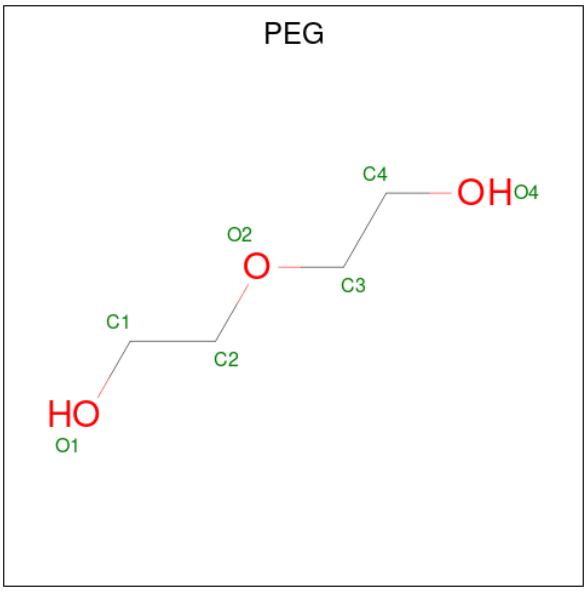
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

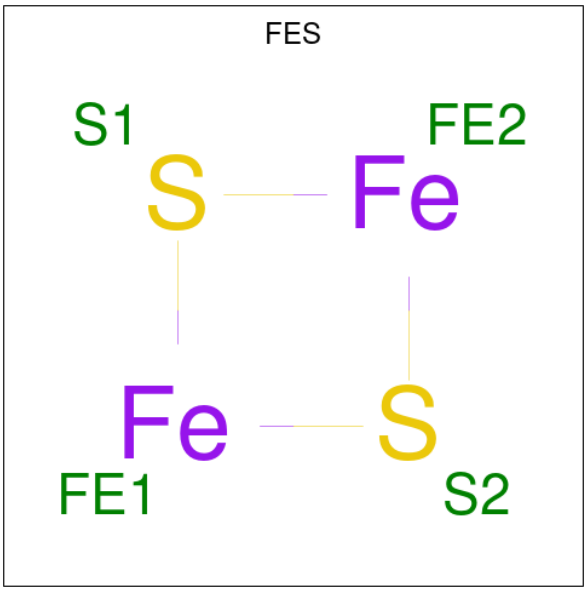
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	29	Total C Mn N O S 80 21 1 20 36 2	0	1
8	B	15	Total C N O S 50 16 12 21 1	0	0
8	C	21	Total C N O S 90 45 6 37 2	0	0
8	D	15	Total C O P 65 32 32 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



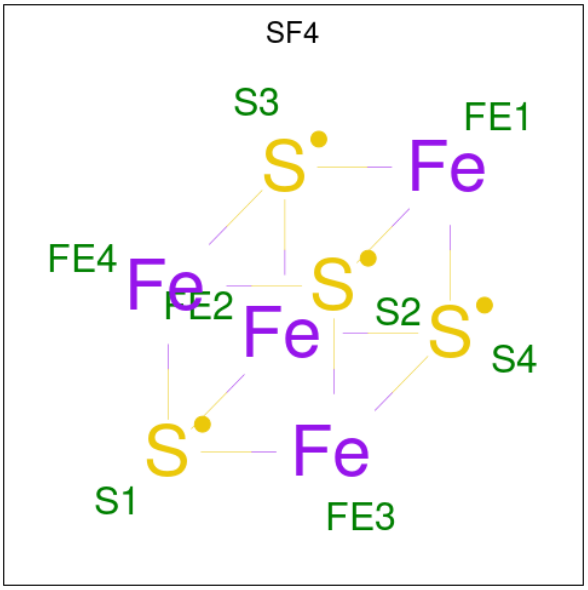
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 5 3 2	0	0

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



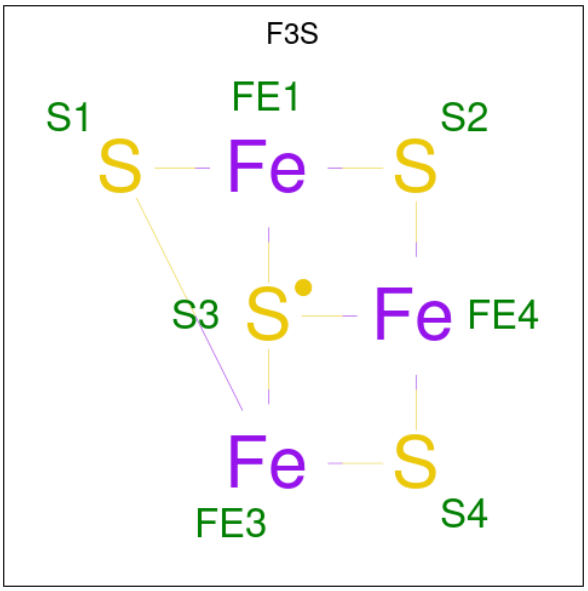
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	B	1	4	2	2	0	0

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



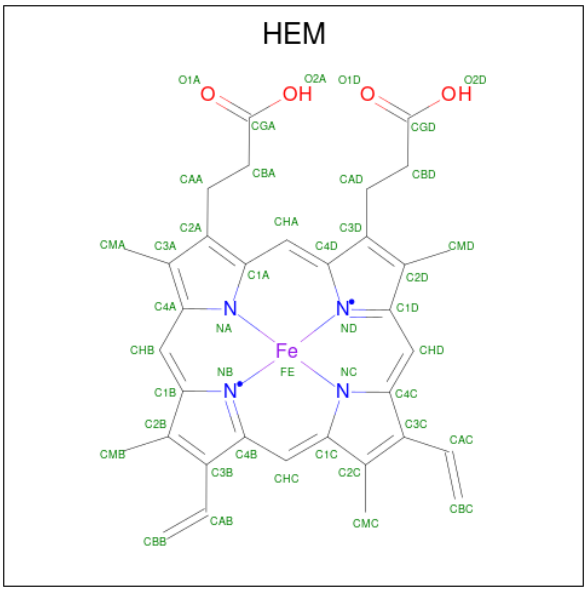
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0

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



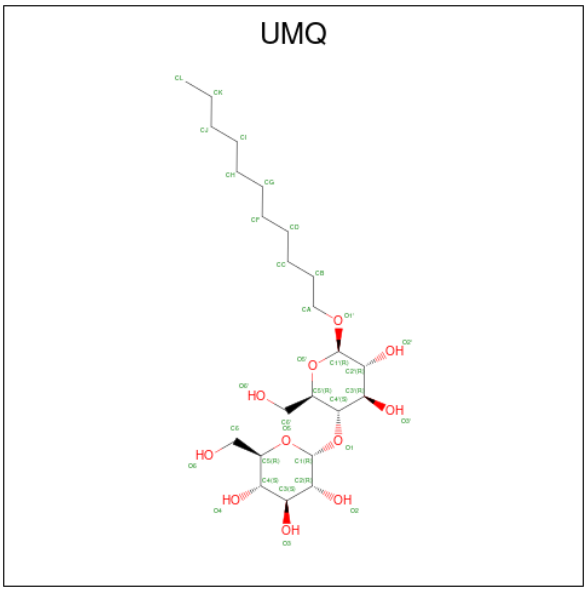
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
12	B	1	7	3	4	0	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



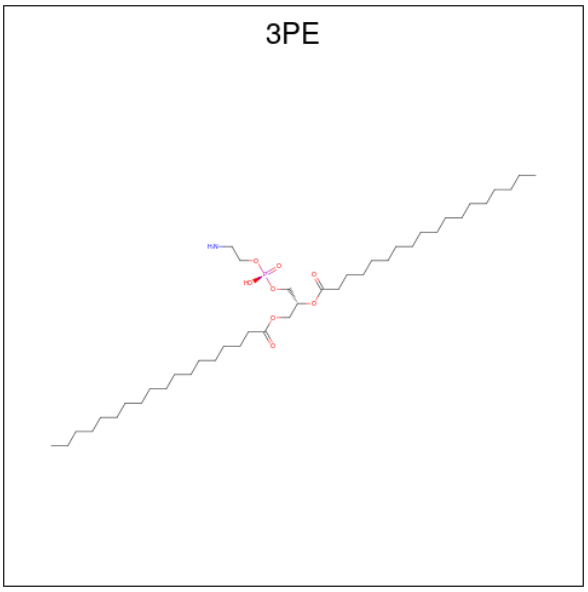
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
13	C	1	41	32	1	4	4	0	0

- Molecule 14 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



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

- Molecule 15 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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

- Molecule 16 is water.

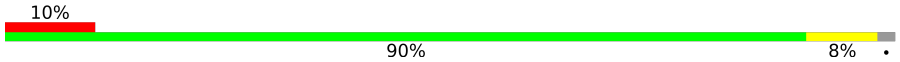
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	A	217	218	218	0	1
			Total	O		
16	B	139	140	140	0	1
			Total	O		
16	C	43	43	43	0	0
			Total	O		
16	D	32	32	32	0	0

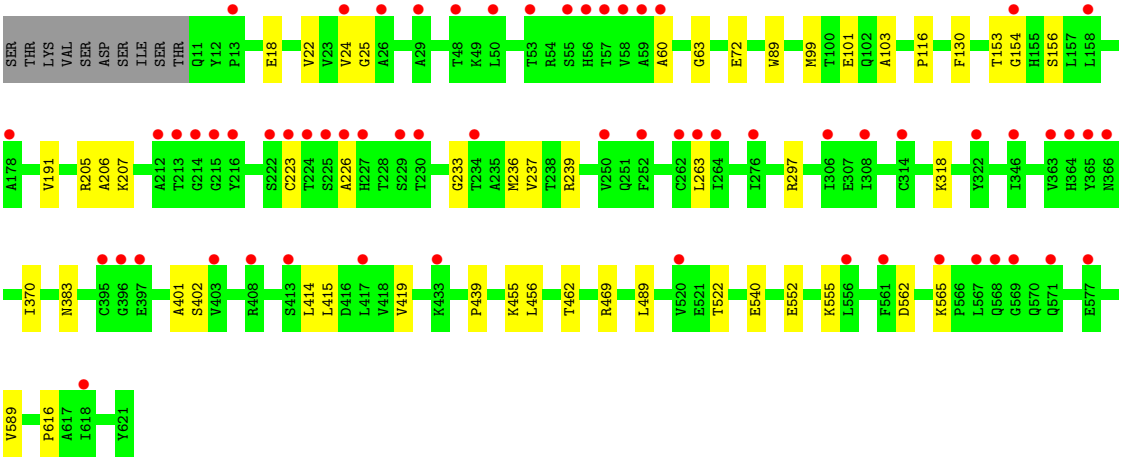
3 Residue-property plots (i)

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

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

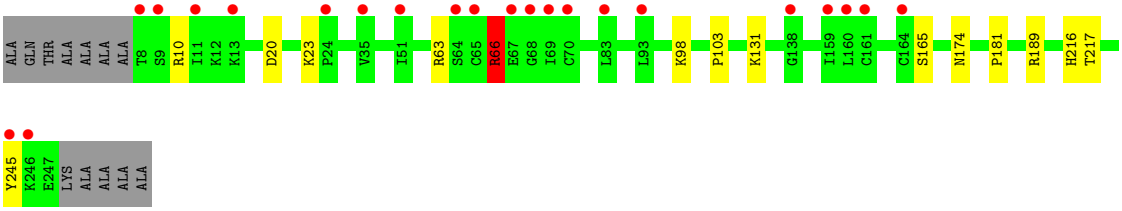
Chain A:





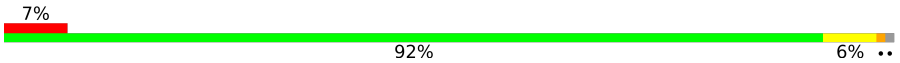
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

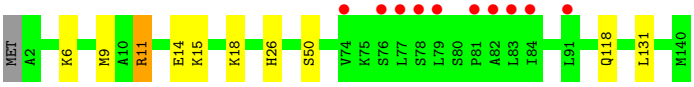
Chain B:



• Molecule 3: Succinate dehydrogenase cytochrome b, large subunit

Chain C:

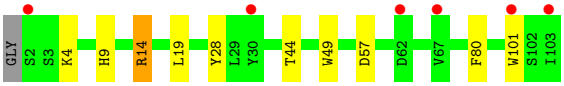




• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:

6%
89%
9%


GLY
S2
S3
K4
H9
R14
L19
Y28
L29
Y30
T44
W49
D57
D62
V67
F80
W101
S102
I103

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.03Å 83.96Å 290.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 1.97 47.78 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.78-1.97) 91.6 (47.78-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.97Å)	Xtriage
Refinement program	PHENIX (DEV_3150: ???)	Depositor
R, R_{free}	0.199 , 0.223 0.199 , 0.223	Depositor DCC
R_{free} test set	2461 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/4824	0.54	0/6531
2	B	0.40	0/1970	0.55	0/2656
3	C	0.36	0/1094	0.50	0/1486
4	D	0.36	0/794	0.48	0/1089
All	All	0.38	0/8682	0.53	0/11762

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	4723	0	4608	39	0
2	B	1928	0	1920	9	0
3	C	1076	0	1116	5	0
4	D	771	0	763	7	0
5	A	53	0	30	7	0
6	A	9	0	2	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	80	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	50	0	0	1	0
8	C	90	0	0	2	0
8	D	65	0	0	1	0
9	A	5	0	5	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	41	0	24	0	0
14	C	34	0	44	1	0
15	D	42	0	61	1	0
16	A	218	0	0	2	0
16	B	140	0	0	4	0
16	C	43	0	0	1	0
16	D	32	0	0	2	0
All	All	9421	0	8573	62	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 (62) 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	1.82	0.91
1:A:297:ARG:HH22	6:A:1002:OAA:H22	1.41	0.83
3:C:118:GLN:OE1	8:C:221:UNL:O	2.08	0.70
1:A:297:ARG:NH2	6:A:1002:OAA:H22	2.08	0.69
2:B:10:ARG:NH2	16:B:1102:HOH:O	2.25	0.69
1:A:18:GLU:OE2	1:A:205:ARG:NH1	2.28	0.67
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.77	0.65
1:A:401:ALA:N	1:A:402:SER:HA	2.12	0.64
4:D:28:TYR:OH	15:D:201:3PE:N	2.33	0.62
8:C:222:UNL:O	8:C:223:UNL:O	2.20	0.60
3:C:6:LYS:HA	3:C:9:MET:HE2	1.84	0.59
1:A:383:ASN:OD1	8:A:1028:UNL:O	2.21	0.58
1:A:297:ARG:HH22	6:A:1002:OAA:C1	2.16	0.58
1:A:237:VAL:HG21	1:A:370:ILE:HG12	1.85	0.57
1:A:239:ARG:HG2	1:A:589:VAL:HG11	1.87	0.57
3:C:11:ARG:NH2	16:C:302:HOH:O	2.38	0.56
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.88	0.56
4:D:14:ARG:NH1	16:D:303:HOH:O	2.40	0.54
1:A:297:ARG:HH22	6:A:1002:OAA:C3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:NE	9:A:1005:PEG:H31	2.24	0.52
9:A:1005:PEG:H32	16:A:1197:HOH:O	2.09	0.52
1:A:60:ALA:HA	5:A:1001:FAD:C5X	2.39	0.52
1:A:462:THR:OG1	8:A:1026:UNL:O	2.25	0.52
1:A:226:ALA:HB2	8:A:1020:UNL:N2	2.25	0.52
1:A:226:ALA:HB2	8:A:1020:UNL:N1	2.25	0.52
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.91	0.51
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.41	0.50
2:B:20:ASP:OD2	2:B:23:LYS:NZ	2.45	0.50
2:B:174:ASN:ND2	16:B:1109:HOH:O	2.44	0.50
1:A:223:CYS:O	2:B:66:ARG:NH2	2.45	0.49
5:A:1001:FAD:C4	6:A:1002:OAA:H21	2.43	0.49
1:A:101:GLU:OE2	16:A:1101:HOH:O	2.20	0.47
1:A:414:LEU:HG	5:A:1001:FAD:C2	2.45	0.47
1:A:207:LYS:HG2	1:A:439:PRO:HD3	1.98	0.46
2:B:103:PRO:HB3	3:C:26:HIS:HA	1.99	0.45
4:D:49:TRP:HE1	8:D:202:UNL:C2	2.29	0.45
1:A:263:LEU:HD22	5:A:1001:FAD:C6	2.46	0.45
1:A:22[A]:VAL:HG23	1:A:206:ALA:HB2	1.99	0.45
1:A:456:LEU:HD13	1:A:522:THR:HG22	1.98	0.45
1:A:552:GLU:O	1:A:555:LYS:NZ	2.50	0.44
2:B:98:LYS:HE2	16:B:1149:HOH:O	2.17	0.44
8:B:1010:UNL:O3	16:B:1101:HOH:O	2.21	0.44
2:B:245:TYR:CE1	4:D:4:LYS:HE3	2.53	0.44
4:D:9:HIS:HE1	16:D:315:HOH:O	2.02	0.43
3:C:14:GLU:O	3:C:18:LYS:HG2	2.19	0.43
1:A:489:LEU:HD13	1:A:540:GLU:HA	2.01	0.43
1:A:89:TRP:CE2	1:A:616:PRO:HA	2.54	0.43
1:A:562:ASP:OD2	1:A:565:LYS:NZ	2.43	0.43
2:B:216:HIS:NE2	4:D:57:ASP:OD2	2.52	0.42
1:A:233:GLY:HA2	1:A:236:MET:CE	2.49	0.42
1:A:233:GLY:HA2	1:A:236:MET:HE3	2.00	0.42
1:A:24:VAL:HG21	1:A:191:VAL:HG11	2.00	0.42
1:A:103:ALA:HB2	1:A:415:LEU:HD21	2.01	0.41
8:A:1010:UNL:O1	8:A:1029:UNL:O	2.37	0.41
1:A:60:ALA:HA	5:A:1001:FAD:N5	2.36	0.41
1:A:99:MET:HA	1:A:419:VAL:HG11	2.02	0.41
1:A:318:LYS:HE3	1:A:318:LYS:HB3	1.90	0.41
14:C:203:UMQ:O3'	14:C:203:UMQ:O2	2.33	0.41
2:B:165:SER:HA	2:B:181:PRO:HD2	2.03	0.41
1:A:63:GLY:HA2	1:A:153:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:HD2	1:A:156:SER:HB3	2.03	0.40
1:A:455:LYS:HE2	1:A:455:LYS:HB3	1.92	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	610/621 (98%)	587 (96%)	23 (4%)	0	100	100
2	B	238/252 (94%)	230 (97%)	7 (3%)	1 (0%)	34	22
3	C	136/140 (97%)	135 (99%)	1 (1%)	0	100	100
4	D	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
All	All	1084/1116 (97%)	1051 (97%)	32 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG

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	496/506 (98%)	494 (100%)	2 (0%)	91	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	216/219 (99%)	211 (98%)	5 (2%)	50	44
3	C	116/117 (99%)	113 (97%)	3 (3%)	46	37
4	D	78/79 (99%)	75 (96%)	3 (4%)	33	21
All	All	906/921 (98%)	893 (99%)	13 (1%)	67	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	130	PHE
2	B	63	ARG
2	B	66	ARG
2	B	131	LYS
2	B	189	ARG
2	B	217	THR
3	C	11	ARG
3	C	50	SER
3	C	131	LEU
4	D	14	ARG
4	D	19	LEU
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 (i)

There are no RNA molecules in this entry.

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

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	0.64	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	-	3/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	15	MLZ	CM-NZ-CE	2.93	120.42	111.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 2 are monoatomic and 81 are unknown - leaving 9 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	$\#\|Z\| > 2$
13	HEM	C	201	3,4	40,48,50	1.41	5 (12%)	46,80,82	1.55	7 (15%)
5	FAD	A	1001	1	53,58,58	0.83	2 (3%)	68,89,89	1.29	8 (11%)
10	FES	B	1001	2	0,4,4	-	-	-		
14	UMQ	C	203	-	35,35,35	0.49	0	46,46,46	0.75	1 (2%)
15	3PE	D	201	-	41,41,50	1.07	2 (4%)	44,46,55	1.08	3 (6%)
12	F3S	B	1003	2	0,9,9	-	-	-		
11	SF4	B	1002	2	0,12,12	-	-	-		
9	PEG	A	1005	-	4,4,6	0.47	0	3,3,5	0.24	0
6	OAA	A	1002	-	8,8,8	2.74	2 (25%)	9,10,10	1.69	2 (22%)

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
13	HEM	C	201	3,4	-	1/10/50/54	-
5	FAD	A	1001	1	-	5/30/50/50	0/6/6/6
14	UMQ	C	203	-	-	10/20/60/60	0/2/2/2
10	FES	B	1001	2	-	-	0/1/1/1
15	3PE	D	201	-	-	14/45/45/54	-
12	F3S	B	1003	2	-	-	0/3/3/3
11	SF4	B	1002	2	-	-	0/6/5/5
9	PEG	A	1005	-	-	0/2/2/4	-
6	OAA	A	1002	-	-	3/8/8/8	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	OAA	O3-C3	5.90	1.35	1.23
15	D	201	3PE	O21-C21	4.43	1.46	1.34
15	D	201	3PE	O31-C31	4.42	1.46	1.33
6	A	1002	OAA	C2-C3	-3.47	1.37	1.51
13	C	201	HEM	FE-NB	2.65	2.10	1.96
13	C	201	HEM	FE-ND	2.53	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	201	HEM	C2C-C3C	-2.25	1.34	1.41
13	C	201	HEM	CMB-C2B	2.14	1.55	1.50
5	A	1001	FAD	C4-N3	-2.11	1.34	1.38
13	C	201	HEM	CAB-C3B	2.08	1.55	1.50
5	A	1001	FAD	C9A-N10	-2.04	1.37	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	201	HEM	C4B-CHC-C1C	3.97	127.79	122.56
5	A	1001	FAD	C4-N3-C2	-3.78	118.65	125.64
15	D	201	3PE	O21-C21-C22	3.66	119.38	111.50
13	C	201	HEM	C4D-ND-C1D	3.42	108.61	105.07
5	A	1001	FAD	C4X-C4-N3	3.33	121.64	113.19
6	A	1002	OAA	O3-C3-C2	3.26	125.29	120.58
15	D	201	3PE	O31-C31-C32	2.95	121.17	111.91
5	A	1001	FAD	O4-C4-C4X	-2.84	119.07	126.60
13	C	201	HEM	C4C-CHD-C1D	2.81	126.27	122.56
13	C	201	HEM	C1B-NB-C4B	2.71	107.87	105.07
5	A	1001	FAD	C4-C4X-N5	2.63	121.97	118.23
5	A	1001	FAD	O2-C2-N1	-2.63	117.48	121.83
5	A	1001	FAD	O5B-C5B-C4B	-2.34	100.93	108.99
14	C	203	UMQ	O5-C5-C6	2.32	112.21	106.44
13	C	201	HEM	CMA-C3A-C4A	-2.29	124.94	128.46
13	C	201	HEM	CAD-C3D-C4D	2.24	128.58	124.66
6	A	1002	OAA	C2-C3-C4	-2.23	114.09	117.85
5	A	1001	FAD	C10-N1-C2	2.23	121.35	116.90
13	C	201	HEM	CBA-CAA-C2A	-2.18	108.90	112.62
5	A	1001	FAD	C4X-C10-N10	2.15	119.63	116.48
15	D	201	3PE	O31-C31-O32	-2.07	118.38	123.59

There are no chirality outliers.

All (33) 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'
6	A	1002	OAA	C2-C3-C4-O4
6	A	1002	OAA	C2-C3-C4-O5
15	D	201	3PE	C1-O11-P-O14
15	D	201	3PE	C22-C21-O21-C2
15	D	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
15	D	201	3PE	C1-O11-P-O13
14	C	203	UMQ	O1'-CA-CB-CC
15	D	201	3PE	C32-C33-C34-C35
14	C	203	UMQ	C4-C5-C6-O6
14	C	203	UMQ	CC-CD-CF-CG
15	D	201	3PE	C21-C22-C23-C24
14	C	203	UMQ	CF-CG-CH-CI
14	C	203	UMQ	C2-C1-O1-C4'
14	C	203	UMQ	O5-C1-O1-C4'
15	D	201	3PE	C32-C31-O31-C3
14	C	203	UMQ	O5-C5-C6-O6
5	A	1001	FAD	PA-O3P-P-O5'
14	C	203	UMQ	CA-CB-CC-CD
15	D	201	3PE	O32-C31-O31-C3
13	C	201	HEM	C2A-CAA-CBA-CGA
15	D	201	3PE	O13-C11-C12-N
6	A	1002	OAA	O3-C3-C4-O4
15	D	201	3PE	C24-C25-C26-C27
14	C	203	UMQ	CG-CH-CI-CJ
14	C	203	UMQ	CH-CI-CJ-CK
15	D	201	3PE	O31-C31-C32-C33
5	A	1001	FAD	P-O3P-PA-O2A
15	D	201	3PE	O32-C31-C32-C33
15	D	201	3PE	C1-O11-P-O12
5	A	1001	FAD	O4B-C4B-C5B-O5B
15	D	201	3PE	C27-C28-C29-C2A

There are no ring outliers.

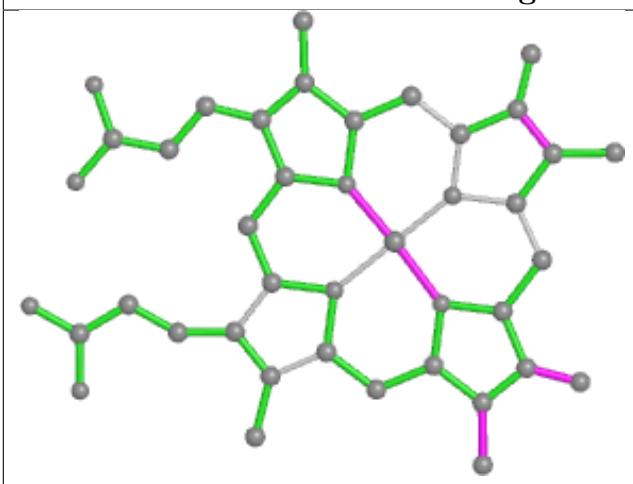
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	FAD	7	0
14	C	203	UMQ	1	0
15	D	201	3PE	1	0
9	A	1005	PEG	2	0
6	A	1002	OAA	6	0

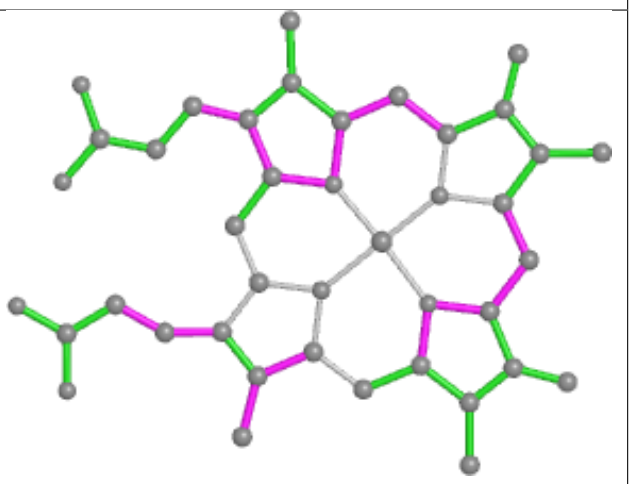
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

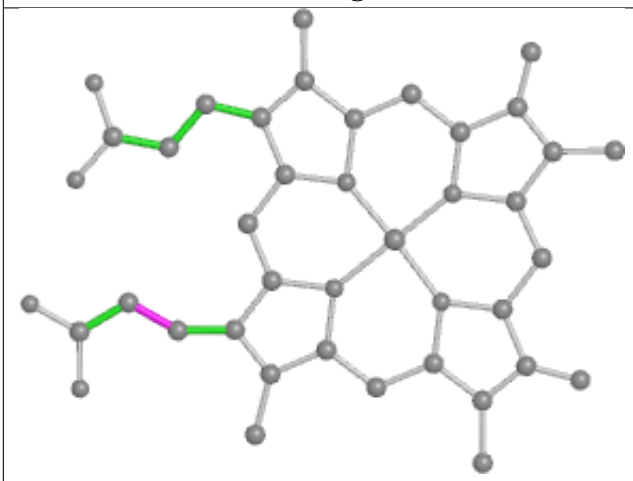
Ligand HEM C 201



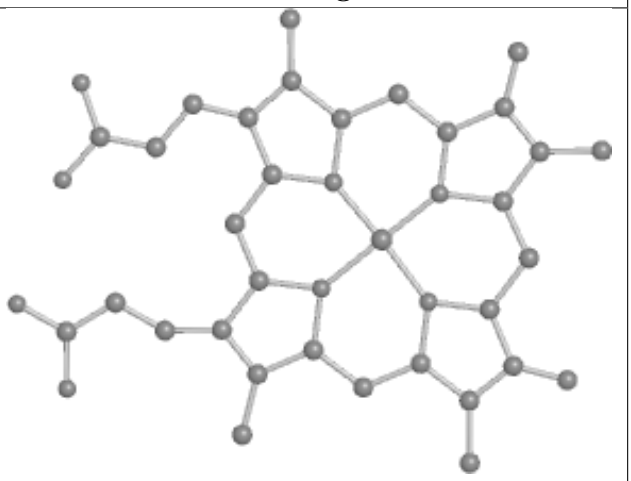
Bond lengths



Bond angles

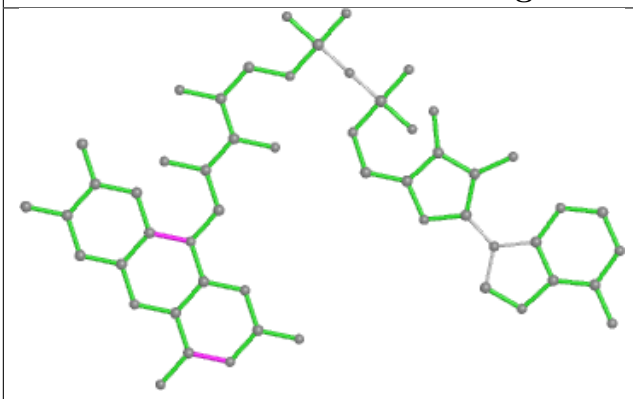


Torsions



Rings

Ligand FAD A 1001



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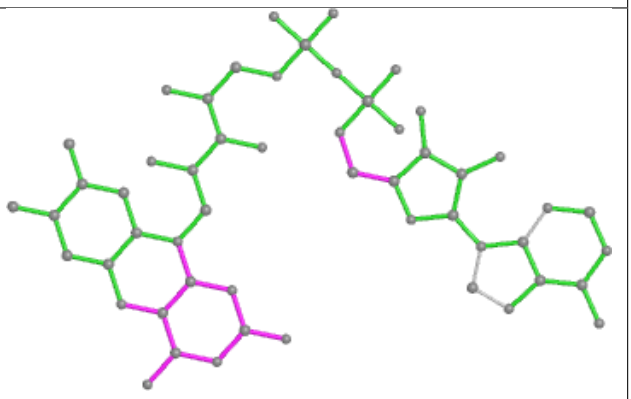

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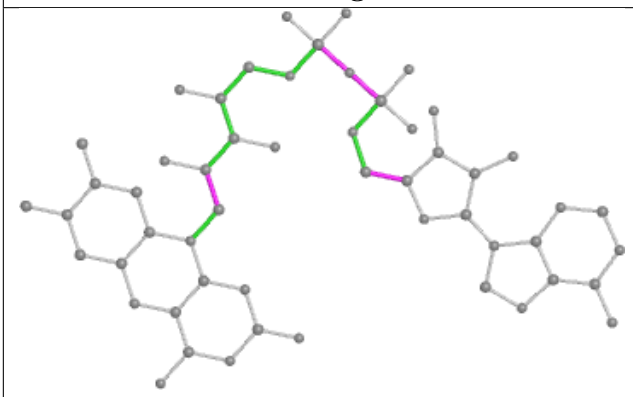
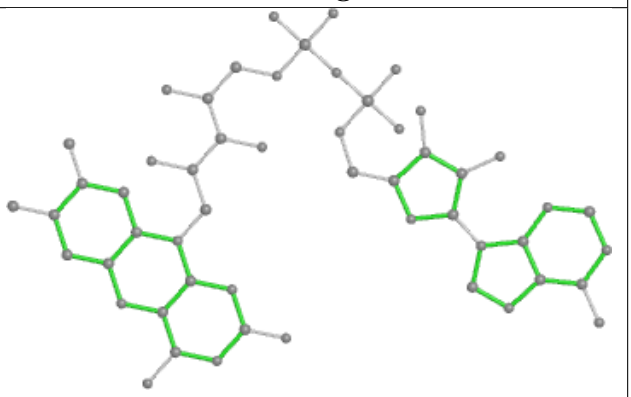
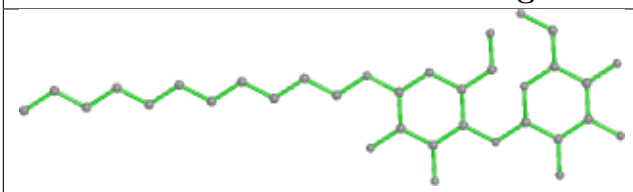


Torsions

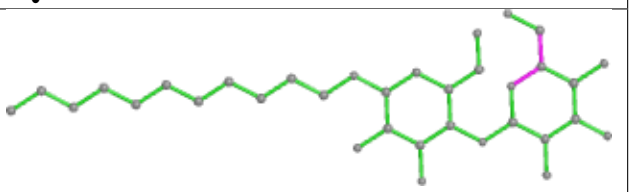


Rings

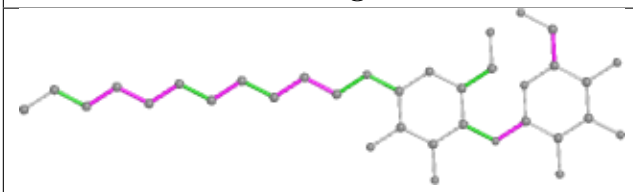
Ligand UMQ C 203



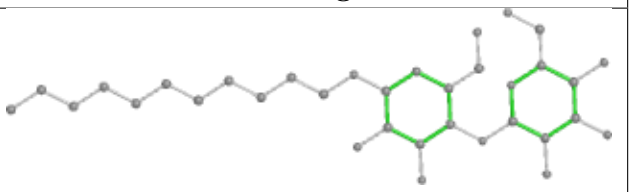
Bond lengths



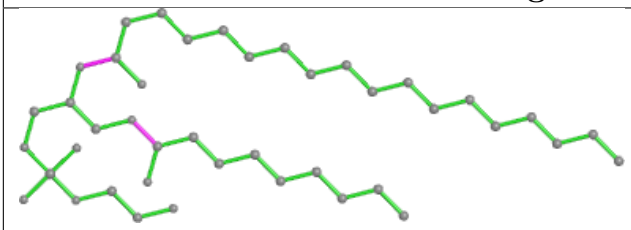
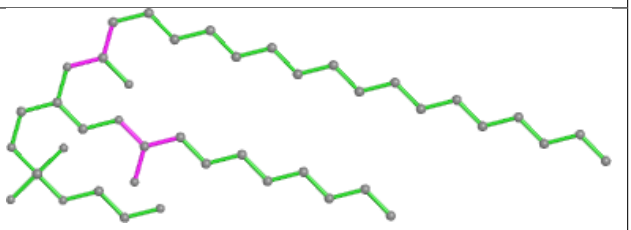
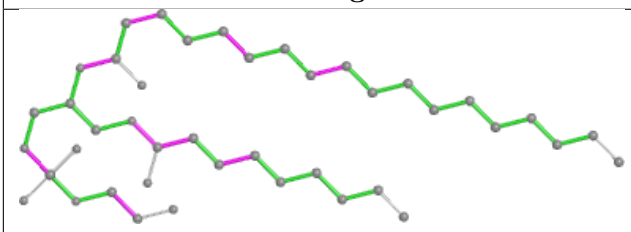
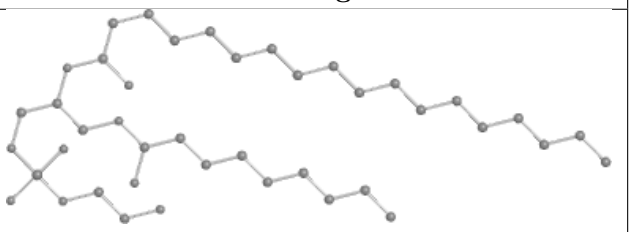
Bond angles



Torsions



Rings

Ligand 3PE D 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (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	611/621 (98%)	0.65	63 (10%) 6 7	31, 49, 74, 93	0
2	B	240/252 (95%)	0.62	22 (9%) 9 10	29, 40, 70, 101	0
3	C	138/140 (98%)	0.40	10 (7%) 15 17	34, 46, 74, 80	0
4	D	102/103 (99%)	0.31	6 (5%) 22 24	35, 46, 65, 77	0
All	All	1091/1116 (97%)	0.58	101 (9%) 8 10	29, 47, 73, 101	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	THR	6.1
3	C	74	VAL	5.3
1	A	59	ALA	4.8
1	A	226	ALA	4.7
2	B	70	CYS	4.7
4	D	30	TYR	4.6
1	A	57	THR	4.5
2	B	9	SER	4.2
1	A	263	LEU	4.2
1	A	365	TYR	4.1
1	A	618	ILE	4.0
2	B	69	ILE	4.0
1	A	53	THR	3.8
1	A	58	VAL	3.8
1	A	56	HIS	3.8
2	B	11	ILE	3.8
1	A	224	THR	3.7
1	A	363	VAL	3.7
2	B	65	CYS	3.7
3	C	84	ILE	3.7
2	B	245	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	79	LEU	3.5
1	A	215	GLY	3.4
3	C	78	SER	3.3
1	A	568	GLN	3.3
1	A	308	ILE	3.3
1	A	556	LEU	3.3
1	A	60	ALA	3.3
4	D	103	ILE	3.2
1	A	262	CYS	3.1
1	A	50	LEU	3.1
1	A	567	LEU	3.1
1	A	561	PHE	3.1
2	B	83	LEU	3.0
1	A	13	PRO	3.0
2	B	159	ILE	3.0
1	A	322	TYR	3.0
1	A	417	LEU	3.0
1	A	213	THR	2.9
1	A	230	THR	2.9
1	A	229	SER	2.8
2	B	35	VAL	2.8
2	B	93	LEU	2.8
1	A	223	CYS	2.8
1	A	252	PHE	2.7
1	A	396	GLY	2.7
1	A	569	GLY	2.7
1	A	154	GLY	2.7
1	A	276	ILE	2.7
3	C	82	ALA	2.7
1	A	225	SER	2.7
1	A	565	LYS	2.7
1	A	216	TYR	2.7
1	A	571	GLN	2.6
3	C	83	LEU	2.6
1	A	48	THR	2.6
2	B	13	LYS	2.6
2	B	24	PRO	2.6
1	A	24	VAL	2.6
4	D	2	SER	2.5
1	A	234	THR	2.5
2	B	51	ILE	2.5
1	A	395	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	ALA	2.5
2	B	68	GLY	2.4
1	A	55	SER	2.4
3	C	81	PRO	2.4
1	A	364	HIS	2.4
1	A	433	LYS	2.4
1	A	222	SER	2.3
1	A	158	LEU	2.3
1	A	264	ILE	2.3
3	C	76	SER	2.3
2	B	138	GLY	2.3
1	A	250	VAL	2.3
4	D	101	TRP	2.3
2	B	67	GLU	2.2
1	A	413	SER	2.2
2	B	64	SER	2.2
3	C	77	LEU	2.2
1	A	403	VAL	2.2
4	D	62	ASP	2.2
1	A	314	CYS	2.2
3	C	91	LEU	2.2
1	A	178	ALA	2.2
1	A	520	VAL	2.2
2	B	160	LEU	2.1
1	A	397	GLU	2.1
1	A	306	ILE	2.1
1	A	29	ALA	2.1
1	A	212	ALA	2.1
2	B	246	LYS	2.1
1	A	366	ASN	2.1
1	A	214	GLY	2.1
2	B	164	CYS	2.1
1	A	408	ARG	2.0
1	A	577	GLU	2.0
1	A	227	HIS	2.0
4	D	67	VAL	2.0
1	A	346	ILE	2.0
2	B	161	CYS	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	0.11	51,55,60,60	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	UNL	A	1011	4/-	0.31	0.46	88,89,90,91	0
8	UNL	A	1012	2/-	0.32	0.53	77,77,77,78	0
8	UNL	A	1025	1/-	0.45	0.19	80,80,80,80	0
8	UNL	D	207	12/-	0.58	0.40	70,87,90,91	0
8	UNL	D	206	5/-	0.60	0.38	78,79,81,82	0
8	UNL	C	214	1/-	0.60	0.32	66,66,66,66	0
8	UNL	C	210	15/-	0.62	0.36	89,95,111,112	0
8	UNL	B	1012	2/-	0.64	0.23	82,82,82,83	0
8	UNL	D	205	1/-	0.64	0.23	55,55,55,55	0
8	UNL	B	1009	3/-	0.65	0.45	62,62,63,63	3
8	UNL	C	208	3/-	0.66	0.23	53,53,58,61	0
8	UNL	B	1014	13/-	0.67	0.27	78,84,86,86	0
8	UNL	A	1031[B]	1/-	0.71	0.48	46,46,46,46	1
8	UNL	A	1031[A]	1/-	0.71	0.48	46,46,46,46	1
9	PEG	A	1005	5/7	0.71	0.40	85,86,88,88	0
8	UNL	D	208	12/-	0.72	0.24	79,83,85,85	0
8	UNL	A	1020	3/-	0.72	0.39	39,39,40,46	0
8	UNL	C	219	1/-	0.73	0.38	52,52,52,52	0
8	UNL	A	1004	6/-	0.73	0.25	71,72,78,89	4
8	UNL	C	207	5/-	0.75	0.21	60,63,68,68	0
8	UNL	C	212	7/-	0.75	0.15	99,100,100,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UNL	B	1018	1/-	0.75	0.30	51,51,51,51	0
8	UNL	D	211	1/-	0.76	0.32	69,69,69,69	0
8	UNL	A	1026	1/-	0.78	0.41	71,71,71,71	0
8	UNL	D	213	1/-	0.78	0.17	49,49,49,49	0
8	UNL	C	205	15/-	0.78	0.85	50,65,67,67	15
15	3PE	D	201	42/51	0.79	0.36	75,84,116,117	0
8	UNL	C	223	1/-	0.80	0.16	58,58,58,58	0
8	UNL	A	1010	4/-	0.80	0.12	71,71,72,74	0
8	UNL	C	220	1/-	0.80	0.49	67,67,67,67	0
8	UNL	A	1014	6/-	0.81	0.53	89,93,95,95	0
8	UNL	A	1013	3/-	0.81	0.36	38,38,39,41	3
8	UNL	A	1032	1/-	0.81	0.32	58,58,58,58	0
8	UNL	B	1011	4/-	0.82	0.22	81,83,84,84	0
8	UNL	A	1030	1/-	0.82	0.42	48,48,48,48	0
8	UNL	C	222	1/-	0.82	0.11	55,55,55,55	0
8	UNL	C	211	4/-	0.84	0.41	80,82,83,85	0
8	UNL	D	202	9/-	0.84	0.12	71,75,79,81	0
8	UNL	A	1017	2/-	0.84	0.58	84,84,84,84	0
8	UNL	D	209	10/-	0.84	0.20	57,68,77,78	0
8	UNL	A	1024	2/-	0.85	0.34	66,66,66,67	0
8	UNL	B	1006	3/-	0.85	0.27	60,60,61,62	0
8	UNL	B	1016	1/-	0.85	0.46	55,55,55,55	0
8	UNL	A	1007	4/-	0.85	0.20	70,70,71,73	0
8	UNL	A	1022	3/-	0.85	0.34	64,64,65,65	0
8	UNL	B	1008	3/-	0.86	0.21	51,51,53,53	0
8	UNL	A	1028	1/-	0.86	0.14	63,63,63,63	0
8	UNL	A	1008	4/-	0.86	0.37	83,83,84,86	0
8	UNL	D	215	1/-	0.86	0.28	63,63,63,63	0
8	UNL	A	1015	3/-	0.86	0.19	81,81,82,82	0
8	UNL	C	206	12/-	0.86	0.19	73,75,78,79	0
8	UNL	C	218	1/-	0.87	0.13	51,51,51,51	0
8	UNL	A	1016	2/-	0.87	0.18	73,73,73,73	0
8	UNL	D	216	1/-	0.87	0.13	56,56,56,56	0
8	UNL	B	1019	1/-	0.87	0.19	57,57,57,57	0
8	UNL	D	212	1/-	0.87	0.10	68,68,68,68	0
8	UNL	C	202	8/-	0.88	0.13	43,47,51,55	0
8	UNL	A	1009	4/-	0.88	0.12	70,70,71,72	0
8	UNL	B	1017	1/-	0.88	0.17	54,54,54,54	0
8	UNL	A	1021	3/-	0.89	0.20	39,39,48,52	0
8	UNL	B	1013	4/-	0.89	0.43	52,52,52,53	4
8	UNL	C	204	3/-	0.89	0.16	47,47,53,56	0
8	UNL	C	215	1/-	0.89	0.18	51,51,51,51	0

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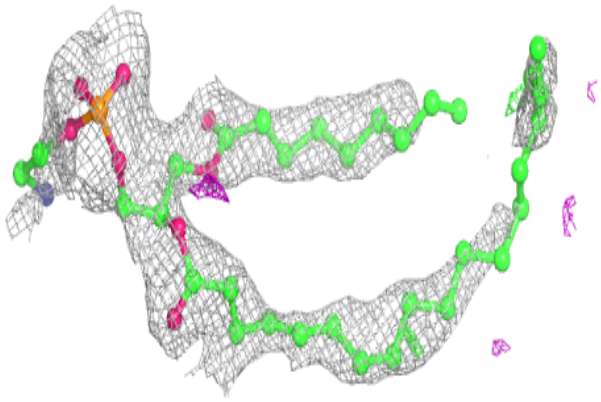
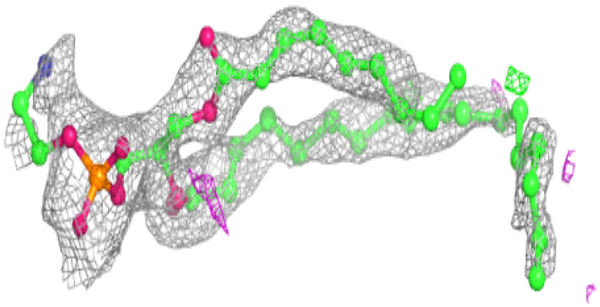
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UNL	B	1005	4/-	0.89	0.13	50,53,57,61	0
8	UNL	D	203	3/-	0.89	0.14	57,57,57,58	0
8	UNL	B	1007	3/-	0.90	0.10	70,70,71,71	0
8	UNL	B	1015	1/-	0.91	0.58	57,57,57,57	0
8	UNL	A	1023	3/-	0.91	0.09	59,59,60,61	0
8	UNL	D	214	1/-	0.91	0.22	44,44,44,44	0
8	UNL	A	1029	1/-	0.91	0.12	61,61,61,61	0
8	UNL	C	209	4/-	0.91	0.19	74,76,77,78	0
8	UNL	C	216	1/-	0.91	0.21	40,40,40,40	0
8	UNL	A	1027	1/-	0.91	0.18	46,46,46,46	0
8	UNL	C	217	1/-	0.92	0.19	37,37,37,37	0
8	UNL	A	1033	1/-	0.92	0.26	49,49,49,49	0
8	UNL	B	1010	6/-	0.92	0.31	45,46,48,48	6
8	UNL	C	221	1/-	0.93	0.09	52,52,52,52	0
8	UNL	C	213	4/-	0.93	0.19	63,64,64,65	0
11	SF4	B	1002	8/8	0.93	0.14	27,33,34,34	0
6	OAA	A	1002	9/9	0.93	0.25	36,42,45,46	0
14	UMQ	C	203	34/34	0.94	0.15	37,61,69,73	0
8	UNL	A	1019	3/-	0.95	0.24	61,61,61,61	0
8	UNL	A	1018	2/-	0.95	0.48	70,70,70,70	0
8	UNL	D	204	5/-	0.95	0.26	61,62,63,64	5
8	UNL	A	1006	7/-	0.96	0.17	37,44,45,47	7
8	UNL	D	210	2/-	0.96	0.14	59,59,59,59	0
12	F3S	B	1003	7/7	0.96	0.16	31,33,35,36	0
7	K	A	1003	1/1	0.96	0.10	41,41,41,41	0
5	FAD	A	1001	53/53	0.96	0.27	31,35,39,42	0
10	FES	B	1001	4/4	0.97	0.15	33,34,34,35	0
13	HEM	C	201	41/43	0.97	0.10	36,40,51,54	0
7	K	B	1004	1/1	0.98	0.16	62,62,62,62	0

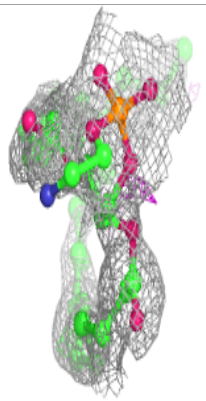
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

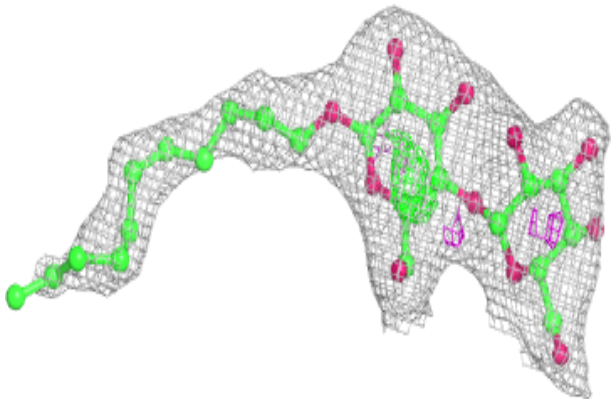


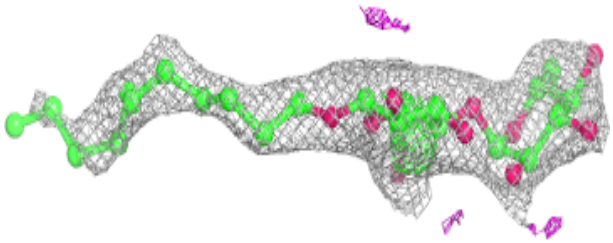


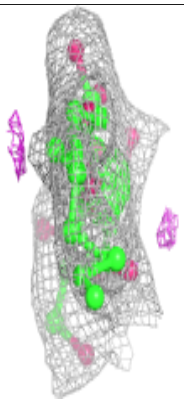


Electron density around UMQ C 203:

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

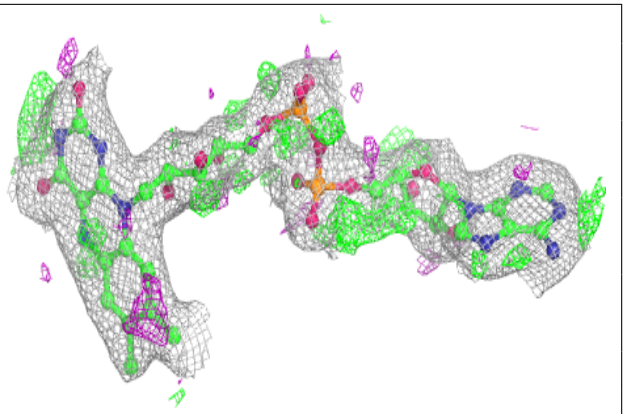


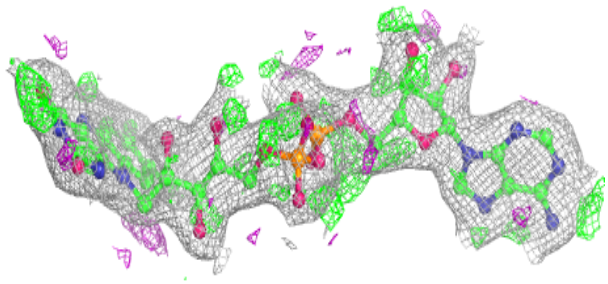


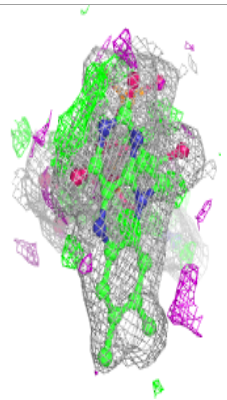


Electron density around FAD A 1001:

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

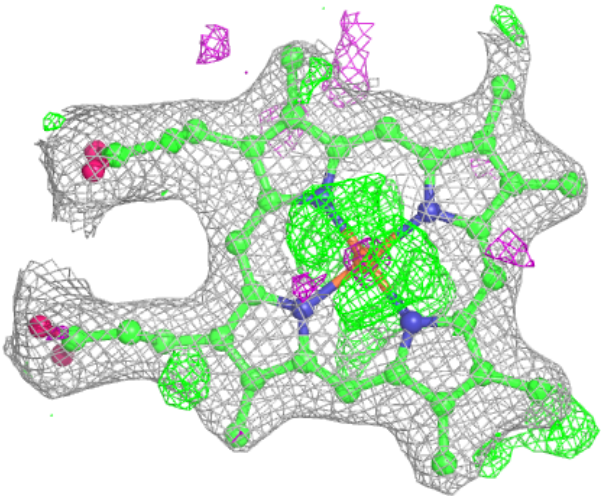


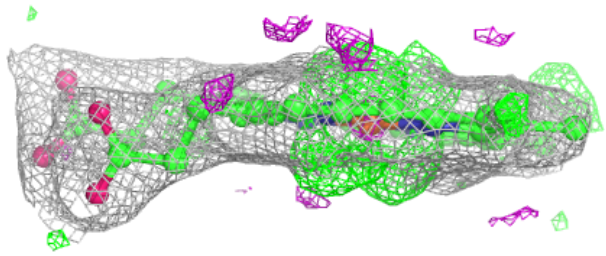


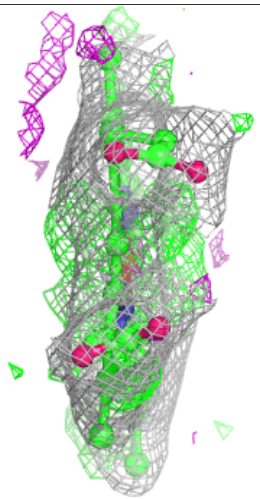


Electron density around HEM C 201:

2mF$_o$-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.