Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:59 PM EDT

PDB ID	:	6MYS
Title	:	Avian mitochondrial complex II with Atpenin A5 bound, sidechain outside
Authors	:	Berry, E.A.; Huang, L.-S.
Deposited on	:	2018-11-02
Resolution	:	2.37 Å(reported)

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

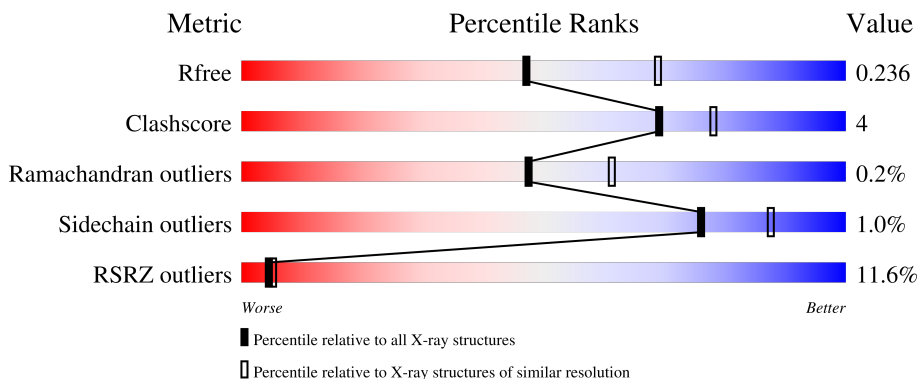|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.37 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.0%
RSRZ outliers		11.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	14% — 87% — 11% •
2	B	252	9% — 86% — 9% — 5%
3	C	140	9% — 92% — 7% •
4	D	103	4% — 95% — • ••

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
15	3PE	D	201	-	-	-	X
7	OAA	A	1003	-	-	X	-
8	UNL	A	1005	-	-	-	X
8	UNL	B	1006	-	-	-	X
8	UNL	C	208	-	-	-	X
8	UNL	C	209	-	-	-	X
8	UNL	D	207	-	-	-	X

2 Entry composition ⓘ

There are 16 unique types of molecules in this entry. The entry contains 9014 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 4737	C 2963	N 848	O 897	S 29	0	2	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total 1076	C 707	N 178	O 186	S 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
4	D	102	Total 771	C 508	N 122	O 138	S 3	0	0	0

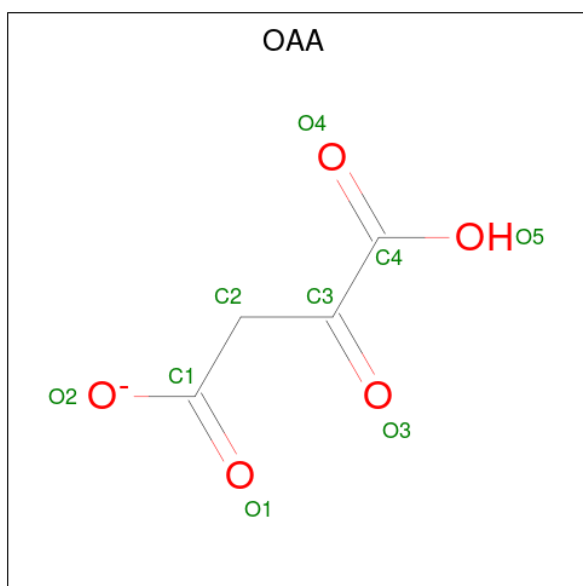- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).

OAA

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	14	Total 48	C 19	N 7	O 19	S 3	0	0
8	B	6	Total 27	C 12	N 5	O 8	S 2	0	0
8	C	6	Total 23	C 13	O 9	S 1		0	0
8	D	14	Total 65	C 37	O 28			0	0

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

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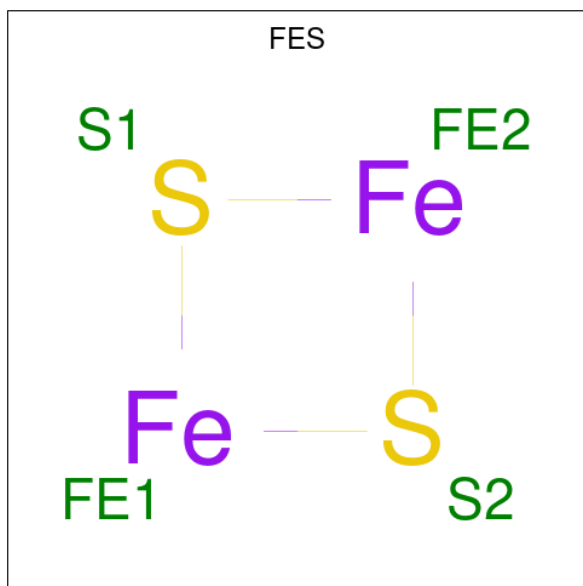
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 4	Fe 2	S 2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

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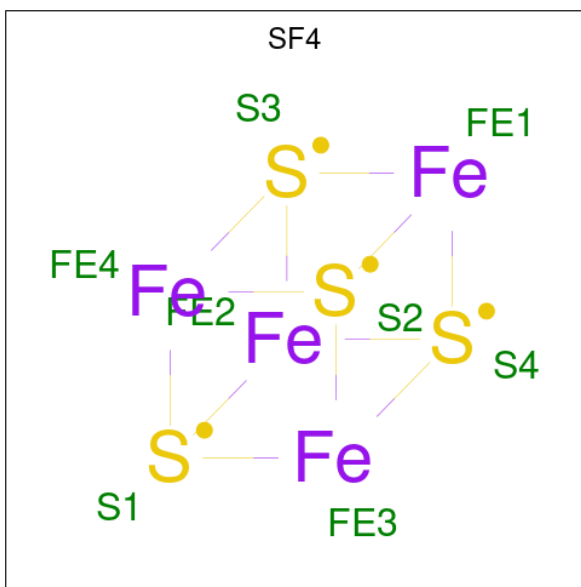
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

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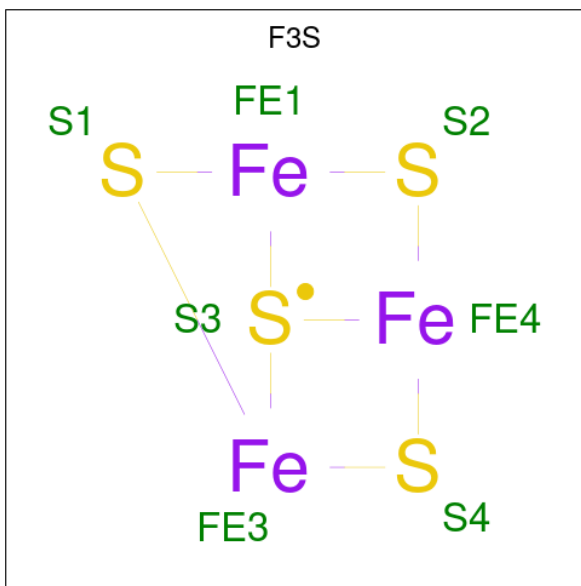
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total 7	Fe 3	S 4	0	0

- Molecule 12 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHEXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (three-letter code: AT5) (formula: $C_{15}H_{21}Cl_2NO_5$).

AT5
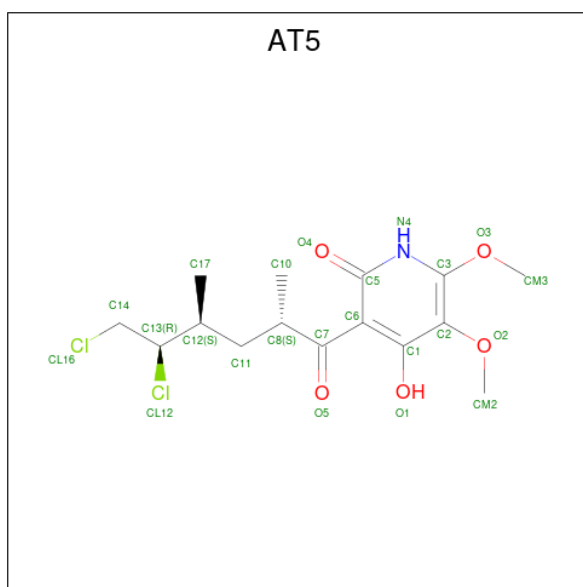
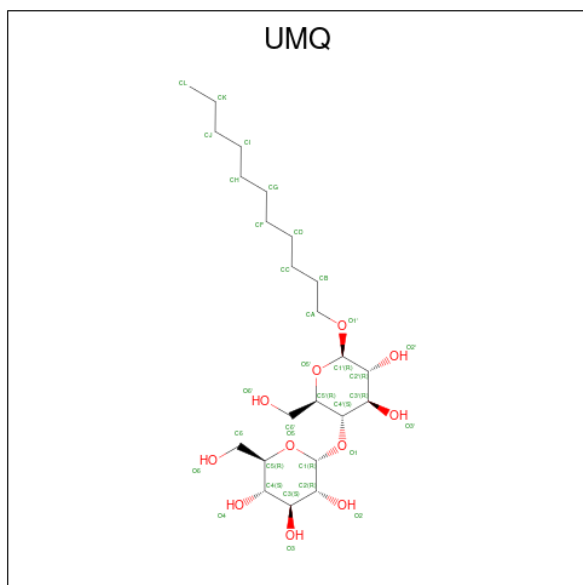| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Cl	N	O	0	0
			23	15	2	1	5		

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

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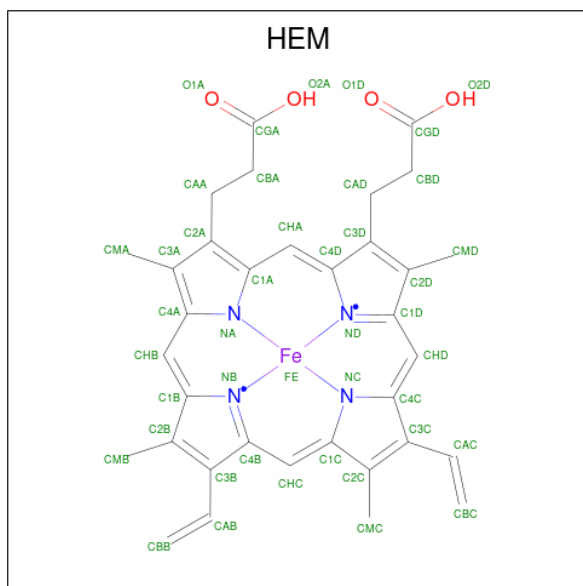
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

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

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

- Molecule 15 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).
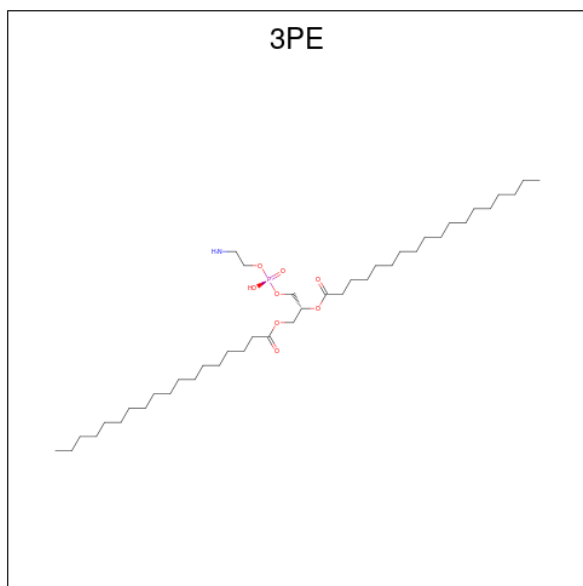
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total 36	C 26	N 1	O 8	P 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	45	Total 45	O 45	0	0
16	B	52	Total 52	O 52	0	0
16	C	17	Total 17	O 17	0	0
16	D	9	Total 9	O 9	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.
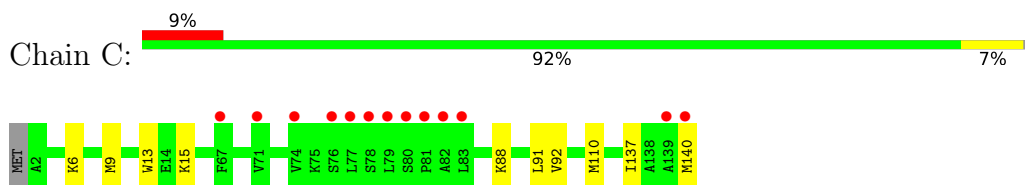
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
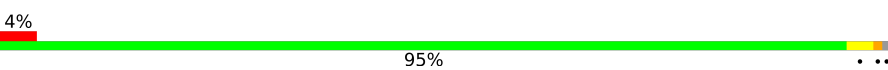
Chain A:
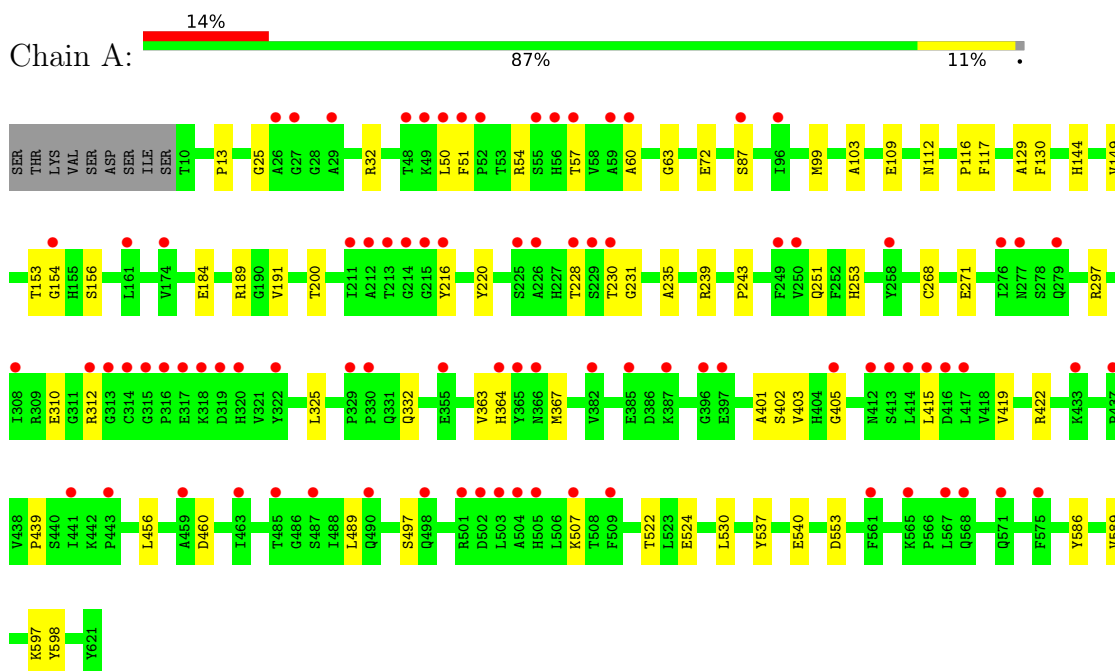
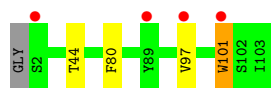- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial
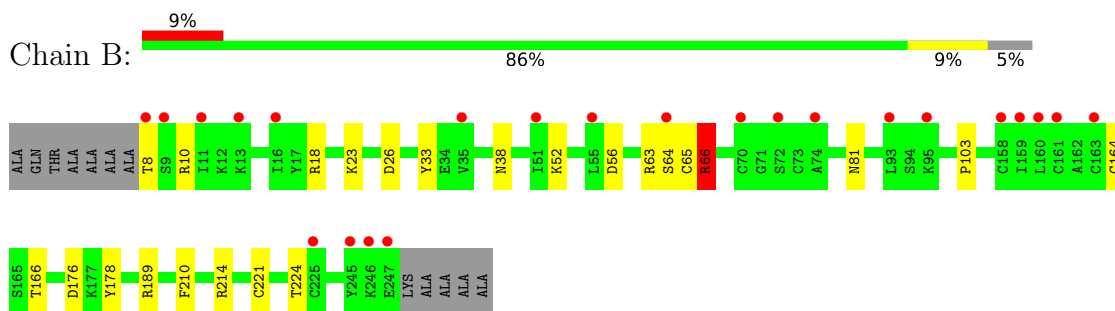
Chain B:

- Molecule 3: Succinate dehydrogenase cytochrome b, large subunit

Chain C:

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

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.68Å 84.42Å 293.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.75 – 2.37 38.75 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.75-2.37) 90.4 (38.75-2.37)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.37Å)	Xtriage
Refinement program	PHENIX (DEV_3150: ???)	Depositor
R, R_{free}	0.211 , 0.237 0.212 , 0.236	Depositor DCC
R_{free} test set	2144 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.9	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
UMQ, MLZ, HEM, AT5, FAD, SF4, FES, 3PE, UNL, K, F3S, OAA

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	0.24	0/4838	0.43	0/6549
2	B	0.24	0/1970	0.41	0/2656
3	C	0.24	0/1094	0.38	0/1486
4	D	0.23	0/794	0.35	0/1089
All	All	0.24	0/8696	0.41	0/11780

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	4737	0	4619	44	0
2	B	1928	0	1921	12	0
3	C	1076	0	1116	5	0
4	D	771	0	763	3	0
5	A	53	0	30	4	0
6	A	1	0	0	0	0
7	A	9	0	2	6	0
8	A	48	0	0	1	0
8	B	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	23	0	0	0	0
8	D	65	0	0	0	0
9	B	4	0	0	0	0
10	B	8	0	0	0	0
11	B	7	0	0	0	0
12	C	23	0	20	1	0
13	C	41	0	24	0	0
14	C	34	0	44	0	0
15	D	36	0	46	2	0
16	A	45	0	0	0	0
16	B	52	0	0	1	0
16	C	17	0	0	0	0
16	D	9	0	0	0	0
All	All	9014	0	8585	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	7:A:1003:OAA:C2	1.69	1.05
1:A:297:ARG:HH22	7:A:1003:OAA:H22	1.27	0.98
1:A:297:ARG:NH2	7:A:1003:OAA:H22	1.89	0.86
1:A:297:ARG:HH22	7:A:1003:OAA:C1	1.97	0.76
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.70	0.73
1:A:401:ALA:N	1:A:402:SER:HA	2.15	0.62
1:A:422[A]:ARG:NH1	8:A:1014:UNL:O	2.32	0.62
3:C:88:LYS:NZ	3:C:140:MET:O	2.35	0.57
3:C:92:VAL:HG21	3:C:137:ILE:HG21	1.86	0.57
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.86	0.57
3:C:6:LYS:HA	3:C:9:MET:HE2	1.85	0.56
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.88	0.56
2:B:10:ARG:NH2	16:B:1104:HOH:O	2.38	0.55
1:A:63:GLY:HA2	1:A:153:THR:HG21	1.87	0.55
2:B:23:LYS:HB2	2:B:26:ASP:HB2	1.90	0.54
2:B:210:PHE:HA	2:B:214:ARG:HG2	1.89	0.54
1:A:253:HIS:NE2	7:A:1003:OAA:O5	2.37	0.54
1:A:13:PRO:HG2	1:A:200:THR:HG22	1.90	0.54
2:B:8:THR:O	2:B:38:ASN:ND2	2.42	0.53
2:B:18:ARG:NH1	2:B:33:TYR:OH	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:OE1	1:A:312:ARG:NH2	2.43	0.52
1:A:401:ALA:HB3	1:A:403:VAL:N	2.26	0.51
4:D:97:VAL:HG21	15:D:201:3PE:H252	1.92	0.50
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.93	0.50
1:A:57:THR:OG1	5:A:1001:FAD:O2A	2.23	0.50
1:A:184:GLU:HB3	1:A:189:ARG:HE	1.77	0.50
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.46	0.50
1:A:189:ARG:HD2	1:A:439:PRO:HB2	1.93	0.50
1:A:401:ALA:HB3	1:A:403:VAL:H	1.75	0.49
1:A:25:GLY:HA2	5:A:1001:FAD:H1B	1.94	0.49
1:A:553:ASP:OD1	1:A:553:ASP:N	2.42	0.49
1:A:239:ARG:HG2	1:A:589:VAL:HG21	1.96	0.47
1:A:235:ALA:HB1	1:A:530:LEU:HD12	1.95	0.47
1:A:297:ARG:NH2	7:A:1003:OAA:C2	2.51	0.47
1:A:87:SER:HB2	1:A:405:GLY:HA3	1.97	0.47
1:A:460:ASP:OD1	1:A:507:LYS:NZ	2.32	0.46
1:A:60:ALA:HA	5:A:1001:FAD:C6	2.46	0.46
1:A:32:ARG:NH2	1:A:109:GLU:OE2	2.45	0.45
1:A:99:MET:HA	1:A:419:VAL:HG11	1.98	0.45
2:B:103:PRO:HD2	2:B:166:THR:HB	1.99	0.45
1:A:497:SER:HG	1:A:537:TYR:HH	1.65	0.44
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.99	0.44
2:B:164:CYS:HB2	2:B:221:CYS:HB2	1.99	0.44
2:B:81:ASN:O	2:B:224:THR:OG1	2.35	0.44
3:C:110:MET:HB2	3:C:110:MET:HE2	1.85	0.44
5:A:1001:FAD:H9	5:A:1001:FAD:H1'1	1.79	0.43
1:A:129:ALA:HB2	1:A:144:HIS:CD2	2.53	0.43
1:A:116:PRO:HD2	1:A:156:SER:HB3	2.01	0.43
1:A:597:LYS:HG2	1:A:598:TYR:H	1.84	0.43
1:A:489:LEU:HD13	1:A:540:GLU:HA	2.01	0.42
12:C:202:AT5:H8	12:C:202:AT5:O1	2.19	0.42
1:A:216:TYR:HB3	1:A:231:GLY:HA3	2.02	0.42
2:B:65:CYS:O	2:B:66:ARG:HG3	2.20	0.42
2:B:176:ASP:HB3	3:C:13:TRP:CZ2	2.56	0.41
1:A:230:THR:HG21	1:A:524:GLU:HB3	2.03	0.41
1:A:271:GLU:HB3	1:A:332:GLN:NE2	2.36	0.41
1:A:103:ALA:HA	1:A:415:LEU:HD11	2.03	0.41
4:D:101:TRP:CH2	15:D:201:3PE:H352	2.56	0.41
1:A:51:PHE:HB3	1:A:54:ARG:HG2	2.02	0.41
1:A:456:LEU:HD13	1:A:522:THR:HG22	2.02	0.41
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:HIS:HB2	1:A:364:HIS:HB2	2.02	0.40
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.56	0.40
1:A:251:GLN:HB2	1:A:367:MET:SD	2.62	0.40
2:B:52:LYS:HA	2:B:56:ASP:O	2.20	0.40

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	612/621 (99%)	584 (95%)	28 (5%)	0	100	100
2	B	238/252 (94%)	229 (96%)	7 (3%)	2 (1%)	19	27
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	1086/1116 (97%)	1047 (96%)	37 (3%)	2 (0%)	47	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	SER
2	B	66	ARG

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%)	493 (99%)	4 (1%)	81	91
2	B	216/219 (99%)	213 (99%)	3 (1%)	67	81
3	C	116/117 (99%)	115 (99%)	1 (1%)	78	89
4	D	78/79 (99%)	77 (99%)	1 (1%)	69	82
All	All	907/921 (98%)	898 (99%)	9 (1%)	76	87

All (9) 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	191	VAL
2	B	63	ARG
2	B	66	ARG
2	B	189	ARG
3	C	91	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 ⓘ

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	0.63	0	4,9,11	1.51	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(^{o})	Ideal(^{o})
3	C	15	MLZ	CM-NZ-CE	2.81	120.06	111.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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 50 ligands modelled in this entry, 1 is monoatomic and 40 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	$\#|Z| > 2$
9	FES	B	1001	2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
15	3PE	D	201	-	35,35,50	1.09	2 (5%)	38,40,55	1.10	3 (7%)
5	FAD	A	1001	-	53,58,58	0.84	1 (1%)	68,89,89	1.24	8 (11%)
14	UMQ	C	203	-	35,35,35	0.41	0	46,46,46	0.70	0
13	HEM	C	201	4,3	40,48,50	1.25	1 (2%)	46,80,82	1.45	6 (13%)
11	F3S	B	1003	2	0,9,9	-	-	-		
7	OAA	A	1003	-	8,8,8	2.51	3 (37%)	9,10,10	1.63	2 (22%)
12	AT5	C	202	-	20,23,23	1.66	3 (15%)	24,32,32	1.35	3 (12%)
10	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
9	FES	B	1001	2	-	-	0/1/1/1
15	3PE	D	201	-	-	4/39/39/54	-
5	FAD	A	1001	-	-	5/30/50/50	0/6/6/6
14	UMQ	C	203	-	-	4/20/60/60	0/2/2/2
13	HEM	C	201	4,3	-	1/10/50/54	-
11	F3S	B	1003	2	-	-	0/3/3/3
7	OAA	A	1003	-	-	3/8/8/8	-
12	AT5	C	202	-	-	5/22/22/22	0/1/1/1
10	SF4	B	1002	2	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	202	AT5	C1-C2	5.40	1.48	1.39
7	A	1003	OAA	O3-C3	5.09	1.33	1.23
15	D	201	3PE	O31-C31	4.18	1.45	1.33
15	D	201	3PE	O21-C21	4.14	1.46	1.34
12	C	202	AT5	C2-C3	3.47	1.48	1.40
7	A	1003	OAA	C2-C3	-3.45	1.37	1.51
5	A	1001	FAD	C4-N3	-2.67	1.33	1.38
12	C	202	AT5	C6-C5	2.32	1.49	1.43
13	C	201	HEM	C2C-C3C	-2.24	1.34	1.41
7	A	1003	OAA	C2-C1	2.15	1.54	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1001	FAD	C4-N3-C2	-3.99	118.26	125.64
12	C	202	AT5	C3-N4-C5	3.88	123.69	117.58
15	D	201	3PE	O21-C21-C22	3.77	119.62	111.50
5	A	1001	FAD	C4X-C4-N3	3.41	121.85	113.19
13	C	201	HEM	C1B-NB-C4B	3.17	108.35	105.07
13	C	201	HEM	C4D-ND-C1D	3.04	108.21	105.07
12	C	202	AT5	CM3-O3-C3	2.76	119.95	117.21
13	C	201	HEM	C4B-CHC-C1C	2.74	126.17	122.56
5	A	1001	FAD	O4-C4-C4X	-2.66	119.54	126.60
7	A	1003	OAA	O3-C3-C2	2.59	124.32	120.58
13	C	201	HEM	C4C-CHD-C1D	2.48	125.83	122.56
5	A	1001	FAD	P-O3P-PA	-2.45	124.41	132.83
15	D	201	3PE	O31-C31-C32	2.40	119.42	111.91
7	A	1003	OAA	O2-C1-C2	2.36	122.09	114.54
13	C	201	HEM	CAD-CBD-CGD	-2.31	108.63	113.60
5	A	1001	FAD	C4X-C10-N1	-2.30	119.40	124.73
12	C	202	AT5	C6-C5-N4	-2.29	122.05	124.09
15	D	201	3PE	C2-O21-C21	-2.25	112.25	117.79
13	C	201	HEM	C3D-C4D-ND	-2.16	107.76	110.17
5	A	1001	FAD	C10-N1-C2	2.14	121.18	116.90
5	A	1001	FAD	C4'-C3'-C2'	-2.13	108.93	113.36
5	A	1001	FAD	O2-C2-N1	-2.02	118.48	121.83

There are no chirality outliers.

All (22) 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'
7	A	1003	OAA	C2-C3-C4-O4
7	A	1003	OAA	C2-C3-C4-O5
12	C	202	AT5	C11-C12-C13-CL12
12	C	202	AT5	C17-C12-C13-CL12
12	C	202	AT5	C12-C13-C14-CL16
15	D	201	3PE	C22-C21-O21-C2
15	D	201	3PE	O22-C21-O21-C2
13	C	201	HEM	C2A-CAA-CBA-CGA
14	C	203	UMQ	CI-CJ-CK-CL
12	C	202	AT5	C17-C12-C13-C14
5	A	1001	FAD	PA-O3P-P-O5'
14	C	203	UMQ	O5-C5-C6-O6
7	A	1003	OAA	O3-C3-C4-O4
14	C	203	UMQ	CA-CB-CC-CD

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Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	P-O3P-PA-O2A
15	D	201	3PE	C22-C23-C24-C25
14	C	203	UMQ	O5'-C1'-O1'-CA
12	C	202	AT5	C11-C12-C13-C14
5	A	1001	FAD	O4B-C4B-C5B-O5B
15	D	201	3PE	C25-C26-C27-C28

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	201	3PE	2	0
5	A	1001	FAD	4	0
7	A	1003	OAA	6	0
12	C	202	AT5	1	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 3PE D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand UMQ C 203

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand AT5 C 202

Bond lengths

Bond angles

Torsions

Rings
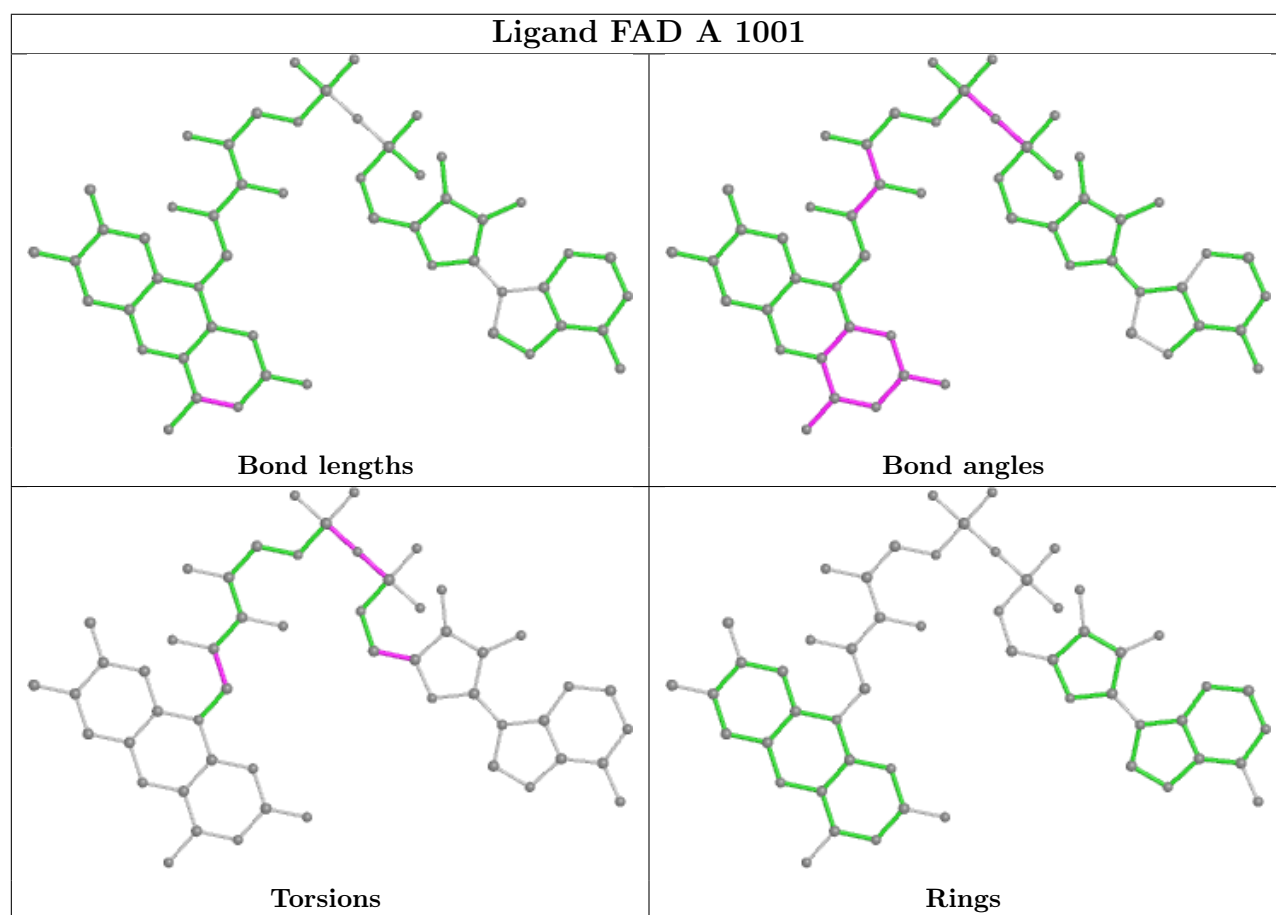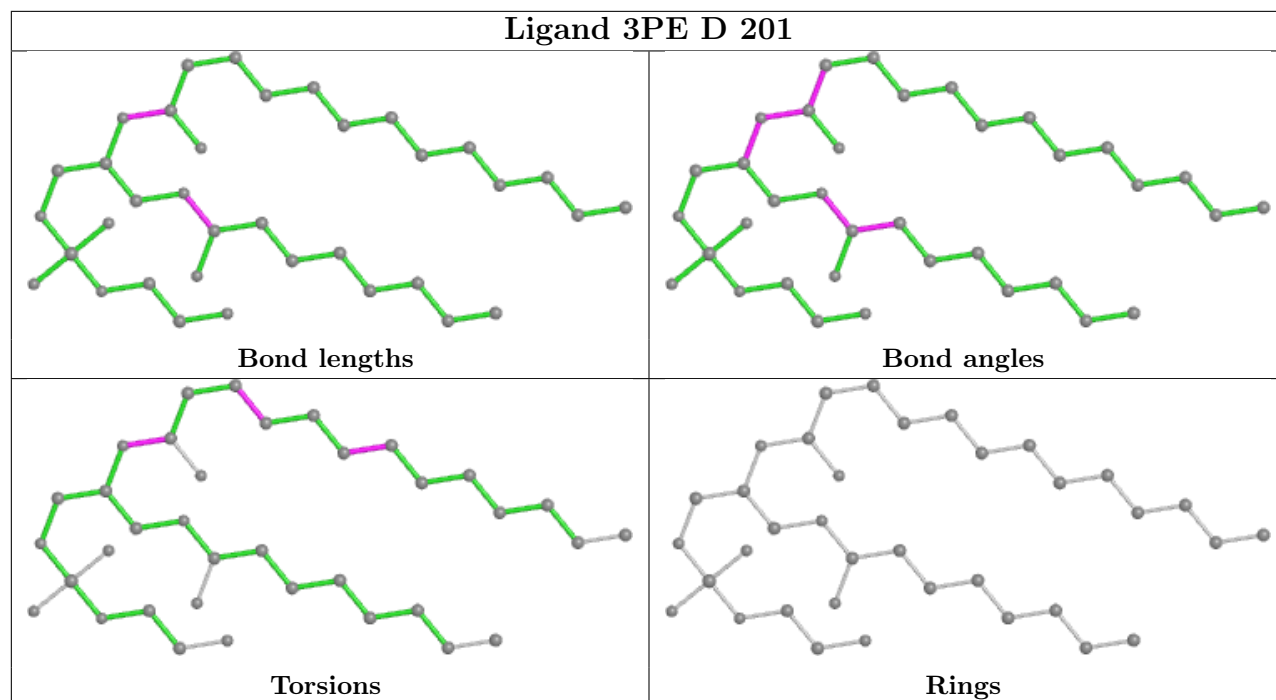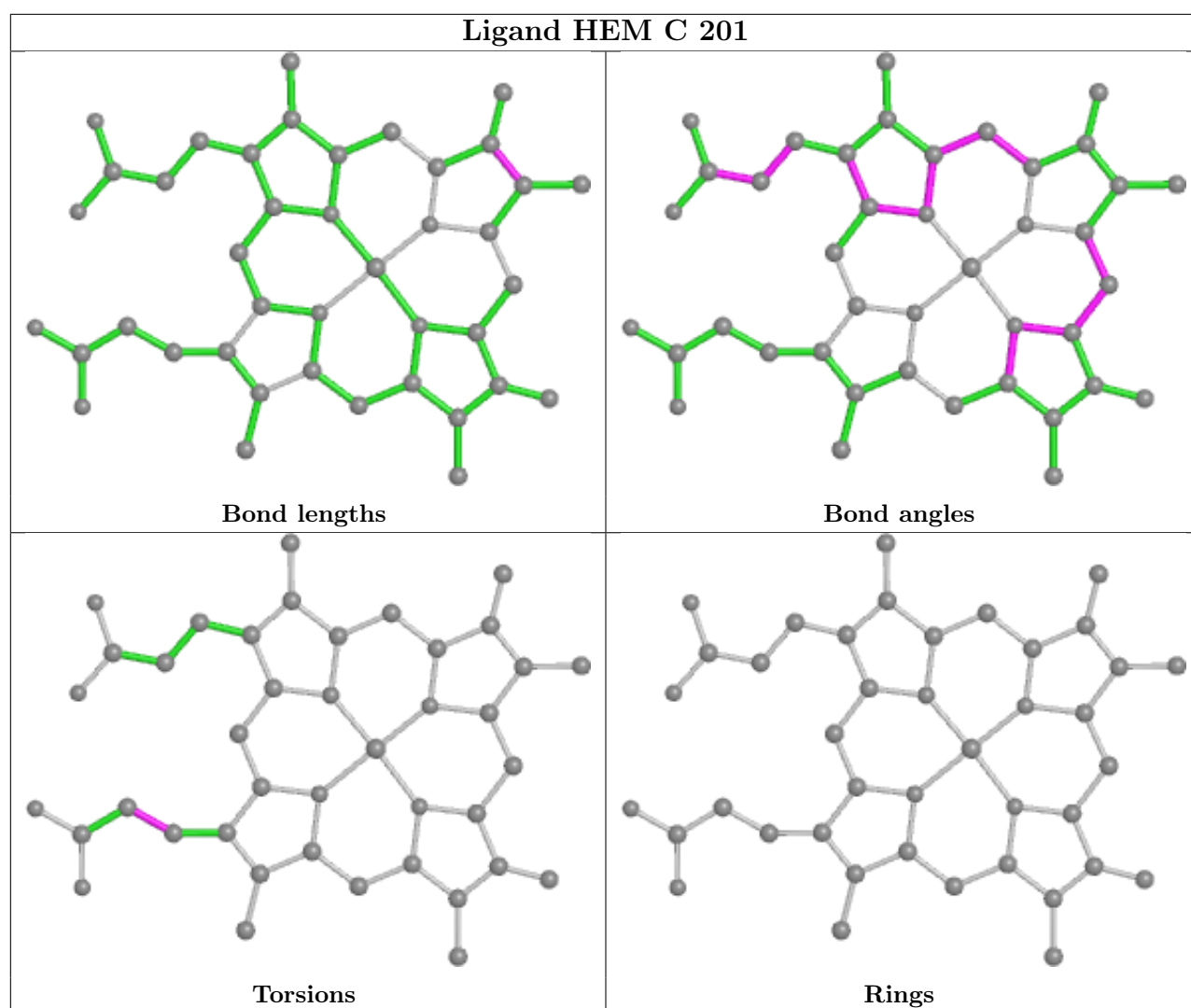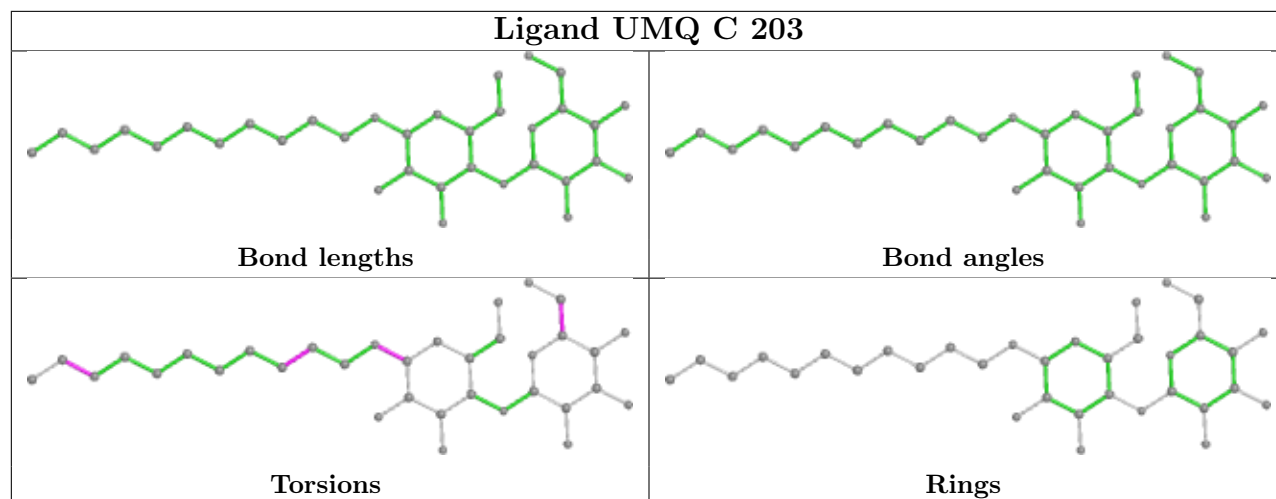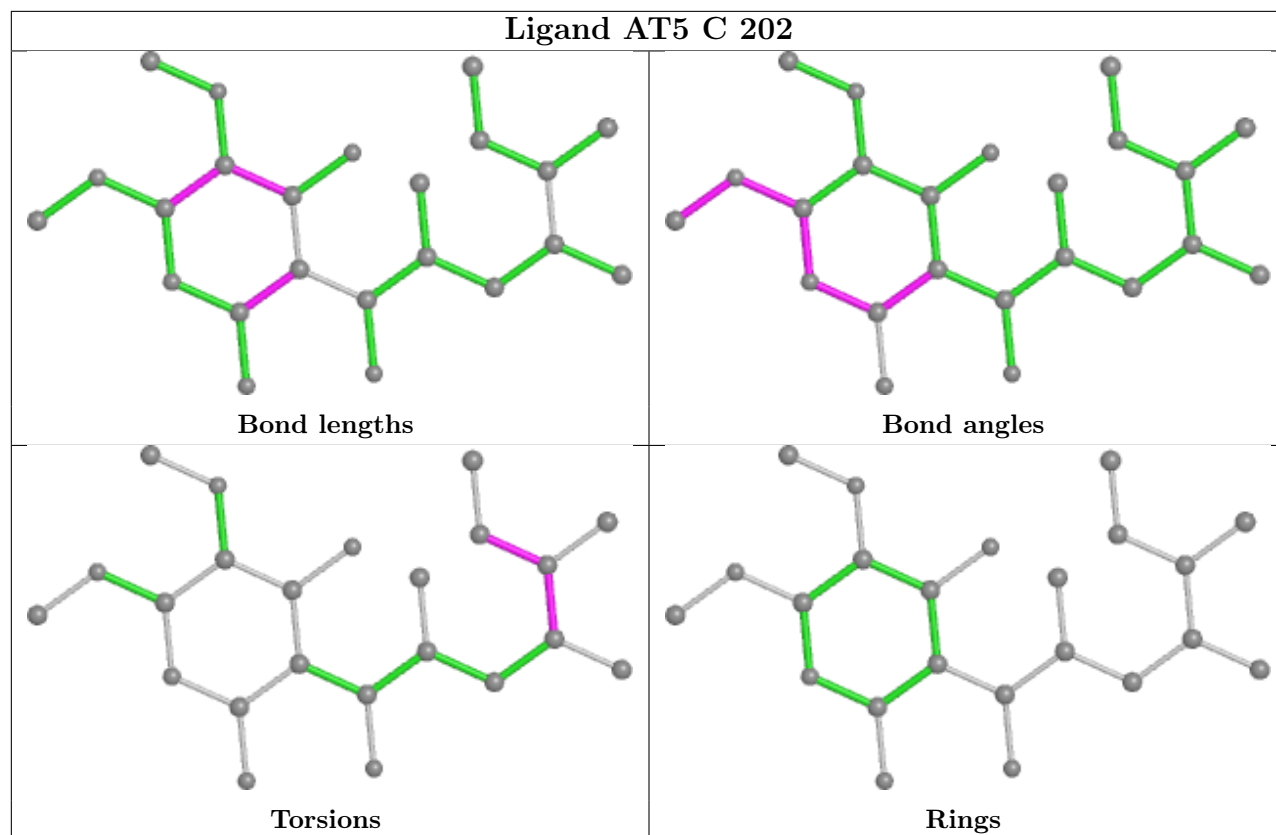
5.7 Other polymers ⓘ

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	612/621 (98%)	0.74	87 (14%)	2	3	47, 74, 110, 132	0
2	B	240/252 (95%)	0.58	23 (9%)	8	9	45, 59, 107, 121	0
3	C	138/140 (98%)	0.31	13 (9%)	8	9	51, 69, 102, 119	0
4	D	102/103 (99%)	0.05	4 (3%)	39	42	51, 68, 92, 105	0
All	All	1092/1116 (97%)	0.59	127 (11%)	4	5	45, 71, 107, 132	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	79	LEU	5.6
2	B	246	LYS	5.4
1	A	314	CYS	5.1
1	A	365	TYR	4.8
4	D	2	SER	4.5
3	C	78	SER	4.4
1	A	413	SER	4.3
1	A	316	PRO	4.1
1	A	414	LEU	4.1
1	A	56	HIS	4.1
1	A	215	GLY	4.0
2	B	35	VAL	3.8
1	A	50	LEU	3.8
2	B	55	LEU	3.7
1	A	228	THR	3.6
1	A	308	ILE	3.5
1	A	417	LEU	3.5
1	A	571	GLN	3.4
3	C	67	PHE	3.4
1	A	226	ALA	3.3
1	A	229	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	3.3
2	B	245	TYR	3.3
3	C	76	SER	3.2
1	A	490	GLN	3.2
1	A	330	PRO	3.2
1	A	567	LEU	3.2
1	A	174	VAL	3.2
1	A	315	GLY	3.1
1	A	415	LEU	3.1
3	C	139	ALA	3.1
1	A	505	HIS	3.1
1	A	48	THR	3.1
1	A	55	SER	3.0
1	A	443	PRO	3.0
3	C	82	ALA	3.0
1	A	230	THR	3.0
2	B	95	LYS	3.0
1	A	60	ALA	3.0
1	A	277	ASN	2.9
1	A	463	ILE	2.9
1	A	276	ILE	2.9
1	A	503	LEU	2.9
2	B	72	SER	2.8
1	A	385	GLU	2.8
1	A	225	SER	2.8
1	A	57	THR	2.8
1	A	382	VAL	2.8
1	A	214	GLY	2.8
2	B	74	ALA	2.7
2	B	161	CYS	2.7
2	B	8	THR	2.7
1	A	502	ASP	2.7
1	A	258	TYR	2.7
1	A	318	LYS	2.7
1	A	405	GLY	2.7
1	A	52	PRO	2.7
1	A	396	GLY	2.7
1	A	387	LYS	2.7
2	B	16	ILE	2.6
1	A	59	ALA	2.6
1	A	575	PHE	2.6
3	C	71	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	247	GLU	2.6
1	A	568	GLN	2.6
1	A	51	PHE	2.6
1	A	27	GLY	2.5
3	C	77	LEU	2.5
3	C	74	VAL	2.5
1	A	87	SER	2.5
1	A	322	TYR	2.5
1	A	279	GLN	2.5
2	B	64	SER	2.5
2	B	163	CYS	2.4
1	A	565	LYS	2.4
1	A	397	GLU	2.4
1	A	312	ARG	2.4
2	B	70	CYS	2.4
1	A	412	ASN	2.4
1	A	441	ILE	2.4
2	B	225	CYS	2.4
1	A	250	VAL	2.3
1	A	487	SER	2.3
1	A	416	ASP	2.3
1	A	26	ALA	2.3
2	B	158	CYS	2.3
2	B	159	ILE	2.3
3	C	83	LEU	2.3
3	C	140	MET	2.3
1	A	507	LYS	2.3
1	A	320	HIS	2.3
1	A	355	GLU	2.3
1	A	459	ALA	2.3
2	B	160	LEU	2.2
1	A	49	LYS	2.2
1	A	501	ARG	2.2
1	A	313	GLY	2.2
1	A	329	PRO	2.2
1	A	561	PHE	2.2
2	B	9	SER	2.2
3	C	80	SER	2.2
1	A	96	ILE	2.2
1	A	212	ALA	2.2
1	A	366	ASN	2.2
1	A	485	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	101	TRP	2.2
1	A	213	THR	2.1
2	B	11	ILE	2.1
1	A	498	GLN	2.1
1	A	216	TYR	2.1
1	A	317	GLU	2.1
1	A	437	PRO	2.1
1	A	364	HIS	2.1
1	A	154	GLY	2.1
1	A	161	LEU	2.1
2	B	13	LYS	2.1
1	A	211	ILE	2.1
1	A	433	LYS	2.1
4	D	89	TYR	2.1
3	C	81	PRO	2.1
1	A	509	PHE	2.1
2	B	51	ILE	2.0
2	B	93	LEU	2.0
4	D	97	VAL	2.0
1	A	249	PHE	2.0
1	A	319	ASP	2.0
1	A	29	ALA	2.0

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

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.
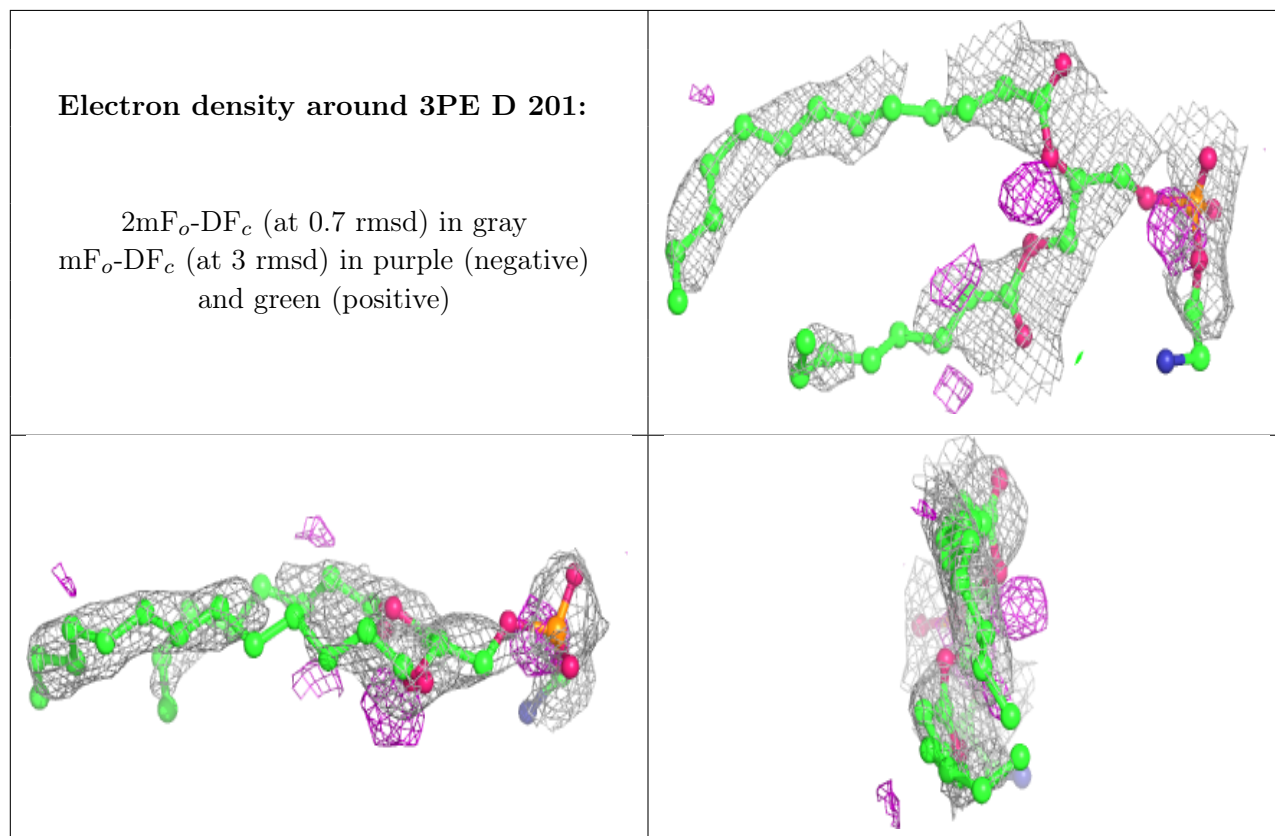
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MLZ	C	15	10/11	0.95	0.14	66,72,84,85	0

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(Å^2)	Q<0.9
8	UNL	C	209	1/-	0.31	0.68	86,86,86,86	0
8	UNL	B	1006	3/-	0.43	0.68	87,87,88,90	0
8	UNL	A	1012	1/-	0.45	0.19	91,91,91,91	0
8	UNL	A	1014	1/-	0.46	0.35	65,65,65,65	0
8	UNL	A	1006	4/-	0.60	0.20	112,116,117,121	0
8	UNL	D	211	1/-	0.60	0.14	80,80,80,80	0
8	UNL	A	1005	15/-	0.65	0.44	111,119,161,162	0
8	UNL	D	210	1/-	0.65	0.26	87,87,87,87	0
8	UNL	C	207	3/-	0.65	0.32	69,69,78,81	0
8	UNL	C	204	12/-	0.66	0.32	87,109,114,114	0
8	UNL	D	214	1/-	0.68	0.09	75,75,75,75	0
8	UNL	D	207	18/-	0.70	0.44	111,129,134,134	0
8	UNL	C	208	1/-	0.70	0.62	91,91,91,91	0
8	UNL	A	1015	1/-	0.71	0.20	106,106,106,106	0
8	UNL	B	1008	1/-	0.73	0.29	62,62,62,62	0
8	UNL	C	205	2/-	0.74	0.24	83,83,83,85	0
8	UNL	D	212	1/-	0.77	0.23	71,71,71,71	0
8	UNL	A	1010	1/-	0.77	0.36	60,60,60,60	0
8	UNL	D	208	9/-	0.80	0.17	77,98,112,113	0
15	3PE	D	201	36/51	0.80	0.40	77,106,170,176	0
8	UNL	D	202	9/-	0.82	0.18	96,99,101,103	0
8	UNL	B	1004	15/-	0.83	0.34	76,87,123,129	15
8	UNL	D	205	2/-	0.83	0.21	54,54,54,57	0
8	UNL	A	1009	4/-	0.83	0.16	80,83,86,97	0
8	UNL	B	1005	4/-	0.84	0.21	57,61,71,85	0
8	UNL	C	206	4/-	0.84	0.23	87,88,89,92	0
8	UNL	D	204	3/-	0.85	0.12	70,70,71,73	0
8	UNL	D	215	1/-	0.86	0.34	76,76,76,76	0
8	UNL	A	1011	3/-	0.86	0.25	82,82,84,84	0
8	UNL	A	1016	1/-	0.89	0.23	62,62,62,62	0
8	UNL	B	1007	3/-	0.90	0.32	57,57,64,68	0
8	UNL	A	1004	7/-	0.91	0.41	97,100,106,108	0
8	UNL	A	1013	1/-	0.91	0.15	61,61,61,61	0
12	AT5	C	202	23/23	0.91	0.20	49,57,109,121	0
14	UMQ	C	203	34/34	0.91	0.26	59,85,115,119	0
8	UNL	D	213	1/-	0.91	0.17	72,72,72,72	0
8	UNL	D	209	10/-	0.92	0.24	81,90,98,99	0
8	UNL	A	1007	4/-	0.93	0.14	83,87,88,91	0
8	UNL	D	206	5/-	0.93	0.33	83,89,97,107	0
8	UNL	D	203	3/-	0.94	0.15	62,62,64,65	0
8	UNL	B	1009	1/-	0.94	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
8	UNL	A	1017	1/-	0.95	0.44	53,53,53,53	0
8	UNL	A	1008	4/-	0.95	0.20	78,79,79,85	0
7	OAA	A	1003	9/9	0.96	0.25	55,63,71,77	0
6	K	A	1002	1/1	0.96	0.30	61,61,61,61	1
13	HEM	C	201	41/43	0.98	0.14	54,59,66,75	0
9	FES	B	1001	4/4	0.98	0.19	50,53,58,63	0
5	FAD	A	1001	53/53	0.98	0.29	48,58,63,66	0
10	SF4	B	1002	8/8	0.99	0.17	51,53,55,58	0
11	F3S	B	1003	7/7	0.99	0.20	46,50,56,58	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.
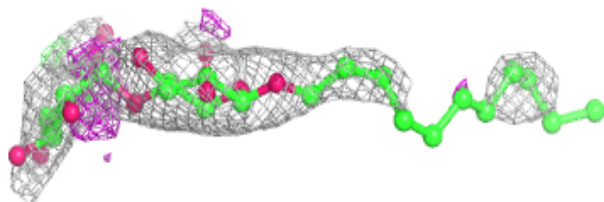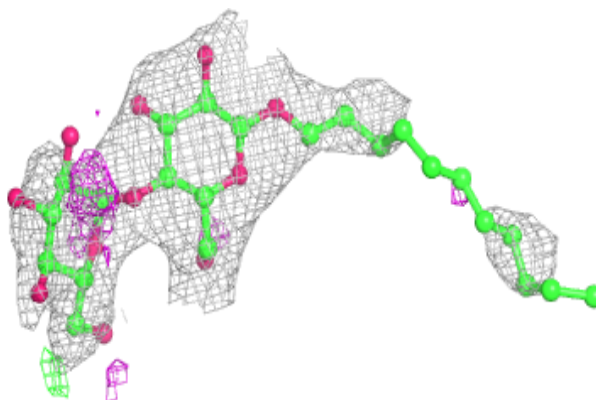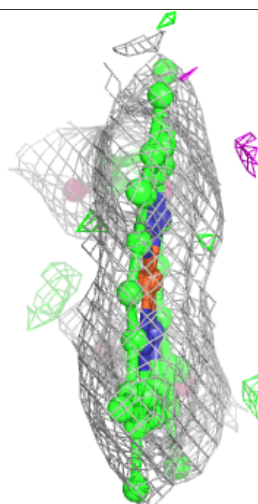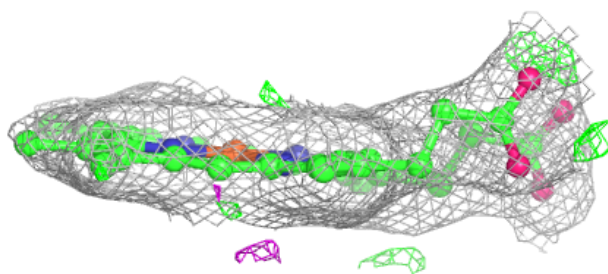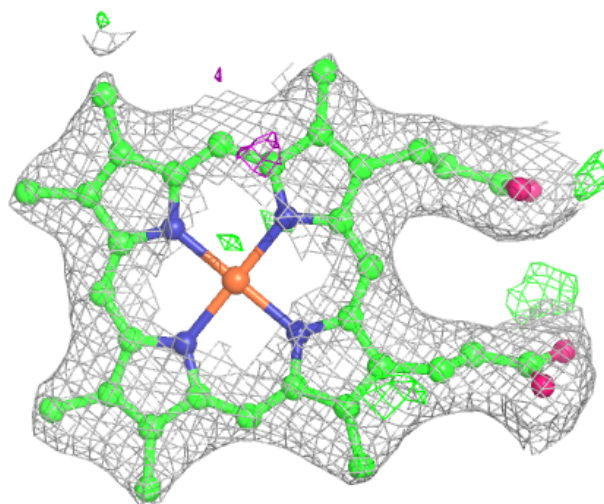

Electron density around 3PE D 201:

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

Electron density around AT5 C 202:

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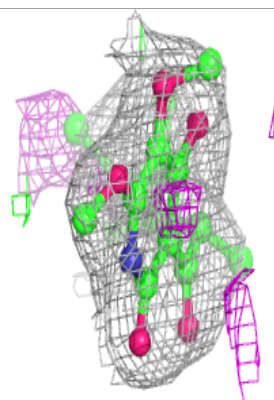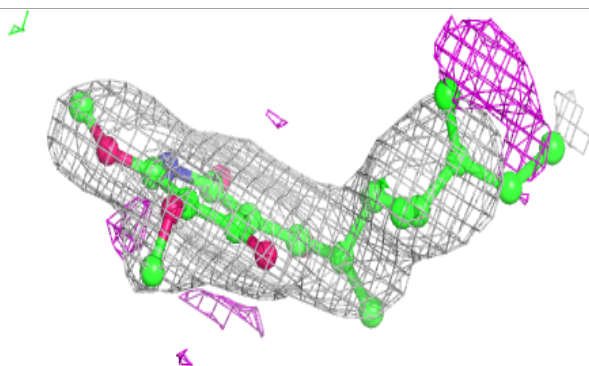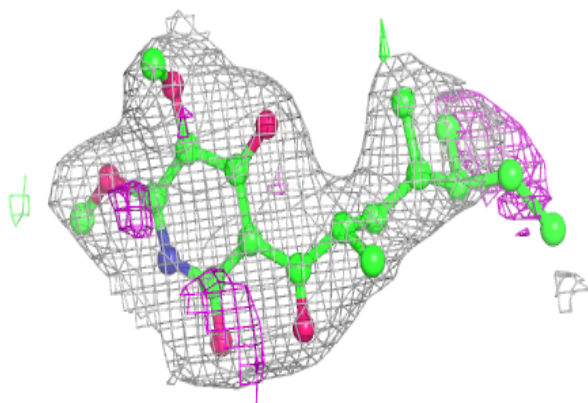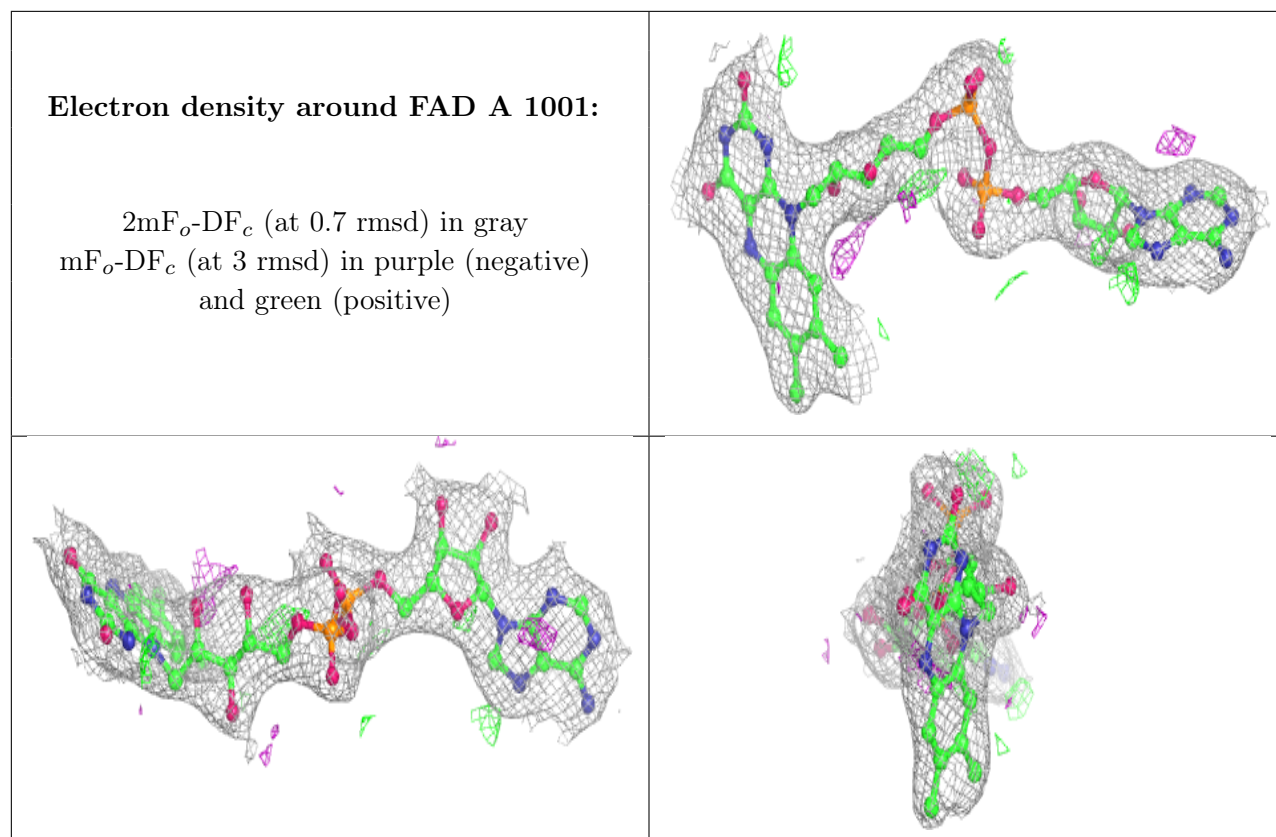

Electron density around UMQ C 203:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
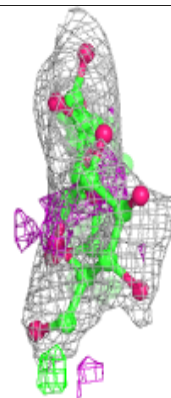
Electron density around HEM C 201:

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

Electron density around FAD A 1001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.