



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 01:28 am BST

PDB ID : 3ETR
Title : Crystal structure of xanthine oxidase in complex with lumazine
Authors : Paufl, J.M.; Cao, H.; Hille, R.
Deposited on : 2008-10-08
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

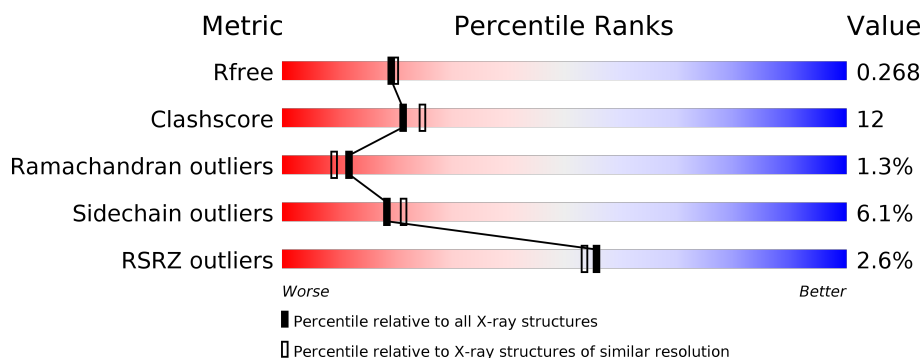
1 Overall quality at a glance

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 on 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	164	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	L	164	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
2	B	305	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
2	M	305	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
3	C	755	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
3	N	755	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>• •</div> </div> </div>

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
7	MOS	N	1327	-	-	X	-
8	LUZ	N	1	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20307 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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			
1	L	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

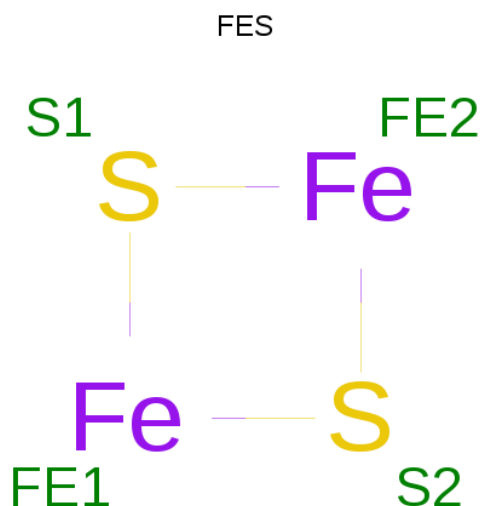
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	M	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called Xanthine dehydrogenase/oxidase.

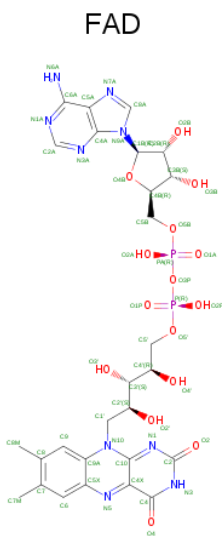
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	N	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



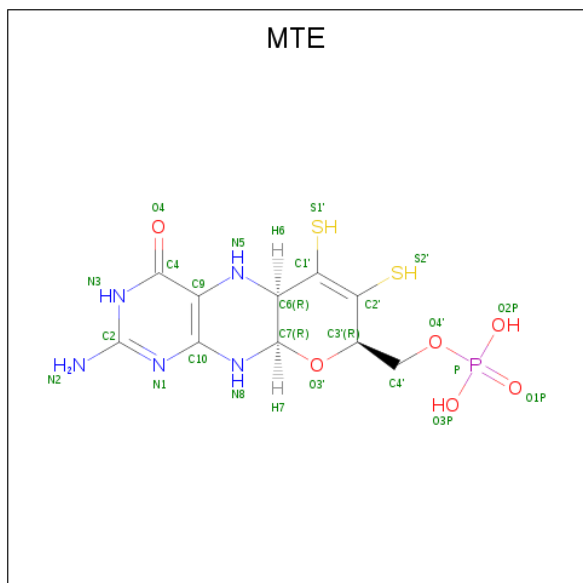
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Fe 2	S 2	0	0
4	A	1	Total 4	Fe 2	S 2	0	0
4	L	1	Total 4	Fe 2	S 2	0	0
4	L	1	Total 4	Fe 2	S 2	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



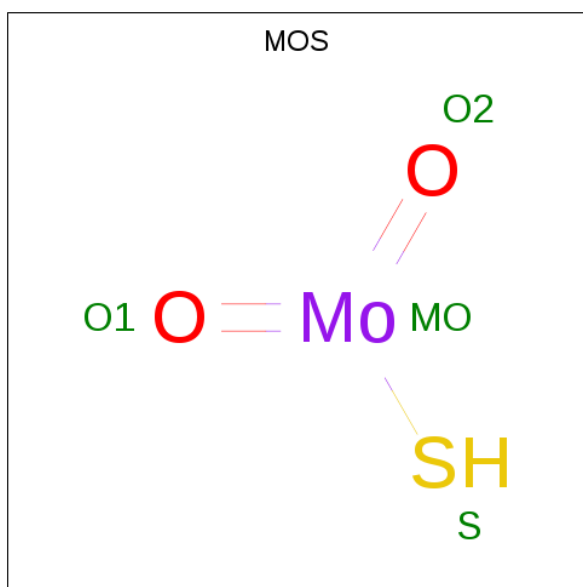
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6P S_2$).



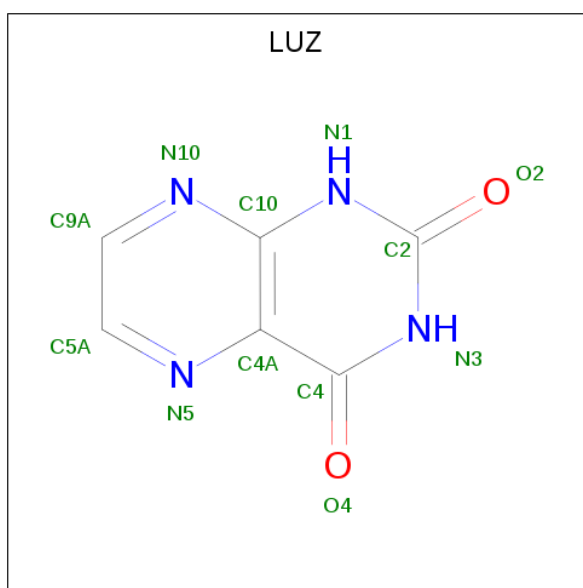
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	N	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
7	N	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is pteridine-2,4(1H,3H)-dione (three-letter code: LUZ) (formula: $C_6H_4N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			12	6	4	2		
8	N	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Ca 1	0	0

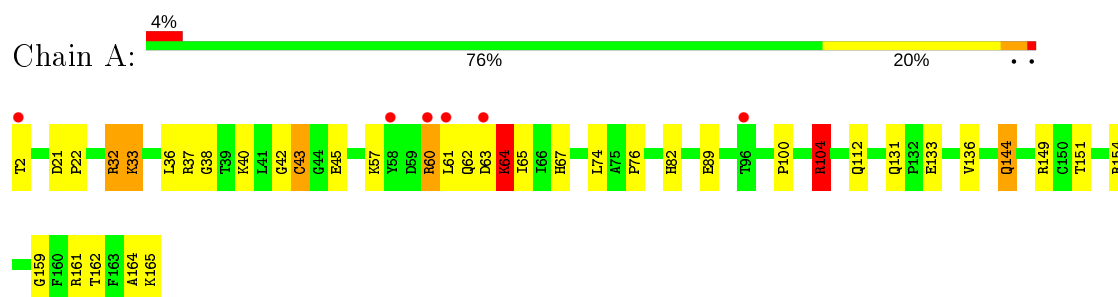
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	101	Total 101	O 101	0	0
10	B	171	Total 171	O 171	0	0
10	C	368	Total 368	O 368	0	0
10	L	116	Total 116	O 116	0	0
10	M	128	Total 128	O 128	0	0
10	N	348	Total 348	O 348	0	0

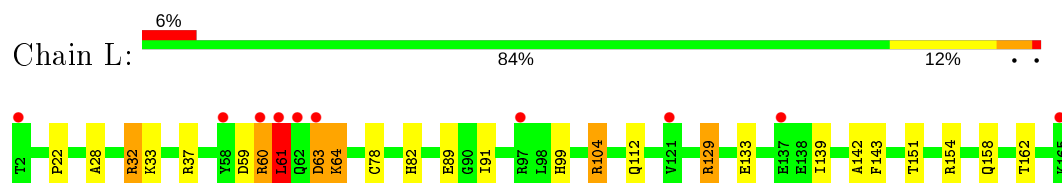
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

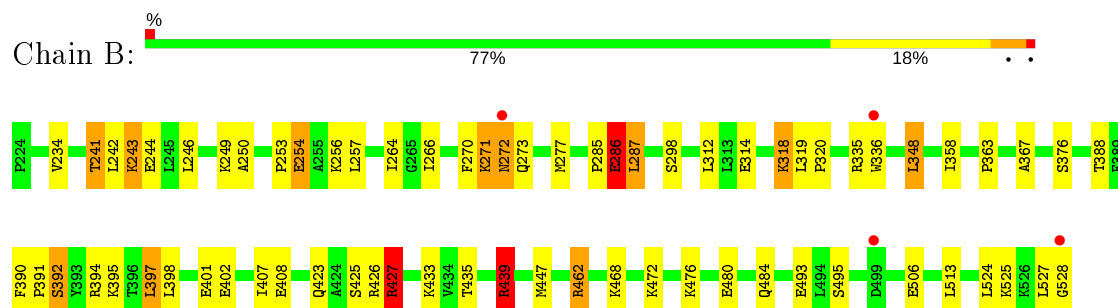
- Molecule 1: Xanthine dehydrogenase/oxidase



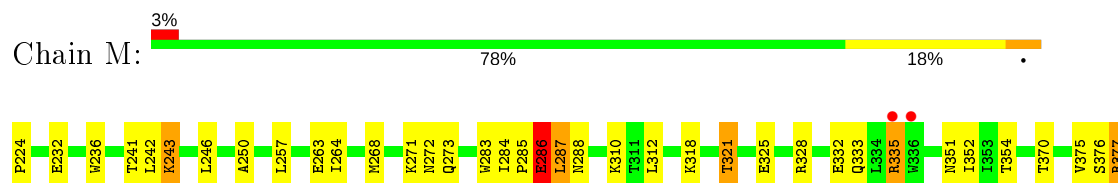
- Molecule 1: Xanthine dehydrogenase/oxidase

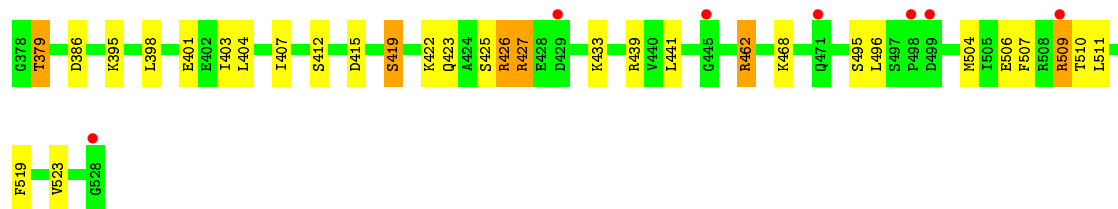


- Molecule 2: Xanthine dehydrogenase/oxidase

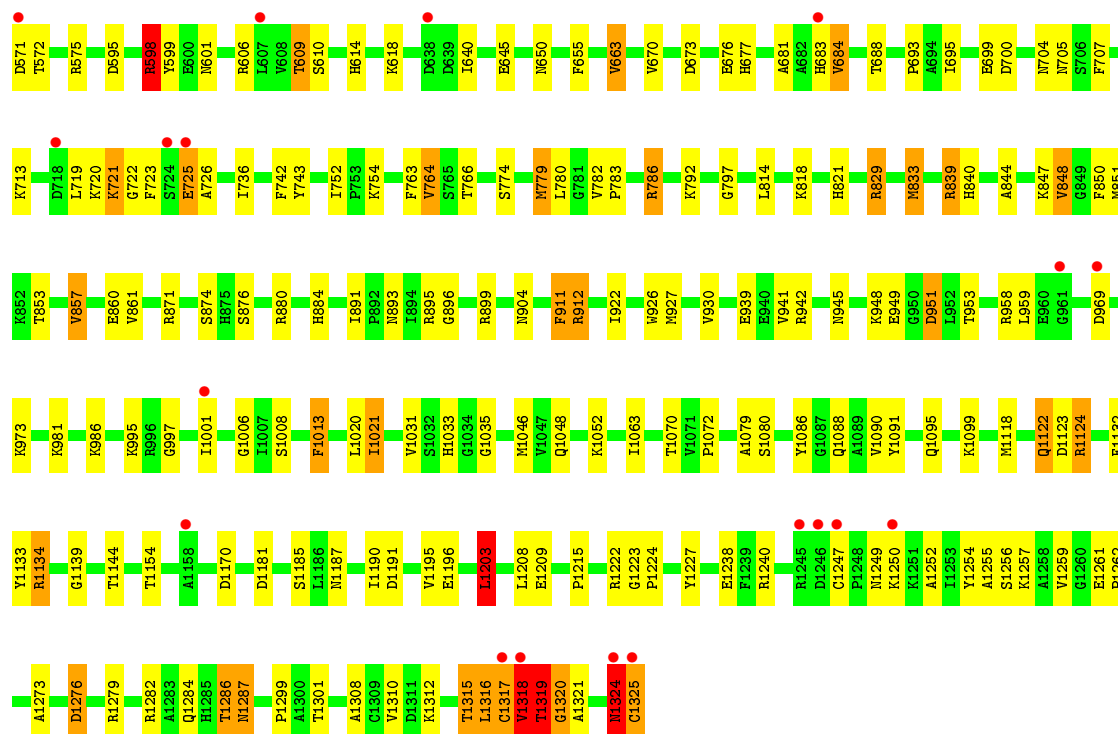


- Molecule 2: Xanthine dehydrogenase/oxidase

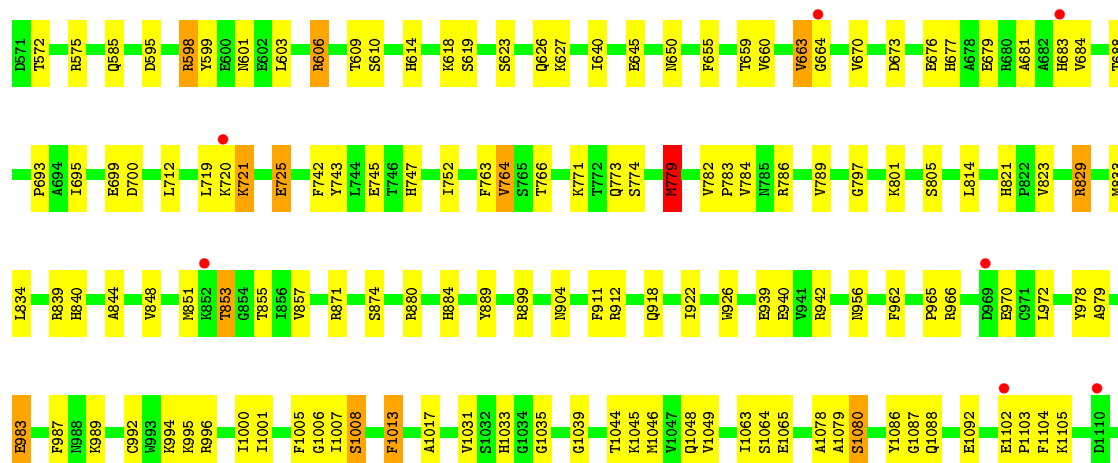


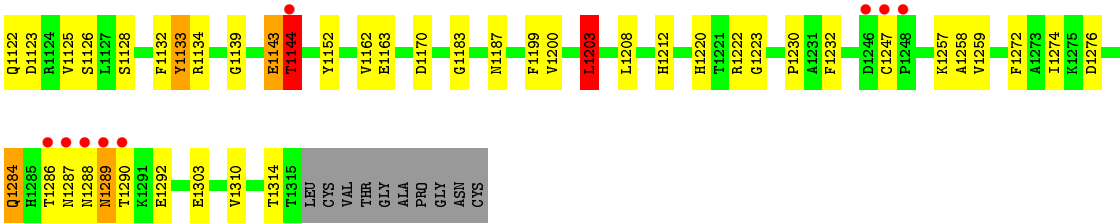


• Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.19Å 73.49Å 146.50Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 26.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.20) 98.8 (26.42-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.267 0.199 , 0.268	Depositor DCC
R_{free} test set	7052 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20307	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: MOS, LUZ, FES, CA, FAD, MTE

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	0.99	0/1277	0.96	5/1723 (0.3%)
1	L	0.87	0/1277	0.87	3/1723 (0.2%)
2	B	0.93	1/2438 (0.0%)	0.92	5/3290 (0.2%)
2	M	0.82	0/2438	0.86	3/3290 (0.1%)
3	C	0.94	2/5951 (0.0%)	0.98	18/8061 (0.2%)
3	N	0.92	5/5888 (0.1%)	0.94	10/7974 (0.1%)
All	All	0.92	8/19269 (0.0%)	0.94	44/26061 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	3
All	All	0	5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	664	GLY	N-CA	5.95	1.54	1.46
3	N	725	GLU	CB-CG	5.88	1.63	1.52
3	N	745	GLU	CB-CG	5.54	1.62	1.52
3	C	1324	ASN	CB-CG	5.53	1.63	1.51
3	N	992	CYS	CB-SG	-5.36	1.73	1.81

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	839	ARG	NE-CZ-NH2	-11.56	114.52	120.30
3	C	839	ARG	NE-CZ-NH2	-11.12	114.74	120.30
2	B	439	ARG	NE-CZ-NH2	-10.69	114.95	120.30
3	N	839	ARG	NE-CZ-NH1	9.69	125.15	120.30
3	N	779	MET	CG-SD-CE	-9.49	85.02	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLN	Peptide
1	A	64	LYS	Peptide
3	C	1316	LEU	Peptide
3	C	1318	VAL	Peptide
3	C	1320	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1255	0	1265	23	0
1	L	1255	0	1265	23	0
2	B	2389	0	2459	55	0
2	M	2389	0	2459	57	0
3	C	5823	0	5746	179	0
3	N	5761	0	5685	149	0
4	A	8	0	0	0	0
4	L	8	0	0	0	0
5	B	53	0	31	2	0
5	M	53	0	31	2	0
6	C	24	0	11	1	0
6	N	24	0	10	0	0
7	C	4	0	0	1	0
7	N	4	0	0	2	0
8	C	12	0	4	0	0
8	N	12	0	4	5	0
9	C	1	0	0	0	0
10	A	101	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	171	0	0	2	0
10	C	368	0	0	12	0
10	L	116	0	0	1	0
10	M	128	0	0	7	0
10	N	348	0	0	11	0
All	All	20307	0	18970	458	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 12.

The worst 5 of 458 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)
3:C:1317:CYS:HB3	3:C:1318:VAL:CB	1.42	1.50
3:C:1317:CYS:HB2	3:C:1319:THR:N	1.09	1.40
3:C:1317:CYS:HB3	3:C:1318:VAL:CA	1.46	1.37
3:C:1317:CYS:CB	3:C:1319:THR:N	2.00	1.24
3:C:618:LYS:HB2	10:C:1551:HOH:O	1.40	1.21

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	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	3
1	L	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	10
2	B	303/305 (99%)	284 (94%)	17 (6%)	2 (1%)	22	22
2	M	303/305 (99%)	284 (94%)	15 (5%)	4 (1%)	12	9
3	C	753/755 (100%)	702 (93%)	41 (5%)	10 (1%)	12	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	743/755 (98%)	701 (94%)	33 (4%)	9 (1%)	13	10
All	All	2426/2448 (99%)	2274 (94%)	121 (5%)	31 (1%)	12	9

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
3	C	1321	ALA
3	C	1324	ASN
1	L	61	LEU
1	L	64	LYS

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	137/137 (100%)	129 (94%)	8 (6%)	20	23
1	L	137/137 (100%)	127 (93%)	10 (7%)	14	15
2	B	261/261 (100%)	240 (92%)	21 (8%)	12	12
2	M	261/261 (100%)	242 (93%)	19 (7%)	14	15
3	C	631/631 (100%)	594 (94%)	37 (6%)	19	23
3	N	624/631 (99%)	594 (95%)	30 (5%)	25	32
All	All	2051/2058 (100%)	1926 (94%)	125 (6%)	18	21

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1144	THR
1	L	63	ASP
3	N	1013	PHE
3	C	1190	ILE
3	C	1286	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1048	GLN
1	L	131	GLN
3	N	1048	GLN
3	C	1212	HIS
3	C	1284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
4	FES	L	601	1	0,4,4	0.00	-	-		
8	LUZ	N	1	-	12,13,13	1.52	2 (16%)	11,18,18	2.15	3 (27%)
4	FES	A	602	1	0,4,4	0.00	-	-		
8	LUZ	C	1	-	12,13,13	1.24	1 (8%)	11,18,18	2.61	5 (45%)
5	FAD	B	606	-	51,58,58	1.51	8 (15%)	60,89,89	2.55	12 (20%)
7	MOS	C	1327	6	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MTE	C	1326	7	21,26,26	1.59	2 (9%)	21,40,40	2.55	12 (57%)
4	FES	A	601	1	0,4,4	0.00	-	-		
6	MTE	N	1326	7	21,26,26	1.34	2 (9%)	21,40,40	2.07	6 (28%)
4	FES	L	602	1	0,4,4	0.00	-	-		
7	MOS	N	1327	6	0,3,3	0.00	-	-		
5	FAD	M	606	-	51,58,58	1.56	7 (13%)	60,89,89	1.87	13 (21%)

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
4	FES	L	601	1	-	-	0/1/1/1
8	LUZ	N	1	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
8	LUZ	C	1	-	-	-	0/2/2/2
5	FAD	B	606	-	-	0/30/50/50	0/6/6/6
6	MTE	C	1326	7	-	1/6/34/34	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
6	MTE	N	1326	7	-	1/6/34/34	0/3/3/3
4	FES	L	602	1	-	-	0/1/1/1
5	FAD	M	606	-	-	0/30/50/50	0/6/6/6

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1326	MTE	C4-C9	5.66	1.49	1.41
6	N	1326	MTE	C4-C9	4.59	1.47	1.41
5	M	606	FAD	C2A-N3A	4.53	1.39	1.32
5	M	606	FAD	C4X-N5	4.52	1.39	1.33
5	M	606	FAD	C4-N3	4.18	1.40	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	C4-N3-C2	10.01	123.59	115.14
5	B	606	FAD	C1'-N10-C9A	9.98	126.15	118.29
5	B	606	FAD	N3A-C2A-N1A	-7.45	117.03	128.68
5	M	606	FAD	N3A-C2A-N1A	-6.63	118.32	128.68
8	C	1	LUZ	C4-N3-C2	5.66	119.92	115.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1326	MTE	C3'-C4'-O4'-P
6	N	1326	MTE	C3'-C4'-O4'-P

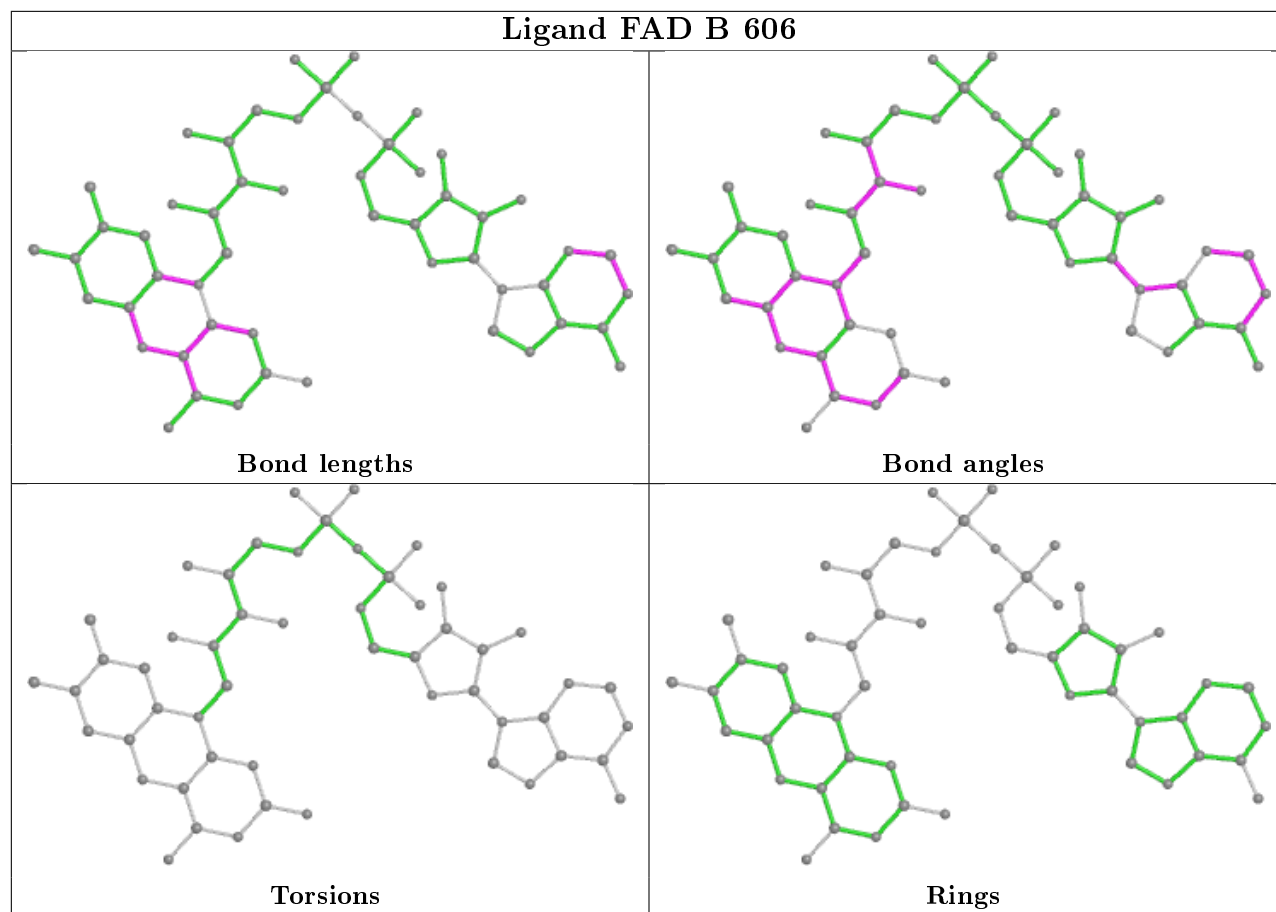
There are no ring outliers.

6 monomers are involved in 11 short contacts:

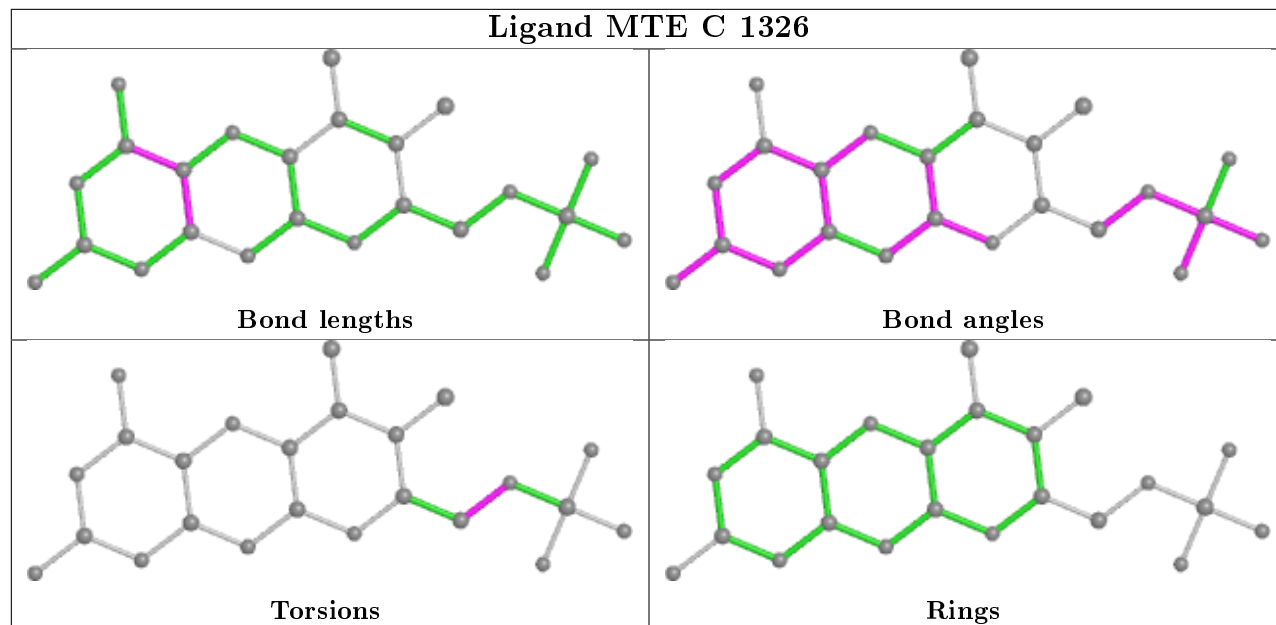
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	1	LUZ	5	0
5	B	606	FAD	2	0
7	C	1327	MOS	1	0
6	C	1326	MTE	1	0
7	N	1327	MOS	2	0
5	M	606	FAD	2	0

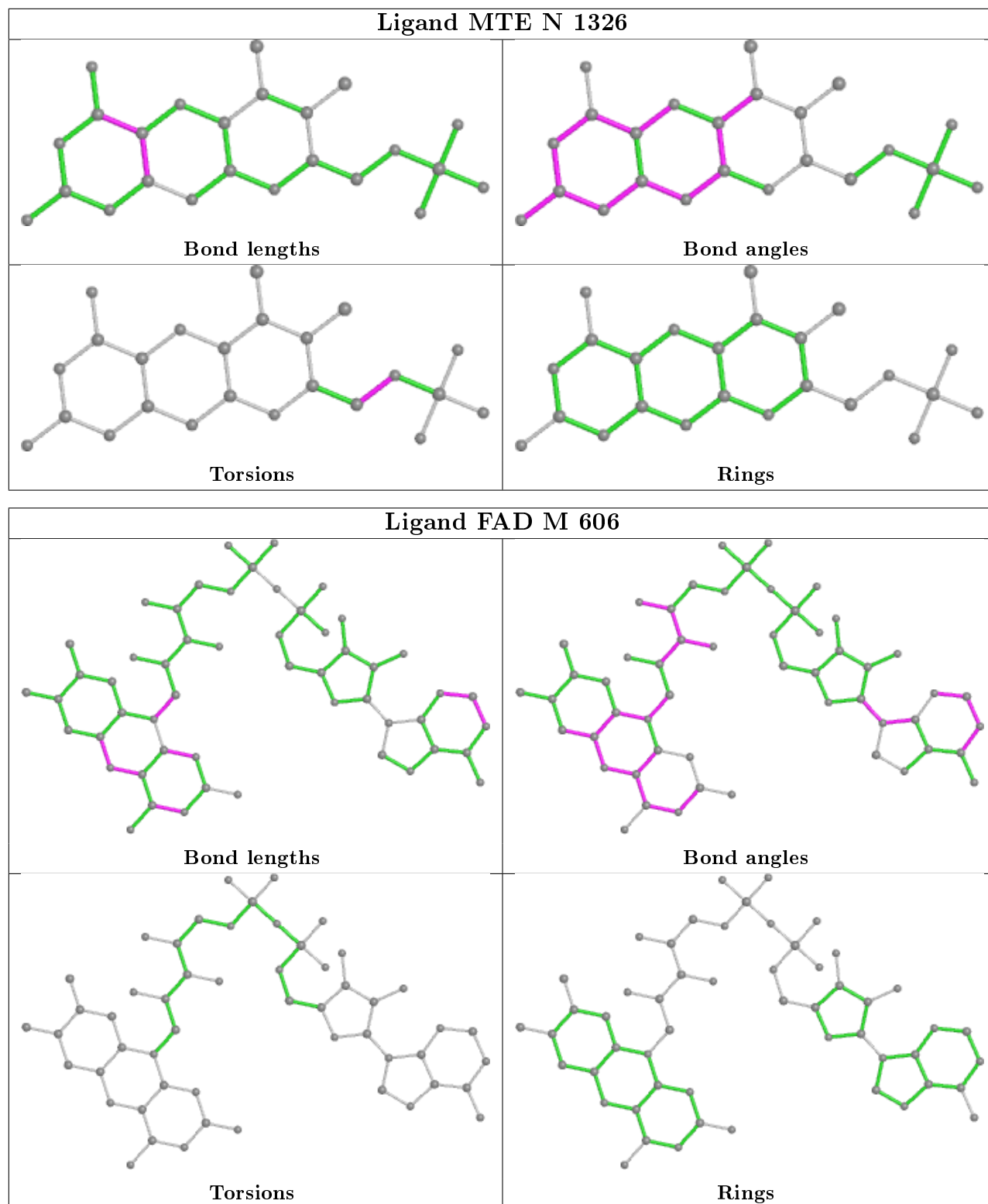
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD B 606



Ligand MTE C 1326





5.7 Other polymers [i](#)

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 [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	164/164 (100%)	-0.08	6 (3%) 41 39	12, 20, 40, 56	0
1	L	164/164 (100%)	0.08	10 (6%) 21 20	16, 28, 54, 67	0
2	B	305/305 (100%)	-0.05	4 (1%) 77 75	15, 27, 40, 45	0
2	M	305/305 (100%)	0.12	9 (2%) 50 48	22, 36, 49, 53	0
3	C	755/755 (100%)	-0.08	19 (2%) 57 55	11, 26, 43, 58	0
3	N	745/755 (98%)	-0.18	16 (2%) 63 61	12, 27, 43, 69	0
All	All	2438/2448 (99%)	-0.07	64 (2%) 56 53	11, 27, 45, 69	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	2	THR	5.7
3	N	1248	PRO	5.7
3	N	1288	ASN	5.2
2	M	429	ASP	4.7
1	L	60	ARG	4.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

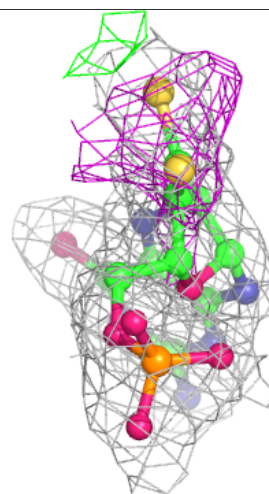
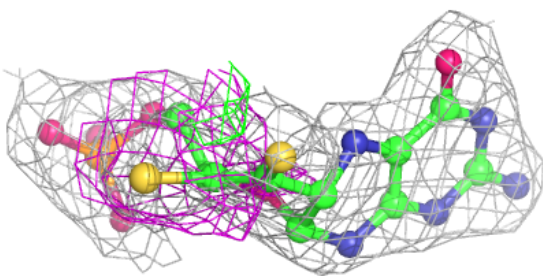
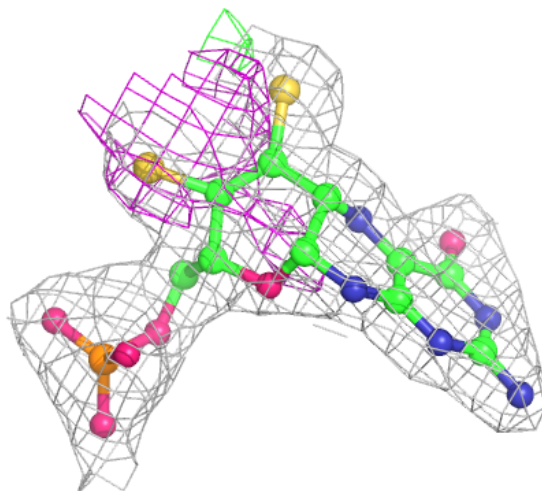
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MOS	C	1327	4/4	0.84	0.26	22,61,61,67	0
8	LUZ	C	1	12/12	0.88	0.16	37,38,39,40	0
8	LUZ	N	1	12/12	0.89	0.15	28,31,32,32	0
6	MTE	C	1326	24/24	0.92	0.13	18,26,34,41	0
9	CA	C	1328	1/1	0.93	0.11	43,43,43,43	0
5	FAD	B	606	53/53	0.96	0.12	15,20,24,28	0
6	MTE	N	1326	24/24	0.96	0.10	26,28,31,33	0
5	FAD	M	606	53/53	0.97	0.11	19,27,36,45	0
7	MOS	N	1327	4/4	0.98	0.12	45,46,48,54	0
4	FES	A	602	4/4	0.99	0.06	13,15,16,16	0
4	FES	L	601	4/4	0.99	0.08	21,22,23,23	0
4	FES	A	601	4/4	0.99	0.08	15,16,17,17	0
4	FES	L	602	4/4	1.00	0.05	19,20,21,24	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.

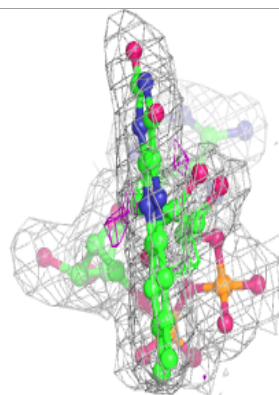
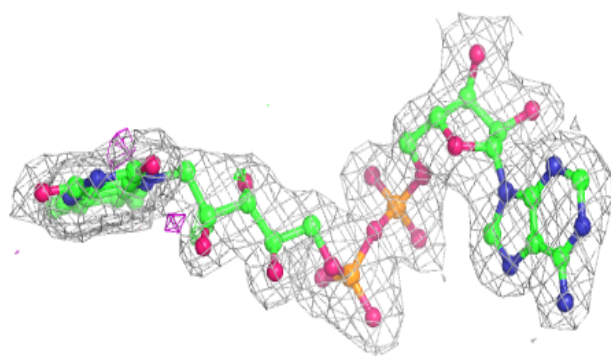
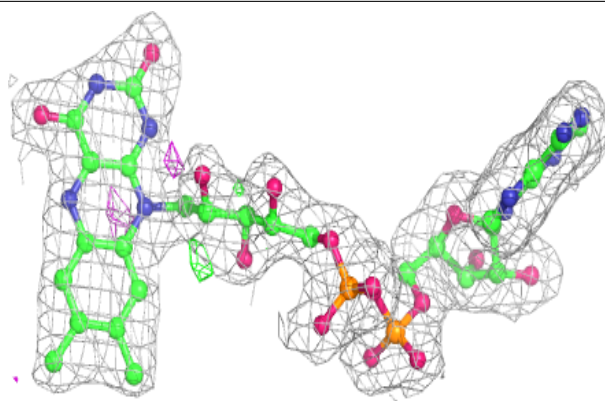
Electron density around MTE C 1326:

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



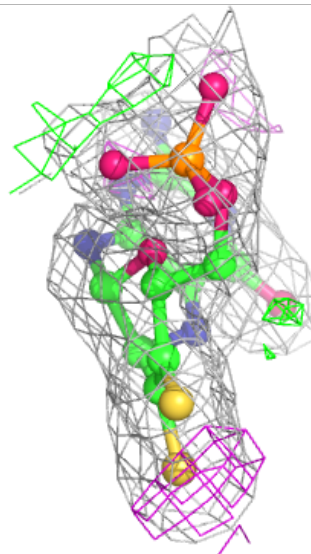
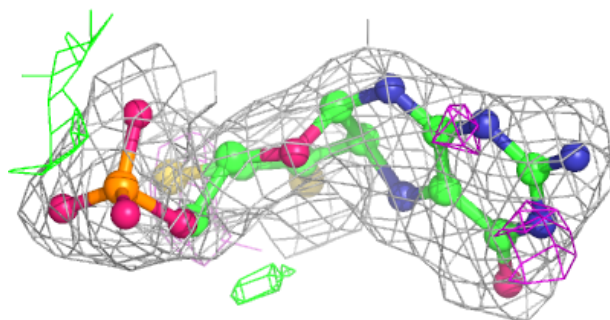
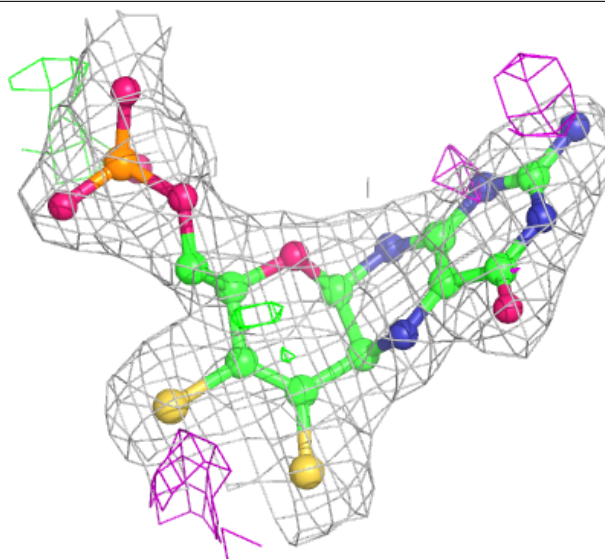
Electron density around FAD B 606:

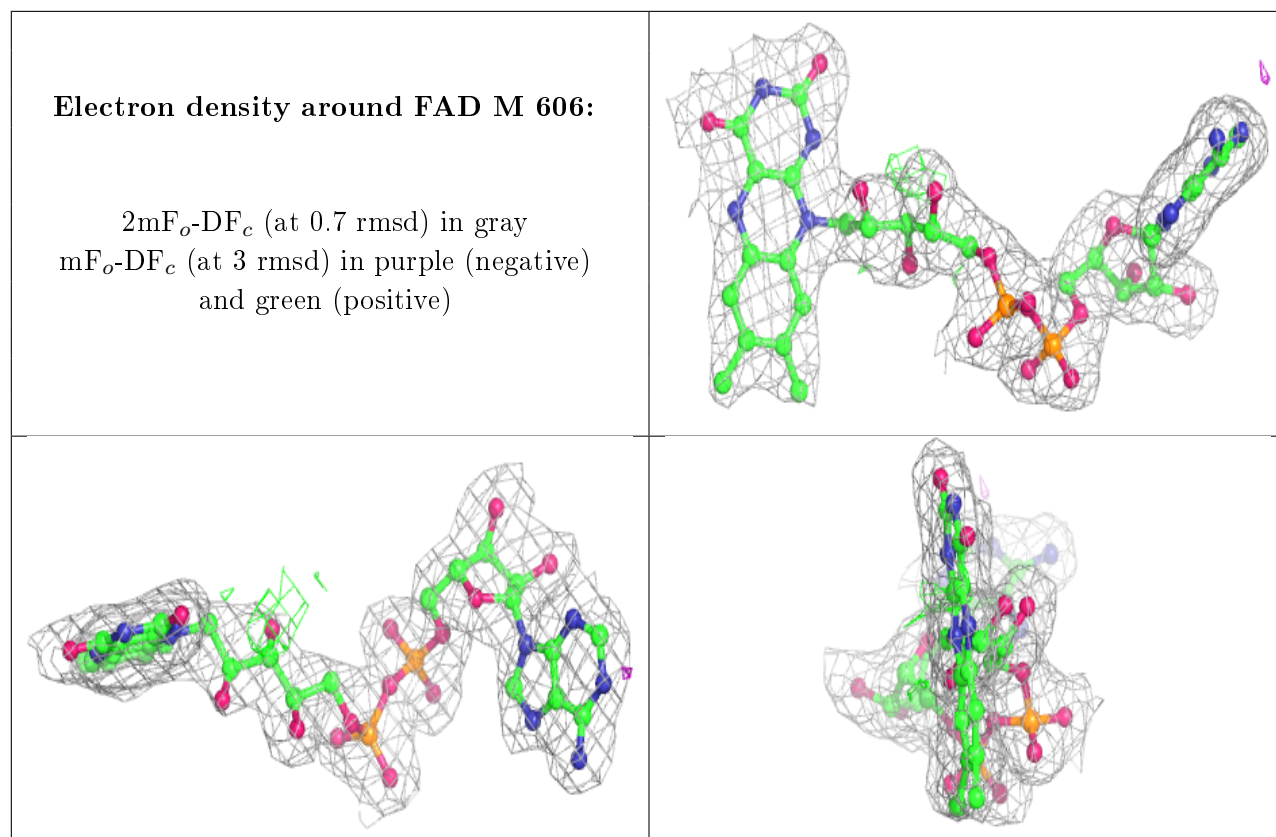
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTE N 1326:

$2mF_o-DF_c$ (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.