



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 11:59 pm BST

PDB ID : 3EUB
Title : Crystal Structure of Desulfo-Xanthine Oxidase with Xanthine
Authors : Paufl, J.M.; Cao, H.; Hille, R.
Deposited on : 2008-10-09
Resolution : 2.60 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

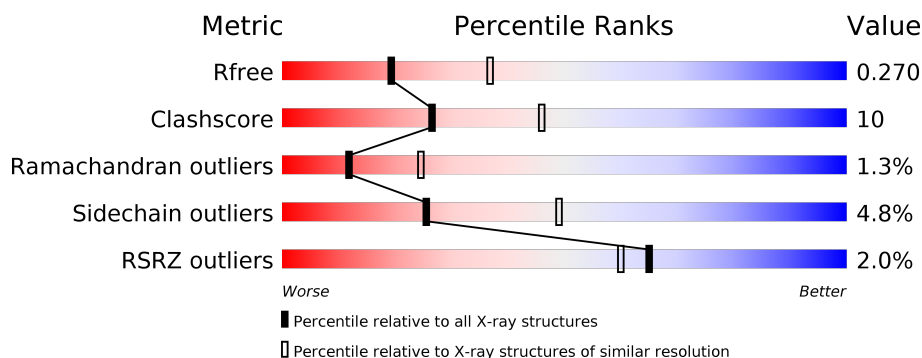
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	2	165	
1	A	165	
1	J	165	
1	S	165	
2	3	305	
2	B	305	

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Mol	Chain	Length	Quality of chain
2	K	305	
2	T	305	
3	4	762	
3	C	762	
3	L	762	
3	U	762	

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	MOM	4	1334	-	-	X	-
7	MOM	C	1334	-	-	X	-
7	MOM	L	1334	-	-	X	-
7	MOM	U	1334	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 38070 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	162	Total	C	N	O	S	0	0	0
			1243	781	223	227	12			
1	J	162	Total	C	N	O	S	0	0	0
			1243	781	223	227	12			
1	S	161	Total	C	N	O	S	0	0	0
			1234	775	221	226	12			
1	2	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

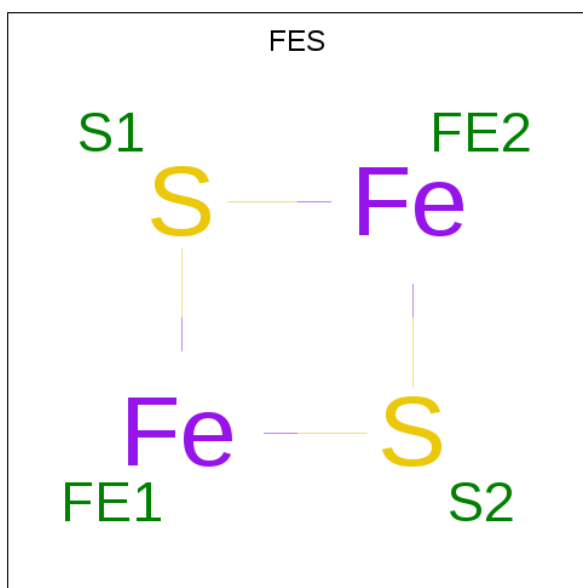
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	0	0
			2385	1537	401	434	13			
2	K	302	Total	C	N	O	S	0	0	0
			2369	1526	398	432	13			
2	T	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	3	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	753	Total	C	N	O	S	0	0	0
			5809	3673	1001	1101	34			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			
3	U	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			
3	4	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



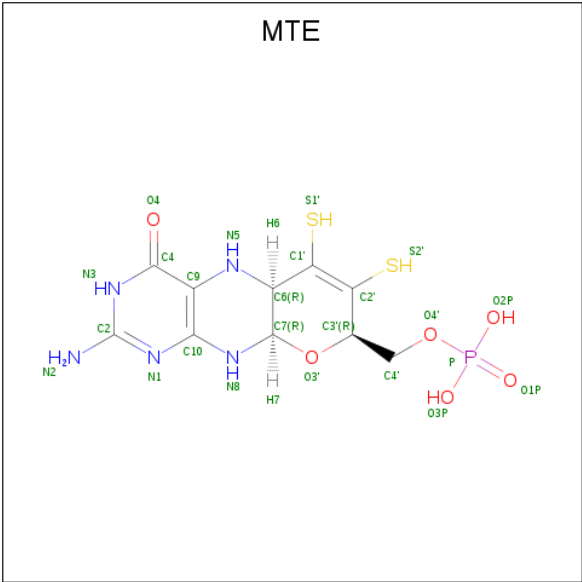
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	S	1	Total	Fe	S	0	0
			4	2	2		
4	S	1	Total	Fe	S	0	0
			4	2	2		
4	2	1	Total	Fe	S	0	0
			4	2	2		
4	2	1	Total	Fe	S	0	0
			4	2	2		

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



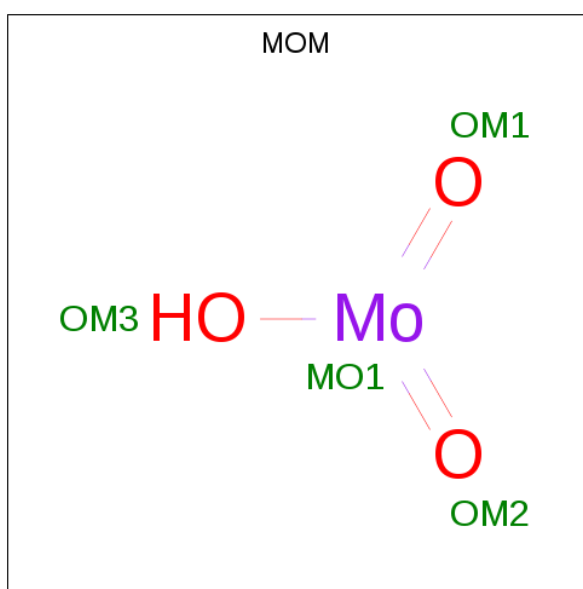
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	T	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	3	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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: C₁₀H₁₄N₅O₆P₂).



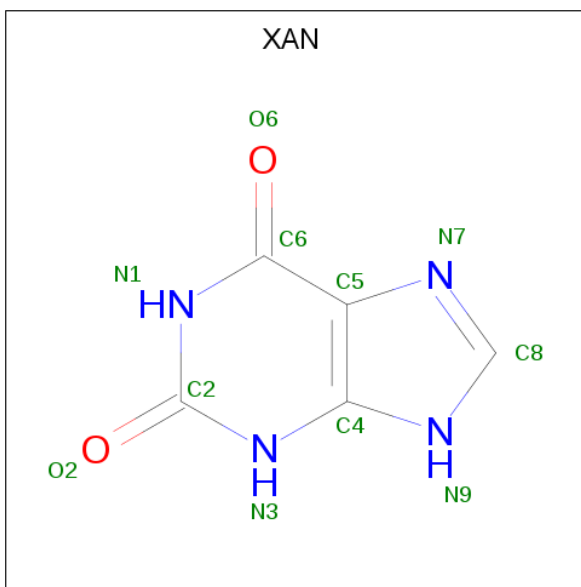
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	L	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	U	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	4	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (three-letter code: MOM) (formula: HMoO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Mo	O		
			4	1	3	0	0
7	L	1	Total	Mo	O		
			4	1	3	0	0
7	U	1	Total	Mo	O		
			4	1	3	0	0
7	4	1	Total	Mo	O		
			4	1	3	0	0

- Molecule 8 is XANTHINE (three-letter code: XAN) (formula: $\text{C}_5\text{H}_4\text{N}_4\text{O}_2$).

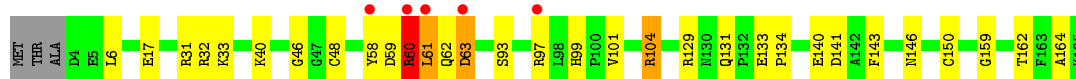
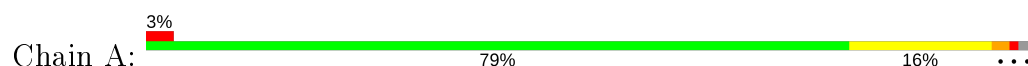


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	5	4	2		
8	L	1	Total	C	N	O	0	0
			11	5	4	2		
8	U	1	Total	C	N	O	0	0
			11	5	4	2		
8	4	1	Total	C	N	O	0	0
			11	5	4	2		

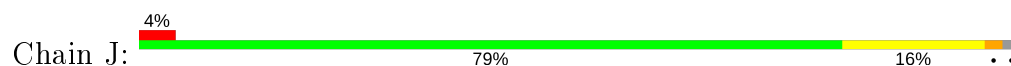
3 Residue-property plots [i](#)

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.

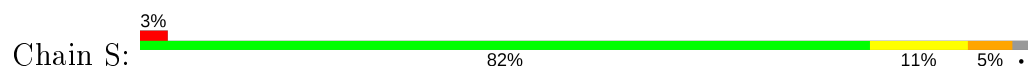
- Molecule 1: Xanthine dehydrogenase/oxidase



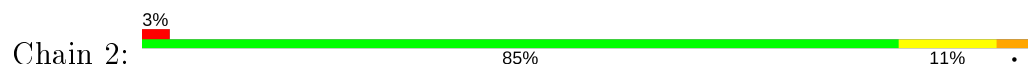
- Molecule 1: Xanthine dehydrogenase/oxidase



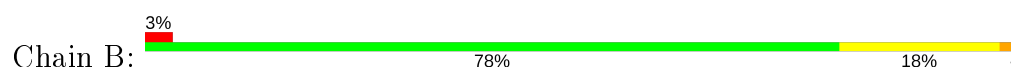
- Molecule 1: Xanthine dehydrogenase/oxidase

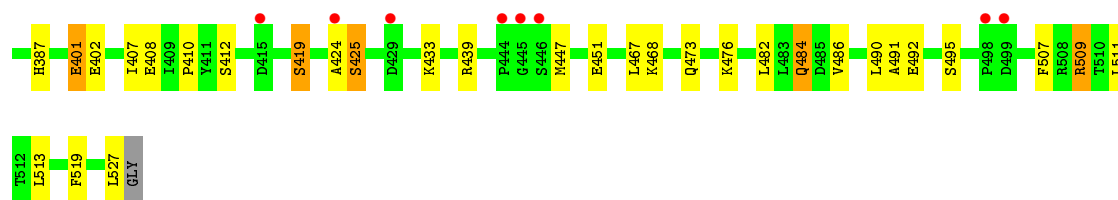


- Molecule 1: Xanthine dehydrogenase/oxidase

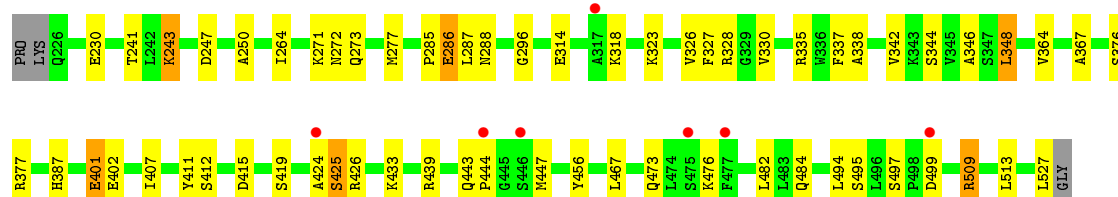
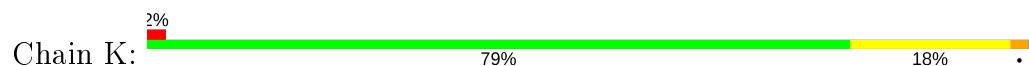


- Molecule 2: Xanthine dehydrogenase/oxidase

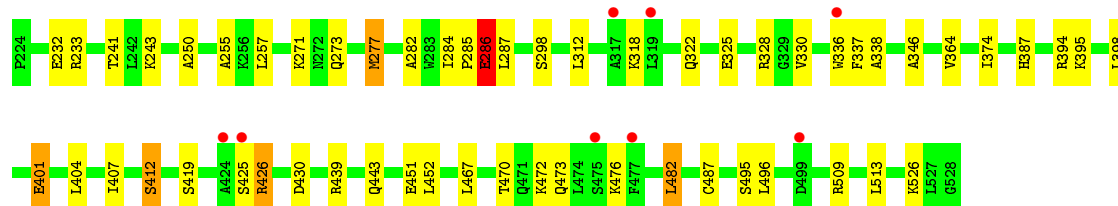
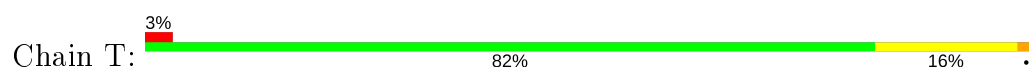




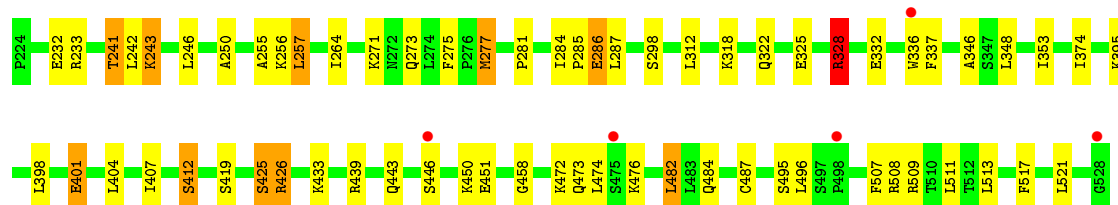
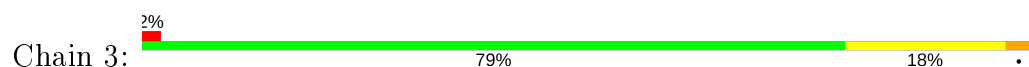
• Molecule 2: Xanthine dehydrogenase/oxidase



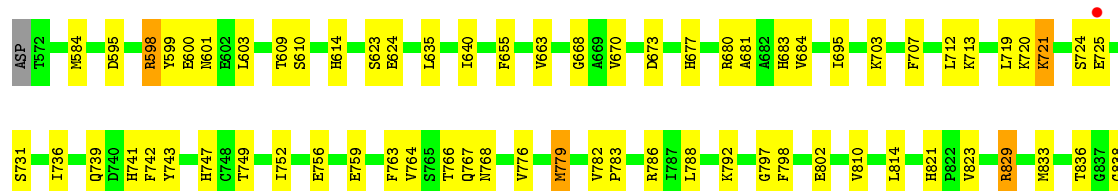
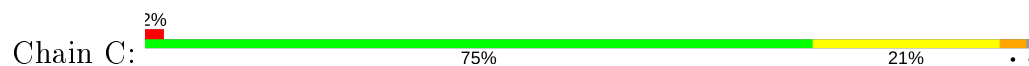
• Molecule 2: Xanthine dehydrogenase/oxidase

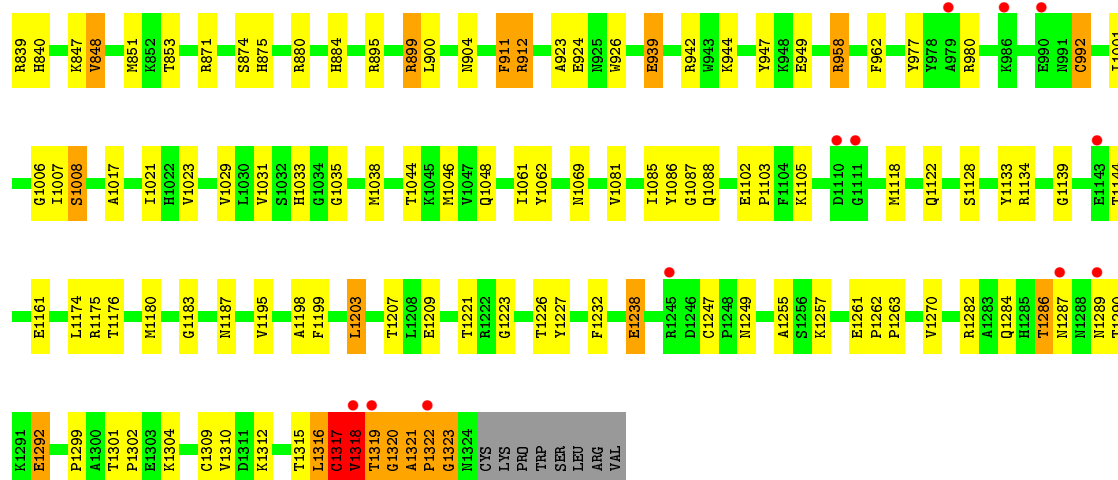


• Molecule 2: Xanthine dehydrogenase/oxidase

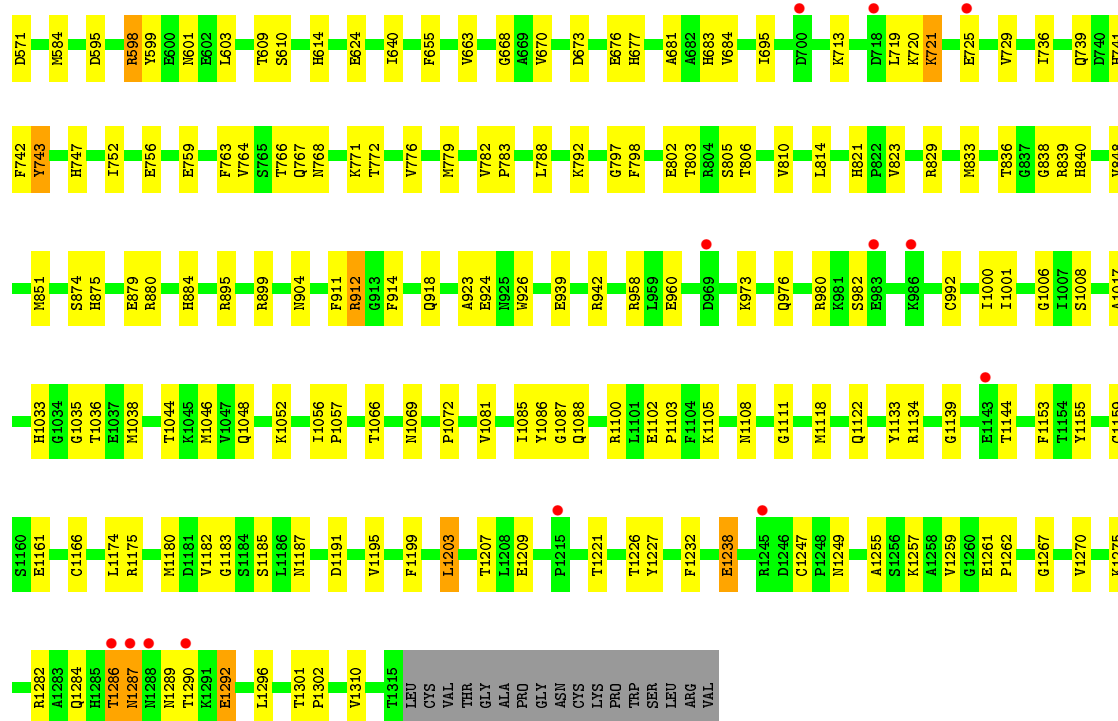
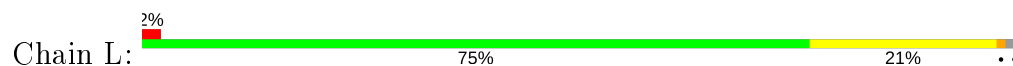


• Molecule 3: Xanthine dehydrogenase/oxidase

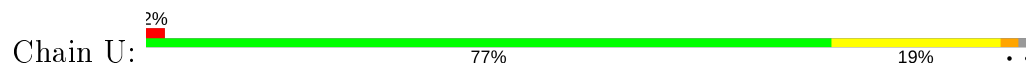


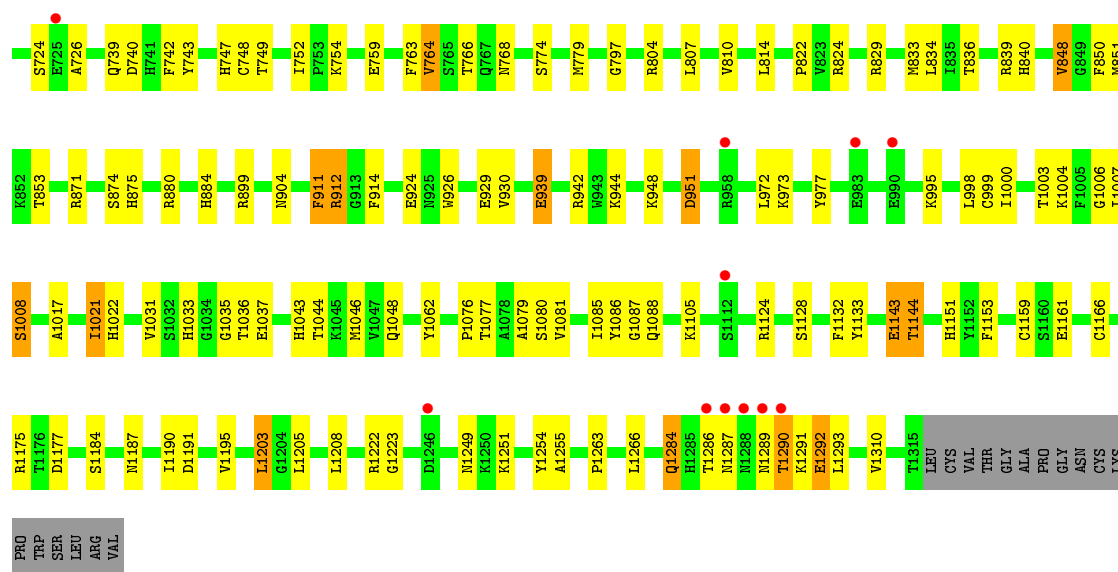


• Molecule 3: Xanthine dehydrogenase/oxidase

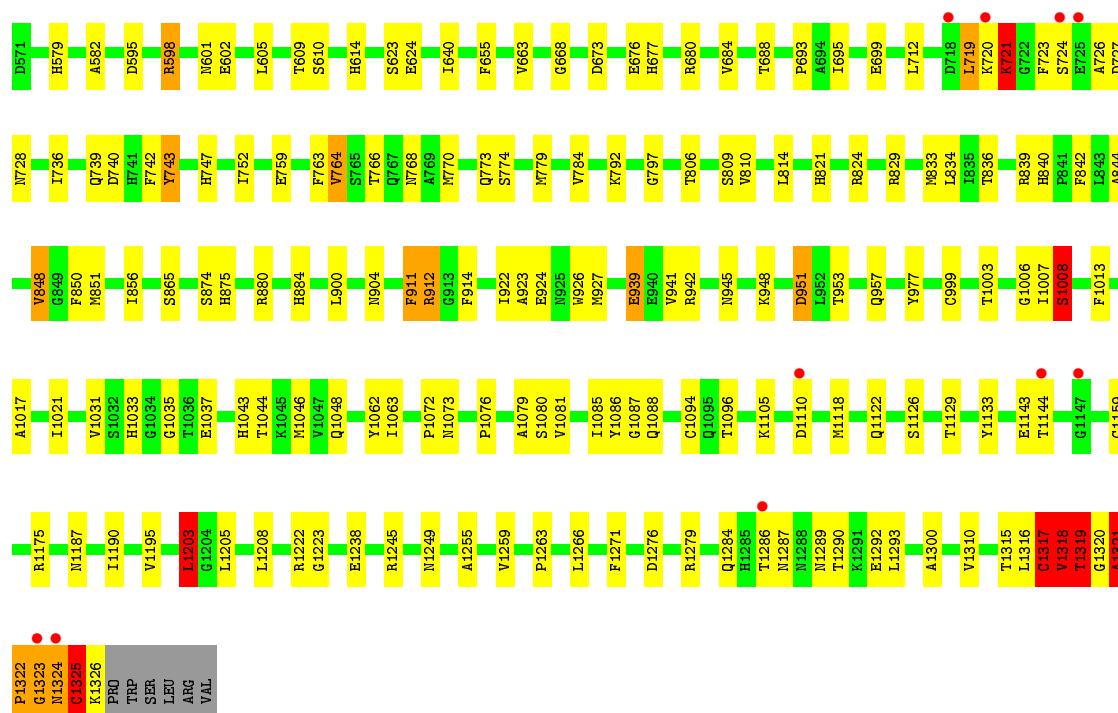
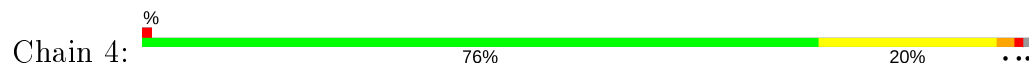


• Molecule 3: Xanthine dehydrogenase/oxidase





• Molecule 3: Xanthine dehydrogenase/oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.30Å 133.18Å 142.63Å 96.88° 93.11° 90.02°	Depositor
Resolution (Å)	33.08 – 2.60 33.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	72.7 (33.08-2.60) 72.7 (33.08-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.268 0.218 , 0.270	Depositor DCC
R_{free} test set	6008 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	38070	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MTE, XAN, FAD, MOM, FES

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	2	0.75	0/1277	0.82	0/1723
1	A	0.76	0/1265	0.80	1/1706 (0.1%)
1	J	0.75	0/1265	0.76	0/1706
1	S	0.72	0/1256	0.79	0/1695
2	3	0.71	0/2438	0.75	1/3290 (0.0%)
2	B	0.73	0/2434	0.76	1/3285 (0.0%)
2	K	0.72	0/2417	0.75	1/3263 (0.0%)
2	T	0.70	0/2438	0.75	1/3290 (0.0%)
3	4	0.77	1/5960 (0.0%)	0.80	6/8072 (0.1%)
3	C	0.76	2/5937 (0.0%)	0.82	6/8042 (0.1%)
3	L	0.76	1/5888 (0.0%)	0.79	1/7974 (0.0%)
3	U	0.76	3/5888 (0.1%)	0.78	3/7974 (0.0%)
All	All	0.75	7/38463 (0.0%)	0.79	21/52020 (0.0%)

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
2	B	0	1
3	4	0	4
3	C	0	2
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	748	CYS	CB-SG	-8.40	1.68	1.82
3	L	1166	CYS	CB-SG	-7.21	1.70	1.82
3	4	1094	CYS	CB-SG	-5.78	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1166	CYS	CB-SG	-5.64	1.72	1.81
3	C	992	CYS	CB-SG	-5.53	1.72	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	871	ARG	NE-CZ-NH2	-8.34	116.13	120.30
3	C	1318	VAL	N-CA-C	-8.09	89.17	111.00
3	4	1323	GLY	N-CA-C	-7.99	93.13	113.10
3	C	1315	THR	C-N-CA	-6.81	104.66	121.70
1	A	31	ARG	NE-CZ-NH1	6.81	123.71	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	1317	CYS	Peptide
3	4	1318	VAL	Peptide
2	B	285	PRO	Peptide
3	C	1317	CYS	Peptide
3	C	1318	VAL	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	2	1255	0	1265	21	0
1	A	1243	0	1253	18	0
1	J	1243	0	1253	18	0
1	S	1234	0	1240	21	0
2	3	2389	0	2459	42	0
2	B	2385	0	2456	49	0
2	K	2369	0	2435	44	0
2	T	2389	0	2459	34	0
3	4	5832	0	5759	172	0
3	C	5809	0	5737	154	0
3	L	5761	0	5685	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	5761	0	5685	132	0
4	2	8	0	0	0	0
4	A	8	0	0	2	0
4	J	8	0	0	0	0
4	S	8	0	0	0	0
5	3	53	0	31	2	0
5	B	53	0	31	1	0
5	K	53	0	31	3	0
5	T	53	0	31	2	0
6	4	24	0	10	0	0
6	C	24	0	10	0	0
6	L	24	0	10	1	0
6	U	24	0	10	0	0
7	4	4	0	0	2	0
7	C	4	0	0	2	0
7	L	4	0	0	2	0
7	U	4	0	0	3	0
8	4	11	0	4	1	0
8	C	11	0	4	1	0
8	L	11	0	4	1	0
8	U	11	0	4	2	0
All	All	38070	0	37866	782	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 10.

The worst 5 of 782 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)
3:4:1318:VAL:HG13	3:4:1319:THR:CG2	1.55	1.34
3:C:1316:LEU:O	3:C:1318:VAL:HB	1.41	1.20
3:L:924:GLU:OE1	3:L:942:ARG:NH1	1.78	1.14
2:K:241:THR:HG22	2:K:243:LYS:HE2	1.28	1.11
1:S:129:ARG:HG3	1:S:129:ARG:HH11	0.98	1.11

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	2	162/165 (98%)	149 (92%)	9 (6%)	4 (2%)	5	9
1	A	160/165 (97%)	150 (94%)	8 (5%)	2 (1%)	12	24
1	J	160/165 (97%)	151 (94%)	6 (4%)	3 (2%)	8	15
1	S	159/165 (96%)	146 (92%)	7 (4%)	6 (4%)	3	4
2	3	303/305 (99%)	283 (93%)	17 (6%)	3 (1%)	15	32
2	B	302/305 (99%)	282 (93%)	17 (6%)	3 (1%)	15	32
2	K	300/305 (98%)	276 (92%)	22 (7%)	2 (1%)	22	43
2	T	303/305 (99%)	284 (94%)	16 (5%)	3 (1%)	15	32
3	4	754/762 (99%)	702 (93%)	42 (6%)	10 (1%)	12	24
3	C	751/762 (99%)	714 (95%)	23 (3%)	14 (2%)	8	15
3	L	743/762 (98%)	707 (95%)	30 (4%)	6 (1%)	19	39
3	U	743/762 (98%)	701 (94%)	37 (5%)	5 (1%)	22	43
All	All	4840/4928 (98%)	4545 (94%)	234 (5%)	61 (1%)	12	24

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	425	SER
3	C	1008	SER
3	C	1318	VAL
3	C	1319	THR
3	C	1321	ALA

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	2	137/138 (99%)	130 (95%)	7 (5%)	24	46
1	A	136/138 (99%)	126 (93%)	10 (7%)	13	28
1	J	136/138 (99%)	126 (93%)	10 (7%)	13	28
1	S	135/138 (98%)	128 (95%)	7 (5%)	23	46
2	3	261/261 (100%)	242 (93%)	19 (7%)	14	28
2	B	261/261 (100%)	245 (94%)	16 (6%)	18	38
2	K	259/261 (99%)	246 (95%)	13 (5%)	24	47
2	T	261/261 (100%)	247 (95%)	14 (5%)	22	44
3	4	632/638 (99%)	606 (96%)	26 (4%)	30	56
3	C	629/638 (99%)	604 (96%)	25 (4%)	31	57
3	L	624/638 (98%)	603 (97%)	21 (3%)	37	63
3	U	624/638 (98%)	597 (96%)	27 (4%)	29	54
All	All	4095/4148 (99%)	3900 (95%)	195 (5%)	25	49

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	1134	ARG
2	T	395	LYS
3	4	848	VAL
3	L	1203	LEU
1	S	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	1048	GLN
2	T	273	GLN
3	4	884	HIS
3	L	1108	ASN
3	L	1285	HIS

5.3.3 RNA ⓘ

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](#)

24 ligands are 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
6	MTE	U	1333	7	21,26,26	1.57	2 (9%)	21,40,40	2.73	12 (57%)
5	FAD	3	606	-	51,58,58	1.67	8 (15%)	60,89,89	1.84	13 (21%)
4	FES	S	601	1	0,4,4	0.00	-	-		
7	MOM	L	1334	6	0,3,3	0.00	-	-		
4	FES	J	601	1	0,4,4	0.00	-	-		
7	MOM	U	1334	6	0,3,3	0.00	-	-		
5	FAD	T	606	-	51,58,58	1.49	5 (9%)	60,89,89	1.70	9 (15%)
8	XAN	4	7319	-	8,12,12	2.14	2 (25%)	4,17,17	5.03	4 (100%)
6	MTE	C	1333	7	21,26,26	1.80	2 (9%)	21,40,40	3.16	9 (42%)
7	MOM	C	1334	6	0,3,3	0.00	-	-		
8	XAN	U	7319	-	8,12,12	1.72	2 (25%)	4,17,17	5.34	3 (75%)
8	XAN	L	7319	-	8,12,12	1.78	2 (25%)	4,17,17	5.19	3 (75%)
6	MTE	L	1333	7	21,26,26	1.45	2 (9%)	21,40,40	2.39	6 (28%)
4	FES	J	602	1	0,4,4	0.00	-	-		
4	FES	S	602	1	0,4,4	0.00	-	-		
6	MTE	4	1333	7	21,26,26	1.82	2 (9%)	21,40,40	2.64	8 (38%)
5	FAD	K	606	-	51,58,58	1.33	6 (11%)	60,89,89	1.75	10 (16%)
8	XAN	C	7319	-	8,12,12	2.02	2 (25%)	4,17,17	5.09	3 (75%)
4	FES	2	601	1	0,4,4	0.00	-	-		
7	MOM	4	1334	6	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	B	606	-	51,58,58	1.53	7 (13%)	60,89,89	1.91	12 (20%)
4	FES	2	602	1	0,4,4	0.00	-	-		
4	FES	A	601	1	0,4,4	0.00	-	-		
4	FES	A	602	1	0,4,4	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MTE	L	1333	7	-	1/6/34/34	0/3/3/3
5	FAD	3	606	-	-	7/30/50/50	0/6/6/6
5	FAD	B	606	-	-	4/30/50/50	0/6/6/6
4	FES	J	602	1	-	-	0/1/1/1
4	FES	S	602	1	-	-	0/1/1/1
4	FES	S	601	1	-	-	0/1/1/1
6	MTE	4	1333	7	-	1/6/34/34	0/3/3/3
6	MTE	U	1333	7	-	3/6/34/34	0/3/3/3
4	FES	J	601	1	-	-	0/1/1/1
8	XAN	L	7319	-	-	-	0/2/2/2
4	FES	2	602	1	-	-	0/1/1/1
5	FAD	T	606	-	-	4/30/50/50	0/6/6/6
8	XAN	4	7319	-	-	-	0/2/2/2
4	FES	2	601	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1
6	MTE	C	1333	7	-	1/6/34/34	0/3/3/3
4	FES	A	602	1	-	-	0/1/1/1
8	XAN	C	7319	-	-	-	0/2/2/2
5	FAD	K	606	-	-	5/30/50/50	0/6/6/6
8	XAN	U	7319	-	-	-	0/2/2/2

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	1333	MTE	C4-C9	6.27	1.50	1.41
6	C	1333	MTE	C4-C9	5.94	1.49	1.41
5	3	606	FAD	C4X-N5	5.77	1.41	1.33
6	U	1333	MTE	C4-C9	5.15	1.48	1.41
8	4	7319	XAN	C6-C5	4.83	1.49	1.41

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	7319	XAN	C6-N1-C2	8.91	122.66	115.14
6	C	1333	MTE	C4-C9-N5	8.85	126.55	119.12
8	L	7319	XAN	C6-N1-C2	8.49	122.31	115.14
8	C	7319	XAN	C6-N1-C2	8.02	121.92	115.14
8	4	7319	XAN	C6-N1-C2	7.88	121.79	115.14

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1333	MTE	C2'-C3'-C4'-O4'
6	U	1333	MTE	O3'-C3'-C4'-O4'
5	3	606	FAD	C5B-O5B-PA-O1A
5	3	606	FAD	C5B-O5B-PA-O2A
5	3	606	FAD	C5B-O5B-PA-O3P

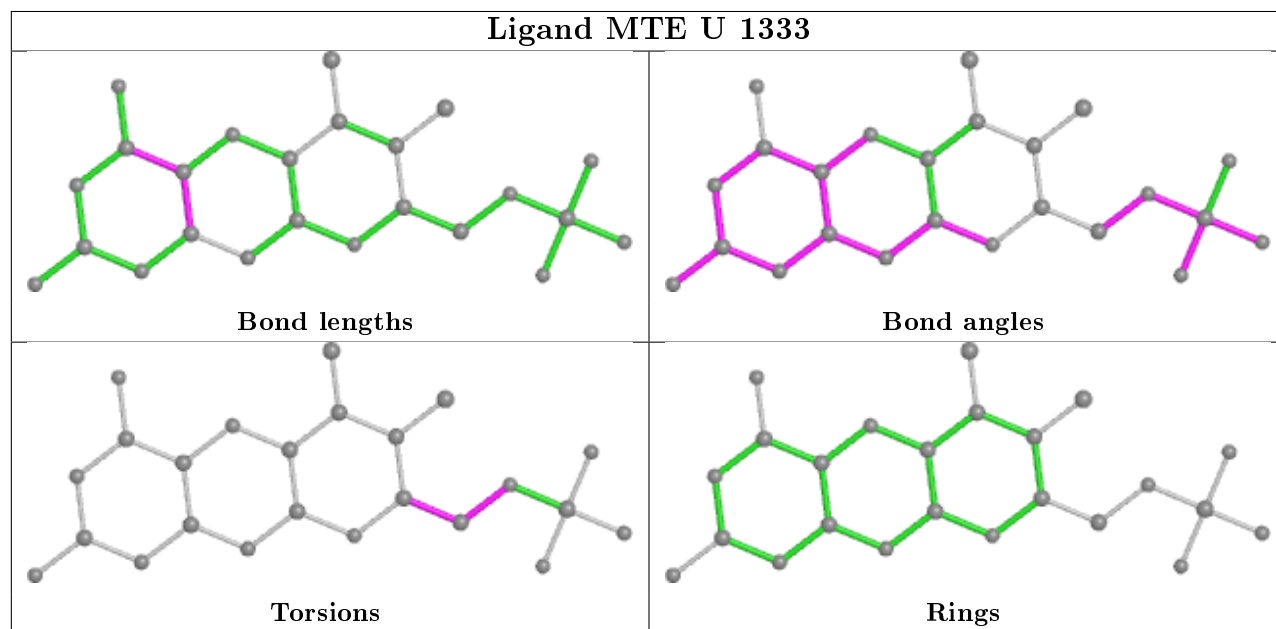
There are no ring outliers.

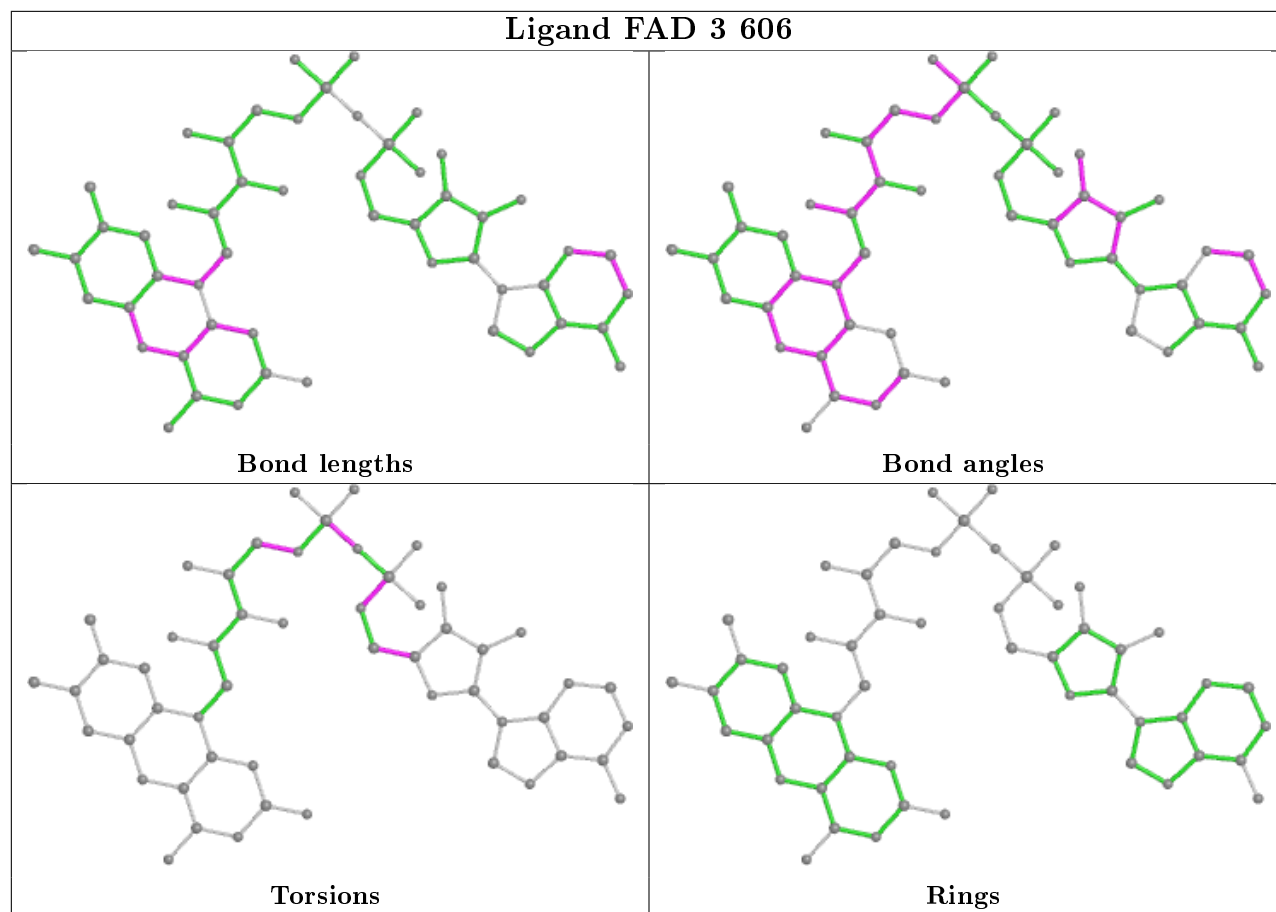
15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	606	FAD	2	0
7	L	1334	MOM	2	0
7	U	1334	MOM	3	0
5	T	606	FAD	2	0
8	4	7319	XAN	1	0
7	C	1334	MOM	2	0
8	U	7319	XAN	2	0
8	L	7319	XAN	1	0
6	L	1333	MTE	1	0
5	K	606	FAD	3	0
8	C	7319	XAN	1	0
7	4	1334	MOM	2	0
5	B	606	FAD	1	0
4	A	601	FES	1	0
4	A	602	FES	1	0

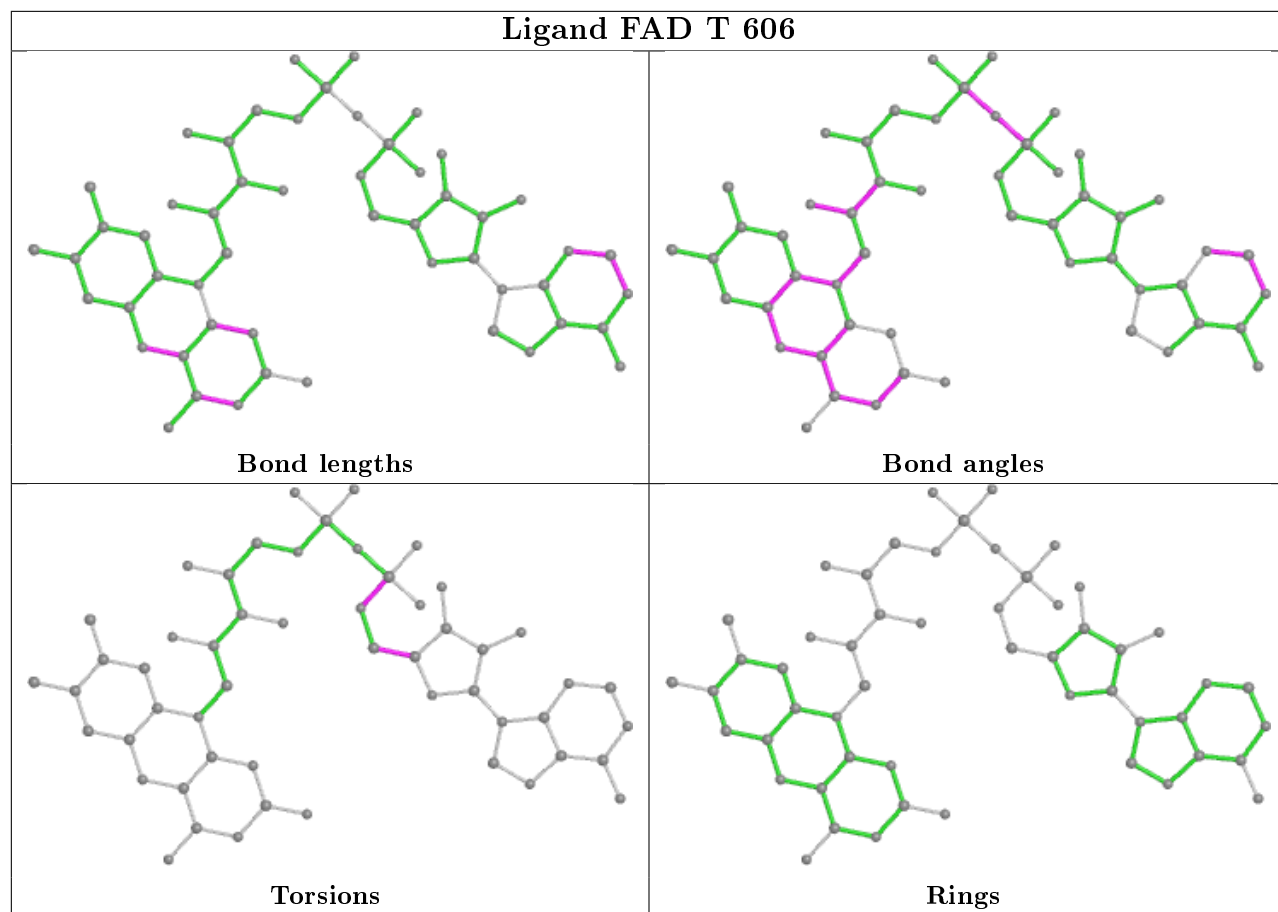
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

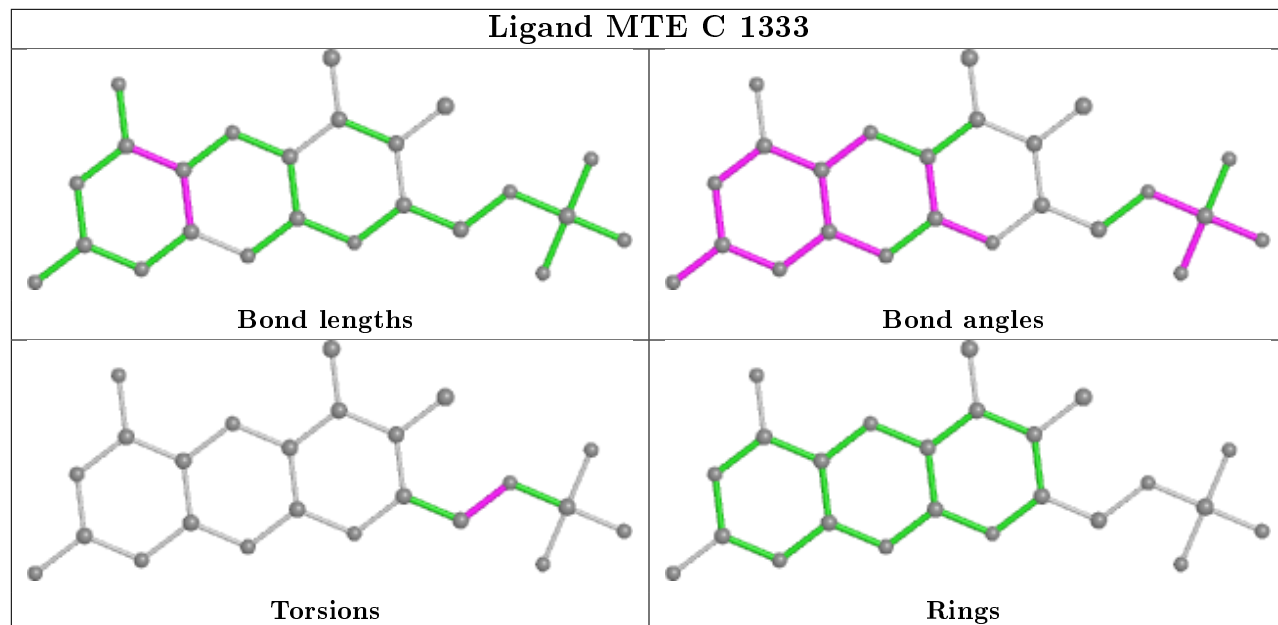




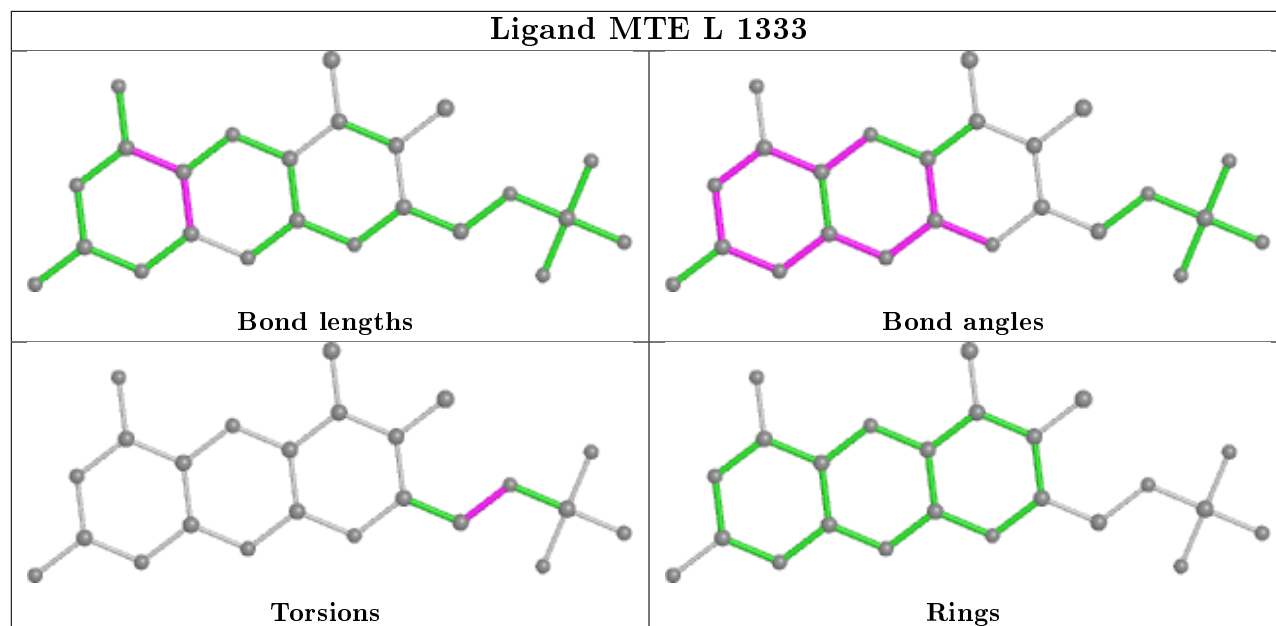
Ligand FAD T 606



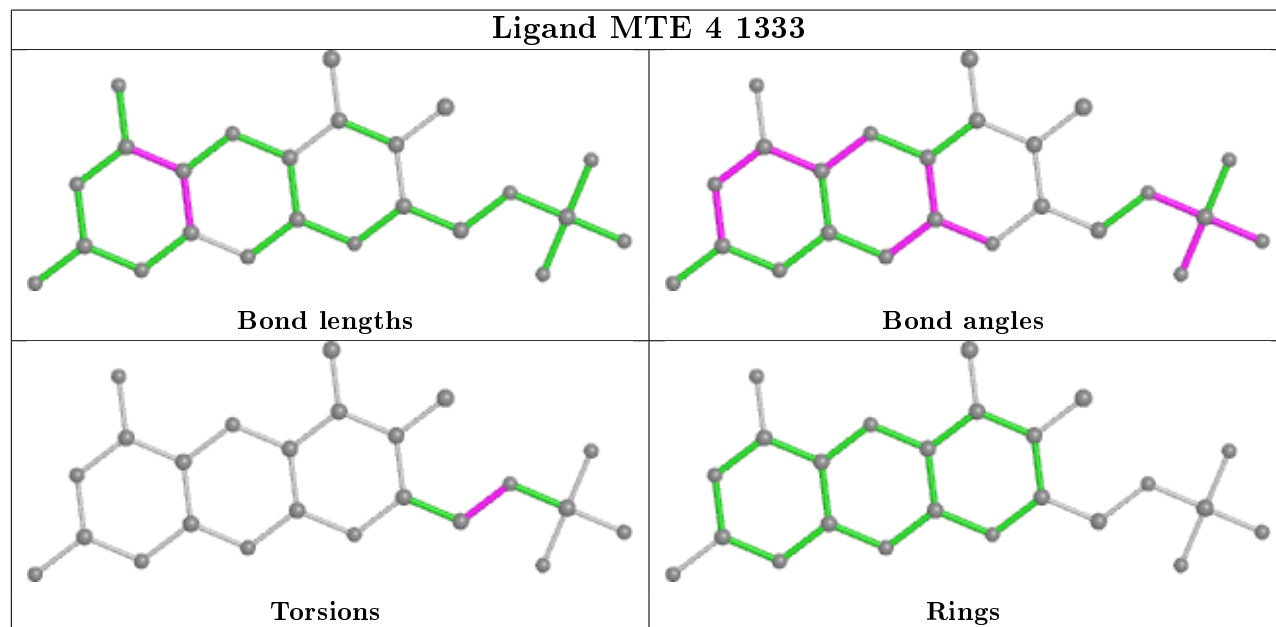
Ligand MTE C 1333

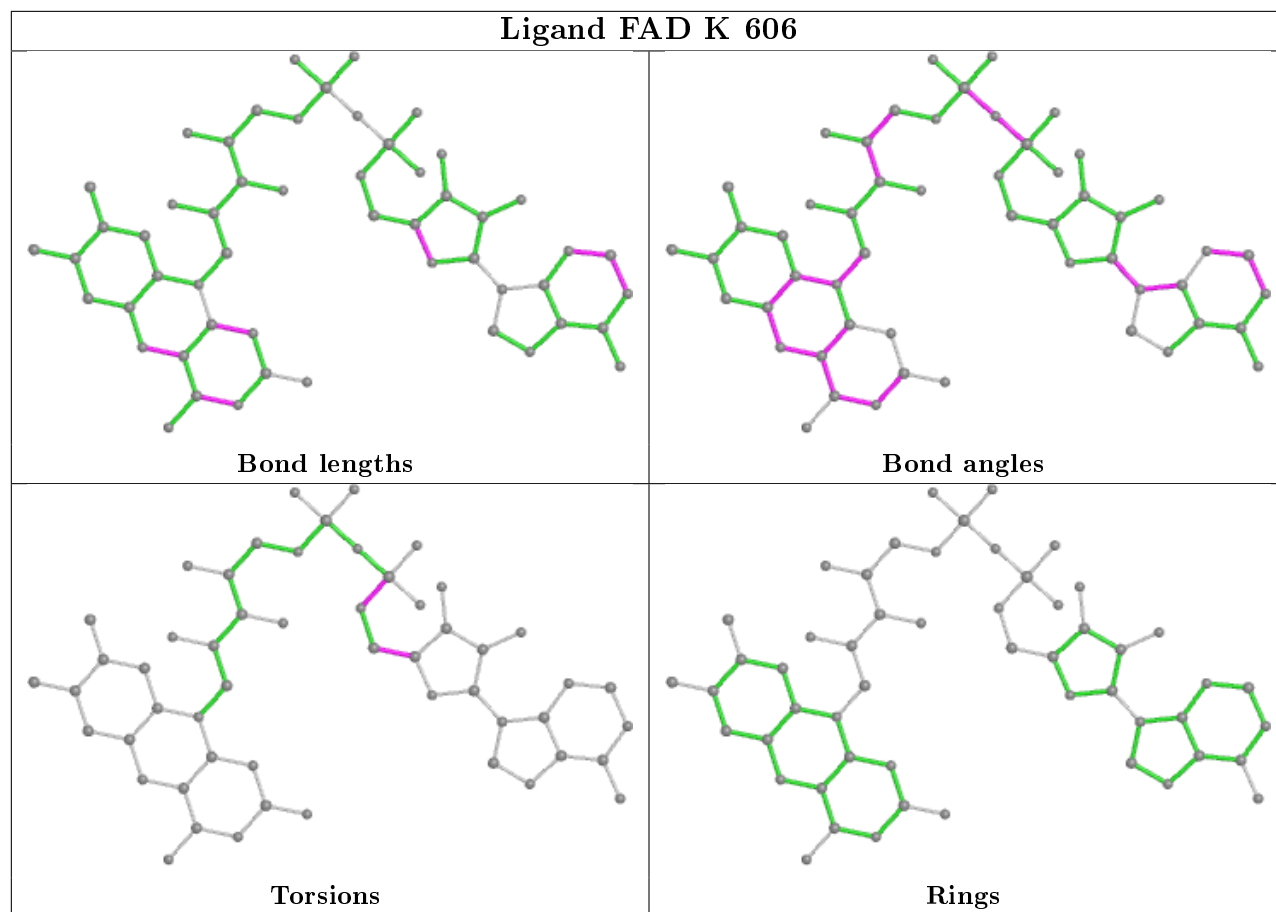


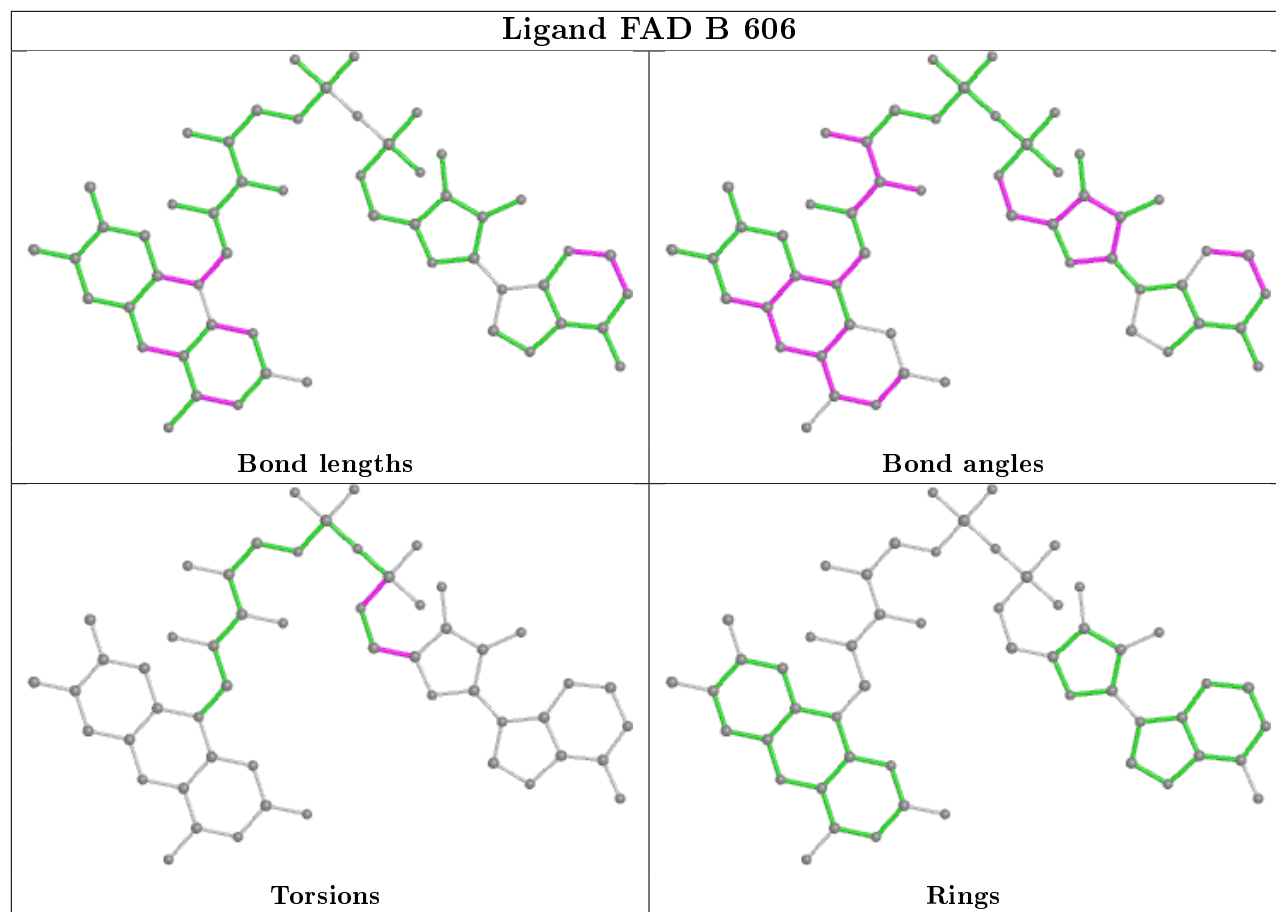
Ligand MTE L 1333



Ligand MTE 4 1333







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	2	164/165 (99%)	-0.21	5 (3%)	50	43	4, 10, 30, 43	0
1	A	162/165 (98%)	-0.20	5 (3%)	49	42	2, 9, 27, 41	0
1	J	162/165 (98%)	-0.25	6 (3%)	41	34	3, 9, 27, 41	0
1	S	161/165 (97%)	-0.22	5 (3%)	49	42	4, 10, 28, 43	0
2	3	305/305 (100%)	-0.08	5 (1%)	72	68	5, 18, 28, 34	0
2	B	304/305 (99%)	-0.02	9 (2%)	50	43	7, 17, 27, 35	0
2	K	302/305 (99%)	-0.06	7 (2%)	60	54	7, 17, 27, 35	0
2	T	305/305 (100%)	-0.03	8 (2%)	56	50	6, 18, 28, 34	0
3	4	756/762 (99%)	-0.13	10 (1%)	77	73	2, 12, 25, 39	0
3	C	753/762 (98%)	-0.19	13 (1%)	70	66	2, 10, 25, 42	0
3	L	745/762 (97%)	-0.21	13 (1%)	70	66	2, 10, 24, 40	0
3	U	745/762 (97%)	-0.19	13 (1%)	70	66	2, 11, 24, 37	0
All	All	4864/4928 (98%)	-0.15	99 (2%)	65	60	2, 12, 26, 43	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1288	ASN	4.9
3	U	1290	THR	4.6
3	L	1290	THR	4.2
3	U	1288	ASN	4.2
3	C	1110	ASP	4.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

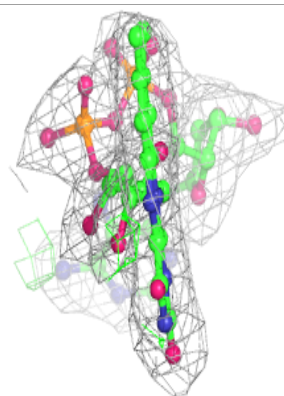
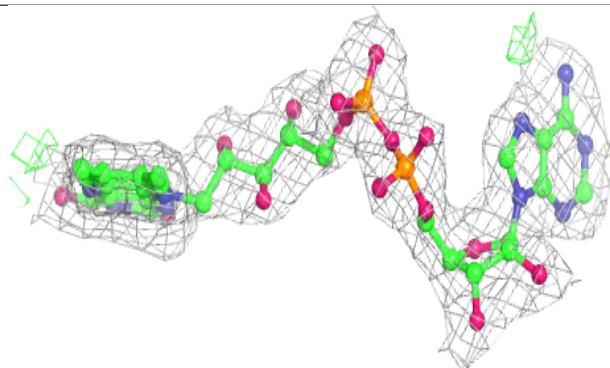
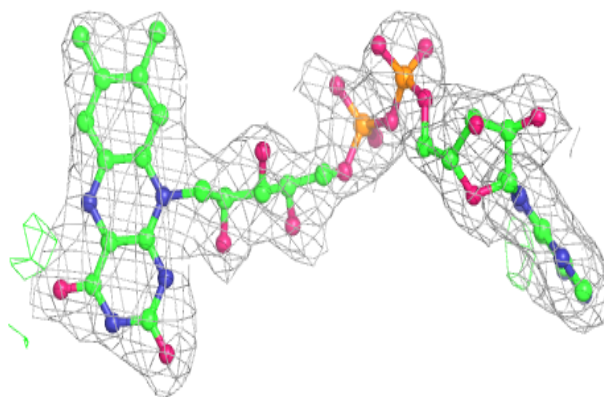
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	XAN	U	7319	11/11	0.87	0.24	40,41,41,41	0
8	XAN	L	7319	11/11	0.91	0.19	31,32,33,33	0
8	XAN	4	7319	11/11	0.94	0.18	33,34,34,35	0
8	XAN	C	7319	11/11	0.94	0.18	26,27,28,28	0
5	FAD	3	606	53/53	0.97	0.12	2,5,9,13	0
6	MTE	U	1333	24/24	0.97	0.14	7,10,15,15	0
6	MTE	L	1333	24/24	0.97	0.12	6,8,13,14	0
6	MTE	4	1333	24/24	0.97	0.13	12,13,15,16	0
6	MTE	C	1333	24/24	0.97	0.13	7,11,15,17	0
5	FAD	B	606	53/53	0.97	0.12	2,4,8,8	0
5	FAD	T	606	53/53	0.98	0.12	2,8,13,16	0
5	FAD	K	606	53/53	0.98	0.11	4,8,12,12	0
4	FES	J	601	4/4	0.99	0.09	2,2,2,2	0
4	FES	J	602	4/4	0.99	0.08	2,3,3,4	0
4	FES	2	601	4/4	0.99	0.08	2,2,3,5	0
4	FES	S	602	4/4	0.99	0.07	4,4,6,9	0
4	FES	S	601	4/4	0.99	0.06	4,5,9,10	0
4	FES	2	602	4/4	0.99	0.07	2,3,5,5	0
4	FES	A	601	4/4	0.99	0.08	2,3,4,8	0
4	FES	A	602	4/4	0.99	0.07	2,2,3,4	0
7	MOM	C	1334	4/4	1.00	0.08	16,16,17,20	0
7	MOM	U	1334	4/4	1.00	0.07	12,14,15,15	0
7	MOM	4	1334	4/4	1.00	0.10	12,12,14,18	0
7	MOM	L	1334	4/4	1.00	0.08	12,15,15,16	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.

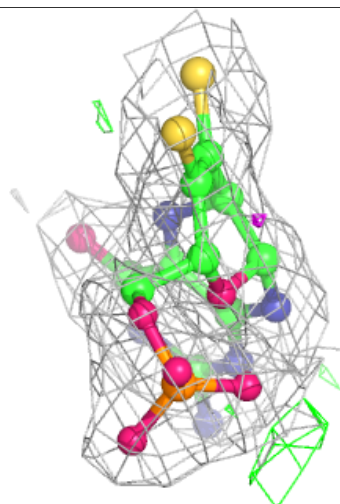
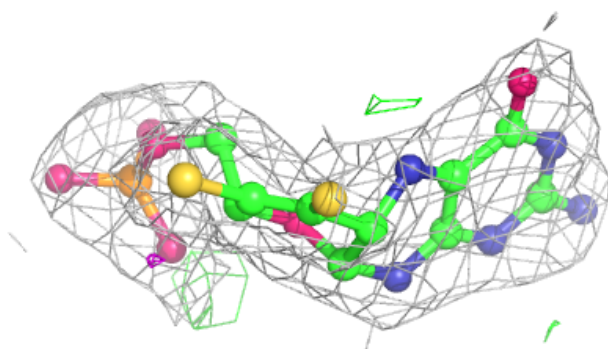
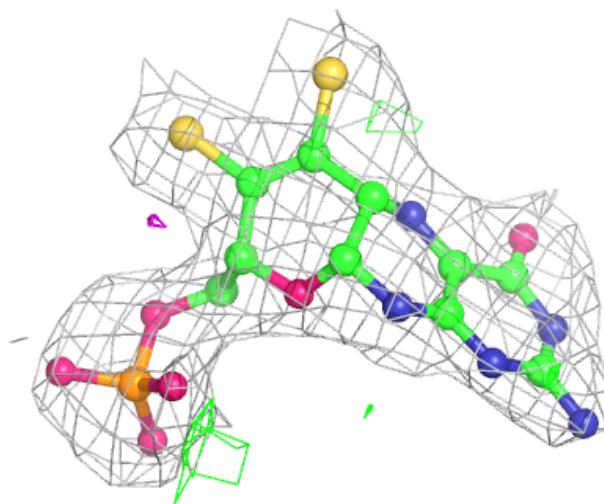
Electron density around FAD 3 606:

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



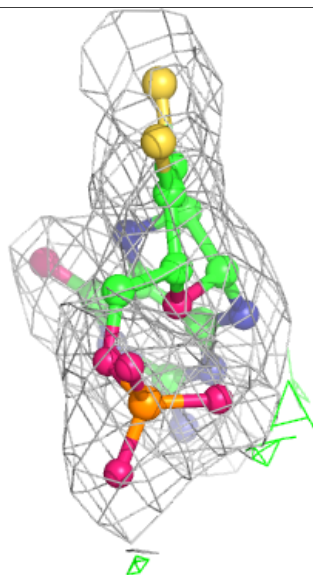
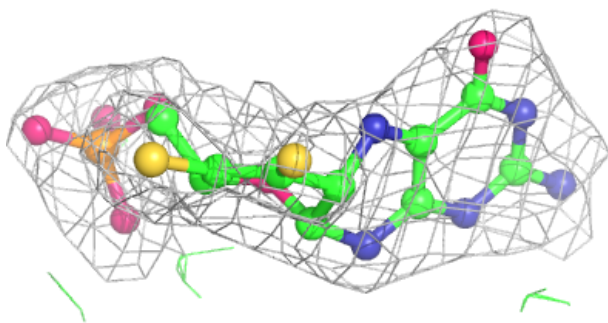
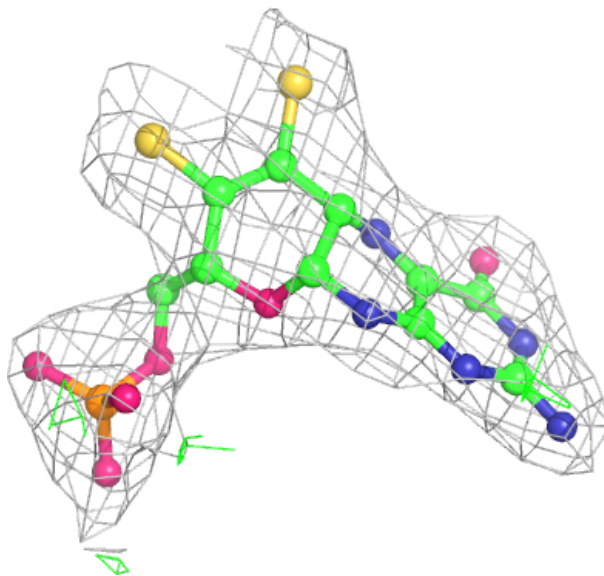
Electron density around MTE U 1333:

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



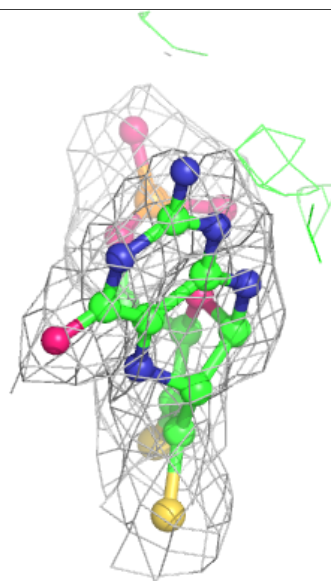
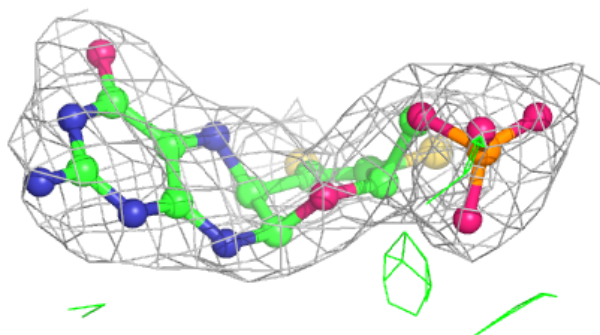
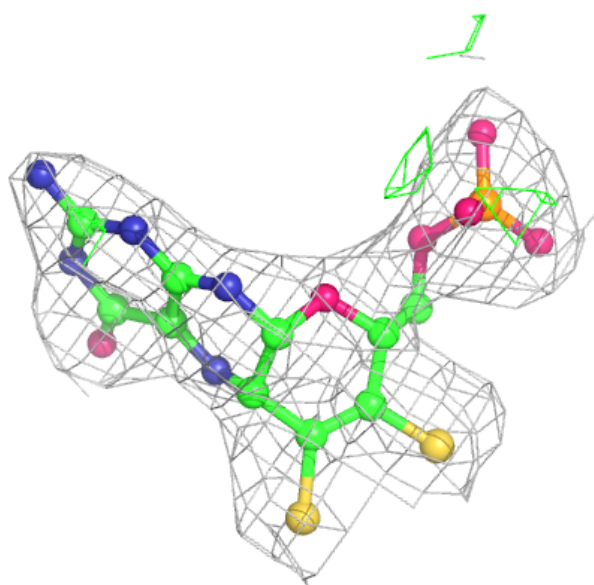
Electron density around MTE L 1333:

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



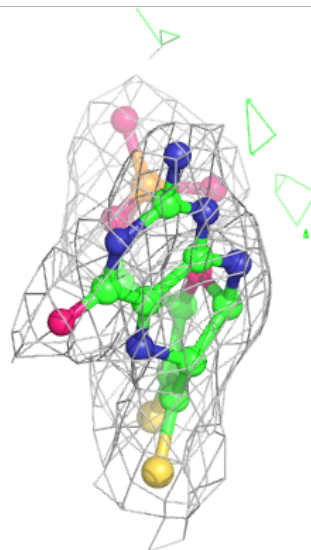
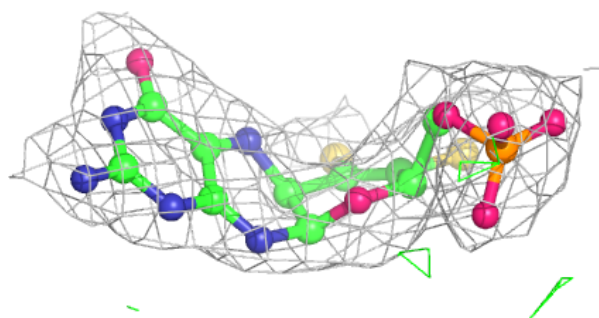
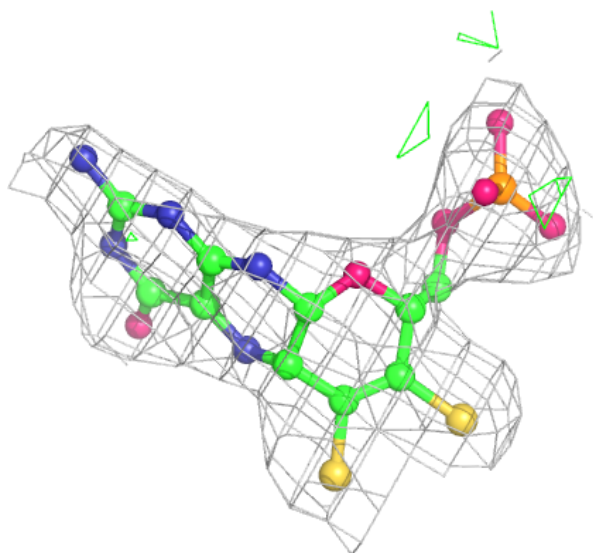
Electron density around MTE 4 1333:

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



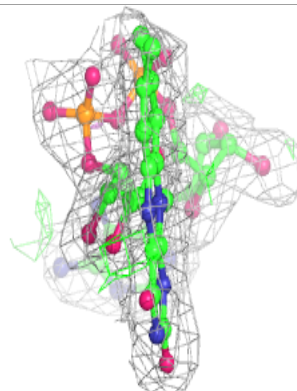
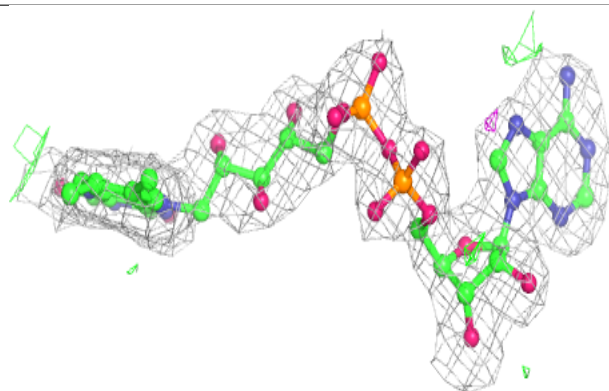
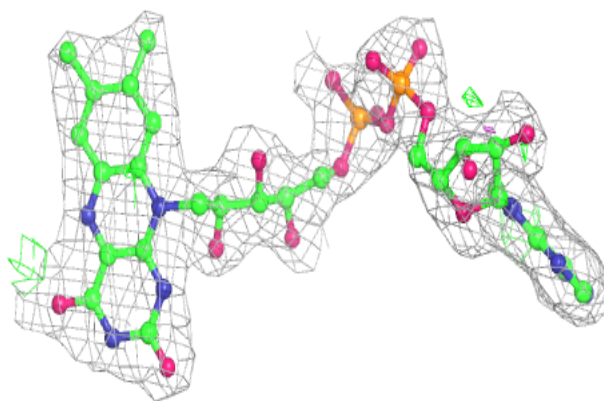
Electron density around MTE C 1333:

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

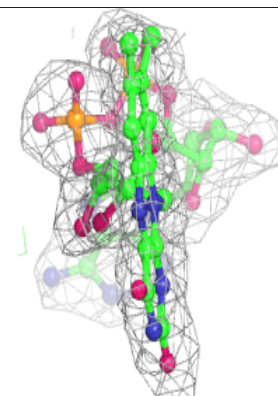
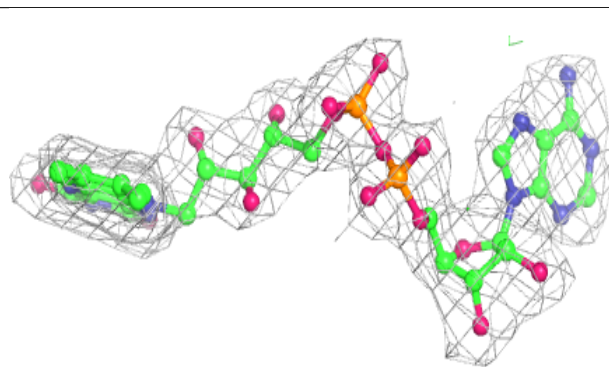
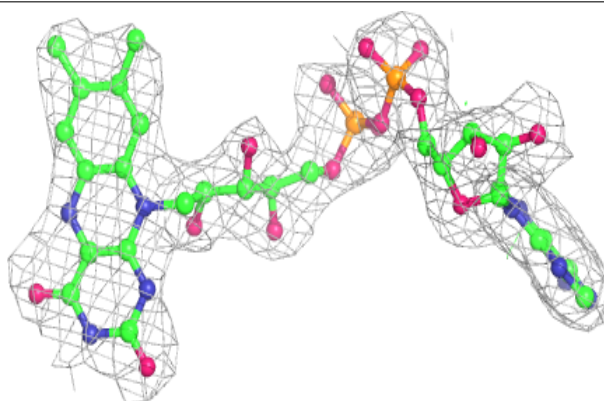


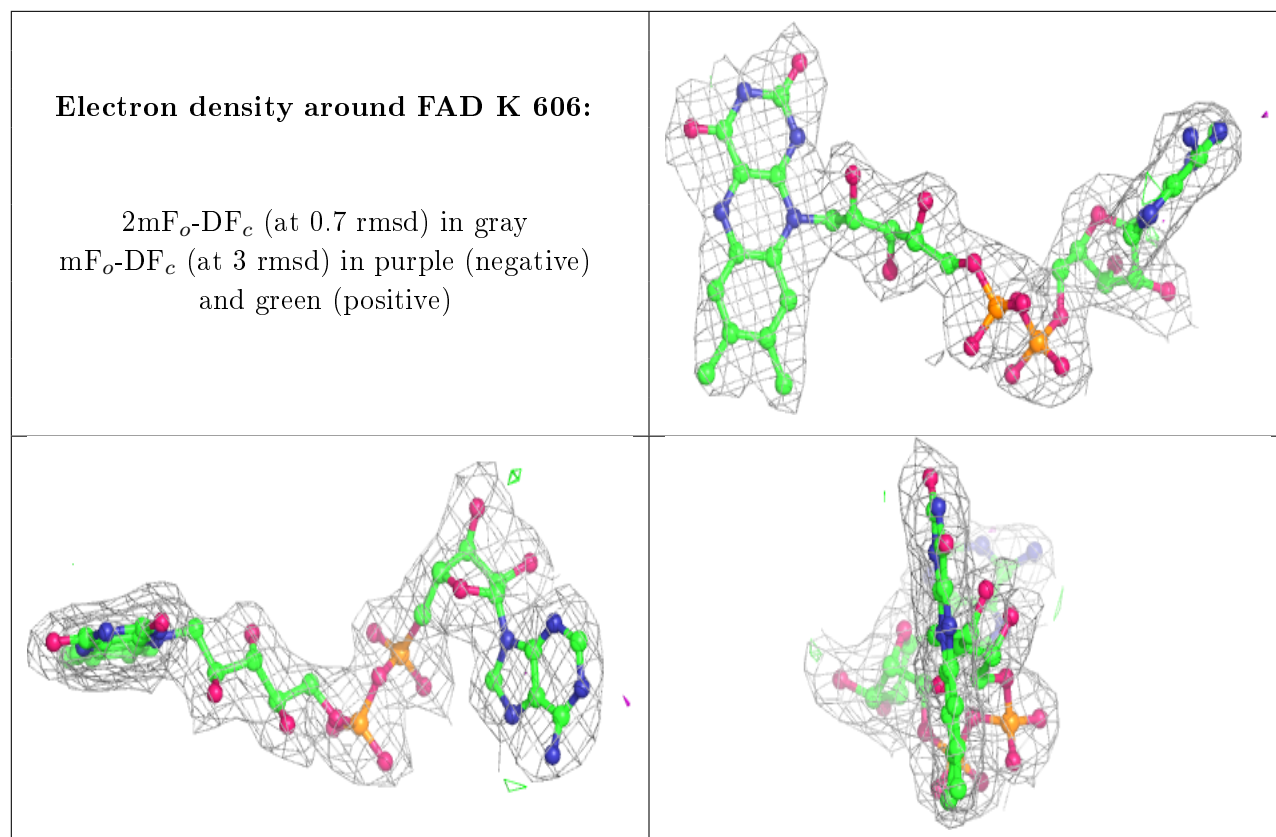
Electron density around FAD B 606:

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

**Electron density around FAD T 606:**

$2mF_o-DF_c$ (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.