



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:25 PM UTC

PDB ID : 3EUB / pdb_00003eub
Title : Crystal Structure of Desulfo-Xanthine Oxidase with Xanthine
Authors : Pauff, 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

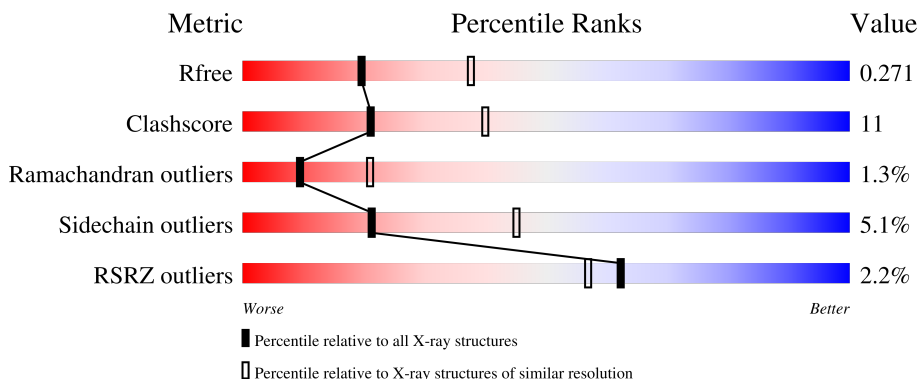
1 Overall quality at a glance

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.





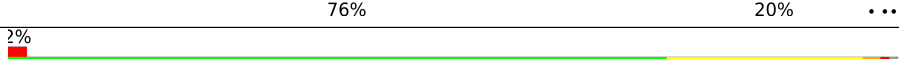
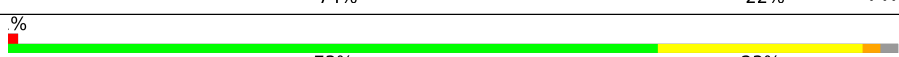
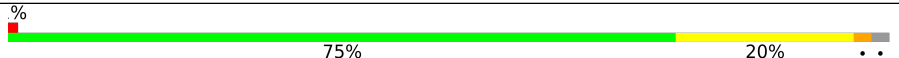
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	165	 5% 79% 16% ...
1	A	165	 5% 78% 18% ...
1	J	165	 % 79% 16% ..
1	S	165	 3% 79% 14% ...
2	3	305	 2% 77% 19% .

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Mol	Chain	Length	Quality of chain	
2	B	305	3% 	76% 20% •
2	K	305	2% 	77% 20% ••
2	T	305	3% 	81% 16% •
3	4	762	2% 	76% 20% •••
3	C	762	2% 	74% 22% •••
3	L	762	% 	73% 23% ••
3	U	762	% 	75% 20% ••

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 [i](#)

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
			Total	C	N	O	S			
1	A	162	1243	781	223	227	12	0	0	0
1	J	162	1243	781	223	227	12	0	0	0
1	S	161	1234	775	221	226	12	0	0	0
1	2	164	1255	788	225	230	12	0	0	0

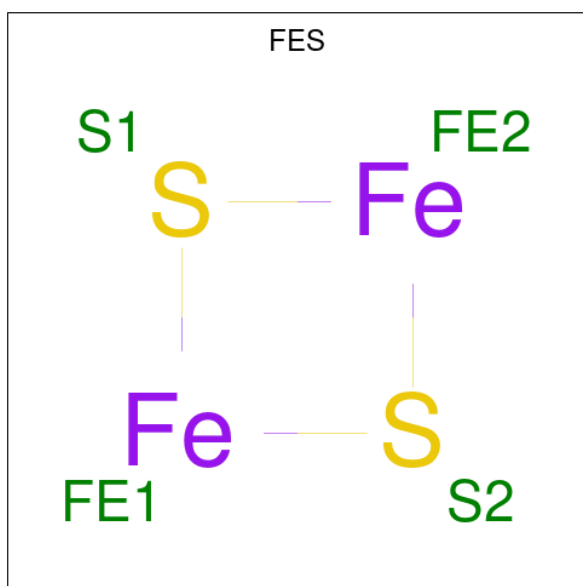
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	304	2385	1537	401	434	13	0	0	0
2	K	302	2369	1526	398	432	13	0	0	0
2	T	305	2389	1539	402	435	13	0	0	0
2	3	305	2389	1539	402	435	13	0	0	0

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

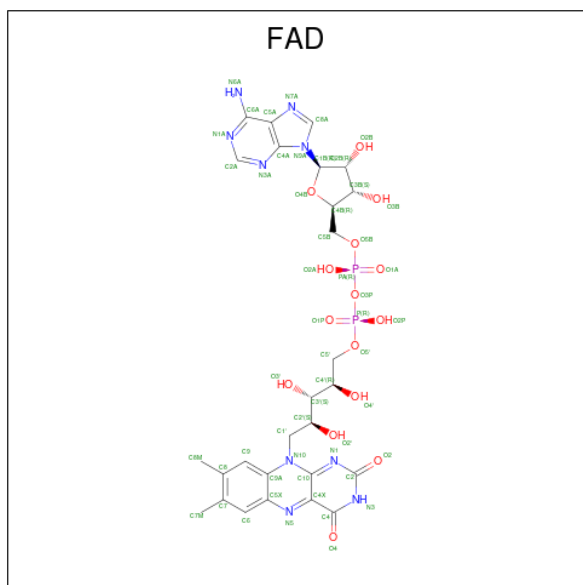
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	753	5809	3673	1001	1101	34	0	0	0
3	L	745	5761	3643	992	1093	33	0	0	0
3	U	745	5761	3643	992	1093	33	0	0	0
3	4	756	5832	3686	1005	1106	35	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



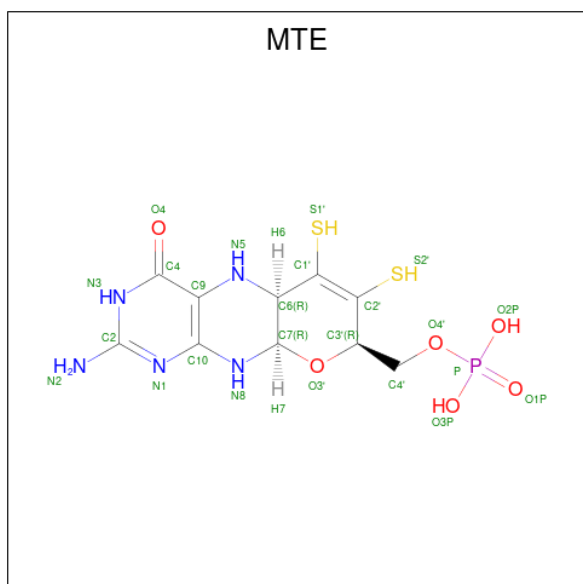
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0
4	S	1	Total Fe S 4 2 2	0	0
4	S	1	Total Fe S 4 2 2	0	0
4	2	1	Total Fe S 4 2 2	0	0
4	2	1	Total Fe S 4 2 2	0	0

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



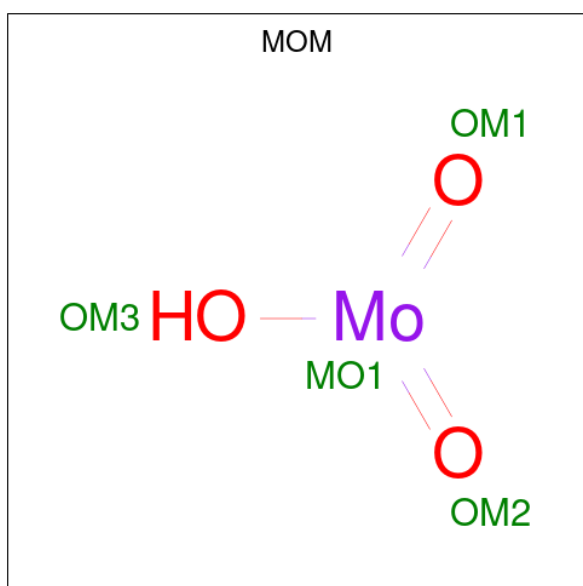
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	T	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	3	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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 (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



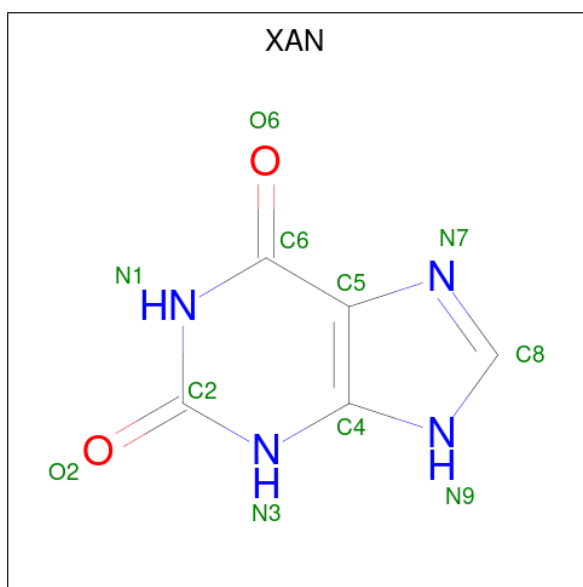
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	L	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	U	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	4	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (CCD ID: MOM) (formula: HMoO₃).



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

- Molecule 8 is XANTHINE (CCD ID: XAN) (formula: C₅H₄N₄O₂).

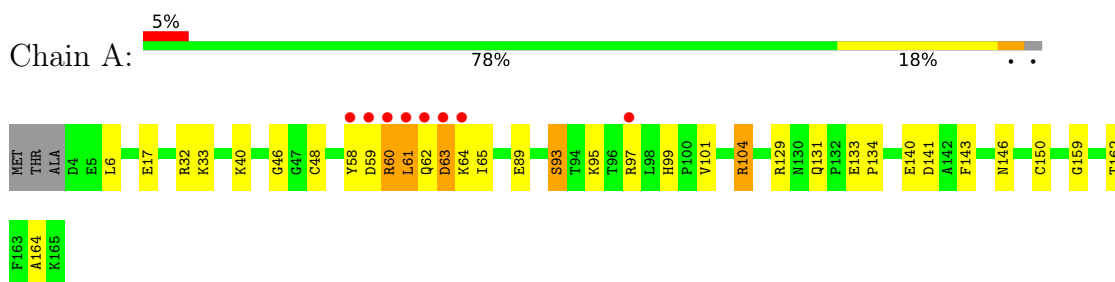


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	C	1	Total 11	5	4	2	0	0
8	L	1	Total 11	5	4	2	0	0
8	U	1	Total 11	5	4	2	0	0
8	4	1	Total 11	5	4	2	0	0

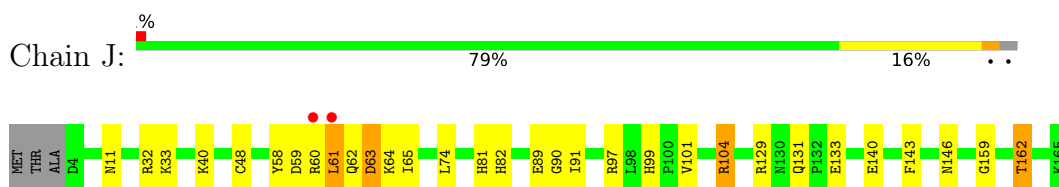
3 Residue-property plots [i](#)

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

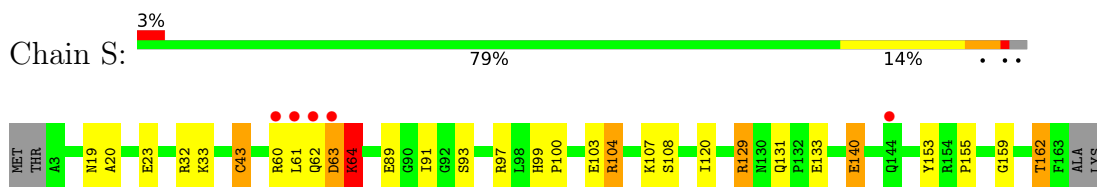
- Molecule 1: Xanthine dehydrogenase/oxidase



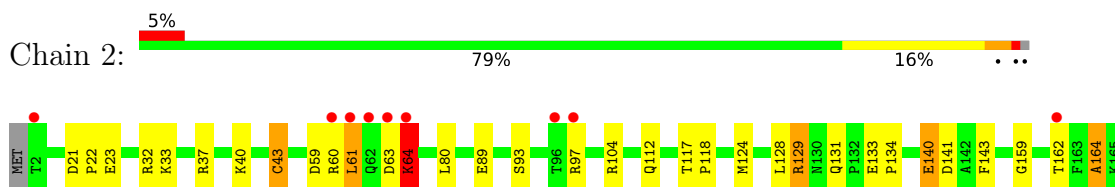
- Molecule 1: Xanthine dehydrogenase/oxidase



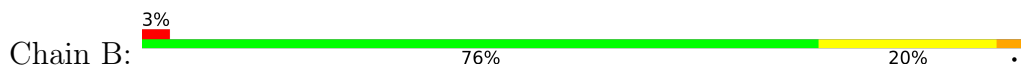
- Molecule 1: Xanthine dehydrogenase/oxidase

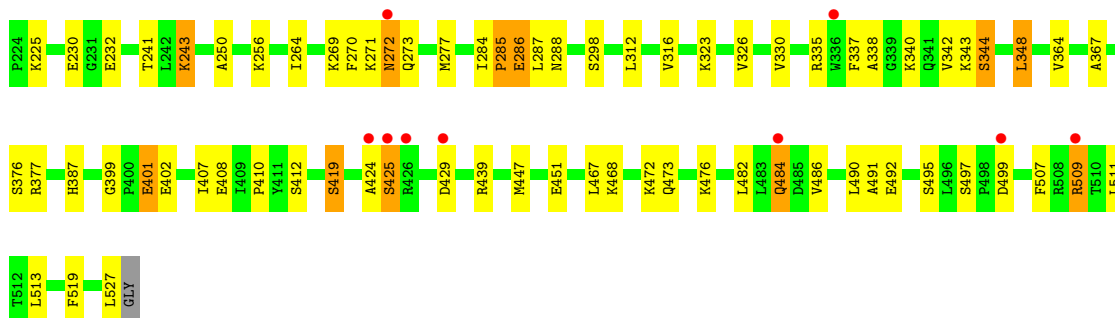


- Molecule 1: Xanthine dehydrogenase/oxidase

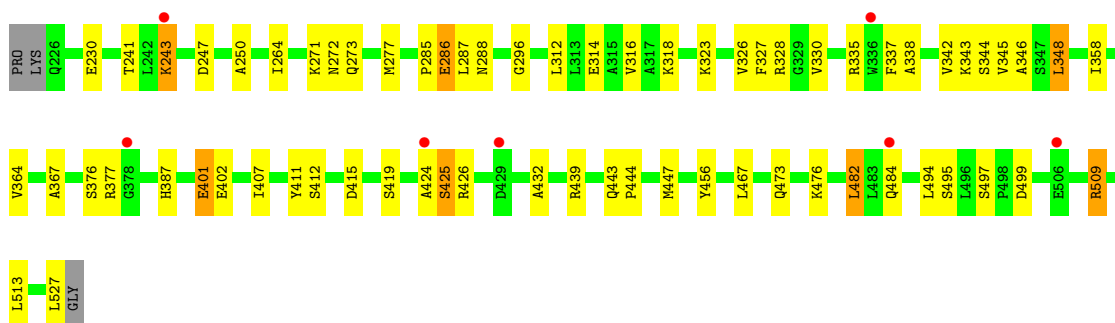
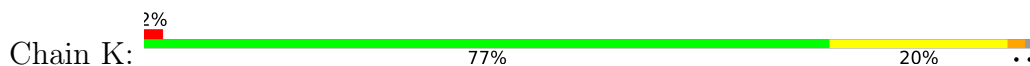


- Molecule 2: Xanthine dehydrogenase/oxidase

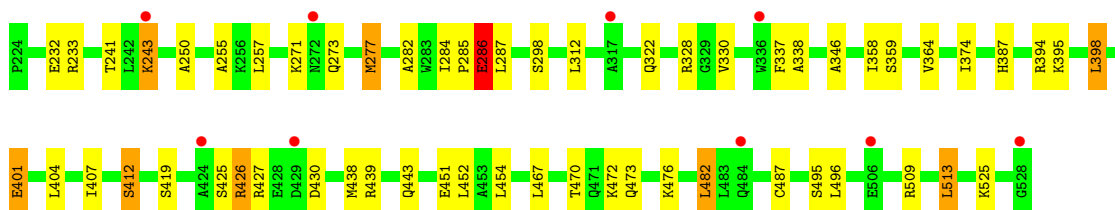
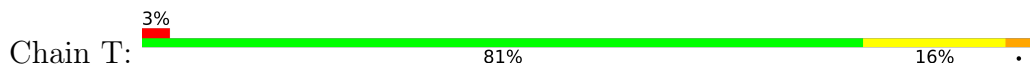




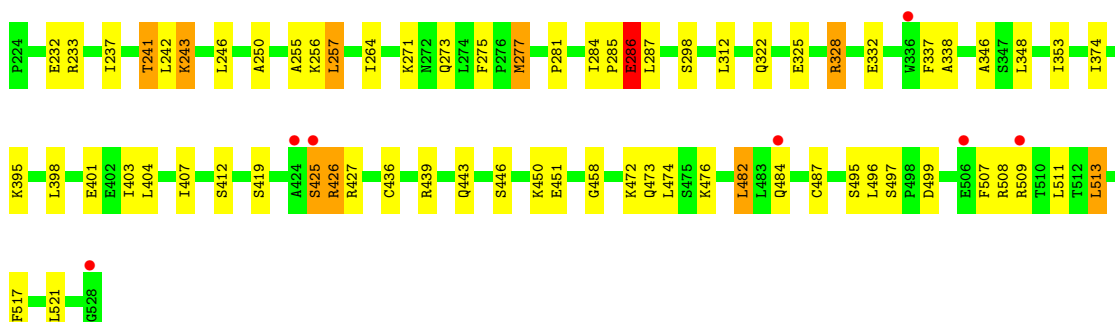
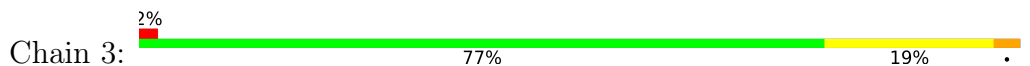
● Molecule 2: Xanthine dehydrogenase/oxidase



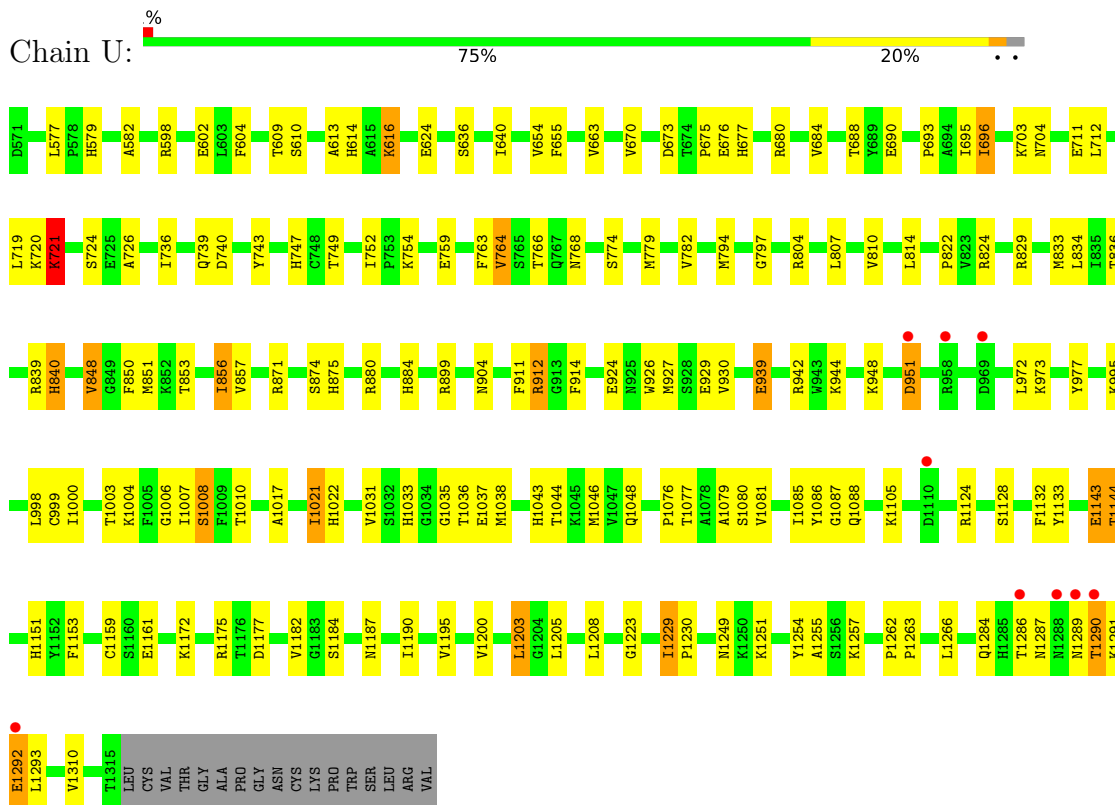
● Molecule 2: Xanthine dehydrogenase/oxidase



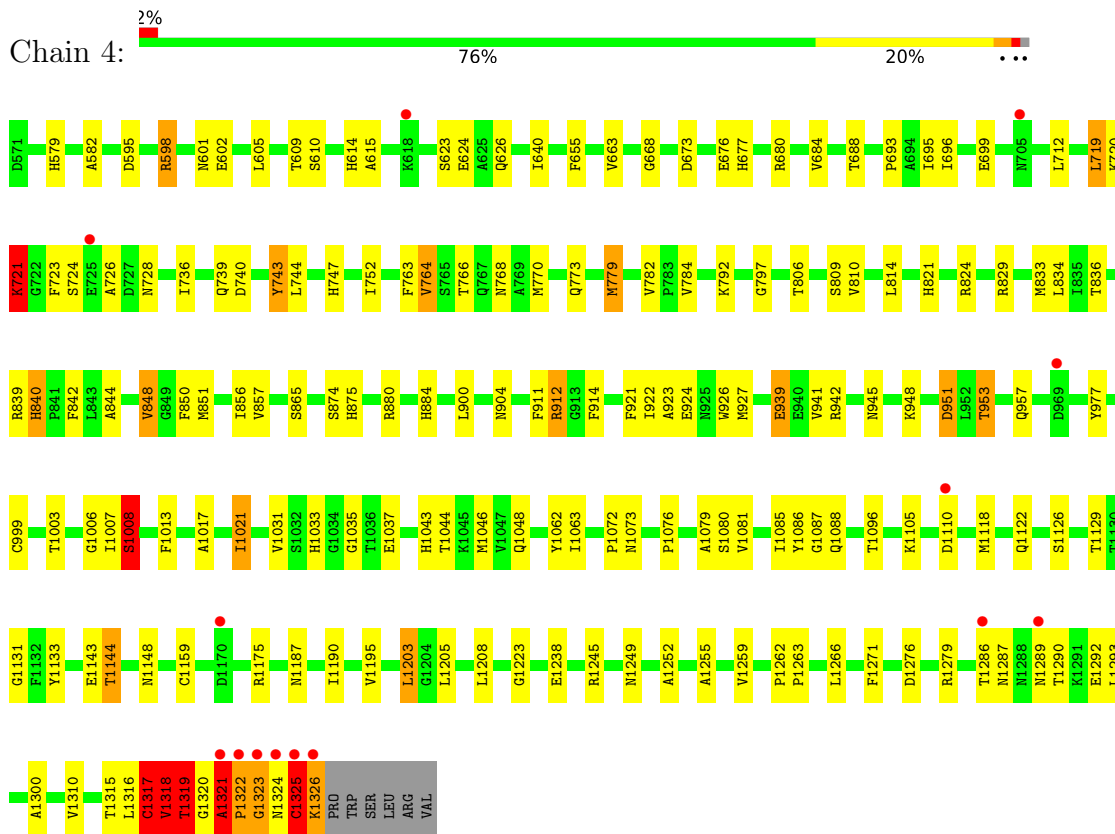
● Molecule 2: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



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)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.268 0.218 , 0.271	Depositor DCC
R_{free} test set	6008 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	38070	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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

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	0.93	1/1277 (0.1%)	1.04	1/1723 (0.1%)
1	A	0.93	0/1265	1.04	1/1706 (0.1%)
1	J	0.89	0/1265	1.00	0/1706
1	S	0.88	0/1256	1.01	0/1695
2	3	0.85	0/2438	1.03	2/3290 (0.1%)
2	B	0.88	0/2434	1.05	4/3285 (0.1%)
2	K	0.85	1/2417 (0.0%)	1.01	2/3263 (0.1%)
2	T	0.85	0/2438	1.04	1/3290 (0.0%)
3	4	0.94	1/5960 (0.0%)	1.09	17/8072 (0.2%)
3	C	0.92	2/5937 (0.0%)	1.11	20/8042 (0.2%)
3	L	0.92	2/5888 (0.0%)	1.09	17/7974 (0.2%)
3	U	0.91	0/5888	1.08	11/7974 (0.1%)
All	All	0.91	7/38463 (0.0%)	1.07	76/52020 (0.1%)

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)
1	2	112	GLN	CA-C	6.72	1.56	1.52
3	C	1319	THR	CA-CB	6.58	1.64	1.53
3	4	1144	THR	CA-CB	6.01	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1322	PRO	N-CA	5.86	1.54	1.47
3	L	1144	THR	CA-CB	5.32	1.62	1.53

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1315	THR	CA-C-N	-9.52	104.66	122.27
3	C	1315	THR	C-N-CA	-9.52	104.66	122.27
3	C	1317	CYS	CA-C-N	9.18	138.22	121.70
3	C	1317	CYS	C-N-CA	9.18	138.22	121.70
3	4	1323	GLY	N-CA-C	-8.46	93.13	113.18

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 [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	2	1255	0	1265	25	0
1	A	1243	0	1253	19	0
1	J	1243	0	1253	21	0
1	S	1234	0	1240	22	0
2	3	2389	0	2459	47	0
2	B	2385	0	2456	50	0
2	K	2369	0	2435	45	0
2	T	2389	0	2459	35	0
3	4	5832	0	5759	175	0
3	C	5809	0	5737	166	0
3	L	5761	0	5685	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	5761	0	5685	138	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	834	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 11.

The worst 5 of 834 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
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.17	1.12
2:K:241:THR:HG22	2:K:243:LYS:HE2	1.28	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%)	4	8
1	A	160/165 (97%)	150 (94%)	8 (5%)	2 (1%)	9	21
1	J	160/165 (97%)	151 (94%)	6 (4%)	3 (2%)	6	13
1	S	159/165 (96%)	146 (92%)	7 (4%)	6 (4%)	2	3
2	3	303/305 (99%)	283 (93%)	17 (6%)	3 (1%)	12	28
2	B	302/305 (99%)	282 (93%)	17 (6%)	3 (1%)	12	28
2	K	300/305 (98%)	276 (92%)	22 (7%)	2 (1%)	18	38
2	T	303/305 (99%)	284 (94%)	16 (5%)	3 (1%)	12	28
3	4	754/762 (99%)	702 (93%)	42 (6%)	10 (1%)	9	21
3	C	751/762 (99%)	714 (95%)	23 (3%)	14 (2%)	6	13
3	L	743/762 (98%)	707 (95%)	30 (4%)	6 (1%)	16	34
3	U	743/762 (98%)	701 (94%)	37 (5%)	5 (1%)	18	38
All	All	4840/4928 (98%)	4545 (94%)	234 (5%)	61 (1%)	9	21

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%)	129 (94%)	8 (6%)	18	39
1	A	136/138 (99%)	125 (92%)	11 (8%)	11	24
1	J	136/138 (99%)	128 (94%)	8 (6%)	18	38
1	S	135/138 (98%)	126 (93%)	9 (7%)	15	33
2	3	261/261 (100%)	245 (94%)	16 (6%)	17	37
2	B	261/261 (100%)	242 (93%)	19 (7%)	13	29
2	K	259/261 (99%)	242 (93%)	17 (7%)	15	34
2	T	261/261 (100%)	244 (94%)	17 (6%)	15	35
3	4	632/638 (99%)	604 (96%)	28 (4%)	25	50
3	C	629/638 (99%)	608 (97%)	21 (3%)	33	61
3	L	624/638 (98%)	599 (96%)	25 (4%)	28	55
3	U	624/638 (98%)	593 (95%)	31 (5%)	22	46
All	All	4095/4148 (99%)	3885 (95%)	210 (5%)	21	45

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	328	ARG
3	U	856	ILE
3	4	953	THR
2	T	412	SER
3	U	636	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
3	U	614	HIS
3	U	1088	GLN
3	4	1173	ASN
3	U	677	HIS
3	U	875	HIS

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 oligosaccharides 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
5	FAD	T	606	-	58,58,58	1.21	6 (10%)	85,89,89	1.72	18 (21%)
8	XAN	C	7319	-	12,12,12	1.88	2 (16%)	14,17,17	2.31	6 (42%)
4	FES	A	602	1	0,4,4	-	-	-	-	-
4	FES	S	602	1	0,4,4	-	-	-	-	-
4	FES	2	602	1	0,4,4	-	-	-	-	-
4	FES	S	601	1	0,4,4	-	-	-	-	-
6	MTE	U	1333	7	21,26,26	1.59	3 (14%)	19,40,40	2.42	9 (47%)
8	XAN	L	7319	-	12,12,12	1.86	1 (8%)	14,17,17	2.26	6 (42%)
7	MOM	4	1334	6	0,3,3	-	-	-	-	-
5	FAD	K	606	-	58,58,58	1.05	5 (8%)	85,89,89	1.75	21 (24%)
8	XAN	4	7319	-	12,12,12	1.95	1 (8%)	14,17,17	2.41	7 (50%)
7	MOM	L	1334	6	0,3,3	-	-	-	-	-
4	FES	J	602	1	0,4,4	-	-	-	-	-
6	MTE	4	1333	7	21,26,26	1.82	3 (14%)	19,40,40	2.52	10 (52%)
8	XAN	U	7319	-	12,12,12	1.97	2 (16%)	14,17,17	2.19	6 (42%)
6	MTE	C	1333	7	21,26,26	1.70	2 (9%)	19,40,40	3.02	8 (42%)
4	FES	2	601	1	0,4,4	-	-	-	-	-
5	FAD	3	606	-	58,58,58	1.27	5 (8%)	85,89,89	1.81	22 (25%)
5	FAD	B	606	-	58,58,58	1.18	5 (8%)	85,89,89	1.87	23 (27%)
7	MOM	U	1334	6	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MTE	L	1333	7	21,26,26	1.62	2 (9%)	19,40,40	2.55	8 (42%)
4	FES	A	601	1	0,4,4	-	-	-		
7	MOM	C	1334	6	0,3,3	-	-	-		
4	FES	J	601	1	0,4,4	-	-	-		

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
5	FAD	T	606	-	-	4/34/50/50	0/6/6/6
8	XAN	C	7319	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
4	FES	S	602	1	-	-	0/1/1/1
4	FES	2	602	1	-	-	0/1/1/1
4	FES	S	601	1	-	-	0/1/1/1
6	MTE	U	1333	7	-	3/6/34/34	0/3/3/3
8	XAN	L	7319	-	-	-	0/2/2/2
5	FAD	K	606	-	-	5/34/50/50	0/6/6/6
8	XAN	4	7319	-	-	-	0/2/2/2
4	FES	J	602	1	-	-	0/1/1/1
6	MTE	4	1333	7	-	1/6/34/34	0/3/3/3
8	XAN	U	7319	-	-	-	0/2/2/2
6	MTE	C	1333	7	-	1/6/34/34	0/3/3/3
5	FAD	3	606	-	-	7/34/50/50	0/6/6/6
4	FES	2	601	1	-	-	0/1/1/1
5	FAD	B	606	-	-	3/34/50/50	0/6/6/6
6	MTE	L	1333	7	-	1/6/34/34	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
4	FES	J	601	1	-	-	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	1333	MTE	C9-C10	6.69	1.50	1.38
6	L	1333	MTE	C9-C10	6.05	1.49	1.38
6	C	1333	MTE	C9-C10	6.03	1.48	1.38
6	U	1333	MTE	C9-C10	5.58	1.48	1.38
8	U	7319	XAN	C5-C4	5.41	1.48	1.38

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1333	MTE	O3'-C7-C6	7.57	114.01	108.96
6	4	1333	MTE	O3'-C7-N8	-6.26	102.92	108.61
5	B	606	FAD	N3A-C2A-N1A	-5.95	119.58	128.58
5	T	606	FAD	N3A-C2A-N1A	-5.86	119.70	128.58
6	C	1333	MTE	C7-C6-N5	5.81	113.58	107.87

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O2A
5	K	606	FAD	C5B-O5B-PA-O3P
5	T	606	FAD	C5B-O5B-PA-O1A

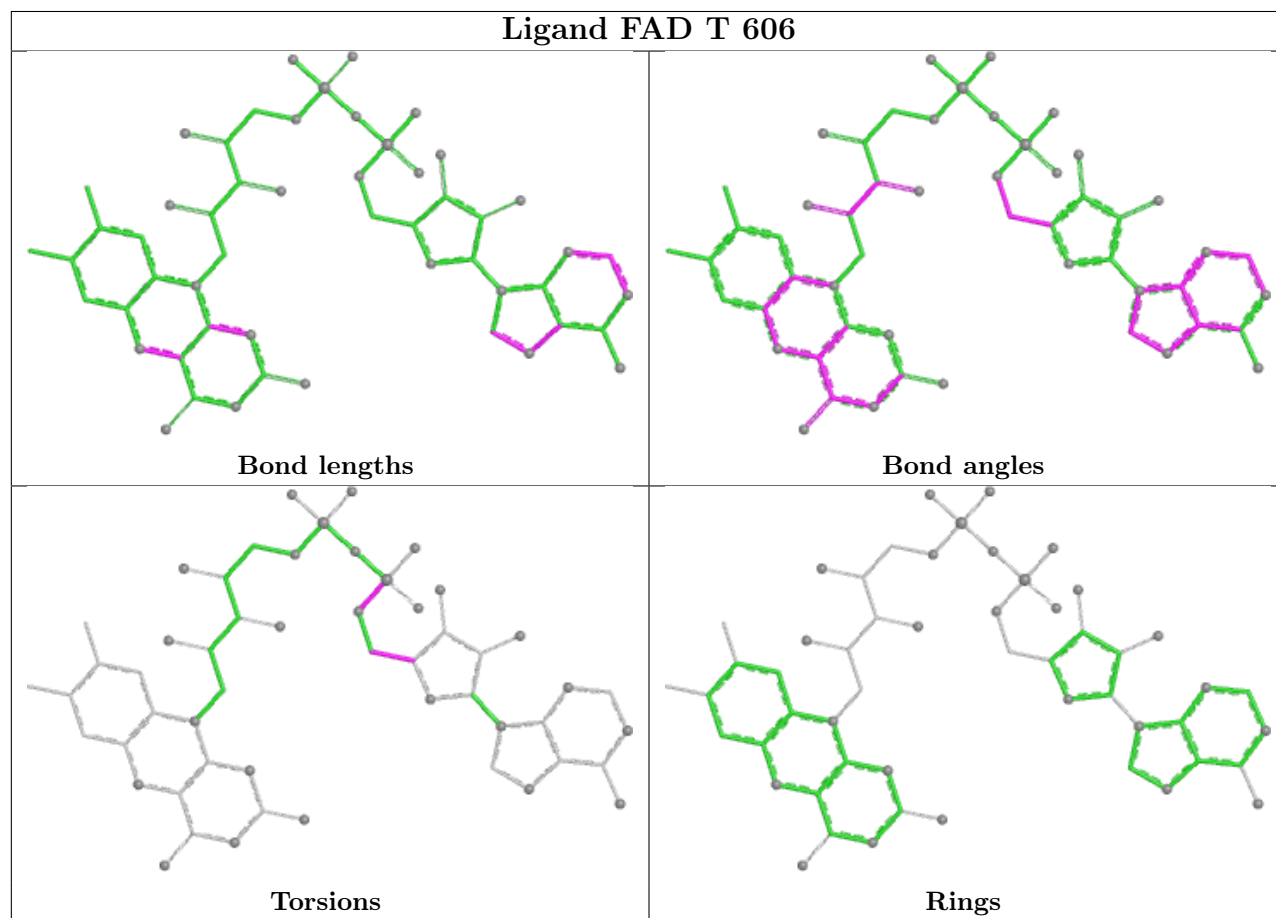
There are no ring outliers.

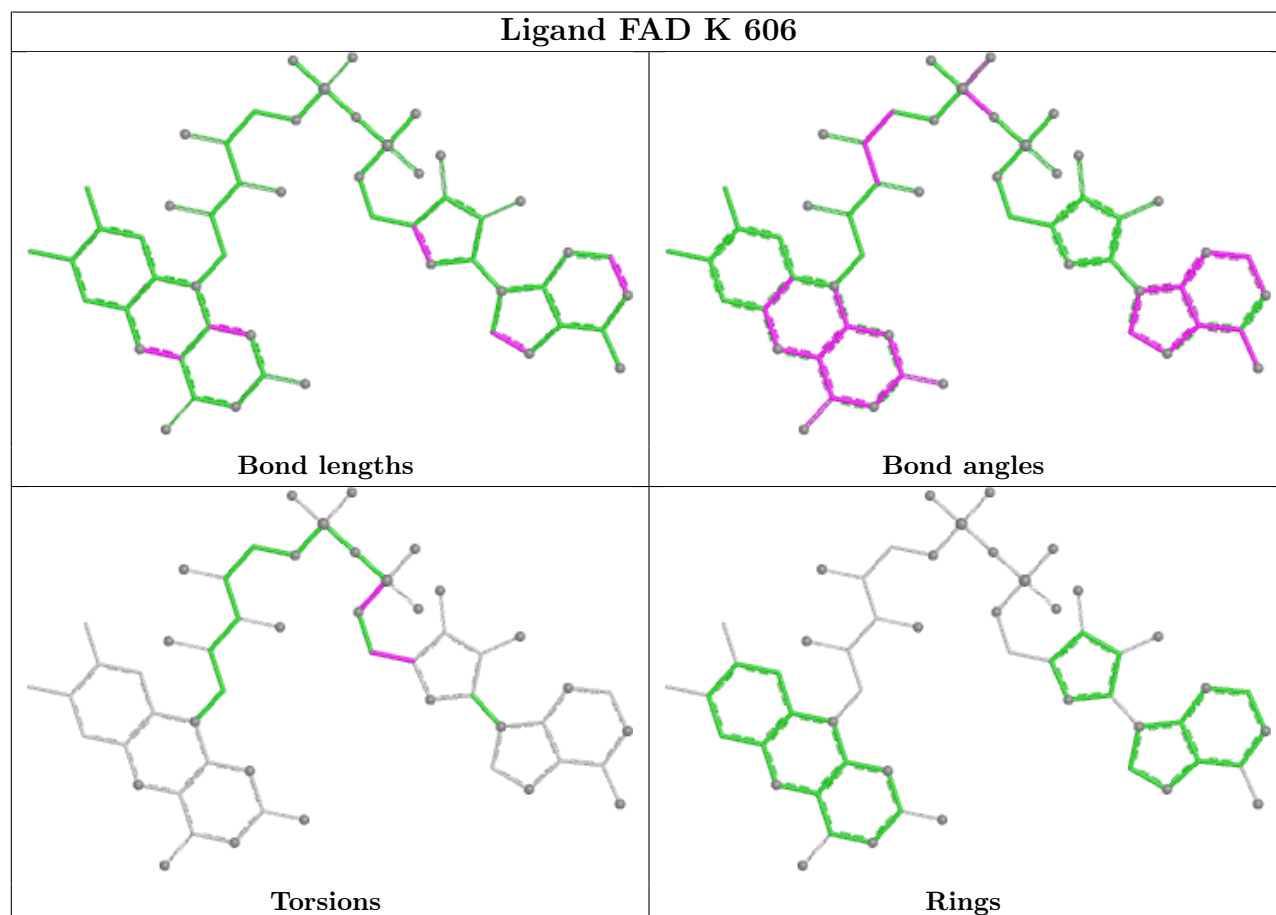
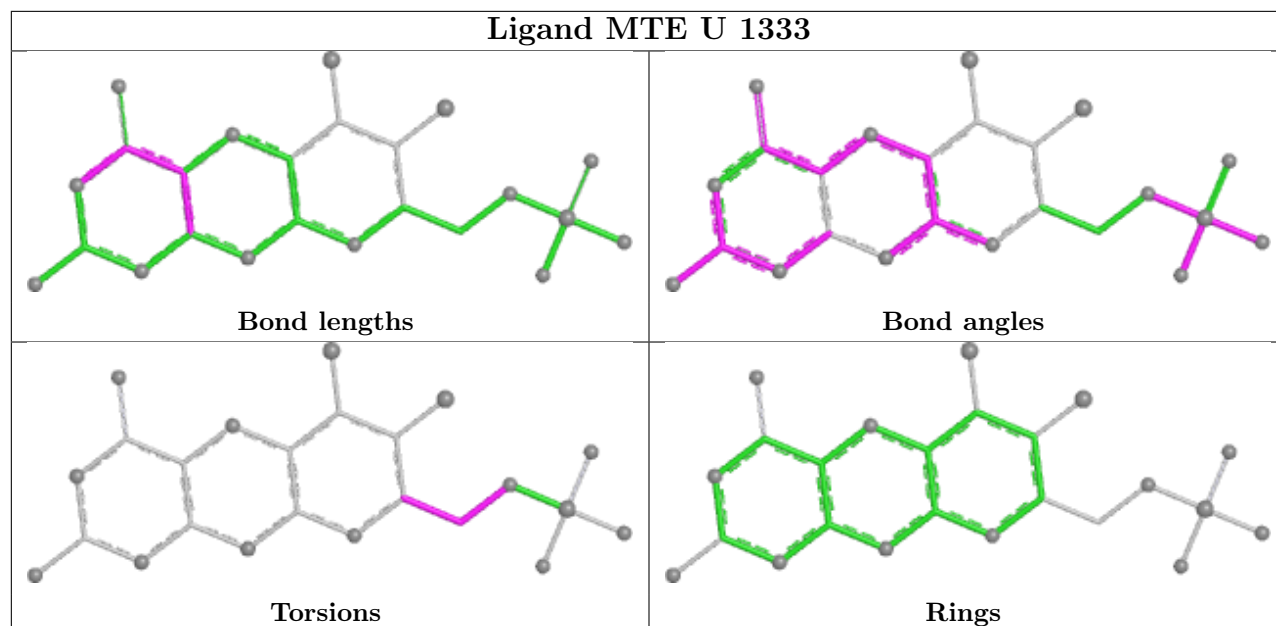
15 monomers are involved in 20 short contacts:

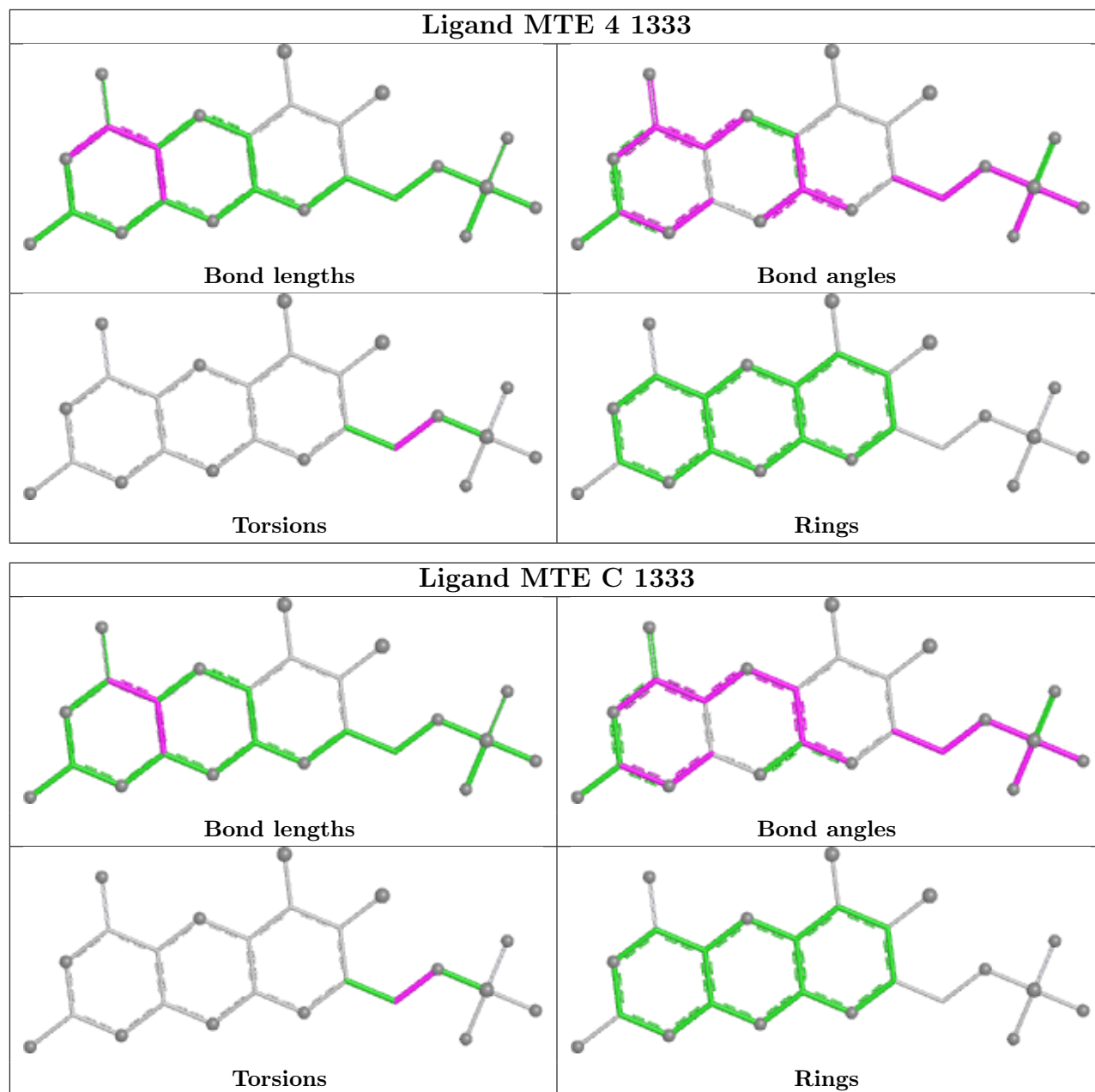
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	606	FAD	2	0
8	C	7319	XAN	1	0
4	A	602	FES	1	0
8	L	7319	XAN	1	0
7	4	1334	MOM	2	0
5	K	606	FAD	3	0
8	4	7319	XAN	1	0
7	L	1334	MOM	2	0
8	U	7319	XAN	2	0
5	3	606	FAD	2	0
5	B	606	FAD	1	0
7	U	1334	MOM	3	0
6	L	1333	MTE	1	0
4	A	601	FES	1	0
7	C	1334	MOM	2	0

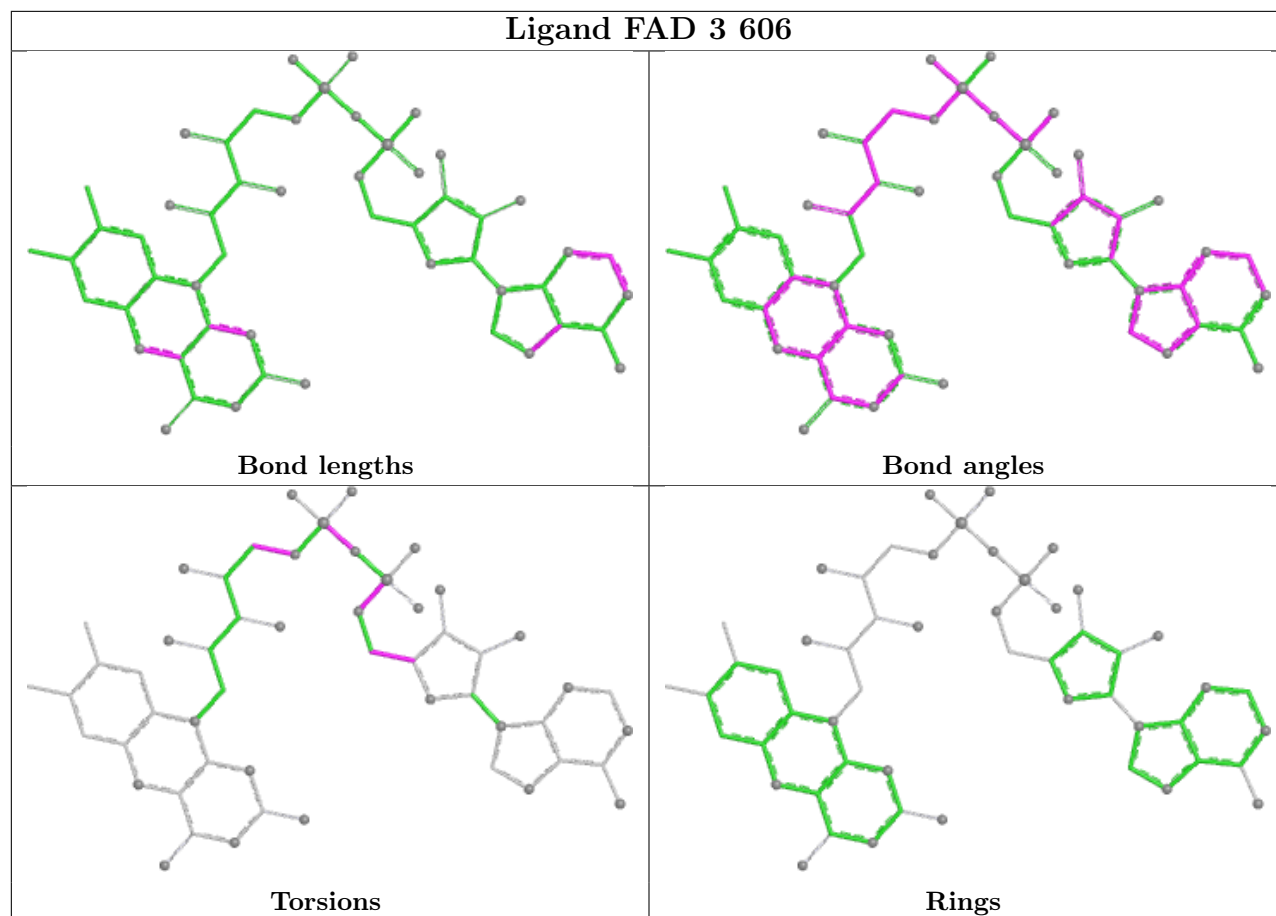
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

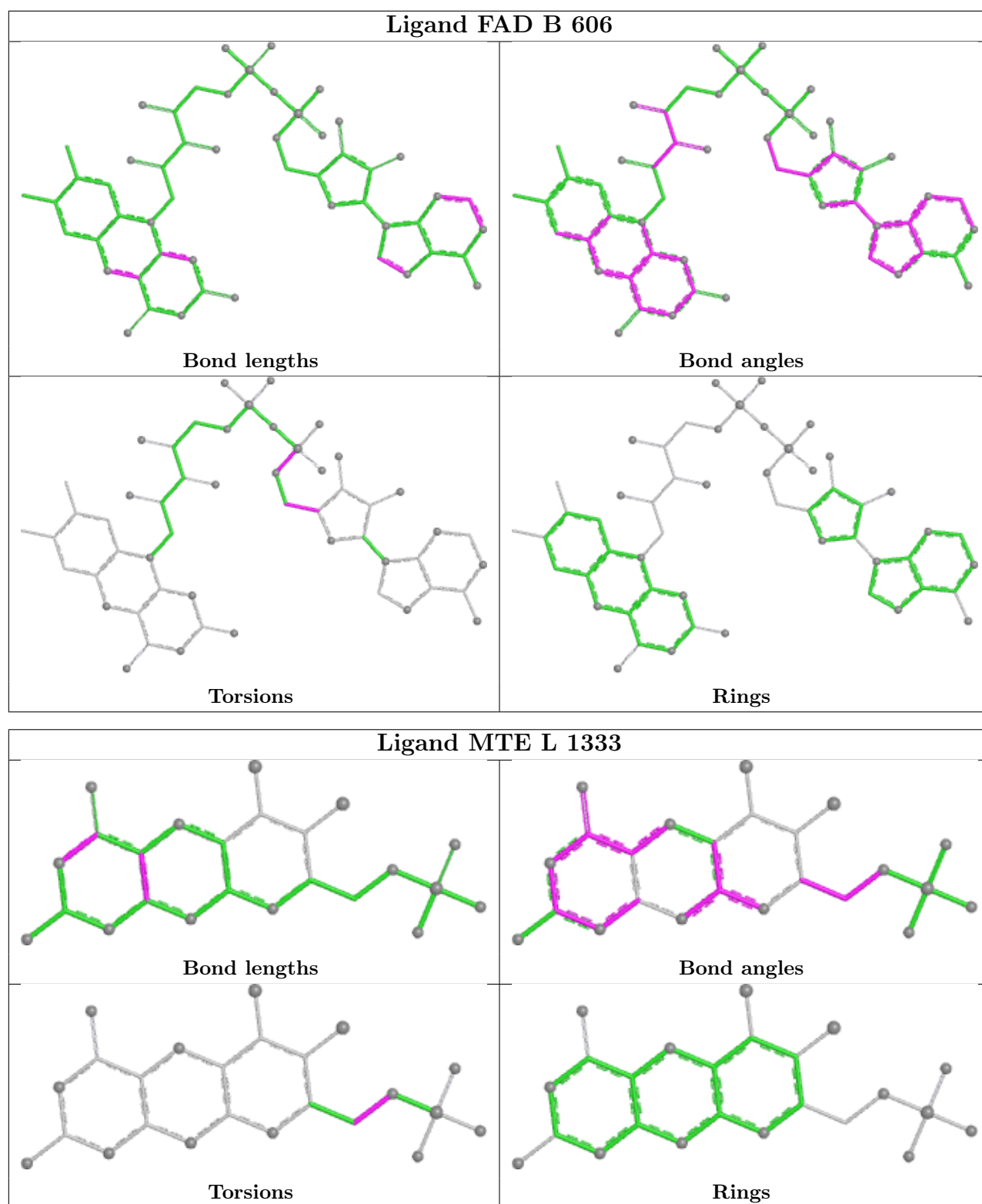
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.











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	2	164/165 (99%)	-0.05	9 (5%) 30 25	4, 10, 30, 43	0
1	A	162/165 (98%)	-0.01	8 (4%) 35 29	2, 9, 27, 41	0
1	J	162/165 (98%)	-0.18	2 (1%) 76 73	3, 9, 27, 41	0
1	S	161/165 (97%)	-0.08	5 (3%) 51 45	4, 10, 28, 43	0
2	3	305/305 (100%)	0.09	7 (2%) 61 55	5, 18, 28, 34	0
2	B	304/305 (99%)	0.10	9 (2%) 52 47	7, 17, 27, 35	0
2	K	302/305 (99%)	0.08	7 (2%) 61 55	7, 17, 27, 35	0
2	T	305/305 (100%)	0.07	9 (2%) 52 47	6, 18, 28, 34	0
3	4	756/762 (99%)	-0.08	14 (1%) 66 61	2, 12, 25, 39	0
3	C	753/762 (98%)	-0.14	18 (2%) 59 54	2, 10, 25, 42	0
3	L	745/762 (97%)	-0.18	10 (1%) 75 71	2, 10, 24, 40	0
3	U	745/762 (97%)	-0.14	9 (1%) 76 73	2, 11, 24, 37	0
All	All	4864/4928 (98%)	-0.07	107 (2%) 62 57	2, 12, 26, 43	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	5.0
3	U	1288	ASN	4.9
3	C	1322	PRO	4.7
3	C	1319	THR	4.6
3	C	1324	ASN	4.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

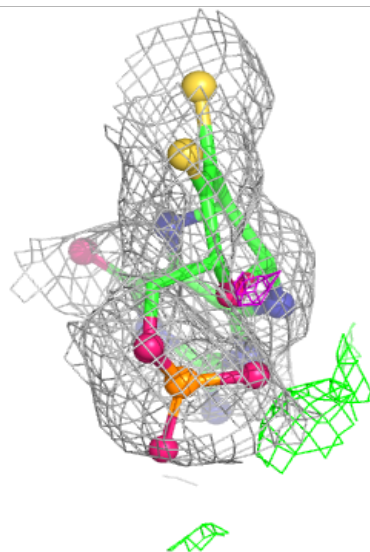
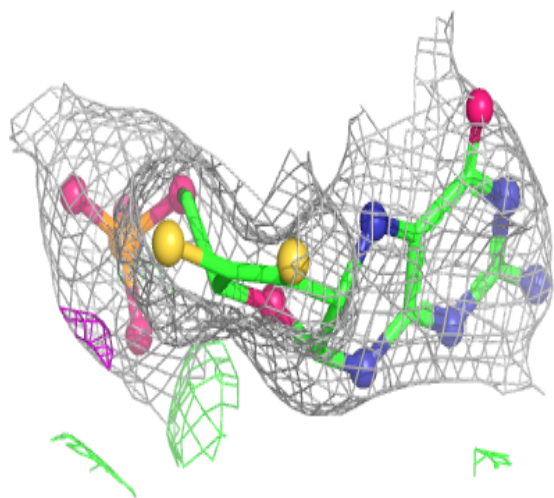
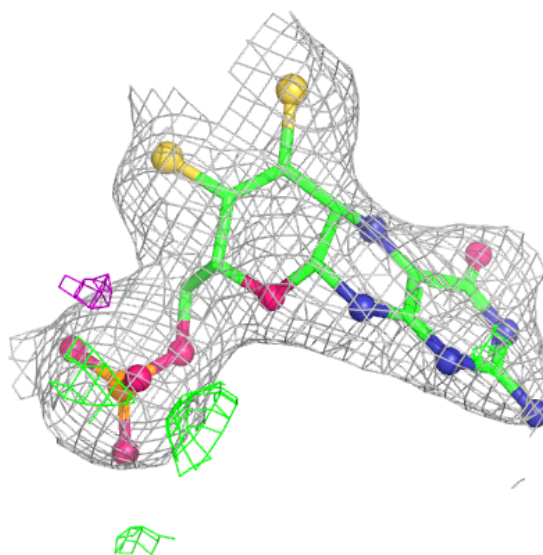
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	XAN	U	7319	11/11	0.80	0.17	40,41,41,41	0
8	XAN	L	7319	11/11	0.83	0.14	31,32,33,33	0
8	XAN	C	7319	11/11	0.88	0.13	26,27,28,28	0
8	XAN	4	7319	11/11	0.88	0.12	33,34,34,35	0
6	MTE	4	1333	24/24	0.97	0.07	12,13,15,16	0
5	FAD	K	606	53/53	0.97	0.06	4,8,12,12	0
5	FAD	3	606	53/53	0.97	0.06	2,5,9,13	0
6	MTE	L	1333	24/24	0.97	0.06	6,8,13,14	0
6	MTE	U	1333	24/24	0.97	0.07	7,10,15,15	0
6	MTE	C	1333	24/24	0.98	0.06	7,11,15,17	0
4	FES	2	602	4/4	0.98	0.03	2,3,5,5	0
5	FAD	T	606	53/53	0.98	0.06	2,8,13,16	0
5	FAD	B	606	53/53	0.98	0.06	2,4,8,8	0
4	FES	2	601	4/4	0.99	0.03	2,2,3,5	0
4	FES	A	601	4/4	0.99	0.03	2,3,4,8	0
4	FES	A	602	4/4	0.99	0.03	2,2,3,4	0
4	FES	J	601	4/4	0.99	0.03	2,2,2,2	0
4	FES	J	602	4/4	0.99	0.04	2,3,3,4	0
4	FES	S	601	4/4	0.99	0.03	4,5,9,10	0
4	FES	S	602	4/4	0.99	0.04	4,4,6,9	0
7	MOM	C	1334	4/4	1.00	0.03	16,16,17,20	0
7	MOM	L	1334	4/4	1.00	0.03	12,15,15,16	0
7	MOM	U	1334	4/4	1.00	0.03	12,14,15,15	0
7	MOM	4	1334	4/4	1.00	0.04	12,12,14,18	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.

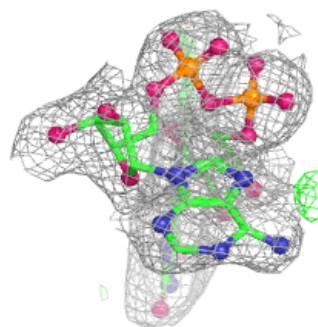
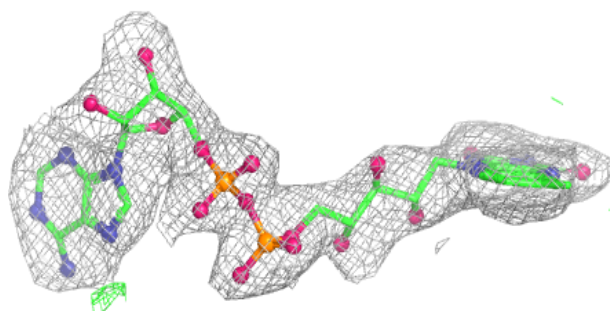
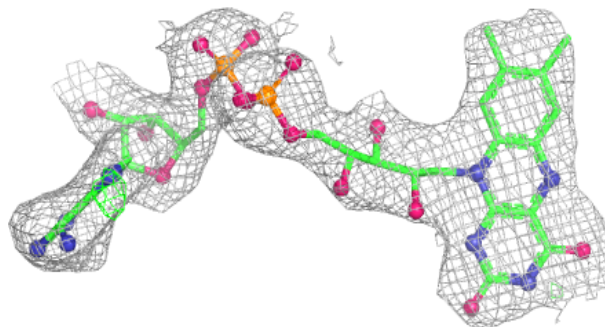
Electron density around MTE 4 1333:

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

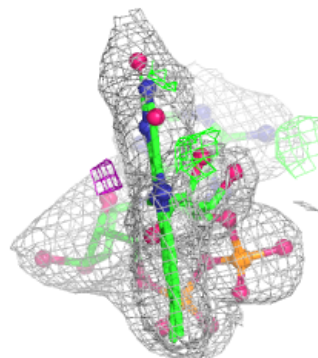
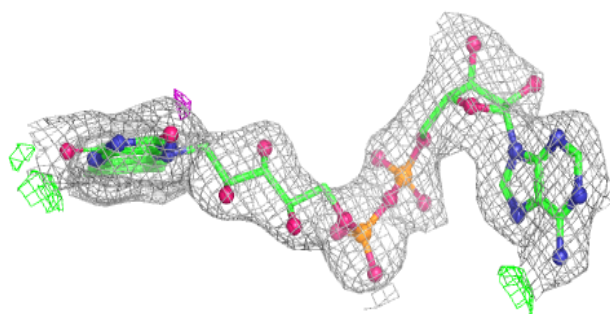
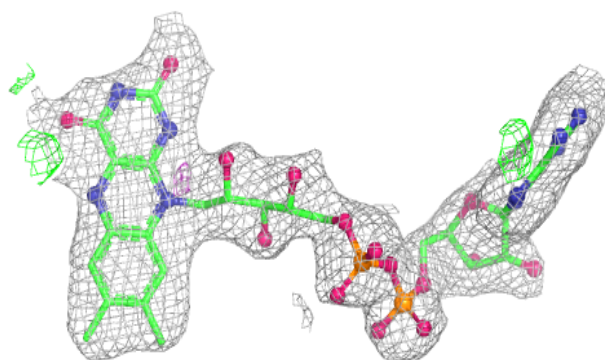


Electron density around FAD K 606:

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

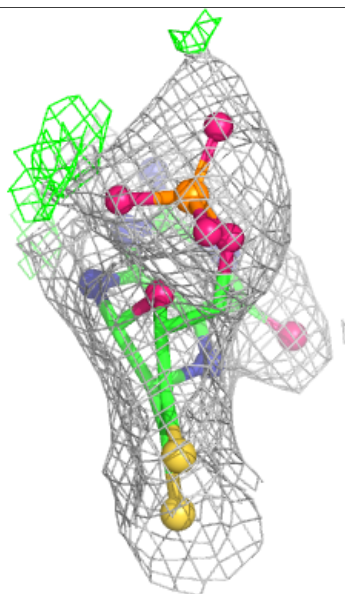
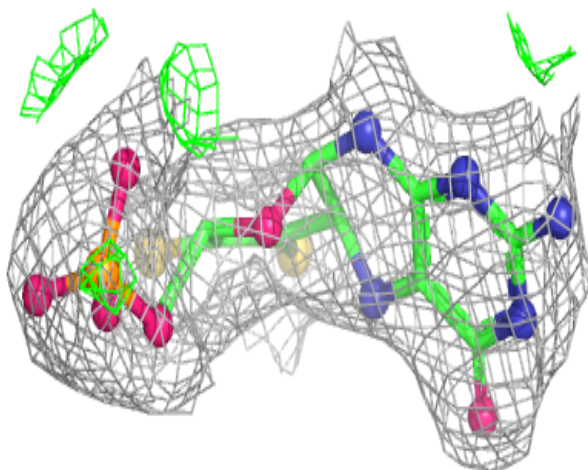
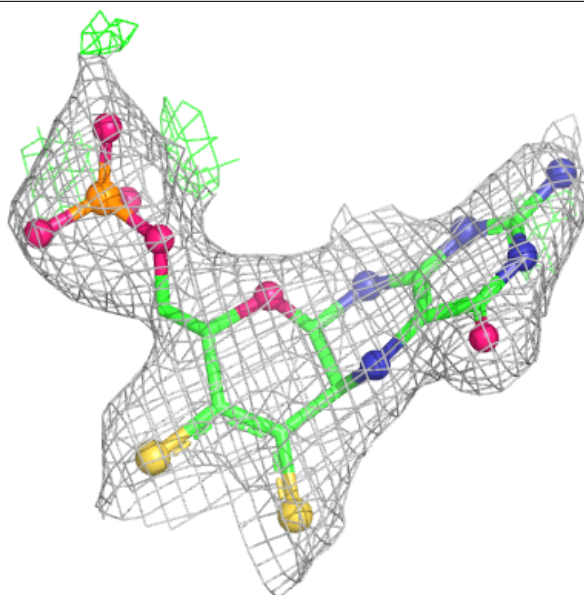
**Electron density around FAD 3 606:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



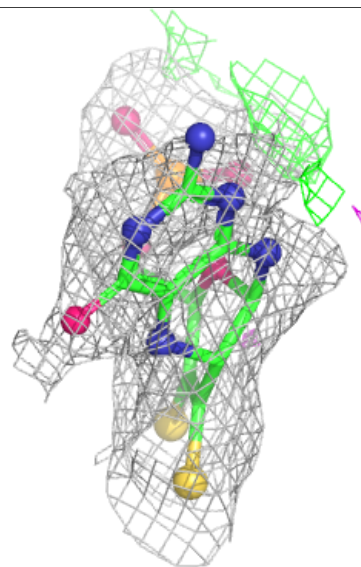
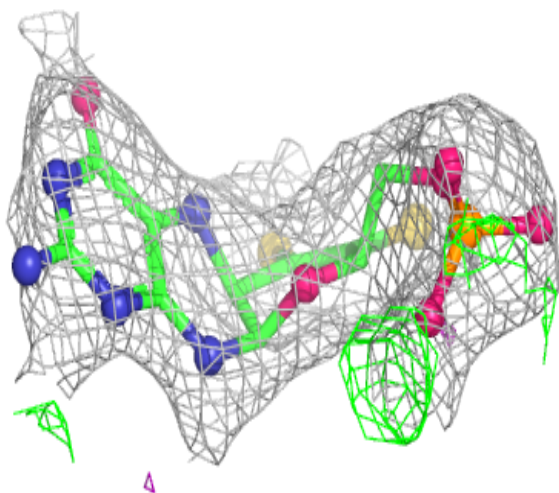
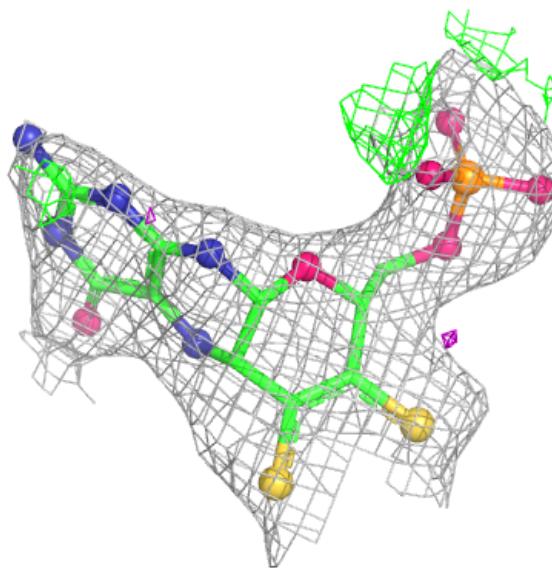
Electron density around MTE L 1333:

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and green (positive)



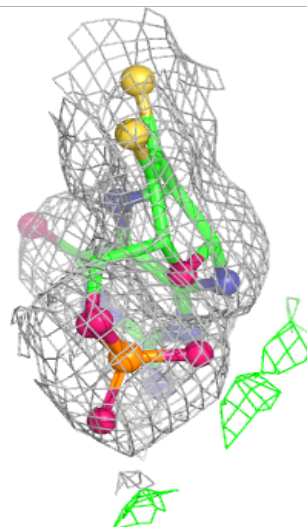
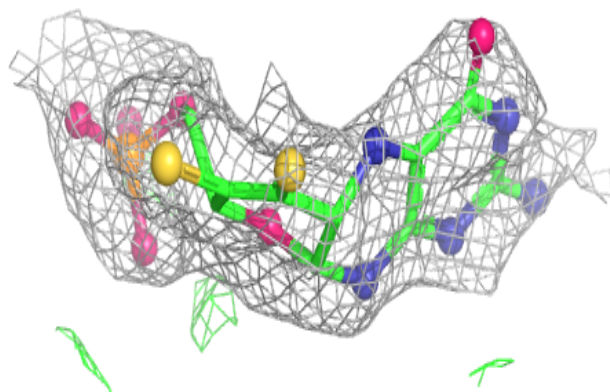
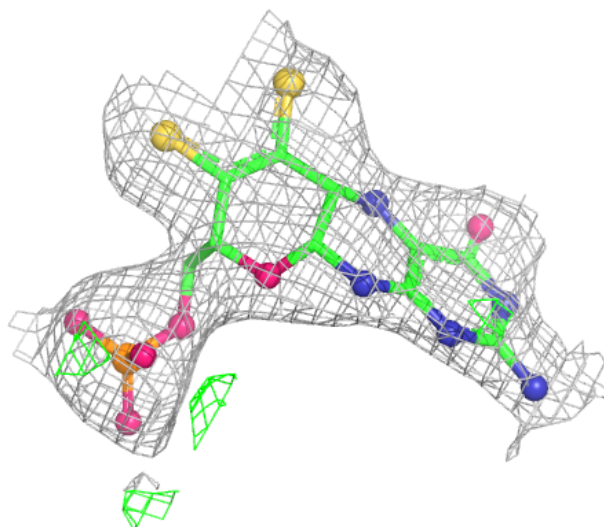
Electron density around MTE U 1333:

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and green (positive)



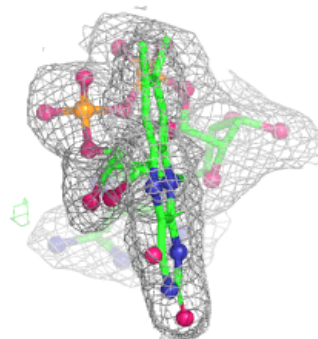
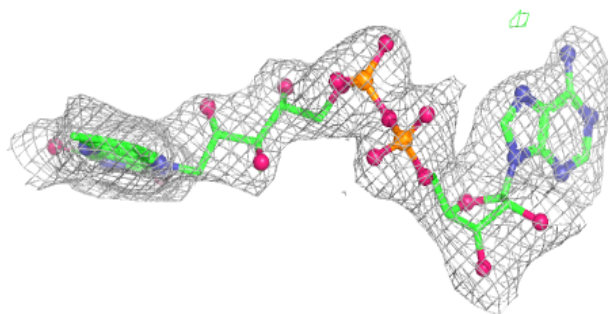
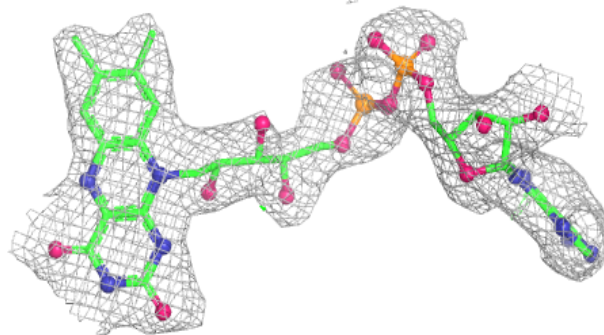
Electron density around MTE C 1333:

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

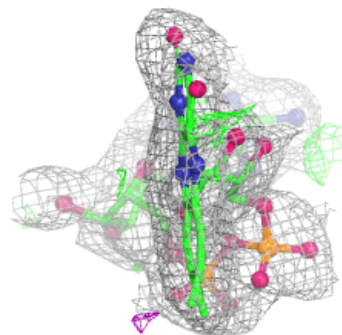
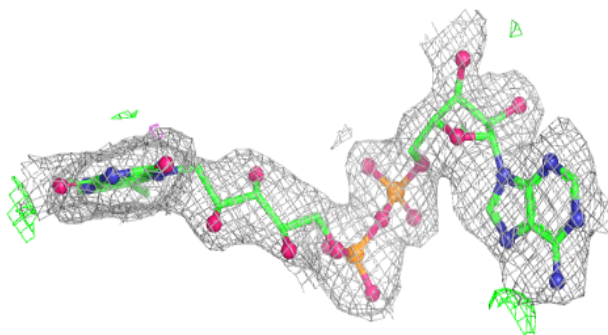
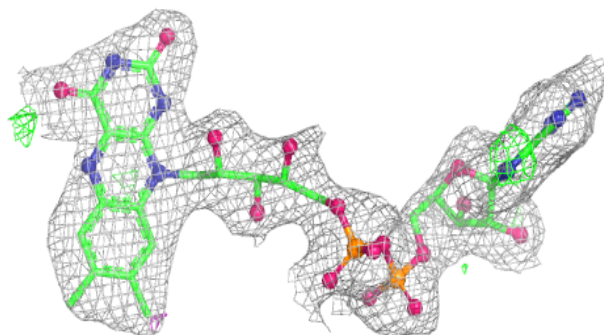


Electron density around FAD T 606:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.