



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2024 – 12:30 AM EST

PDB ID : 3NVY  
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Quercetin  
Authors : Cao, H.; Hille, R.  
Deposited on : 2010-07-08  
Resolution : 2.00 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](mailto: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>.

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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 : 2.36  
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) : 2.36

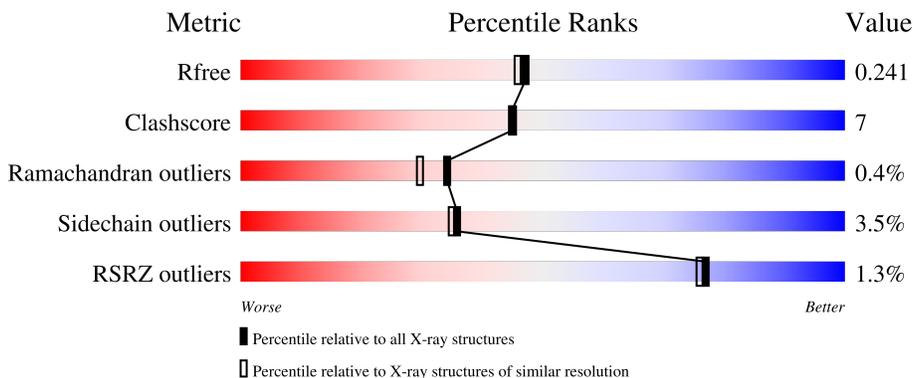
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	 85% 13% 2% 2%
1	J	164	 88% 12% 2%
2	B	334	 86% 12% 2%
2	K	334	 77% 12% 9% 4%
3	C	756	 87% 12%

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Mol	Chain	Length	Quality of chain
3	L	756	

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	C	1328	-	-	X	-
7	MOS	L	1328	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20401 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	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			
1	J	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

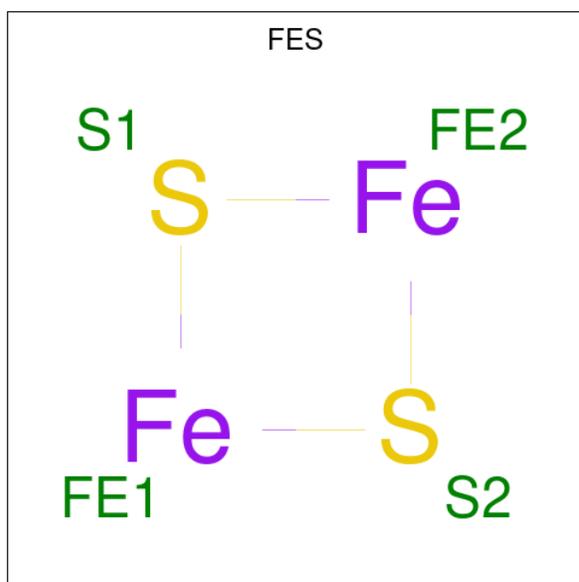
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	334	Total	C	N	O	S	0	0	0
			2630	1700	437	479	14			
2	K	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

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

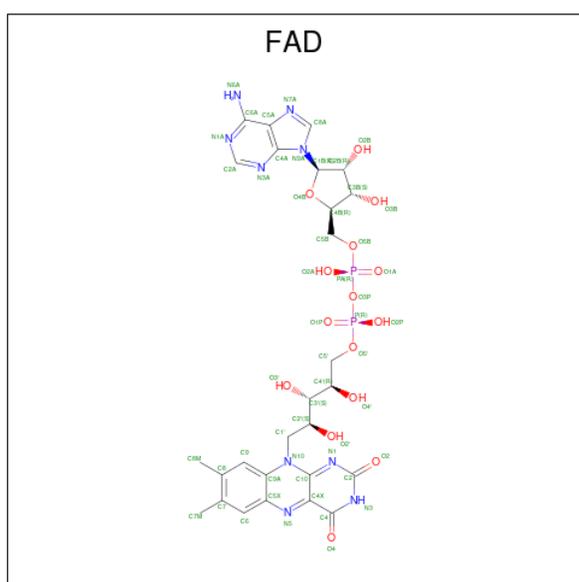
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



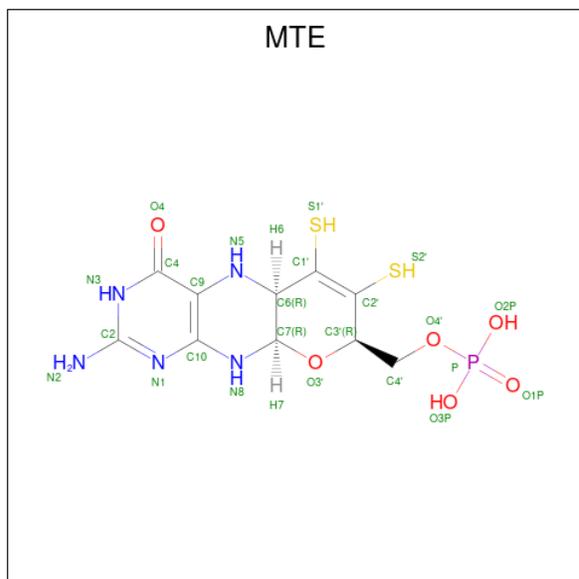
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0

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



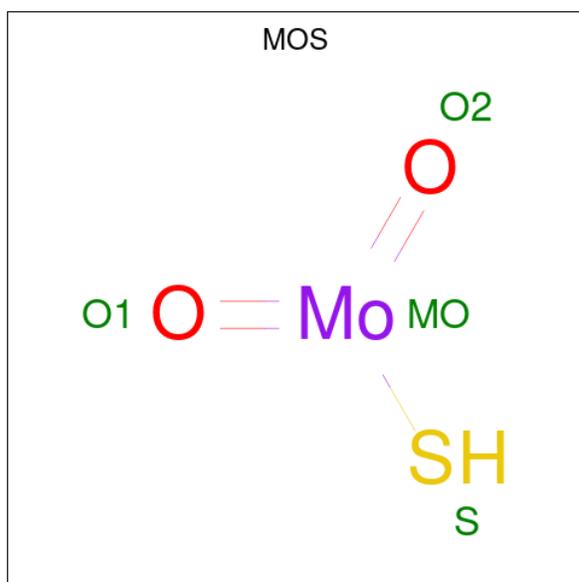
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	53	27	9	15	2	0	0
5	K	1	53	27	9	15	2	0	0

- 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<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).



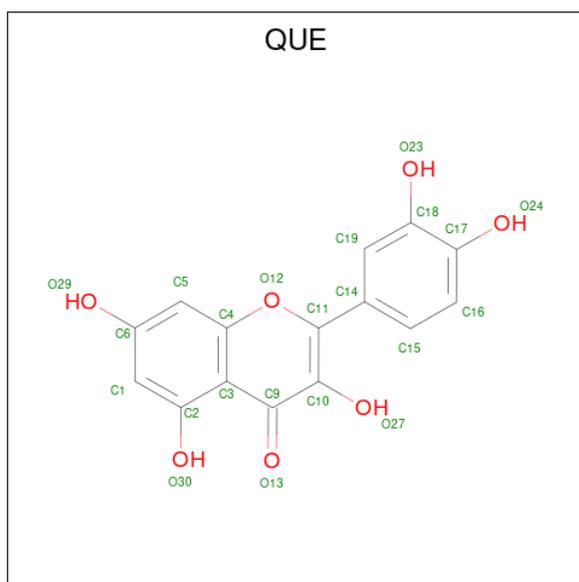
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
6	C	1	24	10	5	6	1	2	0	0
6	L	1	24	10	5	6	1	2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO<sub>2</sub>S).



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

- Molecule 8 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	C	1	22	15	7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			22	15	7		

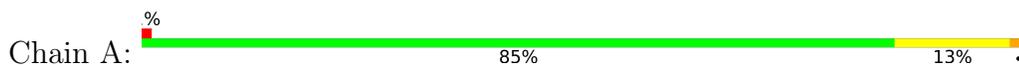
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	79	Total	O	0	0
			79	79		
9	B	114	Total	O	0	0
			114	114		
9	C	369	Total	O	0	0
			369	369		
9	J	84	Total	O	0	0
			84	84		
9	K	66	Total	O	0	0
			66	66		
9	L	345	Total	O	0	0
			345	345		

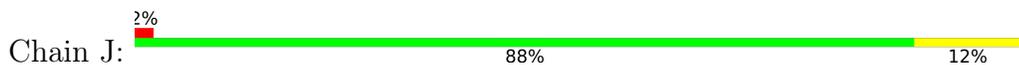
### 3 Residue-property plots

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

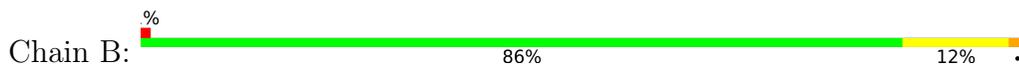
- Molecule 1: Xanthine dehydrogenase/oxidase



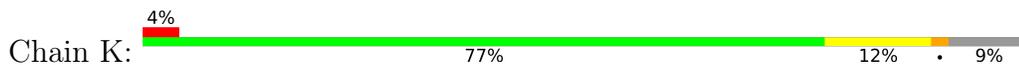
- Molecule 1: Xanthine dehydrogenase/oxidase



- Molecule 2: Xanthine dehydrogenase/oxidase

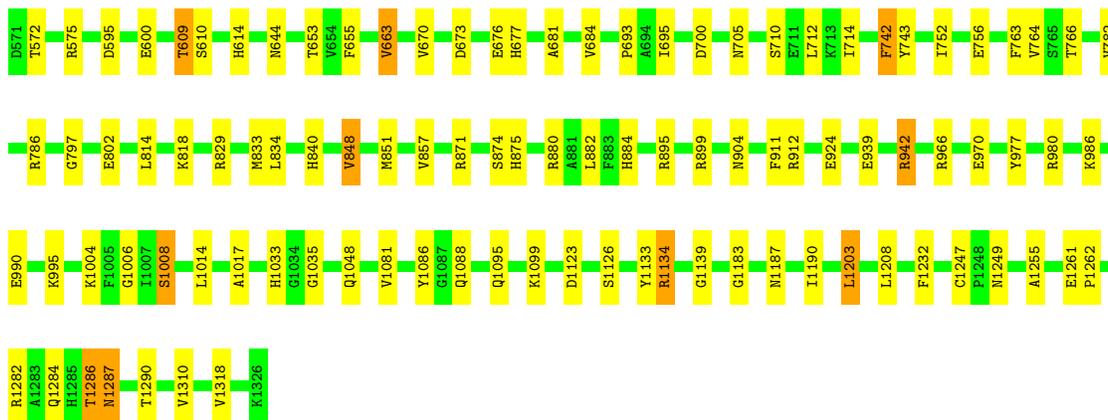


- Molecule 2: Xanthine dehydrogenase/oxidase

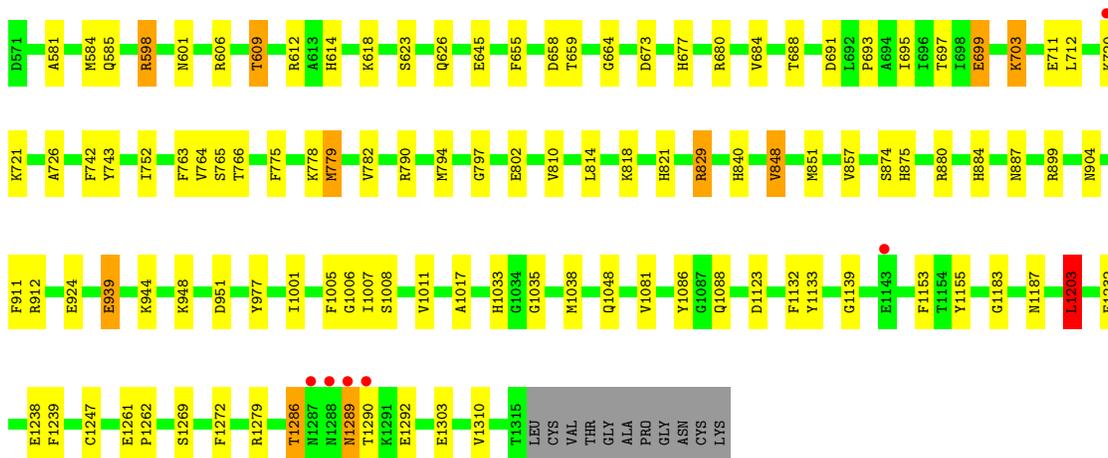
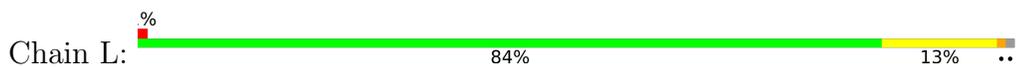




• Molecule 3: Xanthine dehydrogenase/oxidase



• 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, $\alpha$ , $\beta$ , $\gamma$	132.69Å 73.40Å 138.21Å 90.00° 97.13° 90.00°	Depositor
Resolution (Å)	101.50 – 2.00 101.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (101.50-2.00) 98.2 (101.48-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , 0.237 0.194 , 0.241	Depositor DCC
$R_{free}$ test set	8835 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.013 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FAD, QUE, FES, MTE, MOS

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	0.75	0/1277	0.73	0/1723
1	J	0.68	0/1277	0.69	0/1723
2	B	0.60	0/2689	0.69	2/3637 (0.1%)
2	K	0.58	0/2438	0.64	1/3290 (0.0%)
3	C	0.76	0/5960	0.81	11/8072 (0.1%)
3	L	0.71	2/5888 (0.0%)	0.74	5/7974 (0.1%)
All	All	0.70	2/19529 (0.0%)	0.74	19/26419 (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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	699	GLU	CG-CD	6.60	1.61	1.51
3	L	699	GLU	CB-CG	5.61	1.62	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	829	ARG	NE-CZ-NH2	-10.50	115.05	120.30
3	C	942	ARG	NE-CZ-NH1	-9.85	115.37	120.30
3	C	829	ARG	NE-CZ-NH1	8.73	124.67	120.30
3	C	980	ARG	NE-CZ-NH2	-8.40	116.10	120.30
3	C	663	VAL	C-N-CA	-8.11	105.27	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ALA	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	A	1255	0	1265	17	1
1	J	1255	0	1265	16	0
2	B	2630	0	2697	27	0
2	K	2389	0	2459	34	0
3	C	5832	0	5759	78	1
3	L	5761	0	5685	84	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	0	0
5	K	53	0	31	3	0
6	C	24	0	10	1	0
6	L	24	0	10	1	0
7	C	4	0	0	4	0
7	L	4	0	0	3	0
8	C	22	0	7	4	0
8	L	22	0	7	3	0
9	A	79	0	0	2	0
9	B	114	0	0	4	0
9	C	369	0	0	6	0
9	J	84	0	0	2	0
9	K	66	0	0	1	0
9	L	345	0	0	3	0
All	All	20401	0	19226	251	1

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 7.

The worst 5 of 251 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:L:726:ALA:HA	3:L:851:MET:HE1	1.15	1.14
2:K:243:LYS:H	2:K:243:LYS:HD3	0.97	1.11
3:L:779:MET:HG3	3:L:810:VAL:CG1	1.84	1.08
1:J:165:LYS:HD3	9:J:167:HOH:O	1.58	1.04
3:C:742:PHE:CE1	3:C:833:MET:CE	2.44	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:OD2	3:C:871:ARG:NH1[1_545]	2.06	0.14

## 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%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
2	B	332/334 (99%)	315 (95%)	17 (5%)	0	100	100
2	K	303/334 (91%)	289 (95%)	13 (4%)	1 (0%)	41	37
3	C	754/756 (100%)	727 (96%)	23 (3%)	4 (0%)	29	23
3	L	743/756 (98%)	722 (97%)	16 (2%)	5 (1%)	22	16
All	All	2456/2508 (98%)	2365 (96%)	81 (3%)	10 (0%)	34	30

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1008	SER
3	L	1008	SER
3	C	912	ARG
3	L	912	ARG

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Mol	Chain	Res	Type
2	K	426	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	137/137 (100%)	129 (94%)	8 (6%)	20 15
1	J	137/137 (100%)	134 (98%)	3 (2%)	52 55
2	B	290/290 (100%)	278 (96%)	12 (4%)	30 28
2	K	261/290 (90%)	249 (95%)	12 (5%)	27 23
3	C	632/632 (100%)	614 (97%)	18 (3%)	43 44
3	L	624/632 (99%)	604 (97%)	20 (3%)	39 38
All	All	2081/2118 (98%)	2008 (96%)	73 (4%)	36 35

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	684	VAL
3	L	1286	THR
3	L	742	PHE
3	L	911	PHE
3	C	743	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	821	HIS
3	L	1220	HIS
3	L	840	HIS
3	L	1016	GLN
3	C	1016	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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
4	FES	J	601	1	0,4,4	-	-	-		
6	MTE	L	1327	7	21,26,26	1.51	3 (14%)	21,40,40	2.21	7 (33%)
7	MOS	L	1328	6	0,3,3	-	-	-		
5	FAD	B	606	-	53,58,58	1.09	2 (3%)	68,89,89	1.40	5 (7%)
4	FES	J	602	1	0,4,4	-	-	-		
7	MOS	C	1328	6	0,3,3	-	-	-		
4	FES	A	602	1	0,4,4	-	-	-		
5	FAD	K	606	-	53,58,58	1.30	5 (9%)	68,89,89	1.49	11 (16%)
6	MTE	C	1327	7	21,26,26	1.60	3 (14%)	21,40,40	2.47	11 (52%)
8	QUE	C	1356	-	21,24,24	2.12	5 (23%)	27,36,36	1.98	3 (11%)
8	QUE	L	1356	-	21,24,24	2.18	4 (19%)	27,36,36	1.62	4 (14%)
4	FES	A	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
4	FES	J	601	1	-	-	0/1/1/1
6	MTE	L	1327	7	-	2/6/34/34	0/3/3/3
5	FAD	B	606	-	-	0/30/50/50	0/6/6/6
4	FES	J	602	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
5	FAD	K	606	-	-	0/30/50/50	0/6/6/6
8	QUE	C	1356	-	-	0/0/4/4	0/3/3/3
8	QUE	L	1356	-	-	0/0/4/4	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
6	MTE	C	1327	7	-	1/6/34/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1356	QUE	C18-C17	6.11	1.50	1.40
8	L	1356	QUE	C3-C4	5.73	1.49	1.41
8	C	1356	QUE	C3-C4	5.61	1.48	1.41
8	C	1356	QUE	C18-C17	5.17	1.48	1.40
5	K	606	FAD	C2A-N3A	4.69	1.39	1.32

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-6.51	118.51	128.68
6	L	1327	MTE	C2-N3-C4	5.77	125.09	115.93
6	C	1327	MTE	C2-N3-C4	5.60	124.83	115.93
8	C	1356	QUE	O12-C4-C5	5.43	122.47	116.03
8	C	1356	QUE	C5-C4-C3	-5.32	117.16	123.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

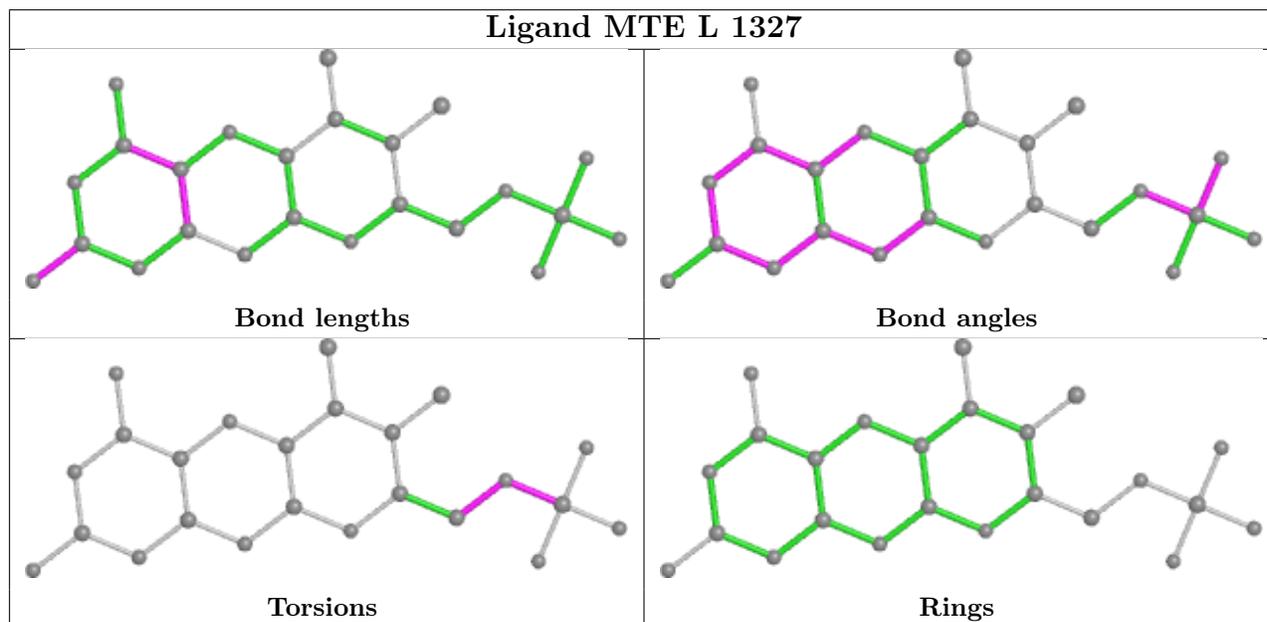
Mol	Chain	Res	Type	Atoms
6	L	1327	MTE	C3'-C4'-O4'-P
6	C	1327	MTE	C3'-C4'-O4'-P
6	L	1327	MTE	C4'-O4'-P-O3P

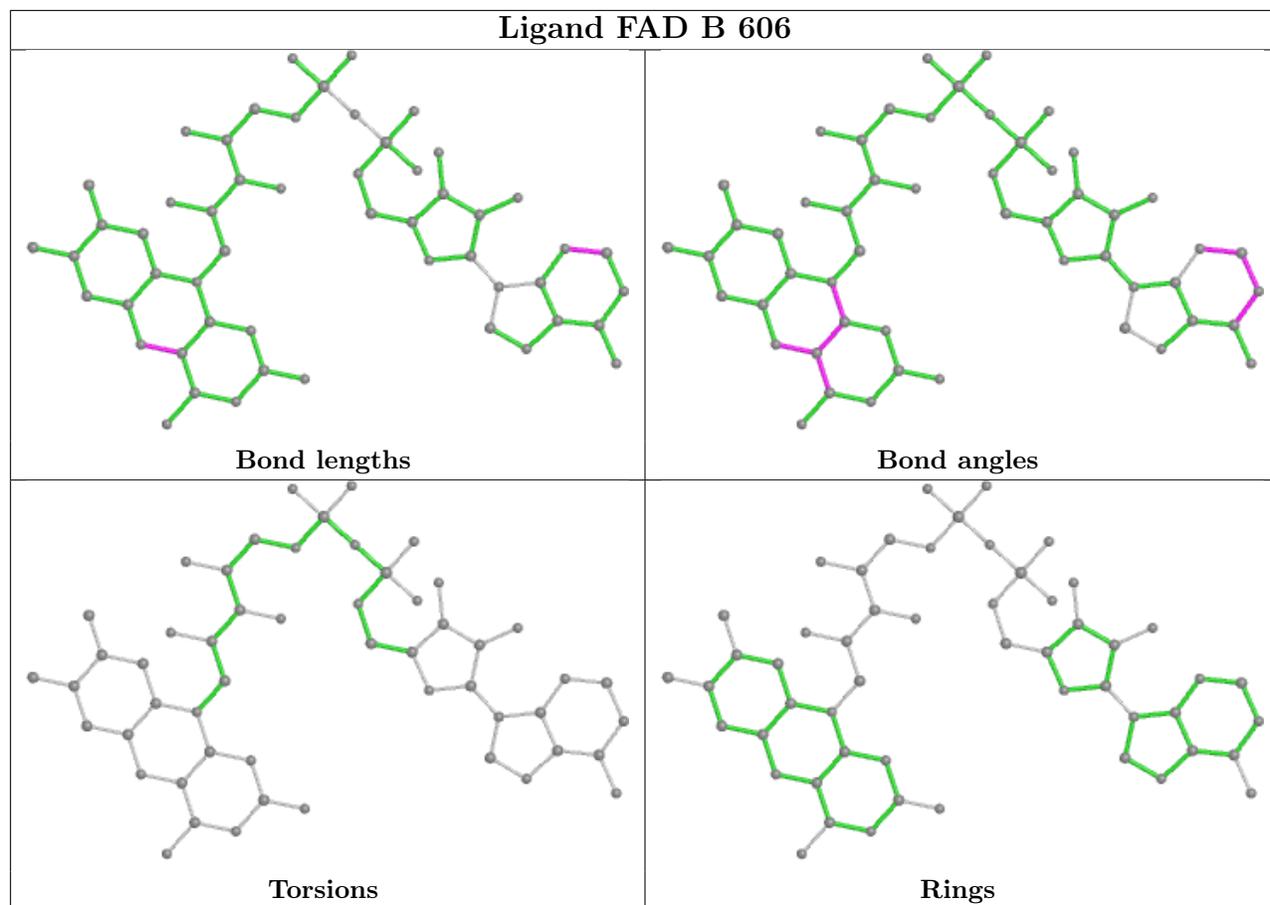
There are no ring outliers.

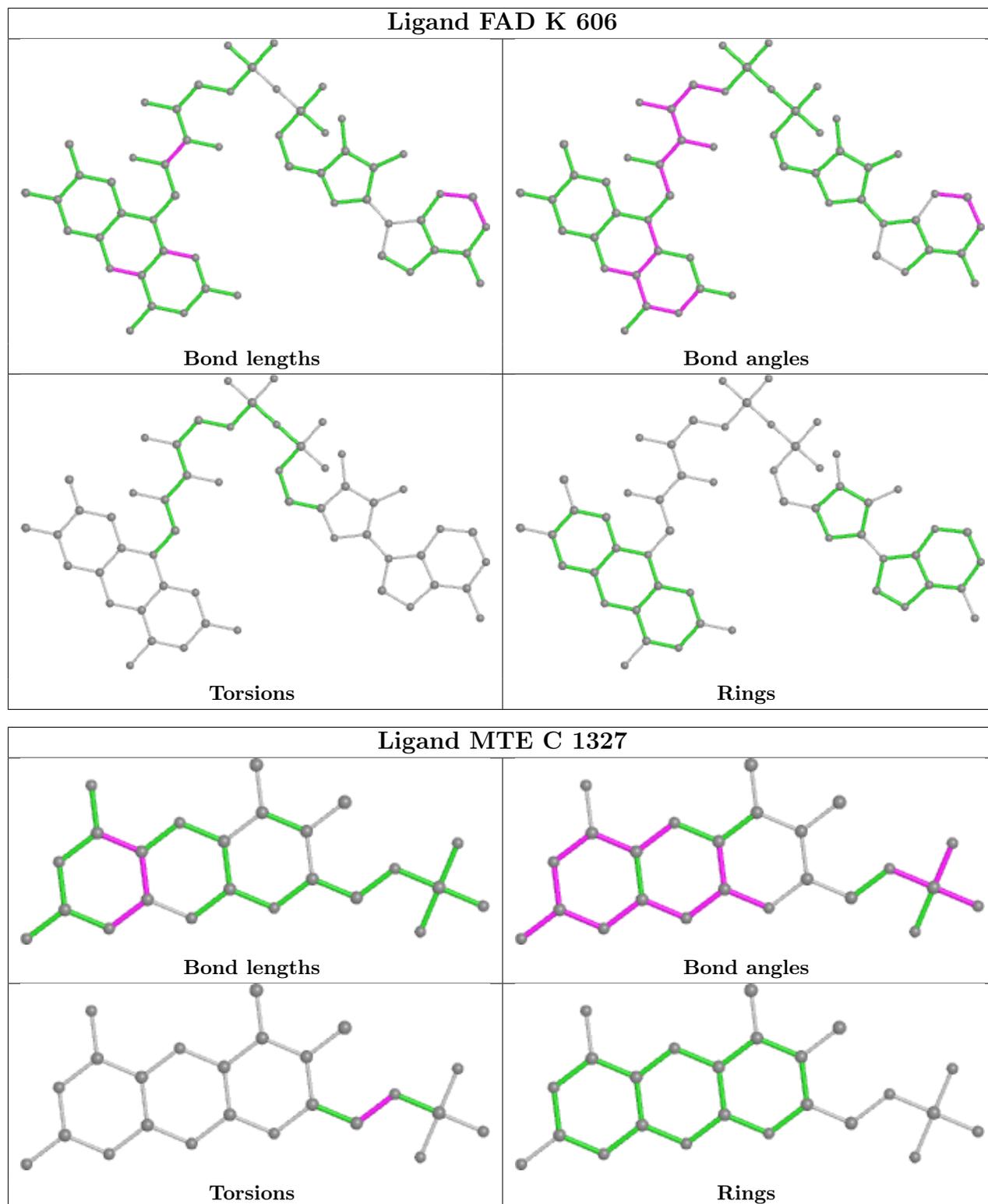
7 monomers are involved in 18 short contacts:

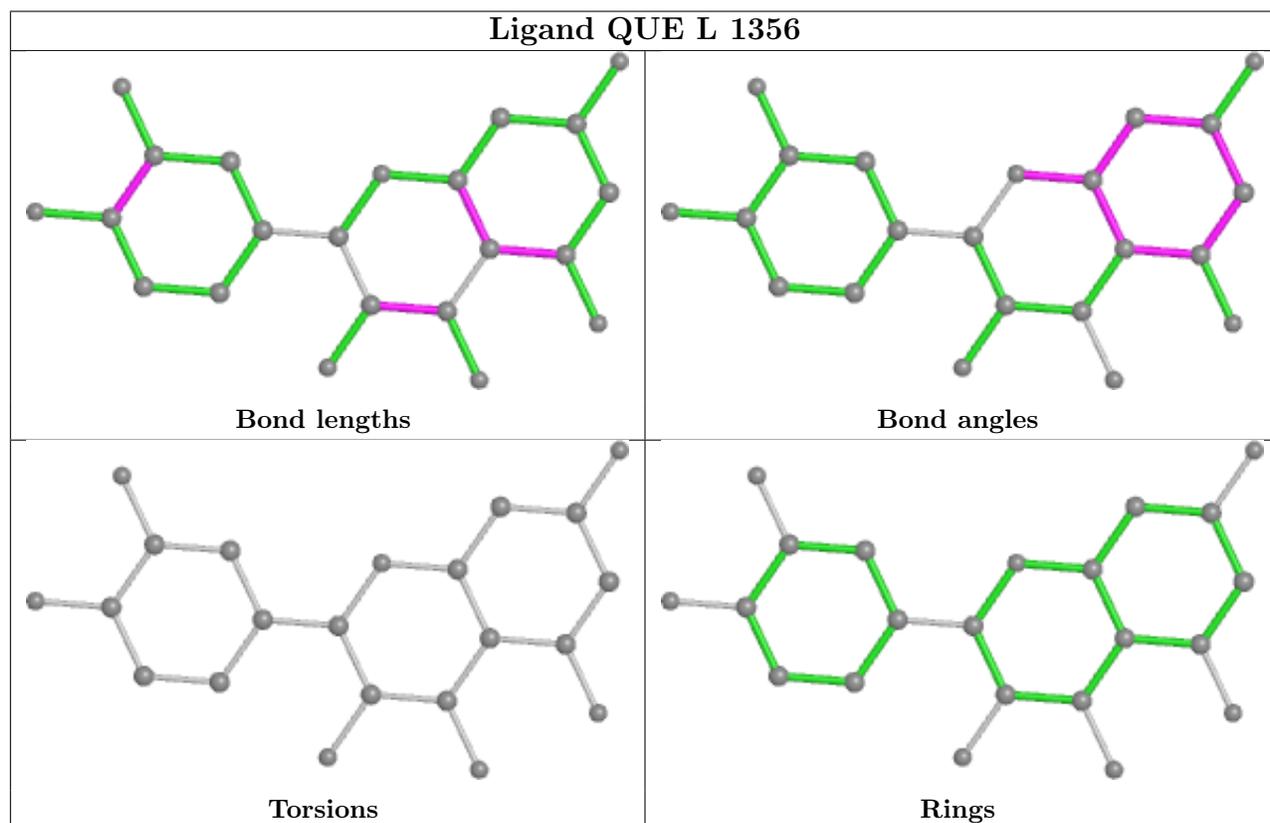
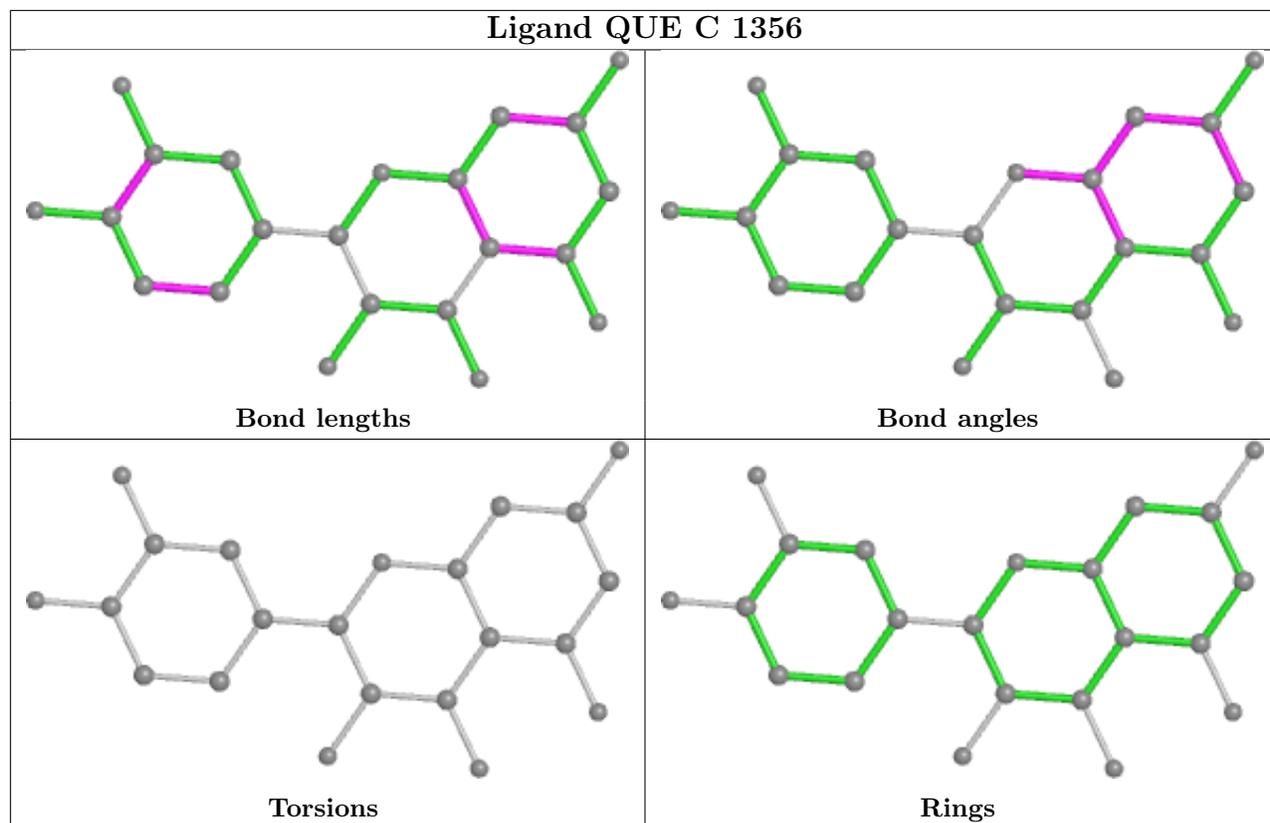
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1327	MTE	1	0
7	L	1328	MOS	3	0
7	C	1328	MOS	4	0
5	K	606	FAD	3	0
6	C	1327	MTE	1	0
8	C	1356	QUE	4	0
8	L	1356	QUE	3	0

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	-0.24	2 (1%) 79 78	11, 21, 38, 46	0
1	J	164/164 (100%)	-0.22	4 (2%) 59 57	15, 25, 44, 59	0
2	B	334/334 (100%)	-0.04	4 (1%) 79 78	18, 31, 46, 57	0
2	K	305/334 (91%)	0.31	15 (4%) 29 28	23, 37, 50, 58	0
3	C	756/756 (100%)	-0.36	0 100 100	11, 20, 31, 37	0
3	L	745/756 (98%)	-0.29	6 (0%) 86 85	12, 22, 37, 68	0
All	All	2468/2508 (98%)	-0.20	31 (1%) 77 76	11, 24, 43, 68	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1288	ASN	5.6
3	L	1287	ASN	5.5
1	A	61	LEU	5.4
2	K	424	ALA	4.9
3	L	1290	THR	4.9

### 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](#)

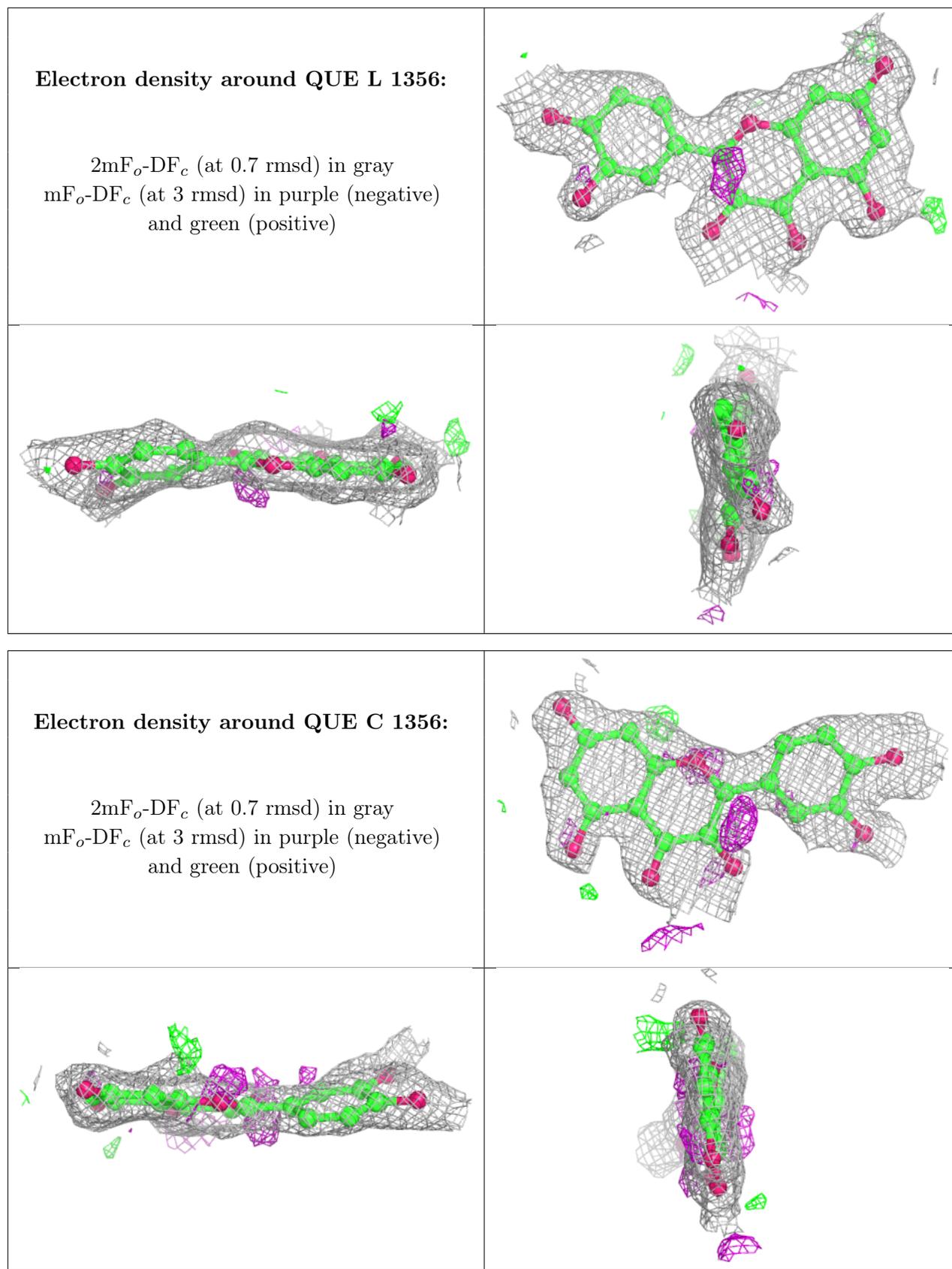
There are no monosaccharides in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

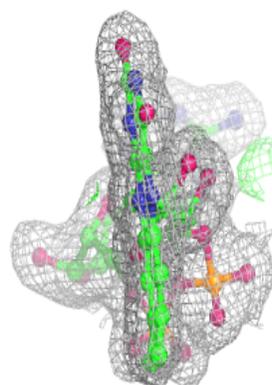
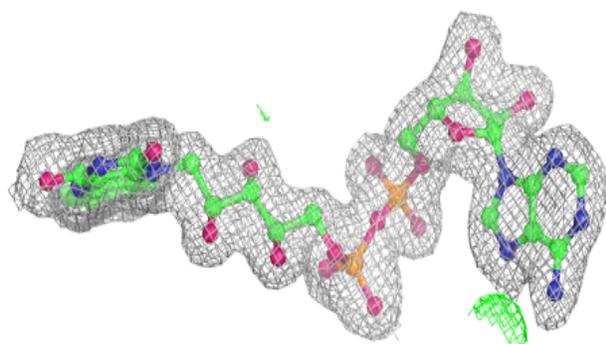
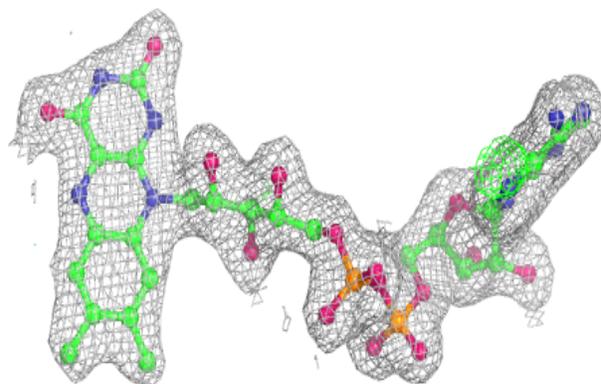
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	QUE	L	1356	22/22	0.85	0.17	37,39,40,41	0
8	QUE	C	1356	22/22	0.87	0.20	35,37,38,40	0
5	FAD	B	606	53/53	0.97	0.10	19,24,27,28	0
5	FAD	K	606	53/53	0.97	0.10	23,30,33,35	0
6	MTE	C	1327	24/24	0.98	0.08	12,13,19,22	0
6	MTE	L	1327	24/24	0.98	0.08	13,16,26,29	0
4	FES	A	602	4/4	0.99	0.09	15,15,17,18	0
7	MOS	C	1328	4/4	0.99	0.13	19,21,21,34	0
7	MOS	L	1328	4/4	0.99	0.11	19,21,26,35	0
4	FES	J	601	4/4	0.99	0.08	15,16,17,18	0
4	FES	J	602	4/4	0.99	0.08	17,17,18,18	0
4	FES	A	601	4/4	1.00	0.11	14,15,15,15	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.

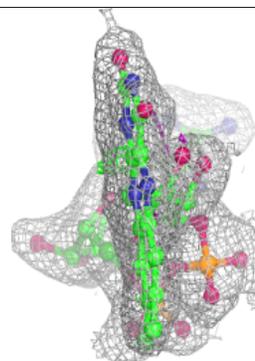
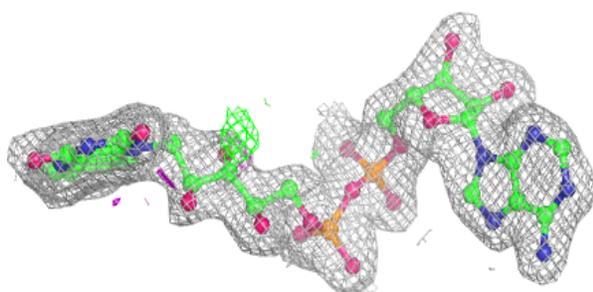
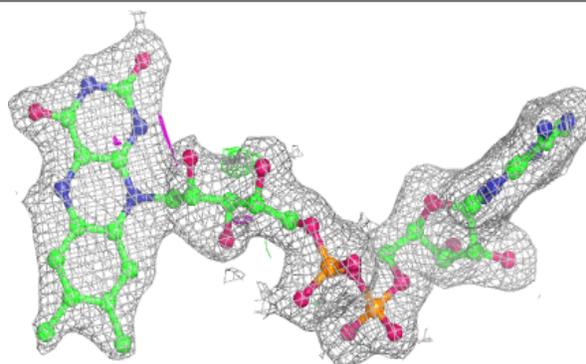


**Electron density around FAD B 606:**

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

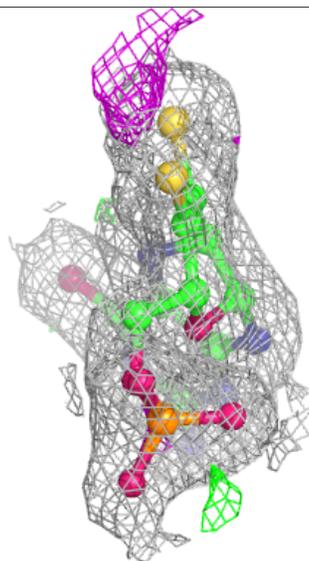
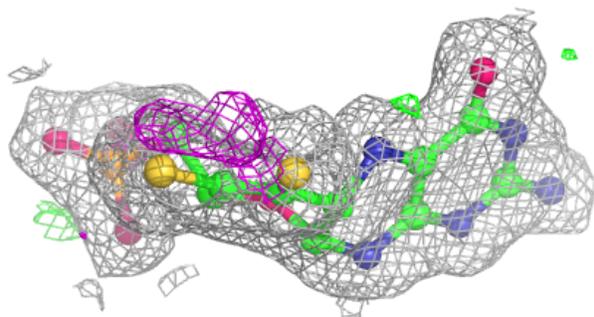
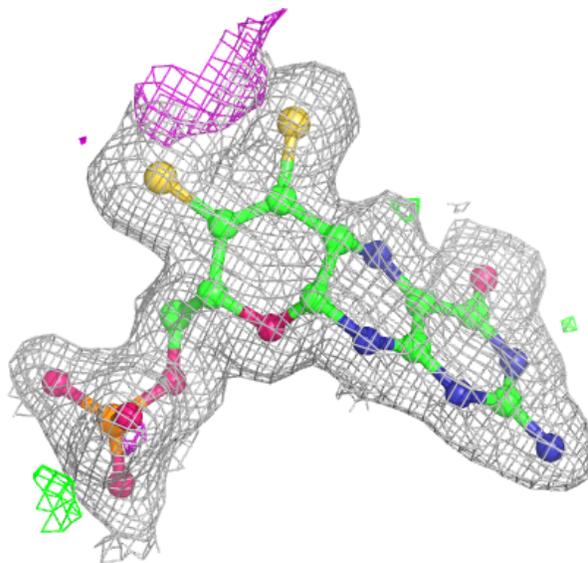
**Electron density around FAD K 606:**

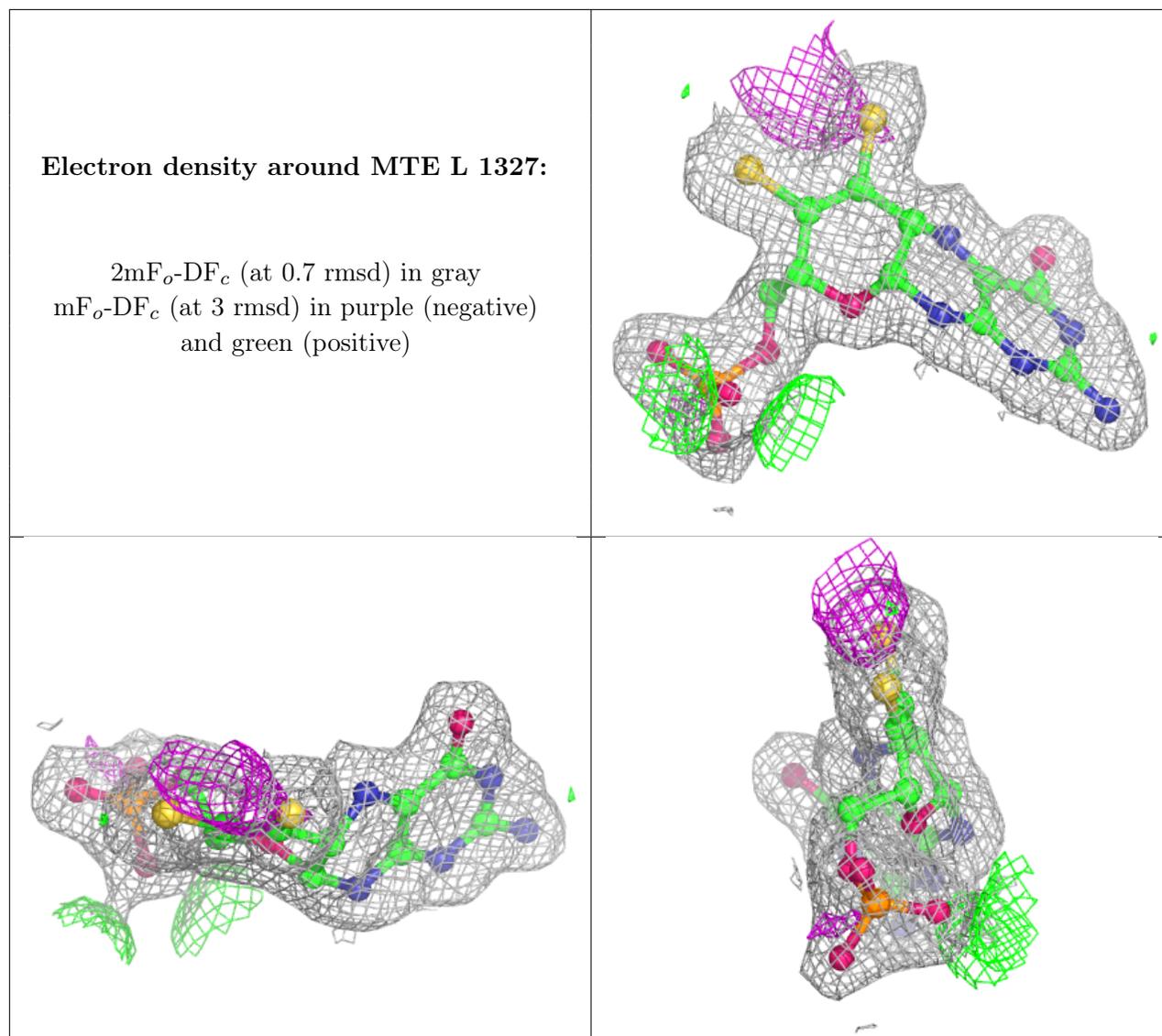
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MTE C 1327:**

$2mF_o-DF_c$  (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.