



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:55 PM EDT

PDB ID : 6GOU  
Title : Development of Alkyl Glycerone Phosphate Synthase Inhibitors: Complex with Inhibitor 2I  
Authors : Mattevi, A.; Piano, V.  
Deposited on : 2018-06-04  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

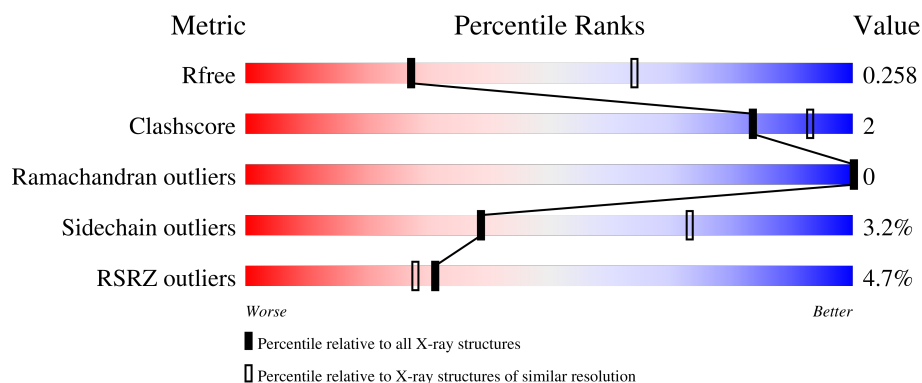
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	658	<div> <div>2%</div> <div>77%</div> <div>7%</div> <div>16%</div> </div>
1	B	658	<div> <div>3%</div> <div>75%</div> <div>6%</div> <div>18%</div> </div>
1	C	658	<div> <div>9%</div> <div>76%</div> <div>5%</div> <div>19%</div> </div>
1	D	658	<div> <div>%</div> <div>76%</div> <div>5%</div> <div>18%</div> </div>

2 Entry composition ⓘ

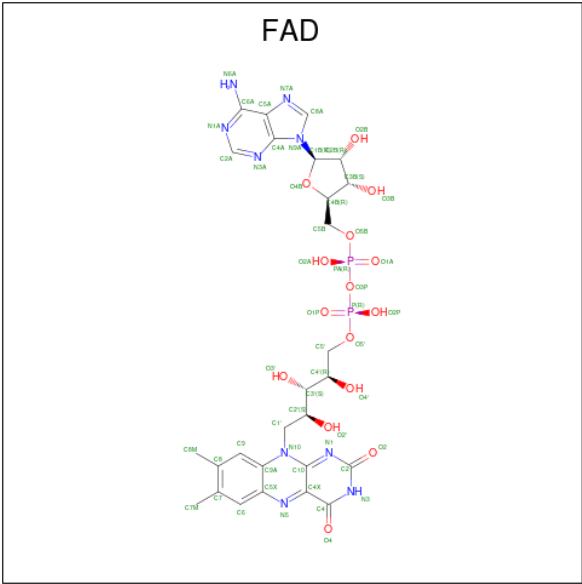
There are 3 unique types of molecules in this entry. The entry contains 17345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alkyldihydroxyacetonephosphate synthase, peroxisomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	540	Total	C	N	O	S	0	0	0
			4247	2697	735	791	24			
1	A	554	Total	C	N	O	S	0	0	0
			4355	2760	755	816	24			
1	B	540	Total	C	N	O	S	0	0	0
			4251	2699	736	792	24			
1	C	535	Total	C	N	O	S	0	0	0
			4205	2667	729	785	24			

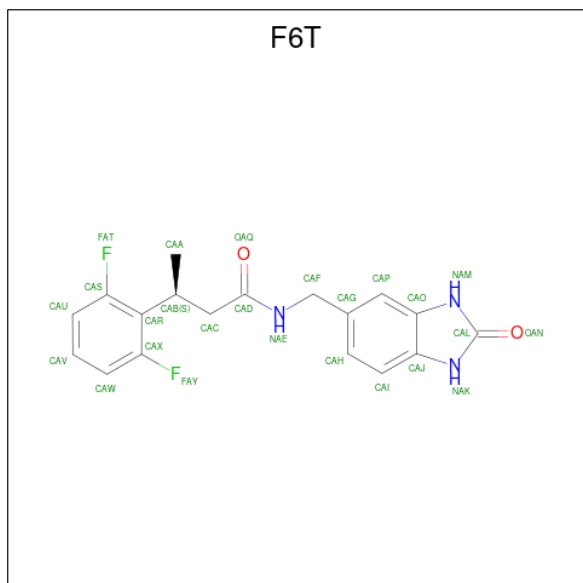
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

- Molecule 3 is (3 {S})-3-[2,6-bis(fluoranyl)phenyl]- {N}-[(2-oxidanylidene-1,3-dihydrobenzimidazol-5-yl)methyl]butanamide (three-letter code: F6T) (formula: C<sub>18</sub>H<sub>17</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total 25	C 18	F 2	N 3	O 2	0	0
3	A	1	Total 25	C 18	F 2	N 3	O 2	0	0
3	B	1	Total 25	C 18	F 2	N 3	O 2	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.96Å 120.64Å 148.16Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	48.00 – 2.90 47.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.90) 100.0 (47.99-2.90)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.219 , 0.258 0.221 , 0.258	Depositor DCC
$R_{free}$ test set	2934 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.31% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6T, 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	A	0.58	0/4454	0.75	2/6030 (0.0%)
1	B	0.56	0/4347	0.74	1/5883 (0.0%)
1	C	0.55	0/4297	0.74	1/5812 (0.0%)
1	D	0.59	0/4343	0.74	0/5878
All	All	0.57	0/17441	0.74	4/23603 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	474	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	572	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	550	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4355	0	4263	25	0
1	B	4251	0	4163	30	0
1	C	4205	0	4114	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4247	0	4157	28	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	25	0	0	1	0
3	B	25	0	0	0	0
3	D	25	0	0	1	0
All	All	17345	0	16821	83	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 2.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:LEU:CD1	1:B:648:PRO:O	2.03	1.06
1:D:478:LEU:HD11	1:B:648:PRO:O	1.57	1.02
1:D:474:ARG:NH1	1:B:649:THR:OG1	2.01	0.94
1:D:474:ARG:HG2	1:B:649:THR:HG21	1.53	0.89
1:D:475:GLU:OE1	1:B:342:ARG:NH2	2.11	0.83
1:D:474:ARG:HH12	1:B:651:ILE:HG13	1.48	0.79
1:D:474:ARG:CZ	1:B:649:THR:OG1	2.33	0.75
1:A:372:GLY:HA2	1:A:652:PHE:CE2	2.27	0.70
1:A:634:VAL:HB	1:C:345:ILE:HG23	1.75	0.68
1:D:478:LEU:HD12	1:B:648:PRO:O	1.92	0.68
2:A:701:FAD:HM72	3:A:702:F6T:CAH	2.26	0.66
1:C:372:GLY:HA2	1:C:652:PHE:CE2	2.34	0.63
1:B:175:TYR:HD2	1:B:208:ILE:HD11	1.65	0.61
1:D:175:TYR:HD2	1:D:208:ILE:HD11	1.66	0.60
1:C:175:TYR:HD2	1:C:208:ILE:HD11	1.66	0.60
1:B:372:GLY:HA2	1:B:652:PHE:CE2	2.37	0.59
1:D:474:ARG:HH12	1:B:651:ILE:CG1	2.14	0.59
1:A:175:TYR:HD2	1:A:208:ILE:HD11	1.68	0.59
1:D:372:GLY:HA2	1:D:652:PHE:CE2	2.39	0.57
1:D:474:ARG:CG	1:B:649:THR:HG21	2.30	0.54
1:A:338:VAL:HB	1:A:345:ILE:HG13	1.90	0.54
1:A:345:ILE:HG23	1:C:634:VAL:HB	1.89	0.54
1:D:474:ARG:NH1	1:B:651:ILE:HD11	2.23	0.54
1:D:338:VAL:HB	1:D:345:ILE:HG13	1.91	0.53
1:C:338:VAL:HB	1:C:345:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:VAL:HB	1:B:345:ILE:HG13	1.92	0.51
1:C:268:TRP:CH2	1:C:277:HIS:HB2	2.47	0.50
1:D:475:GLU:CD	1:B:342:ARG:HH22	2.12	0.49
1:C:268:TRP:CZ3	1:C:277:HIS:HB2	2.47	0.49
1:B:161:ASN:OD1	1:B:163:ASP:N	2.45	0.49
1:C:195:PHE:CD2	1:C:592:LEU:HD21	2.48	0.49
1:A:268:TRP:CZ3	1:A:277:HIS:HB2	2.48	0.48
1:A:268:TRP:CH2	1:A:277:HIS:HB2	2.49	0.48
1:C:470:PHE:HB3	1:C:477:VAL:HG13	1.95	0.47
1:D:475:GLU:HA	1:B:648:PRO:HB2	1.96	0.47
1:D:421:MET:CE	1:D:426:PHE:HA	2.44	0.47
1:A:195:PHE:CD2	1:A:592:LEU:HD21	2.49	0.47
1:A:470:PHE:HB3	1:A:477:VAL:HG13	1.96	0.47
1:B:225:ALA:HA	1:B:230:LEU:HD12	1.97	0.47
1:A:129:LYS:HG3	1:A:140:LEU:HD22	1.97	0.47
1:A:151:ASN:ND2	1:A:154:ASP:OD1	2.48	0.47
1:A:342:ARG:HG3	1:C:634:VAL:HG22	1.97	0.47
1:A:421:MET:CE	1:A:426:PHE:HA	2.45	0.47
2:D:701:FAD:HM72	3:D:702:F6T:CAH	2.46	0.46
1:B:195:PHE:CD2	1:B:592:LEU:HD21	2.51	0.46
1:A:138:ILE:HD13	1:A:140:LEU:HD12	1.97	0.46
1:D:195:PHE:CD2	1:D:592:LEU:HD21	2.50	0.46
1:C:421:MET:CE	1:C:426:PHE:HA	2.46	0.46
1:A:138:ILE:HD13	1:A:140:LEU:CD1	2.46	0.45
1:A:143:LYS:HD2	1:A:521:TYR:CE1	2.51	0.45
1:D:423:ASN:OD1	1:D:427:GLN:NE2	2.49	0.45
1:A:225:ALA:HA	1:A:230:LEU:HD12	1.97	0.45
1:B:421:MET:CE	1:B:426:PHE:HA	2.46	0.45
1:B:470:PHE:HB3	1:B:477:VAL:HG13	1.99	0.45
1:D:470:PHE:HB3	1:D:477:VAL:HG13	1.97	0.45
1:A:132:ILE:HG22	1:A:138:ILE:HD11	1.98	0.45
1:D:225:ALA:HA	1:D:230:LEU:HD12	1.98	0.44
1:A:423:ASN:OD1	1:A:427:GLN:NE2	2.50	0.44
1:C:132:ILE:HG22	1:C:138:ILE:HD11	1.98	0.44
1:D:474:ARG:NH1	1:B:651:ILE:CD1	2.80	0.44
1:C:423:ASN:OD1	1:C:427:GLN:NE2	2.50	0.44
1:C:338:VAL:HB	1:C:345:ILE:CG1	2.48	0.44
1:D:338:VAL:HB	1:D:345:ILE:CG1	2.48	0.43
1:A:338:VAL:HB	1:A:345:ILE:CG1	2.47	0.43
1:A:562:LEU:O	1:A:581:PHE:HA	2.18	0.43
1:D:132:ILE:HG22	1:D:138:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ALA:HA	1:C:230:LEU:HD12	1.99	0.43
1:D:139:ASN:HD22	1:D:139:ASN:HA	1.66	0.43
1:B:132:ILE:HG22	1:B:138:ILE:HD11	2.01	0.42
1:C:161:ASN:OD1	1:C:163:ASP:N	2.52	0.42
1:A:161:ASN:OD1	1:A:163:ASP:N	2.53	0.42
1:B:419:ARG:O	1:B:466:ALA:HA	2.20	0.42
1:A:634:VAL:HB	1:C:345:ILE:CG2	2.49	0.42
1:B:268:TRP:CH2	1:B:277:HIS:HB2	2.54	0.41
1:B:140:LEU:HG	1:B:521:TYR:CE2	2.56	0.41
1:B:139:ASN:HD22	1:B:139:ASN:HA	1.66	0.41
1:B:268:TRP:CZ3	1:B:277:HIS:HB2	2.56	0.41
1:D:268:TRP:CH2	1:D:277:HIS:HB2	2.56	0.41
1:D:474:ARG:HG2	1:B:649:THR:CG2	2.39	0.40
1:B:390:TYR:CD1	1:B:502:GLN:HG3	2.56	0.40
1:D:139:ASN:O	1:D:140:LEU:CB	2.69	0.40
1:A:645:TYR:CZ	1:C:637:GLY:HA3	2.57	0.40
1:A:419:ARG:O	1:A:466:ALA:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/658 (84%)	534 (97%)	16 (3%)	0	100	100
1	B	534/658 (81%)	519 (97%)	15 (3%)	0	100	100
1	C	527/658 (80%)	513 (97%)	14 (3%)	0	100	100
1	D	534/658 (81%)	520 (97%)	14 (3%)	0	100	100
All	All	2145/2632 (82%)	2086 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/545 (86%)	455 (97%)	14 (3%)	41	75
1	B	456/545 (84%)	440 (96%)	16 (4%)	36	70
1	C	450/545 (83%)	436 (97%)	14 (3%)	40	74
1	D	455/545 (84%)	440 (97%)	15 (3%)	38	72
All	All	1830/2180 (84%)	1771 (97%)	59 (3%)	39	73

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	139	ASN
1	D	155	THR
1	D	172	ASN
1	D	174	SER
1	D	175	TYR
1	D	285	GLN
1	D	345	ILE
1	D	349	CYS
1	D	411	GLN
1	D	463	LEU
1	D	480	HIS
1	D	482	LYS
1	D	510	VAL
1	D	529	GLU
1	D	581	PHE
1	A	139	ASN
1	A	153	SER
1	A	172	ASN
1	A	174	SER
1	A	175	TYR
1	A	285	GLN
1	A	345	ILE
1	A	349	CYS
1	A	411	GLN

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Mol	Chain	Res	Type
1	A	480	HIS
1	A	482	LYS
1	A	510	VAL
1	A	529	GLU
1	A	581	PHE
1	B	139	ASN
1	B	140	LEU
1	B	155	THR
1	B	172	ASN
1	B	174	SER
1	B	175	TYR
1	B	285	GLN
1	B	345	ILE
1	B	349	CYS
1	B	411	GLN
1	B	463	LEU
1	B	480	HIS
1	B	482	LYS
1	B	510	VAL
1	B	529	GLU
1	B	581	PHE
1	C	139	ASN
1	C	155	THR
1	C	172	ASN
1	C	174	SER
1	C	175	TYR
1	C	285	GLN
1	C	345	ILE
1	C	349	CYS
1	C	411	GLN
1	C	480	HIS
1	C	482	LYS
1	C	510	VAL
1	C	529	GLU
1	C	581	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	139	ASN
1	D	277	HIS
1	D	300	HIS

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Mol	Chain	Res	Type
1	D	361	HIS
1	D	411	GLN
1	A	139	ASN
1	A	189	HIS
1	A	277	HIS
1	A	300	HIS
1	B	139	ASN
1	B	189	HIS
1	B	277	HIS
1	B	300	HIS
1	B	361	HIS
1	C	139	ASN
1	C	189	HIS
1	C	300	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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
3	F6T	A	702	-	27,27,27	2.21	10 (37%)	38,38,38	1.72	9 (23%)
3	F6T	D	702	-	27,27,27	2.10	8 (29%)	38,38,38	1.48	4 (10%)
2	FAD	A	701	-	54,58,58	1.22	5 (9%)	71,89,89	1.60	16 (22%)
2	FAD	C	701	-	54,58,58	1.39	6 (11%)	71,89,89	1.48	13 (18%)
2	FAD	B	701	-	54,58,58	1.43	8 (14%)	71,89,89	1.56	15 (21%)
2	FAD	D	701	-	54,58,58	1.50	6 (11%)	71,89,89	1.37	10 (14%)
3	F6T	B	702	-	27,27,27	2.14	13 (48%)	38,38,38	1.54	6 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F6T	A	702	-	-	0/13/13/13	0/3/3/3
3	F6T	D	702	-	-	2/13/13/13	0/3/3/3
2	FAD	A	701	-	-	4/30/50/50	0/6/6/6
2	FAD	C	701	-	-	6/30/50/50	0/6/6/6
2	FAD	B	701	-	-	6/30/50/50	0/6/6/6
2	FAD	D	701	-	-	4/30/50/50	0/6/6/6
3	F6T	B	702	-	-	1/13/13/13	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	F6T	CAR-CAB	-6.61	1.42	1.51
2	D	701	FAD	C9A-C5X	5.72	1.50	1.41
2	C	701	FAD	C9A-C5X	5.64	1.50	1.41
3	D	702	F6T	CAR-CAB	-5.17	1.44	1.51
3	D	702	F6T	FAY-CAX	-5.14	1.21	1.35
2	B	701	FAD	C9A-C5X	5.00	1.49	1.41
3	B	702	F6T	FAT-CAS	-4.52	1.23	1.35
2	D	701	FAD	PA-O3P	4.23	1.64	1.59
3	B	702	F6T	CAR-CAB	-3.94	1.46	1.51
3	B	702	F6T	CAF-CAG	-3.74	1.43	1.51
2	A	701	FAD	C9A-C5X	3.60	1.47	1.41
3	A	702	F6T	CAF-CAG	-3.52	1.43	1.51
3	D	702	F6T	CAF-CAG	-3.51	1.43	1.51
3	A	702	F6T	CAI-CAJ	-3.46	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	FAD	C8-C7	3.37	1.49	1.40
2	C	701	FAD	C8-C7	3.17	1.48	1.40
2	B	701	FAD	C8-C7	3.14	1.48	1.40
2	B	701	FAD	C5X-N5	-3.07	1.33	1.39
2	A	701	FAD	C5X-N5	-3.02	1.33	1.39
3	A	702	F6T	CAO-NAM	-2.91	1.33	1.38
3	B	702	F6T	CAL-NAM	-2.89	1.32	1.37
2	D	701	FAD	P-O3P	2.85	1.62	1.59
3	A	702	F6T	FAY-CAX	2.83	1.43	1.35
2	C	701	FAD	PA-O3P	2.79	1.62	1.59
2	B	701	FAD	O4B-C1B	2.76	1.44	1.40
3	A	702	F6T	CAP-CAO	-2.74	1.35	1.39
2	B	701	FAD	C2A-N3A	2.73	1.36	1.32
3	B	702	F6T	CAL-NAK	-2.66	1.33	1.37
3	B	702	F6T	CAR-CAS	2.66	1.42	1.39
3	B	702	F6T	CAP-CAO	-2.64	1.35	1.39
2	A	701	FAD	C8-C7	2.56	1.47	1.40
3	D	702	F6T	CAI-CAJ	-2.51	1.35	1.39
3	B	702	F6T	CAI-CAJ	-2.45	1.35	1.39
3	A	702	F6T	CAR-CAS	2.43	1.41	1.39
2	B	701	FAD	O4-C4	2.38	1.28	1.23
3	B	702	F6T	CAF-NAE	2.37	1.50	1.46
3	D	702	F6T	CAL-NAM	-2.36	1.33	1.37
3	D	702	F6T	CAJ-CAO	-2.34	1.34	1.40
2	C	701	FAD	P-O3P	2.33	1.62	1.59
3	A	702	F6T	CAL-NAM	-2.32	1.33	1.37
3	B	702	F6T	CAO-NAM	-2.30	1.34	1.38
3	B	702	F6T	CAJ-CAO	-2.26	1.35	1.40
2	A	701	FAD	P-O3P	2.23	1.61	1.59
2	B	701	FAD	C4X-N5	2.20	1.35	1.30
2	B	701	FAD	PA-O3P	2.18	1.61	1.59
3	A	702	F6T	CAJ-NAK	-2.18	1.34	1.38
3	B	702	F6T	CAC-CAD	2.17	1.56	1.51
3	B	702	F6T	CAR-CAX	2.17	1.41	1.39
2	A	701	FAD	C4X-N5	2.16	1.35	1.30
2	D	701	FAD	C5A-N7A	-2.10	1.32	1.39
2	C	701	FAD	C5X-N5	-2.10	1.35	1.39
2	D	701	FAD	C10-N10	2.09	1.41	1.37
2	C	701	FAD	C4X-N5	2.08	1.35	1.30
3	D	702	F6T	CAO-NAM	-2.05	1.35	1.38
3	D	702	F6T	CAF-NAE	2.03	1.50	1.46
3	A	702	F6T	CAJ-CAO	-2.02	1.35	1.40



All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	F6T	FAY-CAX-CAR	4.87	124.00	118.14
2	B	701	FAD	N3A-C2A-N1A	-4.81	122.14	128.67
3	B	702	F6T	FAY-CAX-CAR	4.45	123.50	118.14
3	A	702	F6T	CAW-CAX-CAR	-4.30	119.32	123.98
2	A	701	FAD	N3A-C2A-N1A	-4.15	123.04	128.67
2	C	701	FAD	N3A-C2A-N1A	-4.10	123.11	128.67
2	B	701	FAD	O2-C2-N1	-4.03	115.11	121.80
2	A	701	FAD	C9A-C5X-N5	-3.96	118.26	122.45
2	A	701	FAD	C5X-N5-C4X	3.90	124.39	118.09
2	A	701	FAD	C4-C4X-N5	3.76	123.39	118.21
3	A	702	F6T	FAY-CAX-CAR	3.43	122.27	118.14
2	D	701	FAD	O2-C2-N1	-3.30	116.31	121.80
3	D	702	F6T	CAW-CAX-CAR	-3.30	120.41	123.98
2	D	701	FAD	N3A-C2A-N1A	-3.25	124.27	128.67
2	B	701	FAD	C4-C4X-N5	3.24	122.68	118.21
3	B	702	F6T	FAT-CAS-CAR	3.16	121.94	118.14
3	A	702	F6T	CAV-CAW-CAX	3.12	123.33	118.49
2	C	701	FAD	O2-C2-N1	-3.06	116.72	121.80
2	C	701	FAD	C5'-C4'-C3'	3.04	117.95	112.22
2	A	701	FAD	O2-C2-N1	-2.95	116.89	121.80
2	C	701	FAD	C4-C4X-N5	2.93	122.25	118.21
2	C	701	FAD	C9A-C5X-N5	-2.91	119.37	122.45
3	A	702	F6T	CAX-CAR-CAS	2.85	117.89	114.27
2	B	701	FAD	C5X-N5-C4X	2.83	122.67	118.09
2	B	701	FAD	C10-N1-C2	2.82	122.95	116.85
2	C	701	FAD	C4-N3-C2	-2.78	120.70	125.64
3	A	702	F6T	FAT-CAS-CAR	2.76	121.46	118.14
2	B	701	FAD	O4-C4-C4X	-2.73	119.34	126.53
3	D	702	F6T	CAV-CAW-CAX	2.70	122.68	118.49
3	B	702	F6T	CAW-CAX-CAR	-2.68	121.07	123.98
2	A	701	FAD	O4-C4-C4X	-2.68	119.47	126.53
2	D	701	FAD	C4X-C10-N1	-2.67	118.03	124.59
2	C	701	FAD	C4X-C10-N1	-2.66	118.06	124.59
2	C	701	FAD	C5X-N5-C4X	2.66	122.39	118.09
2	D	701	FAD	C4X-C10-N10	2.65	120.28	116.48
2	D	701	FAD	C10-N1-C2	2.62	122.51	116.85
3	A	702	F6T	CAB-CAC-CAD	-2.60	109.42	113.03
2	C	701	FAD	C10-N1-C2	2.58	122.44	116.85
2	A	701	FAD	N6A-C6A-N1A	2.57	123.84	118.33
3	B	702	F6T	CAC-CAB-CAR	2.56	116.87	110.84
2	B	701	FAD	C4X-C10-N1	-2.55	118.33	124.59
3	A	702	F6T	CAC-CAB-CAR	2.53	116.80	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	FAD	O4-C4-C4X	-2.53	119.85	126.53
2	C	701	FAD	O4-C4-C4X	-2.53	119.86	126.53
2	C	701	FAD	C4X-C10-N10	2.48	120.03	116.48
2	D	701	FAD	C4-C4X-N5	2.45	121.59	118.21
2	A	701	FAD	C4X-C10-N1	-2.44	118.62	124.59
2	B	701	FAD	N6A-C6A-N1A	2.42	123.50	118.33
2	A	701	FAD	C10-C4X-N5	-2.38	119.96	124.81
2	A	701	FAD	C10-N1-C2	2.37	121.99	116.85
2	A	701	FAD	O3P-PA-O1A	-2.36	103.60	110.70
3	A	702	F6T	OAN-CAL-NAM	-2.36	123.99	126.68
2	A	701	FAD	C4-N3-C2	-2.35	121.46	125.64
2	D	701	FAD	N6A-C6A-N1A	2.34	123.33	118.33
2	A	701	FAD	O2A-PA-O1A	2.34	123.31	112.44
2	B	701	FAD	C10-C4X-N5	-2.24	120.24	124.81
2	C	701	FAD	C4A-C5A-N7A	-2.23	106.98	109.34
2	B	701	FAD	C4-N3-C2	-2.22	121.70	125.64
2	B	701	FAD	C9A-C5X-N5	-2.21	120.11	122.45
3	B	702	F6T	CAV-CAW-CAX	2.20	121.90	118.49
3	B	702	F6T	CAJ-NAK-CAL	-2.20	107.63	110.03
2	B	701	FAD	O2P-P-O1P	2.18	122.58	112.44
2	C	701	FAD	C4X-C4-N3	2.15	118.73	113.25
2	A	701	FAD	C4X-C4-N3	2.13	118.68	113.25
2	D	701	FAD	C9A-N10-C10	-2.12	117.52	120.75
2	A	701	FAD	C9-C9A-C5X	-2.11	116.31	120.03
2	B	701	FAD	O3'-C3'-C4'	2.11	113.71	108.93
2	B	701	FAD	O3P-P-O1P	-2.10	104.38	110.70
3	D	702	F6T	CAX-CAR-CAS	2.10	116.94	114.27
2	D	701	FAD	C4-N3-C2	-2.09	121.93	125.64
2	B	701	FAD	C4X-C10-N10	2.09	119.47	116.48
3	A	702	F6T	CAW-CAV-CAU	-2.06	117.60	120.24
2	A	701	FAD	C5X-C9A-N10	2.01	119.79	117.97

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	N10-C1'-C2'-O2'
2	A	701	FAD	N10-C1'-C2'-C3'
2	B	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	C	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	N10-C1'-C2'-C3'
3	D	702	F6T	CAR-CAB-CAC-CAD
2	B	701	FAD	C3'-C4'-C5'-O5'
3	D	702	F6T	CAA-CAB-CAC-CAD
2	C	701	FAD	C3'-C4'-C5'-O5'
2	C	701	FAD	PA-O3P-P-O2P
2	B	701	FAD	O4'-C4'-C5'-O5'
2	C	701	FAD	O4'-C4'-C5'-O5'
2	D	701	FAD	PA-O3P-P-O1P
2	A	701	FAD	PA-O3P-P-O1P
2	A	701	FAD	PA-O3P-P-O2P
2	B	701	FAD	PA-O3P-P-O2P
3	B	702	F6T	CAC-CAB-CAR-CAS
2	D	701	FAD	PA-O3P-P-O2P
2	B	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	PA-O3P-P-O1P

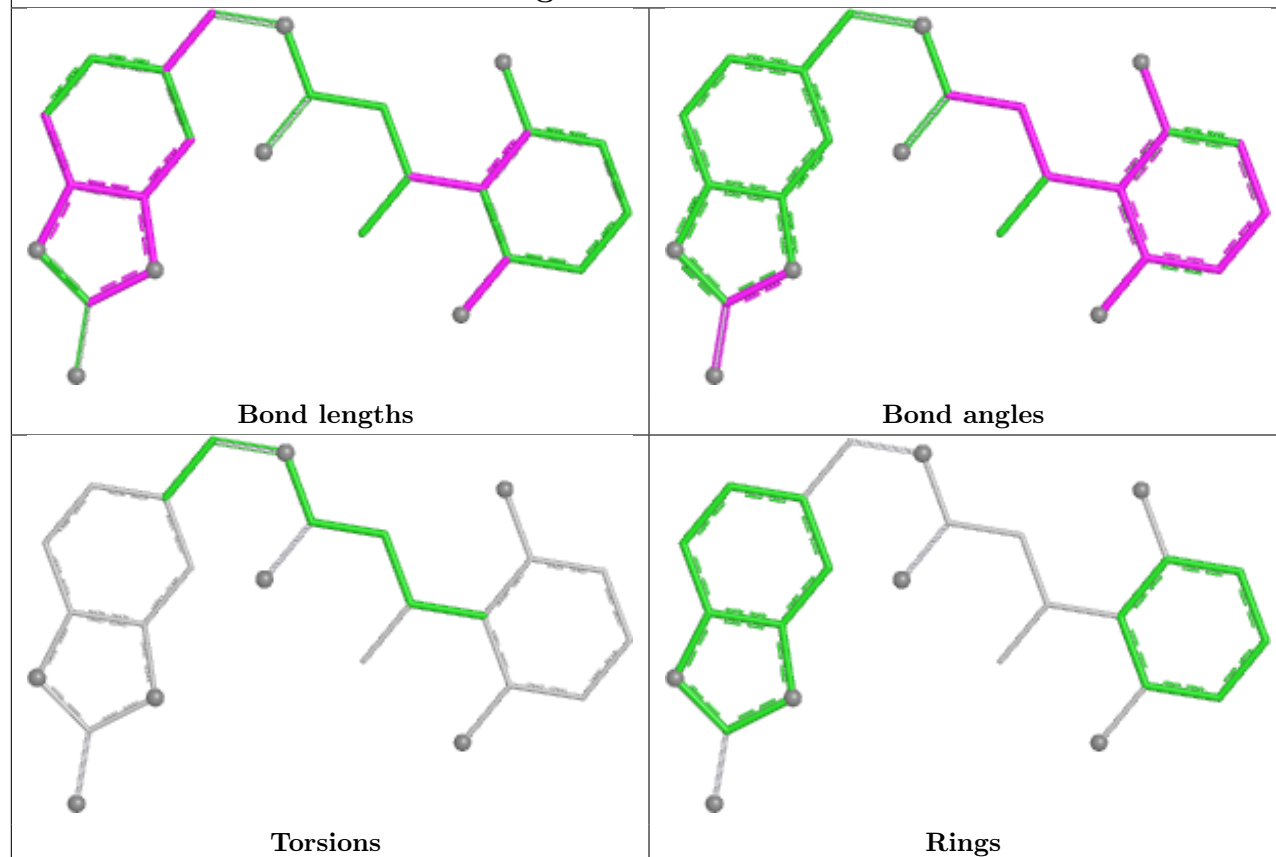
There are no ring outliers.

4 monomers are involved in 2 short contacts:

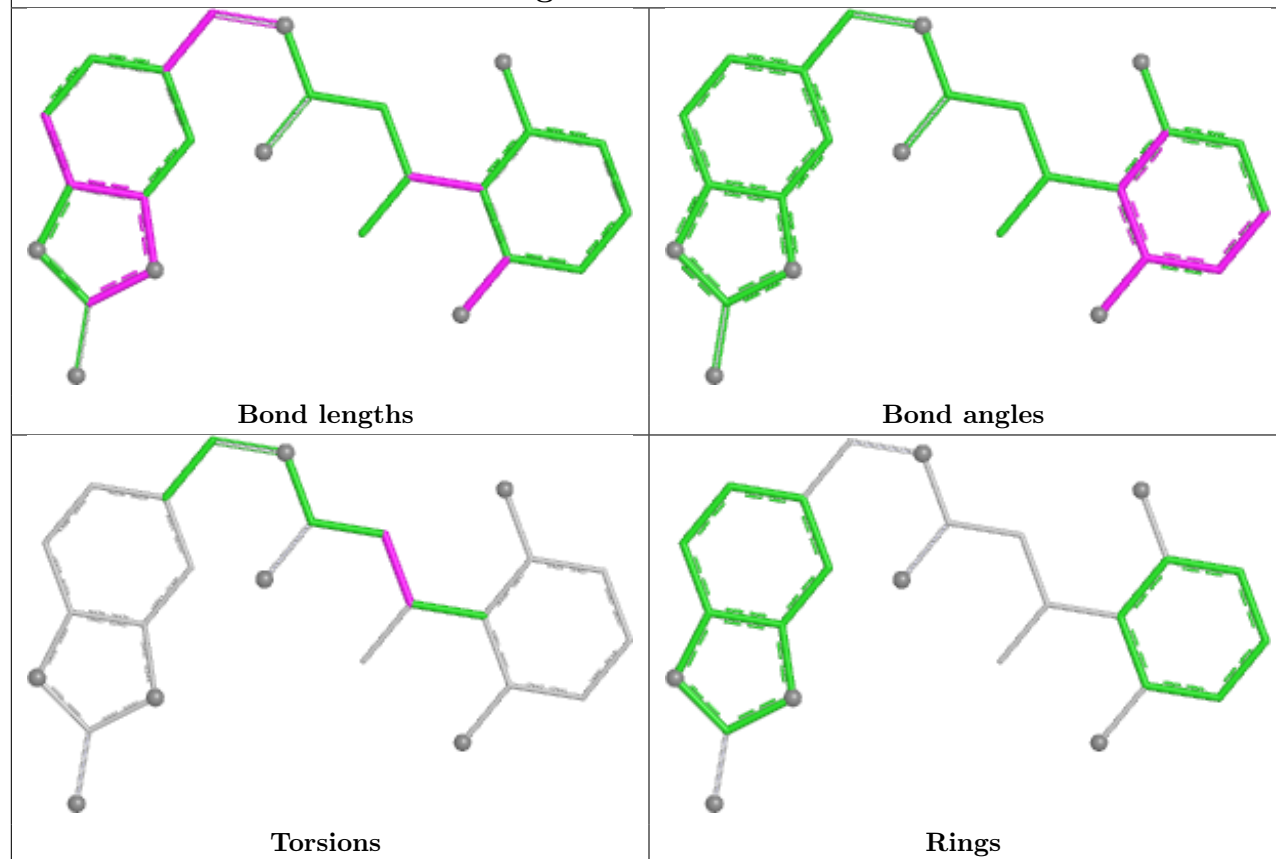
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	F6T	1	0
3	D	702	F6T	1	0
2	A	701	FAD	1	0
2	D	701	FAD	1	0

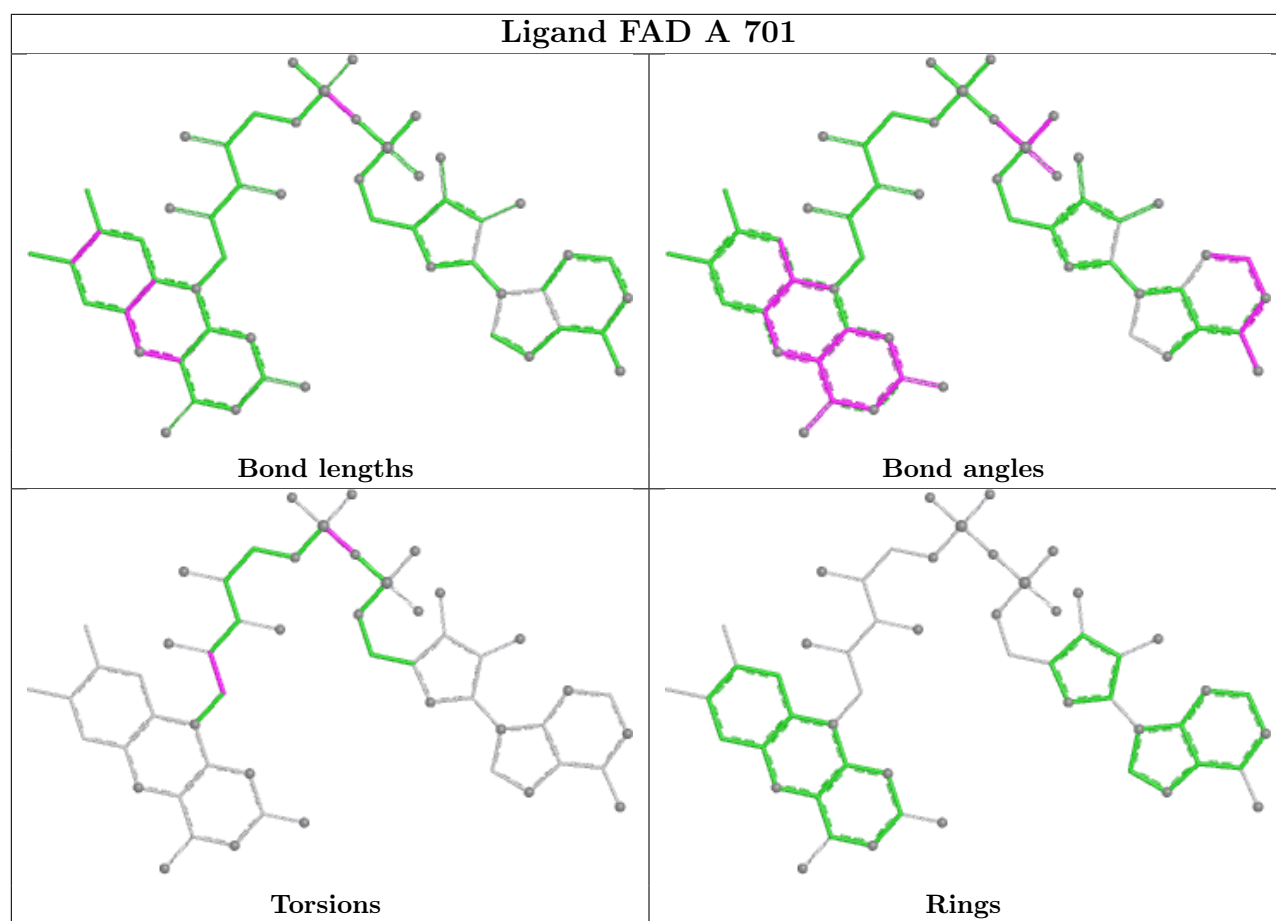
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

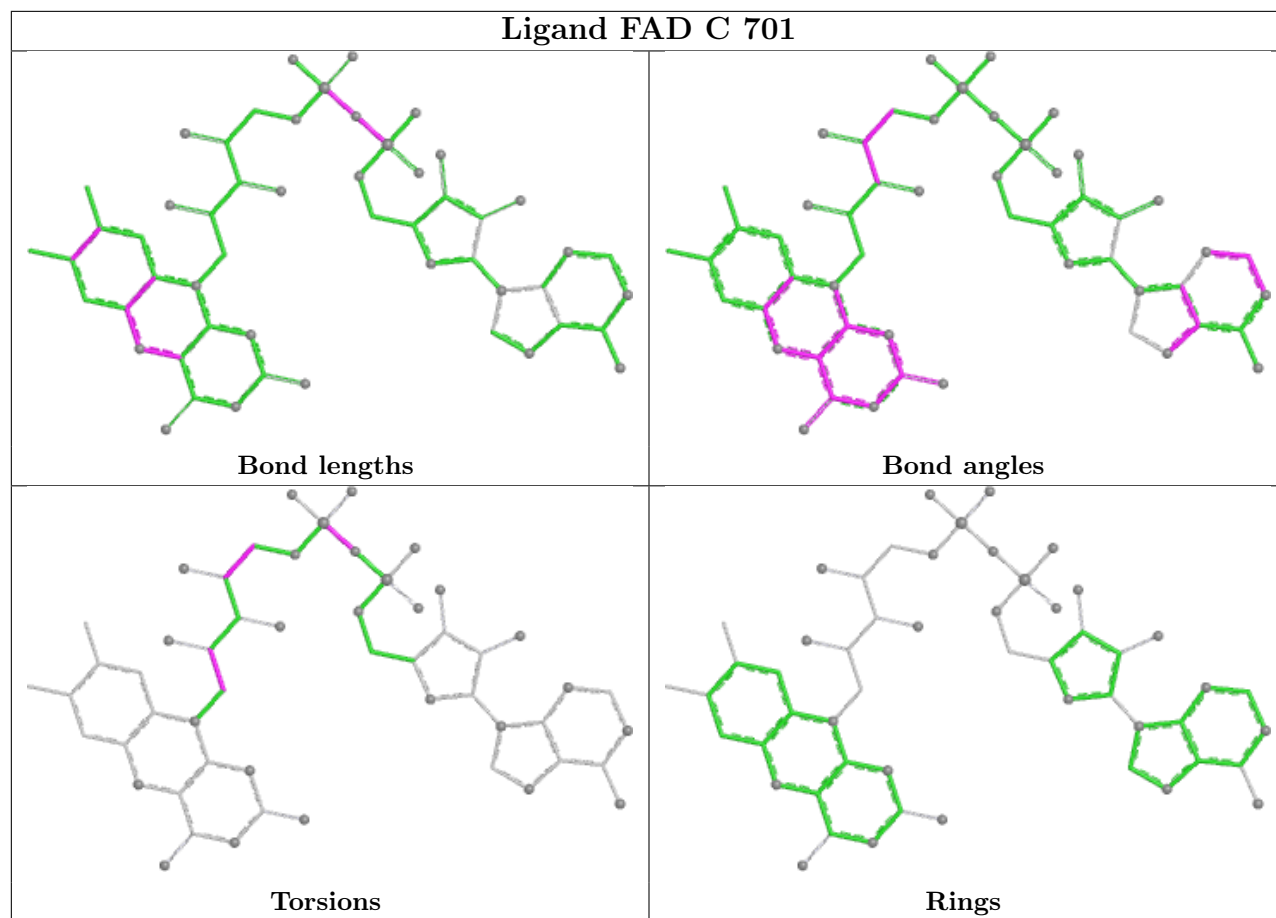
## Ligand F6T A 702

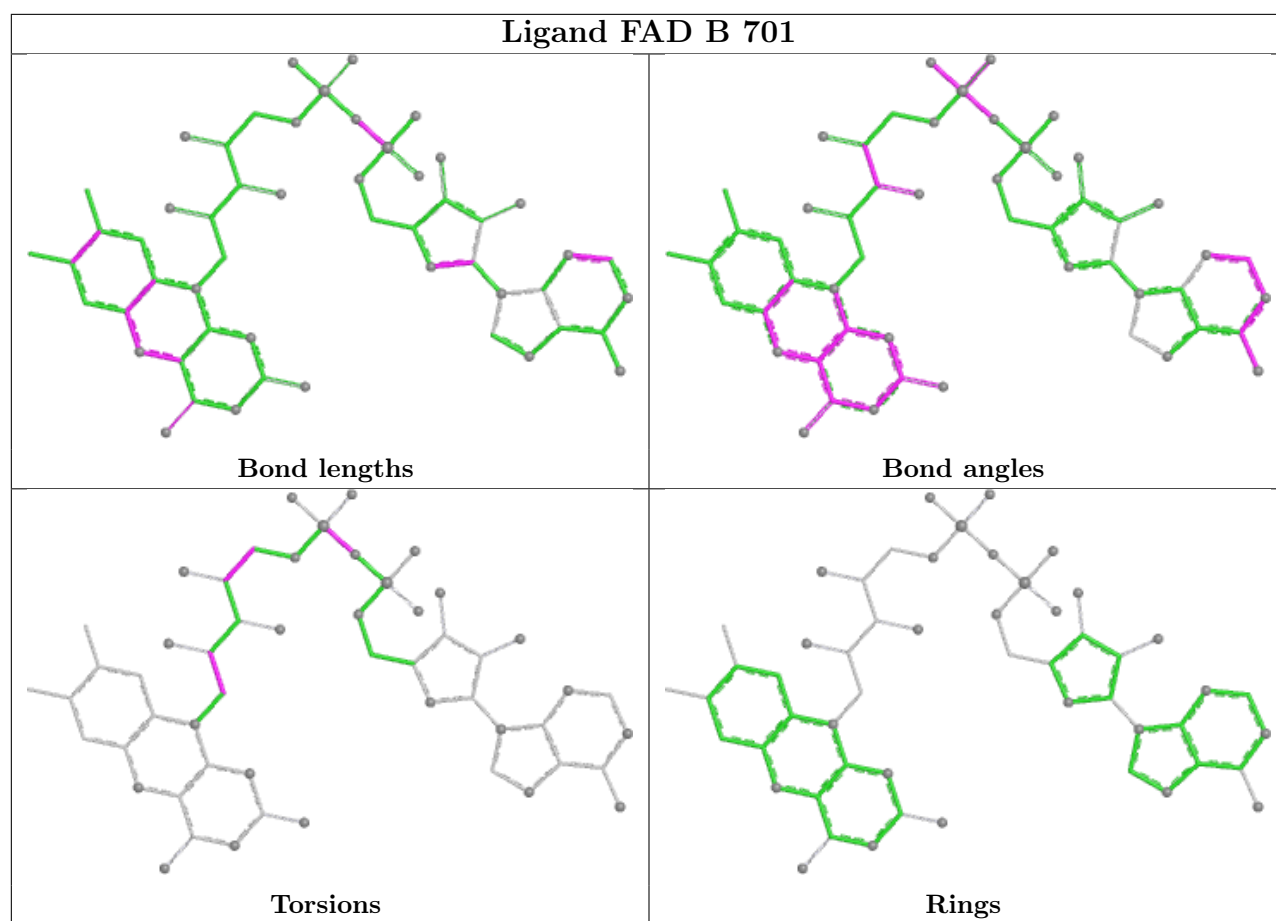


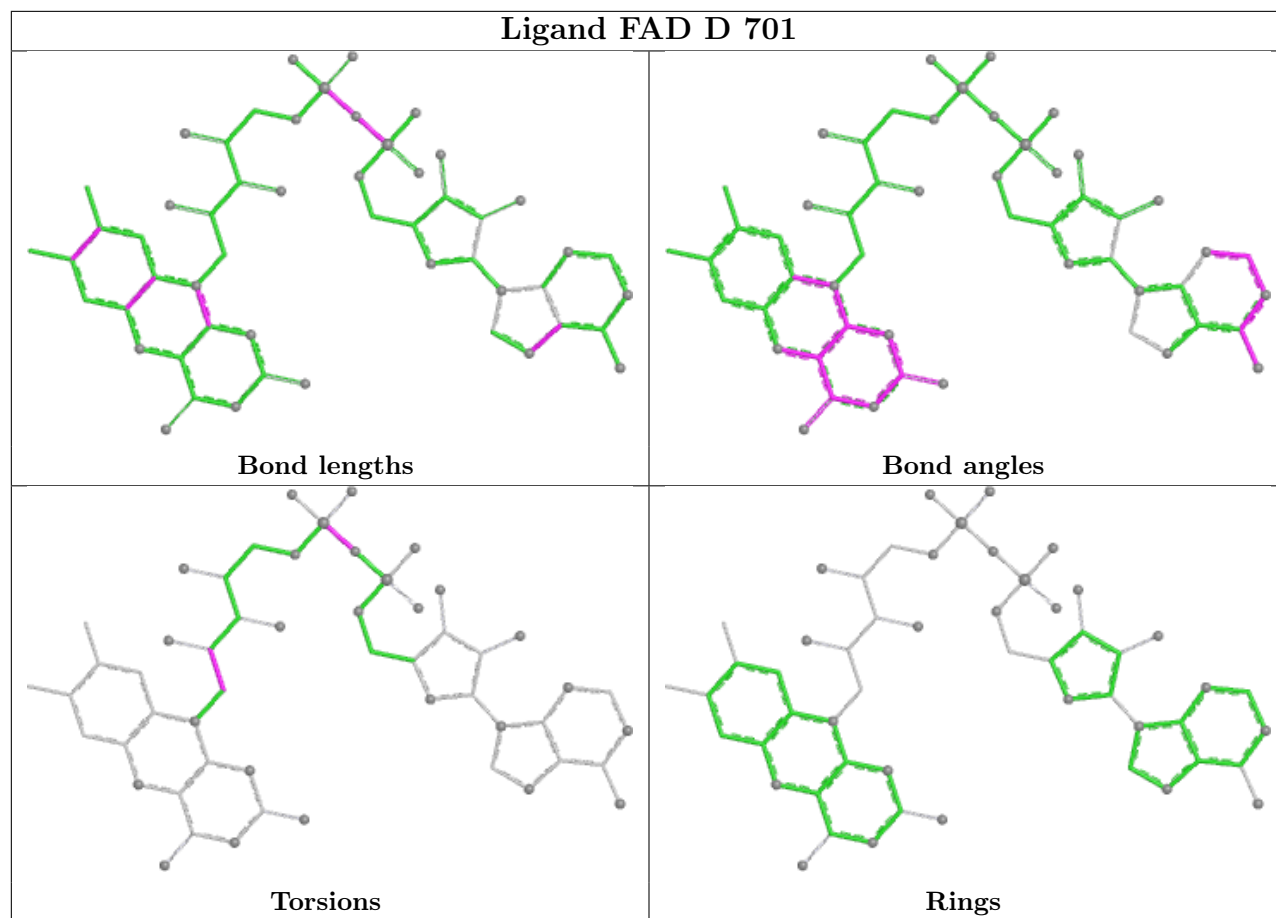
## Ligand F6T D 702



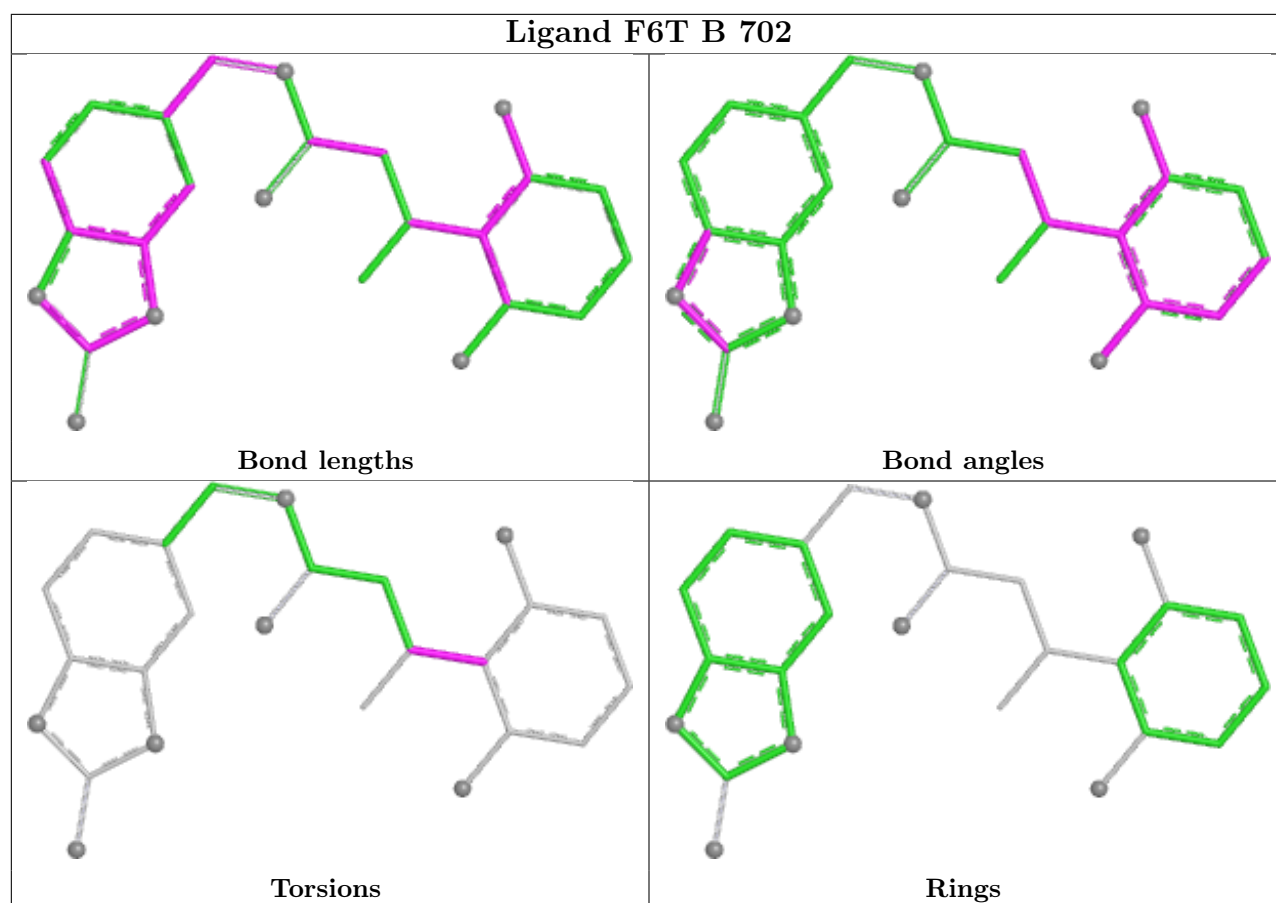












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	554/658 (84%)	-0.05	14 (2%) 57 55	18, 41, 71, 99	0
1	B	540/658 (82%)	0.12	19 (3%) 44 38	21, 48, 80, 122	0
1	C	535/658 (81%)	0.55	59 (11%) 5 4	22, 62, 108, 138	0
1	D	540/658 (82%)	-0.22	9 (1%) 70 69	16, 35, 69, 114	0
All	All	2169/2632 (82%)	0.10	101 (4%) 31 28	16, 44, 90, 138	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	PRO	5.3
1	C	430	HIS	5.2
1	C	135	THR	5.1
1	C	474	ARG	4.7
1	C	137	GLY	4.5
1	C	594	VAL	4.5
1	C	589	SER	4.4
1	C	130	ASP	4.4
1	C	136	PHE	4.3
1	C	106	ASN	4.2
1	C	521	TYR	4.2
1	C	110	GLN	4.2
1	C	427	GLN	4.1
1	B	480	HIS	4.1
1	C	525	GLY	4.1
1	C	111	LEU	4.0
1	C	109	GLY	4.0
1	C	431	ALA	3.7
1	B	159	ILE	3.7
1	C	588	ILE	3.6
1	B	139	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	523	ILE	3.6
1	D	172	ASN	3.6
1	B	157	PRO	3.5
1	C	552	CYS	3.5
1	C	124	ALA	3.4
1	B	459	ASP	3.4
1	C	426	PHE	3.4
1	C	107	LYS	3.3
1	A	107	LYS	3.3
1	B	179	ALA	3.1
1	D	166	HIS	3.0
1	C	387	TYR	3.0
1	C	522	TYR	3.0
1	C	132	ILE	3.0
1	B	462	GLN	2.9
1	C	138	ILE	2.9
1	C	131	TRP	2.9
1	D	159	ILE	2.9
1	C	128	PHE	2.8
1	B	503	ARG	2.8
1	B	474	ARG	2.8
1	C	81	GLY	2.7
1	D	155	THR	2.7
1	C	462	GLN	2.7
1	A	460	PRO	2.7
1	B	492	GLY	2.6
1	C	126	PRO	2.6
1	A	494	LEU	2.6
1	D	474	ARG	2.6
1	C	585	TYR	2.6
1	C	134	ASN	2.6
1	C	591	PRO	2.6
1	C	125	LEU	2.5
1	B	156	PRO	2.5
1	C	172	ASN	2.5
1	C	556	GLY	2.5
1	C	524	ILE	2.5
1	C	120	LEU	2.5
1	A	252	THR	2.5
1	C	105	LEU	2.5
1	A	559	PHE	2.4
1	B	203	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	563	SER	2.4
1	B	552	CYS	2.4
1	C	587	GLY	2.4
1	D	478	LEU	2.4
1	C	505	TYR	2.4
1	A	474	ARG	2.4
1	A	268	TRP	2.4
1	C	127	THR	2.4
1	B	494	LEU	2.3
1	C	396	PRO	2.3
1	B	89	GLU	2.3
1	C	228	TYR	2.3
1	C	494	LEU	2.3
1	A	426	PHE	2.3
1	A	462	GLN	2.3
1	C	584	ASN	2.3
1	C	433	LYS	2.3
1	C	254	THR	2.2
1	B	473	ASP	2.2
1	C	562	LEU	2.2
1	C	583	PHE	2.2
1	D	163	ASP	2.2
1	A	163	ASP	2.2
1	A	475	GLU	2.2
1	B	475	GLU	2.1
1	A	166	HIS	2.1
1	C	123	VAL	2.1
1	B	199	GLU	2.1
1	D	475	GLU	2.1
1	C	230	LEU	2.1
1	B	460	PRO	2.0
1	C	557	VAL	2.0
1	C	461	ASN	2.0
1	A	459	ASP	2.0
1	C	386	GLU	2.0
1	D	156	PRO	2.0
1	C	395	PHE	2.0
1	A	122	GLY	2.0

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

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 [i](#)

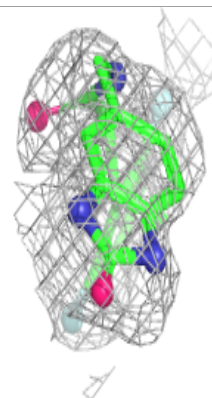
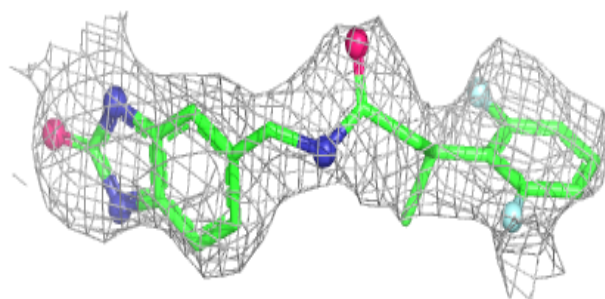
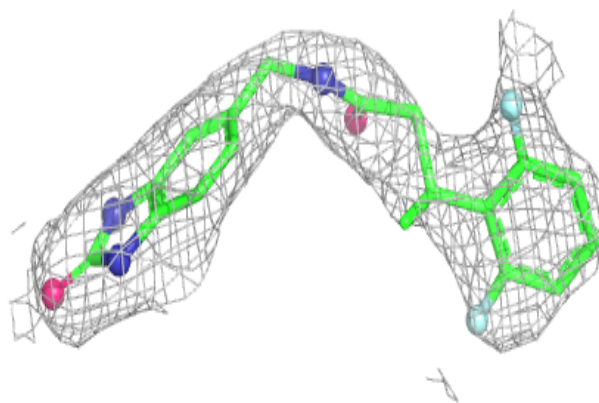
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	F6T	B	702	25/25	0.92	0.21	58,64,83,83	0
3	F6T	A	702	25/25	0.95	0.16	34,41,48,49	0
3	F6T	D	702	25/25	0.95	0.17	34,40,44,47	0
2	FAD	B	701	53/53	0.96	0.14	23,29,32,33	0
2	FAD	D	701	53/53	0.97	0.13	16,20,24,26	0
2	FAD	C	701	53/53	0.98	0.13	26,30,33,37	0
2	FAD	A	701	53/53	0.98	0.14	13,16,26,27	0

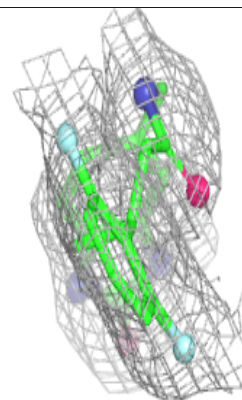
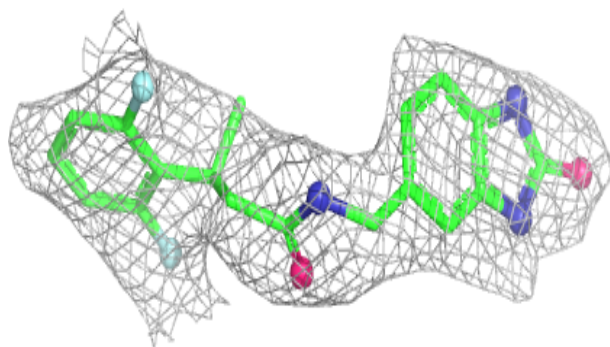
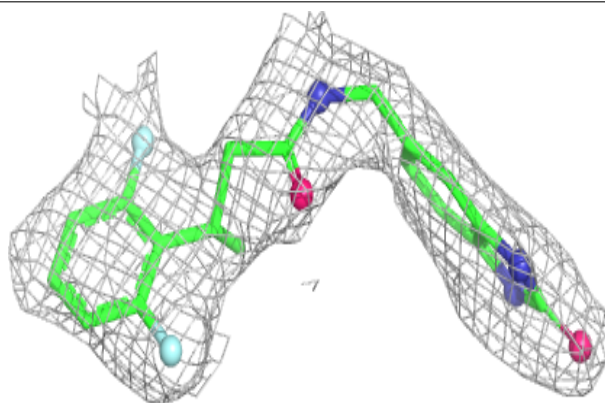
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around F6T B 702:**

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

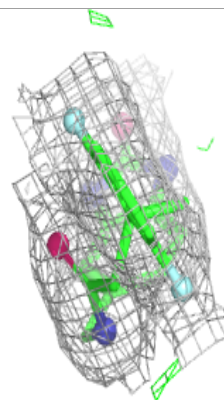
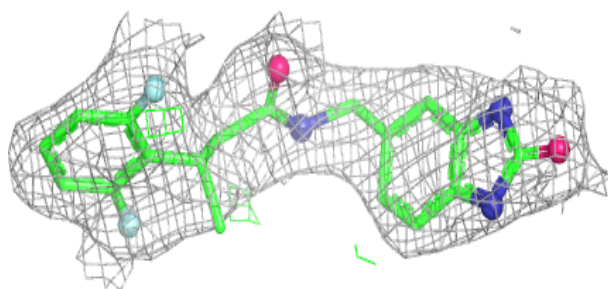
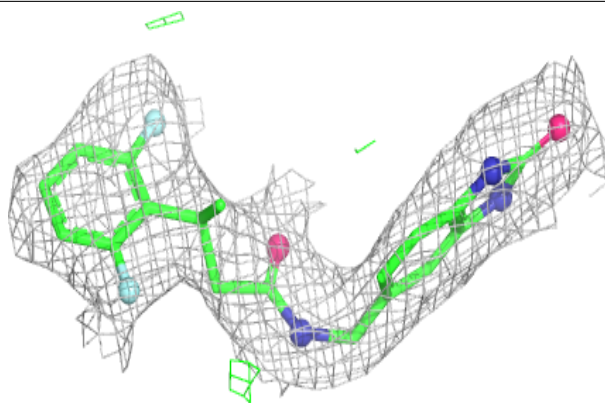
**Electron density around F6T A 702:**

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

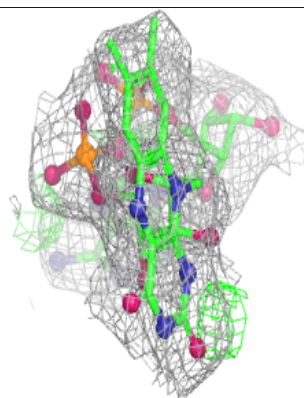
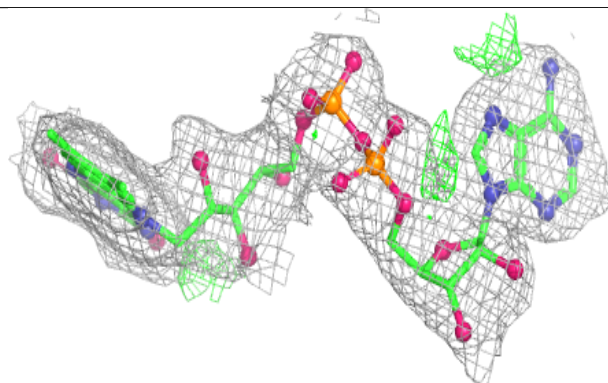
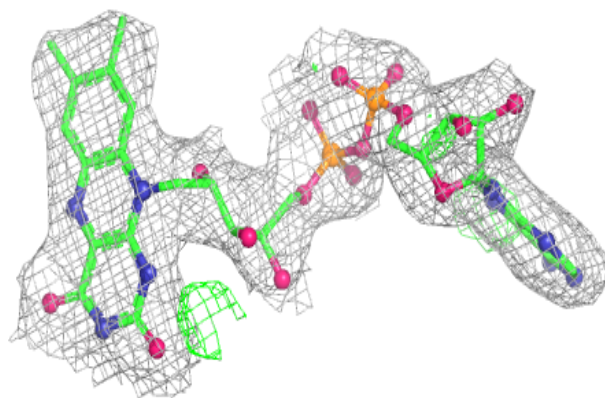


**Electron density around F6T D 702:**

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

**Electron density around FAD B 701:**

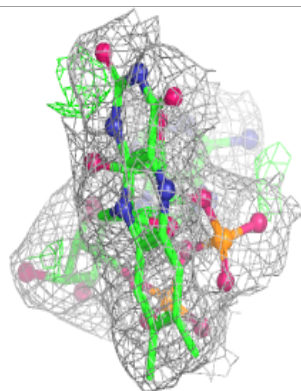
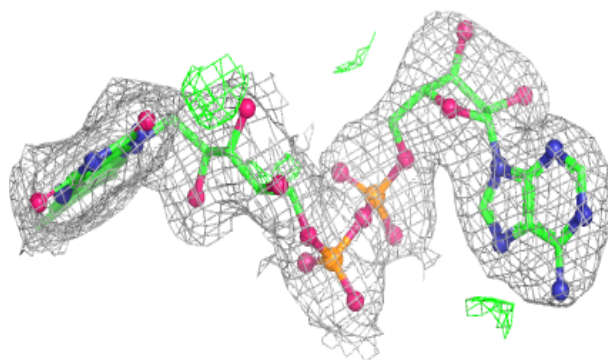
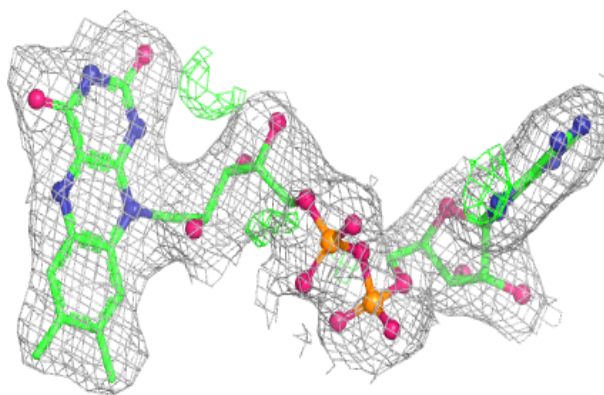
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



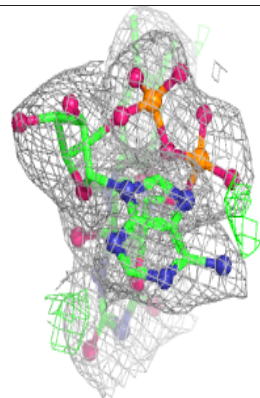
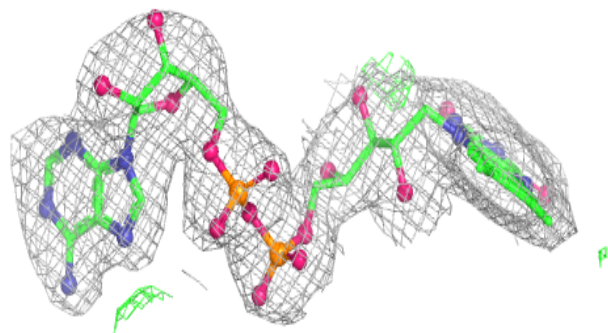
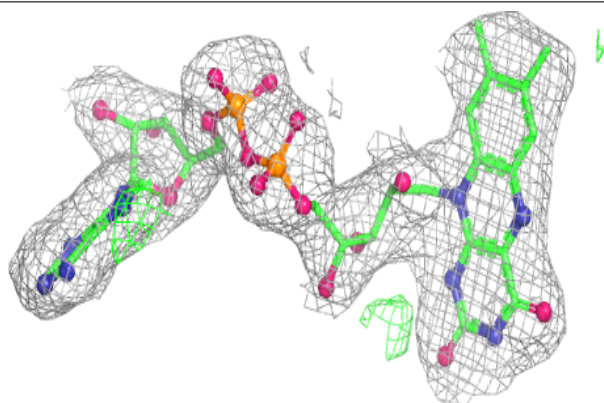


**Electron density around FAD D 701:**

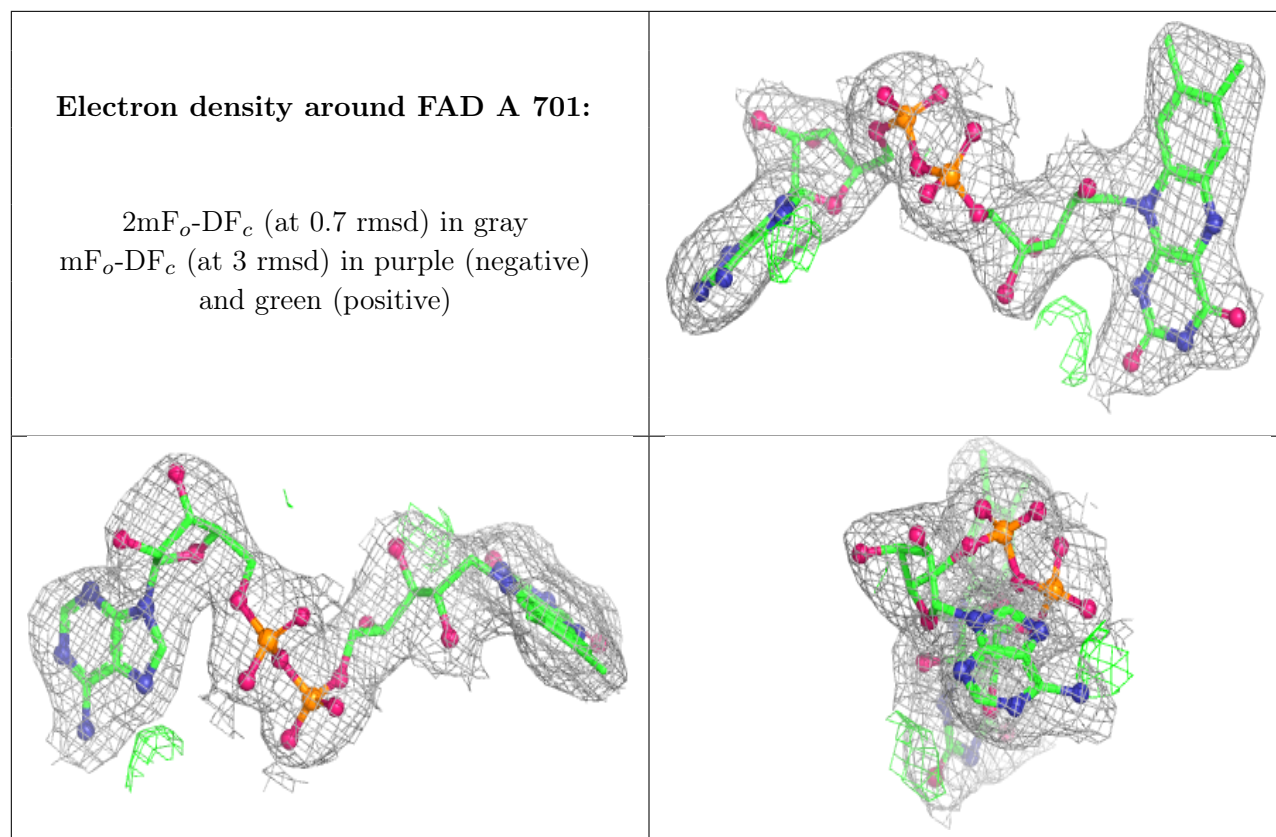
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD C 701:**

$2mF_o - DF_c$  (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.