



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 08:02 AM EDT

PDB ID : 5FEM  
Title : Saccharomyces cerevisiae Acetohydroxyacid Synthase in complex with bensulfuron methyl  
Authors : Guddat, L.W.; Lonhienne, T.  
Deposited on : 2015-12-17  
Resolution : 2.17 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

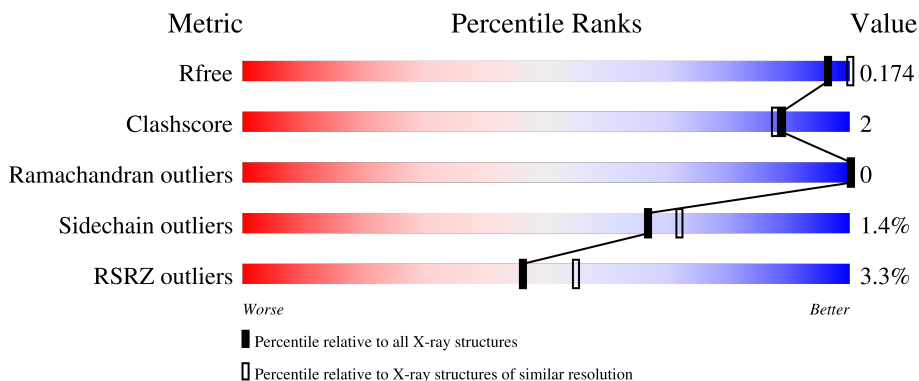
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	677	 2% 85% 12%
1	B	677	 4% 84% 12%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9937 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 Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	599	4584	2901	795	866	22	0	4	0
1	B	599	4578	2898	794	865	21	0	2	0

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P07342
A	12	HIS	-	expression tag	UNP P07342
A	13	HIS	-	expression tag	UNP P07342
A	14	HIS	-	expression tag	UNP P07342
A	15	HIS	-	expression tag	UNP P07342
A	16	HIS	-	expression tag	UNP P07342
A	17	HIS	-	expression tag	UNP P07342
A	18	SER	-	expression tag	UNP P07342
A	19	SER	-	expression tag	UNP P07342
A	20	GLY	-	expression tag	UNP P07342
A	21	LEU	-	expression tag	UNP P07342
A	22	VAL	-	expression tag	UNP P07342
A	23	PRO	-	expression tag	UNP P07342
A	24	ARG	-	expression tag	UNP P07342
A	25	GLY	-	expression tag	UNP P07342
A	26	SER	-	expression tag	UNP P07342
A	27	GLY	-	expression tag	UNP P07342
A	28	MET	-	expression tag	UNP P07342
A	29	LYS	-	expression tag	UNP P07342
A	30	GLU	-	expression tag	UNP P07342
A	31	THR	-	expression tag	UNP P07342
A	32	ALA	-	expression tag	UNP P07342
A	33	ALA	-	expression tag	UNP P07342
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	-	expression tag	UNP P07342
A	37	GLU	-	expression tag	UNP P07342
A	38	ARG	-	expression tag	UNP P07342
A	39	GLN	-	expression tag	UNP P07342
A	40	HIS	-	expression tag	UNP P07342
A	41	MET	-	expression tag	UNP P07342
A	42	ASP	-	expression tag	UNP P07342
A	43	SER	-	expression tag	UNP P07342
A	44	PRO	-	expression tag	UNP P07342
A	45	ASP	-	expression tag	UNP P07342
A	46	LEU	-	expression tag	UNP P07342
A	47	GLY	-	expression tag	UNP P07342
A	48	THR	-	expression tag	UNP P07342
A	49	ASP	-	expression tag	UNP P07342
A	50	ASP	-	expression tag	UNP P07342
A	51	ASP	-	expression tag	UNP P07342
A	52	ASP	-	expression tag	UNP P07342
A	53	LYS	-	expression tag	UNP P07342
A	54	ALA	-	expression tag	UNP P07342
A	55	MET	-	expression tag	UNP P07342
A	56	GLY	-	expression tag	UNP P07342
A	57	SER	-	expression tag	UNP P07342
B	11	MET	-	expression tag	UNP P07342
B	12	HIS	-	expression tag	UNP P07342
B	13	HIS	-	expression tag	UNP P07342
B	14	HIS	-	expression tag	UNP P07342
B	15	HIS	-	expression tag	UNP P07342
B	16	HIS	-	expression tag	UNP P07342
B	17	HIS	-	expression tag	UNP P07342
B	18	SER	-	expression tag	UNP P07342
B	19	SER	-	expression tag	UNP P07342
B	20	GLY	-	expression tag	UNP P07342
B	21	LEU	-	expression tag	UNP P07342
B	22	VAL	-	expression tag	UNP P07342
B	23	PRO	-	expression tag	UNP P07342
B	24	ARG	-	expression tag	UNP P07342
B	25	GLY	-	expression tag	UNP P07342
B	26	SER	-	expression tag	UNP P07342
B	27	GLY	-	expression tag	UNP P07342
B	28	MET	-	expression tag	UNP P07342
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342

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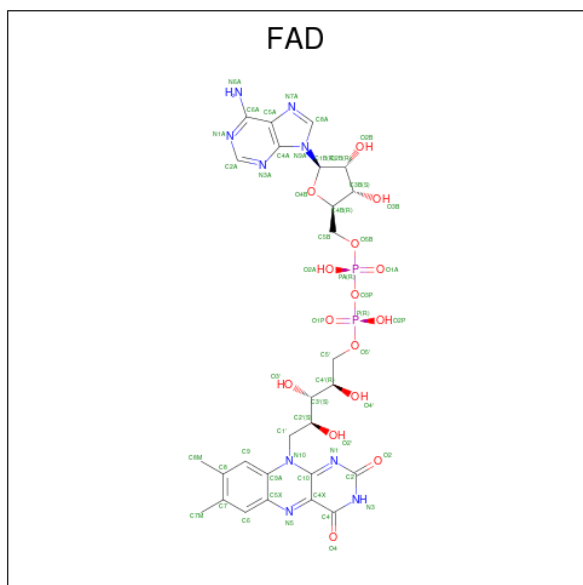
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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
B	38	ARG	-	expression tag	UNP P07342
B	39	GLN	-	expression tag	UNP P07342
B	40	HIS	-	expression tag	UNP P07342
B	41	MET	-	expression tag	UNP P07342
B	42	ASP	-	expression tag	UNP P07342
B	43	SER	-	expression tag	UNP P07342
B	44	PRO	-	expression tag	UNP P07342
B	45	ASP	-	expression tag	UNP P07342
B	46	LEU	-	expression tag	UNP P07342
B	47	GLY	-	expression tag	UNP P07342
B	48	THR	-	expression tag	UNP P07342
B	49	ASP	-	expression tag	UNP P07342
B	50	ASP	-	expression tag	UNP P07342
B	51	ASP	-	expression tag	UNP P07342
B	52	ASP	-	expression tag	UNP P07342
B	53	LYS	-	expression tag	UNP P07342
B	54	ALA	-	expression tag	UNP P07342
B	55	MET	-	expression tag	UNP P07342
B	56	GLY	-	expression tag	UNP P07342
B	57	SER	-	expression tag	UNP P07342

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

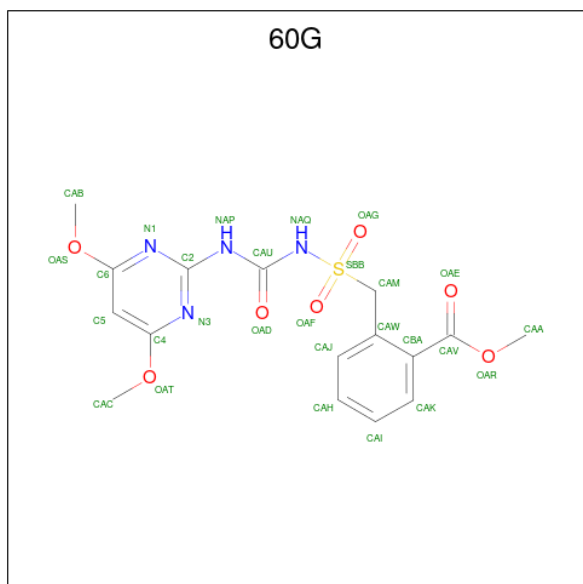
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

- Molecule 3 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>).



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

- Molecule 4 is methyl 2-[(4,6-dimethoxypyrimidin-2-yl)carbamoylsulfamoylmethyl]benzoate (three-letter code: 60G) (formula: C<sub>16</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>S).



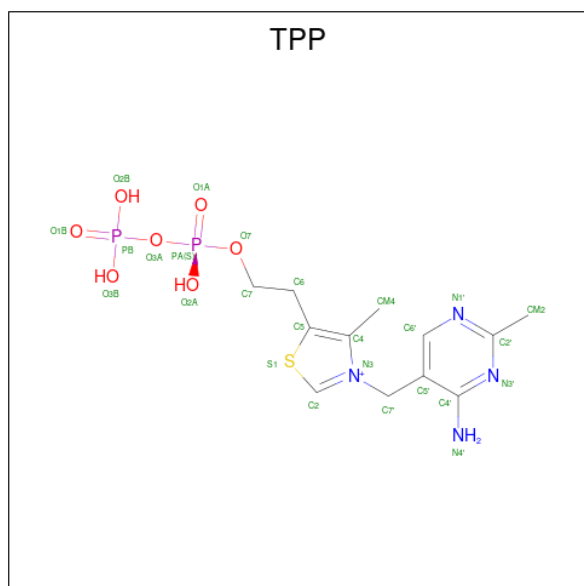
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
4	A	1	Total	C	N	O	S	0	0
			28	16	4	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	28	16	4	7	1	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	26	12	4	7	2	1	0	0
5	B	1	26	12	4	7	2	1	0	0

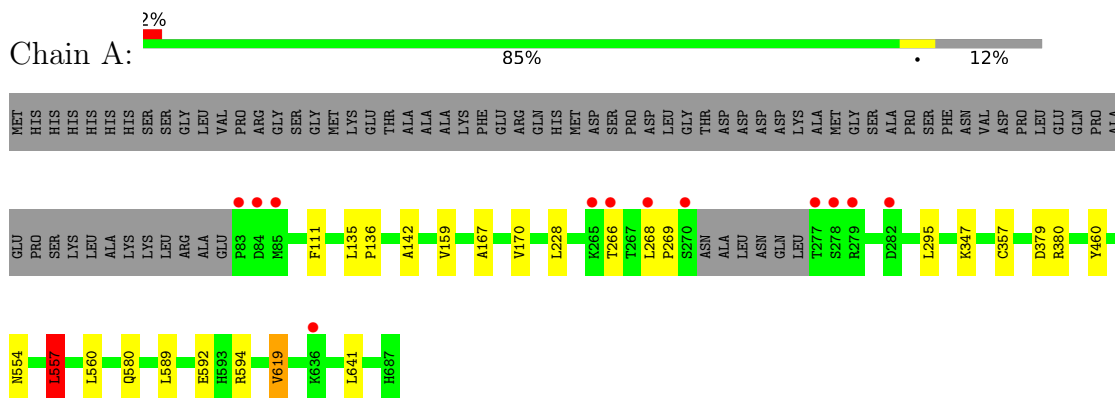
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	329	Total	O	0	0
			329	329		
6	B	228	Total	O	0	0
			228	228		

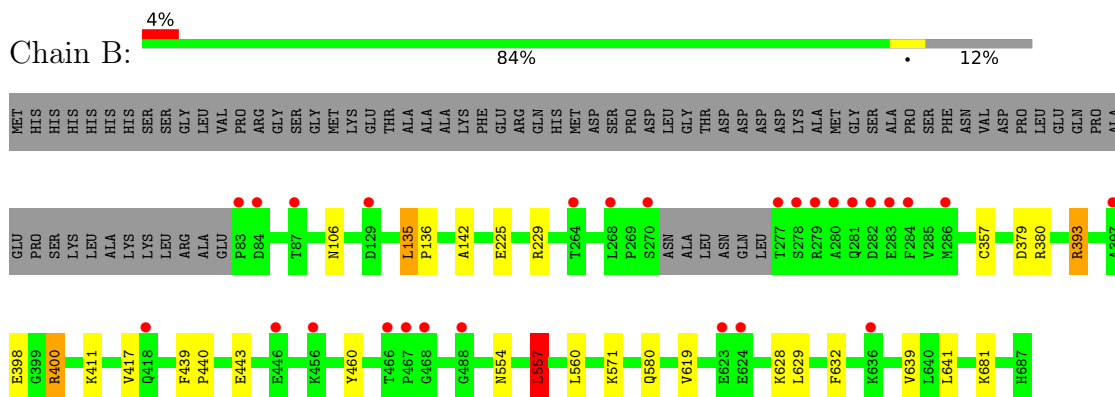
### 3 Residue-property plots [i](#)

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: Acetolactate synthase catalytic subunit, mitochondrial



- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.67Å 154.67Å 178.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.17 48.91 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-2.17) 99.7 (48.91-2.17)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.150 , 0.173 0.152 , 0.174	Depositor DCC
$R_{free}$ test set	2000 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.160	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 6OG, TPP, MG

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	0.32	0/4688	0.50	1/6358 (0.0%)
1	B	0.29	0/4679	0.47	2/6343 (0.0%)
All	All	0.30	0/9367	0.48	3/12701 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	557	LEU	CA-CB-CG	6.04	129.20	115.30
1	B	135	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4584	0	4593	13	0
1	B	4578	0	4598	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	53	0	30	1	0
3	B	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	0	0	0
4	B	28	0	0	0	0
5	A	26	0	16	3	0
5	B	26	0	16	3	0
6	A	329	0	0	0	0
6	B	228	0	0	1	0
All	All	9937	0	9283	35	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 (35) 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:B:681:LYS:NZ	6:B:801:HOH:O	2.27	0.68
1:B:580:GLN:HB3	5:B:705:TPP:H61	1.81	0.63
1:A:379:ASP:OD1	1:A:380:ARG:NE	2.30	0.62
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.80	0.62
5:B:705:TPP:H2	5:B:705:TPP:HN42	1.65	0.61
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.82	0.61
1:B:393:ARG:HH21	1:B:417:VAL:HG23	1.65	0.60
5:A:705:TPP:HN42	5:A:705:TPP:H2	1.66	0.59
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.85	0.59
5:B:705:TPP:HN42	5:B:705:TPP:C2	2.16	0.58
1:B:393:ARG:NH2	1:B:417:VAL:HG23	2.18	0.57
1:A:580:GLN:HB3	5:A:705:TPP:H61	1.85	0.56
5:A:705:TPP:HN42	5:A:705:TPP:C2	2.18	0.56
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.87	0.56
1:B:571:LYS:HD2	1:B:639:VAL:HG12	1.89	0.54
1:A:592:GLU:OE1	1:A:594:ARG:NH2	2.43	0.51
1:B:357:CYS:HB3	1:B:460:TYR:CZ	2.47	0.49
1:B:379:ASP:OD1	1:B:380:ARG:NE	2.46	0.48
1:A:619[A]:VAL:CG2	1:A:641:LEU:HD11	2.44	0.47
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.95	0.47
1:A:357:CYS:HB3	1:A:460:TYR:CZ	2.49	0.47
1:A:619[A]:VAL:HG23	1:A:641:LEU:HD11	1.97	0.47
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.96	0.47
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.97	0.46
3:B:701:FAD:H9	3:B:701:FAD:H1'1	1.82	0.44
1:A:228:LEU:HB2	1:A:266:THR:HB	1.99	0.44
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:O	1:B:632:PHE:HB3	2.18	0.44
1:B:439:PHE:HA	1:B:440:PRO:HD3	1.90	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.88	0.42
1:B:398:GLU:OE1	1:B:400:ARG:HD3	2.20	0.42
1:A:167:ALA:O	1:A:170:VAL:HG22	2.21	0.41
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.56	0.41
3:A:702:FAD:H9	3:A:702:FAD:H1'1	1.81	0.40
1:A:111:PHE:O	1:A:159:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/677 (88%)	592 (99%)	7 (1%)	0	100	100
1	B	597/677 (88%)	590 (99%)	7 (1%)	0	100	100
All	All	1196/1354 (88%)	1182 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	493/556 (89%)	486 (99%)	7 (1%)	67	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	493/556 (89%)	485 (98%)	8 (2%)	62	67
All	All	986/1112 (89%)	971 (98%)	15 (2%)	67	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	347	LYS
1	A	557	LEU
1	A	560	LEU
1	A	589	LEU
1	A	619[A]	VAL
1	A	619[B]	VAL
1	B	106	ASN
1	B	135	LEU
1	B	393	ARG
1	B	400	ARG
1	B	411	LYS
1	B	443	GLU
1	B	557	LEU
1	B	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TPP	A	705	2	22,27,27	1.61	2 (9%)	29,40,40	2.01	9 (31%)
4	60G	A	703	-	28,29,29	1.30	5 (17%)	38,40,40	3.13	16 (42%)
4	60G	B	703	-	28,29,29	1.38	5 (17%)	38,40,40	3.13	15 (39%)
3	FAD	B	701	-	53,58,58	2.13	12 (22%)	68,89,89	1.30	10 (14%)
3	FAD	A	702	-	53,58,58	2.09	12 (22%)	68,89,89	1.36	11 (16%)
5	TPP	B	705	2	22,27,27	1.71	3 (13%)	29,40,40	2.06	11 (37%)

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	TPP	A	705	2	-	1/16/17/17	0/2/2/2
4	60G	A	703	-	-	3/24/24/24	0/2/2/2
4	60G	B	703	-	-	2/24/24/24	0/2/2/2
3	FAD	B	701	-	-	4/30/50/50	0/6/6/6
3	FAD	A	702	-	-	4/30/50/50	0/6/6/6
5	TPP	B	705	2	-	3/16/17/17	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FAD	O2'-C2'	-9.60	1.23	1.43
3	A	702	FAD	O2'-C2'	-9.30	1.23	1.43
5	A	705	TPP	C4-N3	-6.00	1.34	1.39
5	B	705	TPP	C4-N3	-5.72	1.34	1.39
3	B	701	FAD	C10-N1	5.01	1.43	1.33
3	A	702	FAD	C10-N1	4.87	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C4X-N5	4.56	1.39	1.30
3	B	701	FAD	C4X-N5	4.54	1.39	1.30
3	A	702	FAD	C2B-C1B	-4.32	1.47	1.53
3	B	701	FAD	C2B-C1B	-4.24	1.47	1.53
4	B	703	60G	C2-NAP	3.56	1.43	1.38
5	B	705	TPP	C4'-N4'	3.20	1.42	1.34
5	B	705	TPP	C6-C5	3.19	1.52	1.50
4	A	703	60G	C2-NAP	3.07	1.42	1.38
5	A	705	TPP	C4'-N4'	3.03	1.41	1.34
3	B	701	FAD	O4B-C1B	3.00	1.45	1.41
3	A	702	FAD	O4B-C1B	2.93	1.45	1.41
4	B	703	60G	OAR-CAA	-2.91	1.38	1.45
4	A	703	60G	OAR-CAA	-2.84	1.38	1.45
3	A	702	FAD	C1'-C2'	2.82	1.56	1.52
3	A	702	FAD	C2'-C3'	2.73	1.58	1.53
3	B	701	FAD	C2-N1	2.66	1.43	1.36
3	B	701	FAD	C1'-C2'	2.55	1.56	1.52
3	B	701	FAD	C2'-C3'	2.55	1.58	1.53
4	B	703	60G	CAU-NAP	2.55	1.42	1.37
3	B	701	FAD	O3'-C3'	-2.54	1.37	1.43
3	A	702	FAD	O3'-C3'	-2.42	1.37	1.43
3	A	702	FAD	C2-N1	2.35	1.42	1.36
3	B	701	FAD	C1'-N10	-2.30	1.42	1.48
4	A	703	60G	CAU-NAP	2.27	1.42	1.37
4	A	703	60G	C6-N1	2.09	1.36	1.33
4	B	703	60G	C6-N1	2.08	1.36	1.33
4	B	703	60G	OAR-CAV	2.08	1.38	1.33
3	A	702	FAD	C1'-N10	-2.08	1.42	1.48
3	B	701	FAD	C4X-C4	2.04	1.52	1.44
4	A	703	60G	OAR-CAV	2.04	1.37	1.33
3	A	702	FAD	C4X-C4	2.04	1.52	1.44
3	B	701	FAD	C2B-C3B	-2.03	1.47	1.53
3	A	702	FAD	C7M-C7	2.02	1.55	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	60G	OAG-SBB-OAF	-11.06	103.32	119.35
4	A	703	60G	OAG-SBB-OAF	-11.04	103.35	119.35
4	B	703	60G	C6-C5-C4	6.05	120.71	115.21
4	A	703	60G	C2-N3-C4	5.91	121.94	114.99
4	B	703	60G	C2-N3-C4	5.67	121.65	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	60G	C6-C5-C4	5.64	120.34	115.21
4	B	703	60G	NAQ-CAU-NAP	5.54	122.27	114.93
4	A	703	60G	NAQ-CAU-NAP	5.28	121.92	114.93
4	A	703	60G	C5-C4-N3	-4.68	118.62	124.08
4	B	703	60G	C5-C4-N3	-4.64	118.66	124.08
4	B	703	60G	C5-C6-N1	-4.56	118.76	124.08
4	B	703	60G	OAR-CAV-CBA	4.55	119.85	112.30
4	A	703	60G	C5-C6-N1	-4.41	118.94	124.08
4	A	703	60G	OAR-CAV-CBA	4.33	119.49	112.30
3	A	702	FAD	N3A-C2A-N1A	-4.32	121.93	128.68
5	A	705	TPP	N1'-C2'-N3'	-3.96	118.72	125.54
5	B	705	TPP	N1'-C2'-N3'	-3.95	118.74	125.54
5	A	705	TPP	C7'-N3-C2	-3.92	118.26	125.35
3	B	701	FAD	N3A-C2A-N1A	-3.88	122.61	128.68
5	B	705	TPP	C7'-N3-C2	-3.80	118.48	125.35
5	A	705	TPP	CM2-C2'-N1'	3.74	121.26	117.14
4	A	703	60G	CAM-SBB-NAQ	3.67	115.20	105.07
5	B	705	TPP	PA-O3A-PB	-3.63	120.38	132.83
4	B	703	60G	OAD-CAU-NAP	-3.61	117.52	123.62
4	B	703	60G	CAM-SBB-NAQ	3.56	114.91	105.07
5	B	705	TPP	C6'-N1'-C2'	3.55	122.00	115.96
5	A	705	TPP	C6'-N1'-C2'	3.52	121.96	115.96
4	A	703	60G	C2-NAP-CAU	-3.46	126.71	130.40
5	A	705	TPP	PA-O3A-PB	-3.41	121.14	132.83
5	B	705	TPP	CM2-C2'-N1'	3.37	120.85	117.14
4	B	703	60G	C2-N1-C6	3.36	118.95	114.99
4	A	703	60G	OAD-CAU-NAP	-3.36	117.94	123.62
4	A	703	60G	C2-N1-C6	3.22	118.78	114.99
5	B	705	TPP	C5-C4-N3	3.22	114.01	107.57
3	A	702	FAD	C4X-C10-N10	3.15	121.08	116.48
4	B	703	60G	N1-C2-N3	-3.14	121.26	126.23
3	A	702	FAD	C4-N3-C2	-3.09	119.94	125.64
3	B	701	FAD	C4-N3-C2	-3.07	119.97	125.64
4	A	703	60G	N1-C2-N3	-3.07	121.38	126.23
5	B	705	TPP	O2B-PB-O3A	3.04	114.81	104.64
3	B	701	FAD	C4A-C5A-N7A	-2.95	106.32	109.40
3	B	701	FAD	C4X-C10-N10	2.81	120.58	116.48
4	A	703	60G	OAR-CAV-OAE	-2.79	118.00	123.45
3	A	702	FAD	C4X-C4-N3	2.79	120.27	113.19
3	B	701	FAD	C4X-C4-N3	2.78	120.24	113.19
5	A	705	TPP	C5-C4-N3	2.76	113.09	107.57
4	B	703	60G	C2-NAP-CAU	-2.75	127.47	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	705	TPP	C5'-C7'-N3	-2.73	108.73	113.28
4	A	703	60G	NAP-C2-N1	2.71	124.40	116.46
5	B	705	TPP	CM4-C4-C5	-2.70	121.70	127.60
3	B	701	FAD	O4-C4-C4X	-2.61	119.68	126.60
4	B	703	60G	NAP-C2-N1	2.60	124.08	116.46
3	A	702	FAD	C4X-C10-N1	-2.57	118.77	124.73
3	B	701	FAD	C4X-C10-N1	-2.53	118.86	124.73
3	A	702	FAD	O4-C4-C4X	-2.52	119.90	126.60
3	A	702	FAD	C4A-C5A-N7A	-2.50	106.79	109.40
4	B	703	60G	OAR-CAV-OAE	-2.50	118.57	123.45
3	B	701	FAD	C10-C4X-N5	-2.46	119.64	124.86
4	A	703	60G	CAU-NAQ-SBB	-2.39	118.22	123.60
3	A	702	FAD	C9A-N10-C10	-2.39	117.04	120.77
3	A	702	FAD	C10-C4X-N5	-2.38	119.80	124.86
5	A	705	TPP	CM4-C4-C5	-2.38	122.40	127.60
3	B	701	FAD	C4-C4X-N5	2.37	121.60	118.23
3	A	702	FAD	C4-C4X-N5	2.35	121.57	118.23
3	A	702	FAD	C10-N1-C2	2.25	121.41	116.90
5	A	705	TPP	C5'-C6'-N1'	-2.22	120.12	123.82
3	B	701	FAD	C10-N1-C2	2.20	121.31	116.90
4	A	703	60G	OAG-SBB-CAM	2.20	111.65	108.30
5	B	705	TPP	C5'-C6'-N1'	-2.16	120.22	123.82
5	B	705	TPP	C5'-C7'-N3	-2.15	109.69	113.28
4	B	703	60G	OAG-SBB-CAM	2.14	111.56	108.30
5	B	705	TPP	CM2-C2'-N3'	2.09	120.42	117.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	705	TPP	PA-O3A-PB-O2B
4	B	703	60G	OAE-CAV-OAR-CAA
5	B	705	TPP	PA-O3A-PB-O1B
4	A	703	60G	CAW-CAM-SBB-OAF
4	B	703	60G	CAW-CAM-SBB-OAF
3	A	702	FAD	PA-O3P-P-O1P
3	B	701	FAD	PA-O3P-P-O1P
3	A	702	FAD	P-O3P-PA-O5B
4	A	703	60G	N1-C6-OAS-CAB
3	B	701	FAD	P-O3P-PA-O5B
5	B	705	TPP	C4'-C5'-C7'-N3
3	A	702	FAD	O4B-C4B-C5B-O5B

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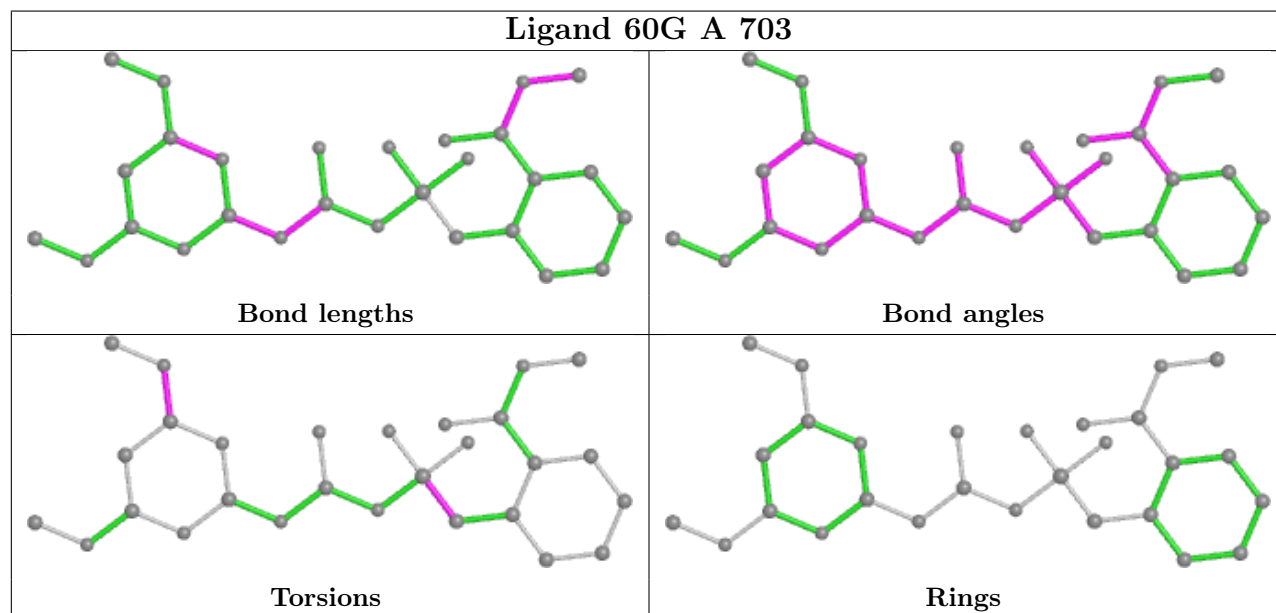
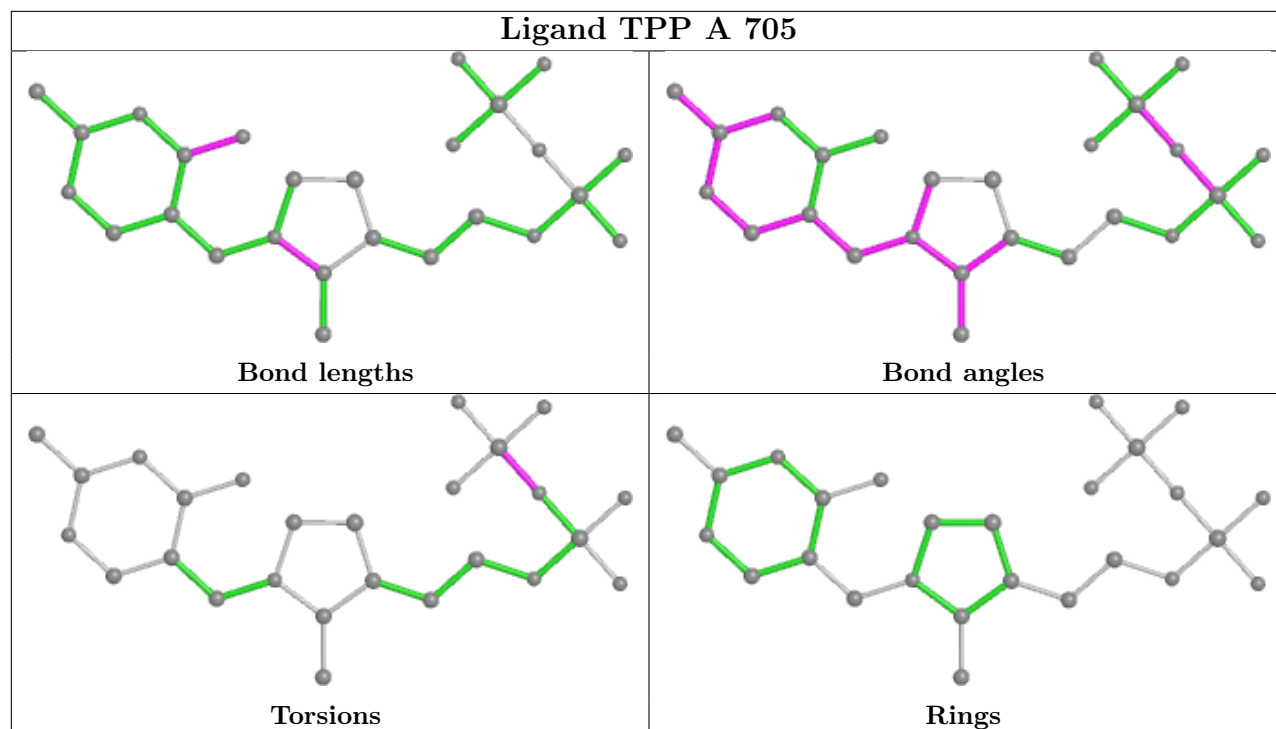
Mol	Chain	Res	Type	Atoms
5	A	705	TPP	PA-O3A-PB-O2B
3	B	701	FAD	O4B-C4B-C5B-O5B
3	A	702	FAD	PA-O3P-P-O2P
3	B	701	FAD	PA-O3P-P-O2P
4	A	703	60G	C5-C6-OAS-CAB

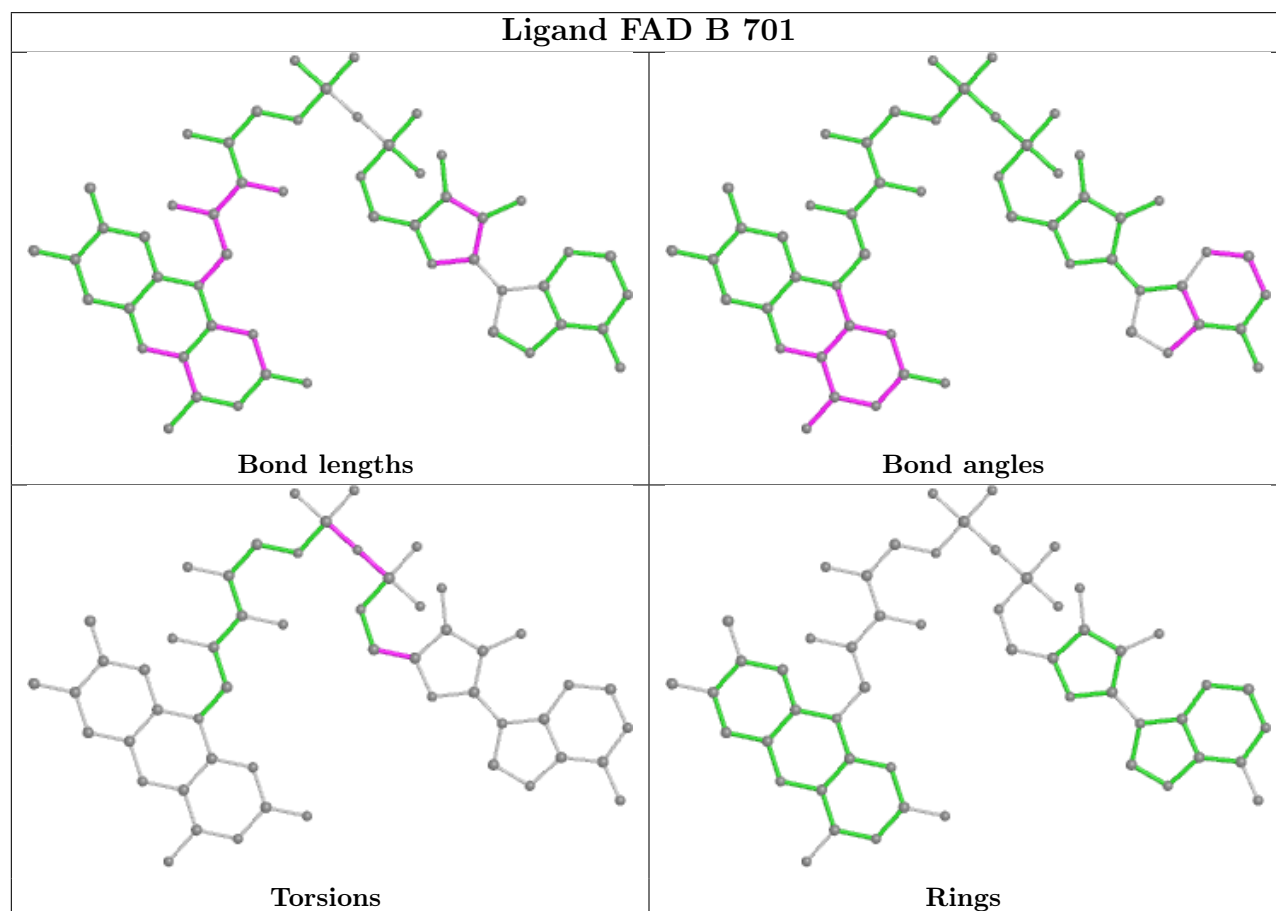
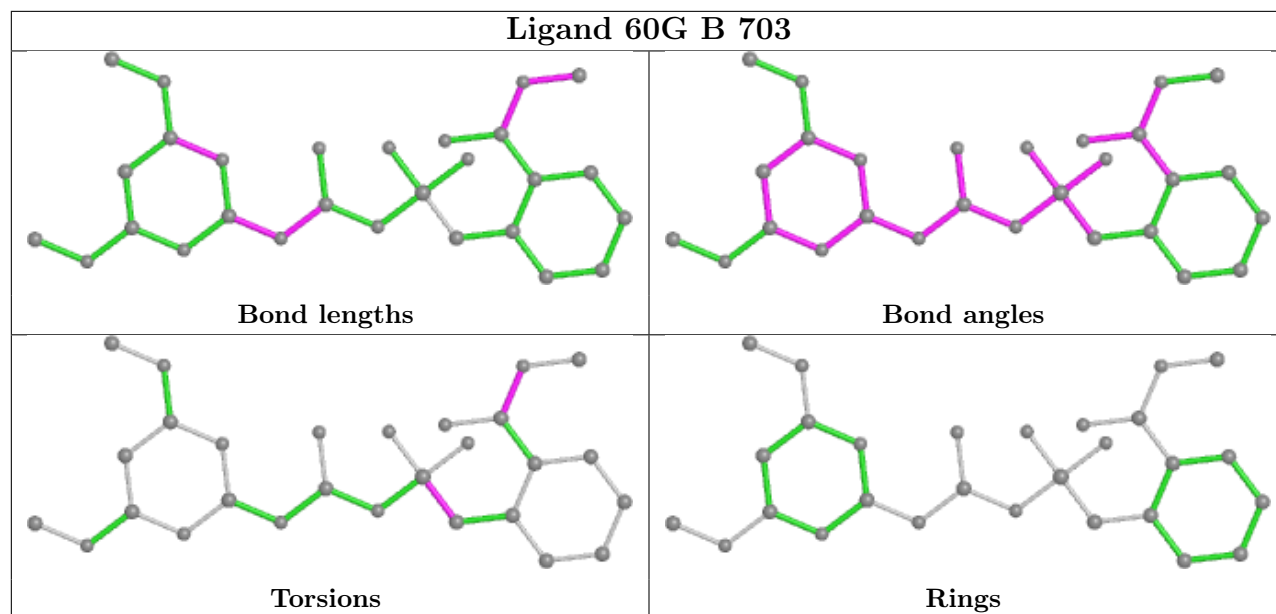
There are no ring outliers.

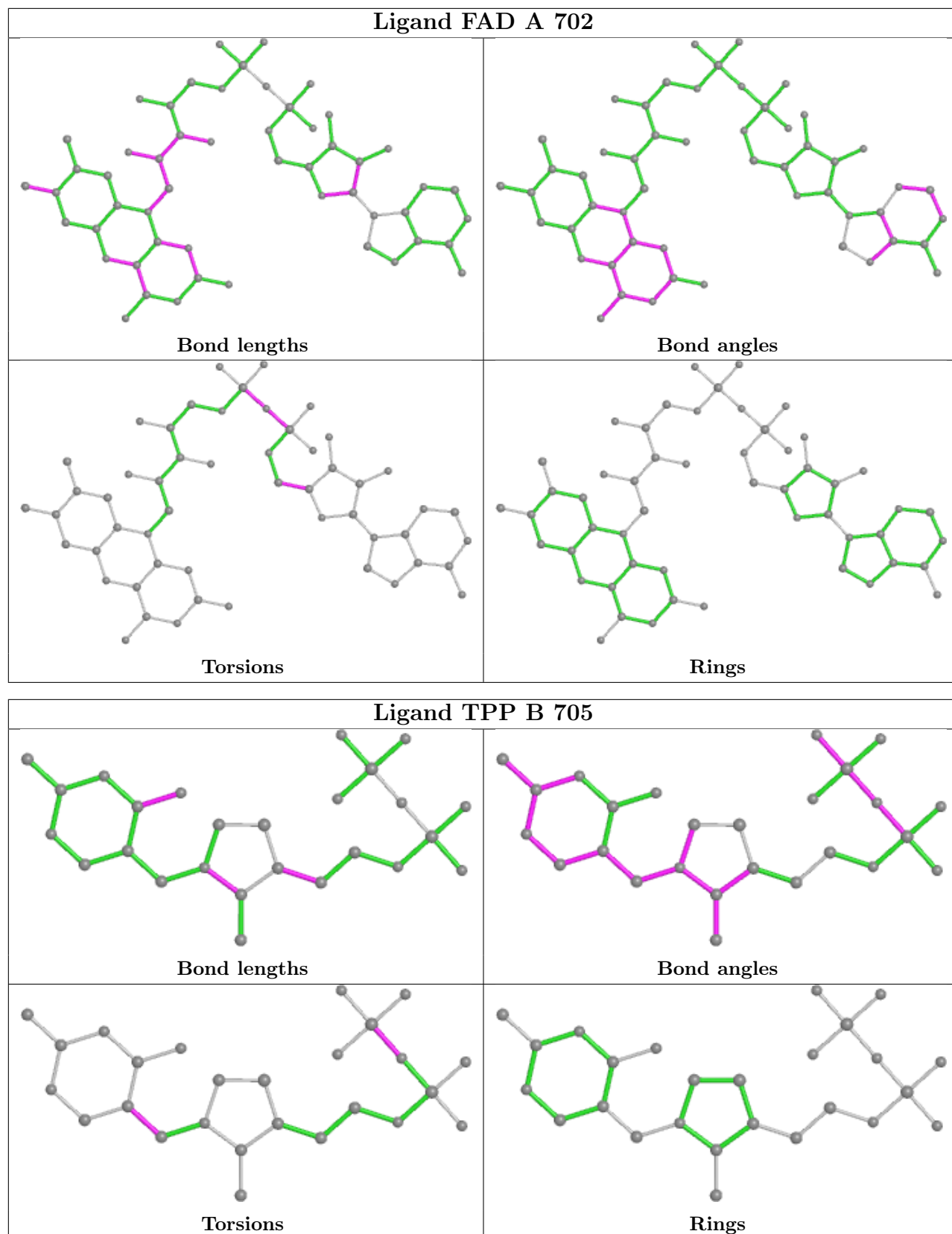
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	TPP	3	0
3	B	701	FAD	1	0
3	A	702	FAD	1	0
5	B	705	TPP	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

### 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	599/677 (88%)	-0.22	12 (2%) 65 72	15, 25, 46, 96	0
1	B	599/677 (88%)	0.00	27 (4%) 33 42	18, 34, 62, 104	0
All	All	1198/1354 (88%)	-0.11	39 (3%) 46 55	15, 29, 57, 104	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	7.6
1	A	83	PRO	6.9
1	B	280	ALA	6.0
1	A	277	THR	5.8
1	B	279	ARG	5.8
1	B	270	SER	5.2
1	A	268	LEU	5.0
1	A	270	SER	4.6
1	B	268	LEU	4.4
1	B	467	PRO	4.3
1	B	281	GLN	4.2
1	B	87	THR	3.9
1	B	278	SER	3.8
1	A	279	ARG	3.8
1	B	282	ASP	3.8
1	B	284	PHE	3.6
1	B	283	GLU	3.5
1	B	277	THR	3.5
1	B	468	GLY	3.3
1	B	84	ASP	3.2
1	B	456	LYS	3.2
1	B	466	THR	3.2
1	A	265	LYS	3.1
1	A	84	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	418	GLN	2.8
1	B	129	ASP	2.7
1	B	636	LYS	2.7
1	B	264	THR	2.6
1	A	266	THR	2.6
1	B	446	GLU	2.4
1	A	278	SER	2.4
1	A	636	LYS	2.4
1	A	282	ASP	2.3
1	B	488	GLY	2.2
1	B	397	ALA	2.2
1	B	624	GLU	2.1
1	B	623	GLU	2.1
1	B	286	MET	2.0
1	A	85	MET	2.0

## 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 [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(Å <sup>2</sup> )	Q<0.9
4	60G	B	703	28/28	0.96	0.09	30,36,42,44	0
4	60G	A	703	28/28	0.97	0.11	21,26,32,34	0
3	FAD	B	701	53/53	0.97	0.09	21,28,36,41	0
5	TPP	A	705	26/26	0.97	0.13	16,20,36,50	0
5	TPP	B	705	26/26	0.97	0.12	17,23,48,54	0
2	MG	B	702	1/1	0.98	0.07	19,19,19,19	0
3	FAD	A	702	53/53	0.99	0.11	13,18,22,23	0
2	MG	A	701	1/1	0.99	0.10	17,17,17,17	0

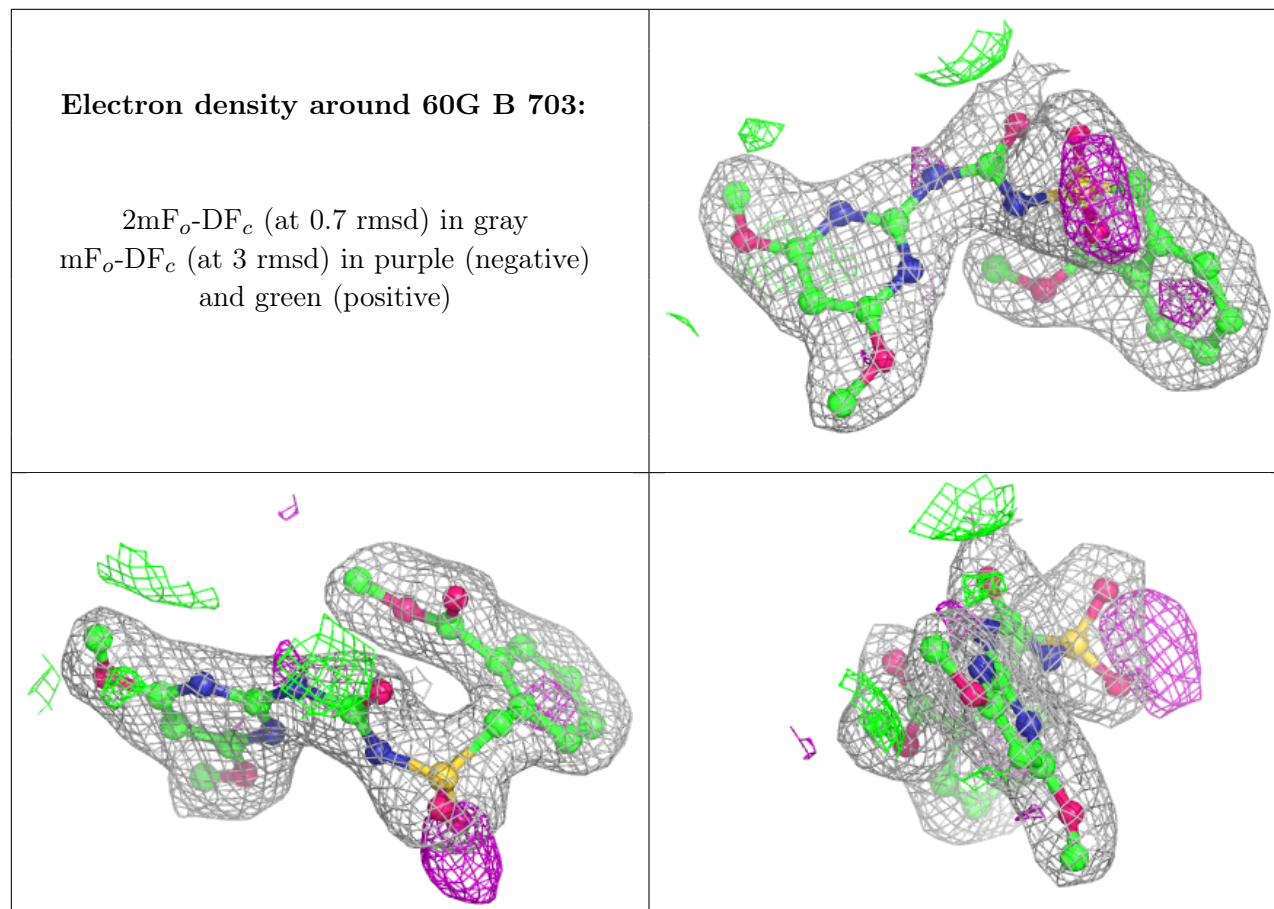
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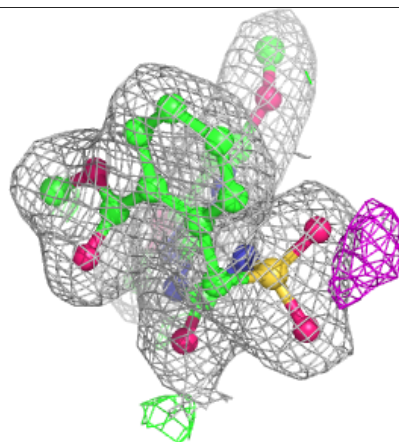
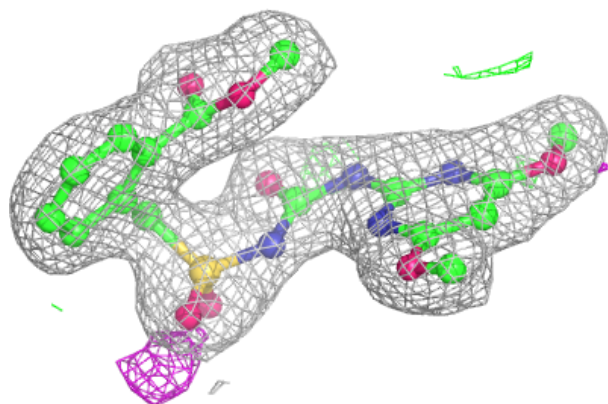
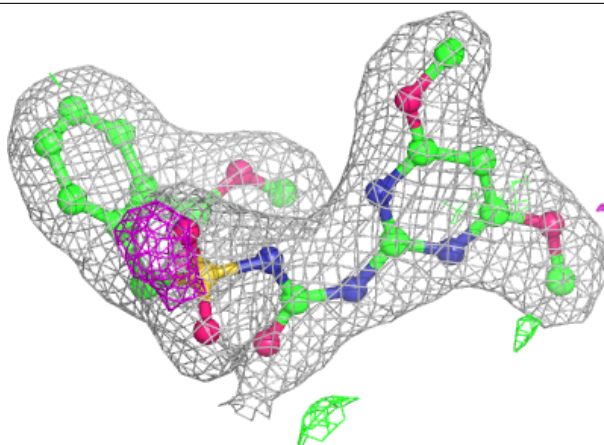
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	704	1/1	0.99	0.13	19,19,19,19	0
2	MG	A	704	1/1	1.00	0.19	12,12,12,12	0

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.

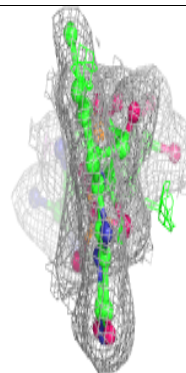
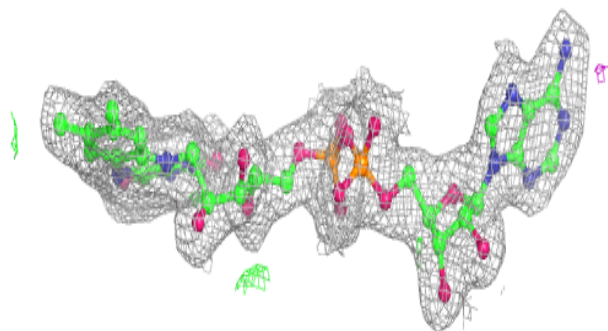
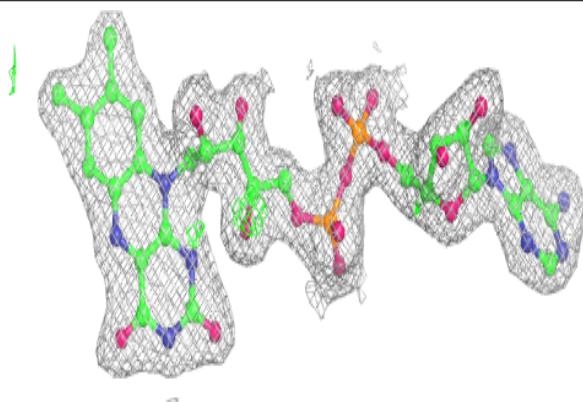


**Electron density around 60G A 703:**

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

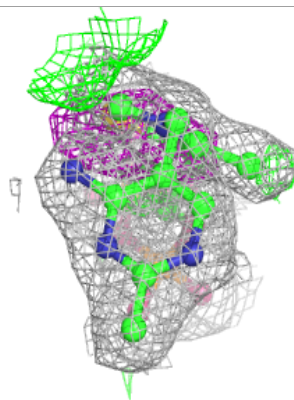
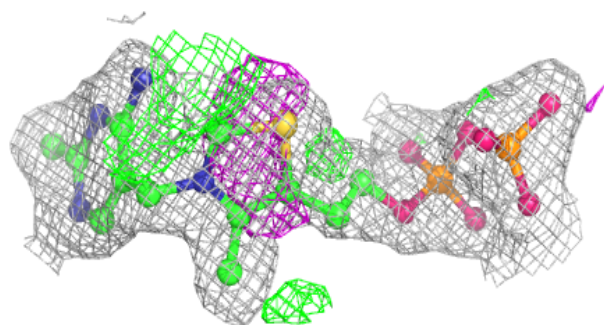
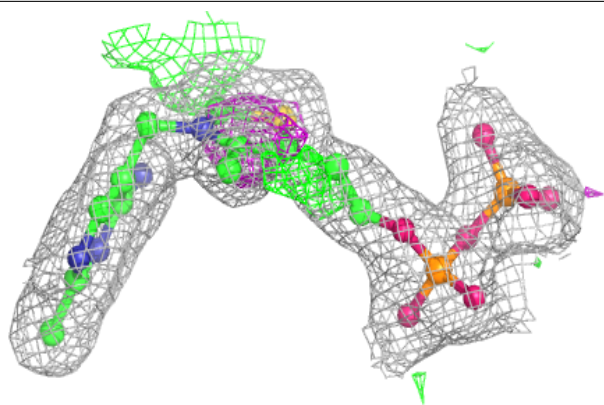
**Electron density around FAD B 701:**

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

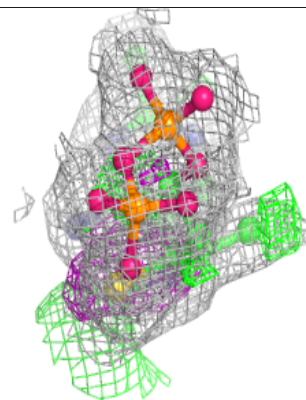
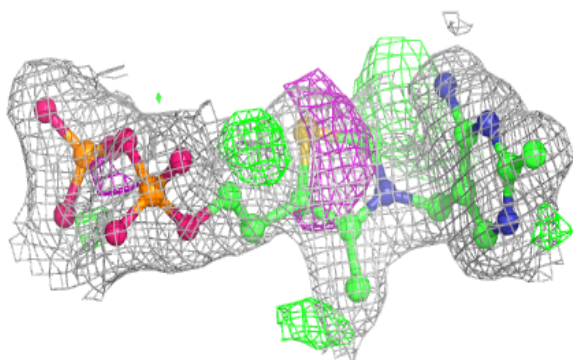
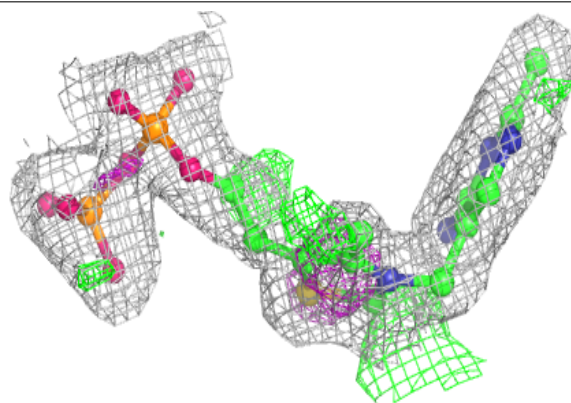


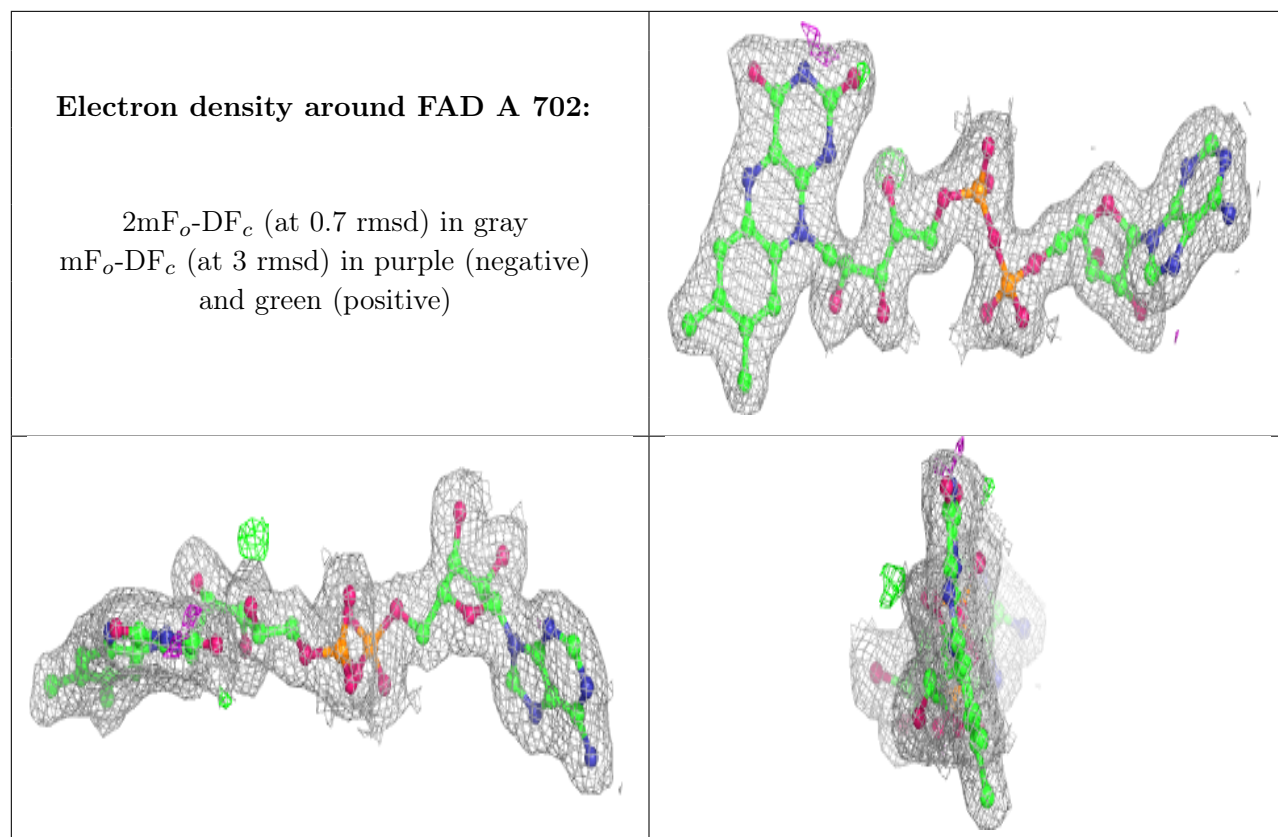
**Electron density around TPP A 705:**

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

**Electron density around TPP B 705:**

$2mF_o-DF_c$  (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.