



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 10, 2020 – 06:11 PM JST

PDB ID : 6LPI  
Title : Crystal Structure of AHAS holo-enzyme  
Authors : Zhang, Y.; Yang, X.; Xi, Z.; Shen, Y.  
Deposited on : 2020-01-10  
Resolution : 2.85 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.

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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 : 2.14.6  
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) : 2.14.6

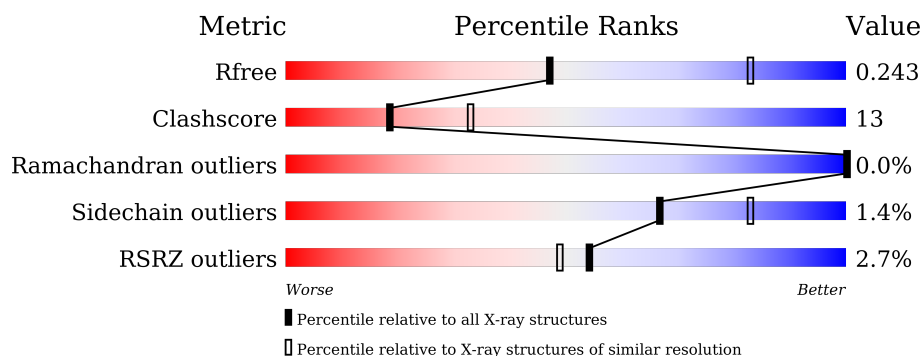
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 62%, yellow 62%, yellow 88%, grey 88%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>62%</span> <span>8%</span> <span>30%</span> </div> </div>
1	F	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 44%, yellow 44%, yellow 70%, grey 70%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>44%</span> <span>25%</span> <span>30%</span> </div> </div>
1	G	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 43%, yellow 43%, yellow 69%, grey 69%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>43%</span> <span>26%</span> <span>31%</span> </div> </div>
1	H	127	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 48%, yellow 48%, yellow 69%, grey 69%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>48%</span> <span>21%</span> <span>31%</span> </div> </div>
2	A	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 66%, yellow 66%, yellow 93%, grey 93%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>66%</span> <span>27%</span> <span>6%</span> </div> </div>
2	B	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 70%, yellow 70%, yellow 95%, grey 95%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>70%</span> <span>25%</span> <span></span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	562	<div><div></div><div>3%</div><div>74%</div><div>20%</div><div>• 5%</div></div>
2	D	562	<div><div></div><div>2%</div><div>71%</div><div>22%</div><div>• 6%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18840 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 isozyme 1 small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	89	Total	C	N	O	S	0	0	0
			689	440	117	127	5			
1	F	89	Total	C	N	O	S	0	0	0
			710	451	124	130	5			
1	G	88	Total	C	N	O	S	0	0	0
			691	441	118	127	5			
1	H	88	Total	C	N	O	S	0	0	0
			707	449	125	128	5			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	PRO	-	expression tag	UNP P0ADF8
E	97	ALA	-	expression tag	UNP P0ADF8
E	98	SER	-	expression tag	UNP P0ADF8
E	99	THR	-	expression tag	UNP P0ADF8
E	100	ALA	-	expression tag	UNP P0ADF8
E	101	ALA	-	expression tag	UNP P0ADF8
E	102	THR	-	expression tag	UNP P0ADF8
E	103	SER	-	expression tag	UNP P0ADF8
E	104	ALA	-	expression tag	UNP P0ADF8
E	105	ALA	-	expression tag	UNP P0ADF8
E	106	ALA	-	expression tag	UNP P0ADF8
E	107	THR	-	expression tag	UNP P0ADF8
E	108	SER	-	expression tag	UNP P0ADF8
E	109	ALA	-	expression tag	UNP P0ADF8
E	110	ALA	-	expression tag	UNP P0ADF8
E	111	ALA	-	expression tag	UNP P0ADF8
E	112	THR	-	expression tag	UNP P0ADF8
E	113	SER	-	expression tag	UNP P0ADF8
E	114	ALA	-	expression tag	UNP P0ADF8
E	115	ALA	-	expression tag	UNP P0ADF8
E	116	ALA	-	expression tag	UNP P0ADF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	117	THR	-	expression tag	UNP P0ADF8
E	118	SER	-	expression tag	UNP P0ADF8
E	119	ALA	-	expression tag	UNP P0ADF8
E	120	ALA	-	expression tag	UNP P0ADF8
E	121	ALA	-	expression tag	UNP P0ADF8
E	122	THR	-	expression tag	UNP P0ADF8
E	123	SER	-	expression tag	UNP P0ADF8
E	124	ALA	-	expression tag	UNP P0ADF8
E	125	ALA	-	expression tag	UNP P0ADF8
E	126	SER	-	expression tag	UNP P0ADF8
F	0	PRO	-	expression tag	UNP P0ADF8
F	97	ALA	-	expression tag	UNP P0ADF8
F	98	SER	-	expression tag	UNP P0ADF8
F	99	THR	-	expression tag	UNP P0ADF8
F	100	ALA	-	expression tag	UNP P0ADF8
F	101	ALA	-	expression tag	UNP P0ADF8
F	102	THR	-	expression tag	UNP P0ADF8
F	103	SER	-	expression tag	UNP P0ADF8
F	104	ALA	-	expression tag	UNP P0ADF8
F	105	ALA	-	expression tag	UNP P0ADF8
F	106	ALA	-	expression tag	UNP P0ADF8
F	107	THR	-	expression tag	UNP P0ADF8
F	108	SER	-	expression tag	UNP P0ADF8
F	109	ALA	-	expression tag	UNP P0ADF8
F	110	ALA	-	expression tag	UNP P0ADF8
F	111	ALA	-	expression tag	UNP P0ADF8
F	112	THR	-	expression tag	UNP P0ADF8
F	113	SER	-	expression tag	UNP P0ADF8
F	114	ALA	-	expression tag	UNP P0ADF8
F	115	ALA	-	expression tag	UNP P0ADF8
F	116	ALA	-	expression tag	UNP P0ADF8
F	117	THR	-	expression tag	UNP P0ADF8
F	118	SER	-	expression tag	UNP P0ADF8
F	119	ALA	-	expression tag	UNP P0ADF8
F	120	ALA	-	expression tag	UNP P0ADF8
F	121	ALA	-	expression tag	UNP P0ADF8
F	122	THR	-	expression tag	UNP P0ADF8
F	123	SER	-	expression tag	UNP P0ADF8
F	124	ALA	-	expression tag	UNP P0ADF8
F	125	ALA	-	expression tag	UNP P0ADF8
F	126	SER	-	expression tag	UNP P0ADF8
G	0	PRO	-	expression tag	UNP P0ADF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	97	ALA	-	expression tag	UNP P0ADF8
G	98	SER	-	expression tag	UNP P0ADF8
G	99	THR	-	expression tag	UNP P0ADF8
G	100	ALA	-	expression tag	UNP P0ADF8
G	101	ALA	-	expression tag	UNP P0ADF8
G	102	THR	-	expression tag	UNP P0ADF8
G	103	SER	-	expression tag	UNP P0ADF8
G	104	ALA	-	expression tag	UNP P0ADF8
G	105	ALA	-	expression tag	UNP P0ADF8
G	106	ALA	-	expression tag	UNP P0ADF8
G	107	THR	-	expression tag	UNP P0ADF8
G	108	SER	-	expression tag	UNP P0ADF8
G	109	ALA	-	expression tag	UNP P0ADF8
G	110	ALA	-	expression tag	UNP P0ADF8
G	111	ALA	-	expression tag	UNP P0ADF8
G	112	THR	-	expression tag	UNP P0ADF8
G	113	SER	-	expression tag	UNP P0ADF8
G	114	ALA	-	expression tag	UNP P0ADF8
G	115	ALA	-	expression tag	UNP P0ADF8
G	116	ALA	-	expression tag	UNP P0ADF8
G	117	THR	-	expression tag	UNP P0ADF8
G	118	SER	-	expression tag	UNP P0ADF8
G	119	ALA	-	expression tag	UNP P0ADF8
G	120	ALA	-	expression tag	UNP P0ADF8
G	121	ALA	-	expression tag	UNP P0ADF8
G	122	THR	-	expression tag	UNP P0ADF8
G	123	SER	-	expression tag	UNP P0ADF8
G	124	ALA	-	expression tag	UNP P0ADF8
G	125	ALA	-	expression tag	UNP P0ADF8
G	126	SER	-	expression tag	UNP P0ADF8
H	0	PRO	-	expression tag	UNP P0ADF8
H	97	ALA	-	expression tag	UNP P0ADF8
H	98	SER	-	expression tag	UNP P0ADF8
H	99	THR	-	expression tag	UNP P0ADF8
H	100	ALA	-	expression tag	UNP P0ADF8
H	101	ALA	-	expression tag	UNP P0ADF8
H	102	THR	-	expression tag	UNP P0ADF8
H	103	SER	-	expression tag	UNP P0ADF8
H	104	ALA	-	expression tag	UNP P0ADF8
H	105	ALA	-	expression tag	UNP P0ADF8
H	106	ALA	-	expression tag	UNP P0ADF8
H	107	THR	-	expression tag	UNP P0ADF8

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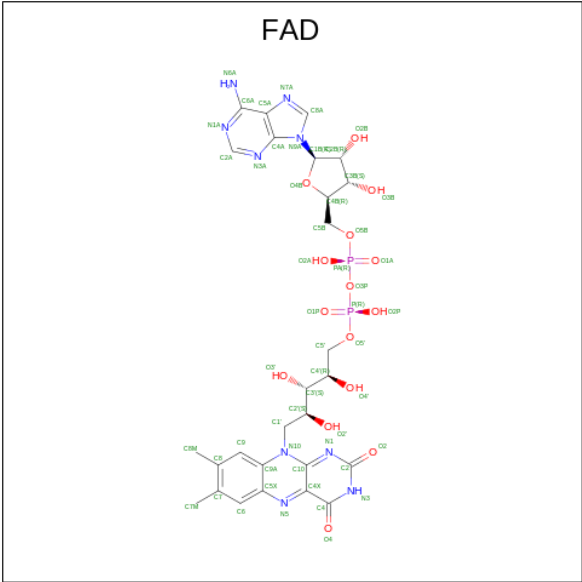
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Chain	Residue	Modelled	Actual	Comment	Reference
H	108	SER	-	expression tag	UNP P0ADF8
H	109	ALA	-	expression tag	UNP P0ADF8
H	110	ALA	-	expression tag	UNP P0ADF8
H	111	ALA	-	expression tag	UNP P0ADF8
H	112	THR	-	expression tag	UNP P0ADF8
H	113	SER	-	expression tag	UNP P0ADF8
H	114	ALA	-	expression tag	UNP P0ADF8
H	115	ALA	-	expression tag	UNP P0ADF8
H	116	ALA	-	expression tag	UNP P0ADF8
H	117	THR	-	expression tag	UNP P0ADF8
H	118	SER	-	expression tag	UNP P0ADF8
H	119	ALA	-	expression tag	UNP P0ADF8
H	120	ALA	-	expression tag	UNP P0ADF8
H	121	ALA	-	expression tag	UNP P0ADF8
H	122	THR	-	expression tag	UNP P0ADF8
H	123	SER	-	expression tag	UNP P0ADF8
H	124	ALA	-	expression tag	UNP P0ADF8
H	125	ALA	-	expression tag	UNP P0ADF8
H	126	SER	-	expression tag	UNP P0ADF8

- Molecule 2 is a protein called Acetolactate synthase isozyme 1 large subunit.

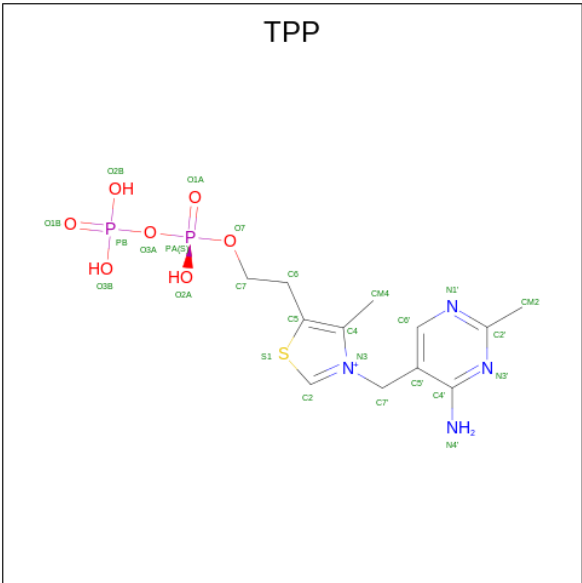
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	531	Total	C	N	O	S	0	0	0
			3971	2519	696	729	27			
2	B	539	Total	C	N	O	S	0	0	0
			3940	2500	677	736	27			
2	C	533	Total	C	N	O	S	0	0	0
			3918	2488	674	729	27			
2	D	529	Total	C	N	O	S	0	0	0
			3889	2467	678	719	25			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 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) (labeled as "Ligand of Interest" by author).





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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg		
			1	1	0	0
5	A	1	Total	Mg		
			1	1	0	0
5	D	1	Total	Mg		
			1	1	0	0
5	C	1	Total	Mg		
			1	1	0	0

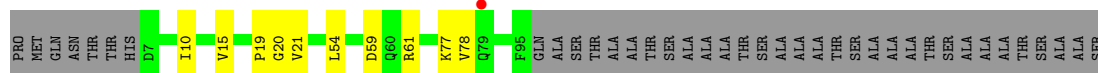
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	O		
			1	1	0	0
6	G	1	Total	O		
			1	1	0	0
6	C	1	Total	O		
			1	1	0	0
6	D	2	Total	O		
			2	2	0	0

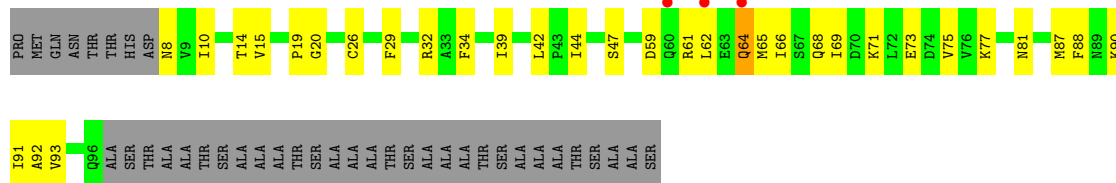
### 3 Residue-property plots [i](#)

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

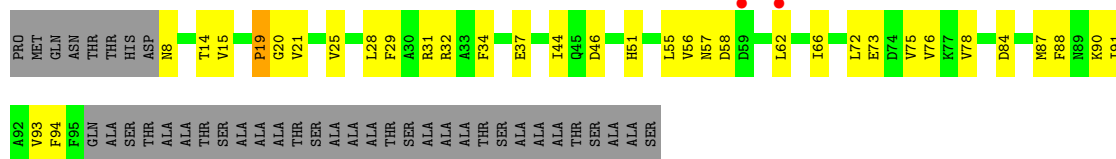
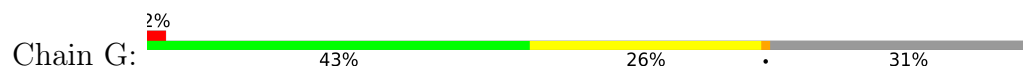
- Molecule 1: Acetolactate synthase isozyme 1 small subunit



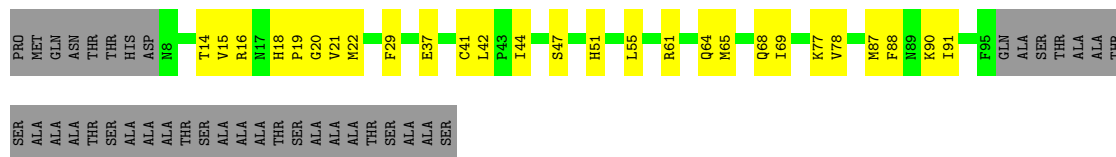
- Molecule 1: Acetolactate synthase isozyme 1 small subunit



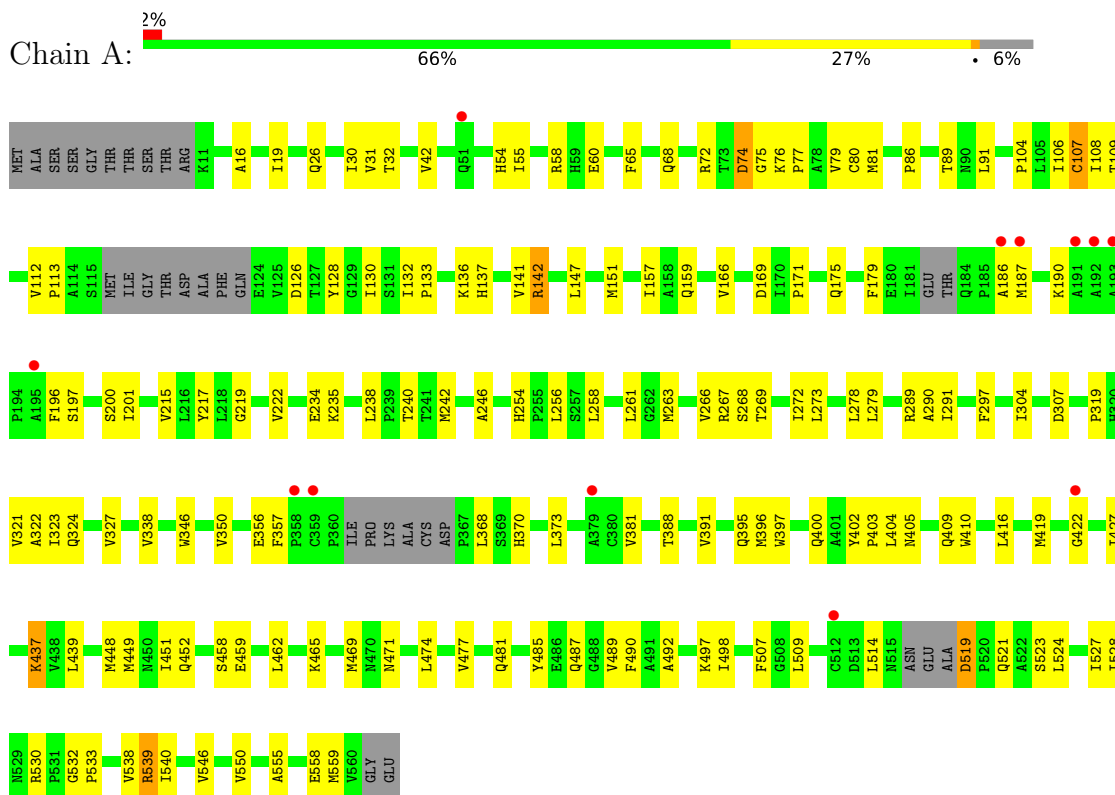
- Molecule 1: Acetolactate synthase isozyme 1 small subunit



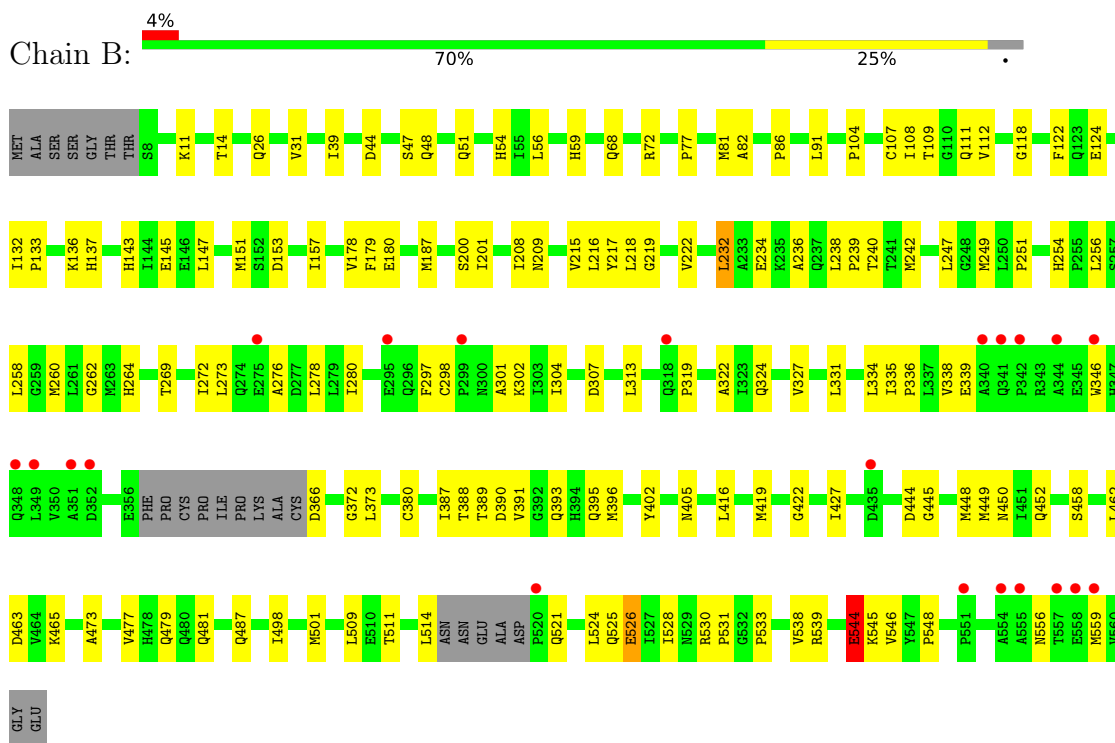
- Molecule 1: Acetolactate synthase isozyme 1 small subunit



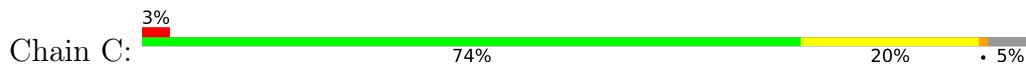
- Molecule 2: Acetolactate synthase isozyme 1 large subunit

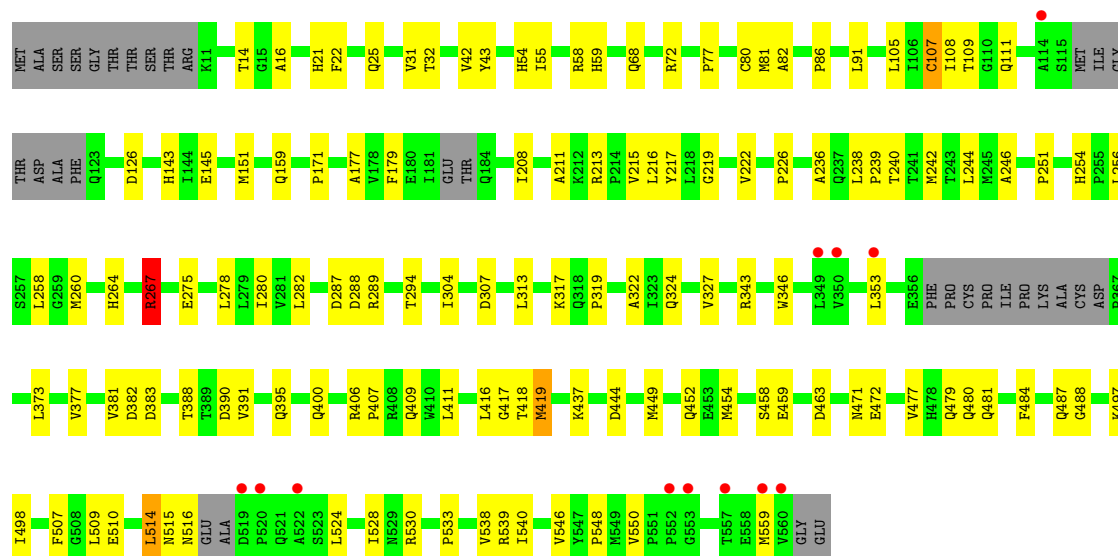


- Molecule 2: Acetolactate synthase isozyme 1 large subunit



- Molecule 2: Acetolactate synthase isozyme 1 large subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.17Å 104.58Å 118.53Å 90.00° 105.68° 90.00°	Depositor
Resolution (Å)	35.93 – 2.85 35.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.2 (35.93-2.85) 95.9 (35.93-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.85Å)	Xtriage
Refinement program	PHENIX dev_2666	Depositor
R, $R_{free}$	0.167 , 0.243 0.167 , 0.243	Depositor DCC
$R_{free}$ test set	2010 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: MG, FAD, TPP

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	E	0.45	0/701	0.66	0/953
1	F	0.42	0/722	0.65	0/978
1	G	0.41	0/703	0.62	0/954
1	H	0.49	0/719	0.66	0/973
2	A	0.48	1/4049 (0.0%)	0.87	10/5508 (0.2%)
2	B	0.45	0/4017	0.72	4/5481 (0.1%)
2	C	0.43	0/3995	0.76	7/5448 (0.1%)
2	D	0.43	0/3965	0.69	5/5405 (0.1%)
All	All	0.45	1/18871 (0.0%)	0.75	26/25700 (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	G	0	1
2	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	356	GLU	CG-CD	5.61	1.60	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	530	ARG	NE-CZ-NH2	-24.21	108.20	120.30
2	A	530	ARG	NE-CZ-NH1	18.92	129.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	250	LEU	CB-CG-CD2	-17.72	80.88	111.00
2	C	406	ARG	CG-CD-NE	9.21	131.13	111.80
2	C	406	ARG	NE-CZ-NH1	8.79	124.69	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	487	GLN	Peptide
2	B	526	GLU	Sidechain
1	G	46	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	689	0	670	7	0
1	F	710	0	708	23	0
1	G	691	0	683	23	0
1	H	707	0	711	26	0
2	A	3971	0	3978	118	0
2	B	3940	0	3875	129	0
2	C	3918	0	3862	100	0
2	D	3889	0	3834	95	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
3	C	53	0	31	0	0
3	D	53	0	31	3	0
4	A	26	0	16	7	0
4	B	26	0	16	1	0
4	C	26	0	16	4	0
4	D	26	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2	0	0	0	0
6	F	1	0	0	1	0
6	G	1	0	0	0	0
All	All	18840	0	18509	491	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 13.

The worst 5 of 491 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)
2:D:22:PHE:CD1	2:D:151:MET:HE2	1.61	1.32
2:B:544:GLU:HG3	2:B:545:LYS:H	1.06	1.09
2:C:406:ARG:CD	2:C:409:GLN:HB2	1.83	1.08
2:C:406:ARG:HD2	2:C:409:GLN:HB2	1.34	1.06
2:D:22:PHE:CE1	2:D:151:MET:HE2	1.99	0.96

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	E	87/127 (68%)	83 (95%)	4 (5%)	0	100	100
1	F	87/127 (68%)	82 (94%)	5 (6%)	0	100	100
1	G	86/127 (68%)	78 (91%)	7 (8%)	1 (1%)	13	28
1	H	86/127 (68%)	78 (91%)	8 (9%)	0	100	100
2	A	521/562 (93%)	505 (97%)	16 (3%)	0	100	100
2	B	533/562 (95%)	515 (97%)	18 (3%)	0	100	100
2	C	525/562 (93%)	507 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	519/562 (92%)	505 (97%)	14 (3%)	0	100	100
All	All	2444/2756 (89%)	2353 (96%)	90 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	19	PRO

### 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	E	76/104 (73%)	76 (100%)	0	100	100
1	F	81/104 (78%)	80 (99%)	1 (1%)	71	85
1	G	78/104 (75%)	78 (100%)	0	100	100
1	H	81/104 (78%)	79 (98%)	2 (2%)	47	71
2	A	410/446 (92%)	405 (99%)	5 (1%)	71	85
2	B	397/446 (89%)	392 (99%)	5 (1%)	69	84
2	C	397/446 (89%)	390 (98%)	7 (2%)	59	78
2	D	393/446 (88%)	387 (98%)	6 (2%)	65	82
All	All	1913/2200 (87%)	1887 (99%)	26 (1%)	67	83

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	107	CYS
2	C	305	HIS
2	D	419	MET
2	C	179	PHE
2	C	217	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	479	GLN
2	C	48	GLN
2	D	393	GLN
1	G	64	GLN
2	C	54	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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	TPP	D	602	5	22,27,27	1.65	4 (18%)	29,40,40	1.92	8 (27%)
4	TPP	B	602	5	22,27,27	1.64	6 (27%)	29,40,40	1.84	9 (31%)
4	TPP	C	602	5	22,27,27	1.56	5 (22%)	29,40,40	1.87	6 (20%)
4	TPP	A	602	5	22,27,27	1.53	4 (18%)	29,40,40	1.84	9 (31%)
3	FAD	D	601	-	51,58,58	1.23	4 (7%)	60,89,89	2.24	9 (15%)
3	FAD	B	601	-	51,58,58	1.28	6 (11%)	60,89,89	2.23	7 (11%)
3	FAD	A	601	-	51,58,58	1.37	6 (11%)	60,89,89	2.23	7 (11%)
3	FAD	C	601	-	51,58,58	1.23	4 (7%)	60,89,89	2.22	7 (11%)

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	TPP	D	602	5	-	5/16/17/17	0/2/2/2
4	TPP	B	602	5	-	2/16/17/17	0/2/2/2
4	TPP	C	602	5	-	7/16/17/17	0/2/2/2
4	TPP	A	602	5	-	5/16/17/17	0/2/2/2
3	FAD	D	601	-	-	10/30/50/50	0/6/6/6
3	FAD	B	601	-	-	9/30/50/50	0/6/6/6
3	FAD	A	601	-	-	10/30/50/50	0/6/6/6
3	FAD	C	601	-	-	6/30/50/50	0/6/6/6

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C4X-C10	5.76	1.44	1.38
3	B	601	FAD	C4X-C10	5.63	1.44	1.38
3	D	601	FAD	C4X-C10	5.62	1.44	1.38
3	C	601	FAD	C4X-C10	5.29	1.44	1.38
4	D	602	TPP	C4-N3	-4.82	1.35	1.39

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	13.12	126.22	115.14
3	C	601	FAD	C4-N3-C2	13.05	126.16	115.14
3	D	601	FAD	C4-N3-C2	13.01	126.13	115.14
3	A	601	FAD	C4-N3-C2	12.78	125.93	115.14
3	B	601	FAD	C4X-C4-N3	-7.34	113.39	123.43

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

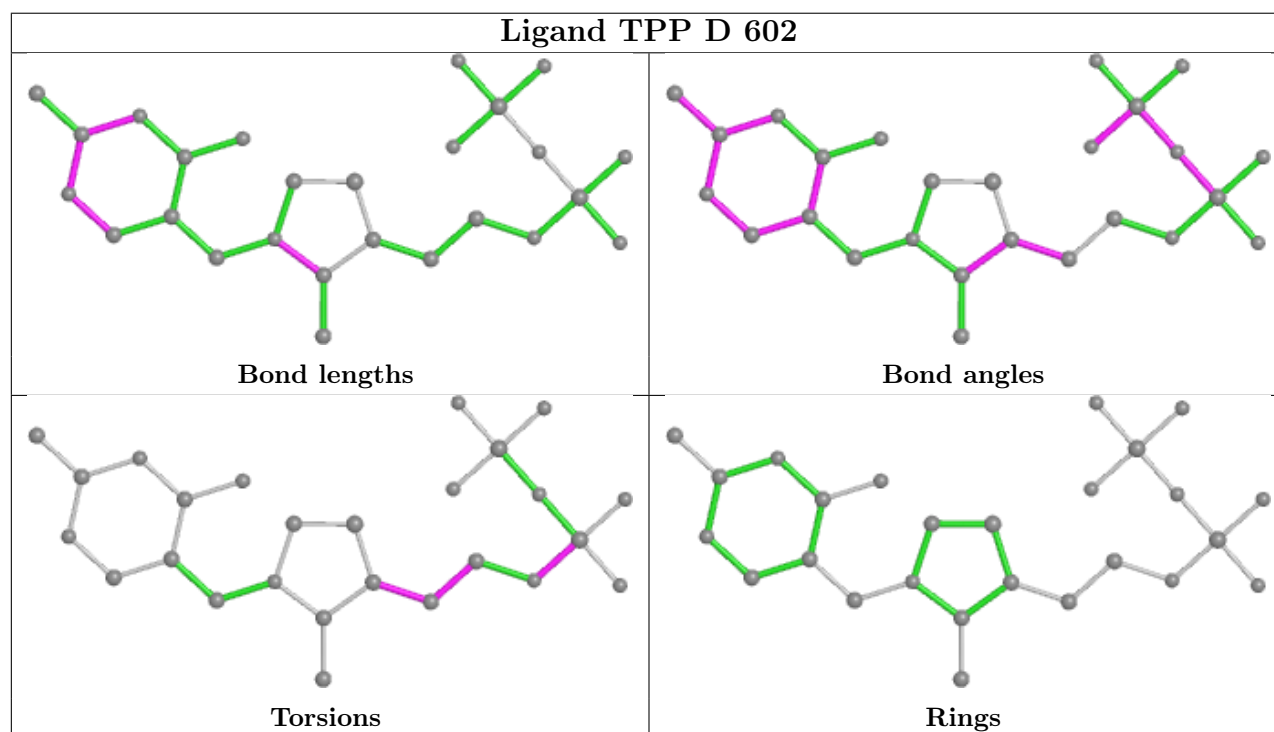
Mol	Chain	Res	Type	Atoms
4	D	602	TPP	C5-C6-C7-O7
4	D	602	TPP	C7-O7-PA-O3A
4	C	602	TPP	C5-C6-C7-O7
4	C	602	TPP	C7-O7-PA-O3A
4	C	602	TPP	PA-O3A-PB-O3B

There are no ring outliers.

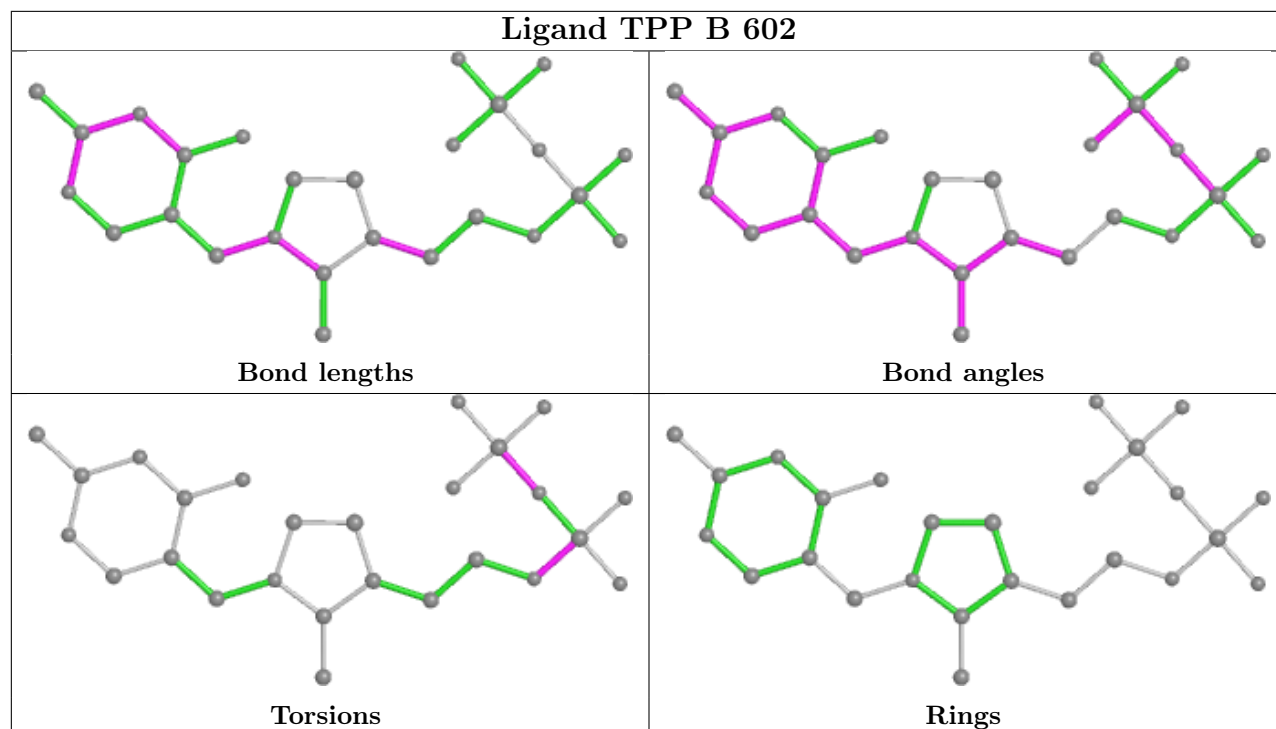
7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	TPP	1	0
4	B	602	TPP	1	0
4	C	602	TPP	4	0
4	A	602	TPP	7	0
3	D	601	FAD	3	0
3	B	601	FAD	1	0
3	A	601	FAD	2	0

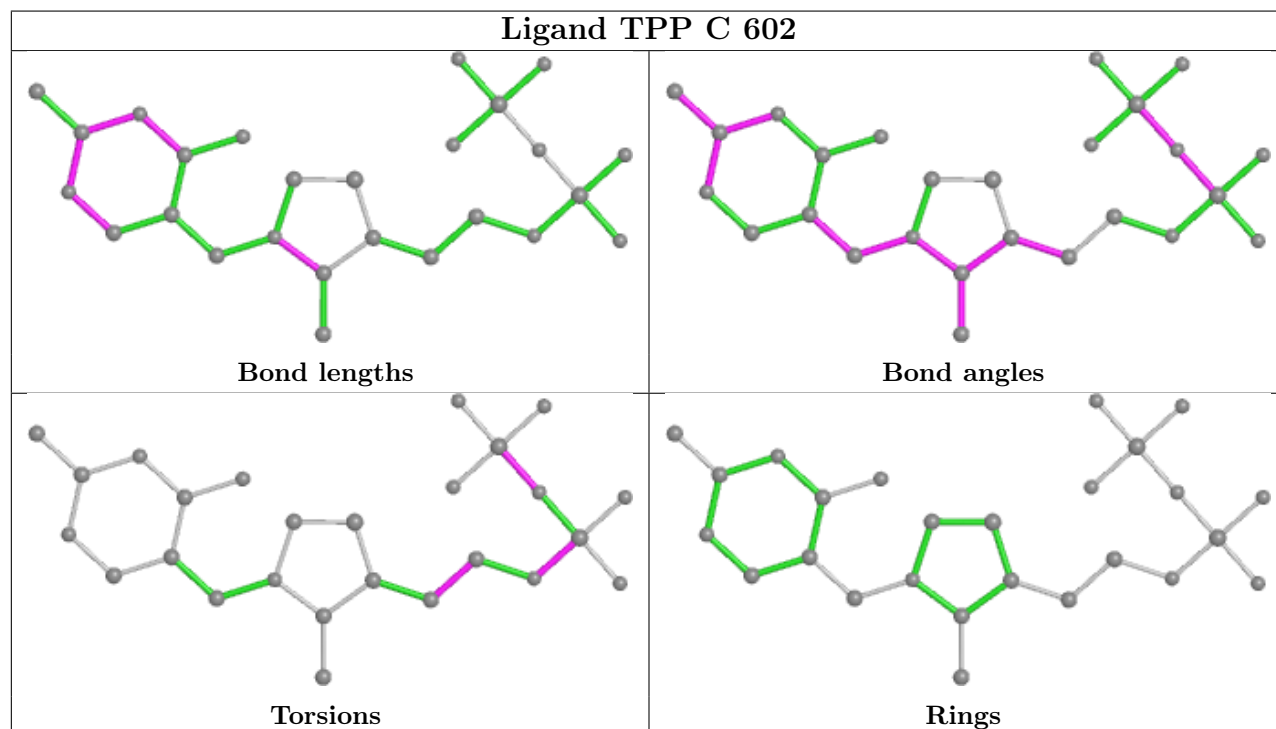
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

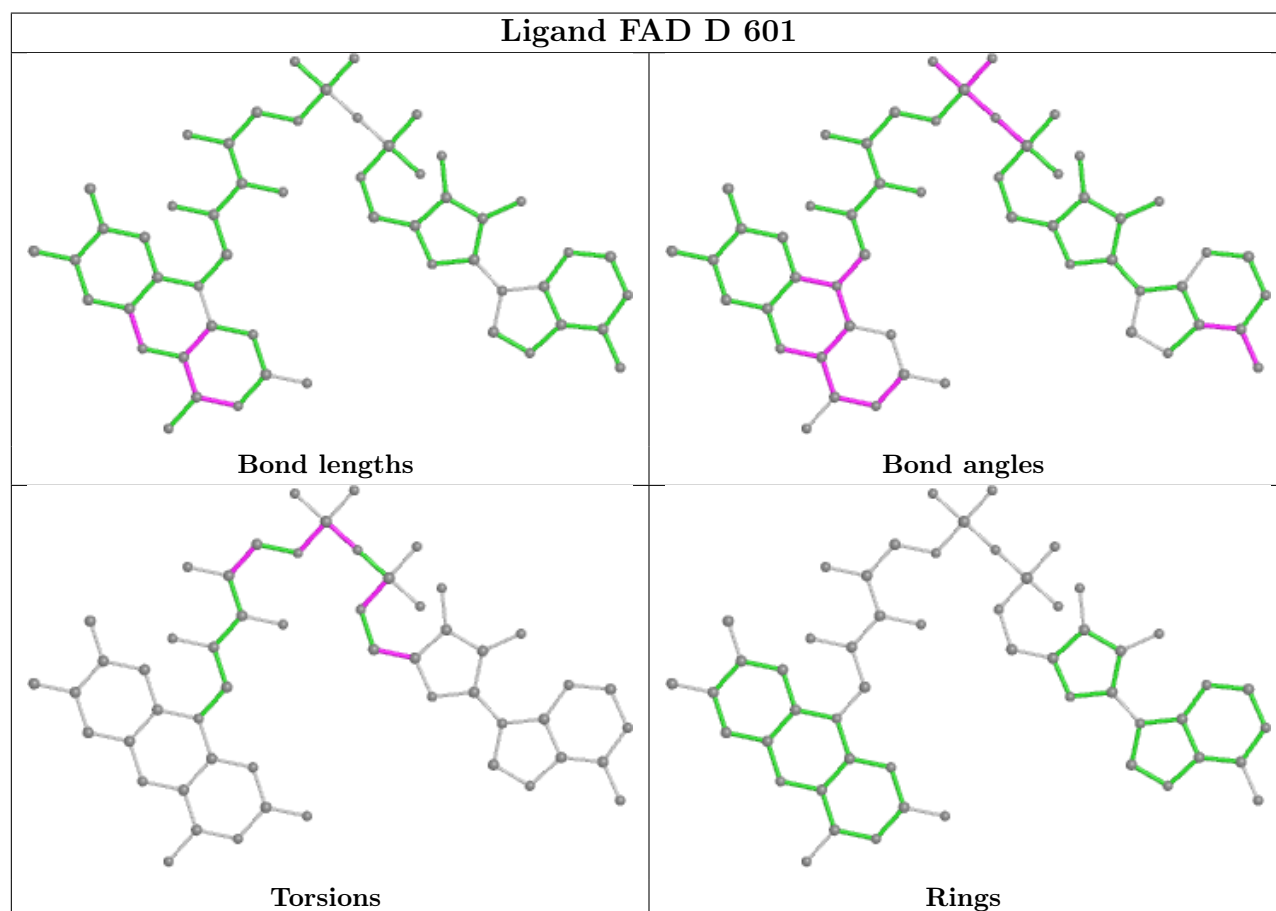
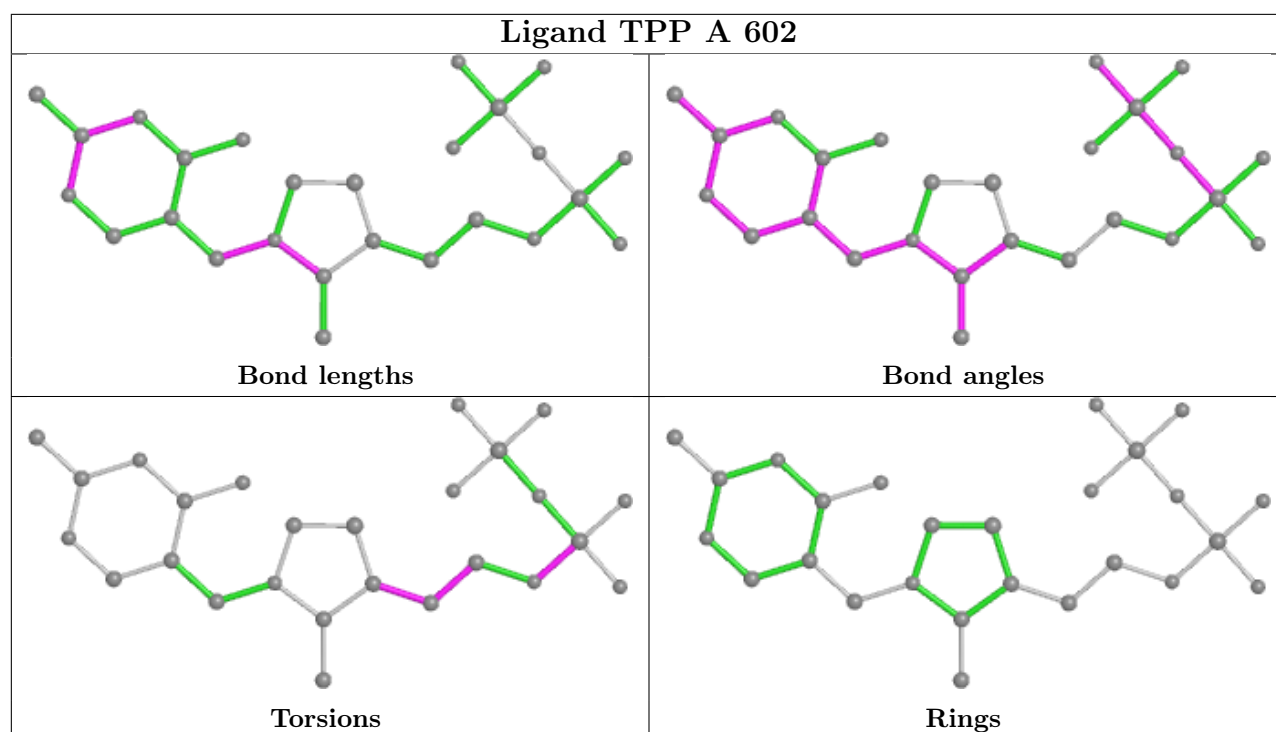


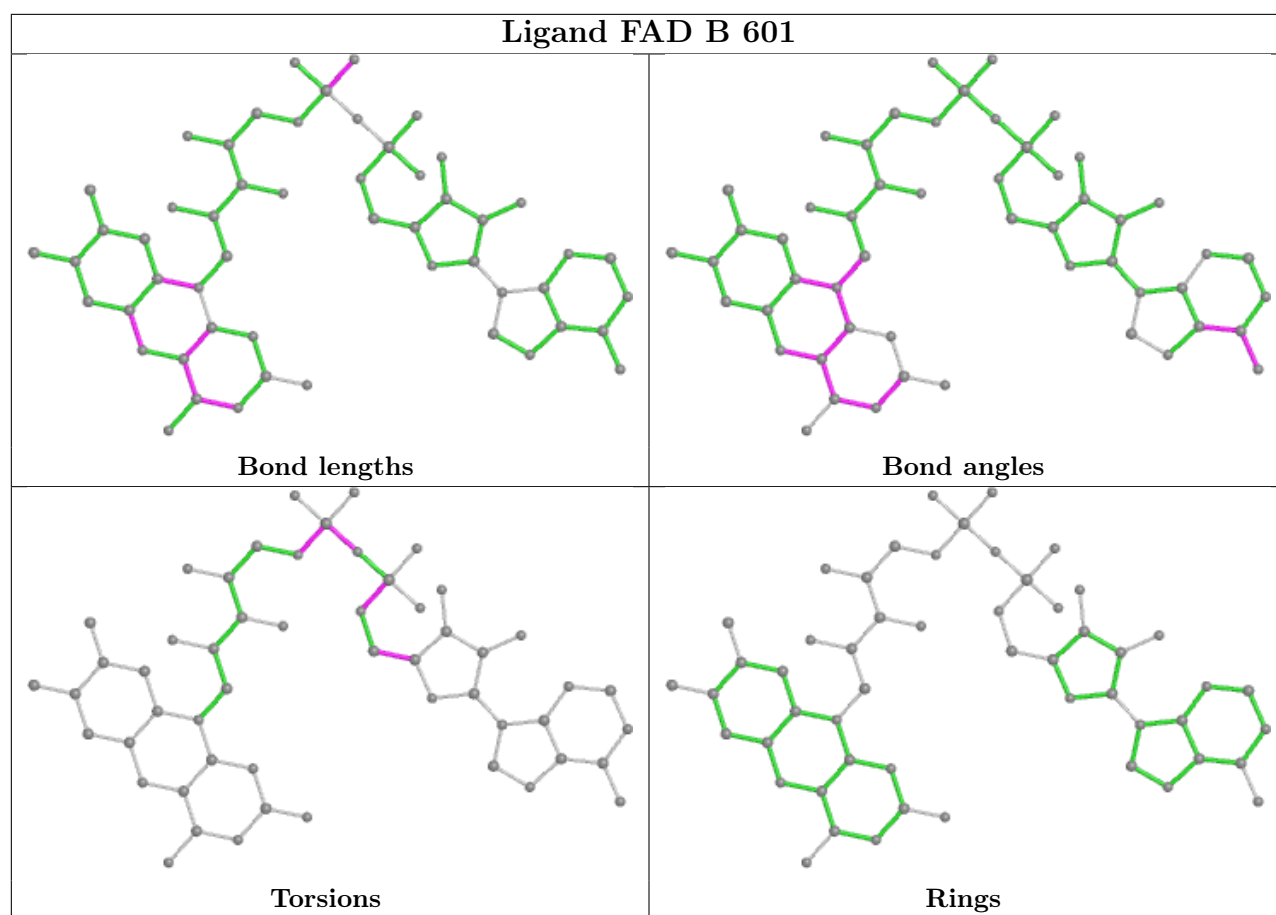
## Ligand TPP B 602

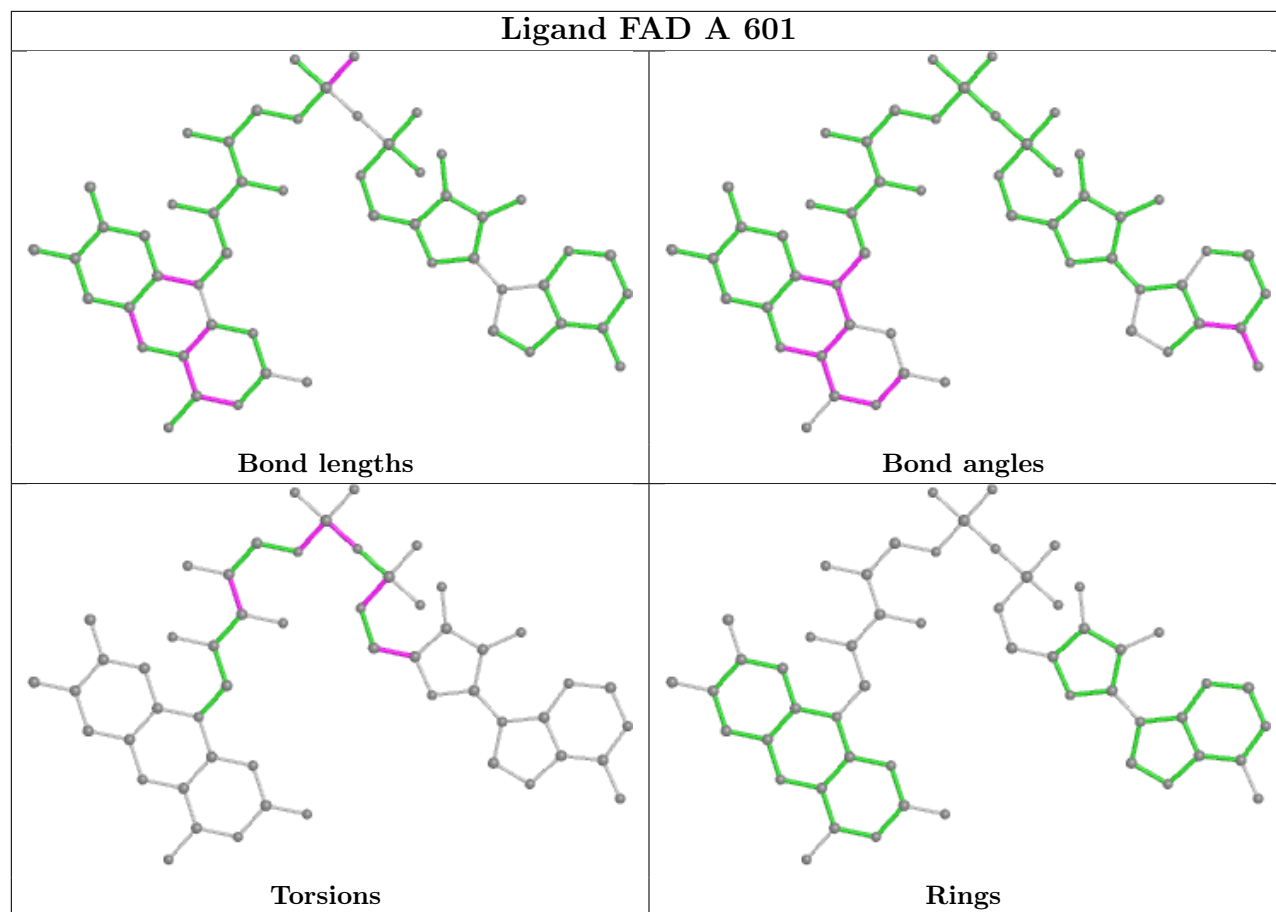


## Ligand TPP C 602

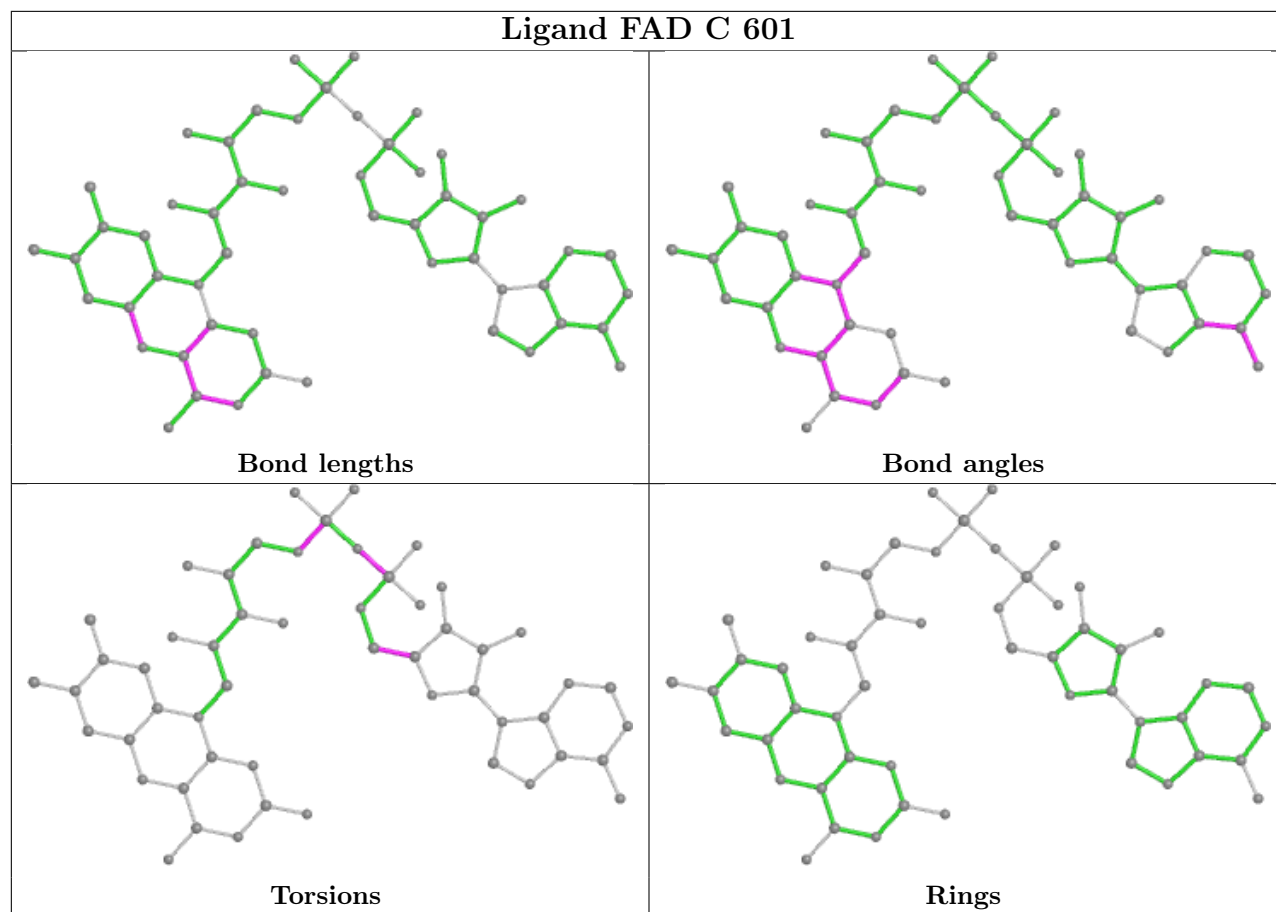












## 5.7 Other polymers [i](#)

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	E	89/127 (70%)	-0.36	1 (1%) 80 78	34, 50, 74, 91	0
1	F	89/127 (70%)	-0.12	3 (3%) 45 37	41, 62, 94, 148	0
1	G	88/127 (69%)	-0.24	2 (2%) 60 55	37, 59, 85, 111	0
1	H	88/127 (69%)	-0.37	0 100 100	36, 55, 83, 101	0
2	A	531/562 (94%)	-0.21	12 (2%) 60 55	34, 57, 84, 137	0
2	B	539/562 (95%)	-0.09	21 (3%) 39 31	31, 65, 110, 135	0
2	C	533/562 (94%)	-0.04	16 (3%) 50 44	31, 66, 100, 115	0
2	D	529/562 (94%)	-0.26	12 (2%) 60 55	27, 63, 99, 132	0
All	All	2486/2756 (90%)	-0.17	67 (2%) 54 49	27, 61, 100, 148	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	193	ALA	4.0
2	D	522	ALA	4.0
2	C	342	PRO	3.9
1	F	60	GLN	3.8
1	G	62	LEU	3.8

### 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

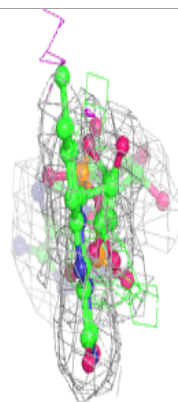
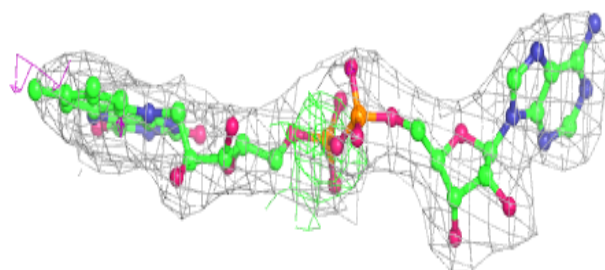
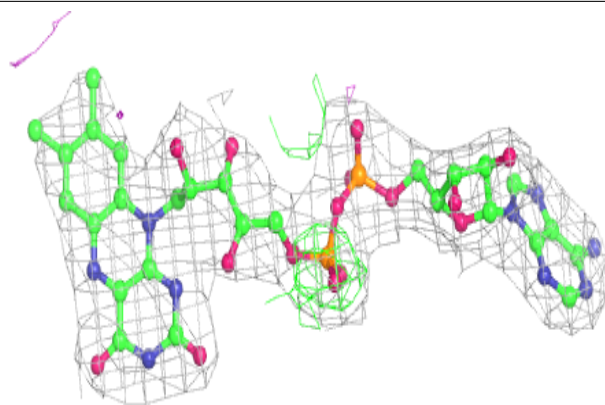
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	FAD	A	601	53/53	0.94	0.17	26,41,61,90	0
5	MG	C	603	1/1	0.94	0.19	56,56,56,56	0
3	FAD	C	601	53/53	0.95	0.18	45,67,78,80	0
3	FAD	B	601	53/53	0.95	0.21	49,65,77,80	0
3	FAD	D	601	53/53	0.96	0.15	50,64,73,78	0
5	MG	D	603	1/1	0.97	0.09	64,64,64,64	0
4	TPP	C	602	26/26	0.97	0.13	35,52,57,63	0
4	TPP	D	602	26/26	0.98	0.12	24,47,63,67	0
5	MG	A	603	1/1	0.98	0.16	50,50,50,50	0
4	TPP	A	602	26/26	0.98	0.15	23,41,54,60	0
4	TPP	B	602	26/26	0.98	0.15	17,43,55,58	0
5	MG	B	603	1/1	0.99	0.11	52,52,52,52	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.

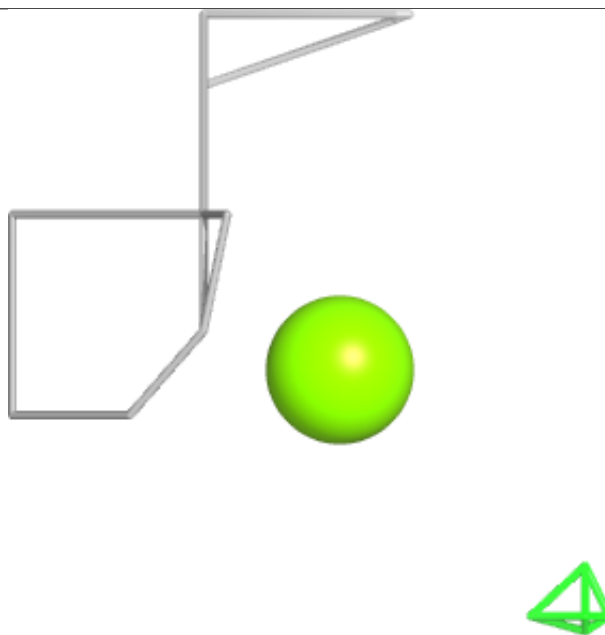
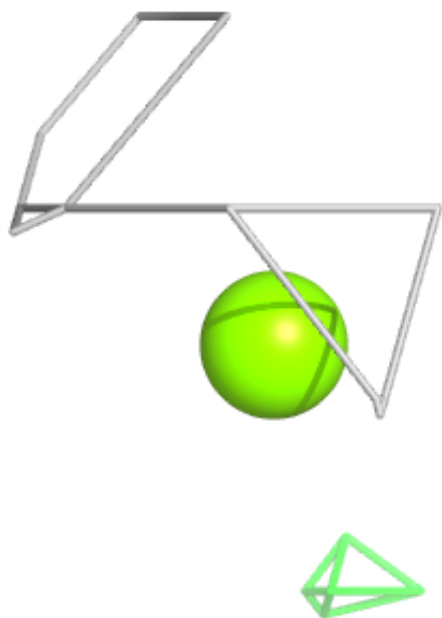
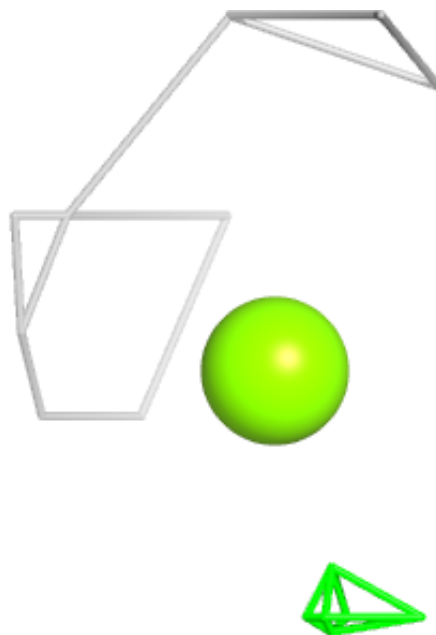
**Electron density around FAD A 601:**

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



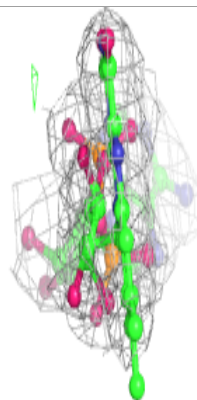
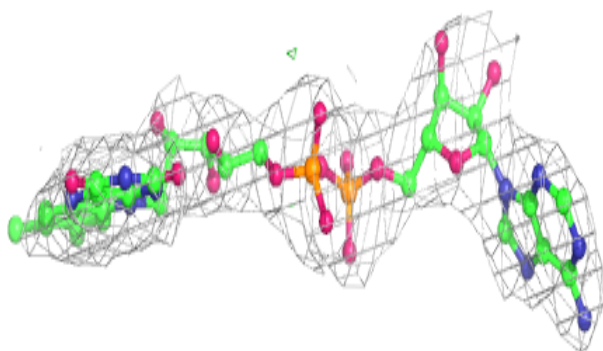
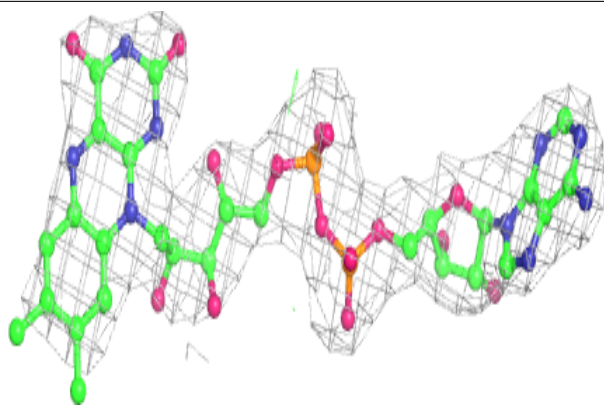
**Electron density around MG C 603:**

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

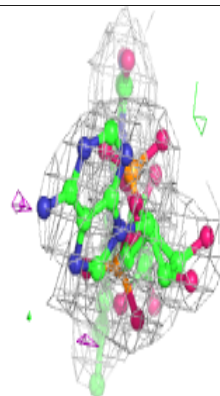
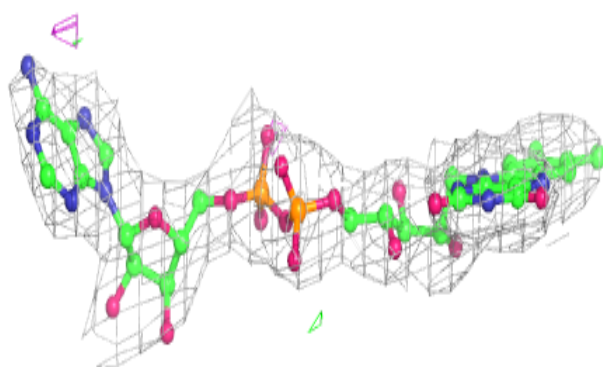
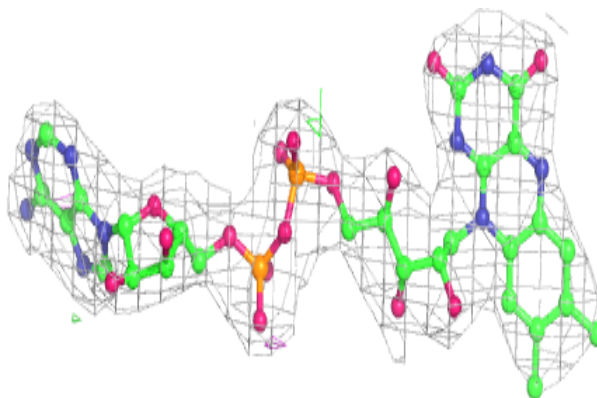


**Electron density around FAD C 601:**

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

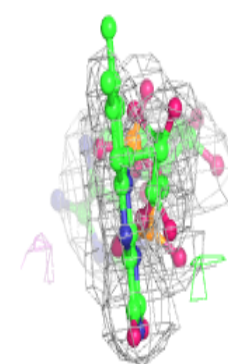
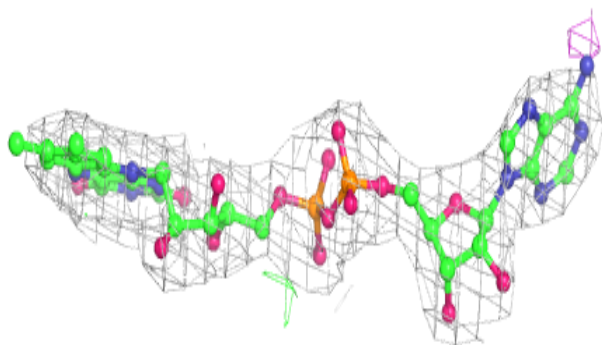
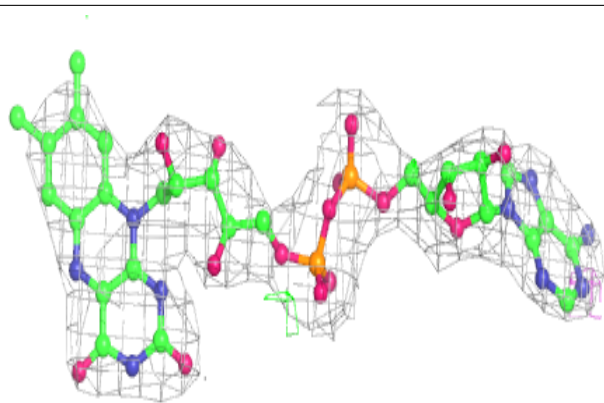
**Electron density around FAD B 601:**

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



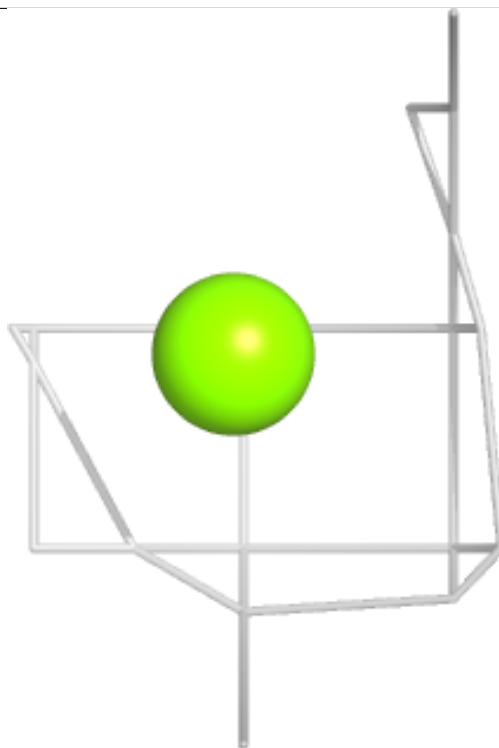
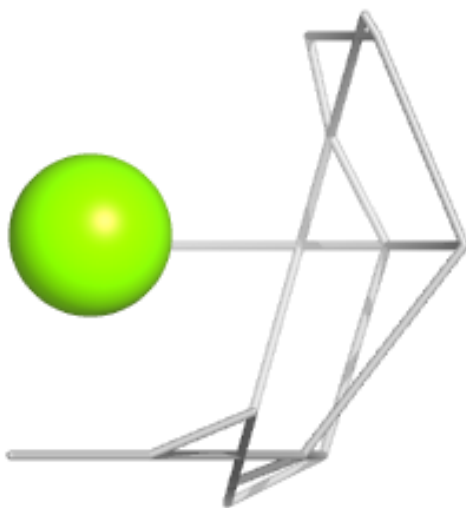
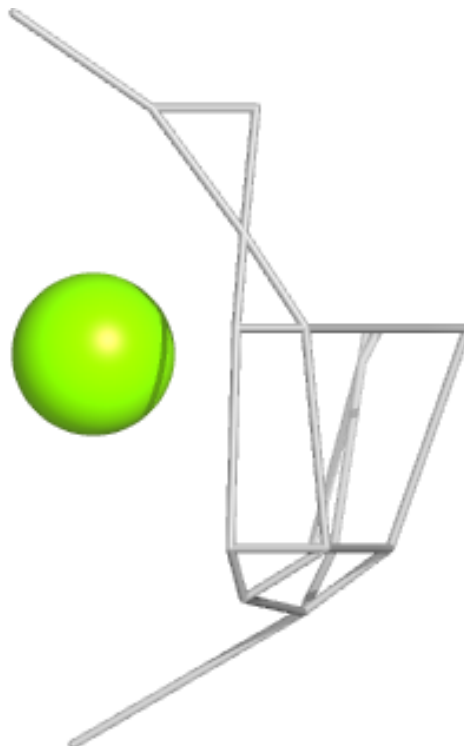
**Electron density around FAD D 601:**

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



**Electron density around MG D 603:**

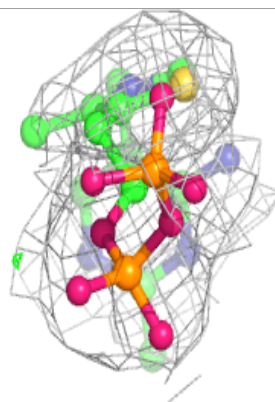
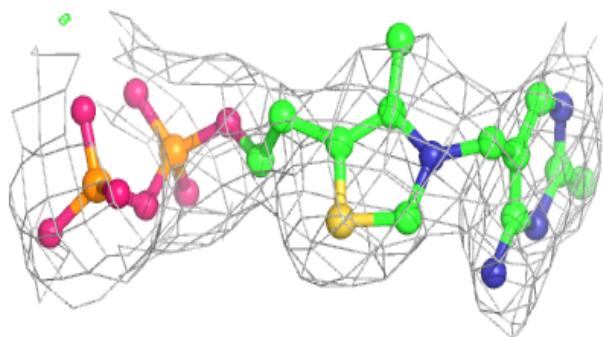
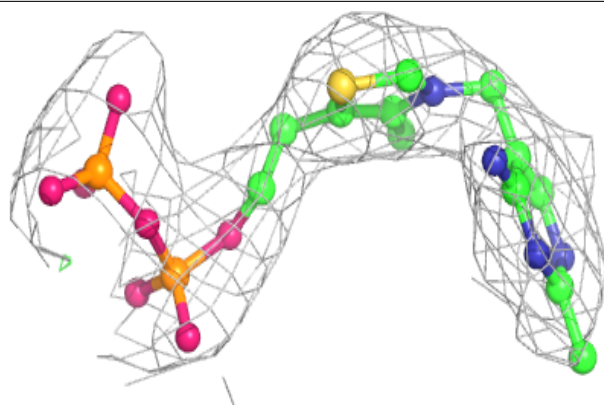
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



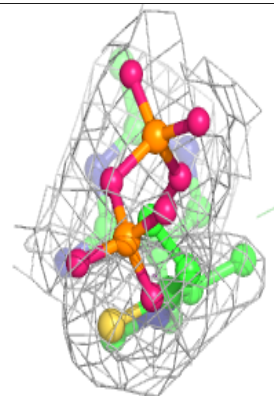
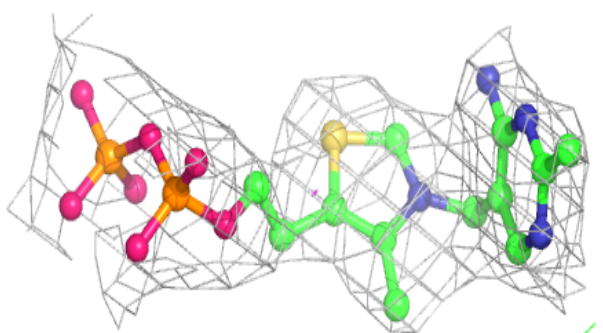
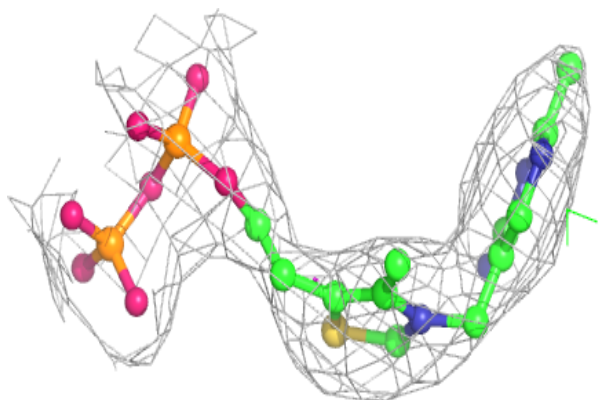


**Electron density around TPP C 602:**

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

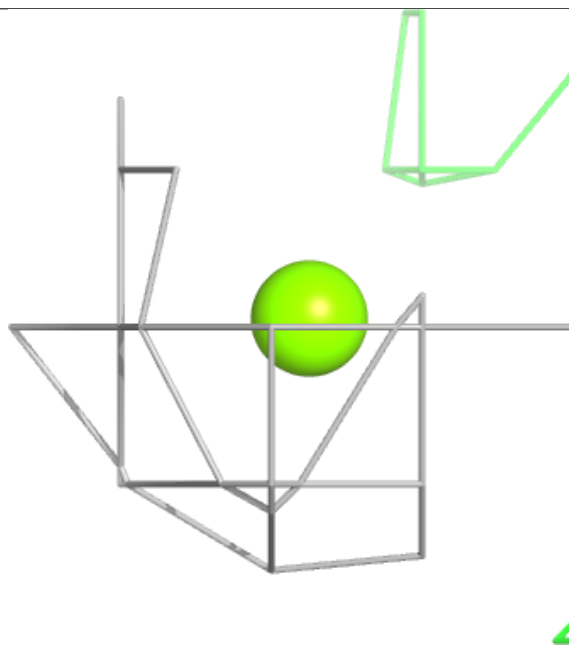
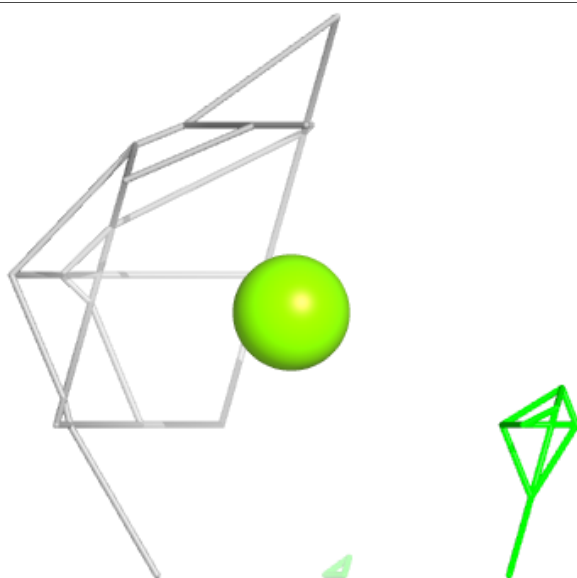
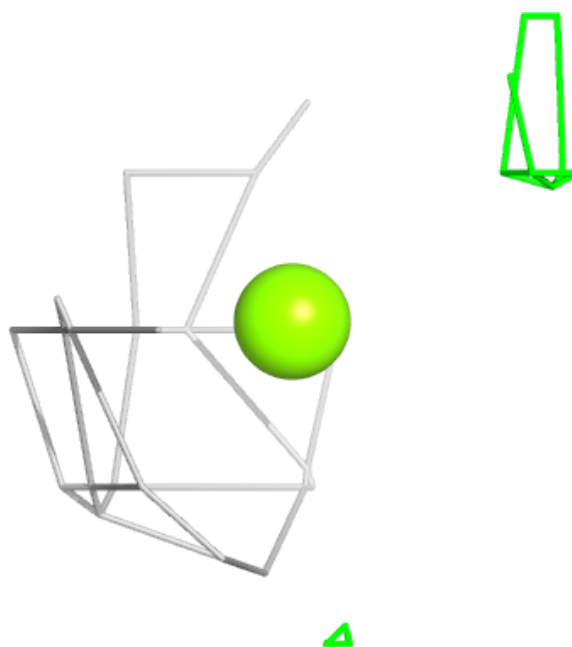
**Electron density around TPP D 602:**

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



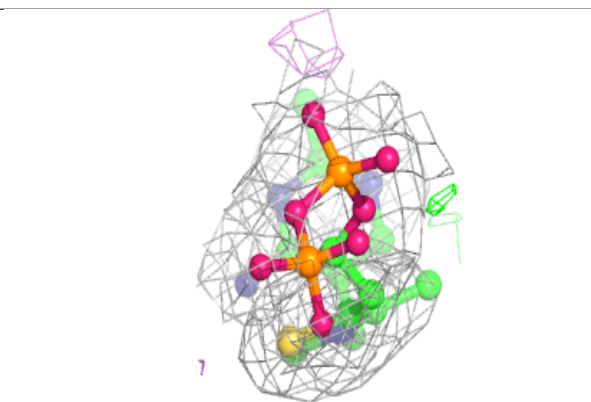
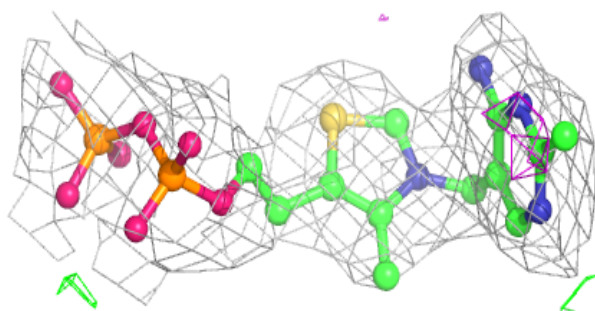
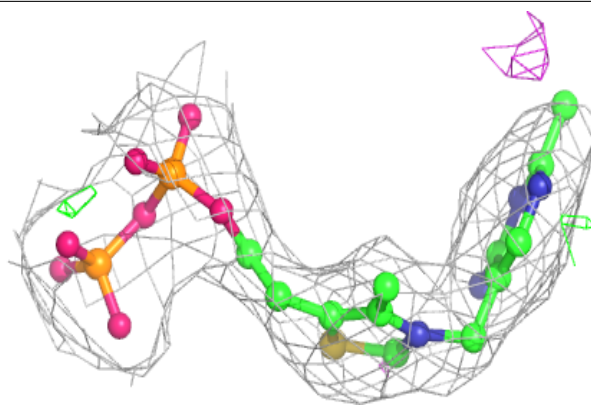
**Electron density around MG A 603:**

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

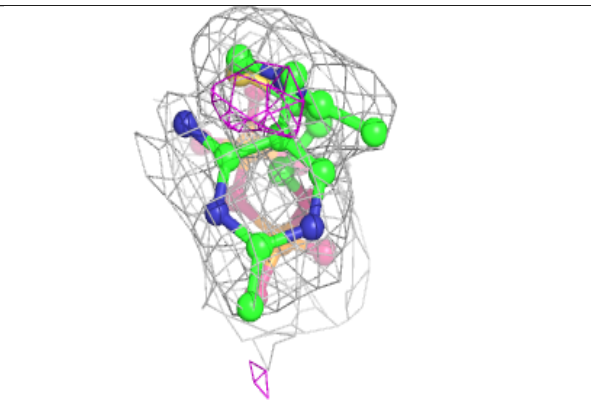
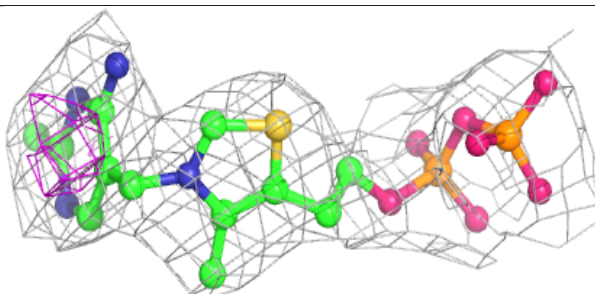
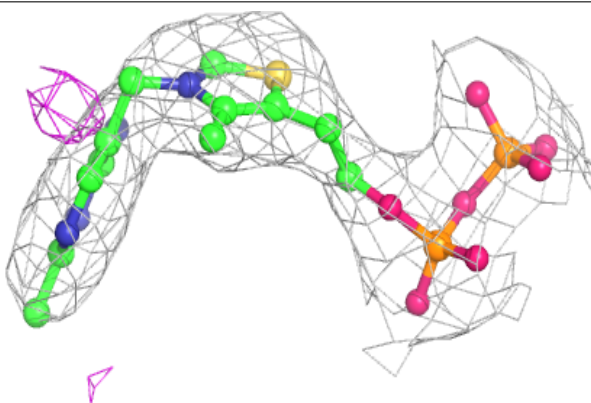


**Electron density around TPP A 602:**

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

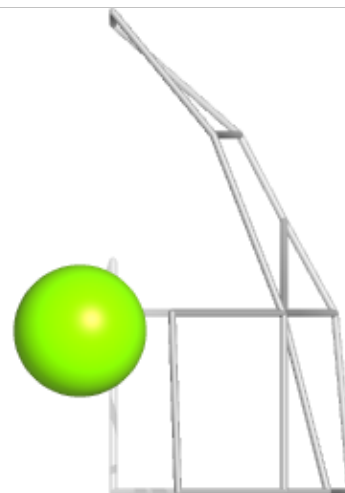
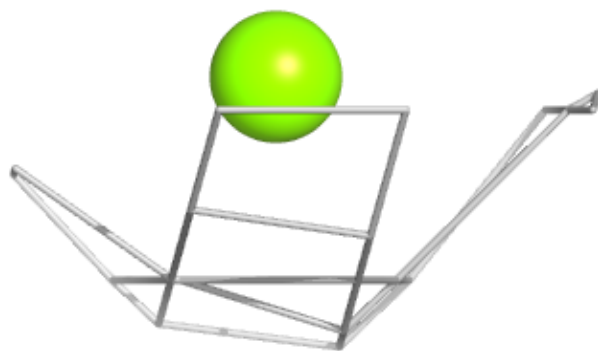
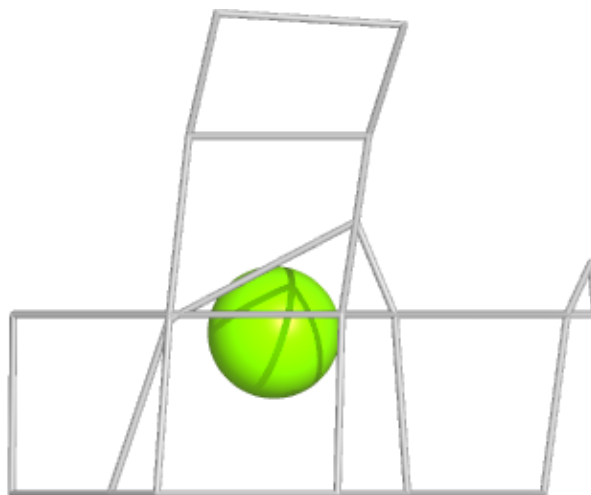
**Electron density around TPP B 602:**

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



**Electron density around MG B 603:**

$2mF_o-DF_c$  (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.