



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 06:36 AM EDT

PDB ID : 3HWX  
Title : Crystal structure of menaquinone synthesis protein MenD from E. coli in complex with ThDP  
Authors : Priyadarshi, A.; Hwang, K.Y.  
Deposited on : 2009-06-19  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 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	:	2.23.2
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)	:	2.23.2

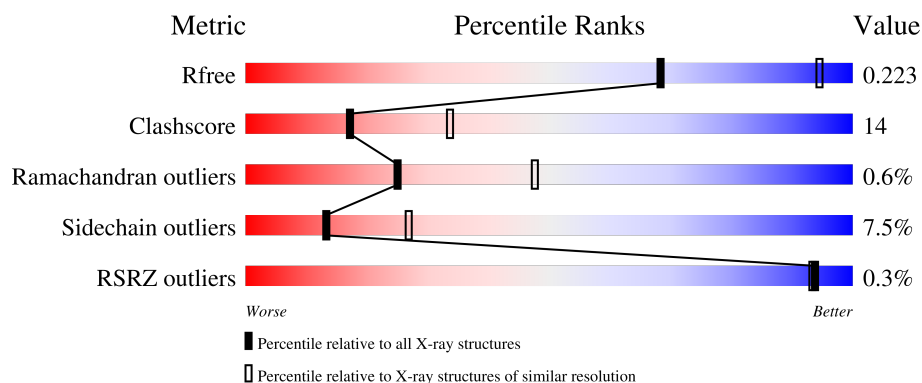
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1	556	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>.</div> </div> </div>
1	A	556	<div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	B	556	<div> <div></div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	I	556	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>..</div> </div> </div>
1	J	556	<div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	R	556	 70% 27% .
1	S	556	%  68% 28% . .
1	Z	556	 65% 30% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35302 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4323	2742	780	786	15			
1	B	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	I	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	J	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	R	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	S	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			
1	Z	554	Total	C	N	O	S	0	0	0
			4319	2740	779	785	15			
1	1	556	Total	C	N	O	S	0	0	0
			4332	2747	781	789	15			

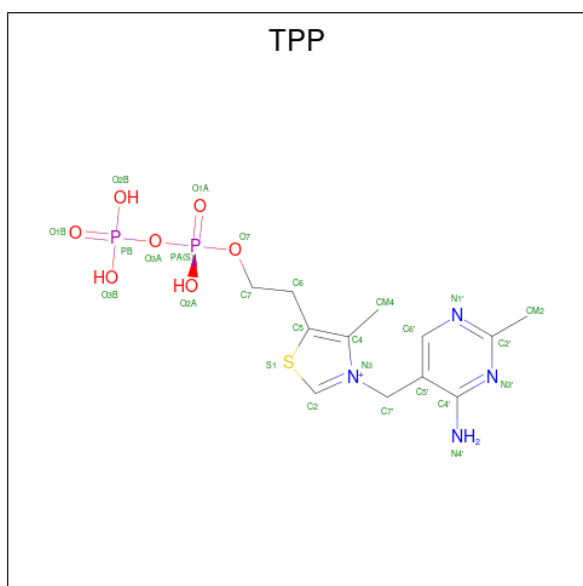
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	engineered mutation	UNP P17109
B	36	LEU	PRO	engineered mutation	UNP P17109
I	36	LEU	PRO	engineered mutation	UNP P17109
J	36	LEU	PRO	engineered mutation	UNP P17109
R	36	LEU	PRO	engineered mutation	UNP P17109
S	36	LEU	PRO	engineered mutation	UNP P17109
Z	36	LEU	PRO	engineered mutation	UNP P17109
1	36	LEU	PRO	engineered mutation	UNP P17109

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	1	Total Na 1 1	0	0
2	I	3	Total Na 3 3	0	0
2	R	3	Total Na 3 3	0	0
2	S	3	Total Na 3 3	0	0
2	Z	2	Total Na 2 2	0	0
2	1	1	Total Na 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$ ).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	S	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
3	Z	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
3	1	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg		
			1	1	0	0
4	B	1	Total	Mg		
			1	1	0	0
4	I	1	Total	Mg		
			1	1	0	0
4	J	1	Total	Mg		
			1	1	0	0
4	R	1	Total	Mg		
			1	1	0	0
4	S	1	Total	Mg		
			1	1	0	0
4	Z	1	Total	Mg		
			1	1	0	0
4	1	1	Total	Mg		
			1	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		
5	1	1	Total	C	O	0	0
			6	3	3		

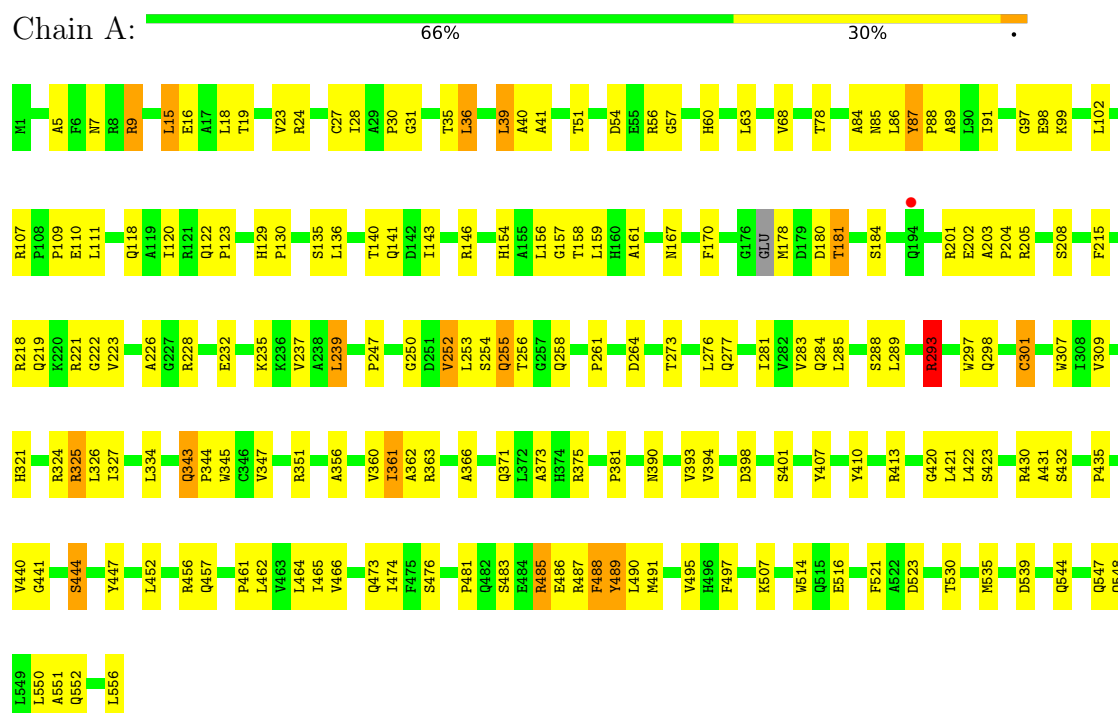
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	56	Total	O	0	0
			56	56		
6	I	53	Total	O	0	0
			53	53		
6	J	43	Total	O	0	0
			43	43		
6	R	55	Total	O	0	0
			55	55		
6	S	76	Total	O	0	0
			76	76		
6	Z	55	Total	O	0	0
			55	55		
6	1	63	Total	O	0	0
			63	63		

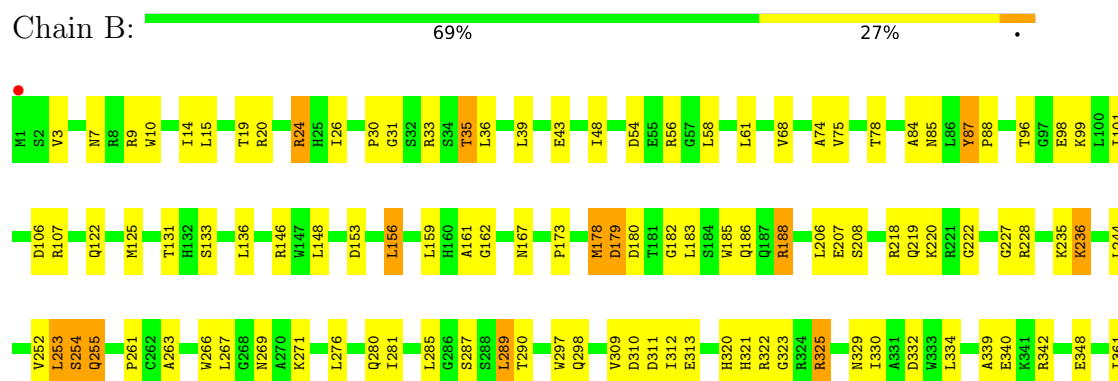
### 3 Residue-property plots [i](#)

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.

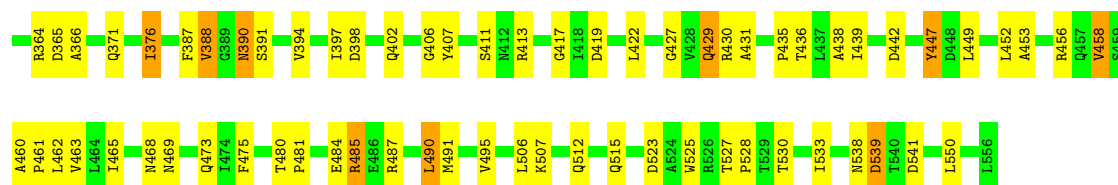
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



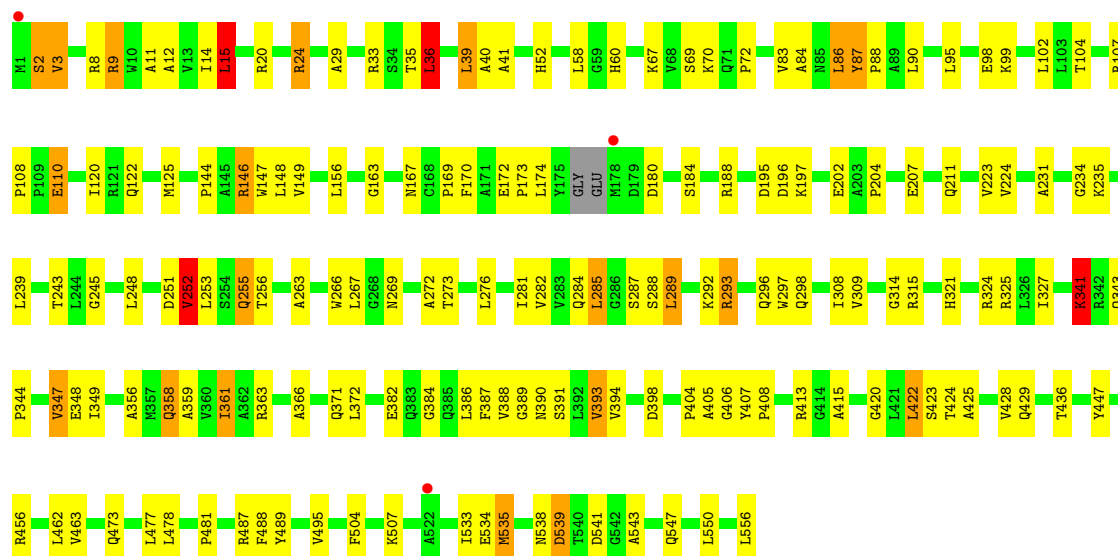
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



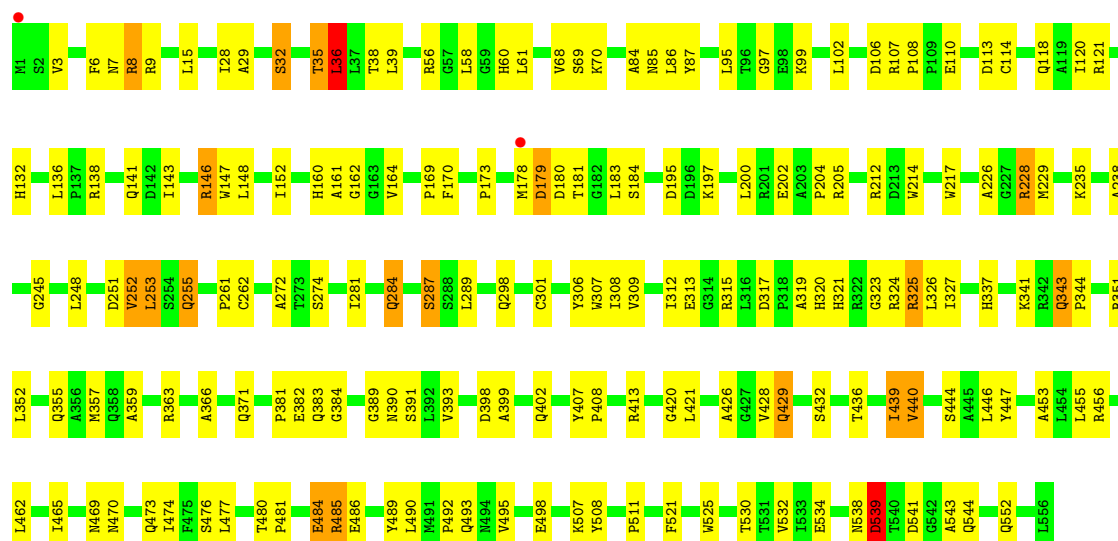




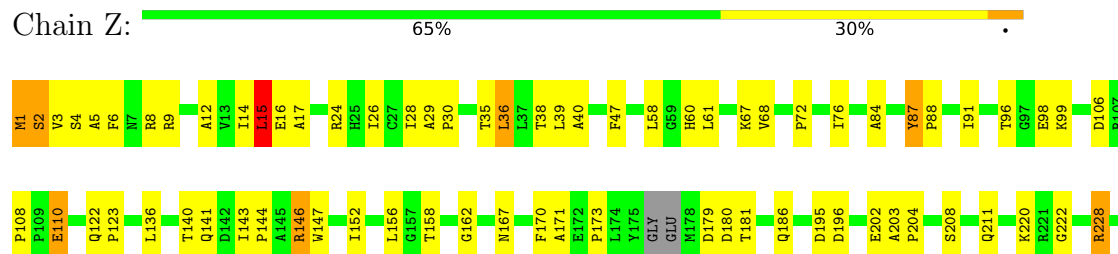
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

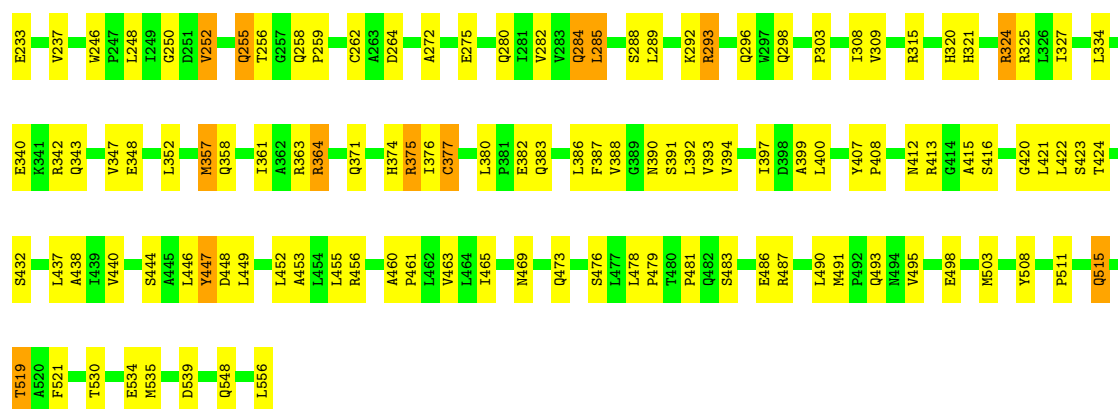


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

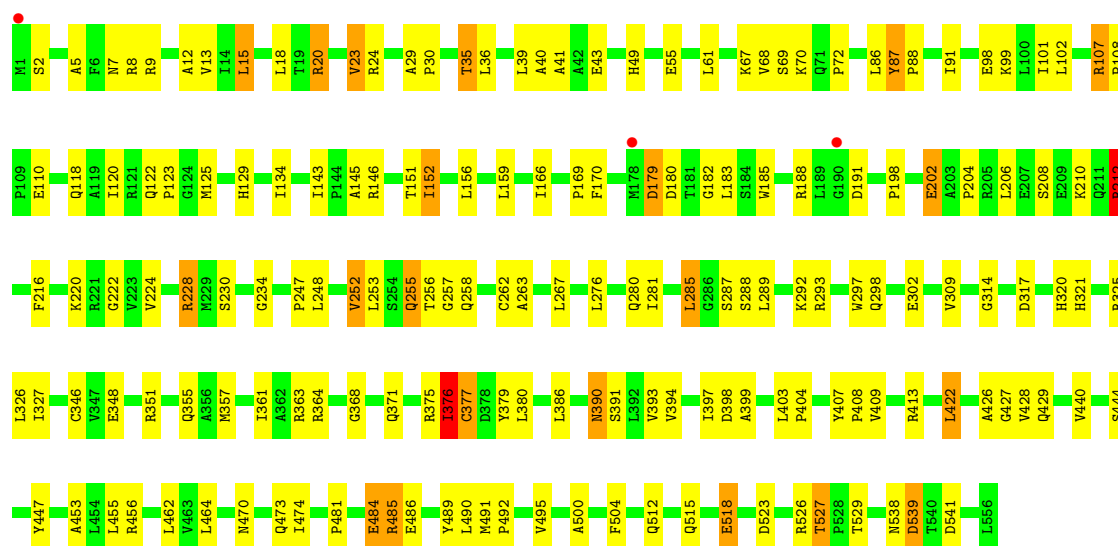


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase





● Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.35Å 90.46Å 169.17Å 75.99° 83.00° 64.15°	Depositor
Resolution (Å)	47.69 – 2.60 47.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.5 (47.69-2.60) 83.5 (47.69-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.197 , 0.253 0.201 , 0.223	Depositor DCC
$R_{free}$ test set	6053 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,-k+1	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	35302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% 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: MG, TPP, GOL, NA

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	1	0.80	0/4439	0.87	4/6053 (0.1%)
1	A	0.83	2/4429 (0.0%)	0.89	5/6038 (0.1%)
1	B	0.79	2/4439 (0.0%)	0.89	7/6053 (0.1%)
1	I	0.79	3/4425 (0.1%)	0.87	6/6033 (0.1%)
1	J	0.72	0/4439	0.85	4/6053 (0.1%)
1	R	0.80	3/4425 (0.1%)	0.87	5/6033 (0.1%)
1	S	0.78	0/4439	0.87	7/6053 (0.1%)
1	Z	0.73	1/4425 (0.0%)	0.86	4/6033 (0.1%)
All	All	0.78	11/35460 (0.0%)	0.87	42/48349 (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	S	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	347	VAL	CB-CG1	-7.42	1.37	1.52
1	R	346	CYS	CB-SG	-7.32	1.69	1.82
1	I	348	GLU	CB-CG	-6.70	1.39	1.52
1	A	489	TYR	CD1-CE1	-6.66	1.29	1.39
1	A	488	PHE	CE1-CZ	-6.51	1.25	1.37

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	Z	36	LEU	CA-CB-CG	-10.65	90.80	115.30
1	A	9	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	R	538	ASN	CB-CA-C	7.60	125.59	110.40
1	B	153	ASP	CB-CG-OD1	7.39	124.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	485	ARG	Sidechain

## 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	1	4332	0	4302	137	0
1	A	4323	0	4295	146	0
1	B	4332	0	4302	128	0
1	I	4319	0	4292	123	0
1	J	4332	0	4302	132	0
1	R	4319	0	4292	114	0
1	S	4332	0	4302	112	0
1	Z	4319	0	4292	141	0
2	1	1	0	0	0	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	I	3	0	0	0	0
2	R	3	0	0	0	0
2	S	3	0	0	0	0
2	Z	2	0	0	0	0
3	1	26	0	16	1	0
3	A	26	0	16	1	0
3	B	26	0	16	7	0
3	I	26	0	16	1	0
3	J	26	0	16	1	0
3	R	26	0	16	3	0
3	S	26	0	16	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	26	0	16	2	0
4	1	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	Z	1	0	0	0	0
5	1	6	0	8	0	0
5	J	6	0	8	0	0
6	1	63	0	0	5	0
6	A	50	0	0	4	0
6	B	56	0	0	5	0
6	I	53	0	0	3	0
6	J	43	0	0	4	0
6	R	55	0	0	3	0
6	S	76	0	0	6	0
6	Z	55	0	0	8	0
All	All	35302	0	34523	956	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 14.

The worst 5 of 956 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:Z:264:ASP:O	1:Z:293:ARG:HG3	1.47	1.12
1:1:7:ASN:HB3	1:1:36:LEU:CD1	1.80	1.12
1:R:293:ARG:HG2	1:R:293:ARG:HH11	1.12	1.12
1:R:39:LEU:HD21	1:S:481:PRO:HG2	1.28	1.12
1:A:39:LEU:HD21	1:B:481:PRO:HG3	1.21	1.11

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	1	554/556 (100%)	511 (92%)	38 (7%)	5 (1%)	17	35
1	A	551/556 (99%)	517 (94%)	32 (6%)	2 (0%)	34	57
1	B	554/556 (100%)	516 (93%)	34 (6%)	4 (1%)	22	43
1	I	550/556 (99%)	494 (90%)	49 (9%)	7 (1%)	12	24
1	J	554/556 (100%)	508 (92%)	44 (8%)	2 (0%)	34	57
1	R	550/556 (99%)	504 (92%)	44 (8%)	2 (0%)	34	57
1	S	554/556 (100%)	506 (91%)	46 (8%)	2 (0%)	34	57
1	Z	550/556 (99%)	509 (92%)	39 (7%)	2 (0%)	34	57
All	All	4417/4448 (99%)	4065 (92%)	326 (7%)	26 (1%)	25	47

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	THR
1	B	179	ASP
1	J	179	ASP
1	1	179	ASP
1	A	181	THR

### 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	1	452/452 (100%)	421 (93%)	31 (7%)	15	31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/452 (100%)	415 (92%)	36 (8%)	12	24
1	B	452/452 (100%)	420 (93%)	32 (7%)	14	29
1	I	451/452 (100%)	415 (92%)	36 (8%)	12	24
1	J	452/452 (100%)	419 (93%)	33 (7%)	14	28
1	R	451/452 (100%)	417 (92%)	34 (8%)	13	27
1	S	452/452 (100%)	415 (92%)	37 (8%)	11	22
1	Z	451/452 (100%)	419 (93%)	32 (7%)	14	29
All	All	3612/3616 (100%)	3341 (92%)	271 (8%)	13	27

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	423	SER
1	Z	535	MET
1	I	429	GLN
1	I	429	GLN
1	I	382	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	355	GLN
1	J	552	GLN
1	I	355	GLN
1	J	544	GLN
1	R	320	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 33 ligands modelled in this entry, 23 are monoatomic - leaving 10 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$
3	TPP	A	601	4	22,27,27	1.50	5 (22%)	29,40,40	1.91	8 (27%)
3	TPP	I	601	4	22,27,27	1.75	7 (31%)	29,40,40	2.39	12 (41%)
5	GOL	1	558	-	5,5,5	0.59	0	5,5,5	0.76	0
3	TPP	B	601	4	22,27,27	1.78	6 (27%)	29,40,40	2.02	10 (34%)
3	TPP	1	601	4	22,27,27	1.27	3 (13%)	29,40,40	2.02	11 (37%)
3	TPP	R	601	4	22,27,27	1.52	6 (27%)	29,40,40	2.21	11 (37%)
3	TPP	J	601	4	22,27,27	1.24	4 (18%)	29,40,40	2.35	10 (34%)
5	GOL	J	557	-	5,5,5	0.38	0	5,5,5	0.55	0
3	TPP	S	601	4	22,27,27	1.83	3 (13%)	29,40,40	1.64	6 (20%)
3	TPP	Z	601	4	22,27,27	1.69	5 (22%)	29,40,40	2.21	7 (24%)

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	TPP	A	601	4	-	0/16/17/17	0/2/2/2
3	TPP	I	601	4	-	3/16/17/17	0/2/2/2
5	GOL	1	558	-	-	2/4/4/4	-
3	TPP	B	601	4	-	1/16/17/17	0/2/2/2
3	TPP	1	601	4	-	5/16/17/17	0/2/2/2
3	TPP	R	601	4	-	0/16/17/17	0/2/2/2
3	TPP	J	601	4	-	0/16/17/17	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	J	557	-	-	2/4/4/4	-
3	TPP	S	601	4	-	1/16/17/17	0/2/2/2
3	TPP	Z	601	4	-	0/16/17/17	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	601	TPP	C4-N3	-5.97	1.34	1.39
3	B	601	TPP	C4-N3	-4.47	1.35	1.39
3	Z	601	TPP	C6-C5	-4.35	1.49	1.50
3	A	601	TPP	C4-N3	-3.53	1.36	1.39
3	I	601	TPP	PB-O3B	-3.45	1.41	1.54

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	601	TPP	C6-C5-C4	7.92	133.79	127.43
3	I	601	TPP	O3B-PB-O3A	7.18	128.70	104.64
3	J	601	TPP	C6-C5-C4	6.59	132.73	127.43
3	I	601	TPP	C6-C5-C4	5.50	131.85	127.43
3	J	601	TPP	CM4-C4-N3	5.47	129.50	122.53

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	601	TPP	PA-O3A-PB-O3B
3	S	601	TPP	PB-O3A-PA-O7
3	1	601	TPP	C7-O7-PA-O1A
3	1	601	TPP	C7-O7-PA-O2A
5	J	557	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

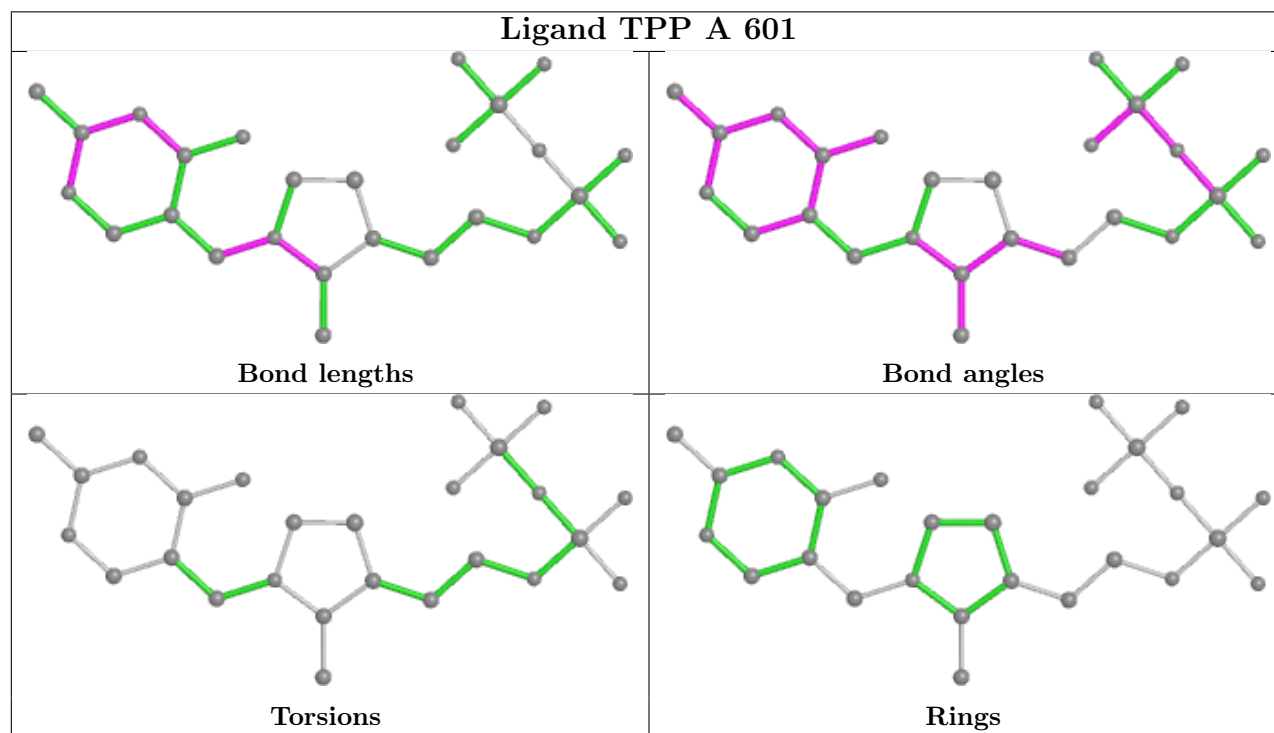
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TPP	1	0
3	I	601	TPP	1	0
3	B	601	TPP	7	0
3	1	601	TPP	1	0
3	R	601	TPP	3	0

*Continued on next page...*

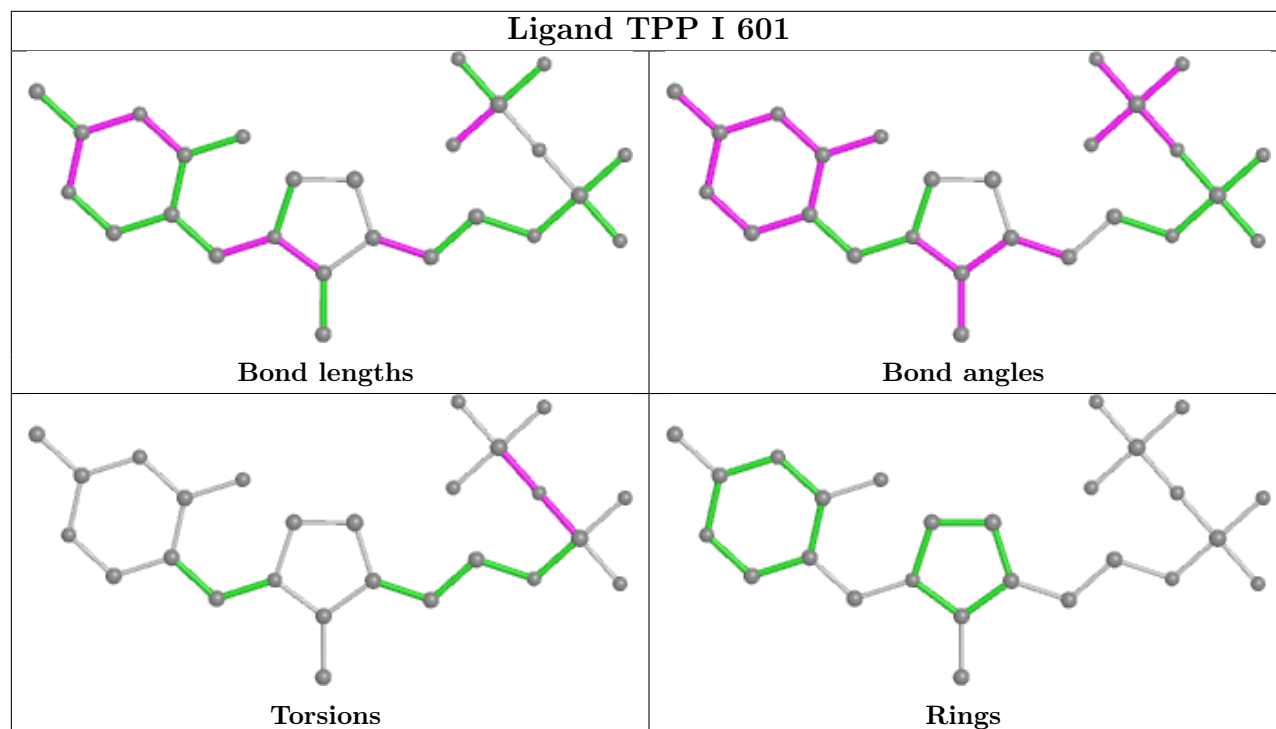
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	601	TPP	1	0
3	S	601	TPP	1	0
3	Z	601	TPP	2	0

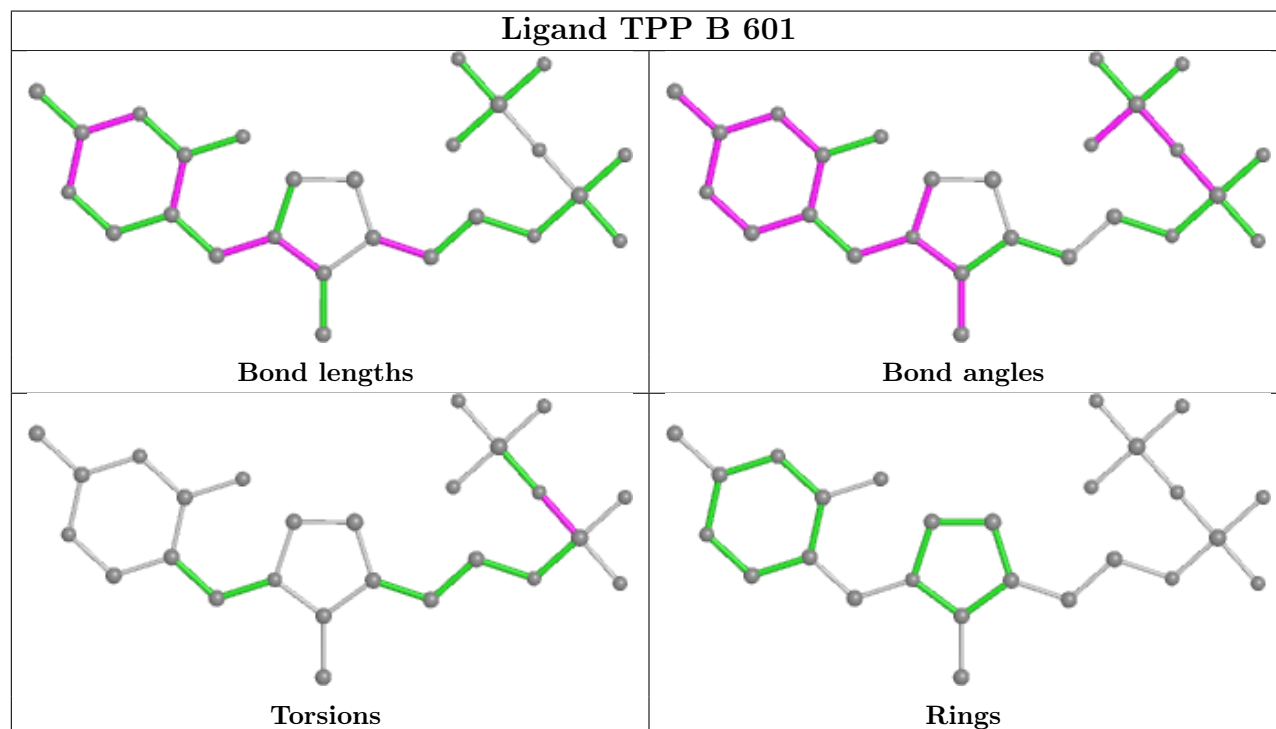
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



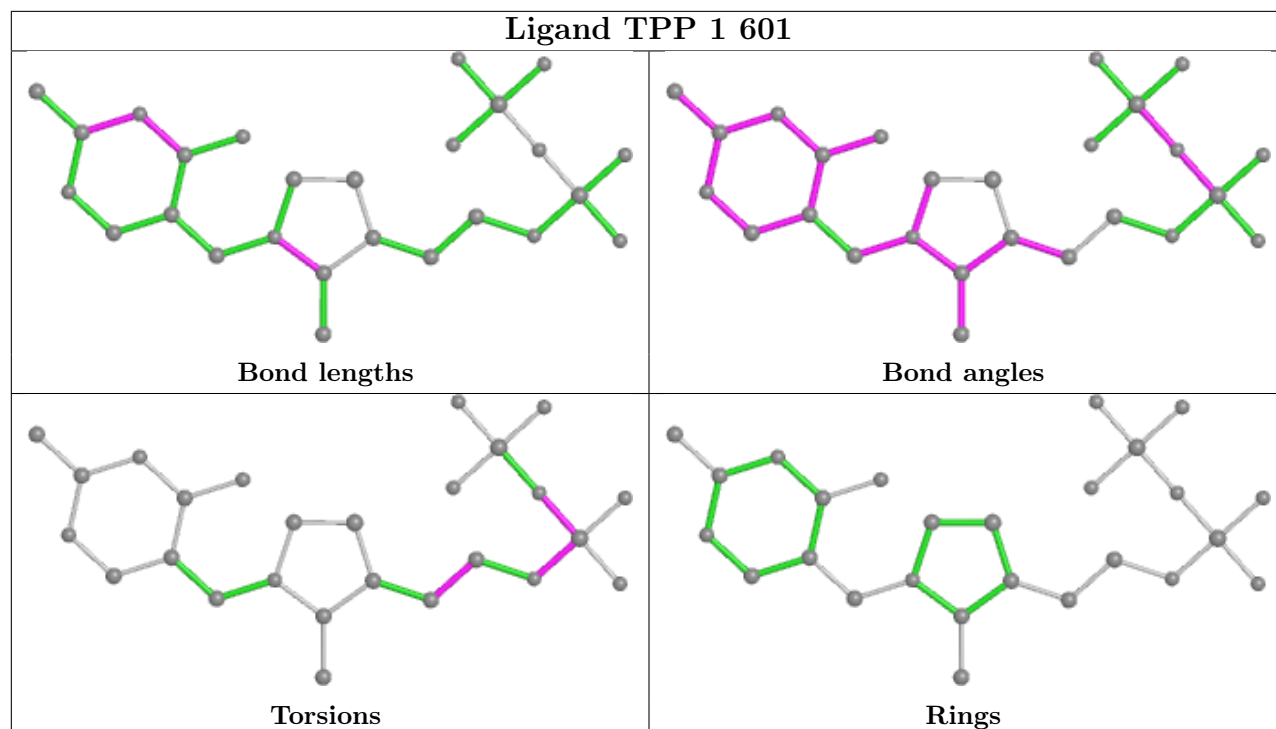
## Ligand TPP I 601



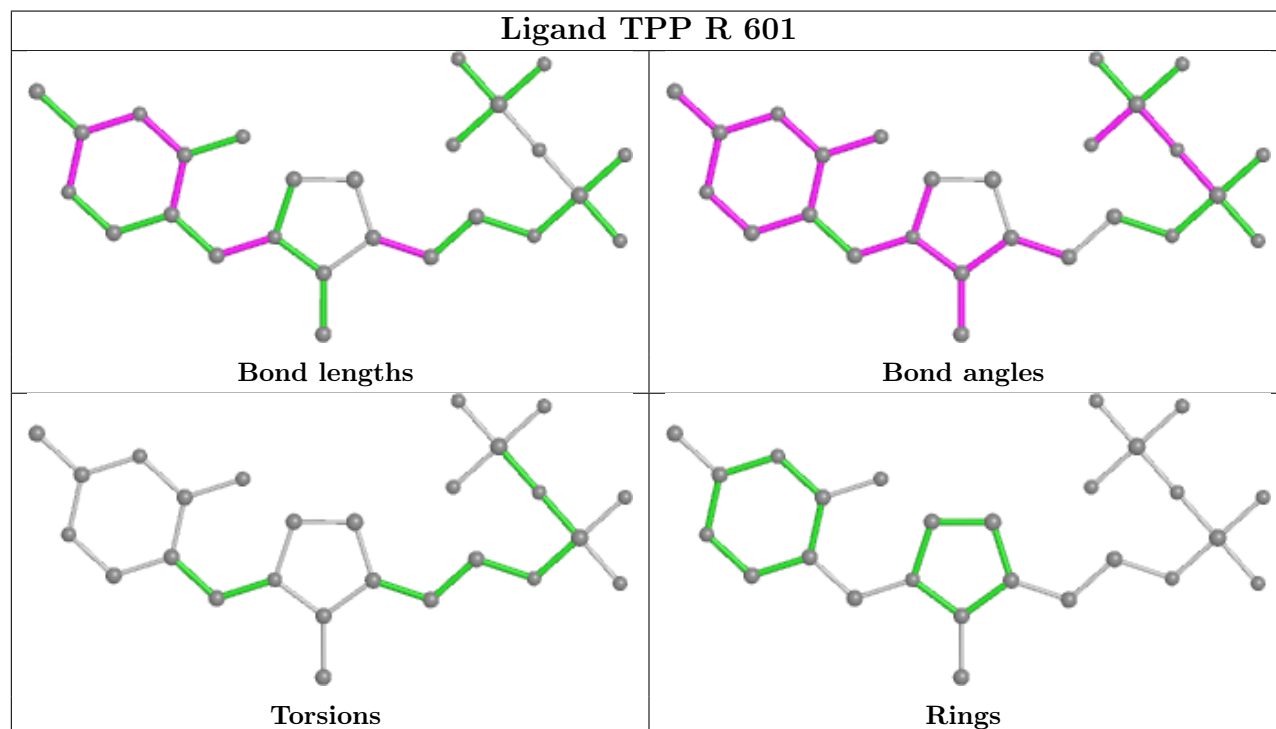
## Ligand TPP B 601



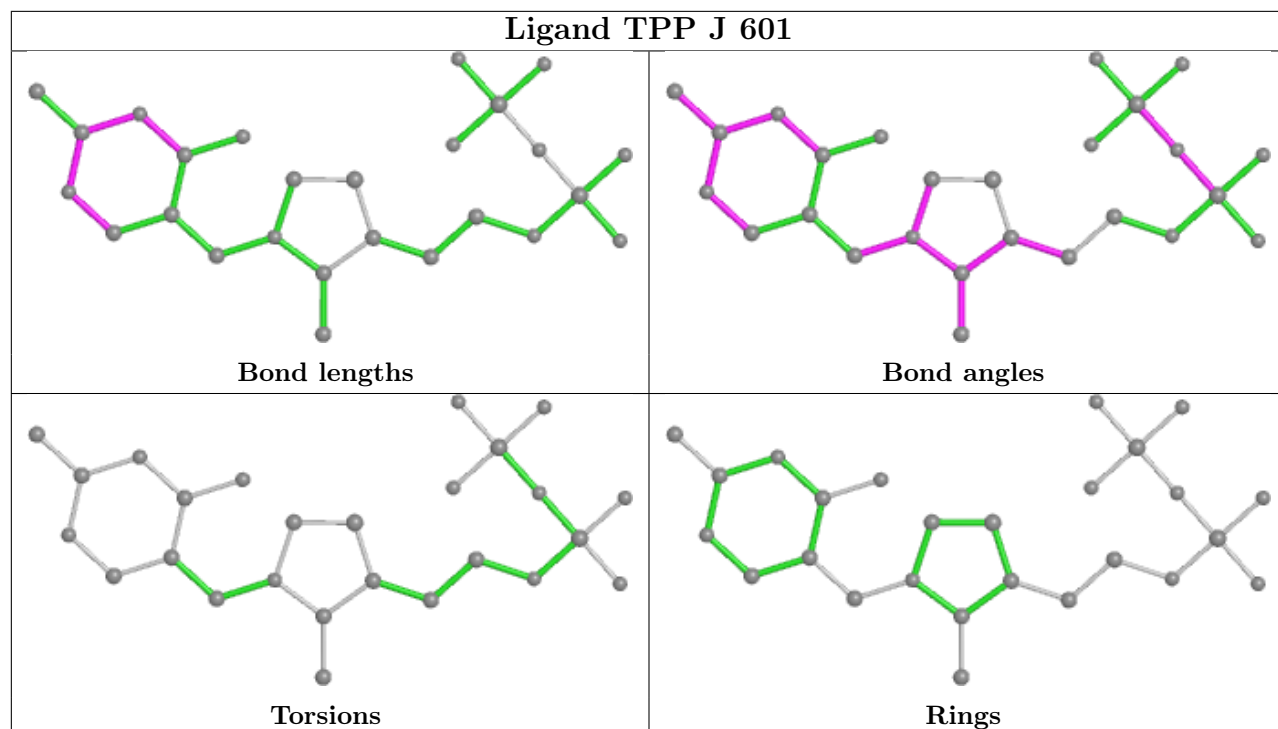
## Ligand TPP 1 601



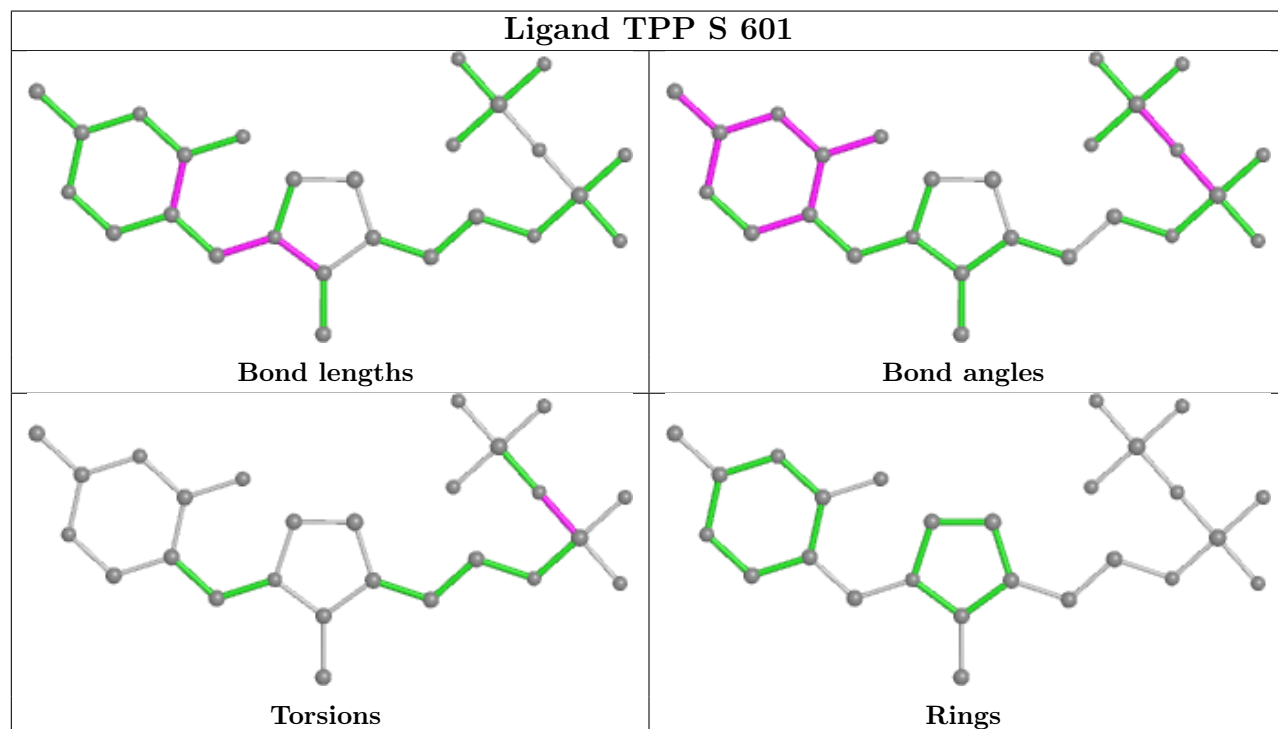
## Ligand TPP R 601

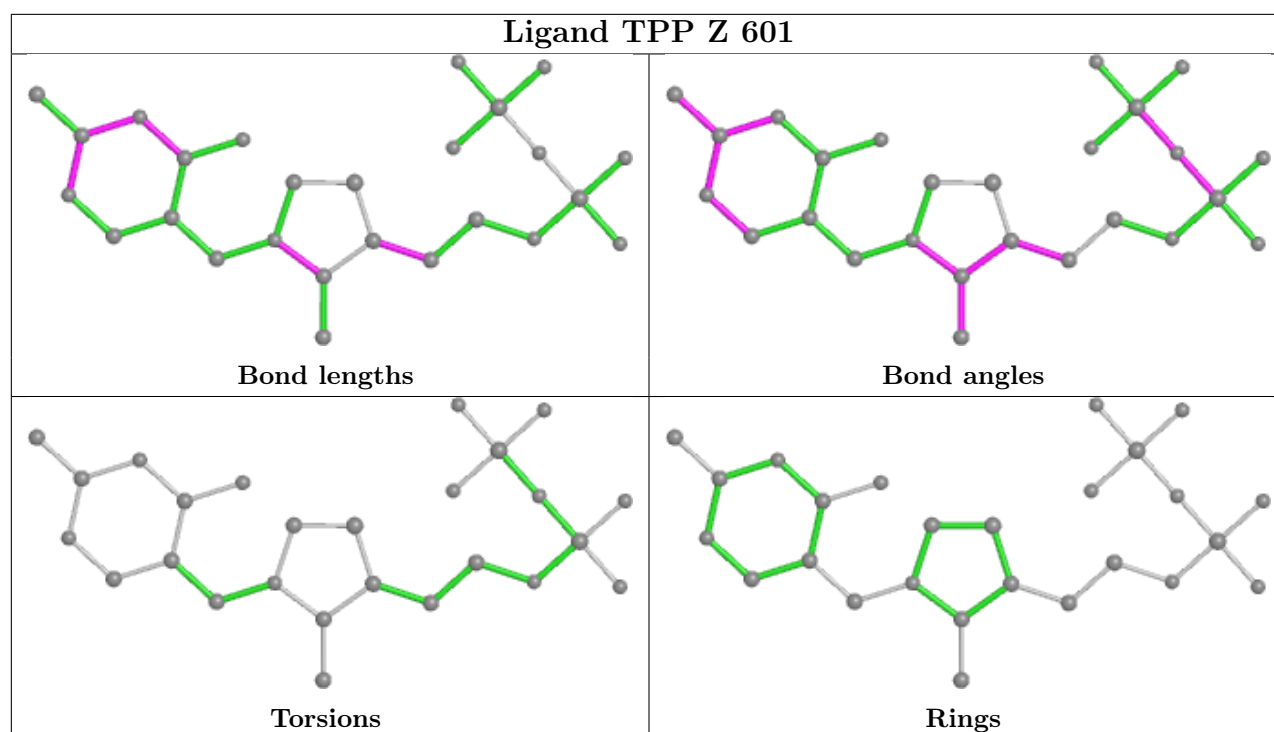


## Ligand TPP J 601



## Ligand TPP S 601





## 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	1	556/556 (100%)	-0.39	3 (0%) 91 89	4, 13, 25, 38	10 (1%)
1	A	555/556 (99%)	-0.50	1 (0%) 95 95	2, 11, 24, 39	11 (1%)
1	B	556/556 (100%)	-0.50	1 (0%) 95 95	3, 12, 22, 35	10 (1%)
1	I	554/556 (99%)	-0.42	3 (0%) 91 89	3, 13, 26, 46	11 (1%)
1	J	556/556 (100%)	-0.25	2 (0%) 92 91	5, 17, 30, 38	10 (1%)
1	R	554/556 (99%)	-0.52	1 (0%) 95 95	4, 12, 22, 42	11 (1%)
1	S	556/556 (100%)	-0.47	3 (0%) 91 89	3, 12, 24, 37	10 (1%)
1	Z	554/556 (99%)	-0.42	0 100 100	4, 15, 29, 43	11 (1%)
All	All	4441/4448 (99%)	-0.44	14 (0%) 94 93	2, 13, 26, 46	84 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.7
1	I	522	ALA	3.4
1	S	1	MET	3.3
1	1	1	MET	3.2
1	R	1	MET	3.1

### 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.

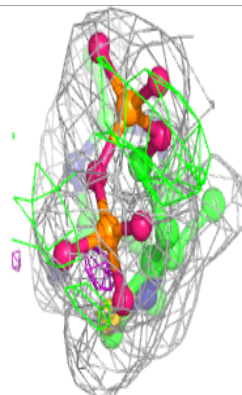
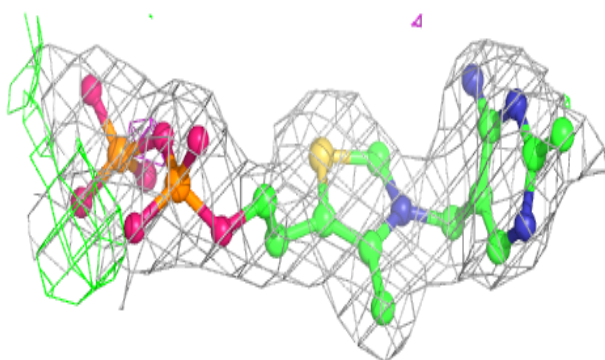
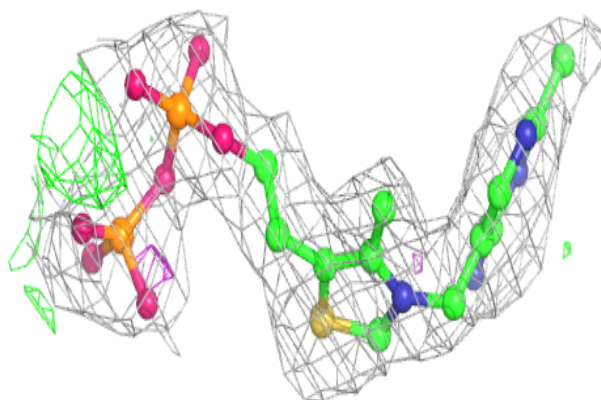
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	1	557	1/1	0.83	0.16	26,26,26,26	0
2	NA	A	558	1/1	0.87	0.16	23,23,23,23	0
2	NA	Z	558	1/1	0.90	0.11	28,28,28,28	0
2	NA	R	558	1/1	0.91	0.11	34,34,34,34	0
5	GOL	J	557	6/6	0.91	0.24	35,37,37,39	0
5	GOL	1	558	6/6	0.91	0.16	29,32,32,33	0
2	NA	B	557	1/1	0.92	0.11	30,30,30,30	0
4	MG	I	602	1/1	0.93	0.23	2,2,2,2	0
2	NA	S	558	1/1	0.94	0.16	25,25,25,25	0
2	NA	I	559	1/1	0.94	0.10	18,18,18,18	0
2	NA	R	559	1/1	0.95	0.10	26,26,26,26	0
2	NA	S	557	1/1	0.95	0.12	19,19,19,19	0
2	NA	A	557	1/1	0.95	0.16	17,17,17,17	0
4	MG	R	602	1/1	0.95	0.22	2,2,2,2	0
2	NA	S	559	1/1	0.95	0.19	18,18,18,18	0
2	NA	Z	557	1/1	0.95	0.25	33,33,33,33	0
2	NA	R	557	1/1	0.96	0.20	29,29,29,29	0
4	MG	S	602	1/1	0.96	0.13	8,8,8,8	0
2	NA	I	558	1/1	0.96	0.12	17,17,17,17	0
4	MG	J	602	1/1	0.96	0.14	2,2,2,2	0
3	TPP	I	601	26/26	0.97	0.13	2,12,14,14	0
3	TPP	J	601	26/26	0.97	0.12	7,13,19,24	0
3	TPP	S	601	26/26	0.97	0.11	2,5,7,12	0
3	TPP	1	601	26/26	0.97	0.13	3,7,10,11	0
3	TPP	B	601	26/26	0.97	0.11	5,8,10,11	0
3	TPP	A	601	26/26	0.98	0.11	2,4,11,12	0
3	TPP	Z	601	26/26	0.98	0.14	4,10,12,13	0
2	NA	I	557	1/1	0.98	0.16	20,20,20,20	0
4	MG	1	602	1/1	0.98	0.23	2,2,2,2	0
4	MG	A	602	1/1	0.98	0.13	2,2,2,2	0
3	TPP	R	601	26/26	0.98	0.10	2,7,11,11	0
4	MG	Z	602	1/1	0.99	0.17	2,2,2,2	0
4	MG	B	602	1/1	0.99	0.18	2,2,2,2	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.

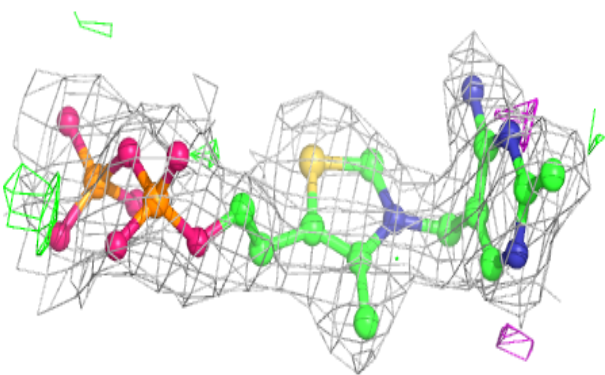
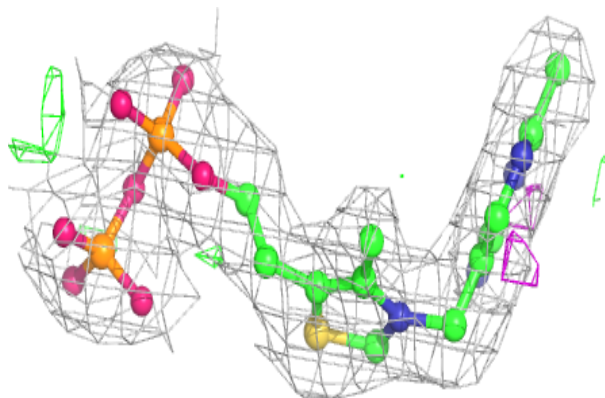
**Electron density around TPP I 601:**

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



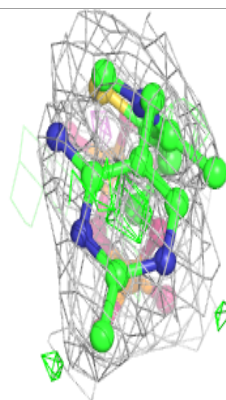
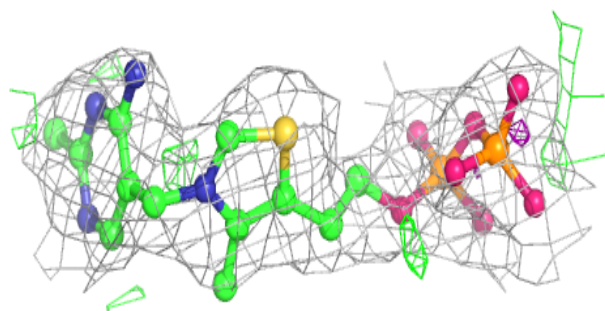
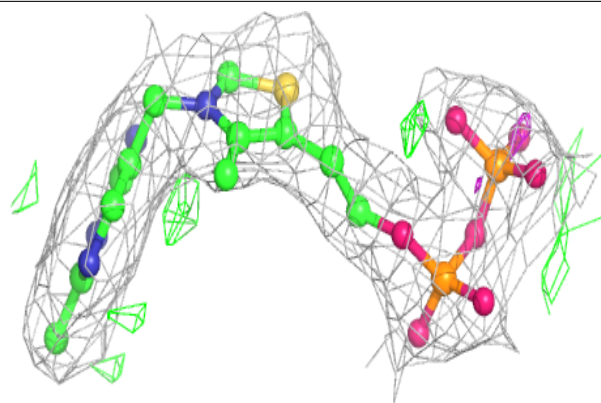
**Electron density around TPP J 601:**

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

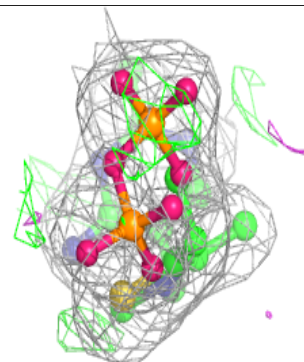
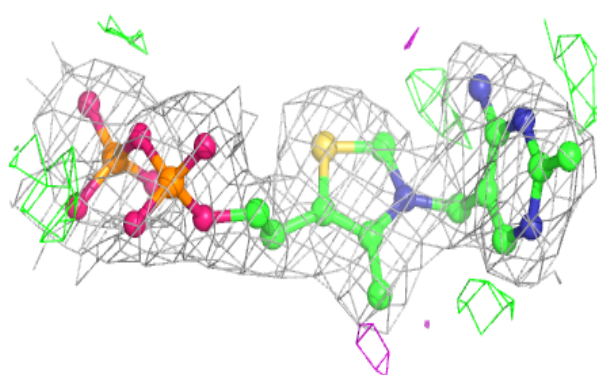
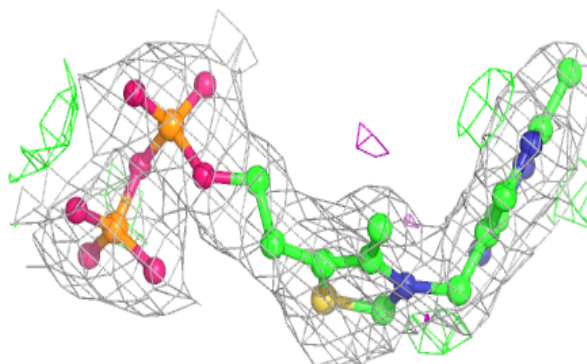


**Electron density around TPP S 601:**

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

**Electron density around TPP 1 601:**

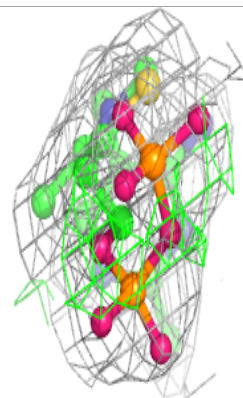
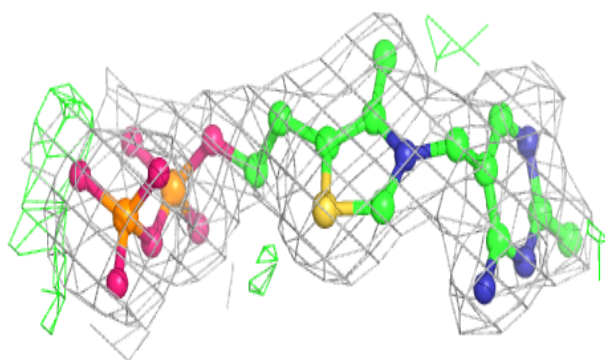
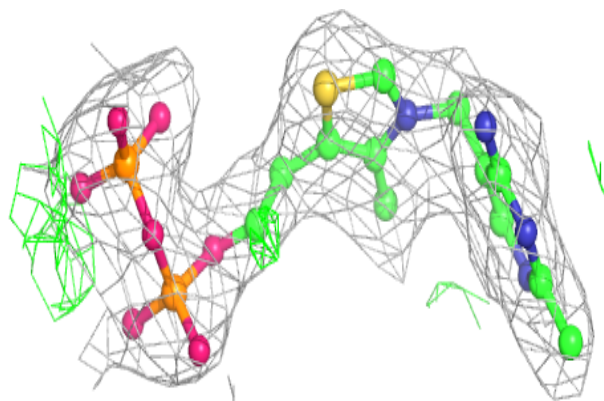
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



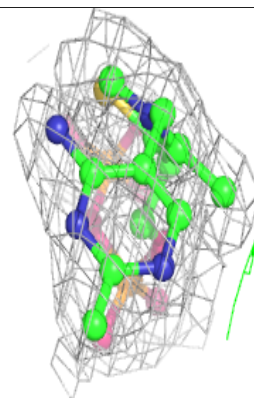
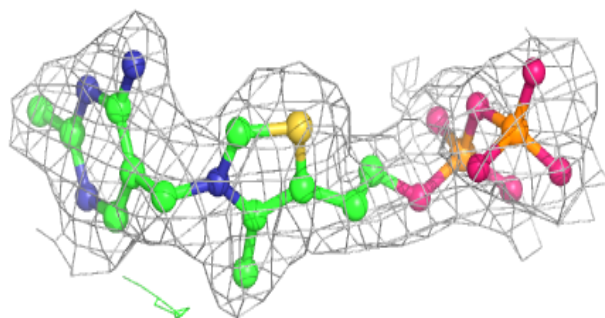
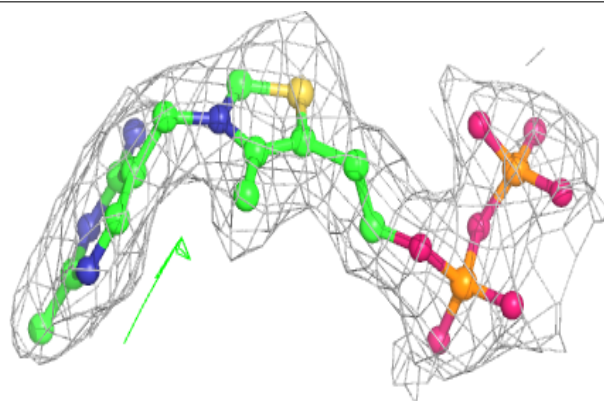


**Electron density around TPP B 601:**

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

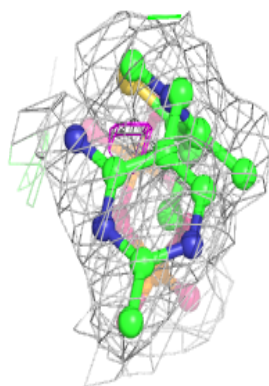
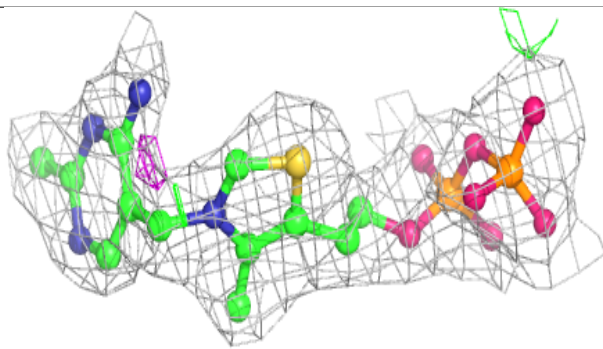
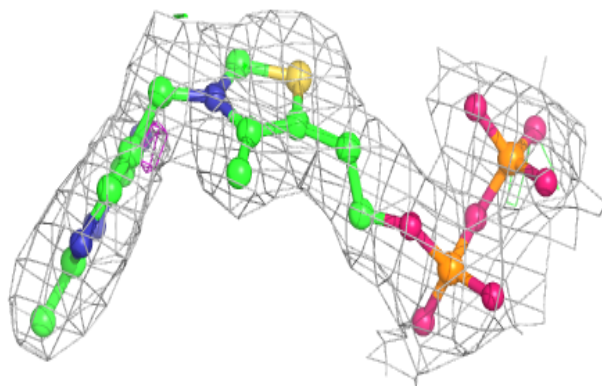
**Electron density around TPP A 601:**

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

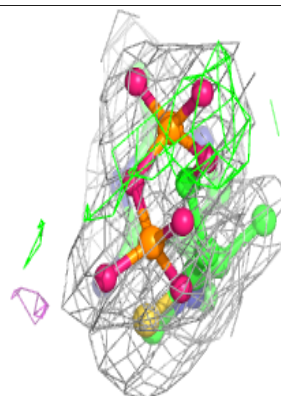
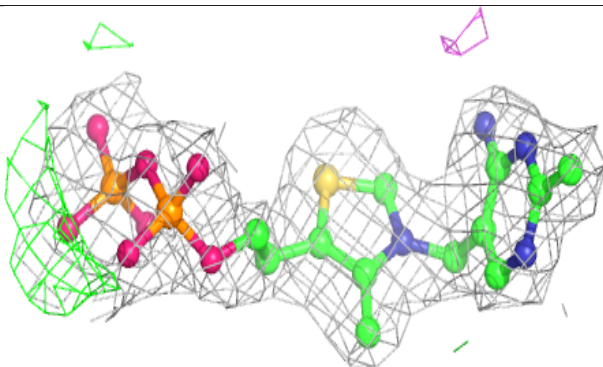
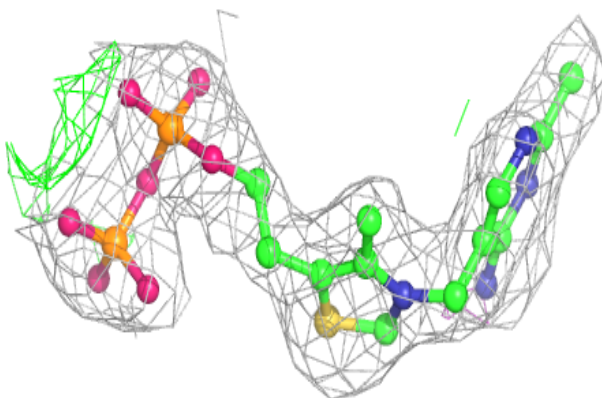


**Electron density around TPP Z 601:**

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

**Electron density around TPP R 601:**

$2mF_o-DF_c$  (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.