



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2021 – 12:22 PM JST

PDB ID : 7C8I  
Title : Ambient temperature structure of Bifidobacterium longum phosphoketolase with thiamine diphosphate and phosphoenol pyruvate  
Authors : Nakata, K.; Kashiwagi, T.; Nango, E.; Miyano, H.; Mizukoshi, T.; Iwata, S.  
Deposited on : 2020-06-01  
Resolution : 2.50 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:

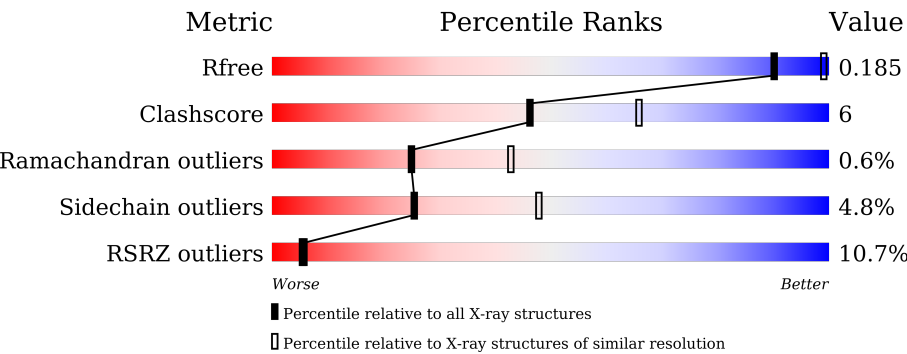
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	831	<div><div>5%</div><div>87%</div><div>9%</div><div>..</div></div>
1	B	831	<div><div>6%</div><div>87%</div><div>10%</div><div>.</div></div>
1	C	831	<div><div>15%</div><div>74%</div><div>21%</div><div>..</div></div>
1	D	831	<div><div>13%</div><div>71%</div><div>24%</div><div>..</div></div>
1	E	831	<div><div>14%</div><div>79%</div><div>17%</div><div>..</div></div>
1	F	831	<div><div>13%</div><div>80%</div><div>16%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	831	
1	H	831	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEP	A	901	-	-	X	-
2	PEP	B	901	-	-	X	-
2	PEP	H	901	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52775 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 Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	1	0
			6436	4085	1098	1234	19			
1	B	811	Total	C	N	O	S	0	1	0
			6458	4099	1103	1237	19			
1	C	806	Total	C	N	O	S	0	0	0
			6411	4071	1093	1228	19			
1	D	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	E	809	Total	C	N	O	S	0	0	0
			6435	4085	1097	1234	19			
1	F	809	Total	C	N	O	S	0	0	0
			6435	4085	1097	1234	19			
1	G	807	Total	C	N	O	S	0	1	0
			6428	4081	1097	1231	19			
1	H	808	Total	C	N	O	S	0	1	0
			6436	4085	1098	1234	19			

There are 48 discrepancies between the modelled and reference sequences:

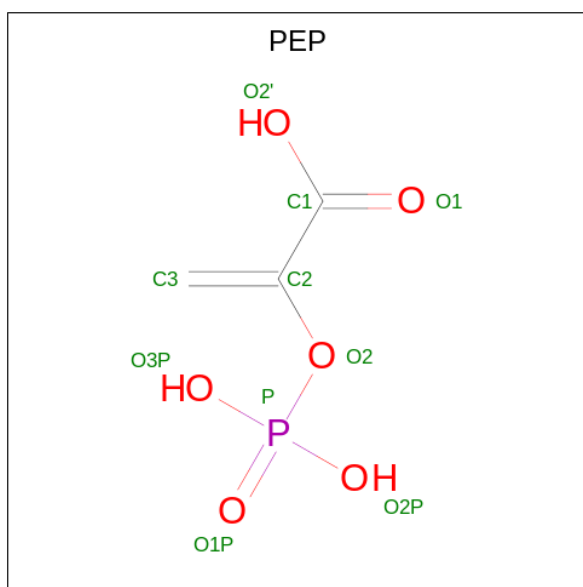
Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	expression tag	UNP Q6R2Q7
A	827	HIS	-	expression tag	UNP Q6R2Q7
A	828	HIS	-	expression tag	UNP Q6R2Q7
A	829	HIS	-	expression tag	UNP Q6R2Q7
A	830	HIS	-	expression tag	UNP Q6R2Q7
A	831	HIS	-	expression tag	UNP Q6R2Q7
B	826	HIS	-	expression tag	UNP Q6R2Q7
B	827	HIS	-	expression tag	UNP Q6R2Q7
B	828	HIS	-	expression tag	UNP Q6R2Q7
B	829	HIS	-	expression tag	UNP Q6R2Q7
B	830	HIS	-	expression tag	UNP Q6R2Q7
B	831	HIS	-	expression tag	UNP Q6R2Q7
C	826	HIS	-	expression tag	UNP Q6R2Q7

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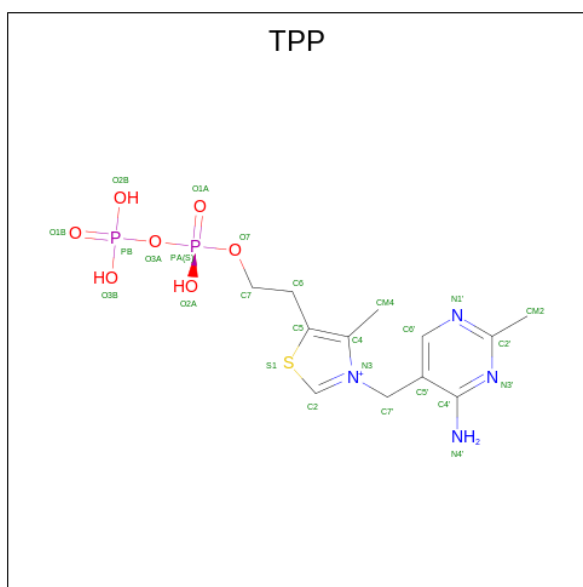
Chain	Residue	Modelled	Actual	Comment	Reference
C	827	HIS	-	expression tag	UNP Q6R2Q7
C	828	HIS	-	expression tag	UNP Q6R2Q7
C	829	HIS	-	expression tag	UNP Q6R2Q7
C	830	HIS	-	expression tag	UNP Q6R2Q7
C	831	HIS	-	expression tag	UNP Q6R2Q7
D	826	HIS	-	expression tag	UNP Q6R2Q7
D	827	HIS	-	expression tag	UNP Q6R2Q7
D	828	HIS	-	expression tag	UNP Q6R2Q7
D	829	HIS	-	expression tag	UNP Q6R2Q7
D	830	HIS	-	expression tag	UNP Q6R2Q7
D	831	HIS	-	expression tag	UNP Q6R2Q7
E	826	HIS	-	expression tag	UNP Q6R2Q7
E	827	HIS	-	expression tag	UNP Q6R2Q7
E	828	HIS	-	expression tag	UNP Q6R2Q7
E	829	HIS	-	expression tag	UNP Q6R2Q7
E	830	HIS	-	expression tag	UNP Q6R2Q7
E	831	HIS	-	expression tag	UNP Q6R2Q7
F	826	HIS	-	expression tag	UNP Q6R2Q7
F	827	HIS	-	expression tag	UNP Q6R2Q7
F	828	HIS	-	expression tag	UNP Q6R2Q7
F	829	HIS	-	expression tag	UNP Q6R2Q7
F	830	HIS	-	expression tag	UNP Q6R2Q7
F	831	HIS	-	expression tag	UNP Q6R2Q7
G	826	HIS	-	expression tag	UNP Q6R2Q7
G	827	HIS	-	expression tag	UNP Q6R2Q7
G	828	HIS	-	expression tag	UNP Q6R2Q7
G	829	HIS	-	expression tag	UNP Q6R2Q7
G	830	HIS	-	expression tag	UNP Q6R2Q7
G	831	HIS	-	expression tag	UNP Q6R2Q7
H	826	HIS	-	expression tag	UNP Q6R2Q7
H	827	HIS	-	expression tag	UNP Q6R2Q7
H	828	HIS	-	expression tag	UNP Q6R2Q7
H	829	HIS	-	expression tag	UNP Q6R2Q7
H	830	HIS	-	expression tag	UNP Q6R2Q7
H	831	HIS	-	expression tag	UNP Q6R2Q7

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C<sub>3</sub>H<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 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 depositor).



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	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0
4	G	1	Total 1	Ca 1	0	0
4	H	1	Total 1	Ca 1	0	0

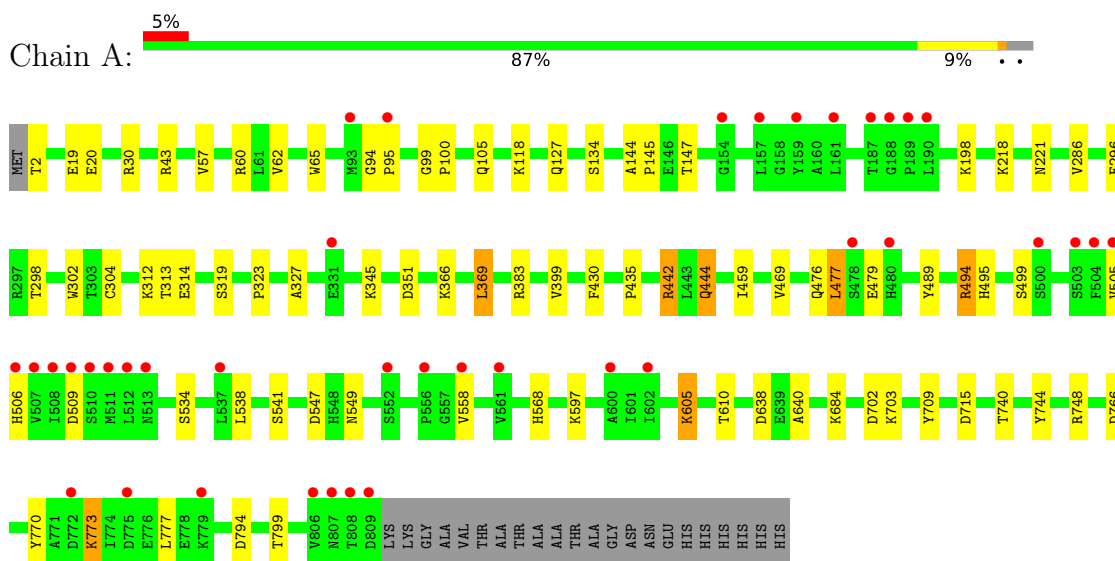
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	208	Total 208	O 208	0	0
5	B	225	Total 225	O 225	0	0
5	C	55	Total 55	O 55	0	0
5	D	53	Total 53	O 53	0	0
5	E	107	Total 107	O 107	0	0
5	F	92	Total 92	O 92	0	0
5	G	153	Total 153	O 153	0	0
5	H	129	Total 129	O 129	0	0

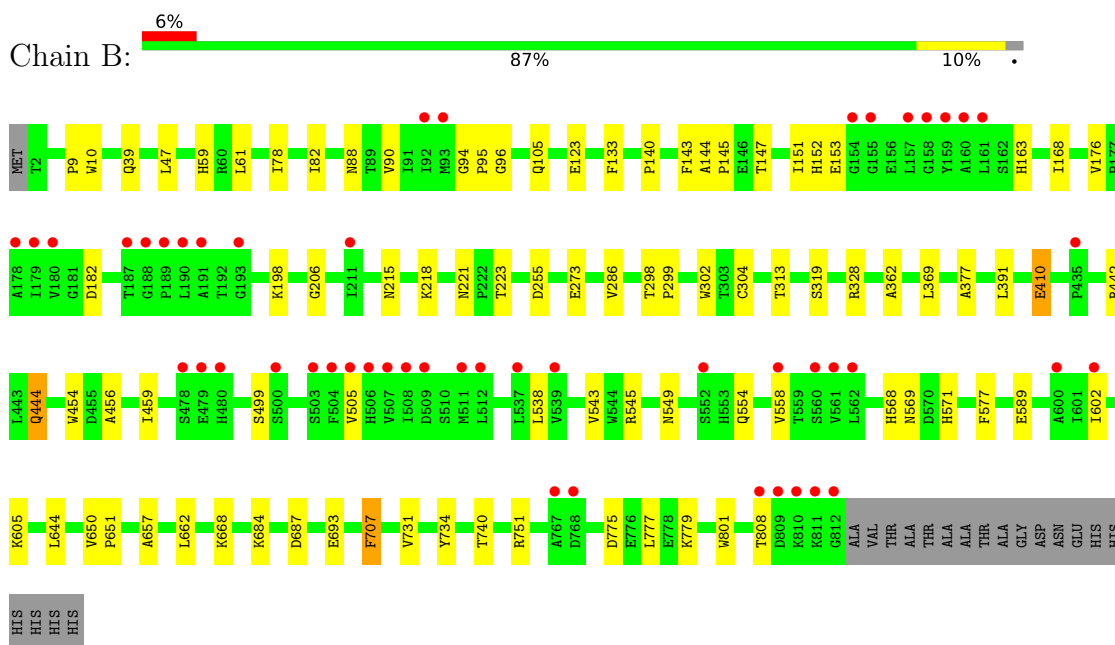
### 3 Residue-property plots [i](#)

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.

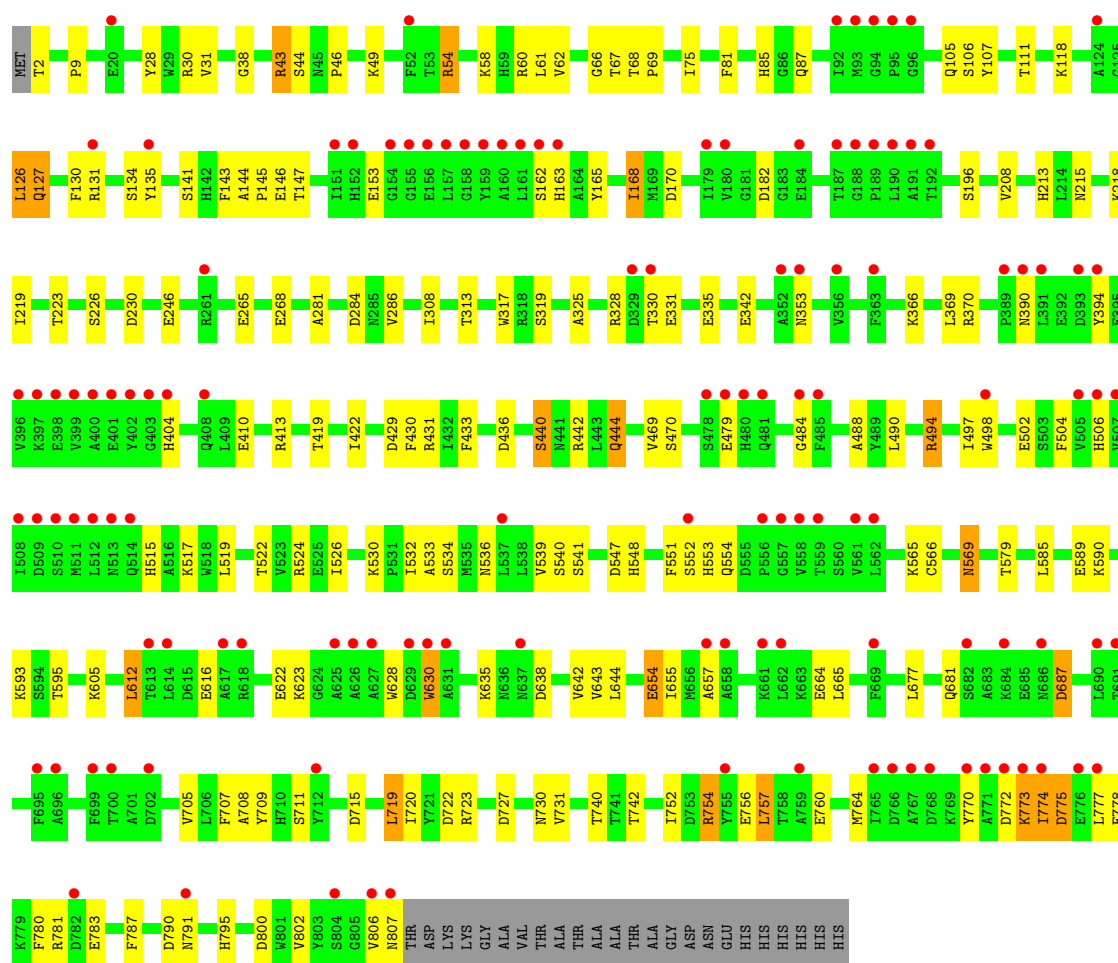
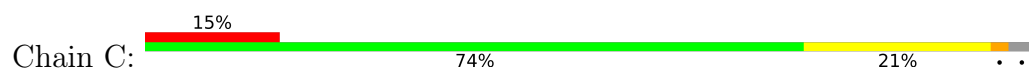
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



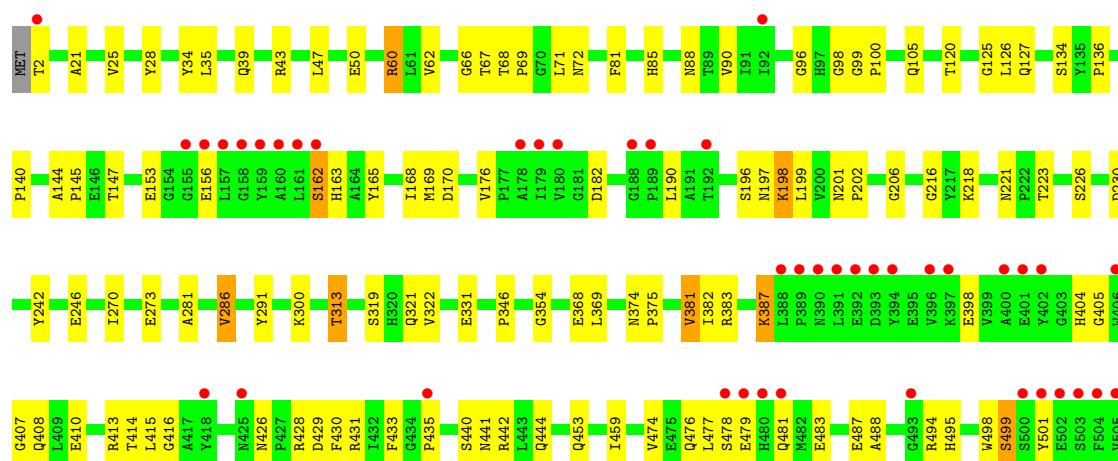
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

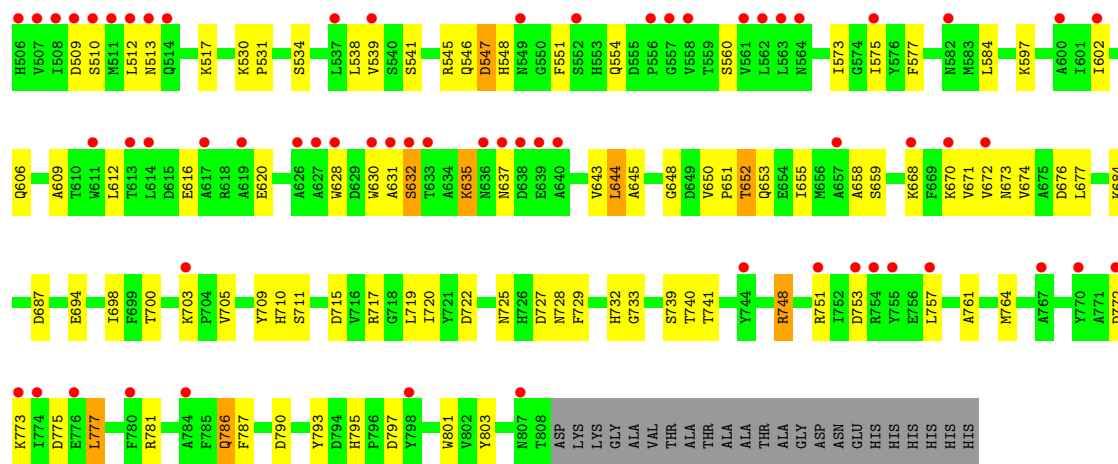


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

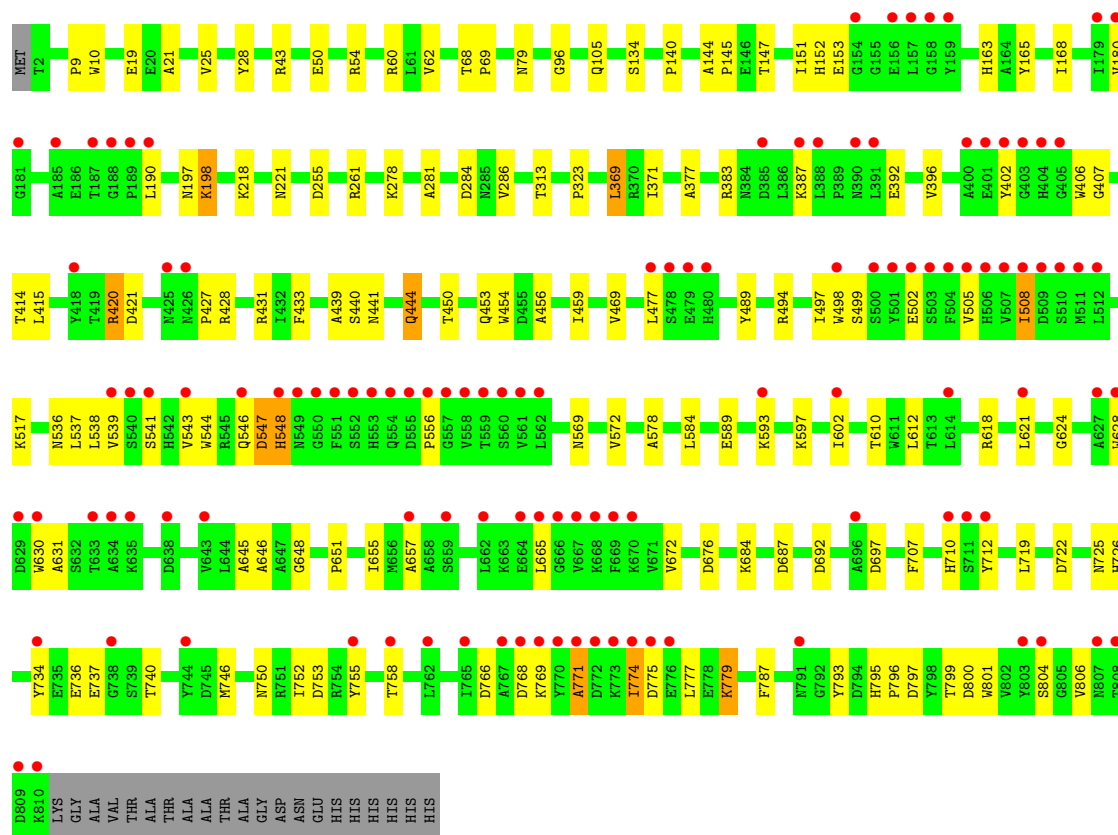
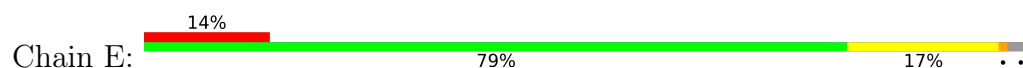


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

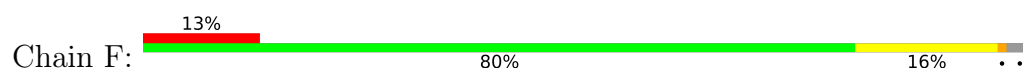


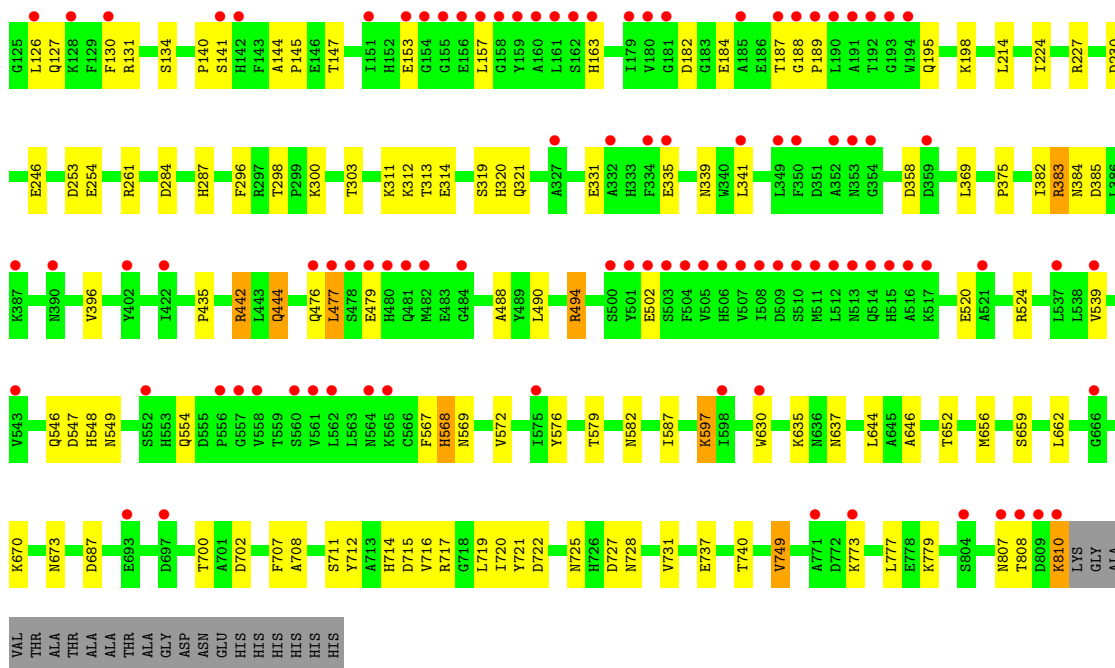


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

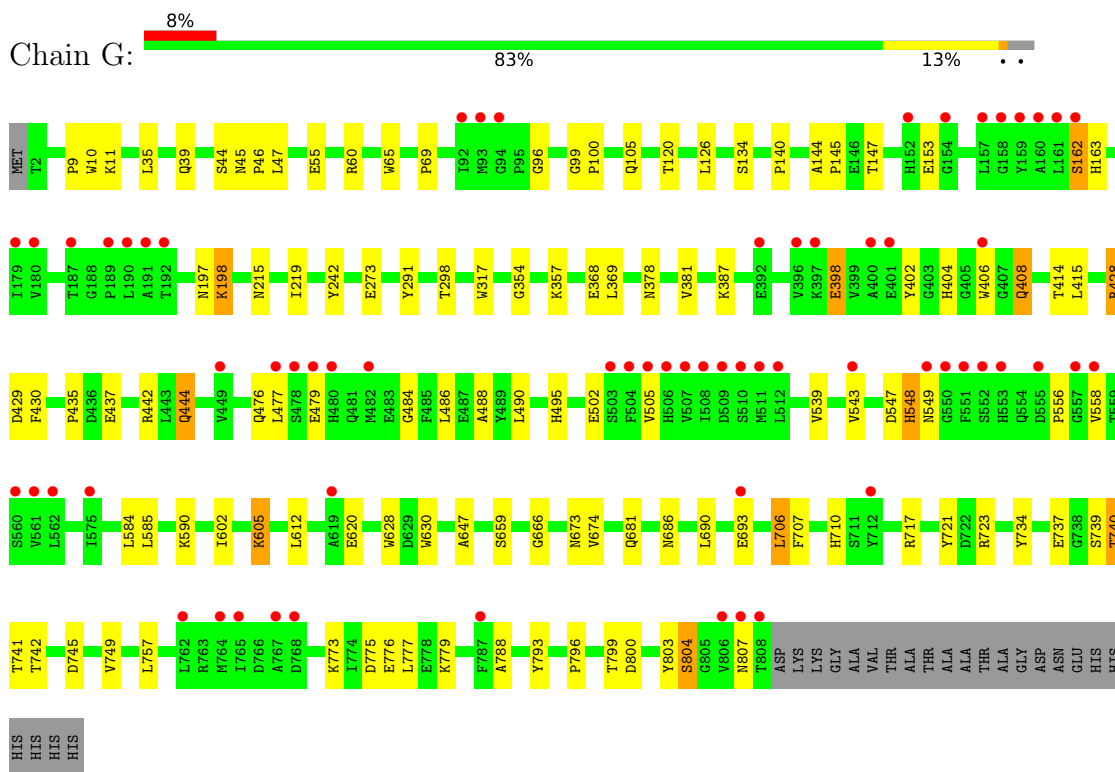


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

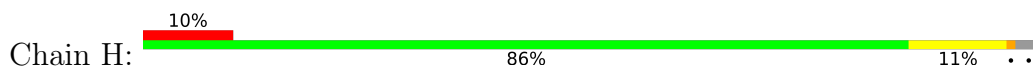


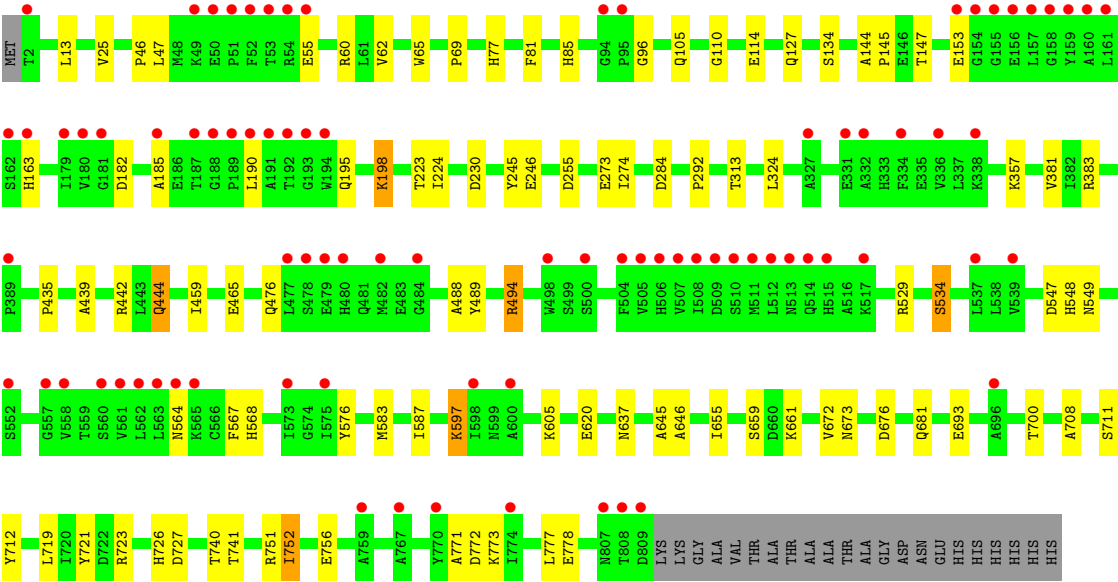


- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.30Å 184.94Å 163.13Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	48.10 – 2.50 48.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.10-2.50) 99.9 (48.05-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.166 , 0.226 0.184 , 0.185	Depositor DCC
$R_{free}$ test set	14632 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: TPP, CA, PEP

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	0.74	0/6614	0.89	1/8996 (0.0%)
1	B	0.72	1/6636 (0.0%)	0.88	0/9023
1	C	0.74	0/6588	0.87	1/8960 (0.0%)
1	D	0.74	0/6595	0.86	0/8970
1	E	0.74	0/6612	0.89	0/8992
1	F	0.72	0/6612	0.88	0/8992
1	G	0.73	0/6606	0.88	0/8985
1	H	0.73	0/6614	0.89	0/8996
All	All	0.73	1/52877 (0.0%)	0.88	2/71914 (0.0%)

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	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	589	GLU	CD-OE1	5.81	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	LYS	CB-CA-C	5.42	121.23	110.40
1	A	383	ARG	NE-CZ-NH1	5.29	122.95	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	597	LYS	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	A	6436	0	6118	47	0
1	B	6458	0	6147	56	0
1	C	6411	0	6101	108	0
1	D	6418	0	6108	128	0
1	E	6435	0	6125	97	0
1	F	6435	0	6125	90	0
1	G	6428	0	6114	76	0
1	H	6436	0	6118	59	0
2	A	10	0	2	4	0
2	B	10	0	2	5	0
2	C	10	0	2	2	0
2	D	10	0	2	1	0
2	E	10	0	2	2	0
2	F	10	0	2	2	0
2	G	10	0	2	3	0
2	H	10	0	2	4	0
3	A	26	0	16	1	0
3	B	26	0	16	4	0
3	C	26	0	16	4	0
3	D	26	0	16	4	0
3	E	26	0	16	4	0
3	F	26	0	16	3	0
3	G	26	0	16	2	0
3	H	26	0	16	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	208	0	0	4	0
5	B	225	0	0	3	0
5	C	55	0	0	1	0
5	D	53	0	0	2	0
5	E	107	0	0	1	0
5	F	92	0	0	1	0
5	G	153	0	0	1	0
5	H	129	0	0	2	0
All	All	52775	0	49100	632	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 6.

The worst 5 of 632 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:902:TPP:H2	3:H:902:TPP:HN42	1.25	0.97
1:G:442:ARG:HA	1:G:444:GLN:HE22	1.28	0.96
1:D:67:THR:OG1	3:D:902:TPP:O2B	1.84	0.95
1:F:442:ARG:HA	1:F:444:GLN:HE22	1.31	0.95
1:B:569:ASN:HD21	1:B:687:ASP:H	1.12	0.92

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	807/831 (97%)	758 (94%)	45 (6%)	4 (0%)	29	48
1	B	810/831 (98%)	766 (95%)	42 (5%)	2 (0%)	47	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	804/831 (97%)	698 (87%)	98 (12%)	8 (1%)	15	28
1	D	805/831 (97%)	715 (89%)	81 (10%)	9 (1%)	14	26
1	E	807/831 (97%)	725 (90%)	78 (10%)	4 (0%)	29	48
1	F	807/831 (97%)	745 (92%)	55 (7%)	7 (1%)	17	31
1	G	806/831 (97%)	737 (91%)	64 (8%)	5 (1%)	25	43
1	H	807/831 (97%)	748 (93%)	57 (7%)	2 (0%)	47	68
All	All	6453/6648 (97%)	5892 (91%)	520 (8%)	41 (1%)	25	43

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	66	GLY
1	D	652	THR
1	F	630	TRP
1	F	721	TYR
1	G	721	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	678/693 (98%)	656 (97%)	22 (3%)	39	65
1	B	680/693 (98%)	664 (98%)	16 (2%)	49	74
1	C	675/693 (97%)	623 (92%)	52 (8%)	13	25
1	D	676/693 (98%)	628 (93%)	48 (7%)	14	28
1	E	678/693 (98%)	647 (95%)	31 (5%)	27	50
1	F	678/693 (98%)	647 (95%)	31 (5%)	27	50
1	G	677/693 (98%)	645 (95%)	32 (5%)	26	49
1	H	678/693 (98%)	652 (96%)	26 (4%)	33	58
All	All	5420/5544 (98%)	5162 (95%)	258 (5%)	25	48

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	779	LYS
1	H	313	THR
1	D	147	THR
1	D	105	GLN
1	H	444	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	444	GLN
1	F	444	GLN
1	H	408	GLN
1	E	480	HIS
1	E	786	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
2	PEP	C	901	-	6,9,9	1.87	1 (16%)	8,13,13	1.38	1 (12%)
2	PEP	F	901	-	6,9,9	1.95	1 (16%)	8,13,13	2.36	4 (50%)
2	PEP	E	901	-	6,9,9	1.68	1 (16%)	8,13,13	3.37	4 (50%)
2	PEP	A	901	-	6,9,9	1.61	1 (16%)	8,13,13	1.59	1 (12%)
3	TPP	B	902	4	22,27,27	0.78	0	29,40,40	1.20	3 (10%)
2	PEP	B	901	-	6,9,9	1.84	1 (16%)	8,13,13	1.85	1 (12%)
3	TPP	C	902	4	22,27,27	0.88	1 (4%)	29,40,40	1.23	4 (13%)
2	PEP	D	901	-	6,9,9	1.87	1 (16%)	8,13,13	2.22	3 (37%)
3	TPP	H	902	4	22,27,27	0.72	0	29,40,40	0.95	0
3	TPP	D	902	4	22,27,27	0.78	0	29,40,40	1.15	3 (10%)
3	TPP	F	902	4	22,27,27	0.63	0	29,40,40	1.02	3 (10%)
3	TPP	A	902	4	22,27,27	0.79	0	29,40,40	0.96	1 (3%)
2	PEP	H	901	-	6,9,9	1.96	1 (16%)	8,13,13	2.13	5 (62%)
3	TPP	G	902	4	22,27,27	0.62	0	29,40,40	1.10	2 (6%)
2	PEP	G	901	-	6,9,9	2.02	1 (16%)	8,13,13	2.05	4 (50%)
3	TPP	E	902	4	22,27,27	0.57	0	29,40,40	0.99	2 (6%)

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
2	PEP	C	901	-	-	0/5/9/9	-
2	PEP	F	901	-	-	0/5/9/9	-
2	PEP	E	901	-	-	0/5/9/9	-
2	PEP	A	901	-	-	0/5/9/9	-
3	TPP	B	902	4	-	3/16/17/17	0/2/2/2
2	PEP	B	901	-	-	0/5/9/9	-
3	TPP	C	902	4	-	3/16/17/17	0/2/2/2
2	PEP	D	901	-	-	0/5/9/9	-
3	TPP	H	902	4	-	6/16/17/17	0/2/2/2
3	TPP	D	902	4	-	3/16/17/17	0/2/2/2
3	TPP	F	902	4	-	5/16/17/17	0/2/2/2
3	TPP	A	902	4	-	3/16/17/17	0/2/2/2
2	PEP	H	901	-	-	0/5/9/9	-
3	TPP	G	902	4	-	6/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEP	G	901	-	-	0/5/9/9	-
3	TPP	E	902	4	-	7/16/17/17	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	901	PEP	C3-C2	4.51	1.41	1.33
2	C	901	PEP	C3-C2	4.50	1.41	1.33
2	G	901	PEP	C3-C2	4.48	1.41	1.33
2	F	901	PEP	C3-C2	4.34	1.41	1.33
2	B	901	PEP	C3-C2	4.06	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	PEP	O2-C2-C3	-7.36	110.62	124.79
2	D	901	PEP	O2-C2-C3	-4.59	115.94	124.79
2	E	901	PEP	C1-C2-C3	4.42	129.34	121.07
2	B	901	PEP	O2-C2-C3	-4.12	116.85	124.79
2	F	901	PEP	O2-C2-C3	-4.05	116.99	124.79

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	TPP	C5-C6-C7-O7
3	D	902	TPP	PA-O3A-PB-O3B
3	E	902	TPP	C4'-C5'-C7'-N3
3	E	902	TPP	C4-C5-C6-C7
3	E	902	TPP	PA-O3A-PB-O2B

There are no ring outliers.

16 monomers are involved in 51 short contacts:

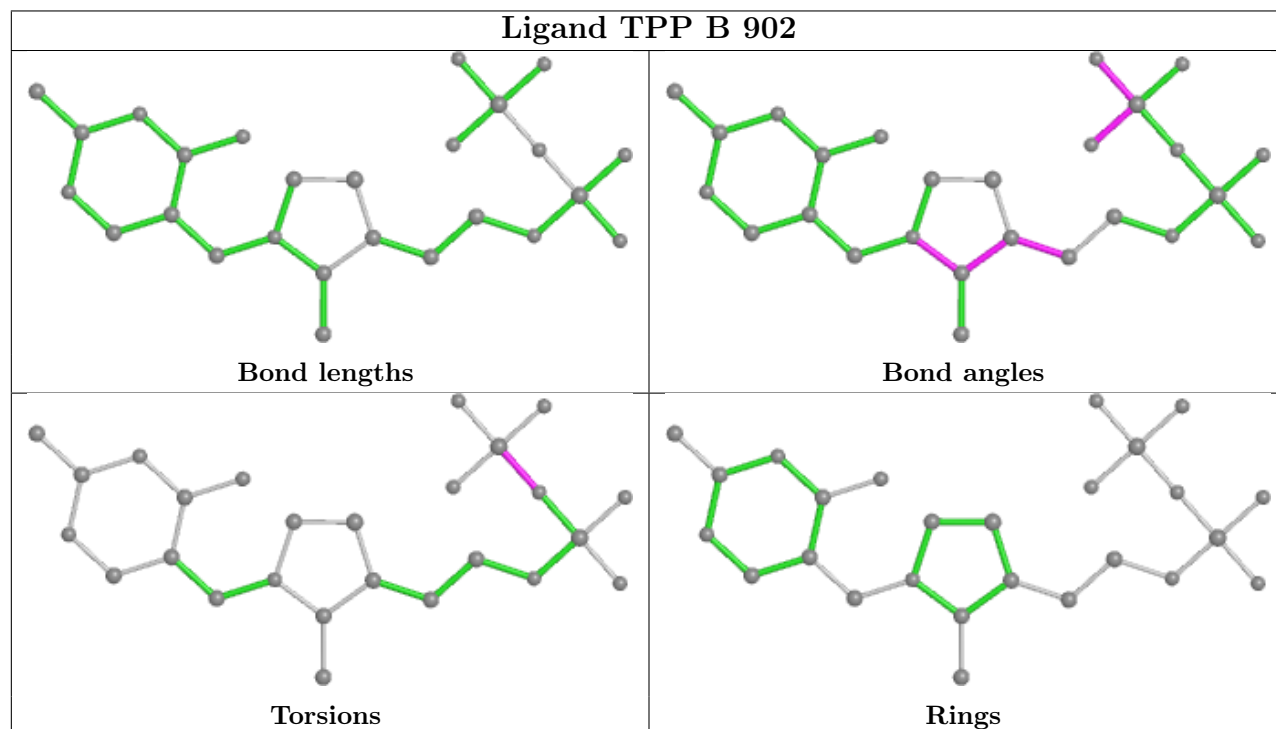
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	PEP	2	0
2	F	901	PEP	2	0
2	E	901	PEP	2	0
2	A	901	PEP	4	0
3	B	902	TPP	4	0
2	B	901	PEP	5	0

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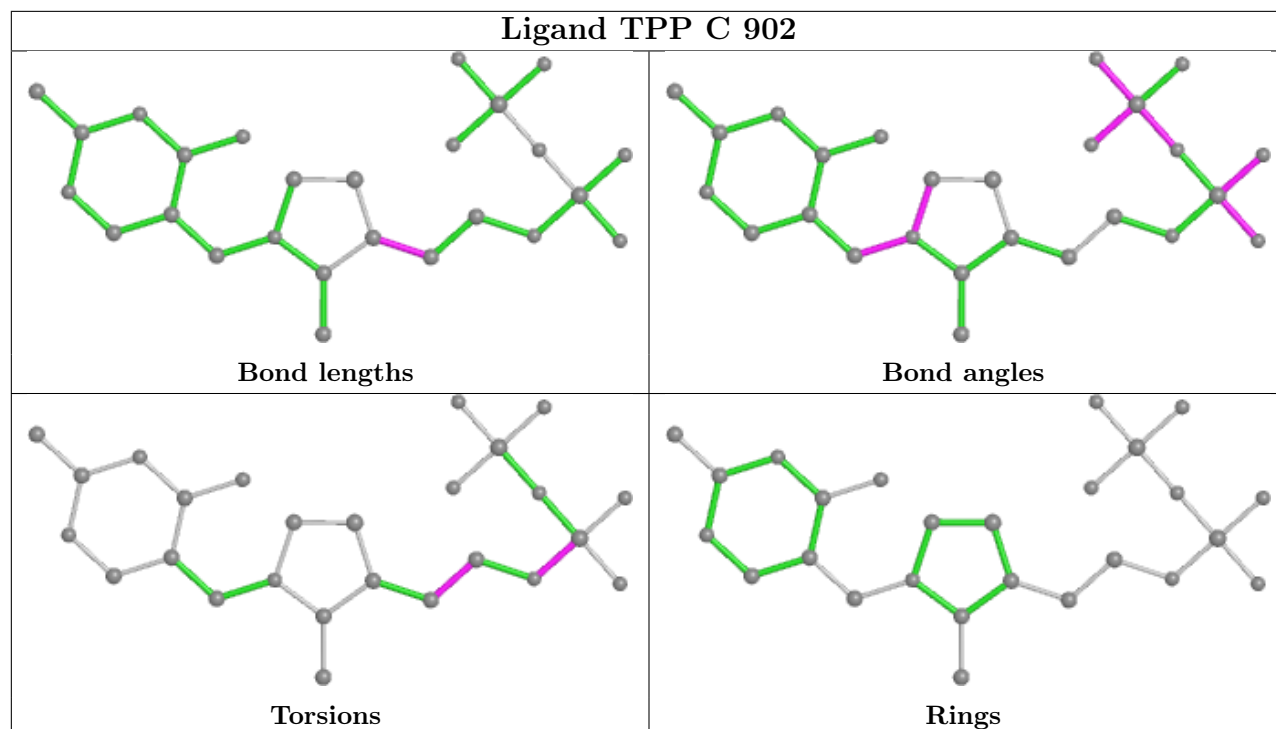
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	902	TPP	4	0
2	D	901	PEP	1	0
3	H	902	TPP	6	0
3	D	902	TPP	4	0
3	F	902	TPP	3	0
3	A	902	TPP	1	0
2	H	901	PEP	4	0
3	G	902	TPP	2	0
2	G	901	PEP	3	0
3	E	902	TPP	4	0

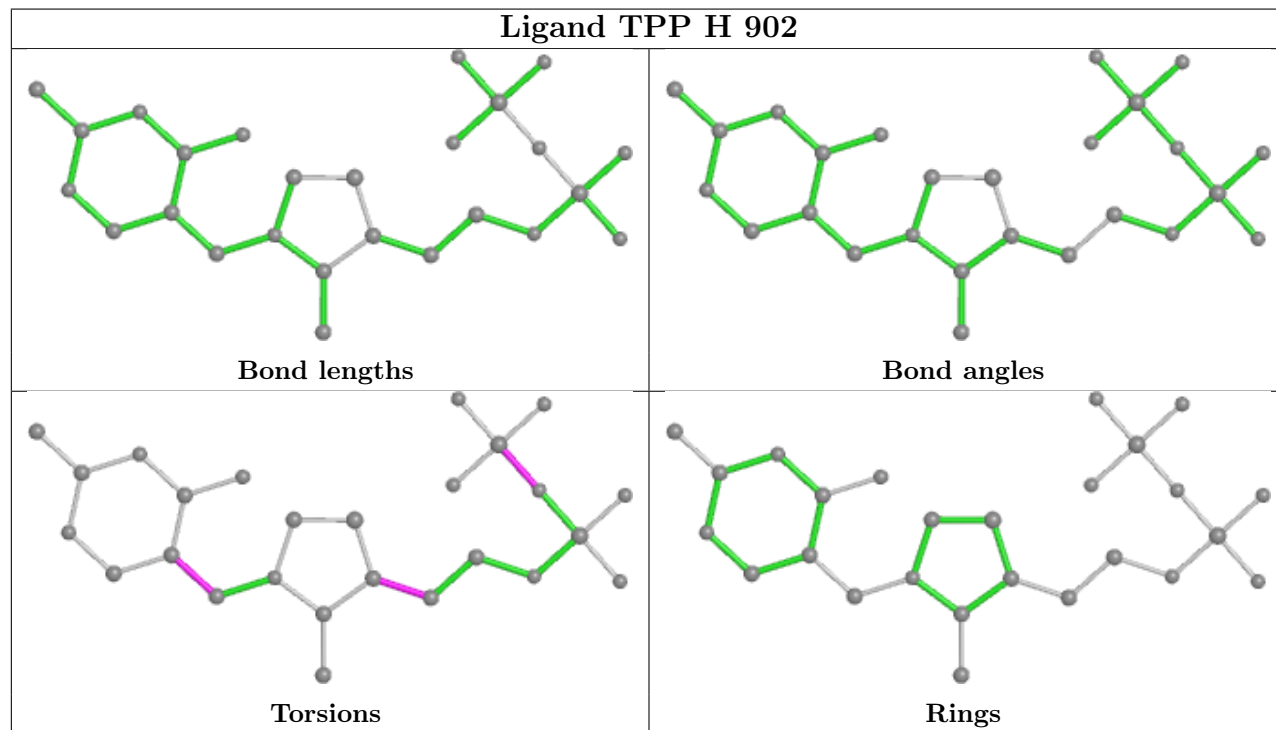
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



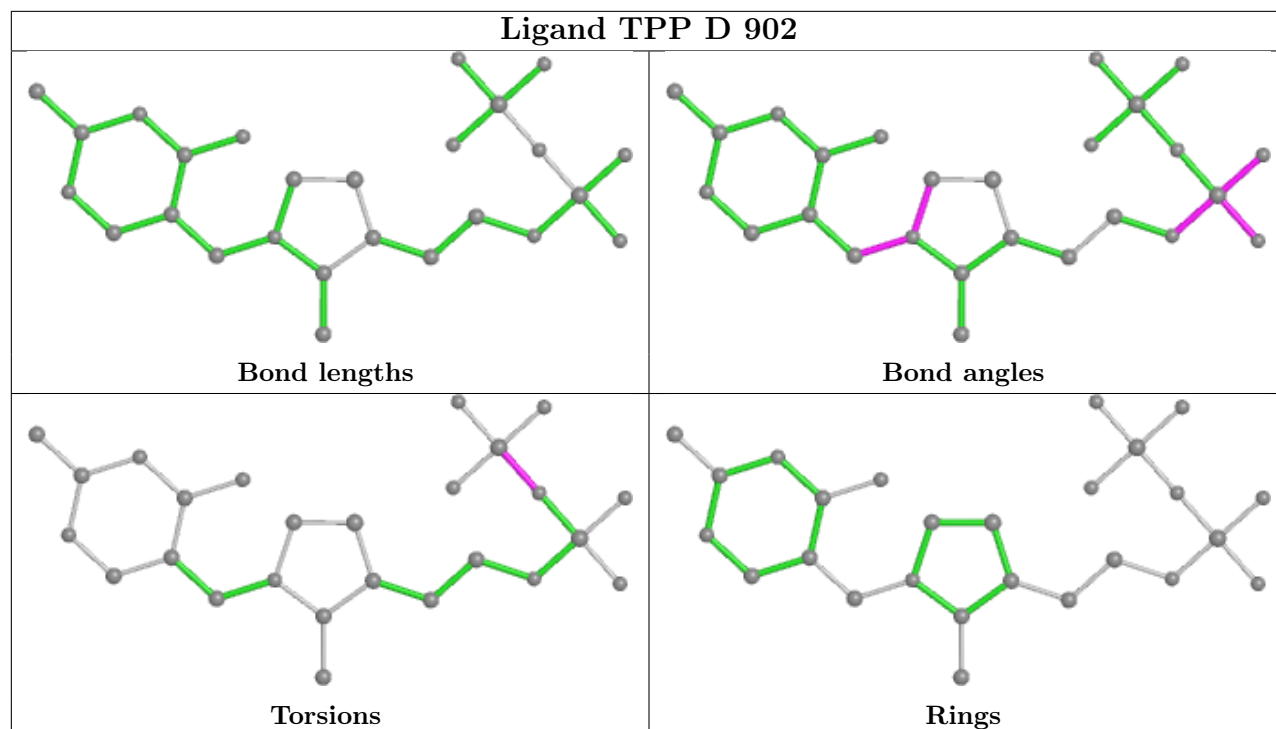
## Ligand TPP C 902



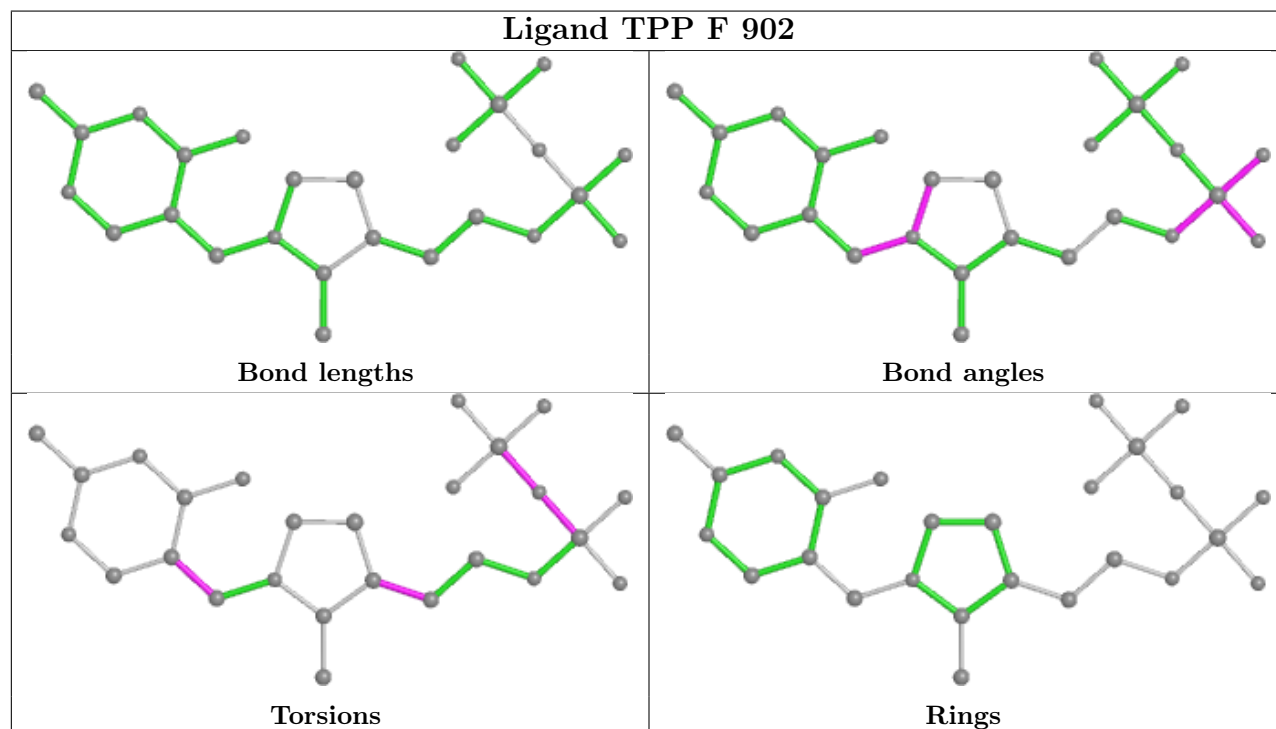
## Ligand TPP H 902



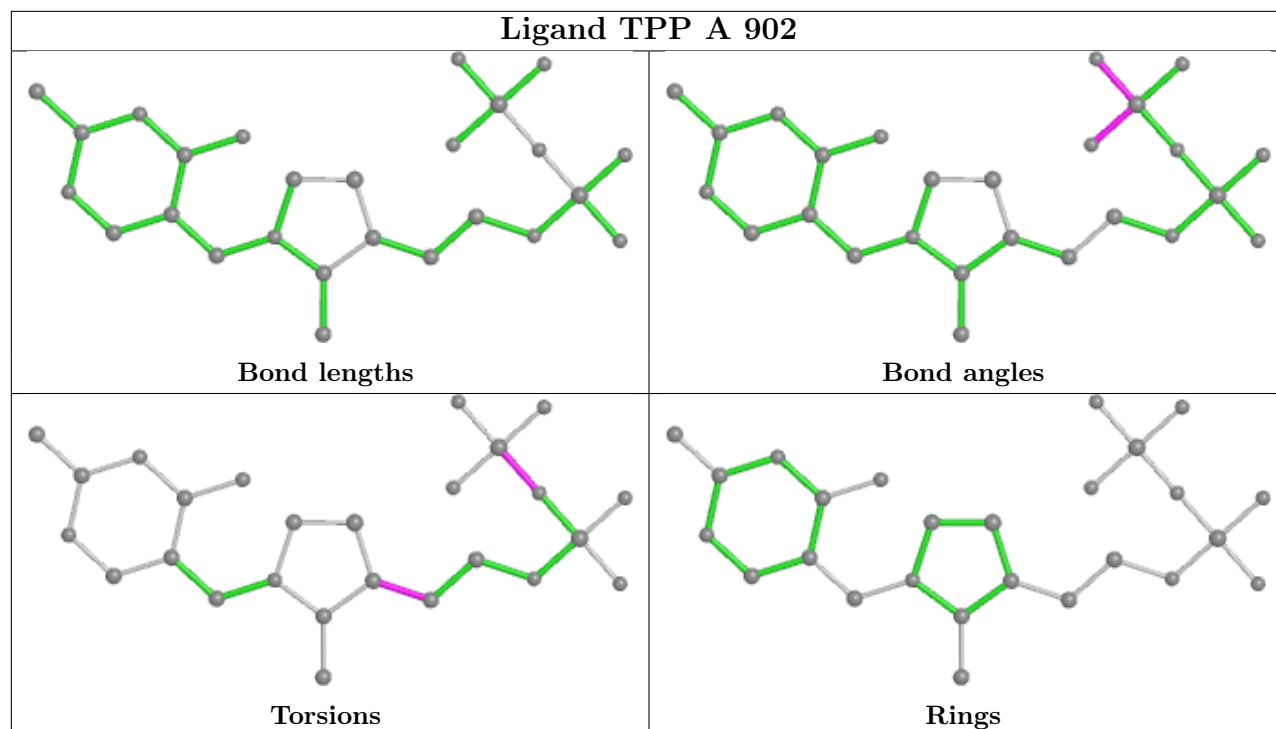
## Ligand TPP D 902



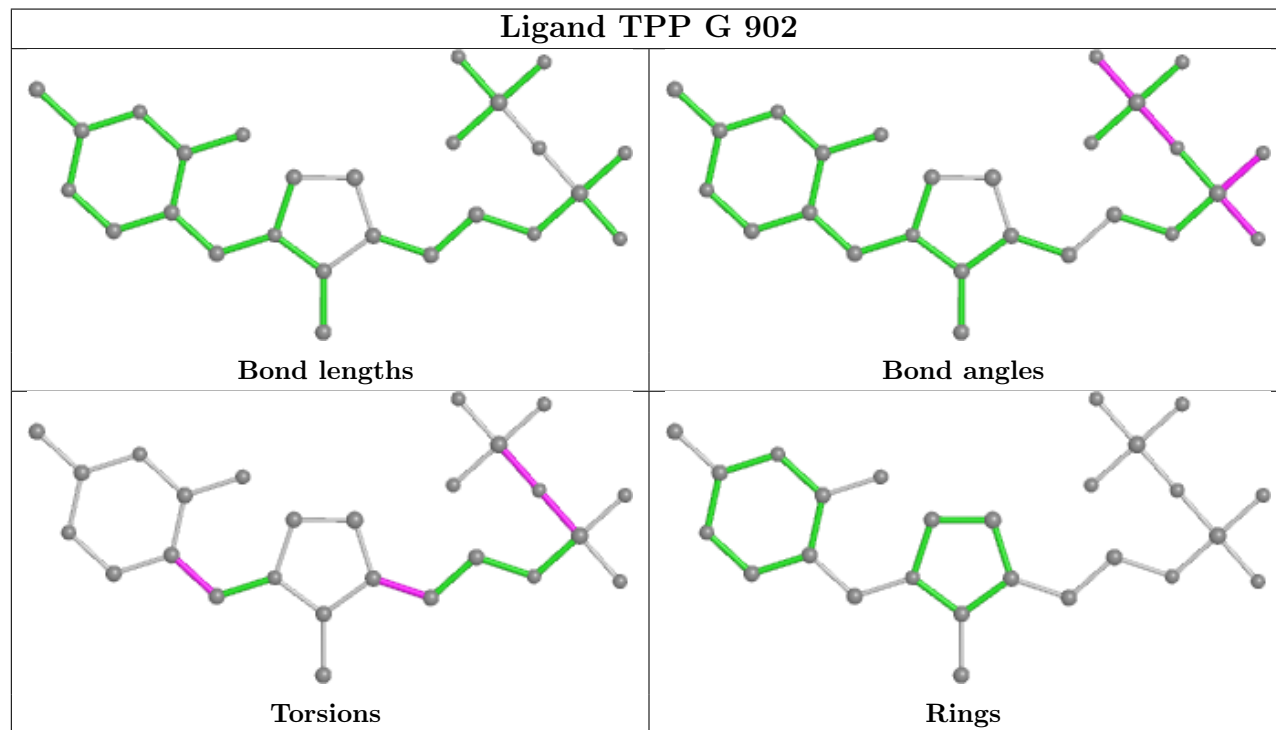
## Ligand TPP F 902

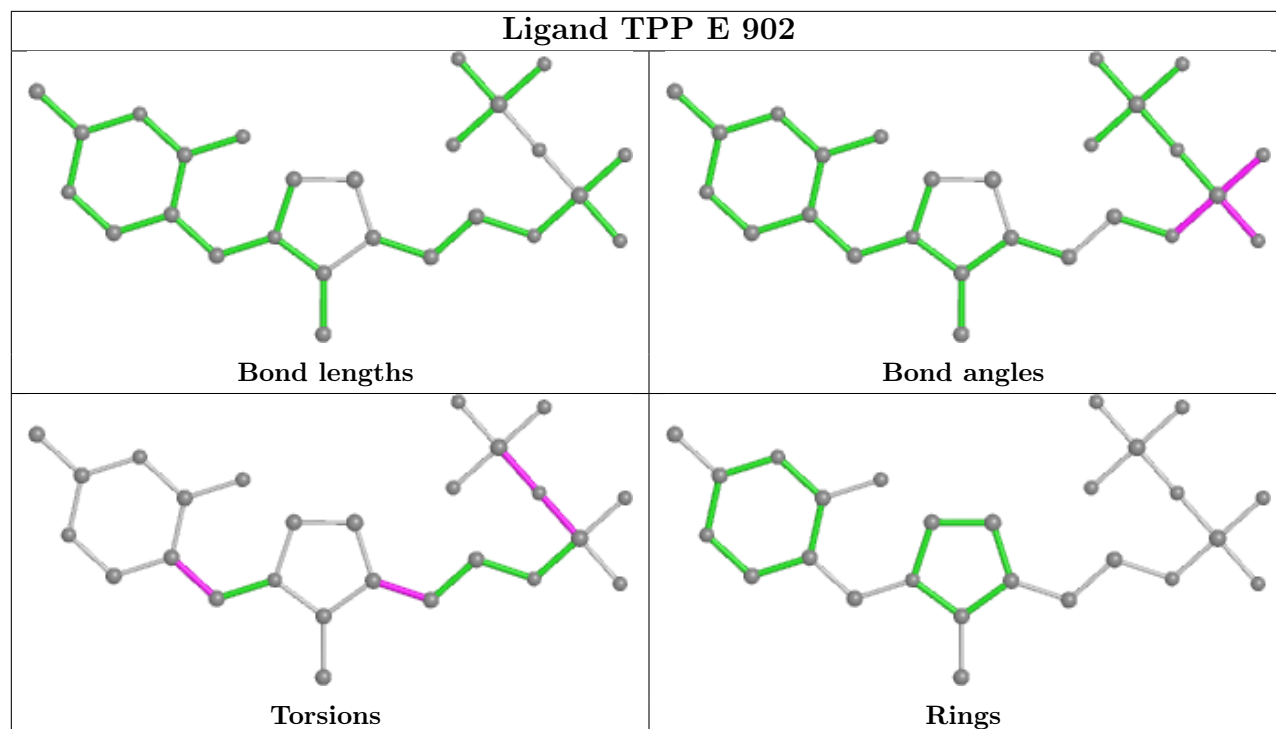


## Ligand TPP A 902



## Ligand TPP G 902





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	808/831 (97%)	0.08	39 (4%) 30 32	29, 44, 68, 135	0
1	B	811/831 (97%)	0.10	49 (6%) 21 22	29, 43, 70, 157	0
1	C	806/831 (96%)	0.66	123 (15%) 2 1	43, 74, 108, 125	0
1	D	807/831 (97%)	0.54	105 (13%) 3 3	43, 71, 109, 132	0
1	E	809/831 (97%)	0.59	116 (14%) 2 2	35, 58, 101, 158	0
1	F	809/831 (97%)	0.60	112 (13%) 2 2	38, 62, 93, 144	0
1	G	807/831 (97%)	0.22	65 (8%) 12 12	29, 51, 86, 119	0
1	H	808/831 (97%)	0.37	84 (10%) 6 6	33, 55, 83, 131	0
All	All	6465/6648 (97%)	0.39	693 (10%) 6 5	29, 57, 99, 158	0

The worst 5 of 693 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	507	VAL	7.6
1	E	808	THR	7.5
1	F	157	LEU	7.1
1	C	399	VAL	7.1
1	F	512	LEU	6.4

### 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 ⓘ

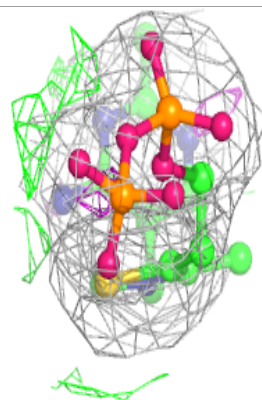
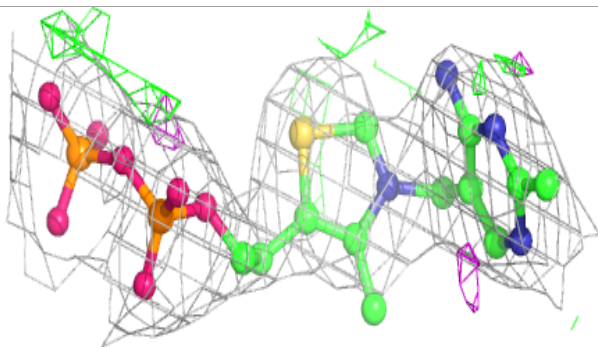
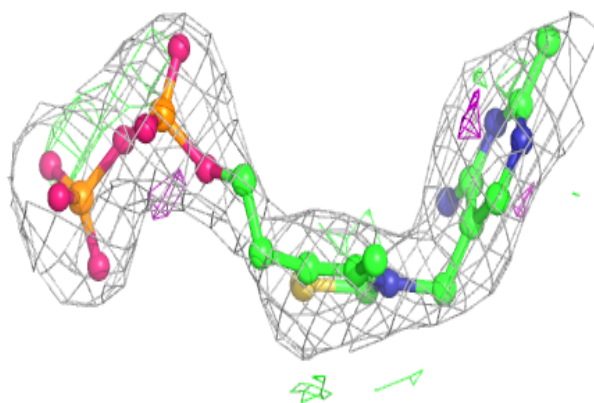
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	PEP	D	901	10/10	0.91	0.60	63,77,83,85	10
2	PEP	E	901	10/10	0.91	0.73	59,66,80,80	10
4	CA	D	903	1/1	0.93	0.06	71,71,71,71	0
2	PEP	A	901	10/10	0.94	0.54	33,50,63,63	10
2	PEP	B	901	10/10	0.94	0.58	26,35,48,55	10
2	PEP	G	901	10/10	0.94	0.54	43,60,73,82	10
2	PEP	C	901	10/10	0.94	0.48	55,65,80,90	10
4	CA	H	903	1/1	0.95	0.10	74,74,74,74	0
3	TPP	C	902	26/26	0.96	0.23	43,55,72,80	0
4	CA	C	903	1/1	0.96	0.09	77,77,77,77	0
2	PEP	F	901	10/10	0.96	0.59	44,49,68,69	10
4	CA	F	903	1/1	0.96	0.04	78,78,78,78	0
2	PEP	H	901	10/10	0.96	0.46	43,46,63,71	10
3	TPP	B	902	26/26	0.97	0.22	29,36,41,43	0
3	TPP	D	902	26/26	0.97	0.16	46,53,65,68	0
4	CA	E	903	1/1	0.97	0.09	60,60,60,60	0
3	TPP	F	902	26/26	0.97	0.25	43,54,63,69	0
4	CA	B	903	1/1	0.97	0.08	52,52,52,52	0
3	TPP	A	902	26/26	0.98	0.21	27,35,48,59	0
3	TPP	G	902	26/26	0.98	0.18	32,44,49,55	0
3	TPP	H	902	26/26	0.98	0.21	38,48,54,56	0
4	CA	A	903	1/1	0.98	0.05	60,60,60,60	0
4	CA	G	903	1/1	0.98	0.06	52,52,52,52	0
3	TPP	E	902	26/26	0.98	0.20	34,46,52,55	0

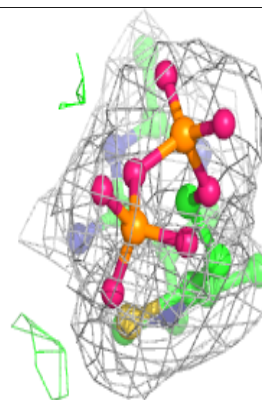
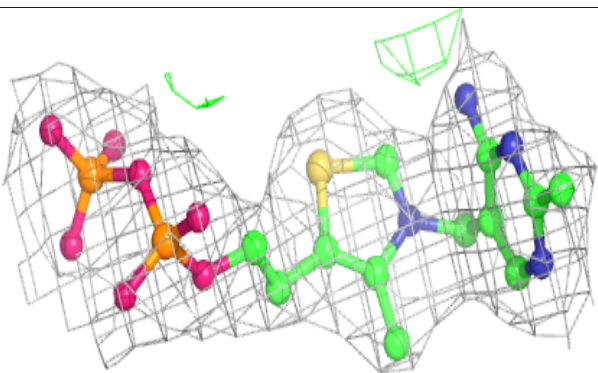
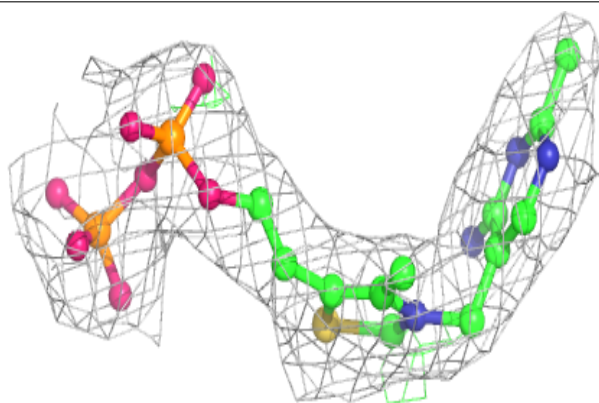
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP C 902:**

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

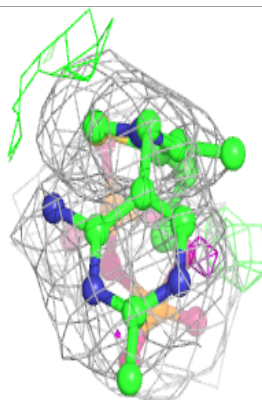
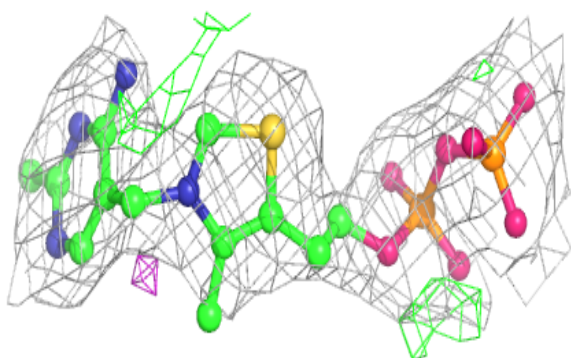
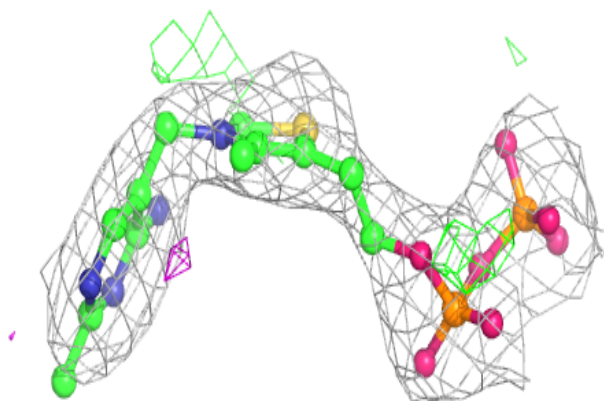
**Electron density around TPP B 902:**

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

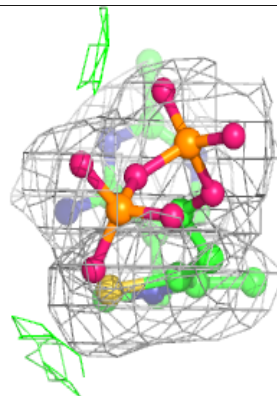
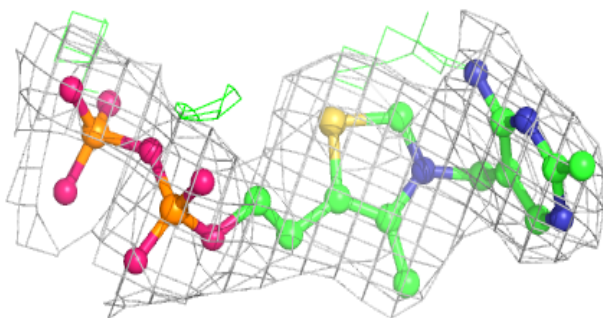
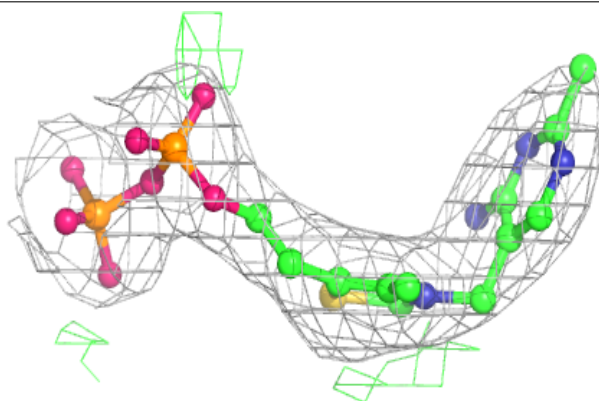


**Electron density around TPP D 902:**

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

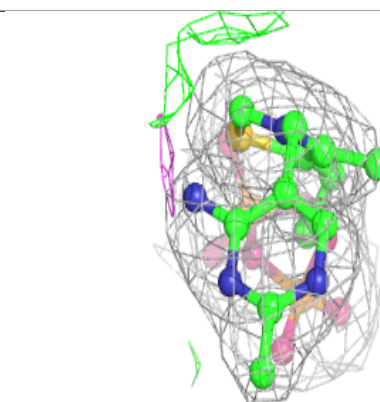
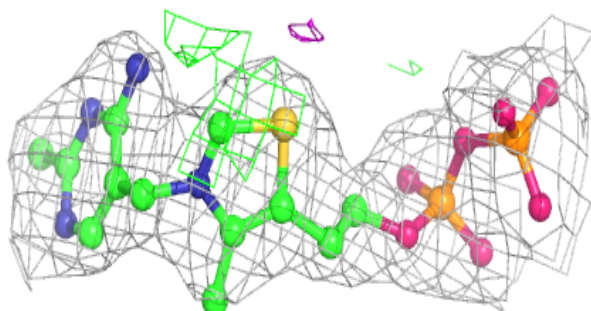
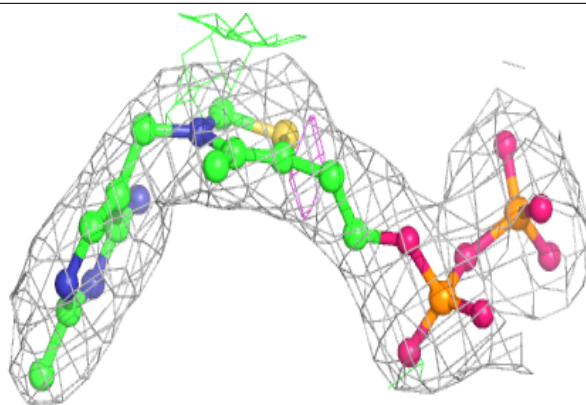
**Electron density around TPP F 902:**

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and green (positive)

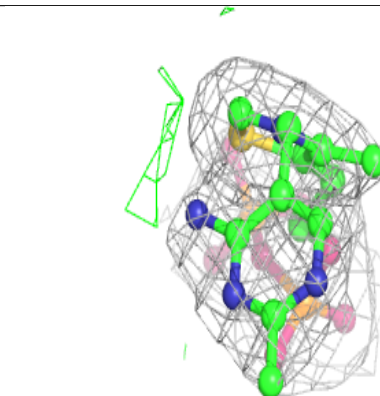
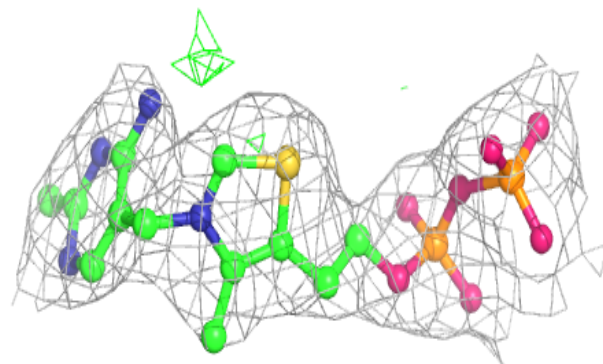
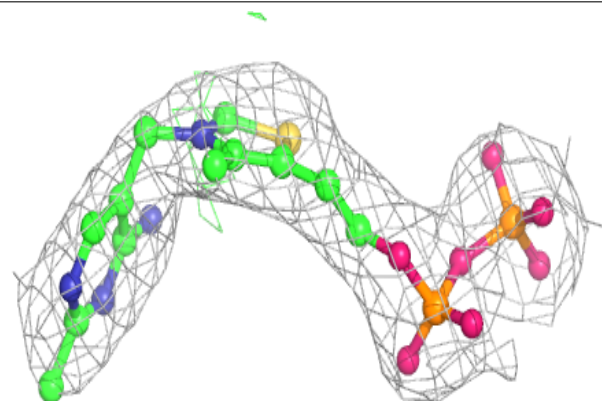


**Electron density around TPP A 902:**

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

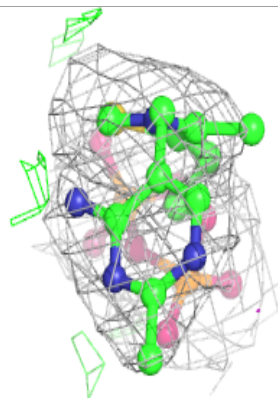
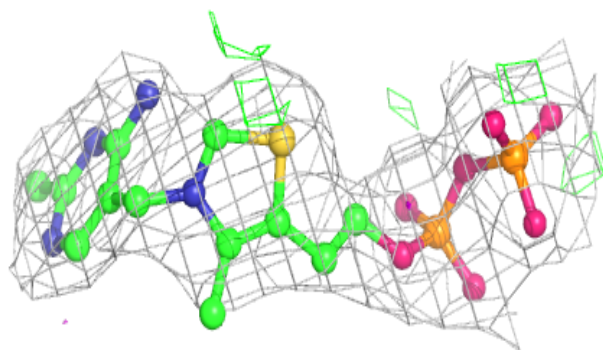
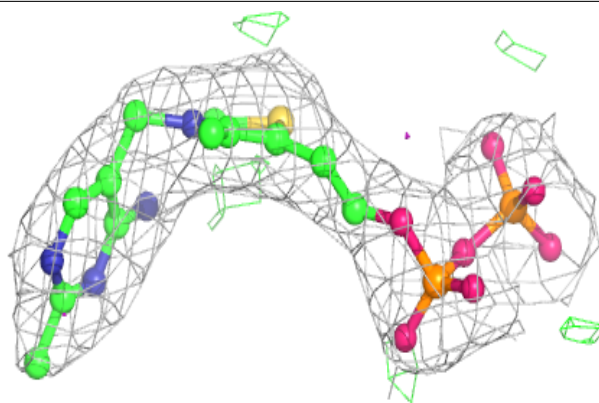
**Electron density around TPP G 902:**

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

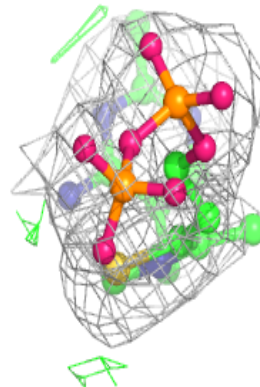
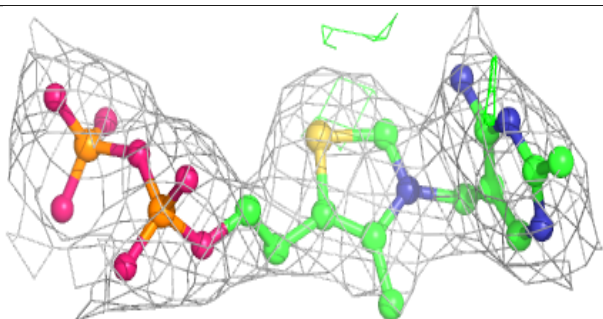
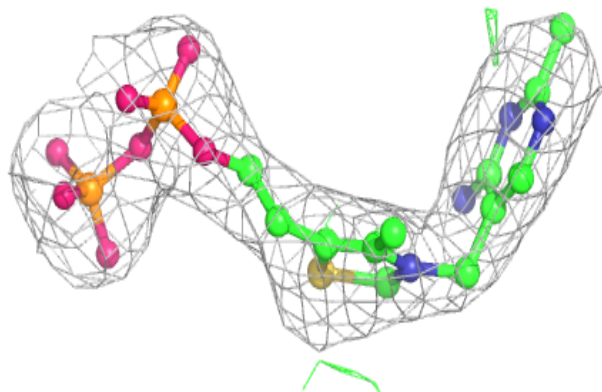


**Electron density around TPP H 902:**

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

**Electron density around TPP E 902:**

$2mF_o-DF_c$  (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.