



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:43 PM UTC

PDB ID : 7C8H / pdb\_00007c8h  
Title : Ambient temperature structure of Bifidobacterium longum phosphoketolase with thiamine diphosphate  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

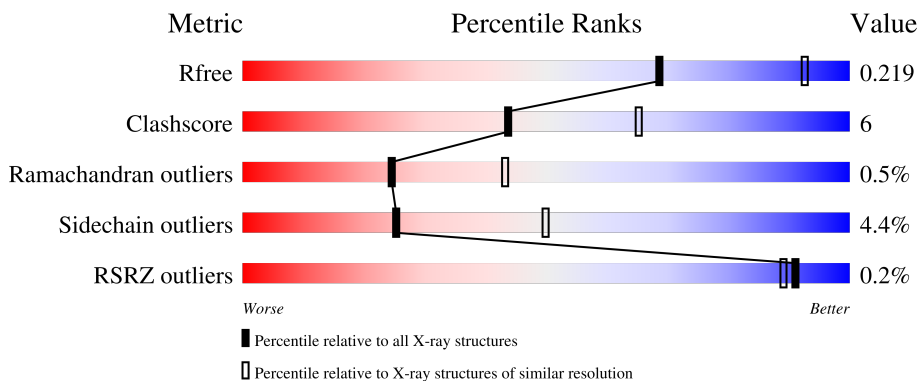
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

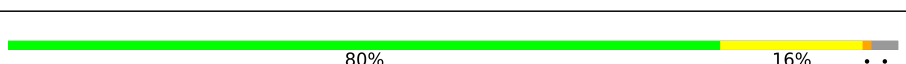
The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	 84% 13% ..
1	B	831	 83% 14% ..
1	C	831	 74% 21% ..
1	D	831	 77% 18% ..
1	E	831	 80% 16% ..

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Mol	Chain	Length	Quality of chain	
1	F	831	 78%	18% ..
1	G	831	 80%	16% ..
1	H	831	 81%	15% ..

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
4	LMR	B	901	-	-	-	X
5	MLA	D	901	-	-	X	-
6	SIN	H	901	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 52781 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
			Total	C	N	O	S			
1	A	807	6418	4075	1094	1230	19	0	0	0
1	B	807	6418	4075	1094	1230	19	0	0	0
1	C	807	6418	4075	1094	1230	19	0	0	0
1	D	808	6433	4084	1097	1233	19	0	1	0
1	E	808	6436	4085	1098	1234	19	0	1	0
1	F	807	6418	4075	1094	1230	19	0	0	0
1	G	806	6427	4081	1096	1231	19	0	2	0
1	H	807	6428	4081	1097	1231	19	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

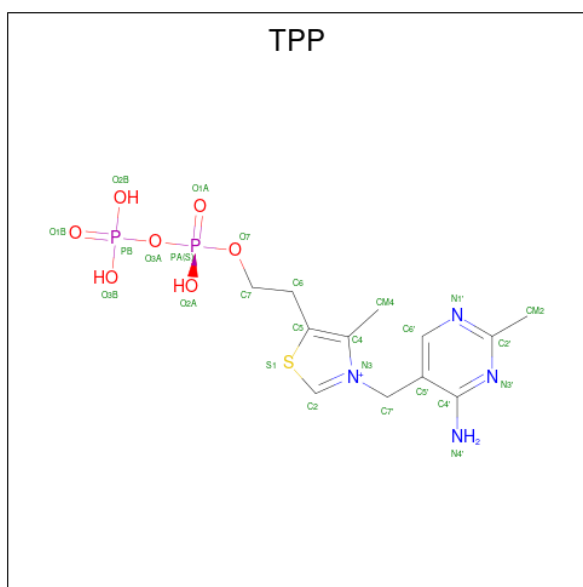
Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	expression tag	UNP Q6R2Q7
A	827	HIS	-	expression tag	UNP Q6R2Q7
A	828	HIS	-	expression tag	UNP Q6R2Q7
A	829	HIS	-	expression tag	UNP Q6R2Q7
A	830	HIS	-	expression tag	UNP Q6R2Q7
A	831	HIS	-	expression tag	UNP Q6R2Q7
B	826	HIS	-	expression tag	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 THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

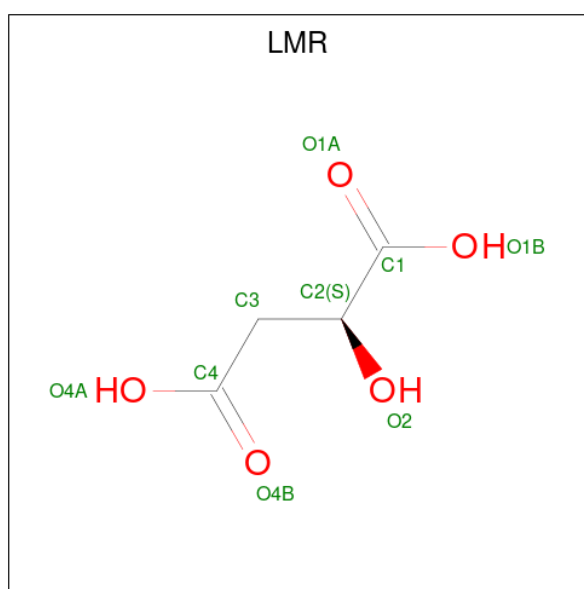
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

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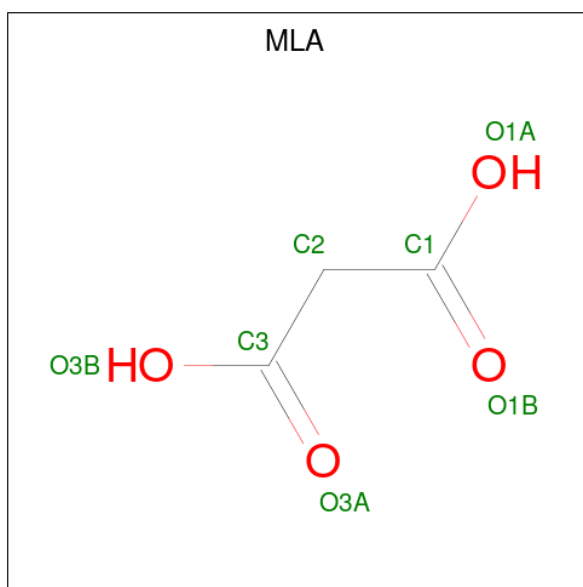
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



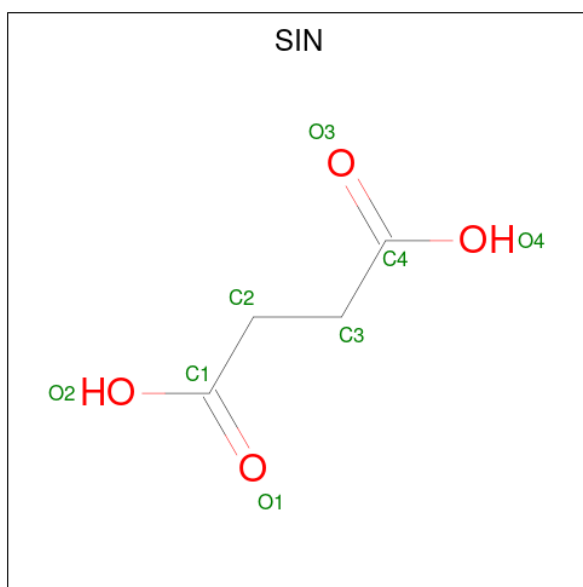
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 9 4 5	0	0
4	B	1	Total C O 9 4 5	0	0

- Molecule 5 is MALONIC ACID (CCD ID: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is SUCCINIC ACID (CCD ID: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			8	4	4		
6	H	1	Total	C	O	0	0
			8	4	4		

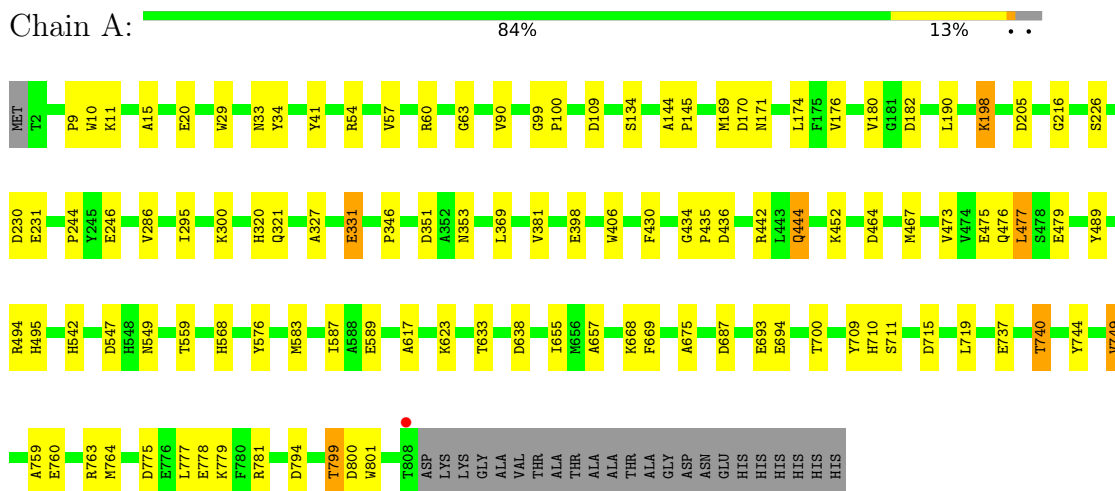
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	215	Total	O	0	0
			215	215		
7	C	92	Total	O	0	0
			92	92		
7	D	77	Total	O	0	0
			77	77		
7	E	126	Total	O	0	0
			126	126		
7	F	93	Total	O	0	0
			93	93		
7	G	160	Total	O	0	0
			160	160		
7	H	132	Total	O	0	0
			132	132		

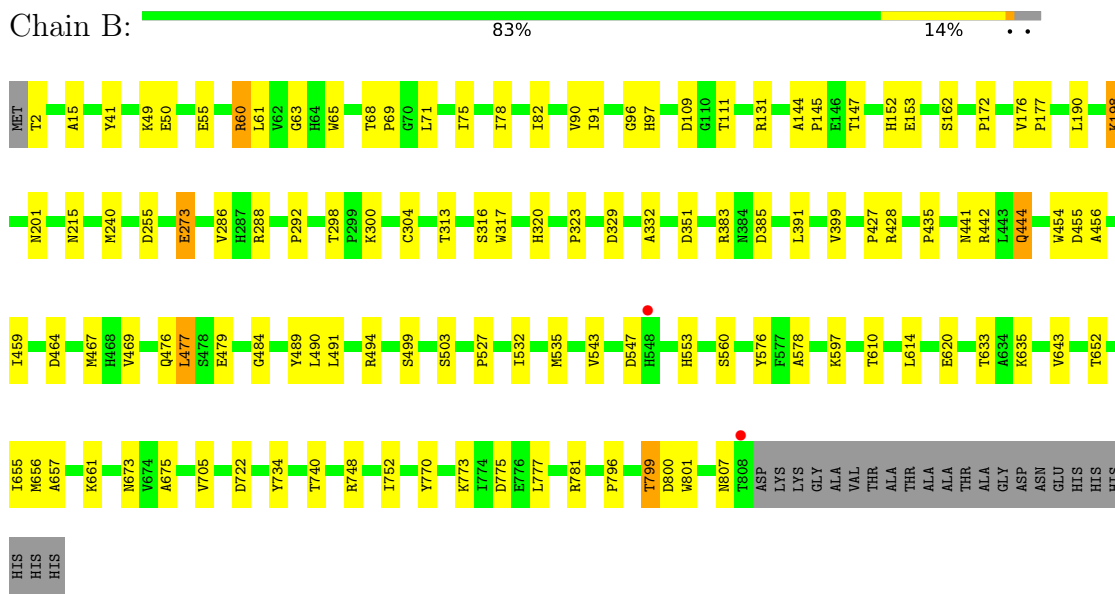
### 3 Residue-property plots [i](#)

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.

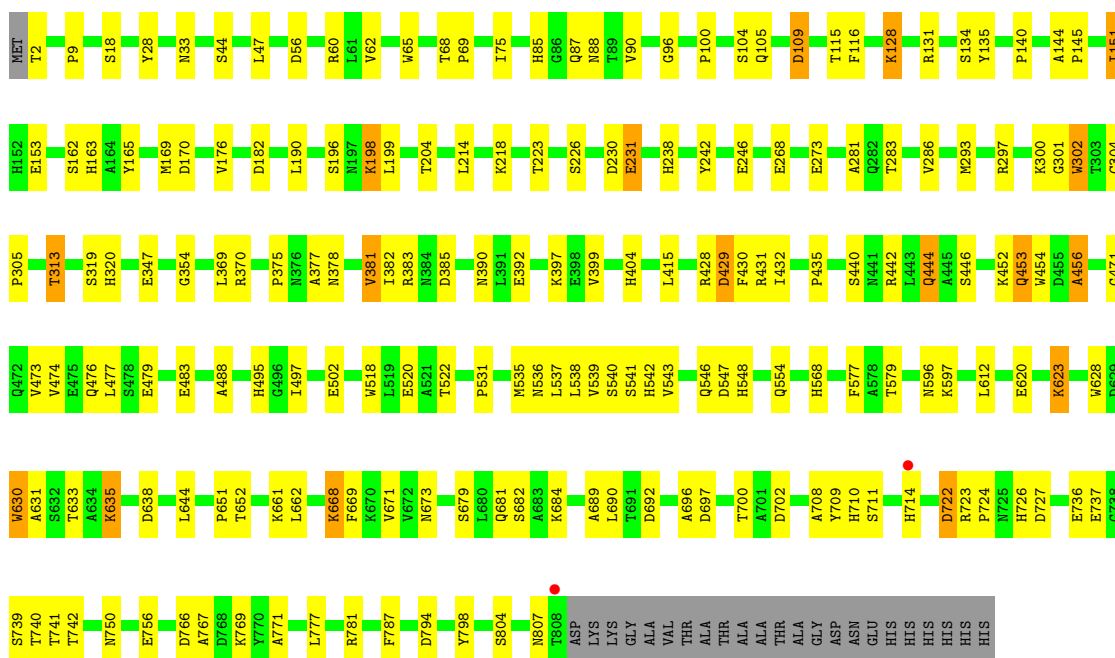
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase




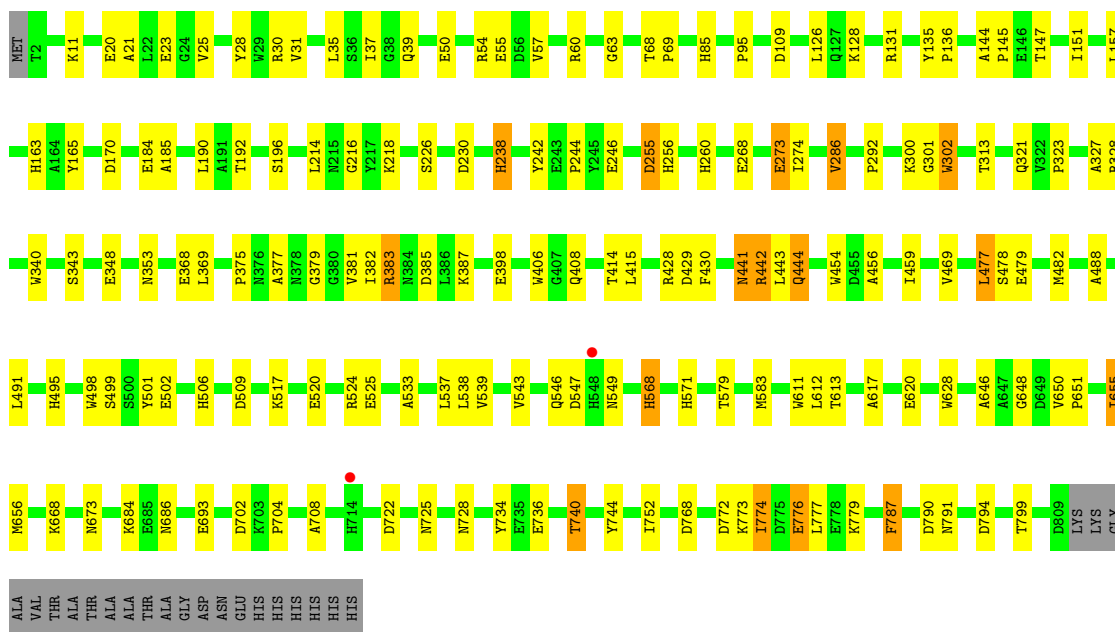
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase




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

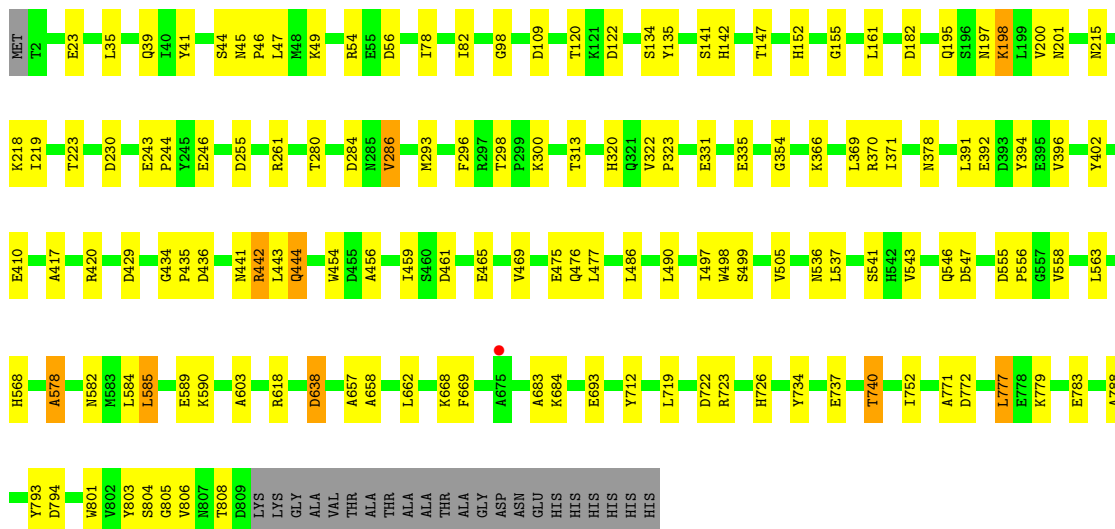
Chain C:  74% 21%

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

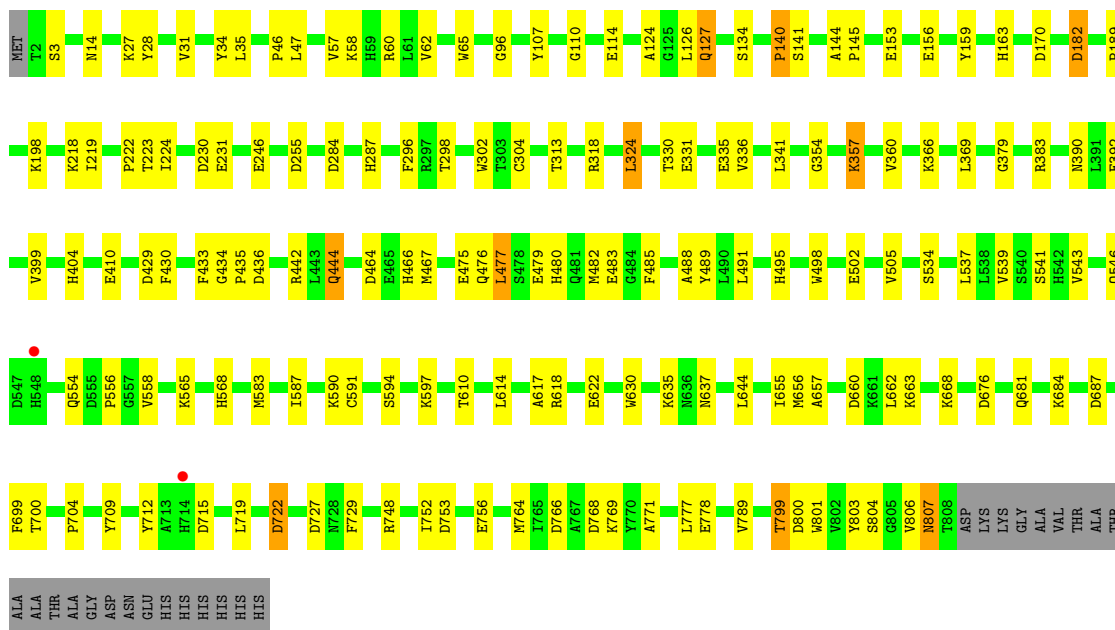
Chain D:  77% 18%

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

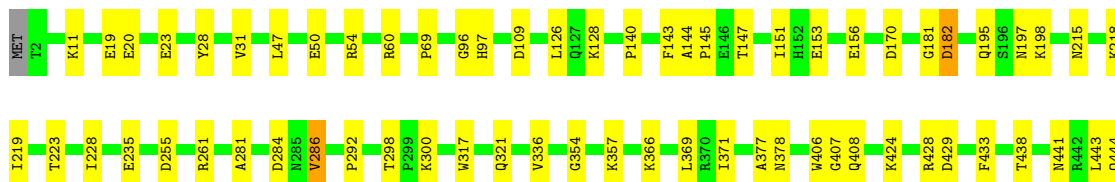
Chain E:  80% 16%



Chain F: 78% 18% ..



Chain G: 80% 16% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.62Å 185.80Å 162.89Å 90.00° 99.61° 90.00°	Depositor
Resolution (Å)	46.80 – 2.50 46.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.80-2.50) 100.0 (46.80-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	16.17 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.161 , 0.218 0.169 , 0.219	Depositor DCC
$R_{free}$ test set	31648 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: LMR, TPP, MLA, SIN, CA

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	1.03	1/6595 (0.0%)	1.42	9/8970 (0.1%)
1	B	1.03	1/6595 (0.0%)	1.44	7/8970 (0.1%)
1	C	1.08	1/6595 (0.0%)	1.49	16/8970 (0.2%)
1	D	1.08	1/6614 (0.0%)	1.48	18/8996 (0.2%)
1	E	1.04	1/6614 (0.0%)	1.46	13/8996 (0.1%)
1	F	1.03	1/6595 (0.0%)	1.46	11/8970 (0.1%)
1	G	1.06	4/6608 (0.1%)	1.46	19/8987 (0.2%)
1	H	1.04	2/6606 (0.0%)	1.45	14/8985 (0.2%)
All	All	1.05	12/52822 (0.0%)	1.46	107/71844 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	PRO	C-O	-7.79	1.16	1.23
1	C	456	ALA	C-O	6.83	1.30	1.23
1	G	456	ALA	C-O	6.06	1.29	1.23
1	B	527	PRO	C-O	-5.67	1.17	1.24
1	H	286	VAL	C-O	-5.65	1.18	1.24

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	740	THR	CB-CA-C	7.51	123.20	110.81
1	H	109	ASP	CA-CB-CG	7.32	119.92	112.60
1	E	98	GLY	CA-C-N	6.76	126.06	121.13
1	E	98	GLY	C-N-CA	6.76	126.06	121.13
1	B	799	THR	CA-CB-OG1	-6.53	99.81	109.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6418	0	6108	56	0
1	B	6418	0	6108	65	0
1	C	6418	0	6108	106	0
1	D	6433	0	6119	86	0
1	E	6436	0	6118	80	0
1	F	6418	0	6108	83	0
1	G	6427	0	6113	74	0
1	H	6428	0	6114	90	0
2	A	26	0	16	6	0
2	B	26	0	16	5	0
2	C	26	0	16	6	0
2	D	26	0	16	7	0
2	E	26	0	16	5	0
2	F	26	0	16	1	0
2	G	26	0	16	6	0
2	H	26	0	16	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	18	0	8	1	0
5	D	14	0	4	5	0
5	E	7	0	2	1	0
6	E	8	0	4	0	0
6	G	8	0	4	0	0
6	H	8	0	4	0	0
7	A	211	0	0	3	0
7	B	215	0	0	3	0
7	C	92	0	0	2	0
7	D	77	0	0	4	0
7	E	126	0	0	4	0
7	F	93	0	0	2	0
7	G	160	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	132	0	0	3	0
All	All	52781	0	49050	617	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 617 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:E:442:ARG:HA	1:E:444:GLN:HE22	1.21	1.00
1:D:441:ASN:HD22	1:D:499:SER:HB2	1.22	0.99
1:D:772:ASP:HA	7:D:1070:HOH:O	1.68	0.91
2:D:903:TPP:H2	2:D:903:TPP:HN42	1.35	0.90
1:E:441:ASN:HD22	1:E:499:SER:HB2	1.37	0.89

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	805/831 (97%)	761 (94%)	43 (5%)	1 (0%)	48 68
1	B	805/831 (97%)	764 (95%)	39 (5%)	2 (0%)	43 63
1	C	805/831 (97%)	735 (91%)	61 (8%)	9 (1%)	11 22
1	D	807/831 (97%)	736 (91%)	65 (8%)	6 (1%)	18 34
1	E	807/831 (97%)	740 (92%)	62 (8%)	5 (1%)	21 38
1	F	805/831 (97%)	752 (93%)	49 (6%)	4 (0%)	24 43
1	G	806/831 (97%)	748 (93%)	53 (7%)	5 (1%)	21 38
1	H	806/831 (97%)	763 (95%)	39 (5%)	4 (0%)	24 43
All	All	6446/6648 (97%)	5999 (93%)	411 (6%)	36 (1%)	24 38

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	714	HIS
1	G	54	ARG
1	C	302	TRP
1	D	774	ILE
1	E	805	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	676/693 (98%)	653 (97%)	23 (3%)	32	60
1	B	676/693 (98%)	657 (97%)	19 (3%)	38	66
1	C	676/693 (98%)	643 (95%)	33 (5%)	22	45
1	D	678/693 (98%)	642 (95%)	36 (5%)	20	42
1	E	678/693 (98%)	642 (95%)	36 (5%)	20	42
1	F	676/693 (98%)	643 (95%)	33 (5%)	22	45
1	G	677/693 (98%)	648 (96%)	29 (4%)	26	51
1	H	677/693 (98%)	648 (96%)	29 (4%)	26	51
All	All	5414/5544 (98%)	5176 (96%)	238 (4%)	25	50

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	255	ASP
1	H	390	ASN
1	E	777	LEU
1	H	369	LEU
1	H	799	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	404	HIS
1	H	127	GLN
1	F	513	ASN
1	G	408	GLN
1	H	444	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 oligosaccharides 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$
6	SIN	E	904	-	7,7,7	1.19	0	8,8,8	1.16	0
6	SIN	H	901	-	7,7,7	1.37	0	8,8,8	1.23	0
4	LMR	B	902	-	8,8,8	1.19	0	10,10,10	1.57	2 (20%)
5	MLA	D	902	-	6,6,6	1.44	0	7,7,7	1.29	1 (14%)
5	MLA	E	901	-	6,6,6	1.28	0	7,7,7	1.16	1 (14%)
2	TPP	F	900	3	26,27,27	0.69	1 (3%)	38,40,40	0.80	0
2	TPP	E	902	3	26,27,27	0.68	0	38,40,40	0.79	1 (2%)
2	TPP	C	900	3	26,27,27	0.77	1 (3%)	38,40,40	0.97	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LMR	B	901	-	8,8,8	1.48	0	10,10,10	1.46	1 (10%)
2	TPP	B	903	3	26,27,27	0.68	0	38,40,40	0.97	2 (5%)
2	TPP	D	903	3	26,27,27	0.57	0	38,40,40	1.21	3 (7%)
2	TPP	G	901	3	26,27,27	0.65	0	38,40,40	0.86	1 (2%)
2	TPP	A	900	3	26,27,27	0.74	0	38,40,40	1.03	3 (7%)
6	SIN	G	903	-	7,7,7	1.23	0	8,8,8	0.91	0
5	MLA	D	901	-	6,6,6	1.10	0	7,7,7	0.95	0
2	TPP	H	902	3	26,27,27	0.57	0	38,40,40	0.83	0

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
6	SIN	E	904	-	-	1/5/5/5	-
6	SIN	H	901	-	-	2/5/5/5	-
4	LMR	B	902	-	-	4/8/8/8	-
5	MLA	D	902	-	-	0/4/4/4	-
5	MLA	E	901	-	-	2/4/4/4	-
2	TPP	F	900	3	-	4/17/17/17	0/2/2/2
2	TPP	E	902	3	-	7/17/17/17	0/2/2/2
2	TPP	C	900	3	-	3/17/17/17	0/2/2/2
4	LMR	B	901	-	-	1/8/8/8	-
2	TPP	B	903	3	-	1/17/17/17	0/2/2/2
2	TPP	D	903	3	-	6/17/17/17	0/2/2/2
2	TPP	G	901	3	-	7/17/17/17	0/2/2/2
2	TPP	A	900	3	-	3/17/17/17	0/2/2/2
6	SIN	G	903	-	-	2/5/5/5	-
5	MLA	D	901	-	-	1/4/4/4	-
2	TPP	H	902	3	-	4/17/17/17	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	TPP	PA-O3A	2.53	1.62	1.59
2	F	900	TPP	PA-O3A	2.09	1.61	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	903	TPP	C2-S1-C5	-4.86	87.99	91.22
2	C	900	TPP	C2-S1-C5	-3.37	88.99	91.22
4	B	901	LMR	C2-C3-C4	2.97	119.84	112.08
2	A	900	TPP	C2-S1-C5	-2.94	89.27	91.22
2	B	903	TPP	O3B-PB-O3A	-2.82	95.17	104.64

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	TPP	PA-O3A-PB-O2B
2	C	900	TPP	PA-O3A-PB-O3B
2	E	902	TPP	PA-O3A-PB-O2B
2	E	902	TPP	PA-O3A-PB-O3B
2	F	900	TPP	PA-O3A-PB-O3B

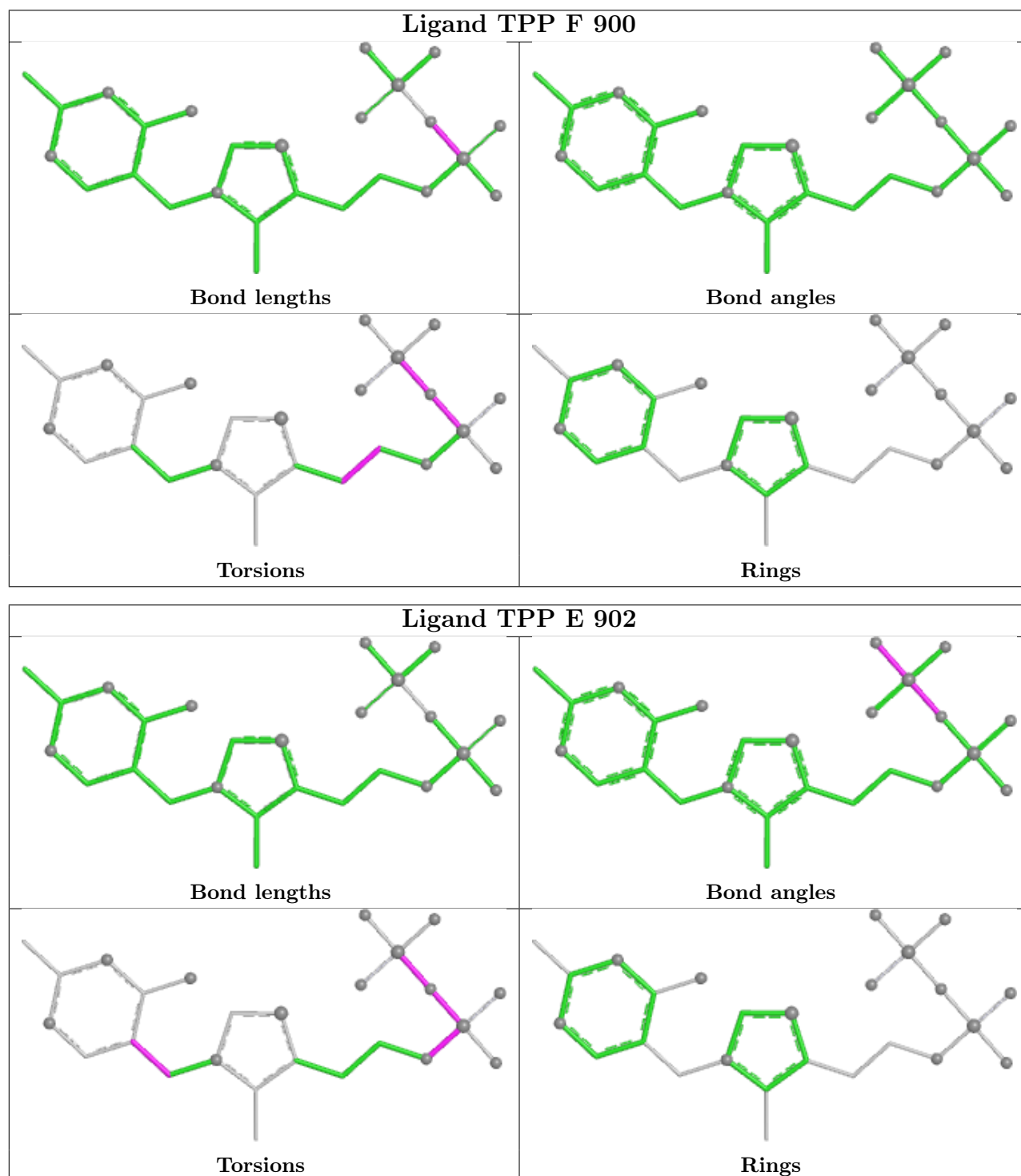
There are no ring outliers.

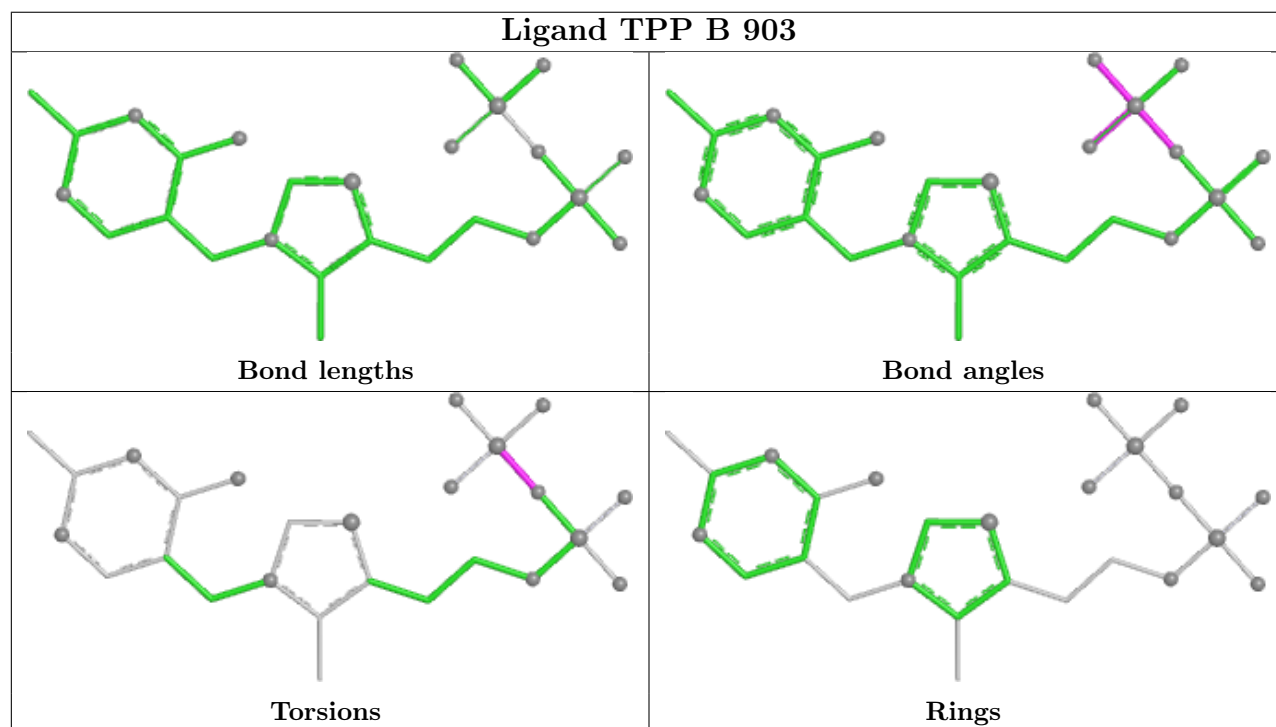
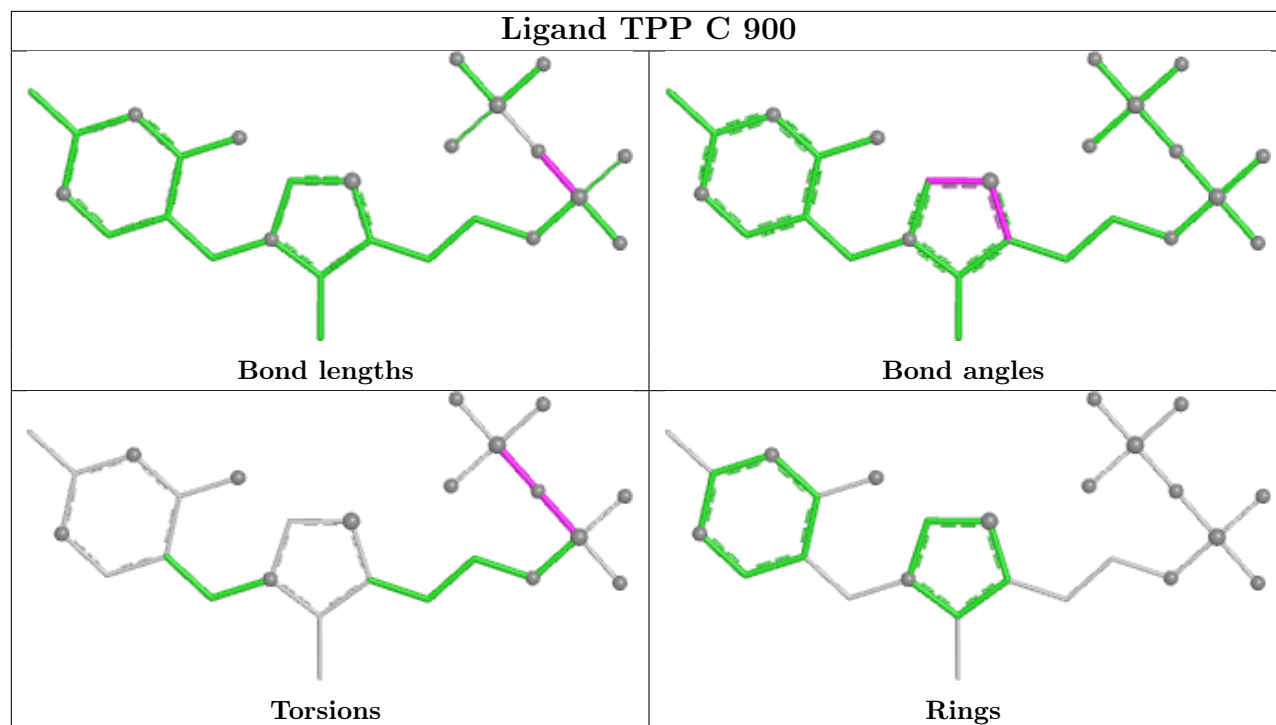
12 monomers are involved in 44 short contacts:

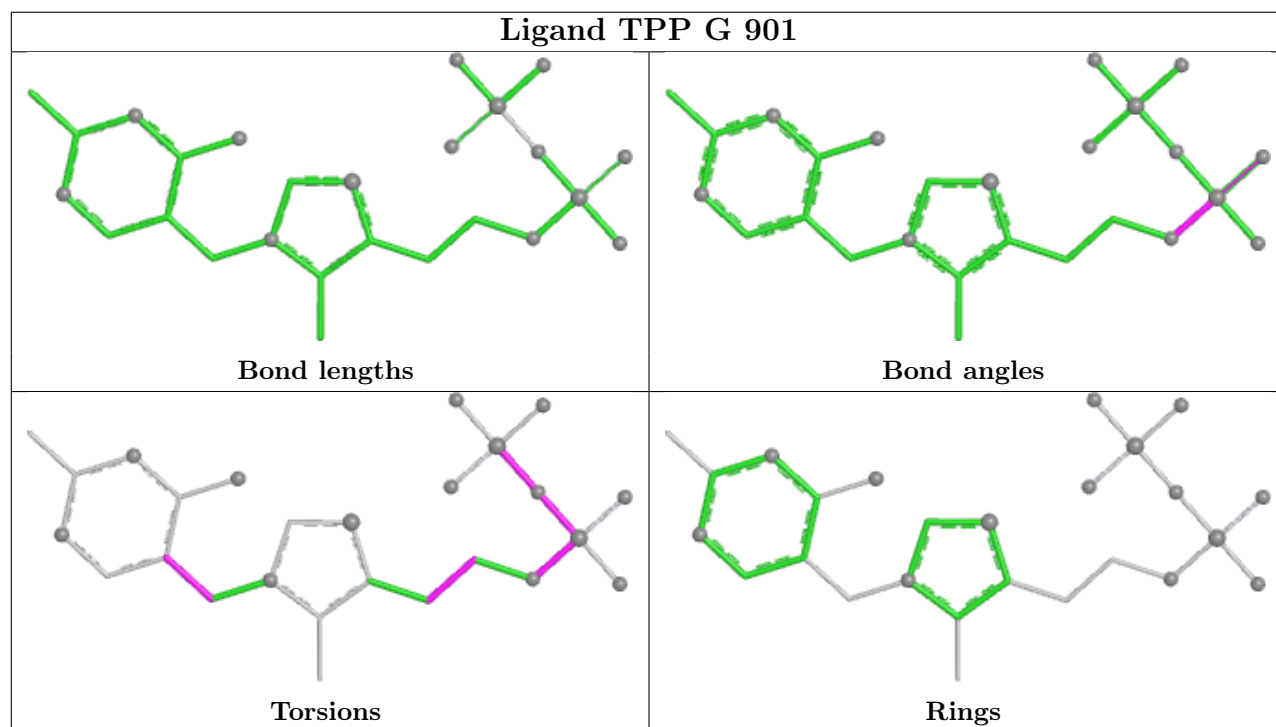
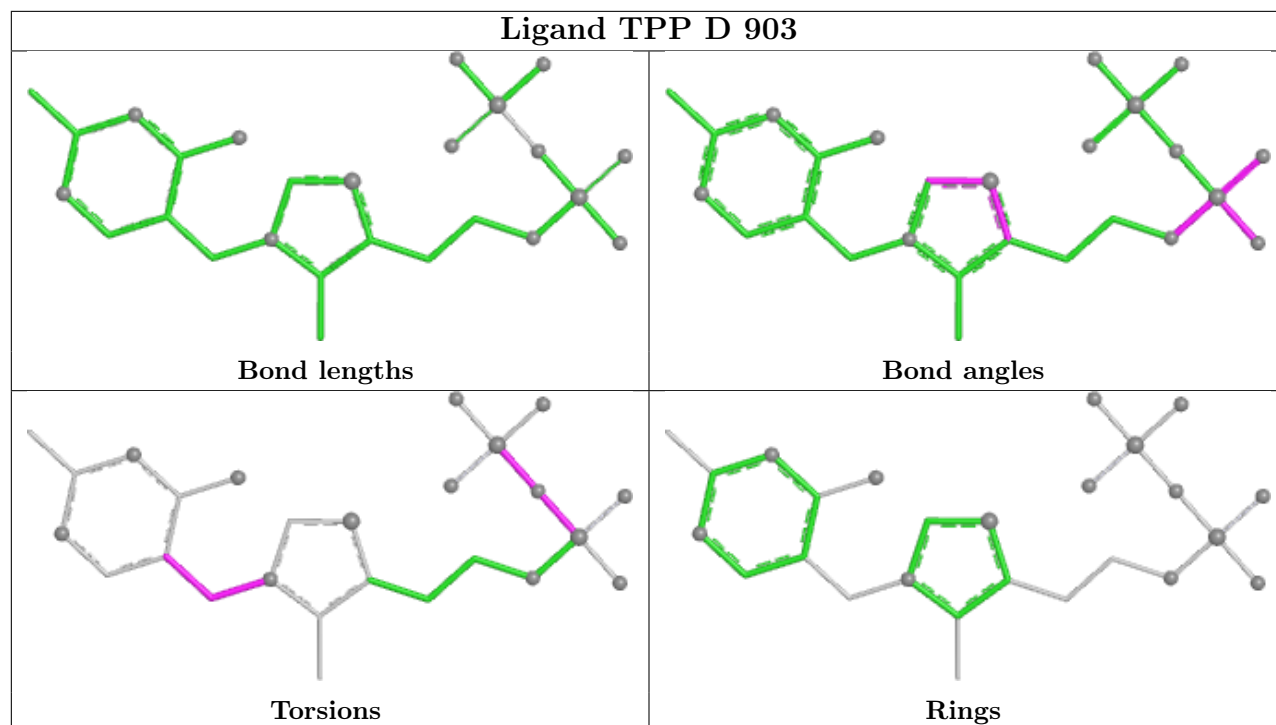
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	LMR	1	0
5	D	902	MLA	1	0
5	E	901	MLA	1	0
2	F	900	TPP	1	0
2	E	902	TPP	5	0
2	C	900	TPP	6	0
2	B	903	TPP	5	0
2	D	903	TPP	7	0
2	G	901	TPP	6	0
2	A	900	TPP	6	0
5	D	901	MLA	4	0
2	H	902	TPP	6	0

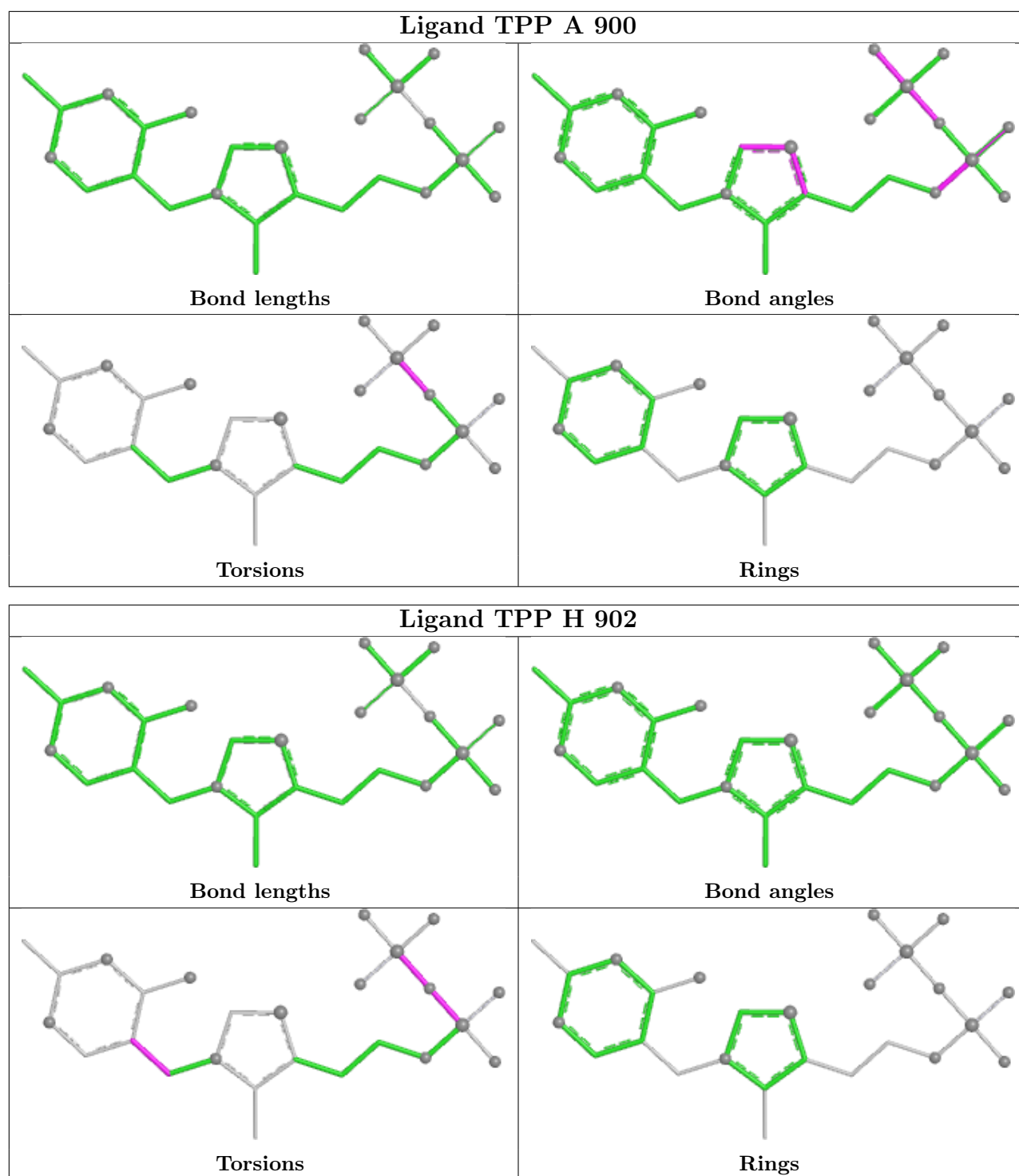
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	807/831 (97%)	-0.64	1 (0%) 92 90	33, 45, 69, 118	0
1	B	807/831 (97%)	-0.64	2 (0%) 91 89	32, 45, 68, 120	0
1	C	807/831 (97%)	-0.12	2 (0%) 91 89	44, 66, 96, 141	0
1	D	808/831 (97%)	-0.08	2 (0%) 91 89	40, 67, 98, 128	1 (0%)
1	E	808/831 (97%)	-0.30	1 (0%) 92 90	31, 57, 95, 129	1 (0%)
1	F	807/831 (97%)	-0.31	2 (0%) 91 89	40, 60, 89, 121	0
1	G	806/831 (96%)	-0.47	0 100 100	25, 50, 77, 104	2 (0%)
1	H	807/831 (97%)	-0.46	0 100 100	29, 53, 77, 118	1 (0%)
All	All	6457/6648 (97%)	-0.38	10 (0%) 91 89	25, 55, 89, 141	5 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	714	HIS	3.9
1	A	808	THR	2.8
1	B	808	THR	2.7
1	C	808	THR	2.5
1	C	714	HIS	2.4

### 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 oligosaccharides in this entry.

## 6.4 Ligands

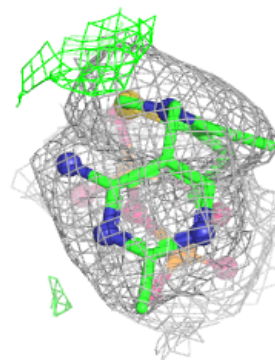
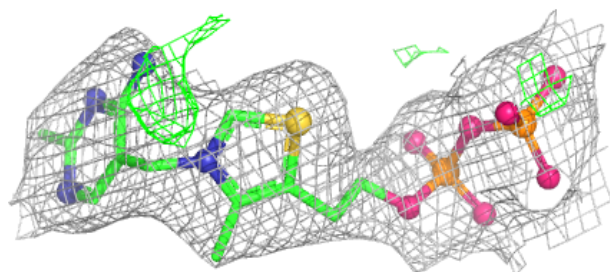
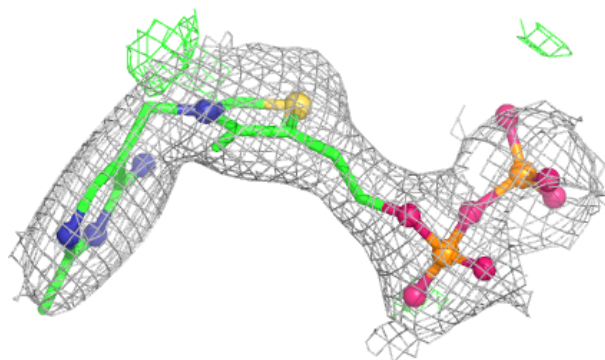
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	LMR	B	901	9/9	0.66	0.49	39,42,48,53	9
6	SIN	H	901	8/8	0.68	0.46	38,46,54,55	8
5	MLA	D	902	7/7	0.69	0.31	42,42,51,53	7
5	MLA	E	901	7/7	0.73	0.38	38,43,53,57	7
6	SIN	E	904	8/8	0.77	0.39	48,55,61,62	8
5	MLA	D	901	7/7	0.80	0.34	42,52,55,56	7
6	SIN	G	903	8/8	0.87	0.30	59,67,70,71	8
4	LMR	B	902	9/9	0.88	0.23	36,49,53,55	9
2	TPP	C	900	26/26	0.97	0.07	49,60,66,90	0
2	TPP	E	902	26/26	0.97	0.06	40,47,54,58	0
2	TPP	F	900	26/26	0.97	0.08	48,60,69,74	0
3	CA	G	902	1/1	0.97	0.05	70,70,70,70	0
2	TPP	H	902	26/26	0.98	0.06	43,50,55,60	0
2	TPP	D	903	26/26	0.98	0.06	42,56,65,83	0
2	TPP	B	903	26/26	0.98	0.06	37,42,46,52	0
2	TPP	A	900	26/26	0.98	0.06	37,44,48,58	0
2	TPP	G	901	26/26	0.98	0.05	38,46,52,54	0
3	CA	C	901	1/1	0.99	0.07	70,70,70,70	0
3	CA	D	904	1/1	0.99	0.07	71,71,71,71	0
3	CA	E	903	1/1	0.99	0.10	62,62,62,62	0
3	CA	F	901	1/1	0.99	0.06	79,79,79,79	0
3	CA	A	901	1/1	0.99	0.05	60,60,60,60	0
3	CA	H	903	1/1	0.99	0.08	69,69,69,69	0
3	CA	B	904	1/1	0.99	0.05	55,55,55,55	0

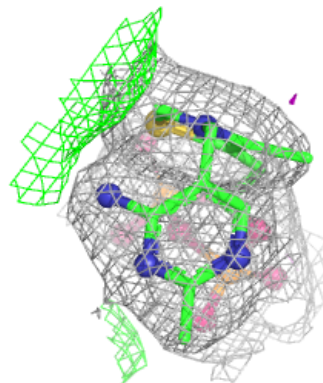
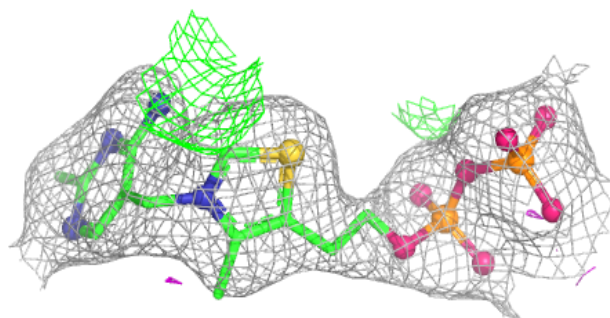
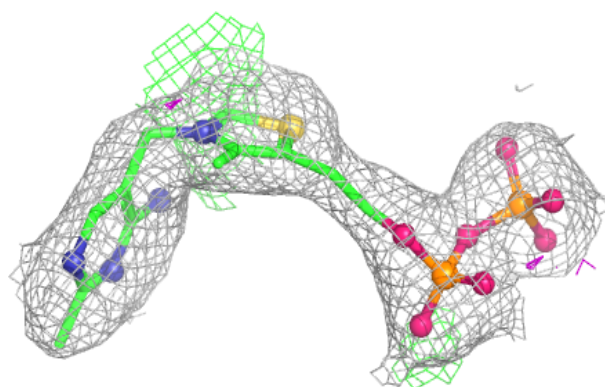
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP C 900:**

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

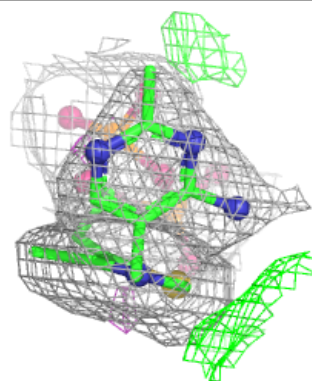
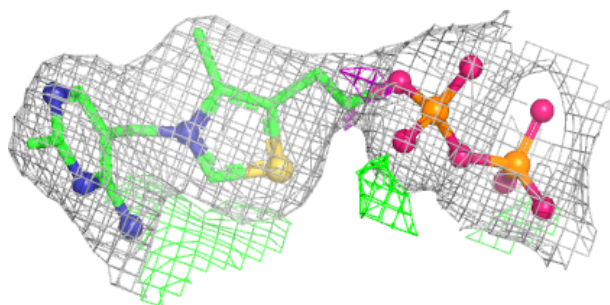
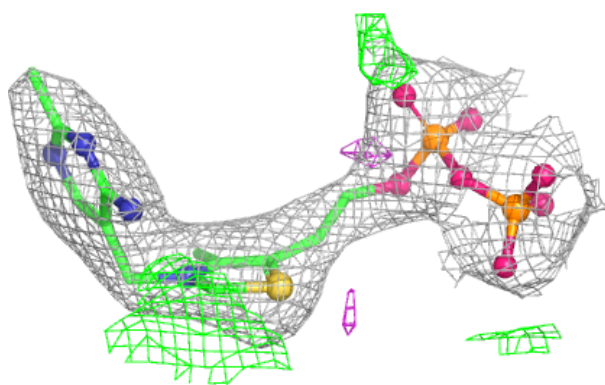
**Electron density around TPP E 902:**

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

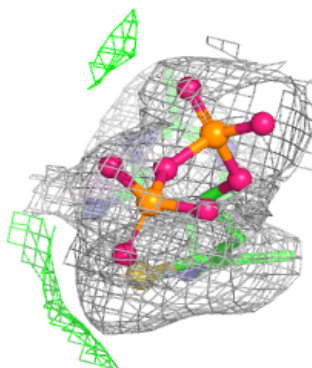
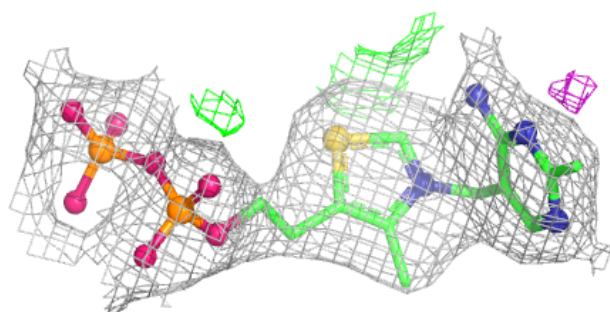
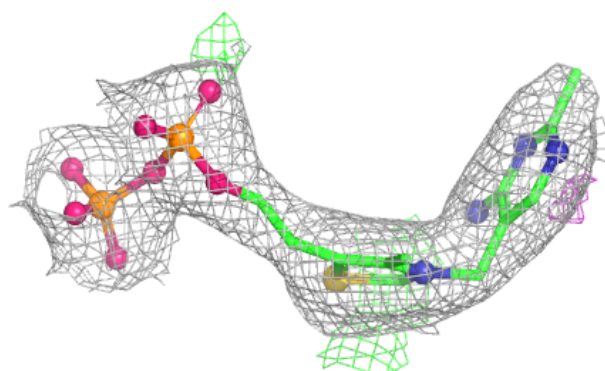


**Electron density around TPP F 900:**

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

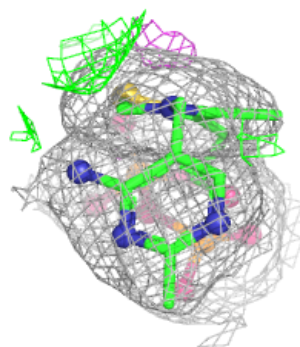
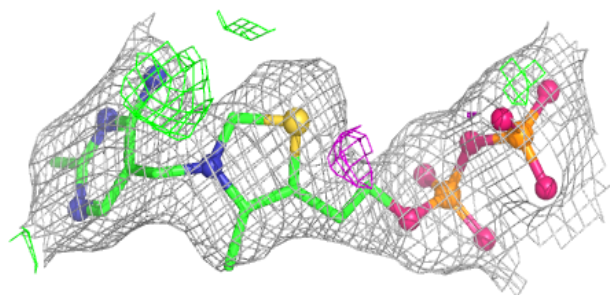
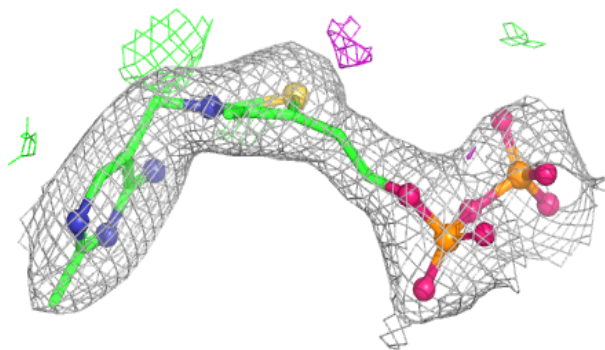
**Electron density around TPP H 902:**

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and green (positive)

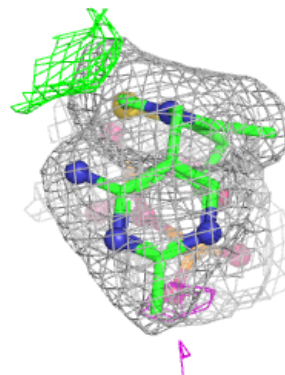
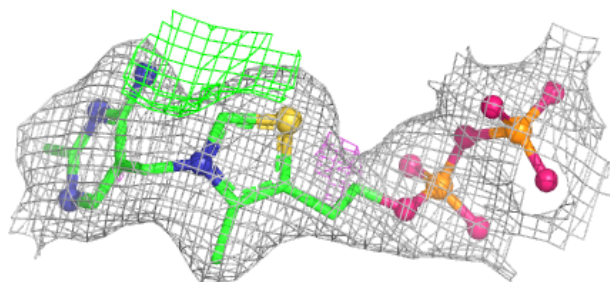
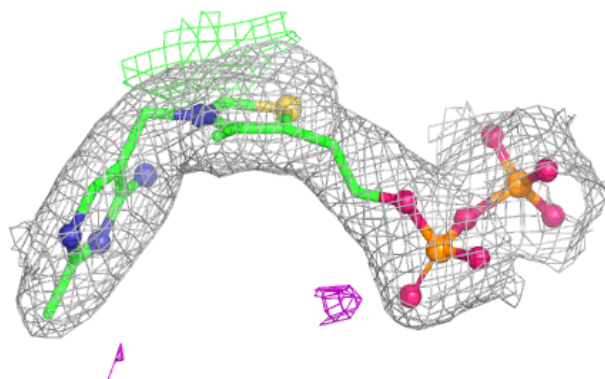


**Electron density around TPP D 903:**

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

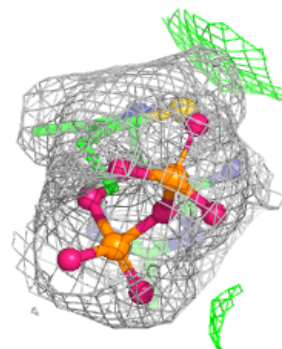
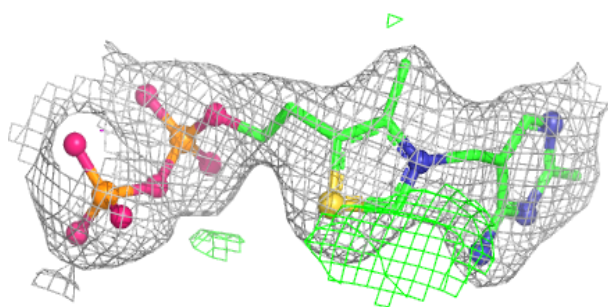
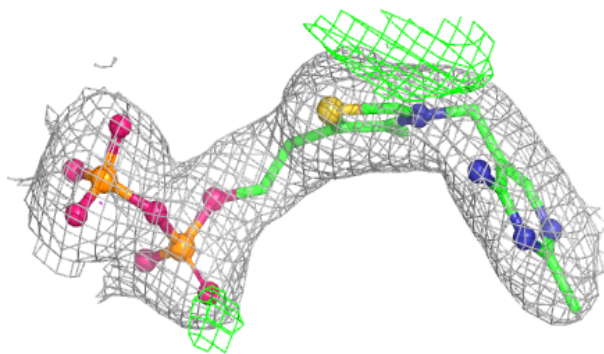
**Electron density around TPP B 903:**

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and green (positive)

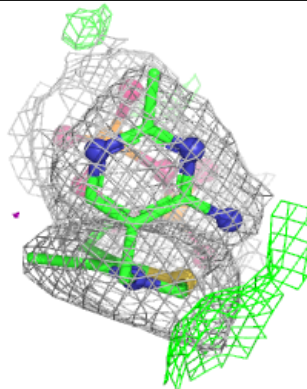
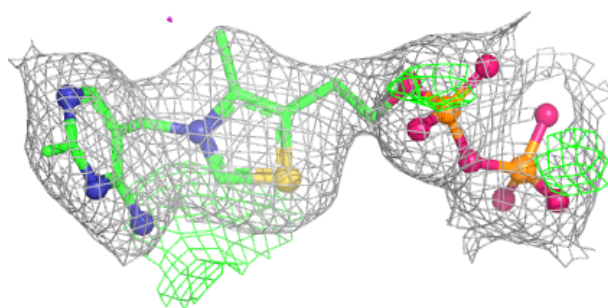
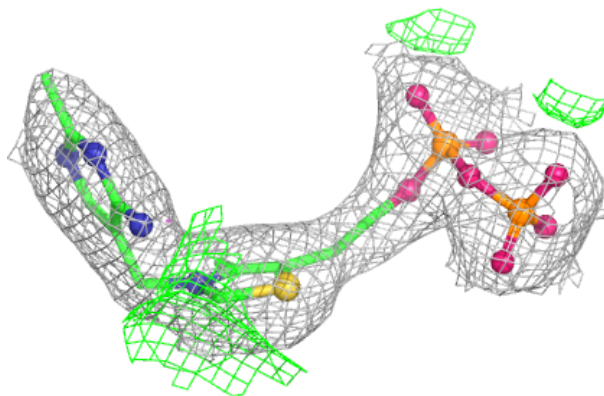


**Electron density around TPP A 900:**

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

**Electron density around TPP G 901:**

$2mF_o-DF_c$  (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.