wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 09:11 PM JST

PDB ID	:	7C8H
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

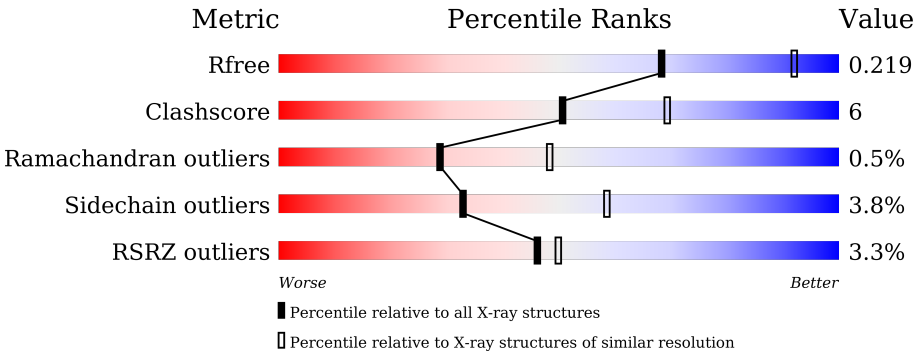
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 >=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 <=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	86% 11%
1	B	831	3% 84% 13%
1	C	831	3% 77% 19%
1	D	831	4% 80% 17%
1	E	831	5% 82% 14%
1	F	831	4% 80% 17%

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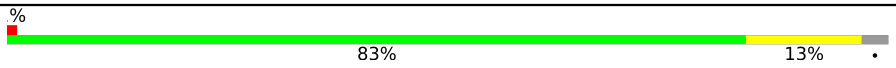
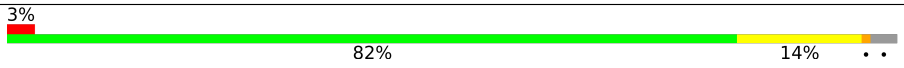
Mol	Chain	Length	Quality of chain
1	G	831	
1	H	831	

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
4	LMR	B	902	-	-	-	X
5	MLA	D	901	-	-	X	-
5	MLA	D	902	-	-	-	X
5	MLA	E	901	-	-	-	X
6	SIN	E	904	-	-	-	X
6	SIN	G	903	-	-	-	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
1	A	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	B	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	C	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	D	808	Total	C	N	O	S	0	1	0
			6433	4084	1097	1233	19			
1	E	808	Total	C	N	O	S	0	1	0
			6436	4085	1098	1234	19			
1	F	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	G	806	Total	C	N	O	S	0	2	0
			6427	4081	1096	1231	19			
1	H	807	Total	C	N	O	S	0	1	0
			6428	4081	1097	1231	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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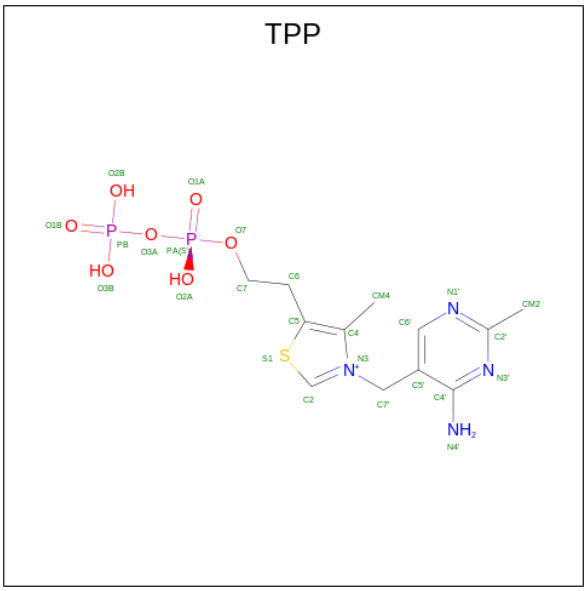
Chain	Residue	Modelled	Actual	Comment	Reference
C	827	HIS	-	expression tag	UNP Q6R2Q7
C	828	HIS	-	expression tag	UNP Q6R2Q7
C	829	HIS	-	expression tag	UNP Q6R2Q7
C	830	HIS	-	expression tag	UNP Q6R2Q7
C	831	HIS	-	expression tag	UNP Q6R2Q7
D	826	HIS	-	expression tag	UNP Q6R2Q7
D	827	HIS	-	expression tag	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 THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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 (three-letter code: CA) (formula: Ca).

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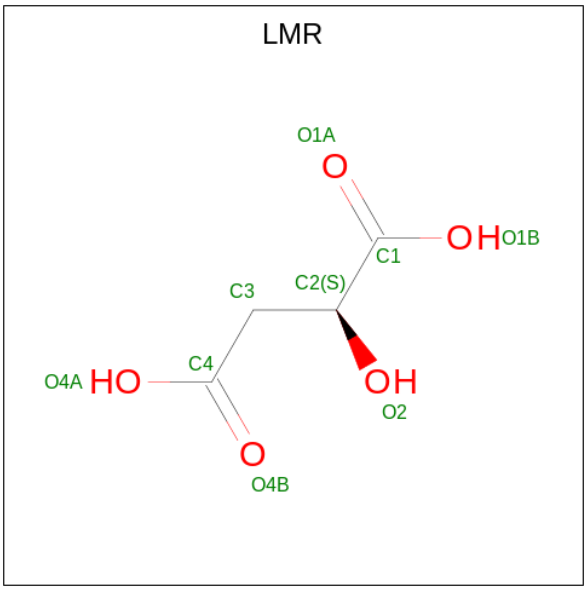
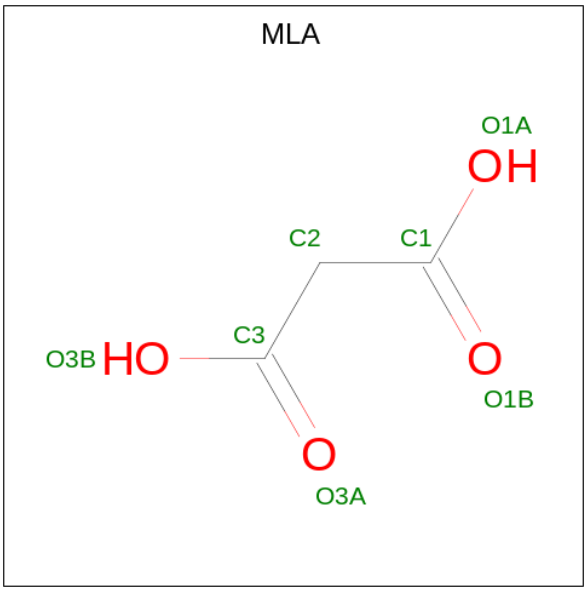
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).



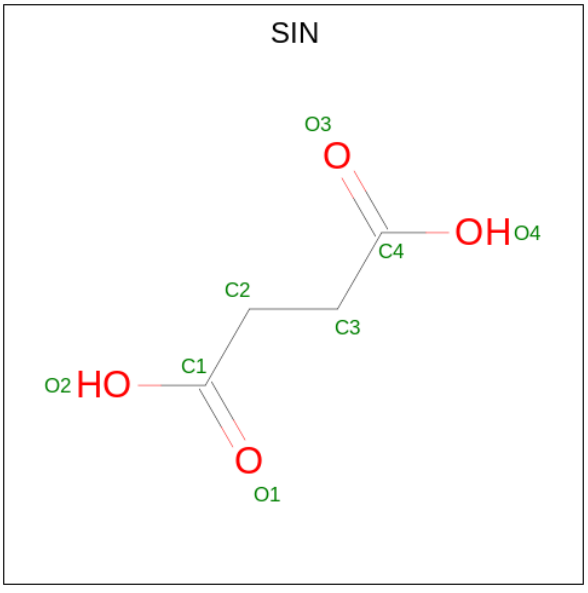
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 9 4 5	0	0
4	B	1	Total C O 9 4 5	0	0

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



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

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

- Molecule 7 is water.

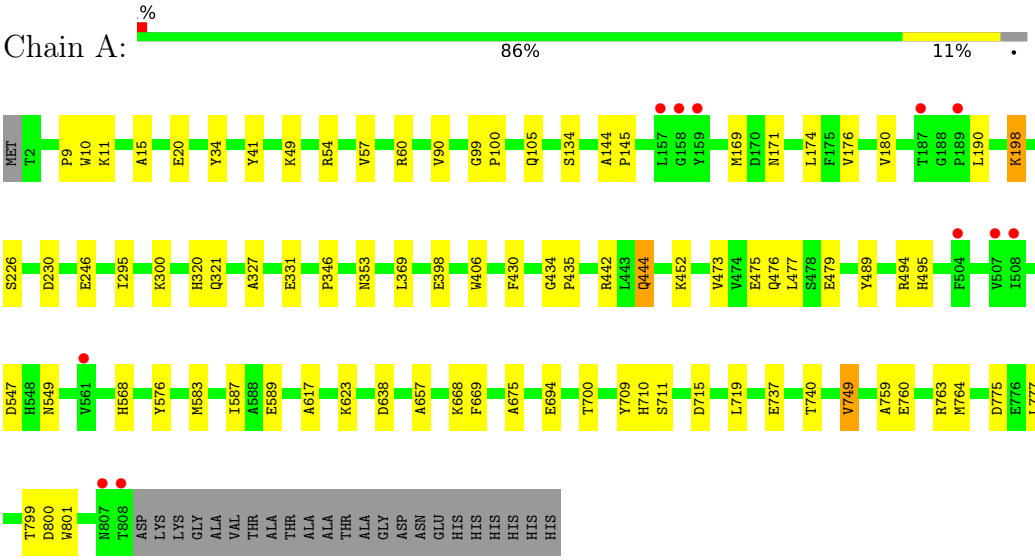
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	211	Total O 211 211	0	0
7	B	215	Total O 215 215	0	0
7	C	92	Total O 92 92	0	0
7	D	77	Total O 77 77	0	0
7	E	126	Total O 126 126	0	0
7	F	93	Total O 93 93	0	0
7	G	160	Total O 160 160	0	0
7	H	132	Total O 132 132	0	0

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.

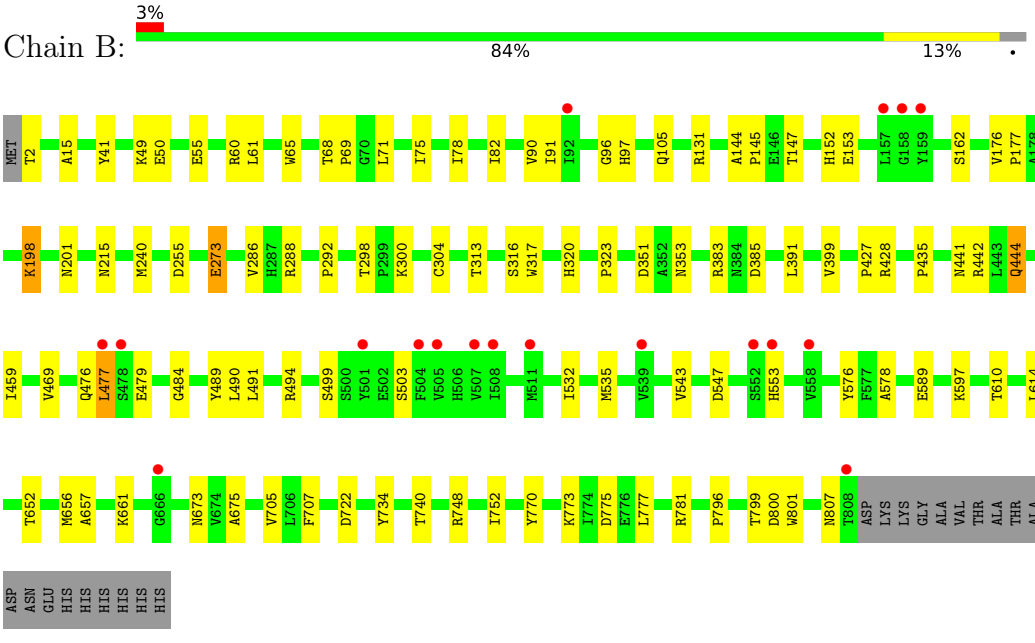
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain A:



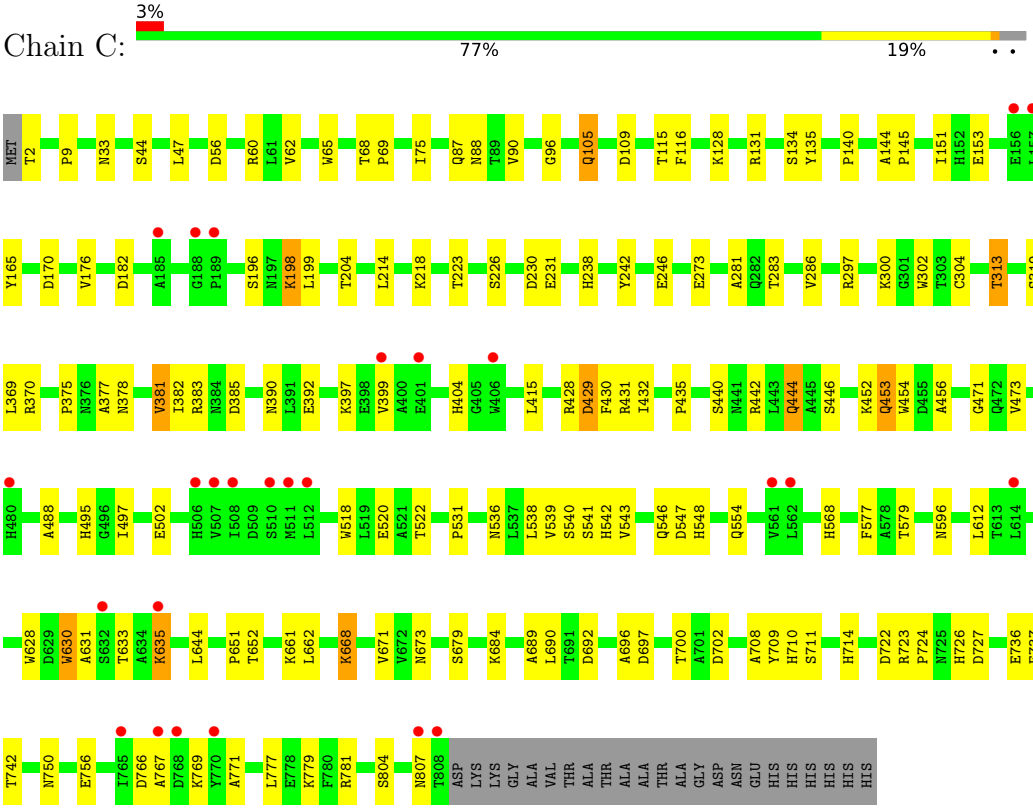
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain B:



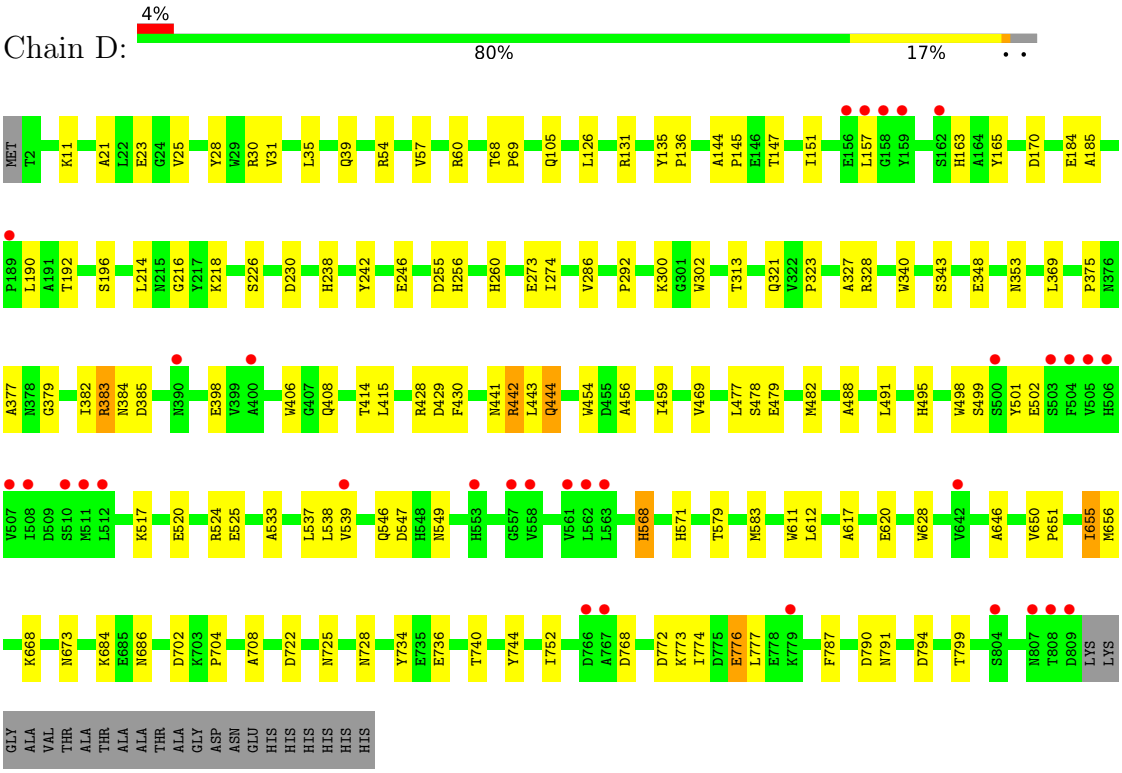
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain C:



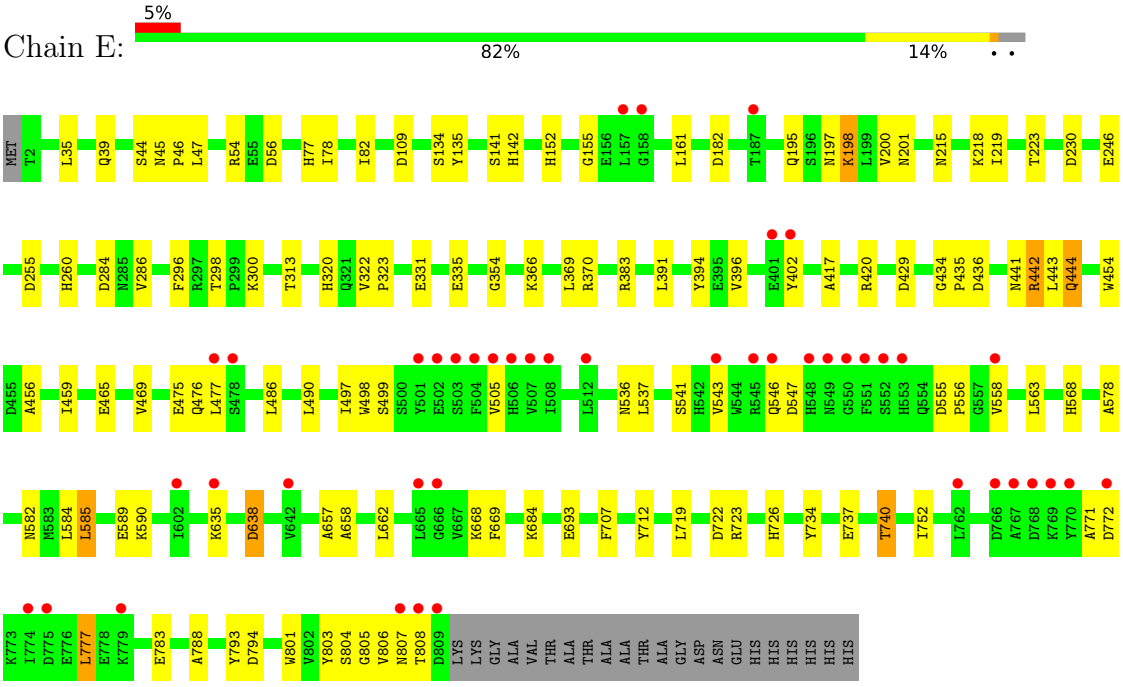
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain D:



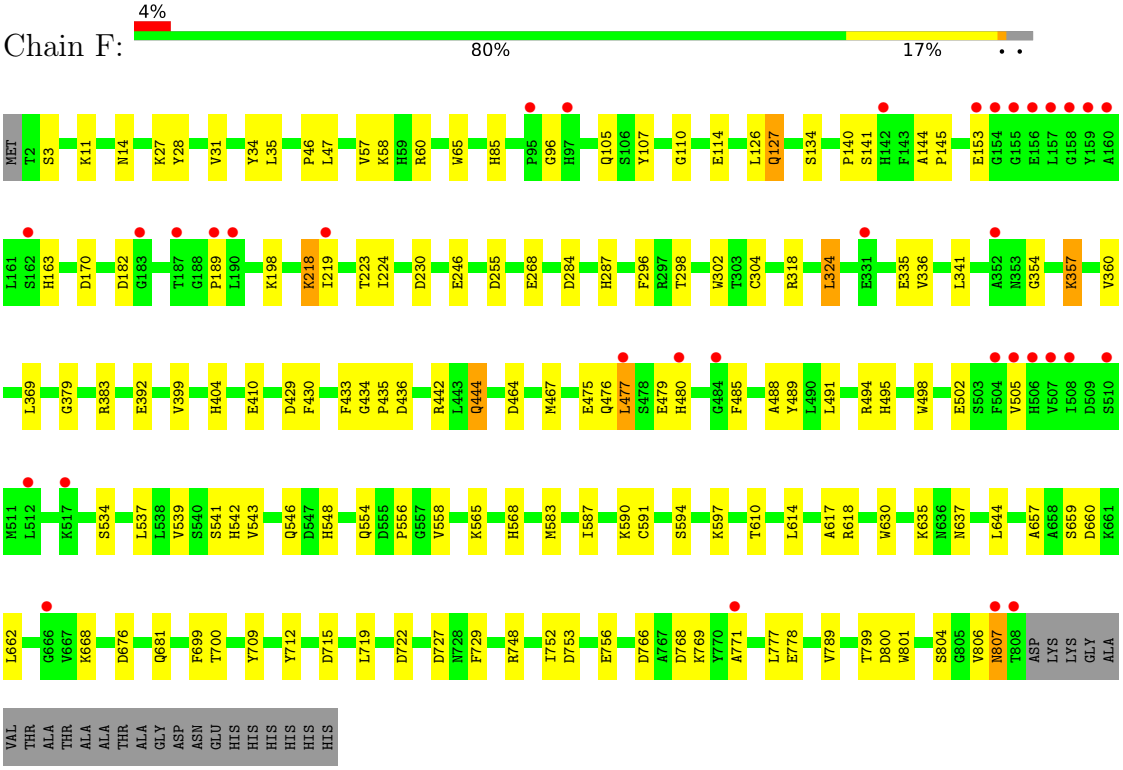
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain E:



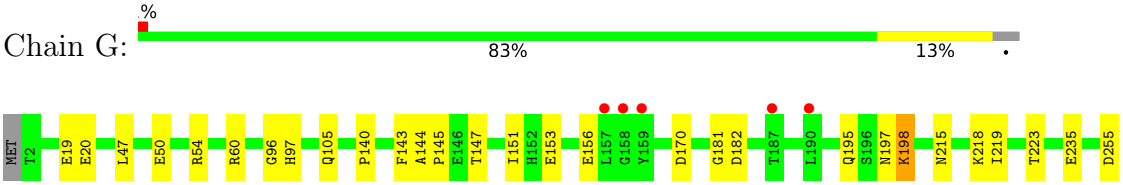
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

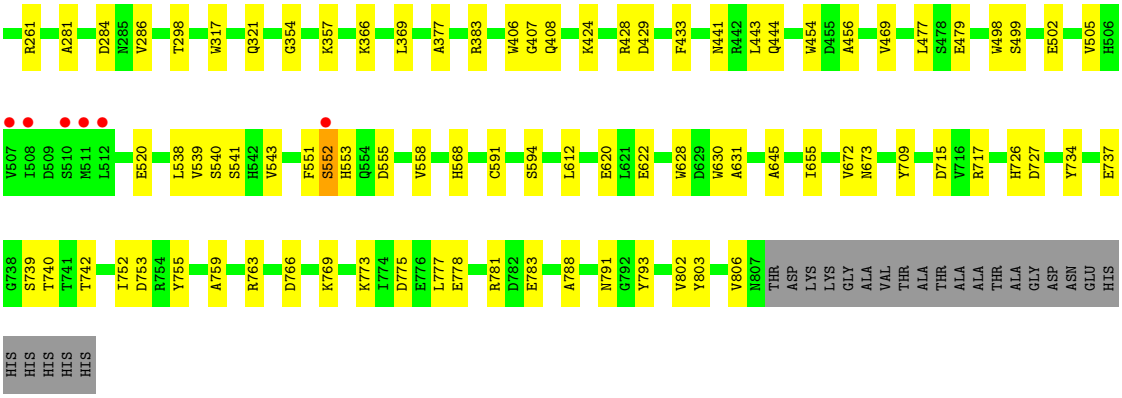
Chain F:



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

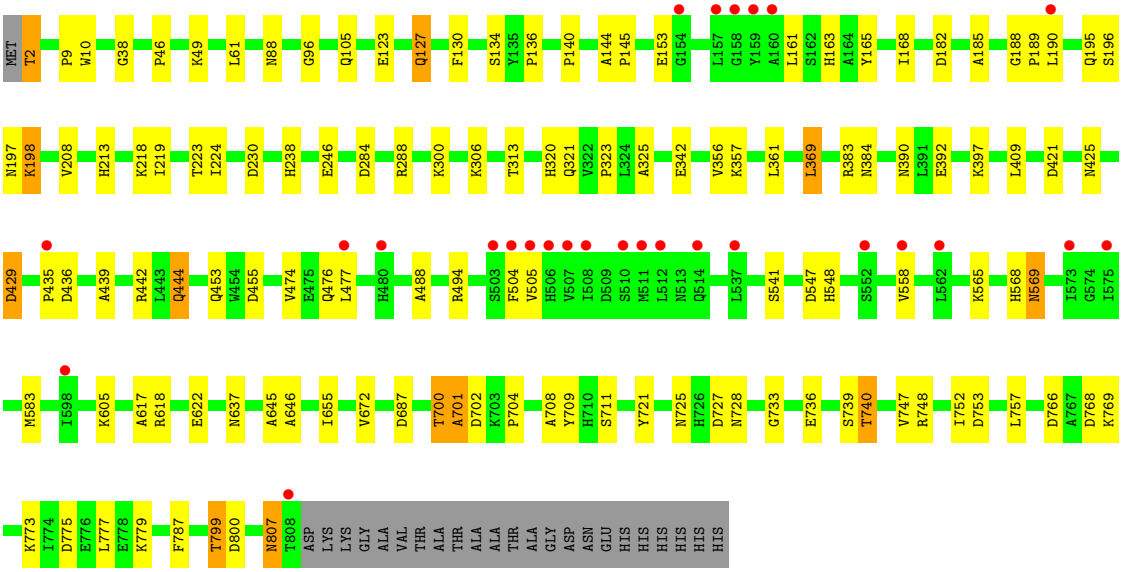
Chain G:





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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.62Å 185.80Å 162.89Å 90.00° 99.61° 90.00°	Depositor
Resolution (Å)	46.80 – 2.50 46.76 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.80-2.50) 62.8 (46.76-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	16.17 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.161 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	21065 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	52781	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, CA, TPP, SIN, MLA

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	0.70	0/6595	0.86	0/8970
1	B	0.71	1/6595 (0.0%)	0.89	0/8970
1	C	0.72	0/6595	0.86	0/8970
1	D	0.72	0/6614	0.85	0/8996
1	E	0.70	0/6614	0.85	0/8996
1	F	0.69	0/6595	0.85	1/8970 (0.0%)
1	G	0.71	0/6608	0.88	1/8987 (0.0%)
1	H	0.69	0/6606	0.86	1/8985 (0.0%)
All	All	0.70	1/52822 (0.0%)	0.86	3/71844 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	589	GLU	CD-OE1	7.17	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	218	LYS	CB-CA-C	5.25	120.90	110.40
1	G	781	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	218	LYS	CB-CA-C	5.05	120.50	110.40

There are no chirality outliers.

There are no planarity outliers.

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	6418	0	6108	49	0
1	B	6418	0	6108	62	0
1	C	6418	0	6108	94	0
1	D	6433	0	6119	79	0
1	E	6436	0	6118	78	0
1	F	6418	0	6108	78	0
1	G	6427	0	6113	69	0
1	H	6428	0	6114	86	0
2	A	26	0	16	5	0
2	B	26	0	16	4	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	5	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	6	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	1	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
7	H	132	0	0	3	0
All	All	52781	0	49050	573	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 573 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%)	51	73
1	B	805/831 (97%)	764 (95%)	39 (5%)	2 (0%)	47	68
1	C	805/831 (97%)	735 (91%)	61 (8%)	9 (1%)	14	26
1	D	807/831 (97%)	736 (91%)	65 (8%)	6 (1%)	22	39
1	E	807/831 (97%)	740 (92%)	62 (8%)	5 (1%)	25	43
1	F	805/831 (97%)	752 (93%)	49 (6%)	4 (0%)	29	48
1	G	806/831 (97%)	748 (93%)	53 (7%)	5 (1%)	25	43
1	H	806/831 (97%)	763 (95%)	39 (5%)	4 (0%)	29	48
All	All	6446/6648 (97%)	5999 (93%)	411 (6%)	36 (1%)	29	43

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	714	HIS
1	G	54	ARG

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Mol	Chain	Res	Type
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%)	657 (97%)	19 (3%)	43	70
1	B	676/693 (98%)	658 (97%)	18 (3%)	44	71
1	C	676/693 (98%)	644 (95%)	32 (5%)	26	49
1	D	678/693 (98%)	650 (96%)	28 (4%)	30	55
1	E	678/693 (98%)	649 (96%)	29 (4%)	29	53
1	F	676/693 (98%)	648 (96%)	28 (4%)	30	55
1	G	677/693 (98%)	655 (97%)	22 (3%)	39	65
1	H	677/693 (98%)	649 (96%)	28 (4%)	30	55
All	All	5414/5544 (98%)	5210 (96%)	204 (4%)	33	58

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	668	LYS
1	F	494	ARG
1	H	775	ASP
1	E	719	LEU
1	F	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	786	GLN
1	G	807	ASN

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Mol	Chain	Res	Type
1	F	321	GLN
1	F	548	HIS
1	H	127	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	TPP	A	900	3	22,27,27	0.76	0	29,40,40	1.22	3 (10%)
4	LMR	B	902	-	8,8,8	1.16	0	10,10,10	1.57	2 (20%)
2	TPP	H	902	3	22,27,27	0.60	0	29,40,40	1.09	1 (3%)
2	TPP	E	902	3	22,27,27	0.72	0	29,40,40	0.96	2 (6%)
2	TPP	B	903	3	22,27,27	0.69	0	29,40,40	1.23	4 (13%)
4	LMR	B	901	-	8,8,8	1.45	0	10,10,10	1.49	1 (10%)
6	SIN	E	904	-	7,7,7	1.16	0	8,8,8	1.17	0
6	SIN	G	903	-	7,7,7	1.20	0	8,8,8	0.92	0
5	MLA	E	901	-	6,6,6	1.25	0	7,7,7	1.13	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TPP	C	900	3	22,27,27	0.73	0	29,40,40	0.88	0
2	TPP	G	901	3	22,27,27	0.60	0	29,40,40	1.06	2 (6%)
5	MLA	D	901	-	6,6,6	1.06	0	7,7,7	0.93	0
2	TPP	F	900	3	22,27,27	0.75	0	29,40,40	0.93	1 (3%)
5	MLA	D	902	-	6,6,6	1.43	0	7,7,7	1.26	1 (14%)
6	SIN	H	901	-	7,7,7	1.35	0	8,8,8	1.30	1 (12%)
2	TPP	D	903	3	22,27,27	0.55	0	29,40,40	1.04	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	TPP	A	900	3	-	4/16/17/17	0/2/2/2
4	LMR	B	902	-	-	4/8/8/8	-
2	TPP	H	902	3	-	3/16/17/17	0/2/2/2
2	TPP	E	902	3	-	7/16/17/17	0/2/2/2
2	TPP	B	903	3	-	1/16/17/17	0/2/2/2
4	LMR	B	901	-	-	2/8/8/8	-
6	SIN	E	904	-	-	1/5/5/5	-
6	SIN	G	903	-	-	3/5/5/5	-
5	MLA	E	901	-	-	2/4/4/4	-
2	TPP	C	900	3	-	4/16/17/17	0/2/2/2
2	TPP	G	901	3	-	8/16/17/17	0/2/2/2
5	MLA	D	901	-	-	2/4/4/4	-
2	TPP	F	900	3	-	3/16/17/17	0/2/2/2
5	MLA	D	902	-	-	0/4/4/4	-
6	SIN	H	901	-	-	2/5/5/5	-
2	TPP	D	903	3	-	6/16/17/17	0/2/2/2

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	LMR	C2-C3-C4	3.12	119.84	112.13
2	B	903	TPP	O3B-PB-O3A	-2.82	95.17	104.64
2	A	900	TPP	O2B-PB-O3A	2.75	113.87	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	LMR	O1A-C1-C2	-2.70	117.26	122.54
2	F	900	TPP	C7'-N3-C2	-2.58	120.69	125.35

There are no chirality outliers.

5 of 52 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	D	903	TPP	C4'-C5'-C7'-N3
2	D	903	TPP	C4-C5-C6-C7
2	E	902	TPP	C4'-C5'-C7'-N3

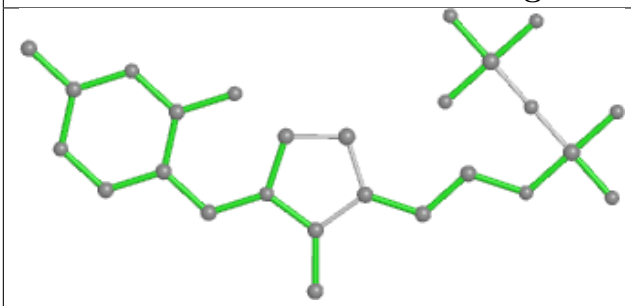
There are no ring outliers.

12 monomers are involved in 42 short contacts:

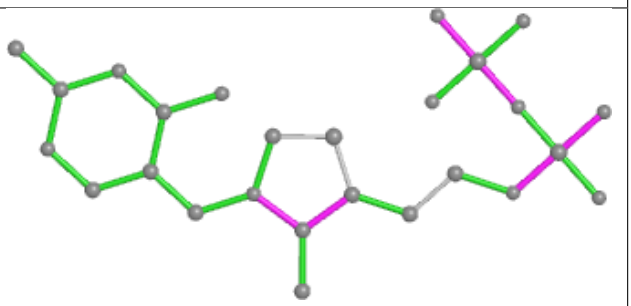
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	TPP	5	0
4	B	902	LMR	1	0
2	H	902	TPP	6	0
2	E	902	TPP	5	0
2	B	903	TPP	4	0
5	E	901	MLA	1	0
2	C	900	TPP	6	0
2	G	901	TPP	5	0
5	D	901	MLA	4	0
2	F	900	TPP	1	0
5	D	902	MLA	2	0
2	D	903	TPP	7	0

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 then 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.

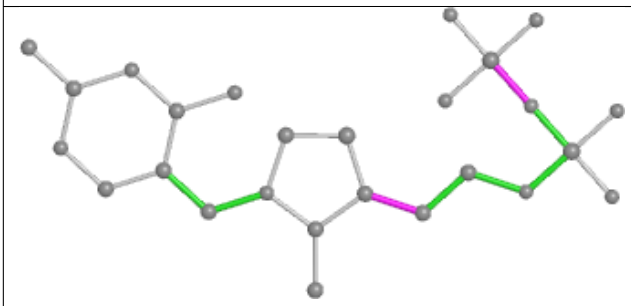
Ligand TPP A 900



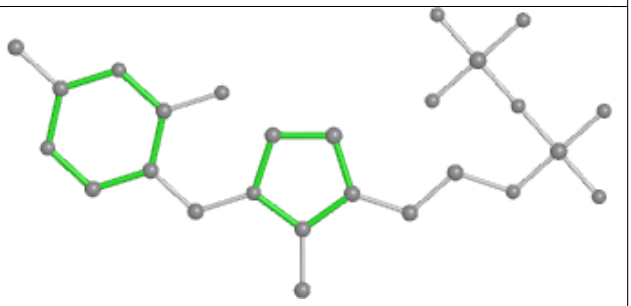
Bond lengths



Bond angles

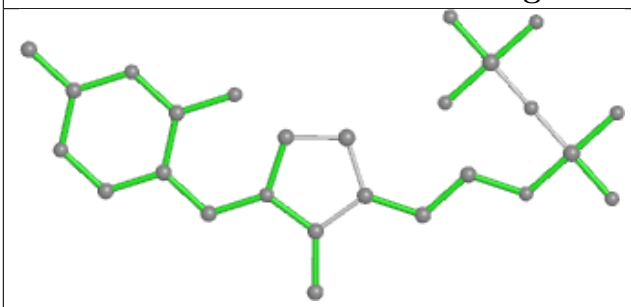


Torsions



Rings

Ligand TPP H 902



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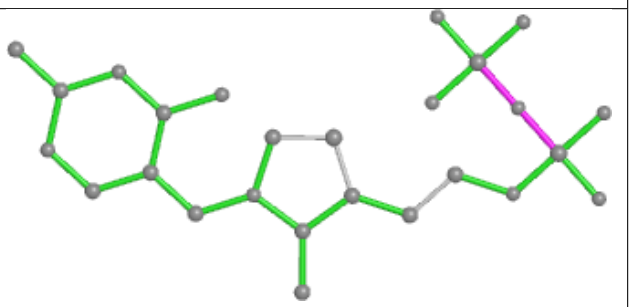

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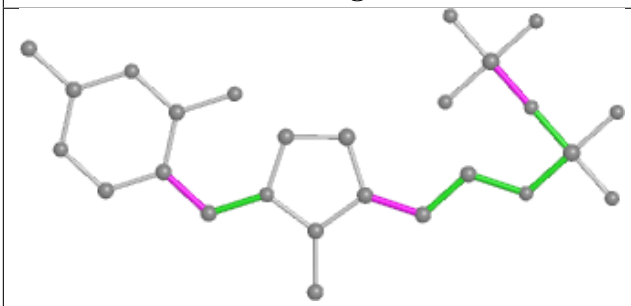

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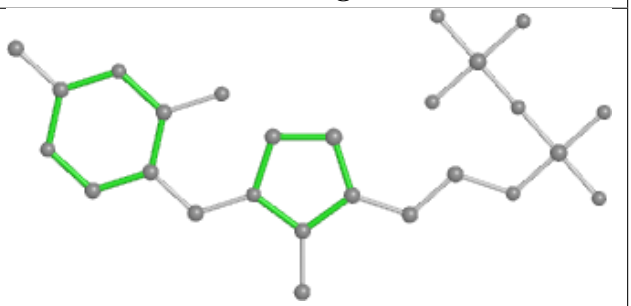
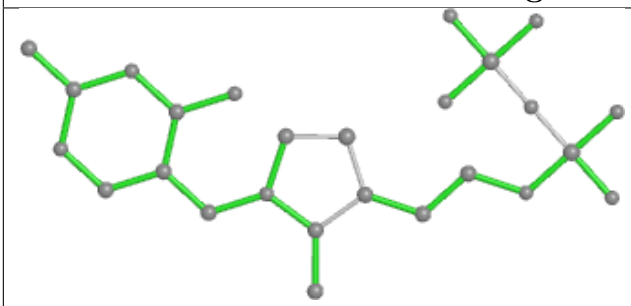


Rings

Ligand TPP E 902



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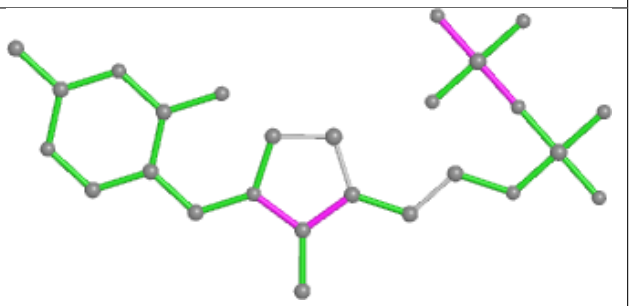

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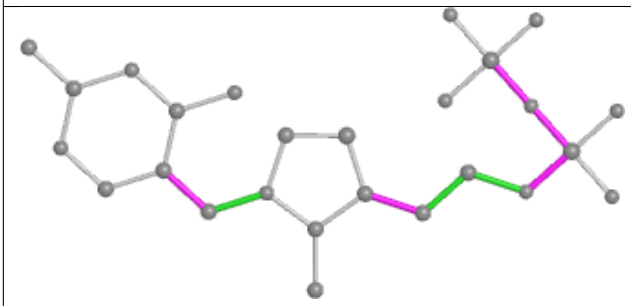

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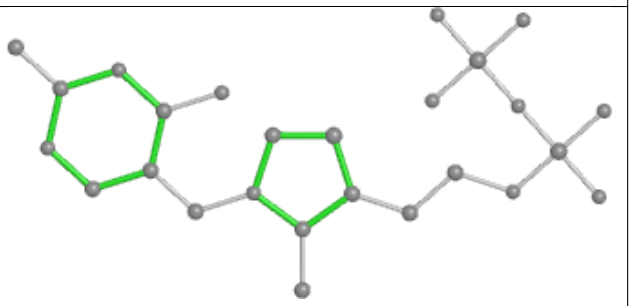

Rings

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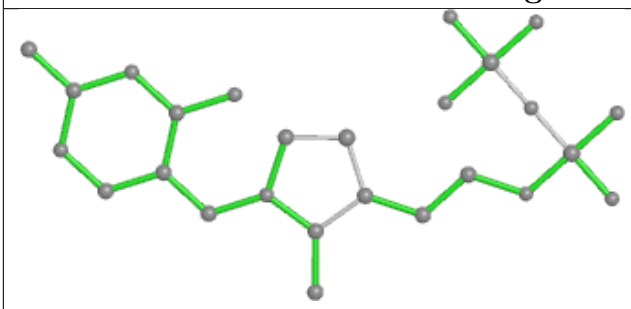

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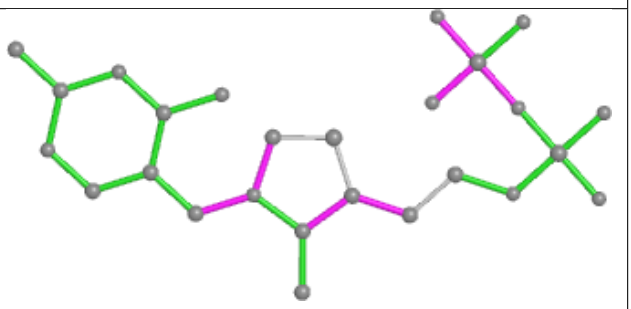

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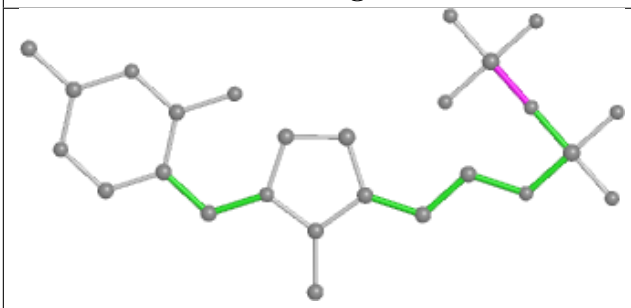

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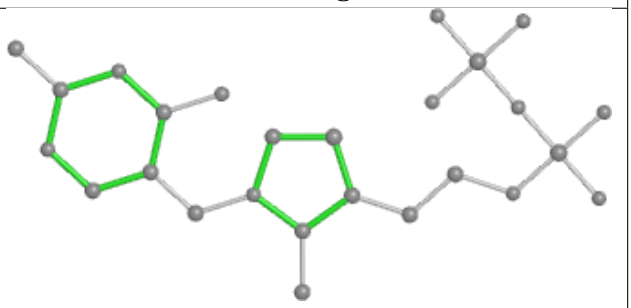
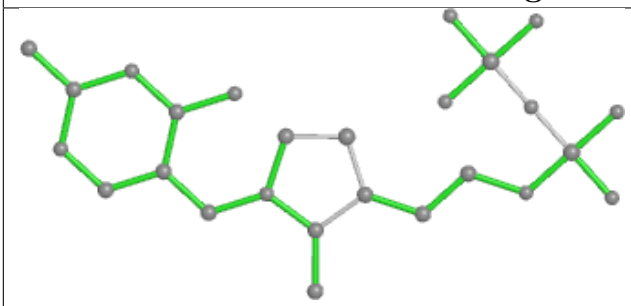


Rings

Ligand TPP C 900



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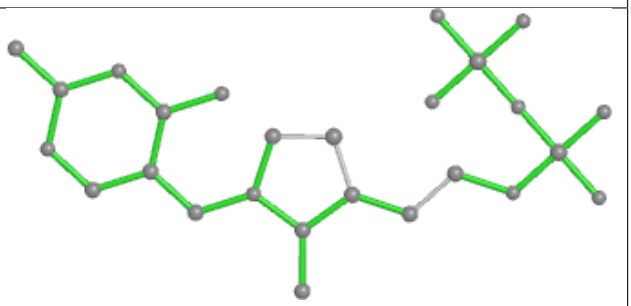

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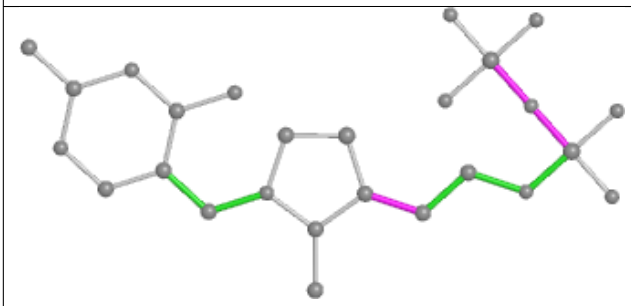

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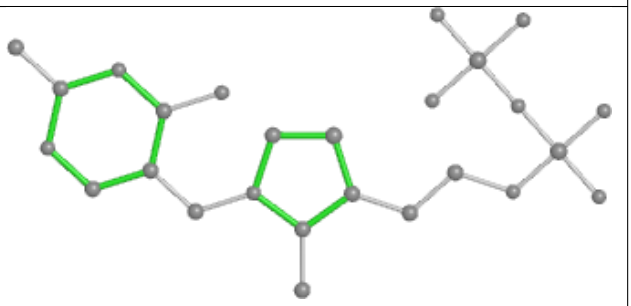
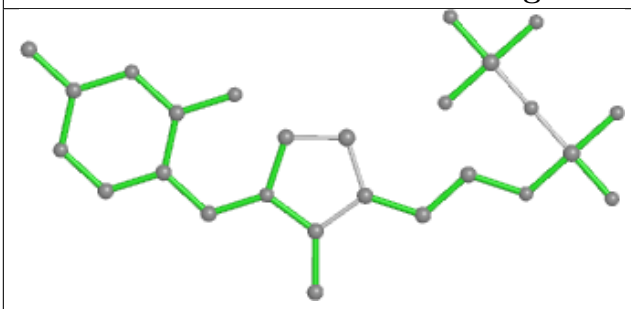
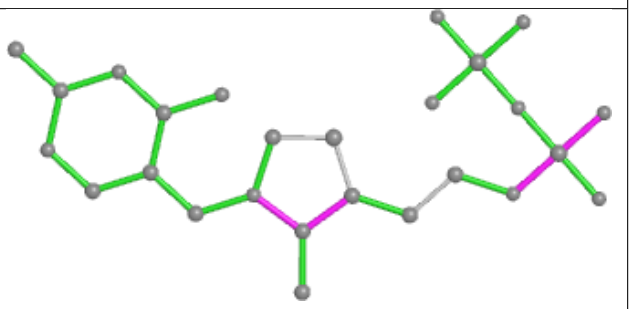


Rings

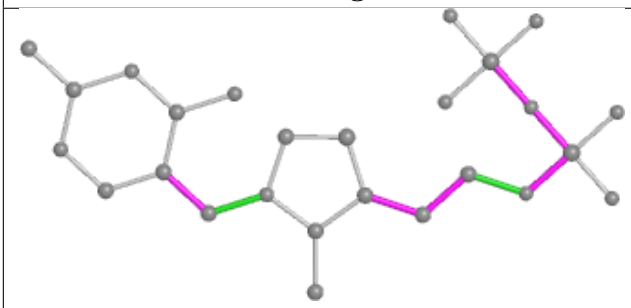
Ligand TPP G 901



Bond lengths



Bond angles



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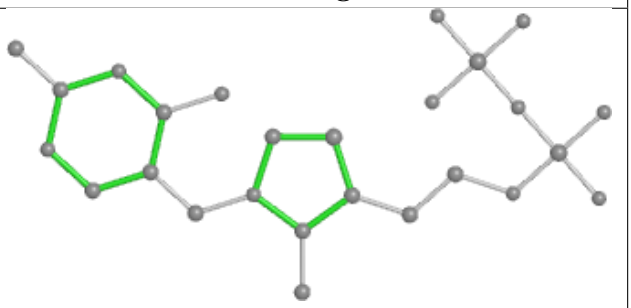
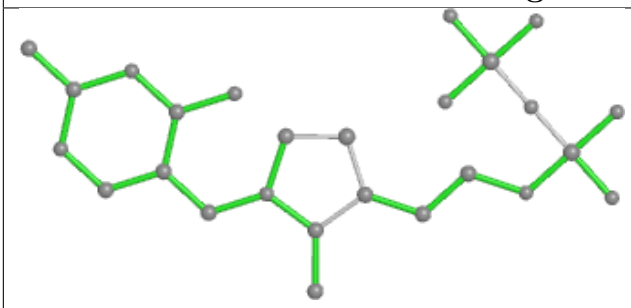


Rings

Ligand TPP F 900



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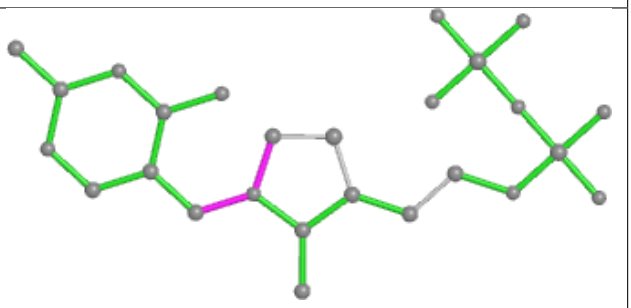
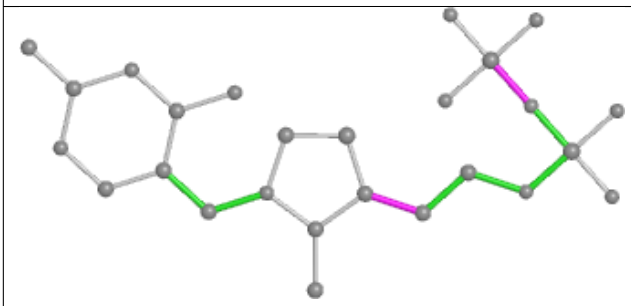
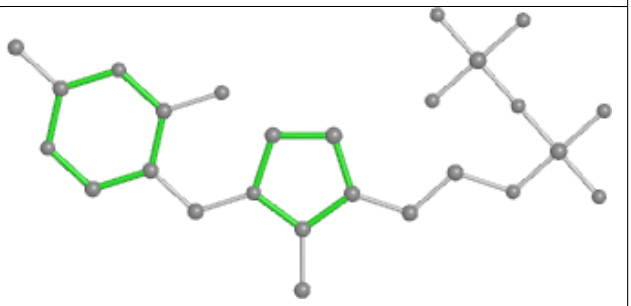


Bond angles

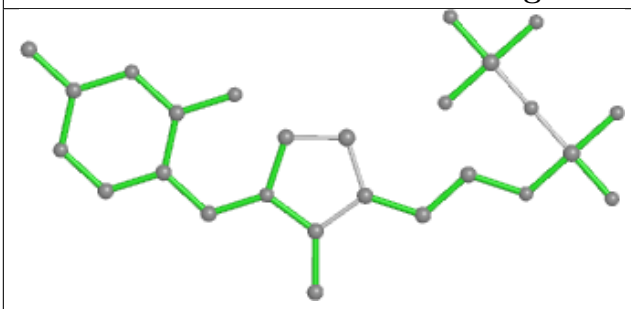


Torsions

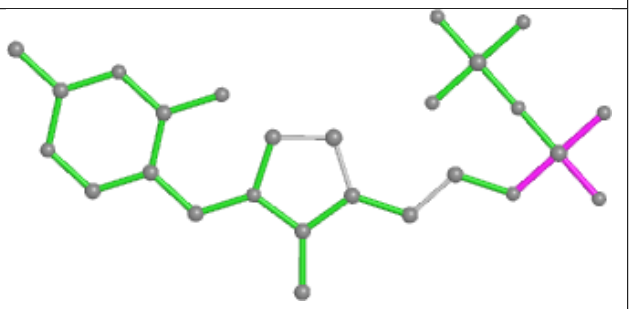


Rings

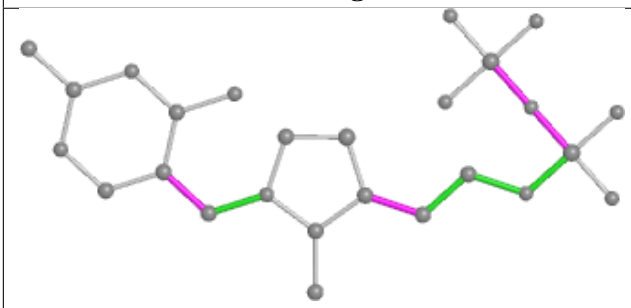
Ligand TPP D 903



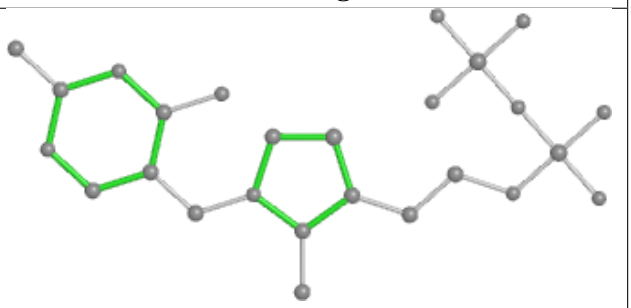
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	807/831 (97%)	-0.51	12 (1%)	73	75	33, 45, 69, 118	0
1	B	807/831 (97%)	-0.46	21 (2%)	56	59	32, 45, 68, 120	0
1	C	807/831 (97%)	-0.18	29 (3%)	42	46	44, 66, 96, 141	0
1	D	808/831 (97%)	-0.14	33 (4%)	37	40	42, 67, 98, 128	0
1	E	808/831 (97%)	-0.22	44 (5%)	25	27	37, 57, 95, 129	0
1	F	807/831 (97%)	-0.21	34 (4%)	36	39	40, 60, 89, 121	0
1	G	806/831 (96%)	-0.47	11 (1%)	75	77	34, 50, 77, 104	0
1	H	807/831 (97%)	-0.34	27 (3%)	46	50	37, 53, 77, 118	0
All	All	6457/6648 (97%)	-0.32	211 (3%)	46	50	32, 55, 89, 141	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	507	VAL	5.6
1	D	507	VAL	5.5
1	F	157	LEU	5.4
1	E	666	GLY	5.2
1	D	808	THR	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

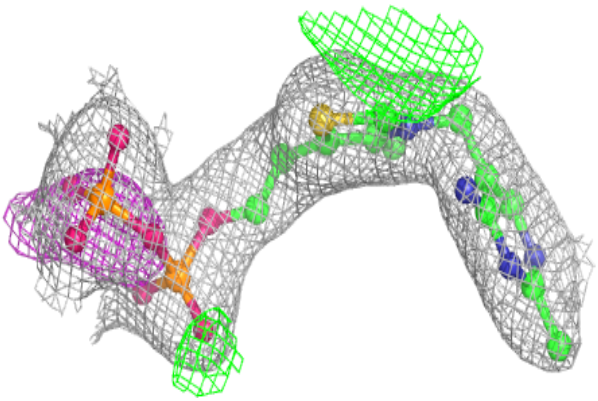
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

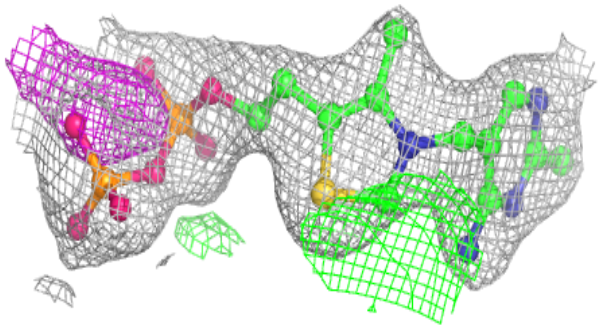
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SIN	G	903	8/8	0.67	1.64	59,67,70,71	8
5	MLA	D	902	7/7	0.72	0.97	42,42,51,53	7
6	SIN	E	904	8/8	0.72	1.61	48,55,61,62	8
4	LMR	B	902	9/9	0.72	1.05	36,49,53,55	9
5	MLA	E	901	7/7	0.74	1.20	38,43,53,57	7
6	SIN	H	901	8/8	0.75	1.31	38,46,54,55	8
3	CA	D	904	1/1	0.81	0.04	71,71,71,71	0
3	CA	H	903	1/1	0.82	0.04	69,69,69,69	0
4	LMR	B	901	9/9	0.86	1.45	39,42,48,53	9
3	CA	G	902	1/1	0.88	0.14	70,70,70,70	0
3	CA	A	901	1/1	0.89	0.04	60,60,60,60	0
3	CA	B	904	1/1	0.89	0.08	55,55,55,55	0
5	MLA	D	901	7/7	0.90	1.14	42,52,55,56	7
3	CA	F	901	1/1	0.91	0.04	79,79,79,79	0
3	CA	E	903	1/1	0.92	0.04	62,62,62,62	0
3	CA	C	901	1/1	0.92	0.05	70,70,70,70	0
2	TPP	A	900	26/26	0.94	0.20	37,44,48,58	0
2	TPP	C	900	26/26	0.95	0.17	49,60,66,90	0
2	TPP	D	903	26/26	0.95	0.14	42,56,65,83	0
2	TPP	E	902	26/26	0.95	0.16	40,47,54,58	0
2	TPP	F	900	26/26	0.95	0.22	48,60,69,74	0
2	TPP	B	903	26/26	0.95	0.18	37,42,46,52	0
2	TPP	G	901	26/26	0.96	0.18	38,46,52,54	0
2	TPP	H	902	26/26	0.96	0.15	43,50,55,60	0

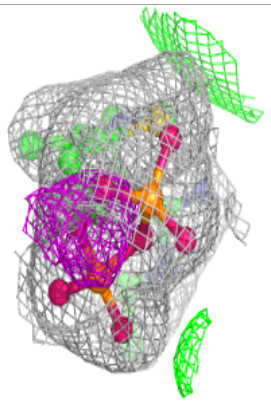
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP 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)

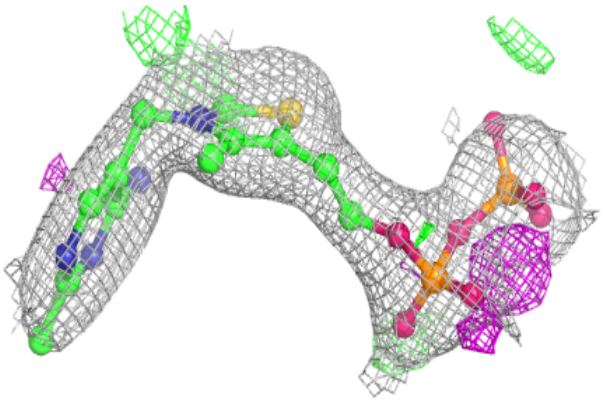


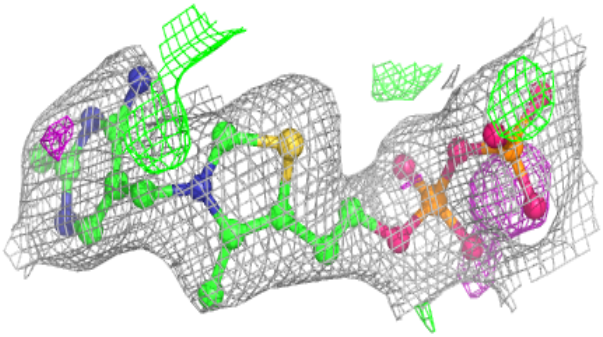


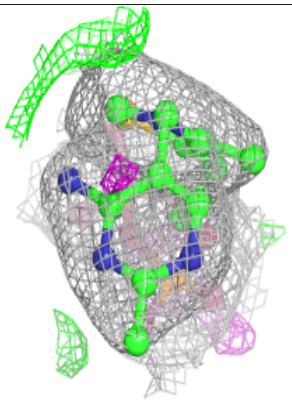


Electron density around TPP C 900:

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

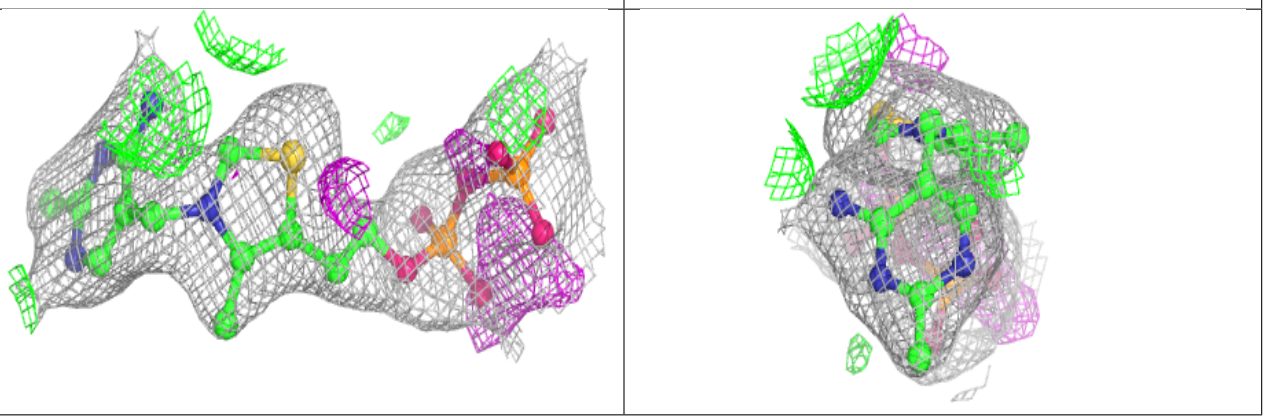






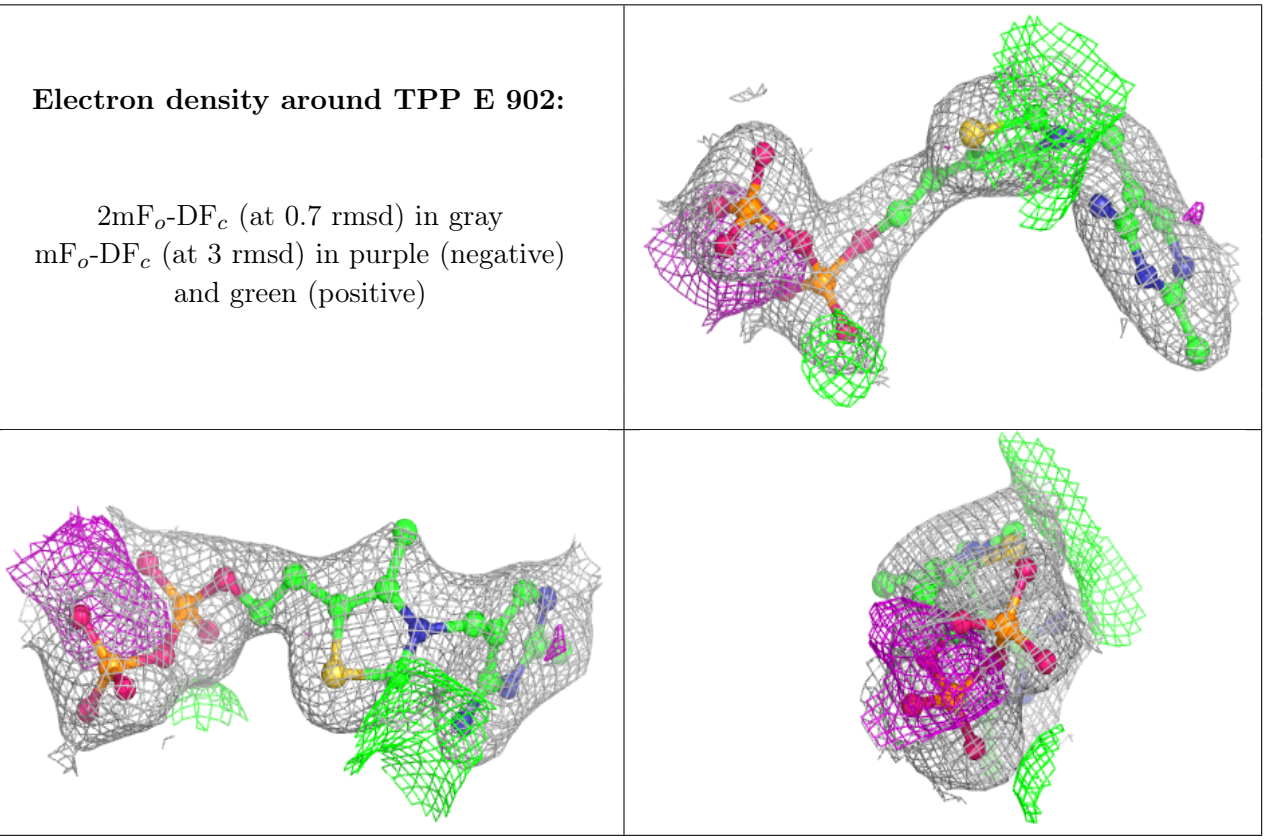
Electron density around TPP D 903:

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



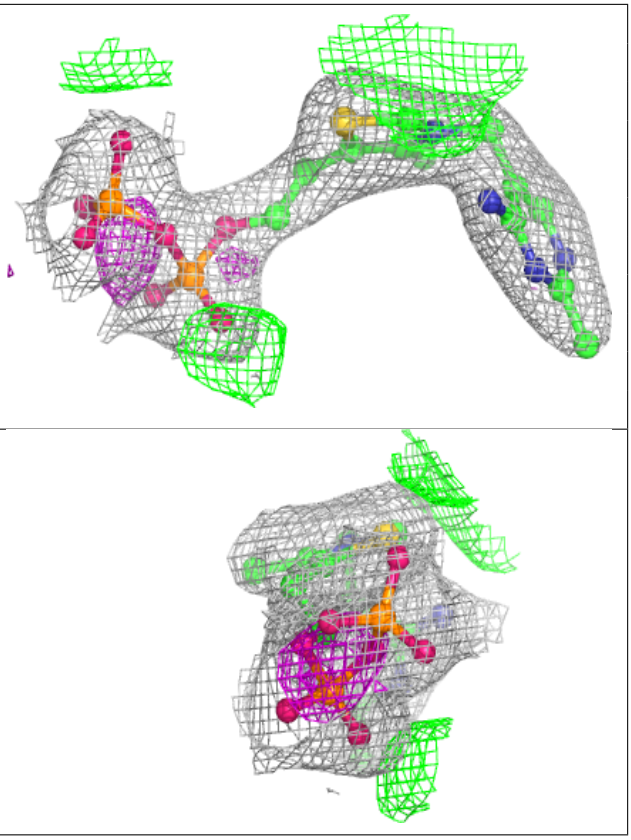
Electron density around TPP E 902:

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



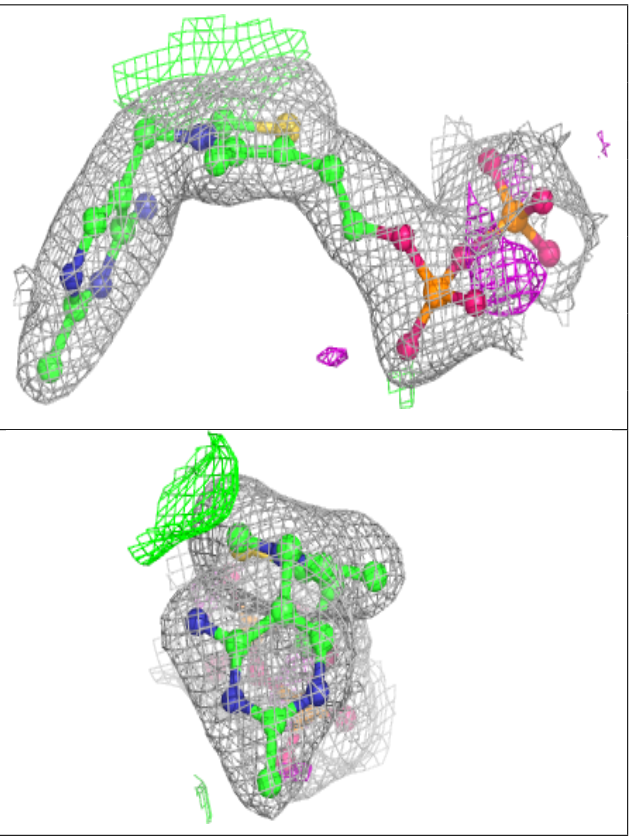
Electron density around TPP F 900:

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



Electron density around TPP B 903:

$2mF_o$-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:

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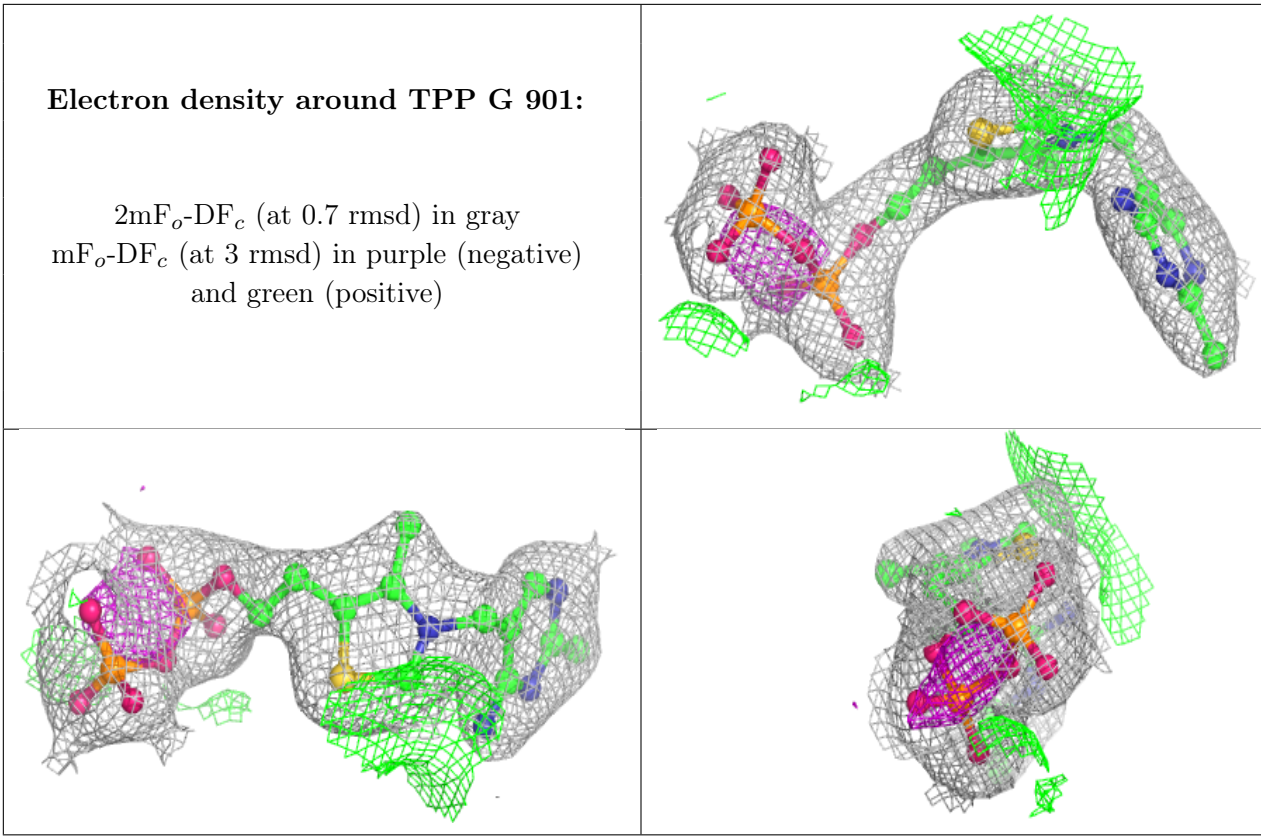
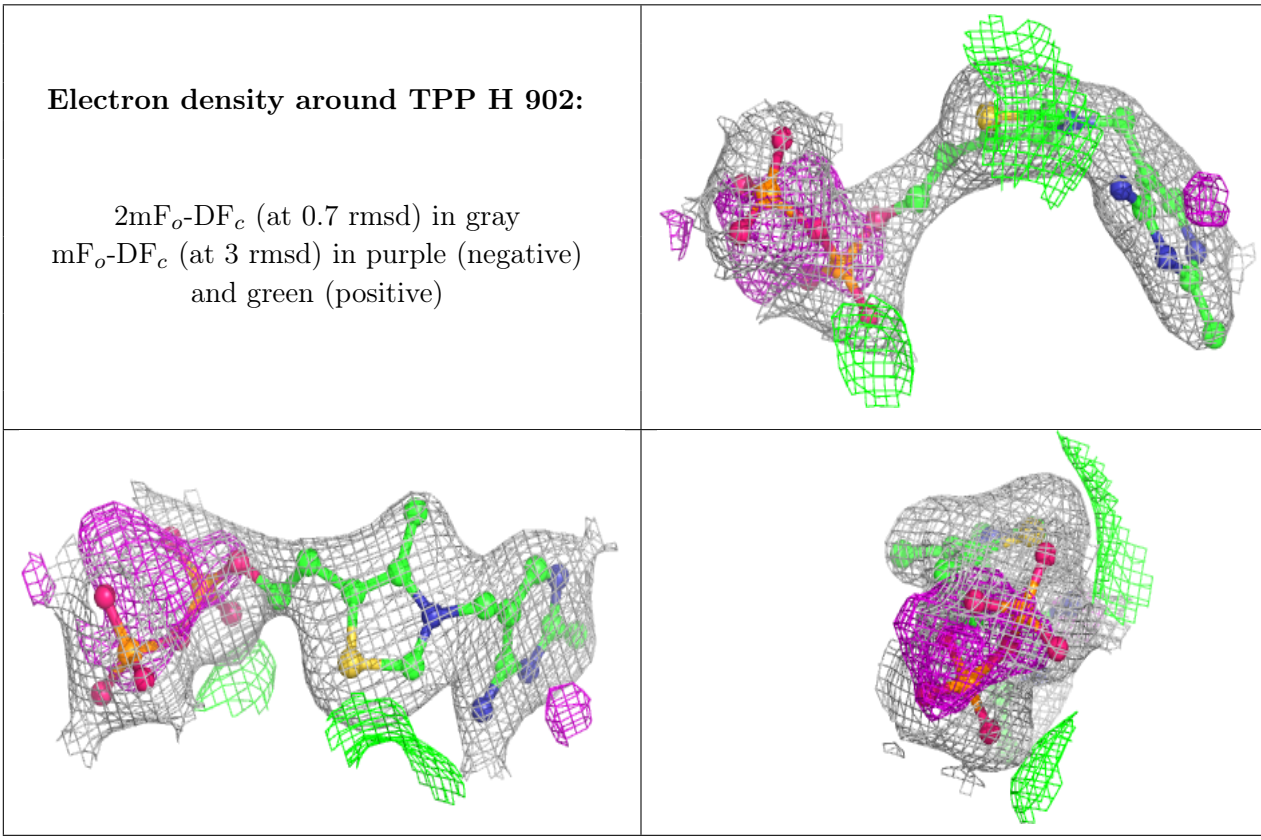
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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)



6.5 Other polymers (i)

There are no such residues in this entry.