



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:51 AM UTC

PDB ID : 8A5K / pdb_00008a5k
Title : Structural analysis of 1-deoxy-D-xylulose 5-phosphate synthase from *Pseudomonas aeruginosa* and *Klebsiella pneumoniae* reveals conformational changes upon cofactor binding
Authors : Hamid, R.; Hirsch, A.
Deposited on : 2022-06-15
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) 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

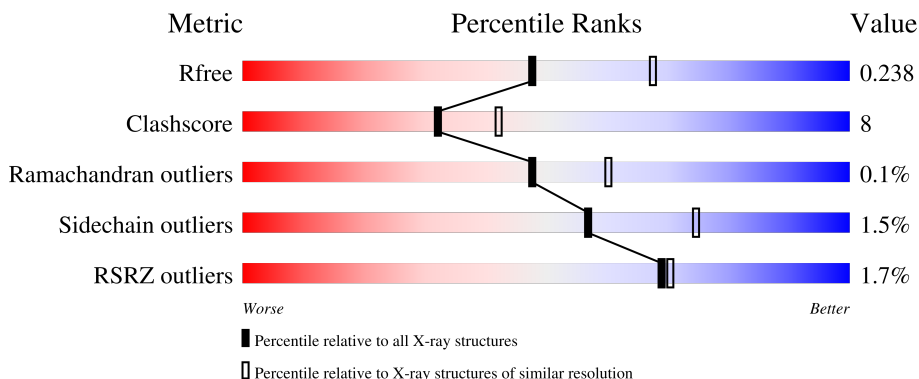
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	622	 2% 77% 13% 10%
1	B	622	 2% 73% 17% 9%
1	C	622	 2% 75% 15% 10%
1	D	622	 % 78% 12% 10%

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Mol	Chain	Length	Quality of chain
1	E	622	 <p>%</p> <p>74% 16% 9%</p>
1	F	622	 <p>2%</p> <p>73% 17% 10%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 27452 atoms, of which 104 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	562	4277	2703	744	809	21	0	0	0
1	B	563	4284	2707	745	811	21	0	0	0
1	C	562	4266	2693	744	808	21	0	0	0
1	D	560	4264	2696	742	805	21	0	0	0
1	E	563	4288	2712	746	809	21	0	0	0
1	F	560	4266	2698	741	806	21	0	0	0

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B7V7R4
A	2	GLY	-	expression tag	UNP B7V7R4
A	3	SER	-	expression tag	UNP B7V7R4
A	4	SER	-	expression tag	UNP B7V7R4
A	5	HIS	-	expression tag	UNP B7V7R4
A	6	HIS	-	expression tag	UNP B7V7R4
A	7	HIS	-	expression tag	UNP B7V7R4
A	8	HIS	-	expression tag	UNP B7V7R4
A	9	HIS	-	expression tag	UNP B7V7R4
A	10	HIS	-	expression tag	UNP B7V7R4
A	11	SER	-	expression tag	UNP B7V7R4
A	12	SER	-	expression tag	UNP B7V7R4
A	13	GLY	-	expression tag	UNP B7V7R4
A	14	LEU	-	expression tag	UNP B7V7R4
A	15	VAL	-	expression tag	UNP B7V7R4
A	16	PRO	-	expression tag	UNP B7V7R4
A	17	ARG	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP B7V7R4
A	19	SER	-	expression tag	UNP B7V7R4
A	20	MET	-	expression tag	UNP B7V7R4
A	21	GLU	-	expression tag	UNP B7V7R4
A	22	ASN	-	expression tag	UNP B7V7R4
A	23	LEU	-	expression tag	UNP B7V7R4
A	24	TYR	-	expression tag	UNP B7V7R4
A	25	PHE	-	expression tag	UNP B7V7R4
A	26	GLN	-	expression tag	UNP B7V7R4
A	27	SER	-	expression tag	UNP B7V7R4
A	28	HIS	-	expression tag	UNP B7V7R4
A	235	GLY	-	linker	UNP B7V7R4
A	236	GLY	-	linker	UNP B7V7R4
A	237	GLY	-	linker	UNP B7V7R4
A	238	GLY	-	linker	UNP B7V7R4
A	239	GLY	-	linker	UNP B7V7R4
A	240	GLY	-	linker	UNP B7V7R4
B	1	MET	-	initiating methionine	UNP B7V7R4
B	2	GLY	-	expression tag	UNP B7V7R4
B	3	SER	-	expression tag	UNP B7V7R4
B	4	SER	-	expression tag	UNP B7V7R4
B	5	HIS	-	expression tag	UNP B7V7R4
B	6	HIS	-	expression tag	UNP B7V7R4
B	7	HIS	-	expression tag	UNP B7V7R4
B	8	HIS	-	expression tag	UNP B7V7R4
B	9	HIS	-	expression tag	UNP B7V7R4
B	10	HIS	-	expression tag	UNP B7V7R4
B	11	SER	-	expression tag	UNP B7V7R4
B	12	SER	-	expression tag	UNP B7V7R4
B	13	GLY	-	expression tag	UNP B7V7R4
B	14	LEU	-	expression tag	UNP B7V7R4
B	15	VAL	-	expression tag	UNP B7V7R4
B	16	PRO	-	expression tag	UNP B7V7R4
B	17	ARG	-	expression tag	UNP B7V7R4
B	18	GLY	-	expression tag	UNP B7V7R4
B	19	SER	-	expression tag	UNP B7V7R4
B	20	MET	-	expression tag	UNP B7V7R4
B	21	GLU	-	expression tag	UNP B7V7R4
B	22	ASN	-	expression tag	UNP B7V7R4
B	23	LEU	-	expression tag	UNP B7V7R4
B	24	TYR	-	expression tag	UNP B7V7R4
B	25	PHE	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLN	-	expression tag	UNP B7V7R4
B	27	SER	-	expression tag	UNP B7V7R4
B	28	HIS	-	expression tag	UNP B7V7R4
B	235	GLY	-	linker	UNP B7V7R4
B	236	GLY	-	linker	UNP B7V7R4
B	237	GLY	-	linker	UNP B7V7R4
B	238	GLY	-	linker	UNP B7V7R4
B	239	GLY	-	linker	UNP B7V7R4
B	240	GLY	-	linker	UNP B7V7R4
C	1	MET	-	initiating methionine	UNP B7V7R4
C	2	GLY	-	expression tag	UNP B7V7R4
C	3	SER	-	expression tag	UNP B7V7R4
C	4	SER	-	expression tag	UNP B7V7R4
C	5	HIS	-	expression tag	UNP B7V7R4
C	6	HIS	-	expression tag	UNP B7V7R4
C	7	HIS	-	expression tag	UNP B7V7R4
C	8	HIS	-	expression tag	UNP B7V7R4
C	9	HIS	-	expression tag	UNP B7V7R4
C	10	HIS	-	expression tag	UNP B7V7R4
C	11	SER	-	expression tag	UNP B7V7R4
C	12	SER	-	expression tag	UNP B7V7R4
C	13	GLY	-	expression tag	UNP B7V7R4
C	14	LEU	-	expression tag	UNP B7V7R4
C	15	VAL	-	expression tag	UNP B7V7R4
C	16	PRO	-	expression tag	UNP B7V7R4
C	17	ARG	-	expression tag	UNP B7V7R4
C	18	GLY	-	expression tag	UNP B7V7R4
C	19	SER	-	expression tag	UNP B7V7R4
C	20	MET	-	expression tag	UNP B7V7R4
C	21	GLU	-	expression tag	UNP B7V7R4
C	22	ASN	-	expression tag	UNP B7V7R4
C	23	LEU	-	expression tag	UNP B7V7R4
C	24	TYR	-	expression tag	UNP B7V7R4
C	25	PHE	-	expression tag	UNP B7V7R4
C	26	GLN	-	expression tag	UNP B7V7R4
C	27	SER	-	expression tag	UNP B7V7R4
C	28	HIS	-	expression tag	UNP B7V7R4
C	235	GLY	-	linker	UNP B7V7R4
C	236	GLY	-	linker	UNP B7V7R4
C	237	GLY	-	linker	UNP B7V7R4
C	238	GLY	-	linker	UNP B7V7R4
C	239	GLY	-	linker	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	GLY	-	linker	UNP B7V7R4
D	1	MET	-	initiating methionine	UNP B7V7R4
D	2	GLY	-	expression tag	UNP B7V7R4
D	3	SER	-	expression tag	UNP B7V7R4
D	4	SER	-	expression tag	UNP B7V7R4
D	5	HIS	-	expression tag	UNP B7V7R4
D	6	HIS	-	expression tag	UNP B7V7R4
D	7	HIS	-	expression tag	UNP B7V7R4
D	8	HIS	-	expression tag	UNP B7V7R4
D	9	HIS	-	expression tag	UNP B7V7R4
D	10	HIS	-	expression tag	UNP B7V7R4
D	11	SER	-	expression tag	UNP B7V7R4
D	12	SER	-	expression tag	UNP B7V7R4
D	13	GLY	-	expression tag	UNP B7V7R4
D	14	LEU	-	expression tag	UNP B7V7R4
D	15	VAL	-	expression tag	UNP B7V7R4
D	16	PRO	-	expression tag	UNP B7V7R4
D	17	ARG	-	expression tag	UNP B7V7R4
D	18	GLY	-	expression tag	UNP B7V7R4
D	19	SER	-	expression tag	UNP B7V7R4
D	20	MET	-	expression tag	UNP B7V7R4
D	21	GLU	-	expression tag	UNP B7V7R4
D	22	ASN	-	expression tag	UNP B7V7R4
D	23	LEU	-	expression tag	UNP B7V7R4
D	24	TYR	-	expression tag	UNP B7V7R4
D	25	PHE	-	expression tag	UNP B7V7R4
D	26	GLN	-	expression tag	UNP B7V7R4
D	27	SER	-	expression tag	UNP B7V7R4
D	28	HIS	-	expression tag	UNP B7V7R4
D	235	GLY	-	linker	UNP B7V7R4
D	236	GLY	-	linker	UNP B7V7R4
D	237	GLY	-	linker	UNP B7V7R4
D	238	GLY	-	linker	UNP B7V7R4
D	239	GLY	-	linker	UNP B7V7R4
D	240	GLY	-	linker	UNP B7V7R4
E	1	MET	-	initiating methionine	UNP B7V7R4
E	2	GLY	-	expression tag	UNP B7V7R4
E	3	SER	-	expression tag	UNP B7V7R4
E	4	SER	-	expression tag	UNP B7V7R4
E	5	HIS	-	expression tag	UNP B7V7R4
E	6	HIS	-	expression tag	UNP B7V7R4
E	7	HIS	-	expression tag	UNP B7V7R4

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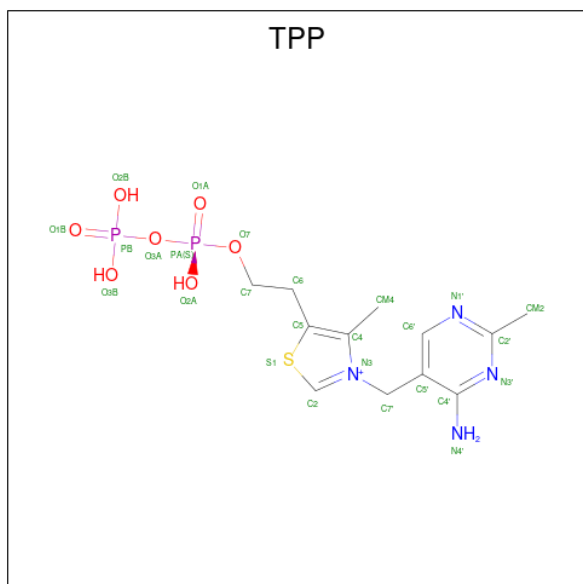
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	HIS	-	expression tag	UNP B7V7R4
E	9	HIS	-	expression tag	UNP B7V7R4
E	10	HIS	-	expression tag	UNP B7V7R4
E	11	SER	-	expression tag	UNP B7V7R4
E	12	SER	-	expression tag	UNP B7V7R4
E	13	GLY	-	expression tag	UNP B7V7R4
E	14	LEU	-	expression tag	UNP B7V7R4
E	15	VAL	-	expression tag	UNP B7V7R4
E	16	PRO	-	expression tag	UNP B7V7R4
E	17	ARG	-	expression tag	UNP B7V7R4
E	18	GLY	-	expression tag	UNP B7V7R4
E	19	SER	-	expression tag	UNP B7V7R4
E	20	MET	-	expression tag	UNP B7V7R4
E	21	GLU	-	expression tag	UNP B7V7R4
E	22	ASN	-	expression tag	UNP B7V7R4
E	23	LEU	-	expression tag	UNP B7V7R4
E	24	TYR	-	expression tag	UNP B7V7R4
E	25	PHE	-	expression tag	UNP B7V7R4
E	26	GLN	-	expression tag	UNP B7V7R4
E	27	SER	-	expression tag	UNP B7V7R4
E	28	HIS	-	expression tag	UNP B7V7R4
E	235	GLY	-	linker	UNP B7V7R4
E	236	GLY	-	linker	UNP B7V7R4
E	237	GLY	-	linker	UNP B7V7R4
E	238	GLY	-	linker	UNP B7V7R4
E	239	GLY	-	linker	UNP B7V7R4
E	240	GLY	-	linker	UNP B7V7R4
F	1	MET	-	initiating methionine	UNP B7V7R4
F	2	GLY	-	expression tag	UNP B7V7R4
F	3	SER	-	expression tag	UNP B7V7R4
F	4	SER	-	expression tag	UNP B7V7R4
F	5	HIS	-	expression tag	UNP B7V7R4
F	6	HIS	-	expression tag	UNP B7V7R4
F	7	HIS	-	expression tag	UNP B7V7R4
F	8	HIS	-	expression tag	UNP B7V7R4
F	9	HIS	-	expression tag	UNP B7V7R4
F	10	HIS	-	expression tag	UNP B7V7R4
F	11	SER	-	expression tag	UNP B7V7R4
F	12	SER	-	expression tag	UNP B7V7R4
F	13	GLY	-	expression tag	UNP B7V7R4
F	14	LEU	-	expression tag	UNP B7V7R4
F	15	VAL	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	PRO	-	expression tag	UNP B7V7R4
F	17	ARG	-	expression tag	UNP B7V7R4
F	18	GLY	-	expression tag	UNP B7V7R4
F	19	SER	-	expression tag	UNP B7V7R4
F	20	MET	-	expression tag	UNP B7V7R4
F	21	GLU	-	expression tag	UNP B7V7R4
F	22	ASN	-	expression tag	UNP B7V7R4
F	23	LEU	-	expression tag	UNP B7V7R4
F	24	TYR	-	expression tag	UNP B7V7R4
F	25	PHE	-	expression tag	UNP B7V7R4
F	26	GLN	-	expression tag	UNP B7V7R4
F	27	SER	-	expression tag	UNP B7V7R4
F	28	HIS	-	expression tag	UNP B7V7R4
F	235	GLY	-	linker	UNP B7V7R4
F	236	GLY	-	linker	UNP B7V7R4
F	237	GLY	-	linker	UNP B7V7R4
F	238	GLY	-	linker	UNP B7V7R4
F	239	GLY	-	linker	UNP B7V7R4
F	240	GLY	-	linker	UNP B7V7R4

- 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	H	N	O			P	S
2	A	1	42	12	16	4	7	2	1	0	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

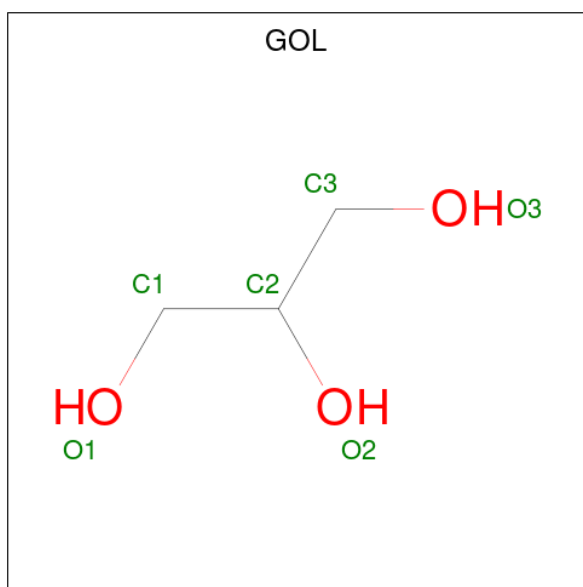
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

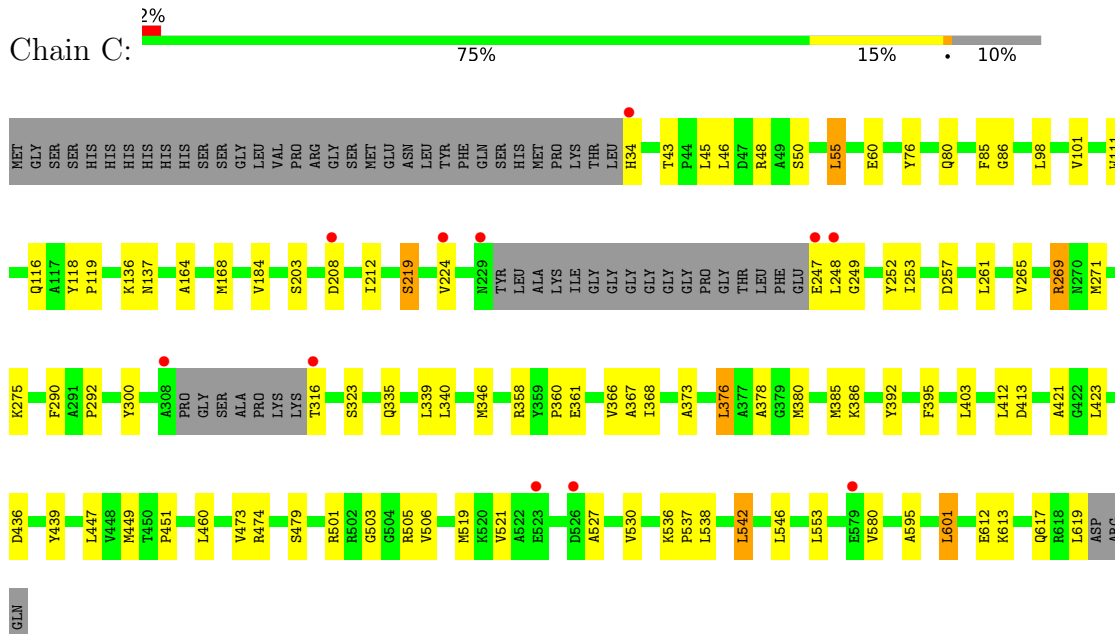


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	D	1	14	3	8	3	0	0

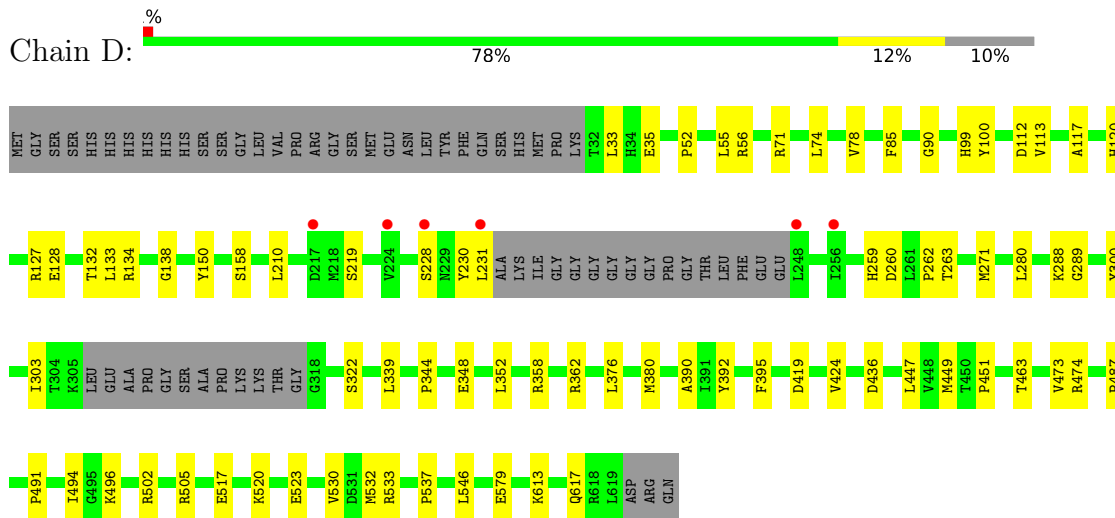
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	271	Total	O	0	0
			271	271		
6	B	238	Total	O	0	0
			238	238		
6	C	249	Total	O	0	0
			249	249		
6	D	262	Total	O	0	0
			262	262		
6	E	253	Total	O	0	0
			253	253		
6	F	254	Total	O	0	0
			254	254		

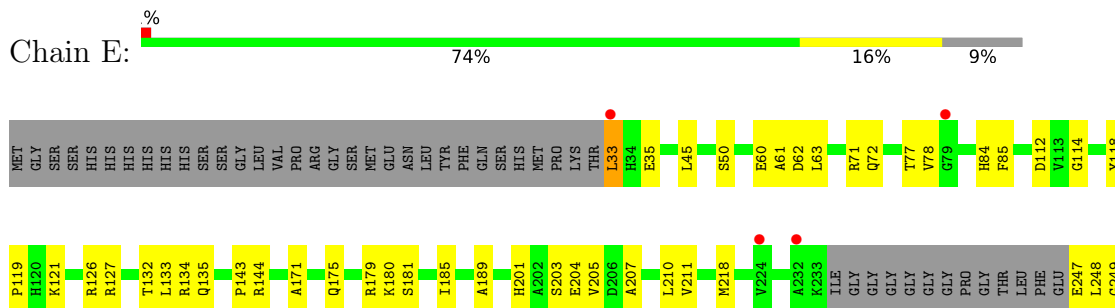
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

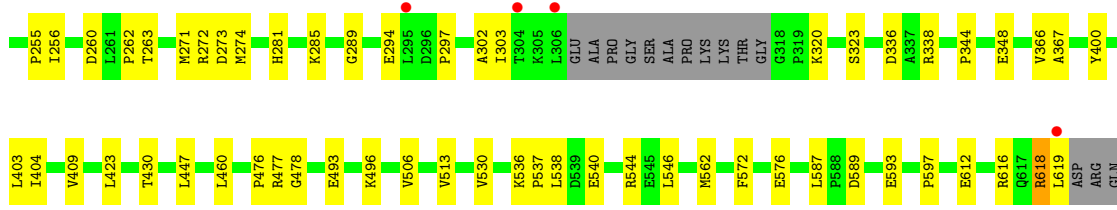


• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

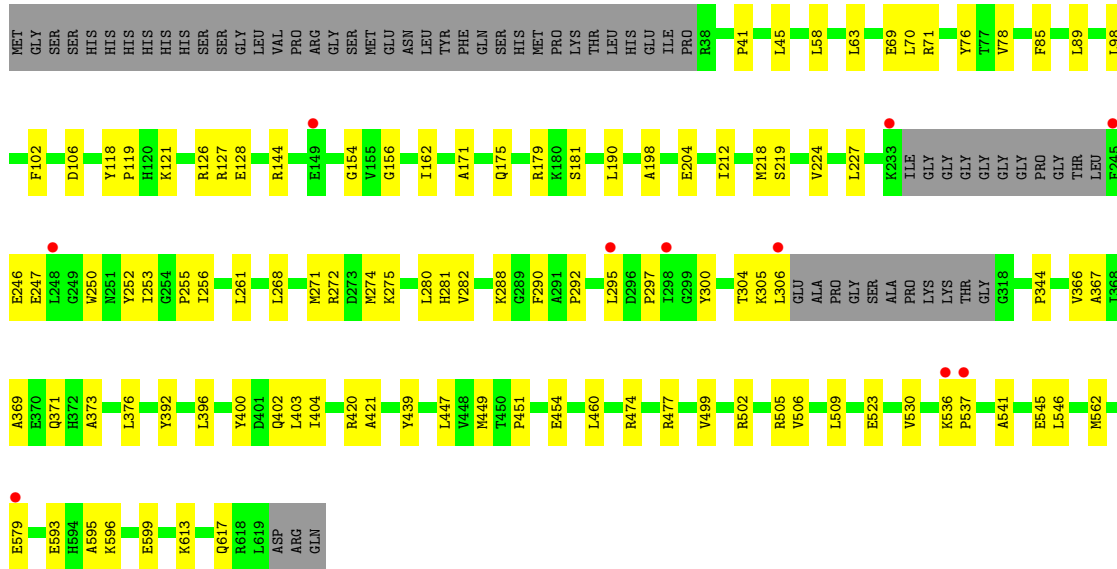
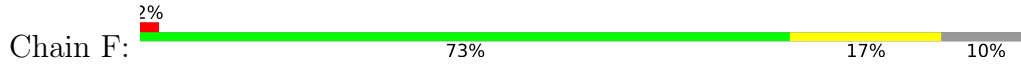


• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase





● Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.82Å 137.06Å 231.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.92 – 2.30 46.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.92-2.30) 99.5 (46.92-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.238 0.183 , 0.238	Depositor DCC
R_{free} test set	8418 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.843	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27452	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6657e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, TPP, 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	0.36	0/4362	0.54	0/5915
1	B	0.35	0/4369	0.52	0/5924
1	C	0.36	0/4350	0.54	0/5898
1	D	0.37	0/4349	0.53	0/5898
1	E	0.36	0/4373	0.52	0/5929
1	F	0.35	0/4350	0.52	0/5896
All	All	0.36	0/26153	0.53	0/35460

There are no bond length outliers.

There are no bond angle outliers.

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	4277	0	4246	73	0
1	B	4284	0	4250	75	0
1	C	4266	0	4232	71	0
1	D	4264	0	4237	51	0
1	E	4288	0	4265	70	0
1	F	4266	0	4238	72	0
2	A	26	16	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	16	16	4	0
2	C	26	16	16	3	0
2	D	26	16	16	3	0
2	E	26	16	16	1	0
2	F	26	16	16	1	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
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	F	4	0	0	0	0
5	D	6	8	7	1	0
6	A	271	0	0	8	0
6	B	238	0	0	4	0
6	C	249	0	0	4	0
6	D	262	0	0	9	0
6	E	253	0	0	6	0
6	F	254	0	0	4	0
All	All	27348	104	25571	410	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 8.

The worst 5 of 410 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:C:60:GLU:OE2	1:C:269:ARG:NH2	1.91	1.04
1:B:271:MET:HA	1:B:274:MET:HE3	1.37	1.03
1:A:33:LEU:HD11	1:A:72:GLN:OE1	1.63	0.98
1:A:108:ARG:HB3	1:A:168:MET:HE2	1.40	0.97
1:B:455:ASP:OD2	1:B:459:LYS:HE3	1.69	0.93

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	556/622 (89%)	532 (96%)	24 (4%)	0	100	100
1	B	557/622 (90%)	532 (96%)	25 (4%)	0	100	100
1	C	556/622 (89%)	530 (95%)	26 (5%)	0	100	100
1	D	554/622 (89%)	532 (96%)	21 (4%)	1 (0%)	43	55
1	E	557/622 (90%)	531 (95%)	26 (5%)	0	100	100
1	F	554/622 (89%)	529 (96%)	24 (4%)	1 (0%)	43	55
All	All	3334/3732 (89%)	3186 (96%)	146 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	344	PRO
1	F	156	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	444/490 (91%)	438 (99%)	6 (1%)	59	76
1	B	444/490 (91%)	439 (99%)	5 (1%)	65	81
1	C	442/490 (90%)	431 (98%)	11 (2%)	42	60
1	D	443/490 (90%)	440 (99%)	3 (1%)	76	87
1	E	445/490 (91%)	439 (99%)	6 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	442/490 (90%)	432 (98%)	10 (2%)	44	63
All	All	2660/2940 (90%)	2619 (98%)	41 (2%)	57	75

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	181	SER
1	F	288	LYS
1	E	506	VAL
1	F	219	SER
1	F	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	251	ASN
1	E	72	GLN
1	D	584	GLN
1	E	270	ASN
1	B	229	ASN

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 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 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	B	701	3	26,27,27	2.08	6 (23%)	38,40,40	2.23	12 (31%)
2	TPP	E	701	3	26,27,27	2.27	7 (26%)	38,40,40	1.94	8 (21%)
5	GOL	D	702	-	5,5,5	1.21	1 (20%)	5,5,5	0.75	0
2	TPP	C	701	3	26,27,27	1.84	5 (19%)	38,40,40	2.13	11 (28%)
2	TPP	A	701	3	26,27,27	1.89	5 (19%)	38,40,40	2.13	10 (26%)
2	TPP	F	701	3	26,27,27	2.02	7 (26%)	38,40,40	1.94	9 (23%)
2	TPP	D	701	3	26,27,27	1.92	5 (19%)	38,40,40	2.11	10 (26%)

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	B	701	3	-	8/17/17/17	0/2/2/2
2	TPP	E	701	3	-	3/17/17/17	0/2/2/2
5	GOL	D	702	-	-	2/4/4/4	-
2	TPP	C	701	3	-	4/17/17/17	0/2/2/2
2	TPP	A	701	3	-	3/17/17/17	0/2/2/2
2	TPP	F	701	3	-	5/17/17/17	0/2/2/2
2	TPP	D	701	3	-	6/17/17/17	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	TPP	PA-O3A	6.05	1.66	1.59
2	B	701	TPP	PA-O3A	5.41	1.65	1.59
2	A	701	TPP	PA-O3A	5.06	1.65	1.59
2	B	701	TPP	PB-O1B	4.75	1.65	1.50
2	E	701	TPP	PB-O1B	4.71	1.65	1.50

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	TPP	C2-S1-C5	7.85	96.42	91.22
2	C	701	TPP	C2-S1-C5	7.80	96.38	91.22
2	B	701	TPP	C2-S1-C5	7.50	96.19	91.22
2	D	701	TPP	C2-S1-C5	7.26	96.02	91.22
2	E	701	TPP	C2-S1-C5	7.15	95.95	91.22

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

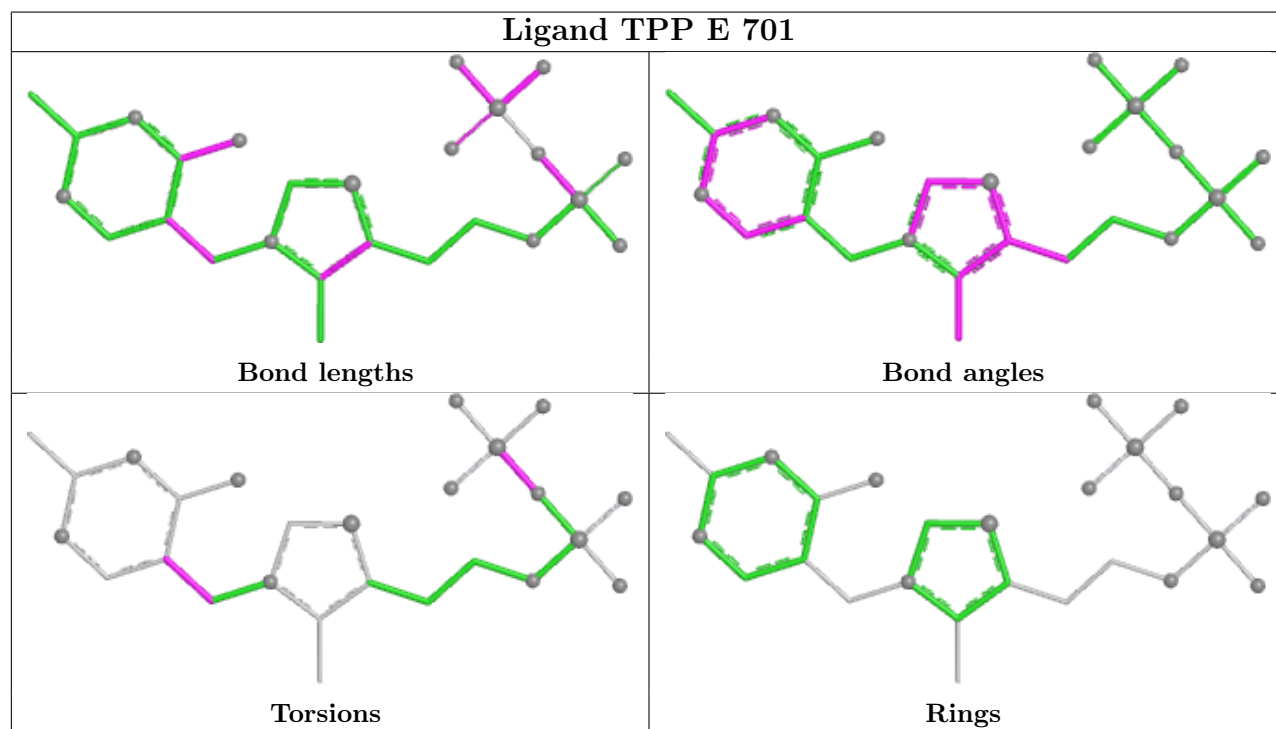
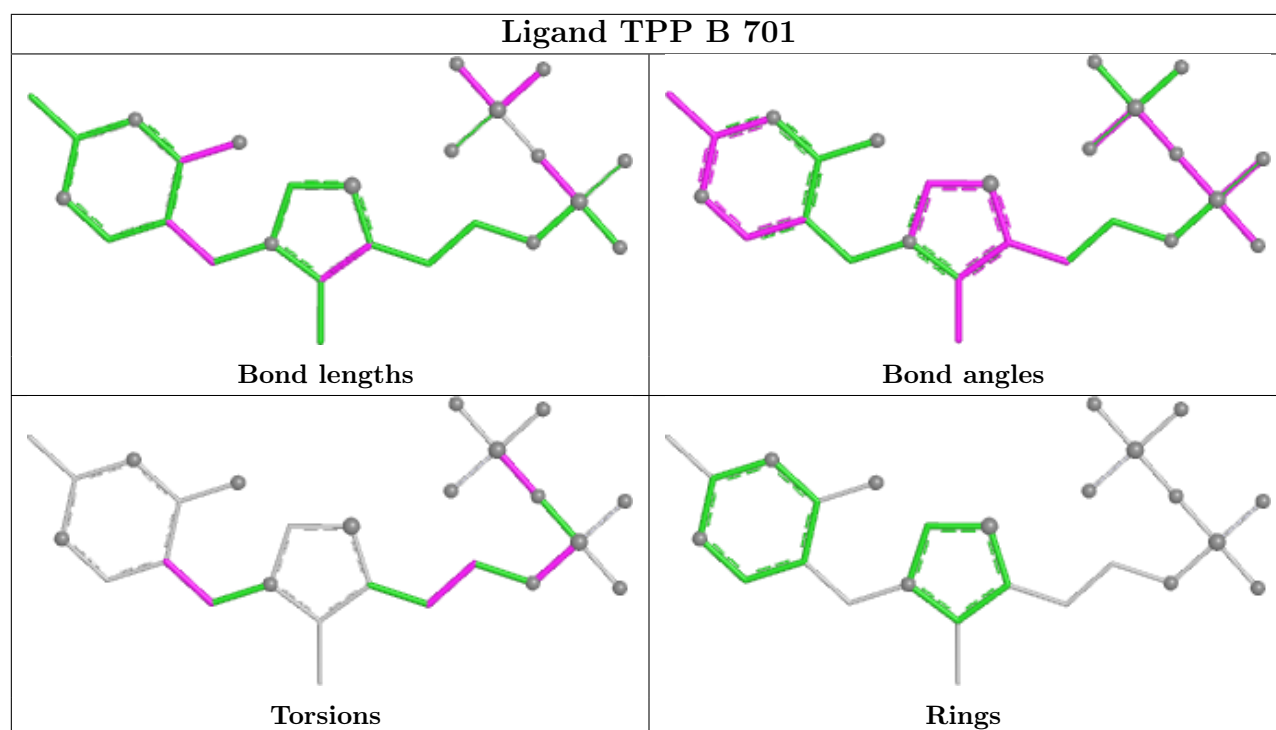
Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C6'-C5'-C7'-N3
2	B	701	TPP	C6'-C5'-C7'-N3
2	B	701	TPP	C7-O7-PA-O2A
2	B	701	TPP	C7-O7-PA-O3A
2	B	701	TPP	PA-O3A-PB-O3B

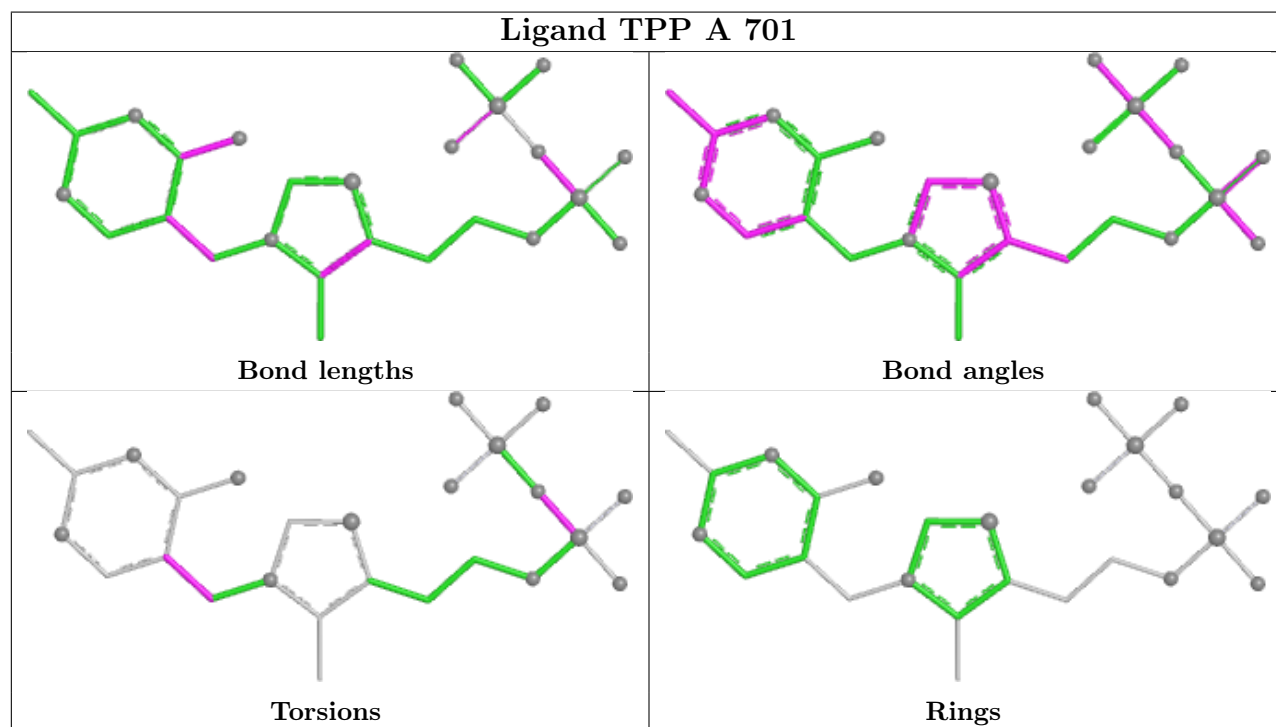
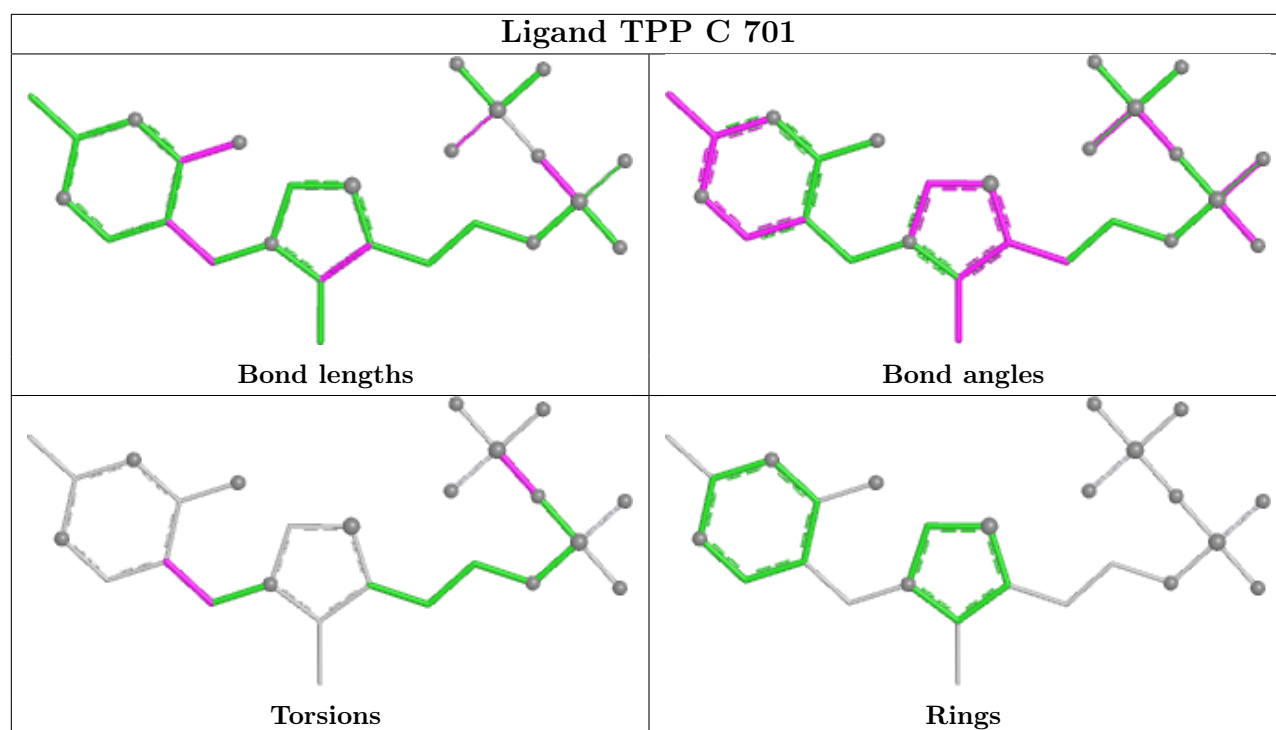
There are no ring outliers.

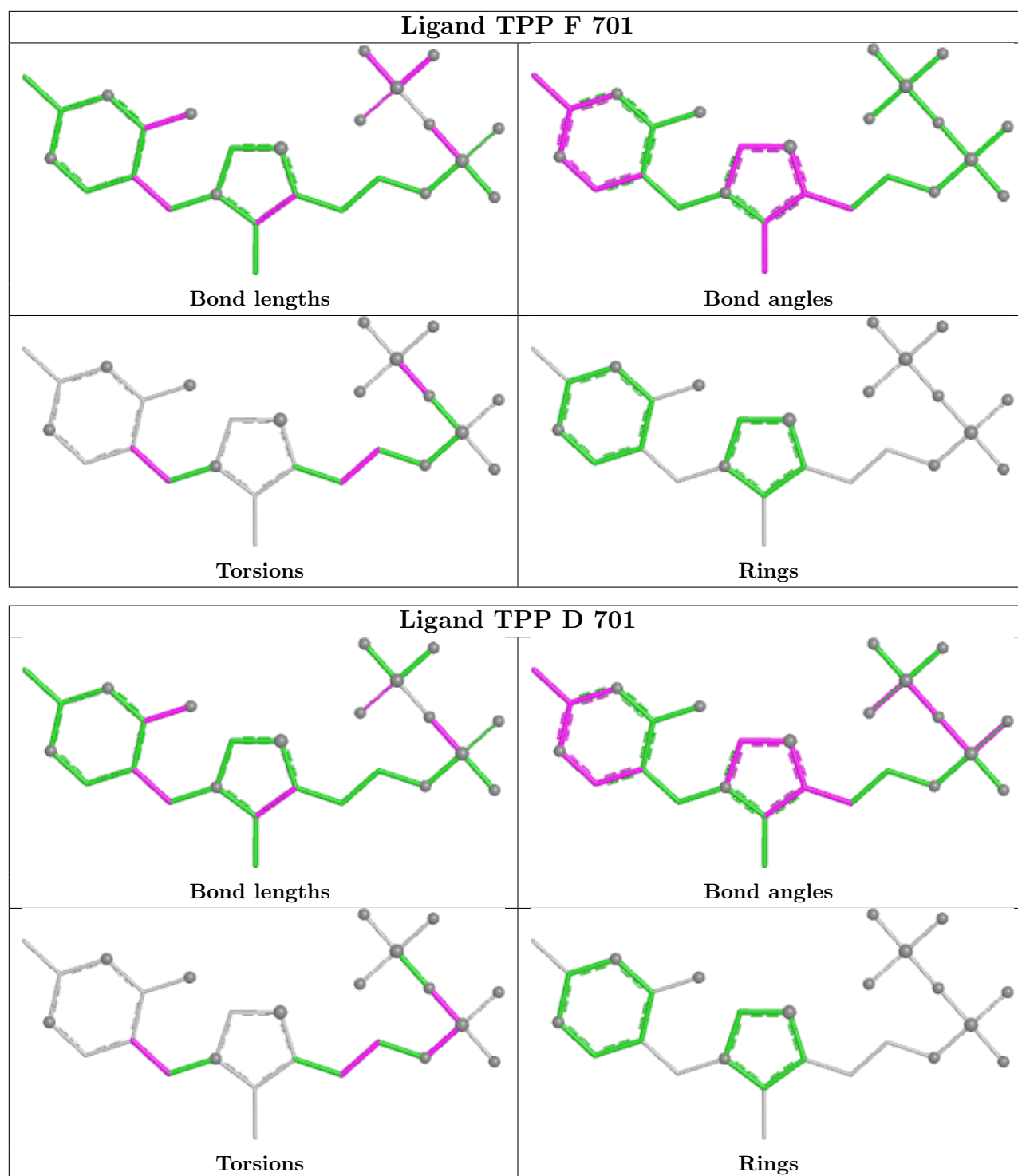
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	TPP	4	0
2	E	701	TPP	1	0
5	D	702	GOL	1	0
2	C	701	TPP	3	0
2	A	701	TPP	1	0
2	F	701	TPP	1	0
2	D	701	TPP	3	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, 95th 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	562/622 (90%)	-0.05	11 (1%) 65 66	17, 28, 46, 93	0
1	B	563/622 (90%)	0.02	10 (1%) 67 69	18, 30, 49, 94	0
1	C	562/622 (90%)	-0.07	11 (1%) 65 66	16, 27, 46, 80	0
1	D	560/622 (90%)	-0.10	6 (1%) 78 79	16, 27, 47, 68	0
1	E	563/622 (90%)	-0.02	8 (1%) 73 75	18, 29, 46, 66	0
1	F	560/622 (90%)	0.02	10 (1%) 67 69	18, 29, 52, 68	1 (0%)
All	All	3370/3732 (90%)	-0.03	56 (1%) 69 70	16, 28, 49, 94	1 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	6.6
1	E	79	GLY	5.2
1	A	224	VAL	5.1
1	C	308	ALA	4.2
1	E	224	VAL	4.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

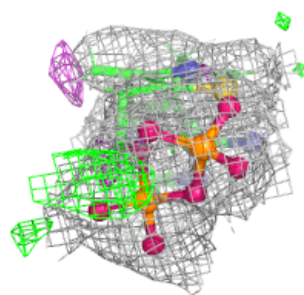
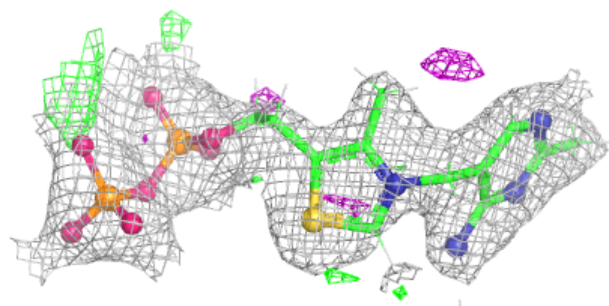
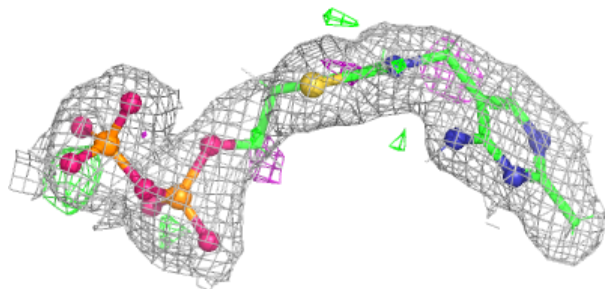
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	A	703	1/1	0.76	0.17	70,70,70,70	0
4	CA	F	705	1/1	0.81	0.15	66,66,66,66	0
5	GOL	D	702	6/6	0.86	0.12	27,36,48,49	0
4	CA	F	704	1/1	0.94	0.06	44,44,44,44	0
2	TPP	D	701	26/26	0.94	0.09	23,35,50,53	0
2	TPP	A	701	26/26	0.94	0.08	20,32,41,47	0
2	TPP	E	701	26/26	0.95	0.08	24,31,42,47	0
2	TPP	F	701	26/26	0.95	0.07	25,33,45,49	0
2	TPP	C	701	26/26	0.95	0.07	20,25,35,41	0
4	CA	B	703	1/1	0.96	0.05	43,43,43,43	0
2	TPP	B	701	26/26	0.96	0.07	18,27,37,39	0
4	CA	F	706	1/1	0.97	0.04	53,53,53,53	0
4	CA	D	704	1/1	0.97	0.11	62,62,62,62	0
3	MG	E	702	1/1	0.98	0.11	22,22,22,22	0
4	CA	C	703	1/1	0.98	0.19	38,38,38,38	0
3	MG	C	702	1/1	0.98	0.12	18,18,18,18	0
4	CA	F	703	1/1	0.98	0.06	60,60,60,60	0
3	MG	D	703	1/1	0.99	0.15	22,22,22,22	0
3	MG	B	702	1/1	0.99	0.14	18,18,18,18	0
3	MG	F	702	1/1	0.99	0.08	23,23,23,23	0
3	MG	A	702	1/1	0.99	0.12	21,21,21,21	0

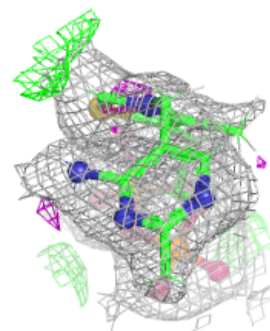
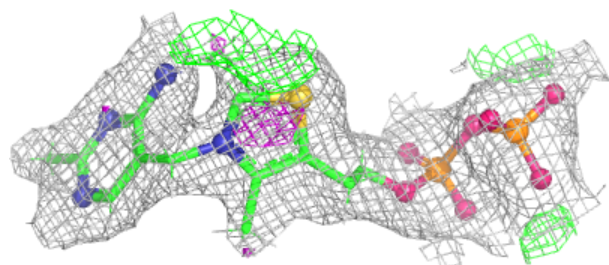
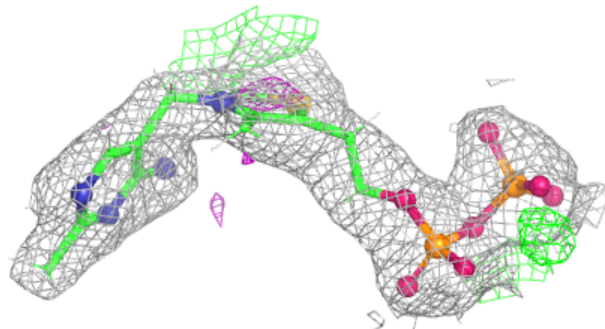
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP D 701:

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

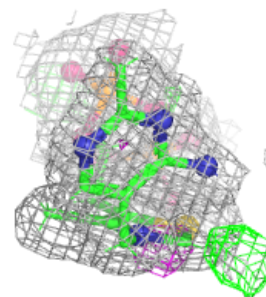
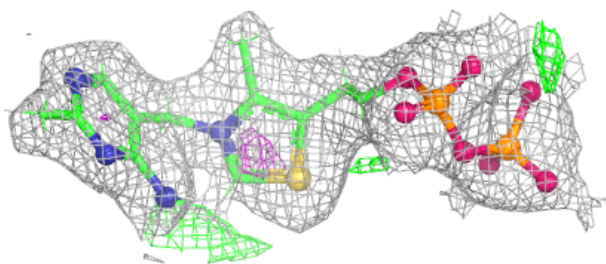
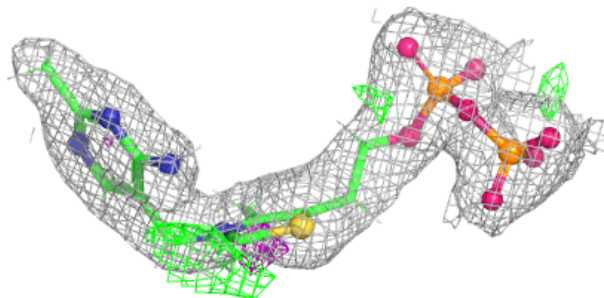
**Electron density around TPP A 701:**

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

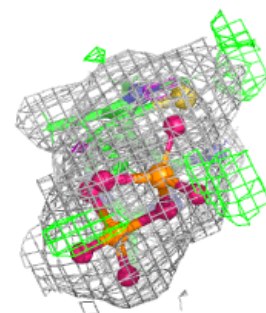
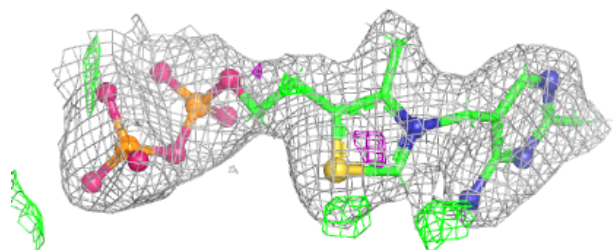
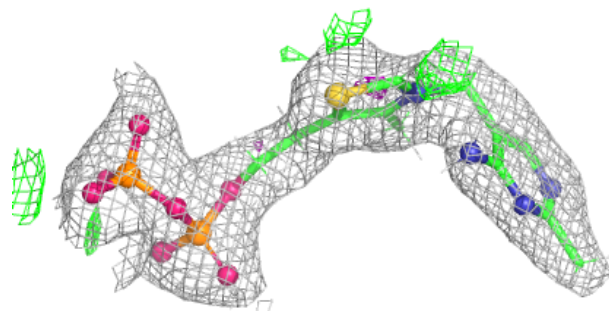


Electron density around TPP E 701:

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

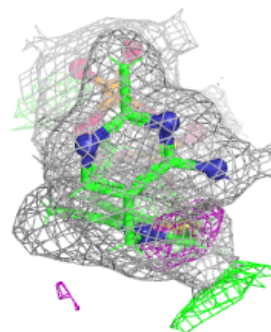
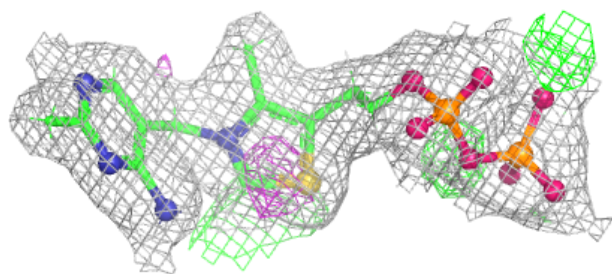
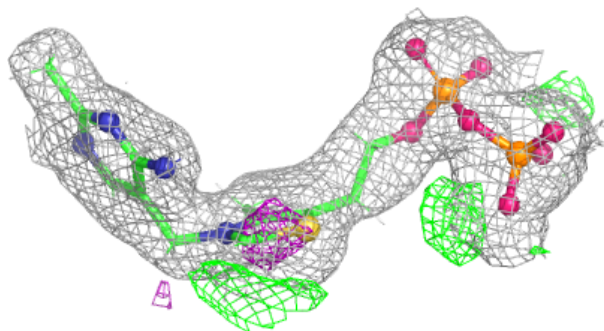
**Electron density around TPP F 701:**

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

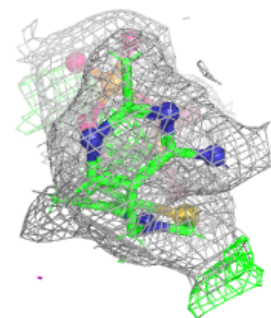
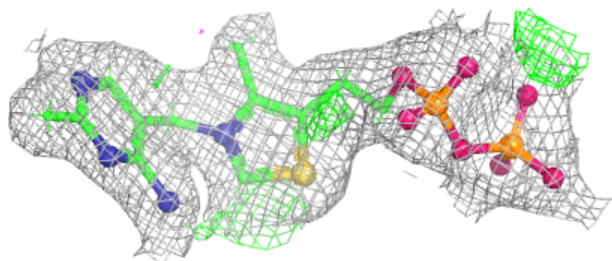
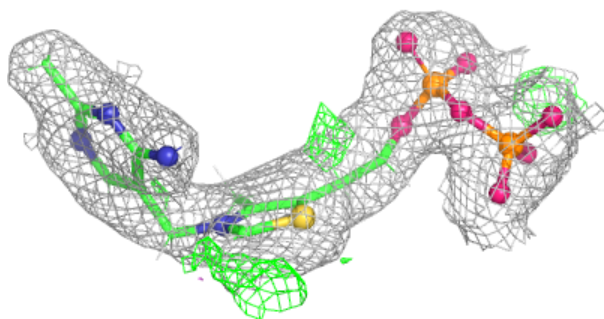


Electron density around TPP C 701:

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

**Electron density around TPP B 701:**

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



6.5 Other polymers

There are no such residues in this entry.