



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:51 PM UTC

PDB ID : 8R3S / pdb_00008r3s
Title : Transketolase from Staphylococcus aureus in complex with thiamin pyrophosphate
Authors : Ballut, L.; Georges, N.; Aghajari, N.; Hecquet, L.; Charmantray, F.; Doumeche, B.
Deposited on : 2023-11-10
Resolution : 2.80 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)
Xtriage (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

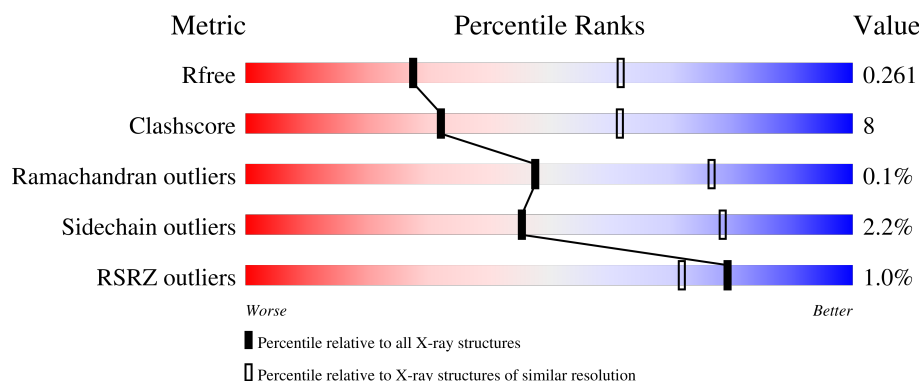
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	677	80% 17% ..
1	B	677	% 76% 21% ..
1	C	677	% 76% 22% .
1	D	677	% 79% 19% .

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Mol	Chain	Length	Quality of chain
1	E	677	% 75% 22% .
1	F	677	% 78% 19% ..
1	G	677	% 77% 21% .
1	H	677	% 77% 20% ..
1	I	677	% 80% 18% .
1	J	677	% 79% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51300 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5107	3226	857	1011	13			
1	B	662	Total	C	N	O	S	0	0	0
			5098	3221	856	1008	13			
1	C	663	Total	C	N	O	S	0	0	0
			5107	3226	857	1011	13			
1	D	663	Total	C	N	O	S	0	1	0
			5121	3237	859	1012	13			
1	E	662	Total	C	N	O	S	0	1	0
			5106	3225	860	1009	12			
1	F	662	Total	C	N	O	S	0	0	0
			5095	3219	856	1008	12			
1	G	662	Total	C	N	O	S	0	0	0
			5099	3221	856	1010	12			
1	H	662	Total	C	N	O	S	0	0	0
			5098	3221	856	1008	13			
1	I	663	Total	C	N	O	S	0	0	0
			5104	3224	857	1011	12			
1	J	662	Total	C	N	O	S	0	0	0
			5095	3219	856	1008	12			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	663	GLU	-	expression tag	UNP P99161
A	664	ASN	-	expression tag	UNP P99161
A	665	LEU	-	expression tag	UNP P99161
A	666	TYR	-	expression tag	UNP P99161
A	667	PHE	-	expression tag	UNP P99161
A	668	GLN	-	expression tag	UNP P99161
A	669	GLY	-	expression tag	UNP P99161
A	670	LEU	-	expression tag	UNP P99161
A	671	GLU	-	expression tag	UNP P99161

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Chain	Residue	Modelled	Actual	Comment	Reference
A	672	HIS	-	expression tag	UNP P99161
A	673	HIS	-	expression tag	UNP P99161
A	674	HIS	-	expression tag	UNP P99161
A	675	HIS	-	expression tag	UNP P99161
A	676	HIS	-	expression tag	UNP P99161
A	677	HIS	-	expression tag	UNP P99161
B	663	GLU	-	expression tag	UNP P99161
B	664	ASN	-	expression tag	UNP P99161
B	665	LEU	-	expression tag	UNP P99161
B	666	TYR	-	expression tag	UNP P99161
B	667	PHE	-	expression tag	UNP P99161
B	668	GLN	-	expression tag	UNP P99161
B	669	GLY	-	expression tag	UNP P99161
B	670	LEU	-	expression tag	UNP P99161
B	671	GLU	-	expression tag	UNP P99161
B	672	HIS	-	expression tag	UNP P99161
B	673	HIS	-	expression tag	UNP P99161
B	674	HIS	-	expression tag	UNP P99161
B	675	HIS	-	expression tag	UNP P99161
B	676	HIS	-	expression tag	UNP P99161
B	677	HIS	-	expression tag	UNP P99161
C	663	GLU	-	expression tag	UNP P99161
C	664	ASN	-	expression tag	UNP P99161
C	665	LEU	-	expression tag	UNP P99161
C	666	TYR	-	expression tag	UNP P99161
C	667	PHE	-	expression tag	UNP P99161
C	668	GLN	-	expression tag	UNP P99161
C	669	GLY	-	expression tag	UNP P99161
C	670	LEU	-	expression tag	UNP P99161
C	671	GLU	-	expression tag	UNP P99161
C	672	HIS	-	expression tag	UNP P99161
C	673	HIS	-	expression tag	UNP P99161
C	674	HIS	-	expression tag	UNP P99161
C	675	HIS	-	expression tag	UNP P99161
C	676	HIS	-	expression tag	UNP P99161
C	677	HIS	-	expression tag	UNP P99161
D	663	GLU	-	expression tag	UNP P99161
D	664	ASN	-	expression tag	UNP P99161
D	665	LEU	-	expression tag	UNP P99161
D	666	TYR	-	expression tag	UNP P99161
D	667	PHE	-	expression tag	UNP P99161
D	668	GLN	-	expression tag	UNP P99161

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Chain	Residue	Modelled	Actual	Comment	Reference
D	669	GLY	-	expression tag	UNP P99161
D	670	LEU	-	expression tag	UNP P99161
D	671	GLU	-	expression tag	UNP P99161
D	672	HIS	-	expression tag	UNP P99161
D	673	HIS	-	expression tag	UNP P99161
D	674	HIS	-	expression tag	UNP P99161
D	675	HIS	-	expression tag	UNP P99161
D	676	HIS	-	expression tag	UNP P99161
D	677	HIS	-	expression tag	UNP P99161
E	663	GLU	-	expression tag	UNP P99161
E	664	ASN	-	expression tag	UNP P99161
E	665	LEU	-	expression tag	UNP P99161
E	666	TYR	-	expression tag	UNP P99161
E	667	PHE	-	expression tag	UNP P99161
E	668	GLN	-	expression tag	UNP P99161
E	669	GLY	-	expression tag	UNP P99161
E	670	LEU	-	expression tag	UNP P99161
E	671	GLU	-	expression tag	UNP P99161
E	672	HIS	-	expression tag	UNP P99161
E	673	HIS	-	expression tag	UNP P99161
E	674	HIS	-	expression tag	UNP P99161
E	675	HIS	-	expression tag	UNP P99161
E	676	HIS	-	expression tag	UNP P99161
E	677	HIS	-	expression tag	UNP P99161
F	663	GLU	-	expression tag	UNP P99161
F	664	ASN	-	expression tag	UNP P99161
F	665	LEU	-	expression tag	UNP P99161
F	666	TYR	-	expression tag	UNP P99161
F	667	PHE	-	expression tag	UNP P99161
F	668	GLN	-	expression tag	UNP P99161
F	669	GLY	-	expression tag	UNP P99161
F	670	LEU	-	expression tag	UNP P99161
F	671	GLU	-	expression tag	UNP P99161
F	672	HIS	-	expression tag	UNP P99161
F	673	HIS	-	expression tag	UNP P99161
F	674	HIS	-	expression tag	UNP P99161
F	675	HIS	-	expression tag	UNP P99161
F	676	HIS	-	expression tag	UNP P99161
F	677	HIS	-	expression tag	UNP P99161
G	663	GLU	-	expression tag	UNP P99161
G	664	ASN	-	expression tag	UNP P99161
G	665	LEU	-	expression tag	UNP P99161

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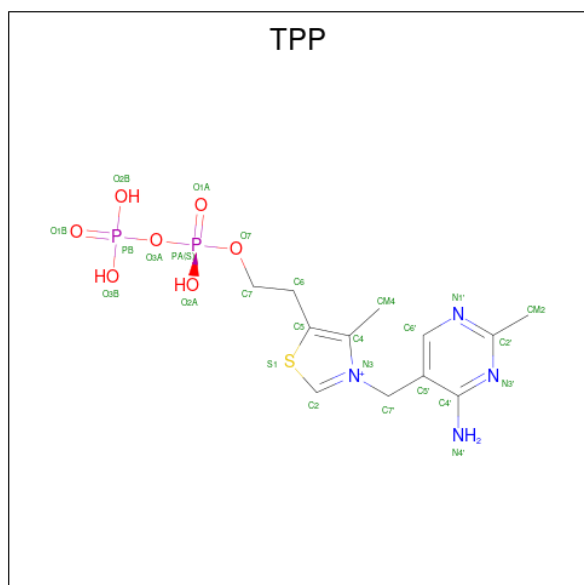
Chain	Residue	Modelled	Actual	Comment	Reference
G	666	TYR	-	expression tag	UNP P99161
G	667	PHE	-	expression tag	UNP P99161
G	668	GLN	-	expression tag	UNP P99161
G	669	GLY	-	expression tag	UNP P99161
G	670	LEU	-	expression tag	UNP P99161
G	671	GLU	-	expression tag	UNP P99161
G	672	HIS	-	expression tag	UNP P99161
G	673	HIS	-	expression tag	UNP P99161
G	674	HIS	-	expression tag	UNP P99161
G	675	HIS	-	expression tag	UNP P99161
G	676	HIS	-	expression tag	UNP P99161
G	677	HIS	-	expression tag	UNP P99161
H	663	GLU	-	expression tag	UNP P99161
H	664	ASN	-	expression tag	UNP P99161
H	665	LEU	-	expression tag	UNP P99161
H	666	TYR	-	expression tag	UNP P99161
H	667	PHE	-	expression tag	UNP P99161
H	668	GLN	-	expression tag	UNP P99161
H	669	GLY	-	expression tag	UNP P99161
H	670	LEU	-	expression tag	UNP P99161
H	671	GLU	-	expression tag	UNP P99161
H	672	HIS	-	expression tag	UNP P99161
H	673	HIS	-	expression tag	UNP P99161
H	674	HIS	-	expression tag	UNP P99161
H	675	HIS	-	expression tag	UNP P99161
H	676	HIS	-	expression tag	UNP P99161
H	677	HIS	-	expression tag	UNP P99161
I	663	GLU	-	expression tag	UNP P99161
I	664	ASN	-	expression tag	UNP P99161
I	665	LEU	-	expression tag	UNP P99161
I	666	TYR	-	expression tag	UNP P99161
I	667	PHE	-	expression tag	UNP P99161
I	668	GLN	-	expression tag	UNP P99161
I	669	GLY	-	expression tag	UNP P99161
I	670	LEU	-	expression tag	UNP P99161
I	671	GLU	-	expression tag	UNP P99161
I	672	HIS	-	expression tag	UNP P99161
I	673	HIS	-	expression tag	UNP P99161
I	674	HIS	-	expression tag	UNP P99161
I	675	HIS	-	expression tag	UNP P99161
I	676	HIS	-	expression tag	UNP P99161
I	677	HIS	-	expression tag	UNP P99161

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Chain	Residue	Modelled	Actual	Comment	Reference
J	663	GLU	-	expression tag	UNP P99161
J	664	ASN	-	expression tag	UNP P99161
J	665	LEU	-	expression tag	UNP P99161
J	666	TYR	-	expression tag	UNP P99161
J	667	PHE	-	expression tag	UNP P99161
J	668	GLN	-	expression tag	UNP P99161
J	669	GLY	-	expression tag	UNP P99161
J	670	LEU	-	expression tag	UNP P99161
J	671	GLU	-	expression tag	UNP P99161
J	672	HIS	-	expression tag	UNP P99161
J	673	HIS	-	expression tag	UNP P99161
J	674	HIS	-	expression tag	UNP P99161
J	675	HIS	-	expression tag	UNP P99161
J	676	HIS	-	expression tag	UNP P99161
J	677	HIS	-	expression tag	UNP P99161

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

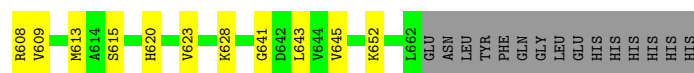
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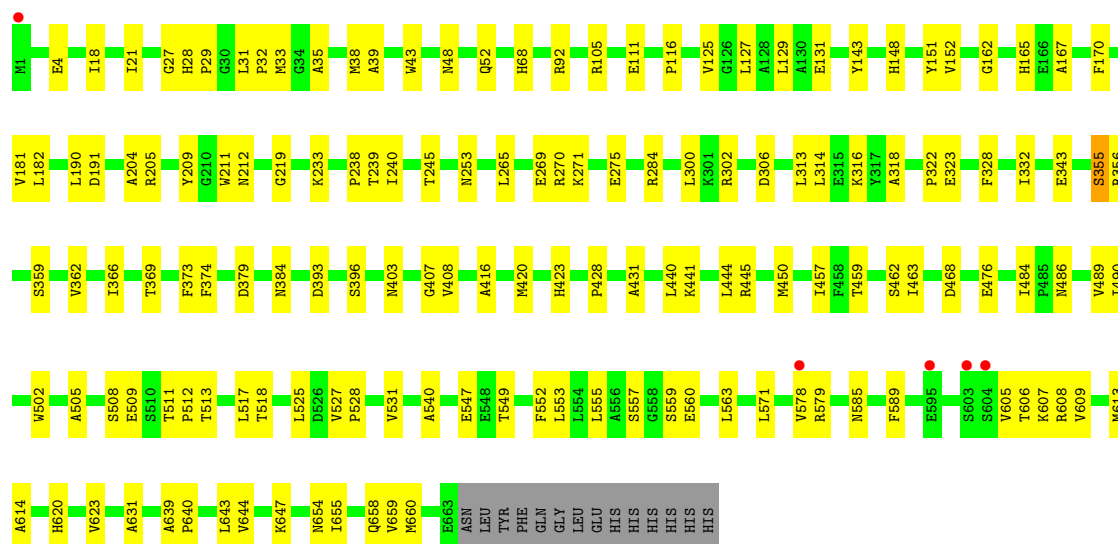
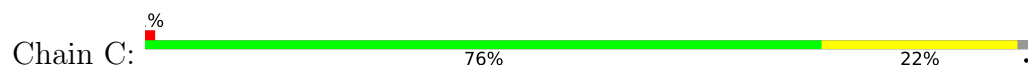
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	H	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	I	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	J	1	Total	C	N	O	P	S	0	0
			26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

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

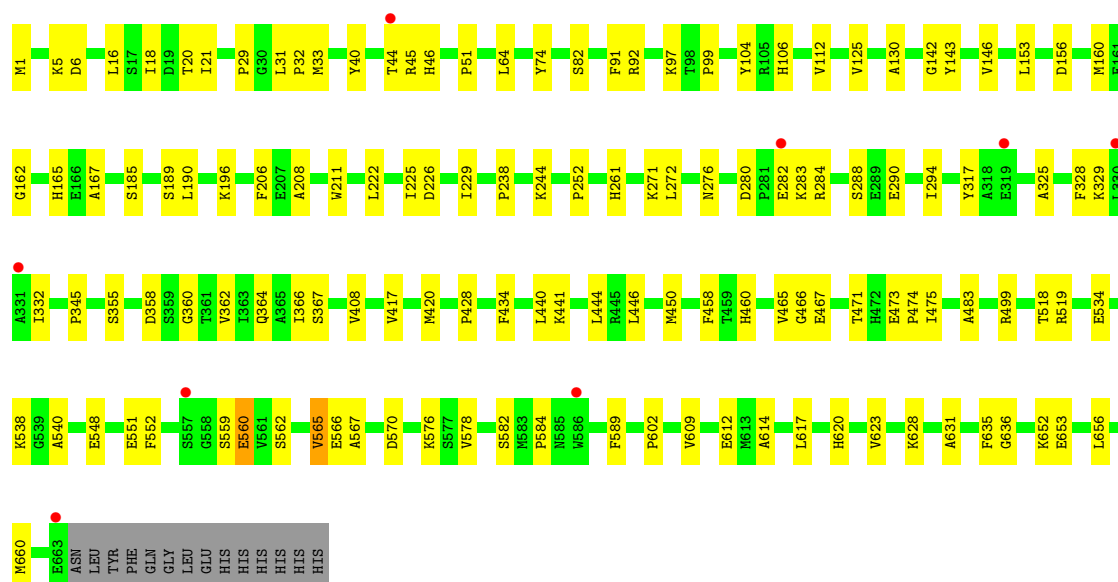
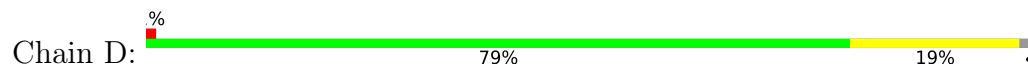
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	J	1	Total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



• Molecule 1: Transketolase

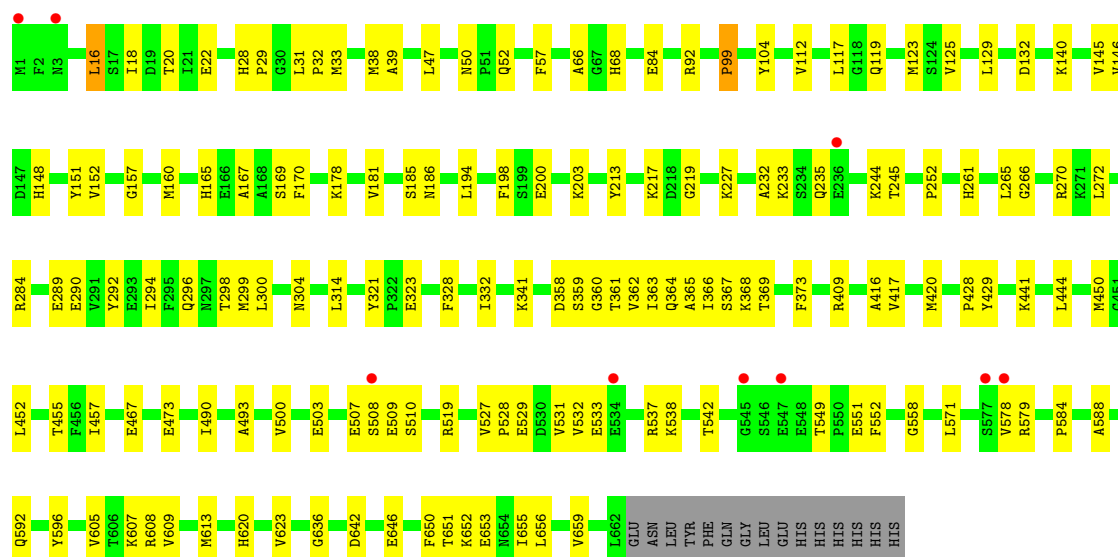


• Molecule 1: Transketolase

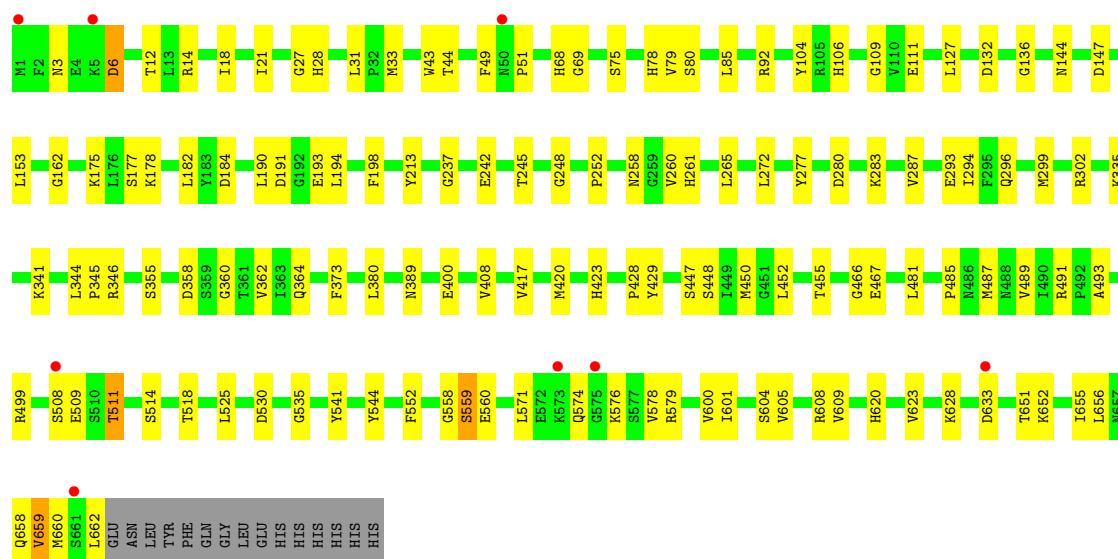
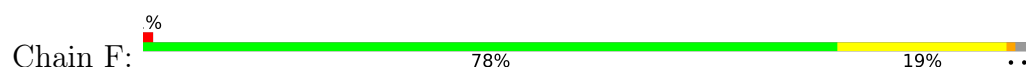


• Molecule 1: Transketolase

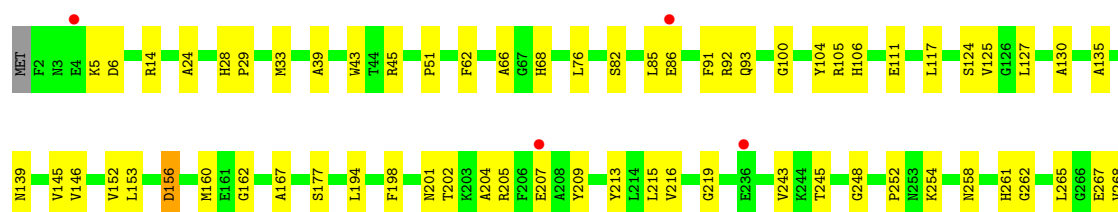
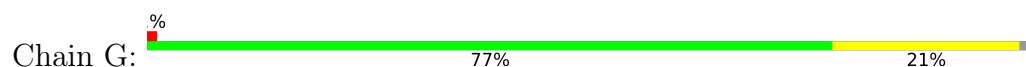


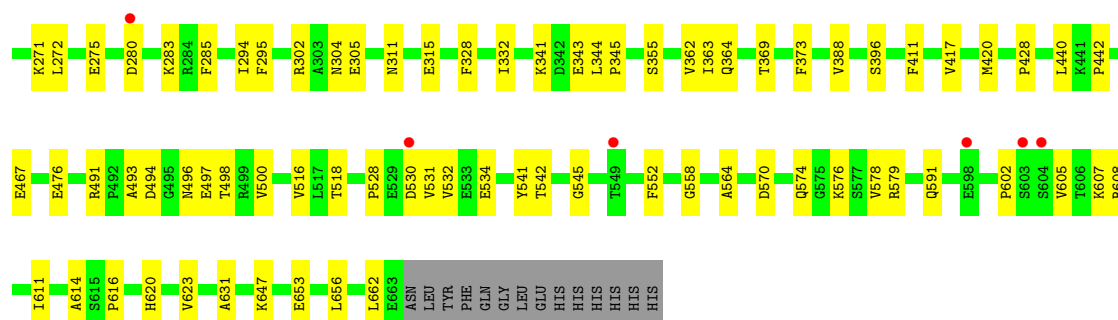


• Molecule 1: Transketolase

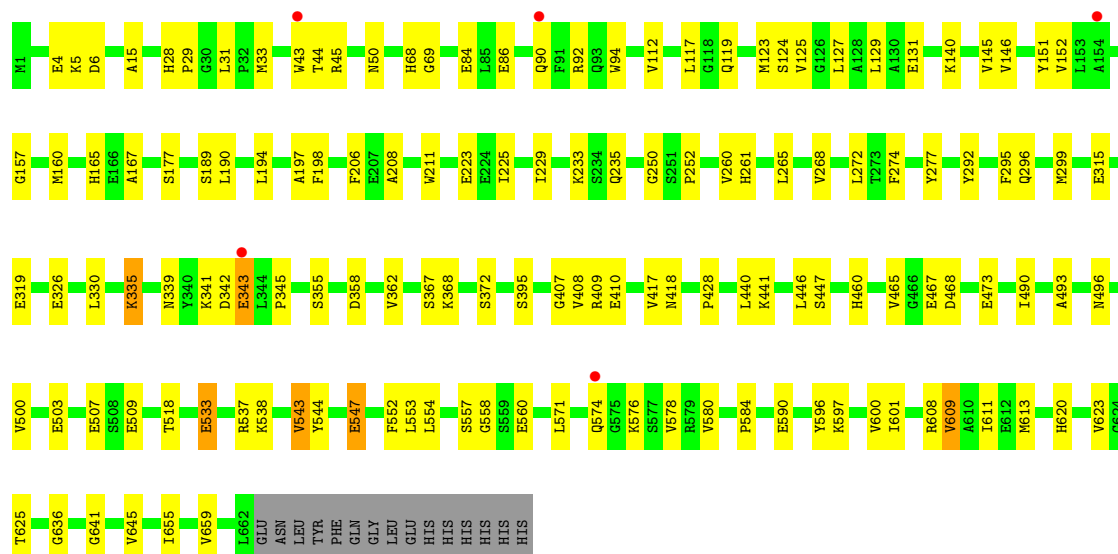
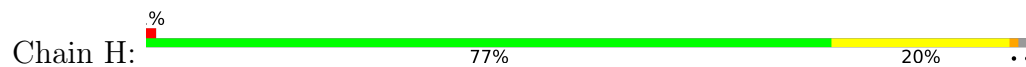


• Molecule 1: Transketolase

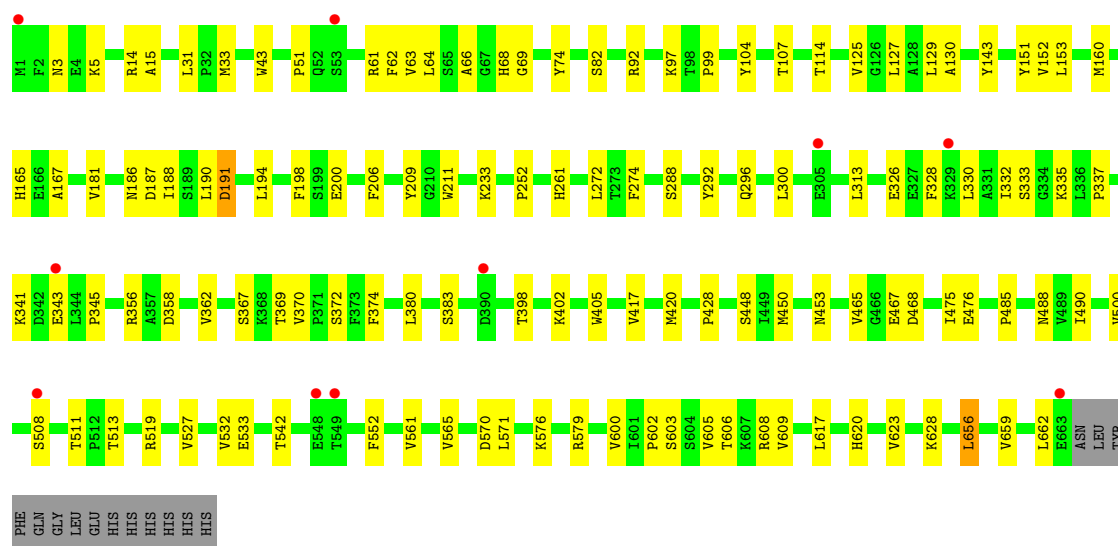




• Molecule 1: Transketolase

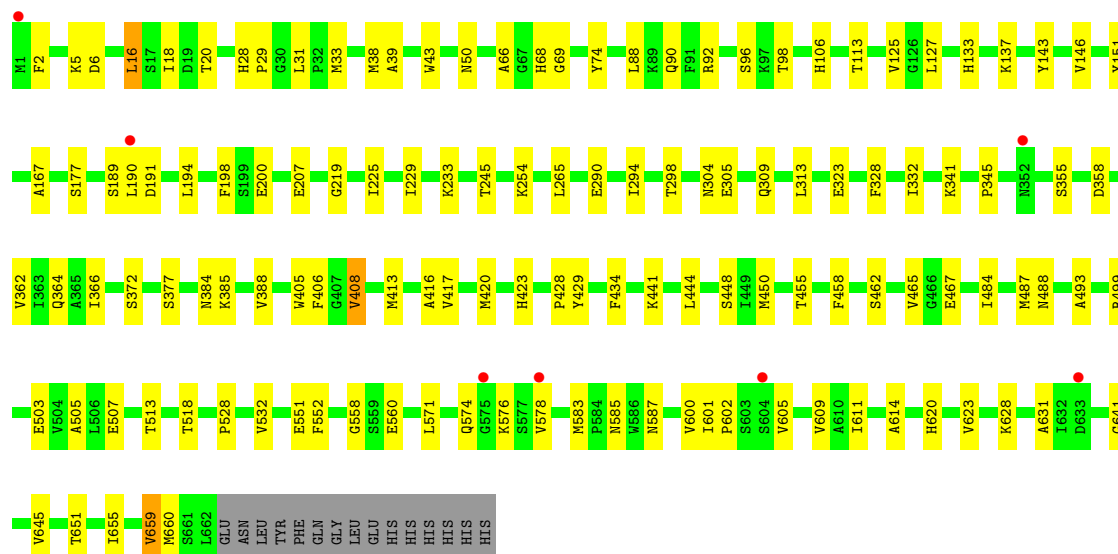


• Molecule 1: Transketolase



● Molecule 1: Transketolase

Chain J:  79% 19% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 149.90Å 253.30Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	34.86 – 2.80 34.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (34.86-2.80) 96.1 (34.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.260 0.219 , 0.261	Depositor DCC
R_{free} test set	8376 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	51300	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, MG

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	0.17	0/5221	0.38	0/7080
1	B	0.16	0/5212	0.36	0/7068
1	C	0.19	0/5221	0.39	0/7080
1	D	0.18	0/5237	0.39	1/7103 (0.0%)
1	E	0.22	1/5220 (0.0%)	0.48	3/7079 (0.0%)
1	F	0.17	0/5209	0.39	1/7065 (0.0%)
1	G	0.16	0/5213	0.37	0/7070
1	H	0.20	1/5212 (0.0%)	0.38	0/7068
1	I	0.20	0/5218	0.42	0/7077
1	J	0.17	0/5209	0.37	0/7065
All	All	0.18	2/52172 (0.0%)	0.39	5/70755 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	99	PRO	CG-CD	-7.29	1.25	1.50
1	H	335	LYS	C-N	-5.54	1.22	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	PRO	N-CD-CG	-13.99	82.21	103.20
1	E	99	PRO	CA-CB-CG	-13.89	78.10	104.50
1	E	99	PRO	CA-N-CD	-6.94	102.28	112.00
1	D	466	GLY	N-CA-C	6.53	117.68	111.67
1	F	466	GLY	N-CA-C	6.42	117.58	111.67

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	5107	0	4947	79	0
1	B	5098	0	4941	94	1
1	C	5107	0	4947	87	0
1	D	5121	0	4956	87	0
1	E	5106	0	4946	97	1
1	F	5095	0	4934	77	0
1	G	5099	0	4935	93	0
1	H	5098	0	4941	85	0
1	I	5104	0	4940	78	0
1	J	5095	0	4934	82	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	0	0
2	E	26	0	16	4	0
2	F	26	0	16	2	0
2	G	26	0	16	2	0
2	H	26	0	16	2	0
2	I	26	0	16	3	0
2	J	26	0	16	3	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
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	51300	0	49581	810	1

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 810 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:J:113:THR:H	1:J:450:MET:HE3	1.31	0.95
1:C:52:GLN:HE22	1:F:574:GLN:HE22	1.19	0.87
1:G:355:SER:HB2	1:G:518:THR:H	1.43	0.84
1:F:355:SER:HB2	1:F:518:THR:H	1.44	0.81
1:H:355:SER:HB2	1:H:518:THR:H	1.47	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:O	1:E:217:LYS:NZ[1_455]	2.18	0.02

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	661/677 (98%)	633 (96%)	26 (4%)	2 (0%)	36	66
1	B	660/677 (98%)	637 (96%)	23 (4%)	0	100	100
1	C	661/677 (98%)	642 (97%)	18 (3%)	1 (0%)	43	72
1	D	662/677 (98%)	644 (97%)	17 (3%)	1 (0%)	43	72
1	E	661/677 (98%)	634 (96%)	26 (4%)	1 (0%)	43	72
1	F	660/677 (98%)	636 (96%)	24 (4%)	0	100	100
1	G	660/677 (98%)	633 (96%)	27 (4%)	0	100	100
1	H	660/677 (98%)	634 (96%)	24 (4%)	2 (0%)	36	66
1	I	661/677 (98%)	638 (96%)	23 (4%)	0	100	100
1	J	660/677 (98%)	641 (97%)	19 (3%)	0	100	100
All	All	6606/6770 (98%)	6372 (96%)	227 (3%)	7 (0%)	48	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	509	GLU
1	A	408	VAL
1	H	197	ALA
1	H	408	VAL
1	C	408	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	544/557 (98%)	533 (98%)	11 (2%)	48	80
1	B	543/557 (98%)	527 (97%)	16 (3%)	37	73
1	C	544/557 (98%)	529 (97%)	15 (3%)	38	73
1	D	545/557 (98%)	536 (98%)	9 (2%)	53	83
1	E	543/557 (98%)	534 (98%)	9 (2%)	53	83
1	F	542/557 (97%)	525 (97%)	17 (3%)	35	70
1	G	543/557 (98%)	535 (98%)	8 (2%)	57	84
1	H	543/557 (98%)	523 (96%)	20 (4%)	30	65
1	I	543/557 (98%)	533 (98%)	10 (2%)	51	82
1	J	542/557 (97%)	535 (99%)	7 (1%)	61	86
All	All	5432/5570 (98%)	5310 (98%)	122 (2%)	45	78

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	367	SER
1	I	511	THR
1	F	525	LEU
1	I	372	SER
1	J	207	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	384	ASN
1	G	286	ASN
1	J	309	GLN
1	F	574	GLN
1	F	658	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPP	B	701	3	26,27,27	0.27	0	38,40,40	0.33	0
2	TPP	I	701	3	26,27,27	0.27	0	38,40,40	0.27	0
2	TPP	H	701	3	26,27,27	0.42	0	38,40,40	0.34	0
2	TPP	J	701	3	26,27,27	0.30	0	38,40,40	0.27	0
2	TPP	F	701	3	26,27,27	0.37	0	38,40,40	0.28	0
2	TPP	E	701	3	26,27,27	0.41	0	38,40,40	0.29	0
2	TPP	C	701	3	26,27,27	0.47	1 (3%)	38,40,40	0.29	0
2	TPP	G	701	3	26,27,27	0.25	0	38,40,40	0.31	0
2	TPP	D	701	3	26,27,27	0.31	0	38,40,40	0.29	0
2	TPP	A	701	3	26,27,27	0.39	0	38,40,40	0.28	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
2	TPP	B	701	3	-	7/17/17/17	0/2/2/2
2	TPP	I	701	3	-	5/17/17/17	0/2/2/2
2	TPP	H	701	3	-	9/17/17/17	0/2/2/2
2	TPP	J	701	3	-	4/17/17/17	0/2/2/2
2	TPP	F	701	3	-	6/17/17/17	0/2/2/2
2	TPP	E	701	3	-	6/17/17/17	0/2/2/2
2	TPP	C	701	3	-	4/17/17/17	0/2/2/2
2	TPP	G	701	3	-	6/17/17/17	0/2/2/2
2	TPP	D	701	3	-	11/17/17/17	0/2/2/2
2	TPP	A	701	3	-	5/17/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	TPP	PA-O3A	2.08	1.61	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C5-C6-C7-O7
2	A	701	TPP	C7-O7-PA-O1A
2	A	701	TPP	C7-O7-PA-O3A
2	B	701	TPP	C7-O7-PA-O1A
2	B	701	TPP	C7-O7-PA-O2A

There are no ring outliers.

9 monomers are involved in 20 short contacts:

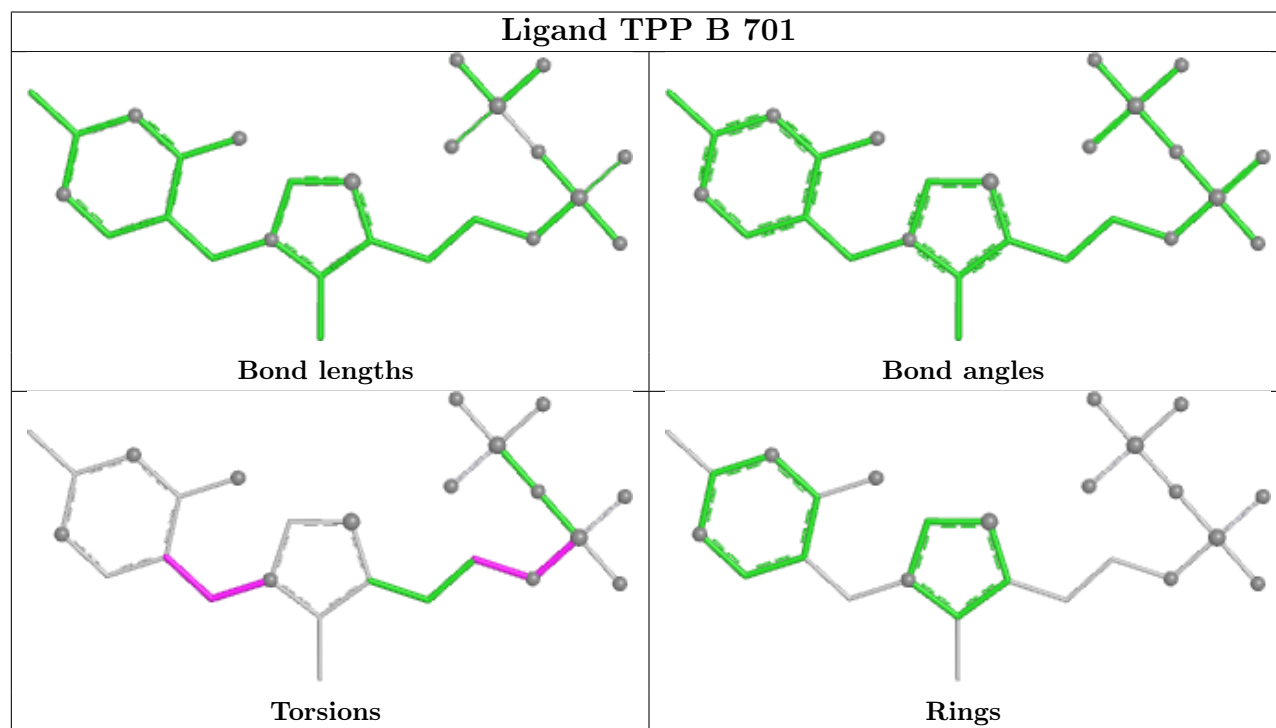
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	TPP	1	0
2	I	701	TPP	3	0
2	H	701	TPP	2	0
2	J	701	TPP	3	0

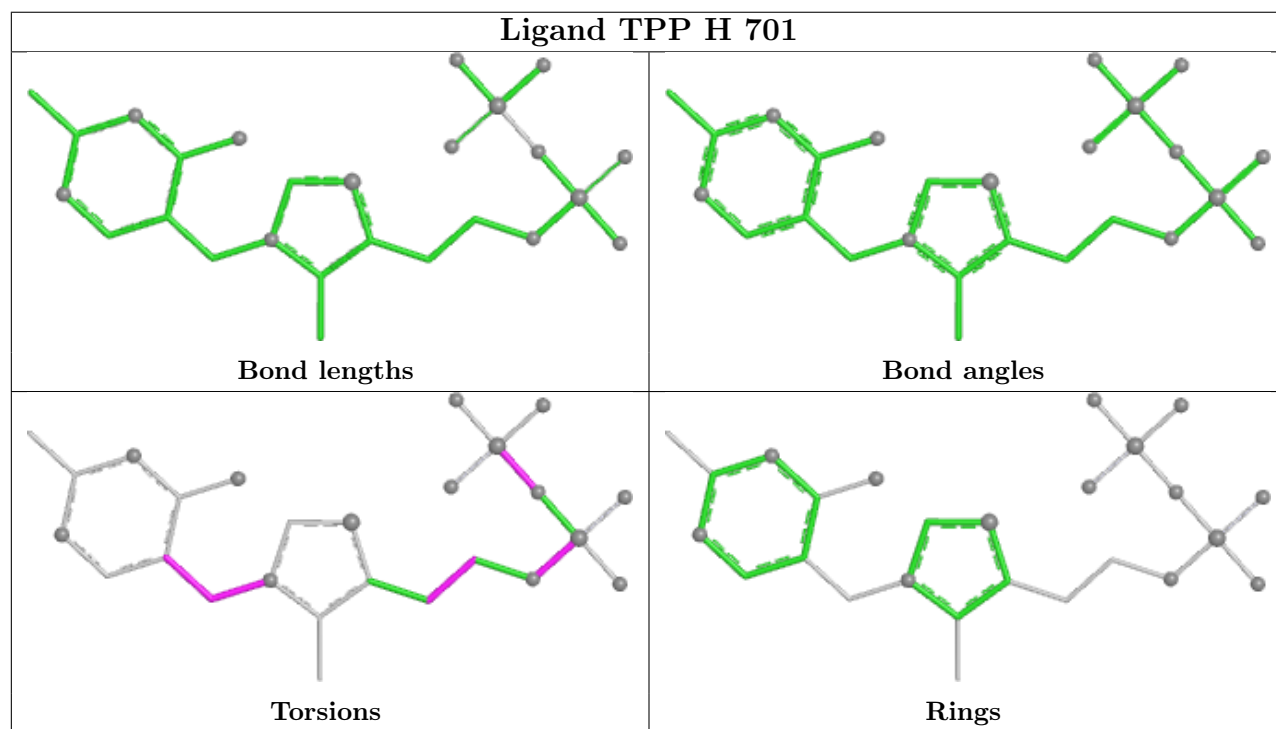
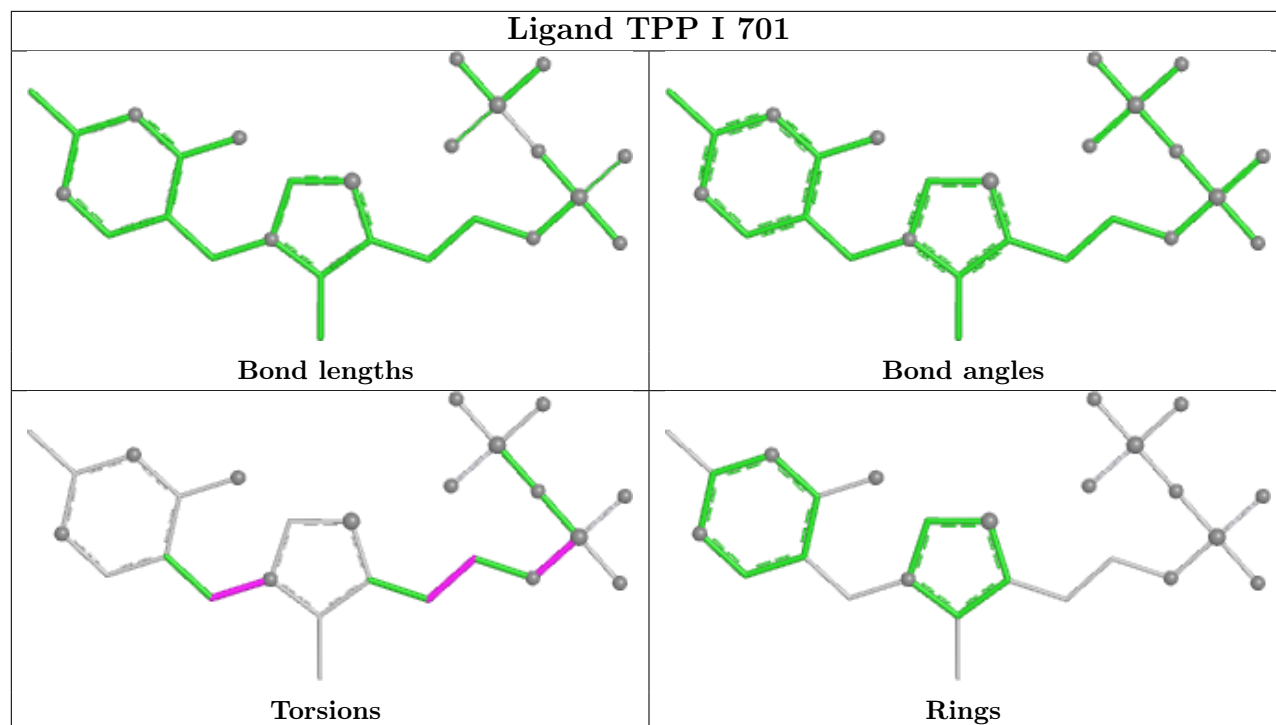
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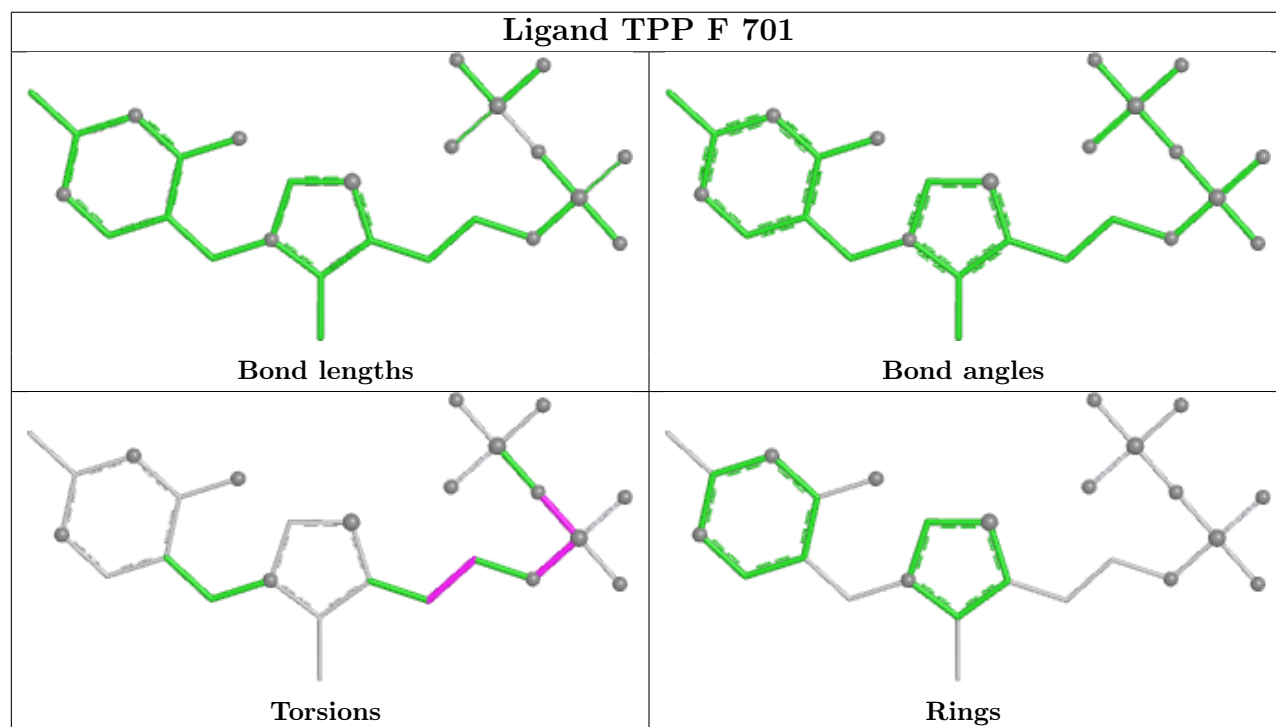
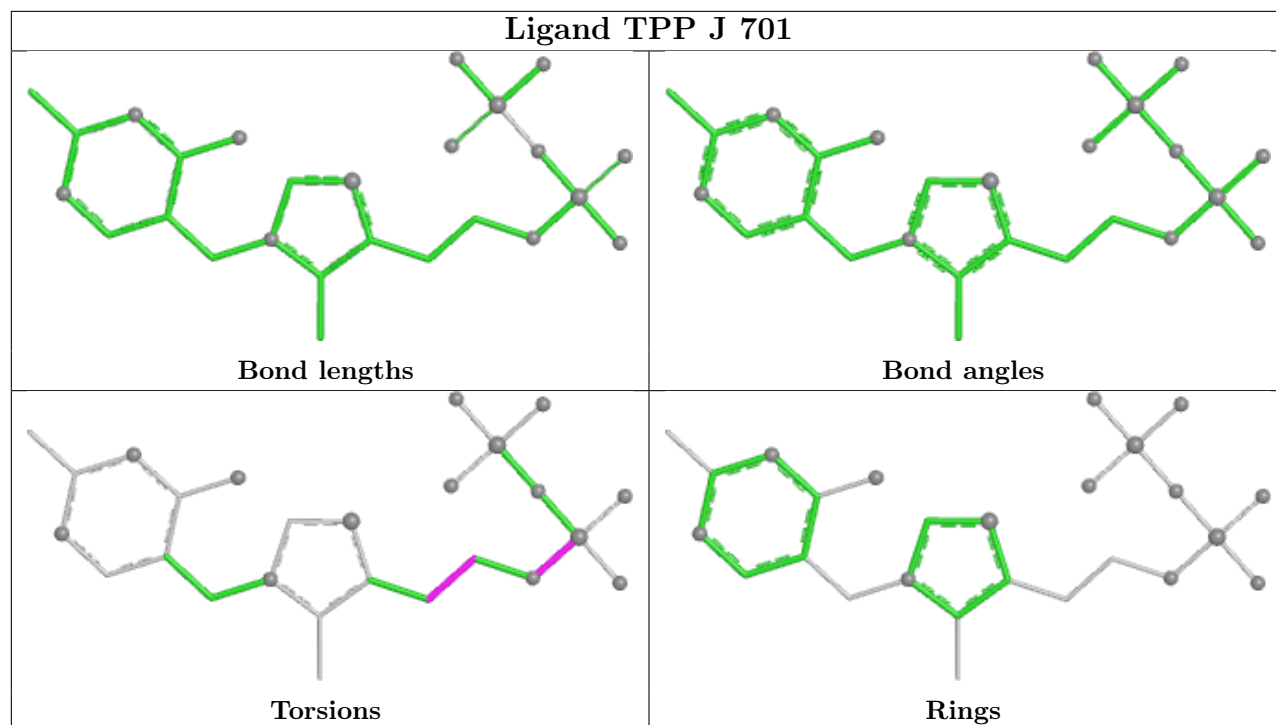
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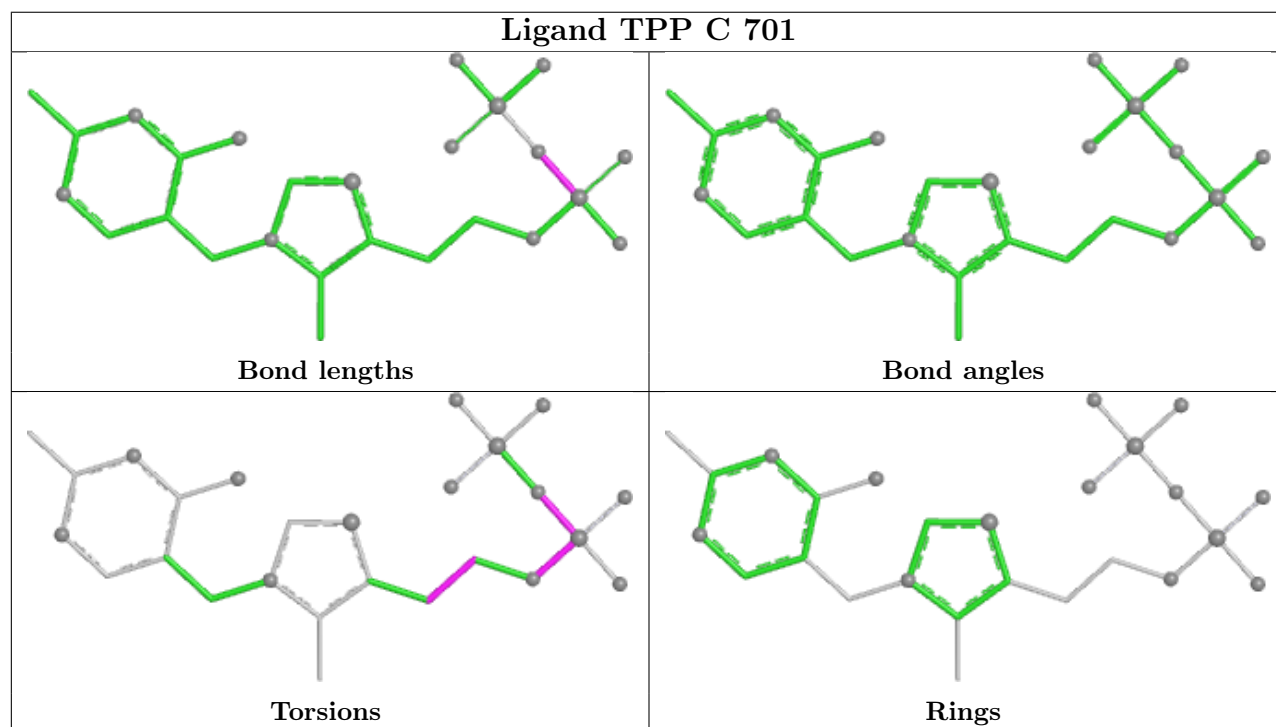
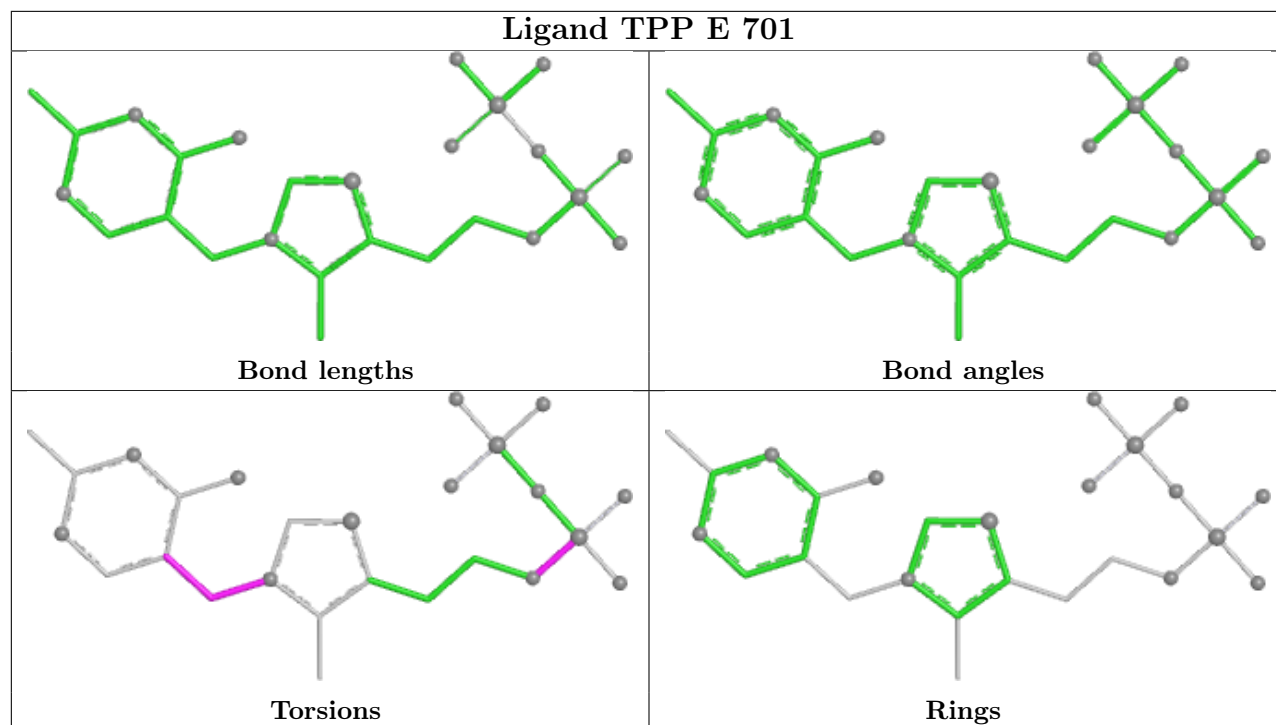
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	TPP	2	0
2	E	701	TPP	4	0
2	C	701	TPP	1	0
2	G	701	TPP	2	0
2	A	701	TPP	2	0

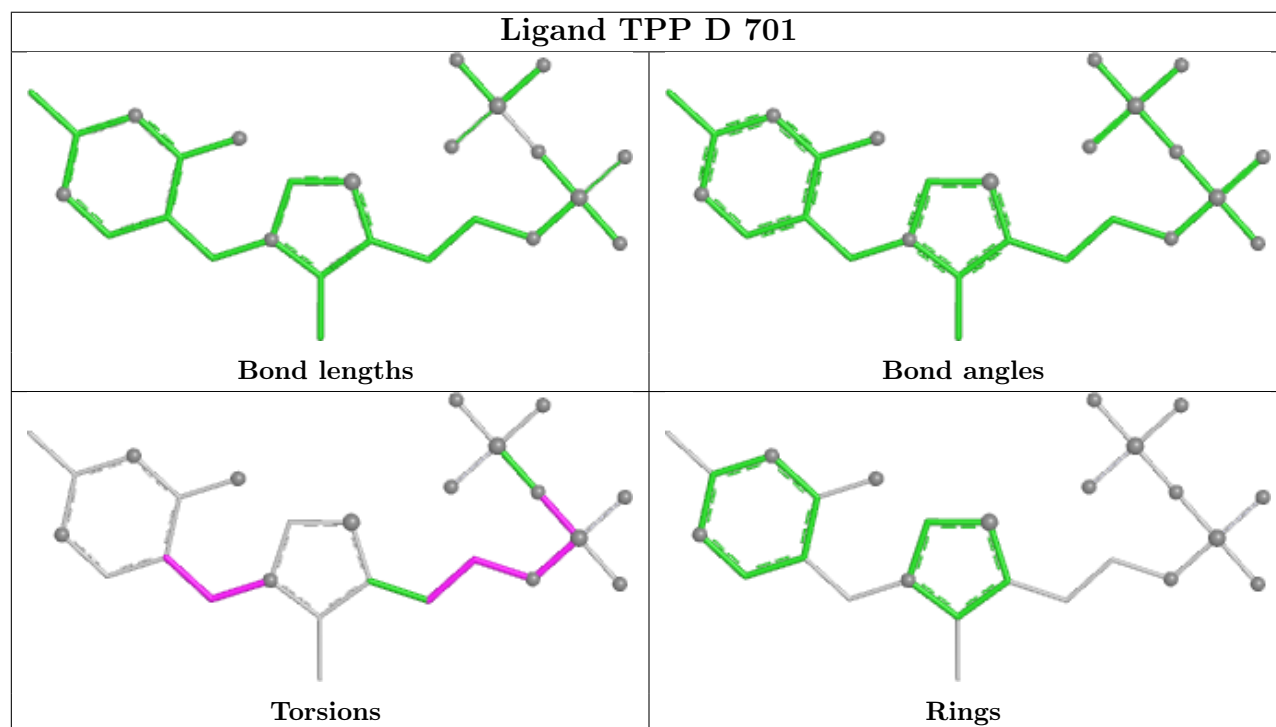
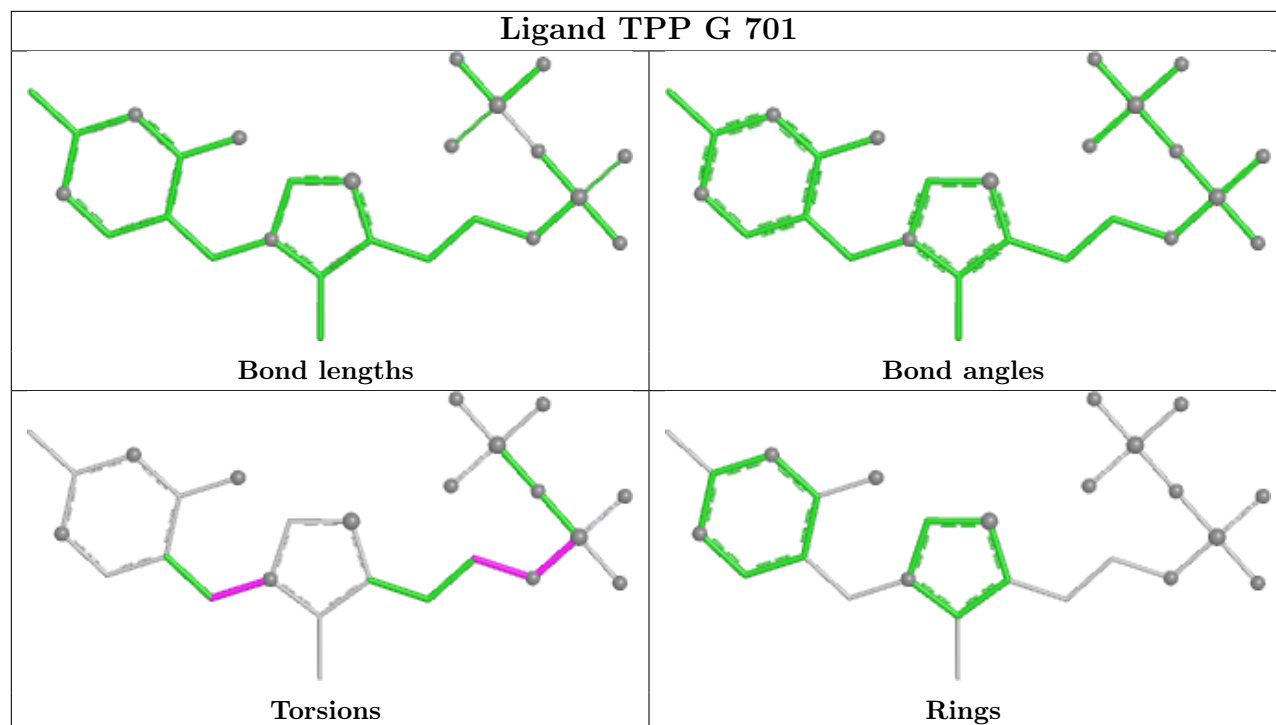
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

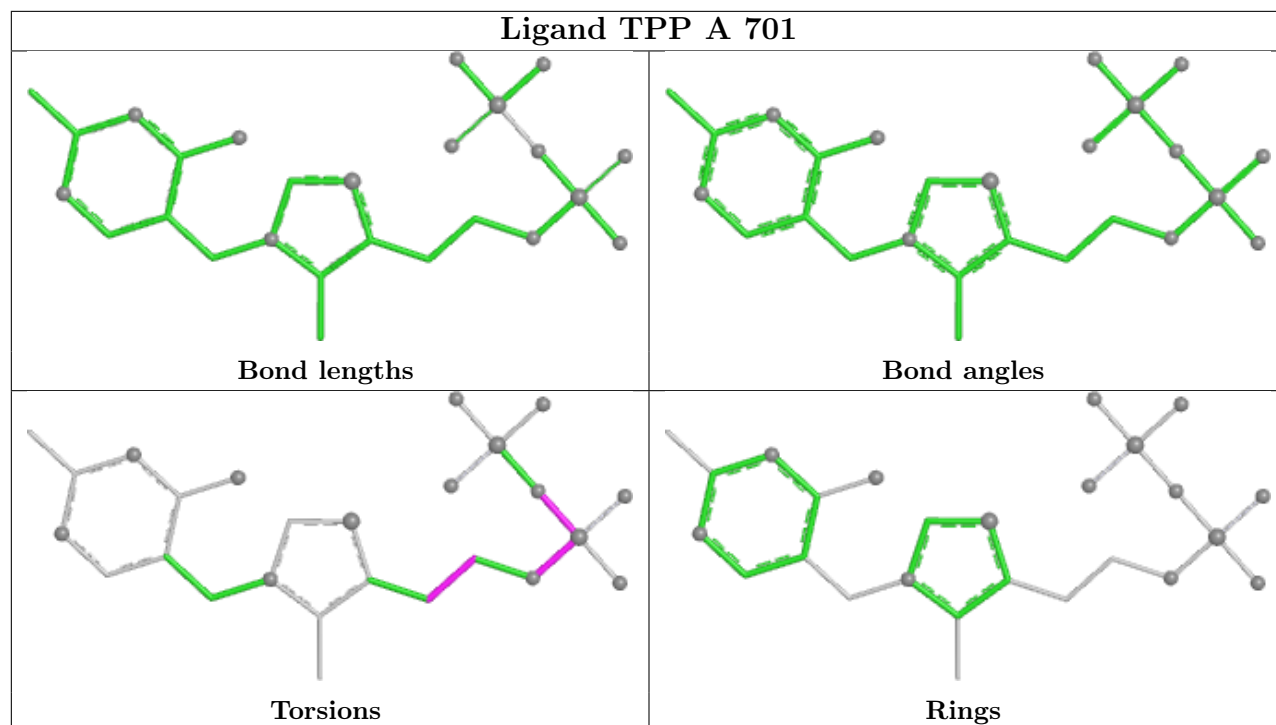












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	663/677 (97%)	0.12	1 (0%) 91 88	20, 31, 46, 68	0
1	B	662/677 (97%)	0.13	4 (0%) 85 80	20, 31, 49, 76	0
1	C	663/677 (97%)	0.03	5 (0%) 82 75	18, 28, 44, 74	0
1	D	663/677 (97%)	0.14	8 (1%) 76 68	19, 29, 52, 79	1 (0%)
1	E	662/677 (97%)	0.14	9 (1%) 73 64	18, 30, 51, 82	1 (0%)
1	F	662/677 (97%)	0.19	8 (1%) 76 68	19, 32, 52, 82	0
1	G	662/677 (97%)	0.23	10 (1%) 72 63	19, 34, 56, 84	0
1	H	662/677 (97%)	0.22	5 (0%) 82 75	22, 34, 53, 76	0
1	I	663/677 (97%)	0.20	10 (1%) 72 63	21, 33, 52, 84	0
1	J	662/677 (97%)	0.17	7 (1%) 78 70	21, 31, 55, 86	0
All	All	6624/6770 (97%)	0.16	67 (1%) 79 72	18, 31, 52, 86	2 (0%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	661	SER	4.0
1	D	586[A]	TRP	3.8
1	E	547	GLU	3.7
1	G	280	ASP	3.5
1	I	343	GLU	3.4

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

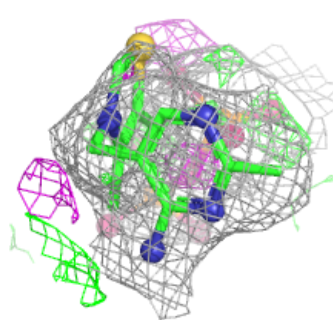
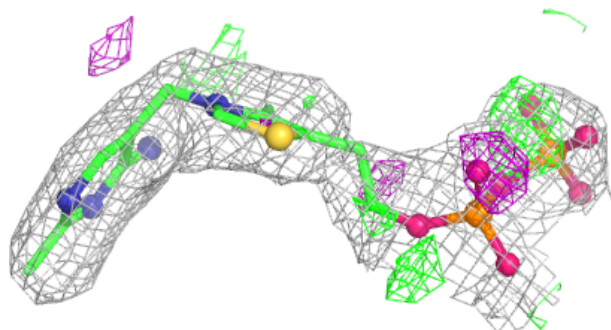
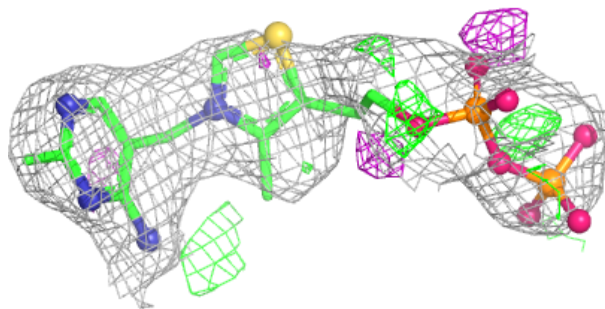
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPP	H	701	26/26	0.82	0.18	36,61,82,92	0
2	TPP	E	701	26/26	0.86	0.17	36,53,71,96	0
2	TPP	G	701	26/26	0.87	0.17	41,64,84,86	0
2	TPP	F	701	26/26	0.87	0.16	42,58,73,86	0
2	TPP	B	701	26/26	0.88	0.15	36,60,76,95	0
2	TPP	D	701	26/26	0.88	0.15	37,54,63,75	0
2	TPP	A	701	26/26	0.88	0.14	37,55,70,77	0
2	TPP	I	701	26/26	0.91	0.13	39,57,72,86	0
2	TPP	J	701	26/26	0.91	0.13	37,59,69,73	0
2	TPP	C	701	26/26	0.92	0.12	31,48,60,78	0
3	MG	G	702	1/1	0.92	0.10	54,54,54,54	0
3	MG	J	702	1/1	0.92	0.09	58,58,58,58	0
3	MG	H	702	1/1	0.93	0.09	52,52,52,52	0
3	MG	A	702	1/1	0.93	0.08	49,49,49,49	0
3	MG	C	702	1/1	0.94	0.07	46,46,46,46	0
3	MG	E	702	1/1	0.94	0.07	43,43,43,43	0
3	MG	F	702	1/1	0.94	0.07	52,52,52,52	0
3	MG	B	702	1/1	0.96	0.06	50,50,50,50	0
3	MG	I	702	1/1	0.97	0.10	53,53,53,53	0
3	MG	D	702	1/1	0.99	0.06	43,43,43,43	0

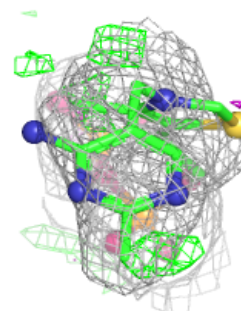
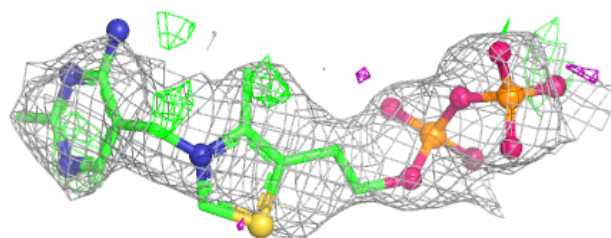
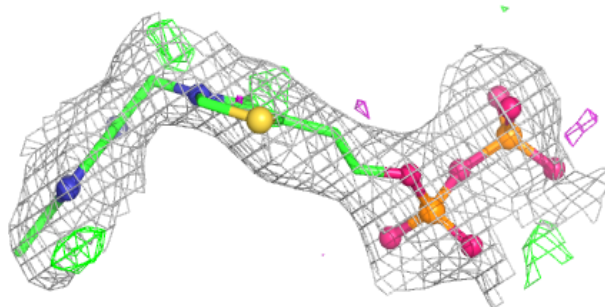
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP H 701:

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

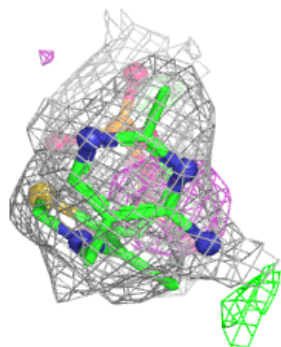
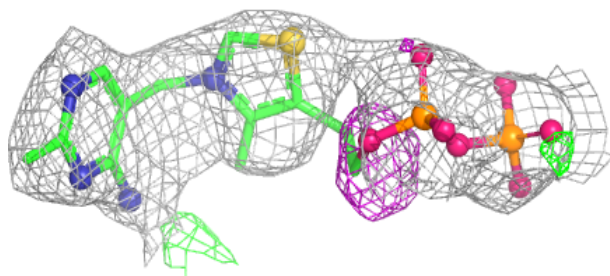
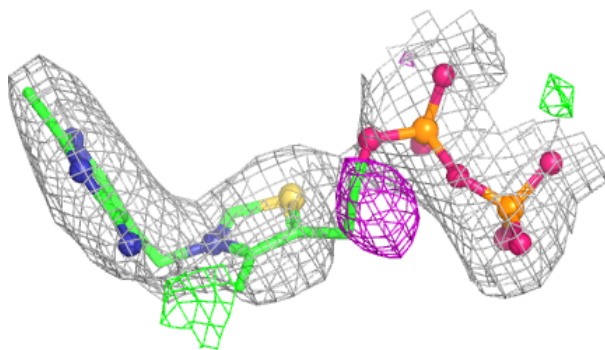
**Electron density around TPP E 701:**

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

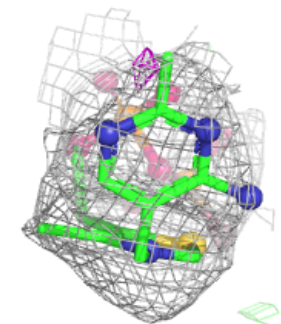
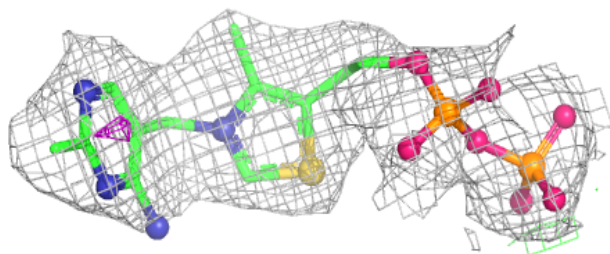
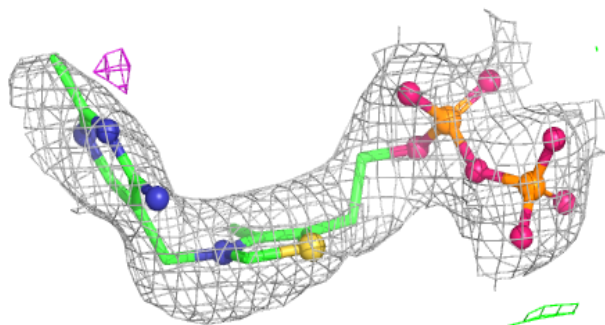


Electron density around TPP G 701:

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

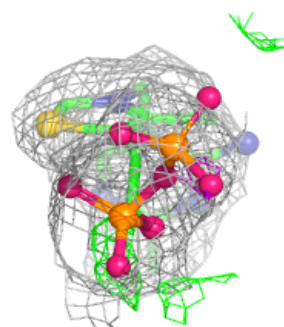
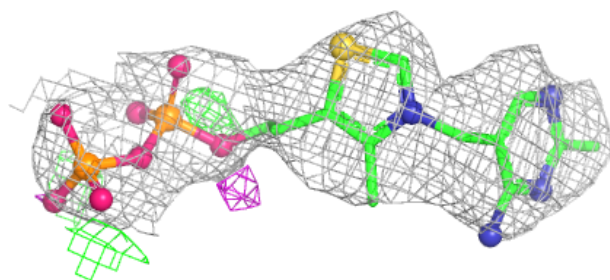
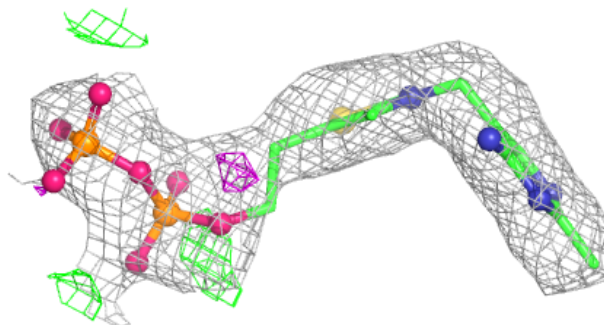
**Electron density around TPP F 701:**

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

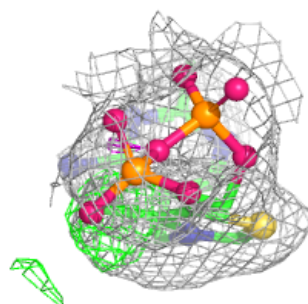
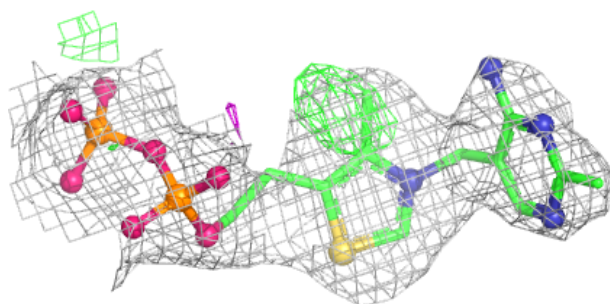
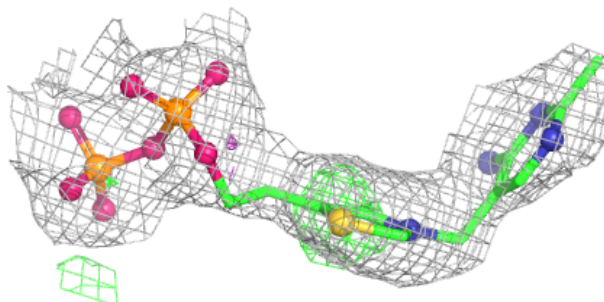


Electron density around TPP B 701:

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

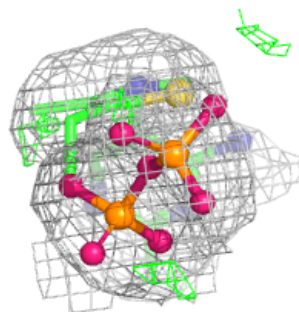
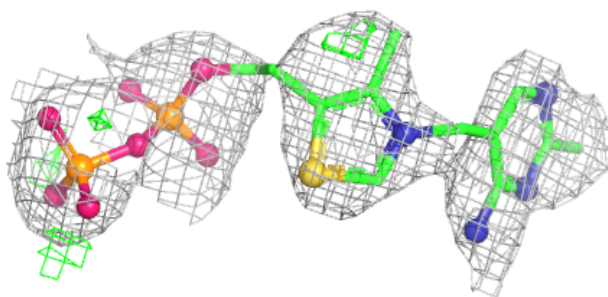
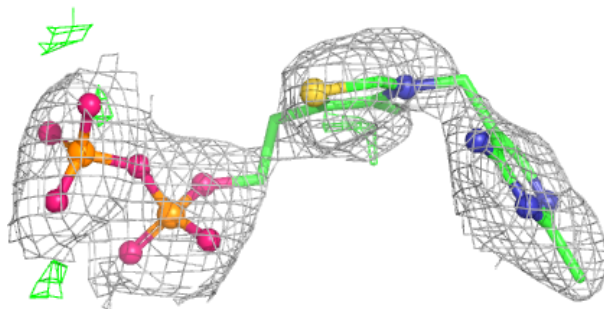
**Electron density around TPP D 701:**

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

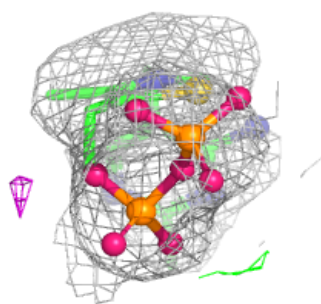
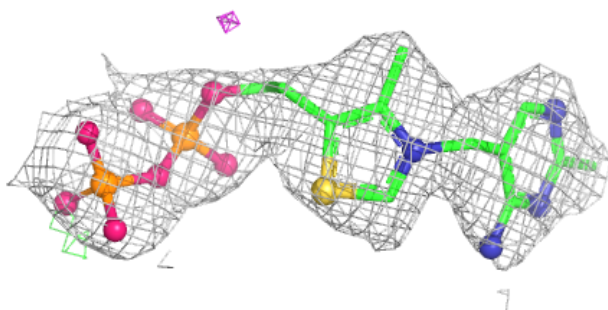
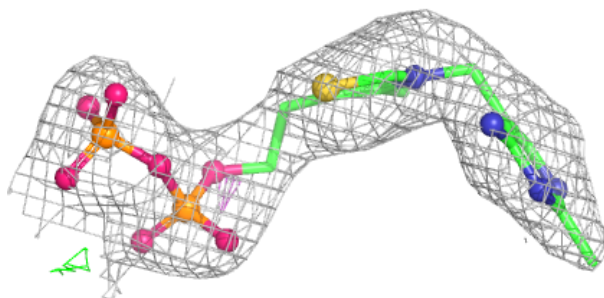


Electron density around TPP A 701:

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

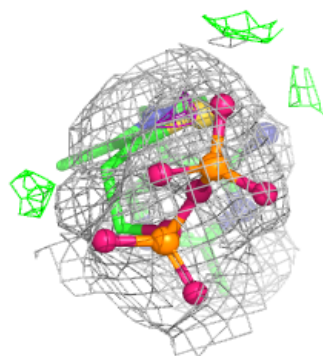
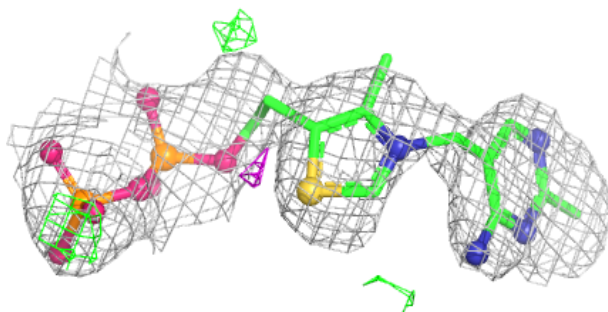
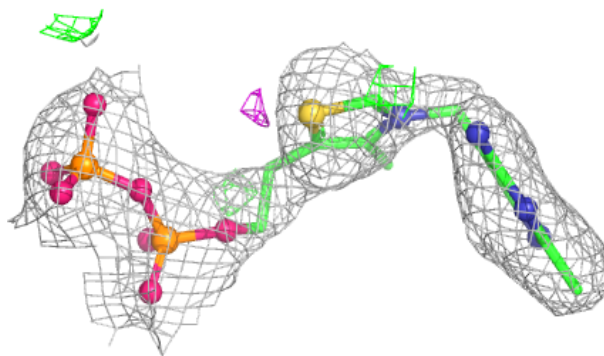
**Electron density around TPP I 701:**

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

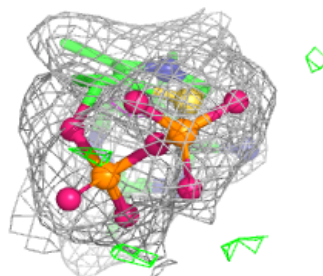
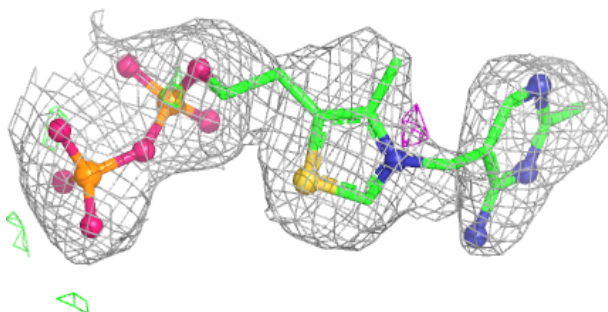
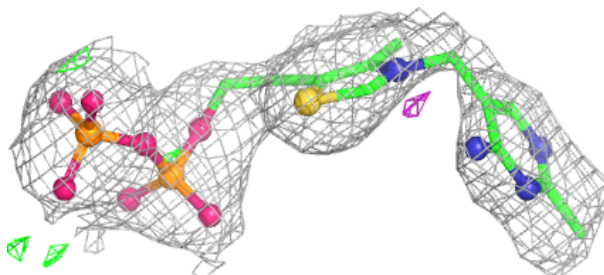


Electron density around TPP J 701:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.