



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:43 am BST

PDB ID : 4RJJ
Title : Acetolactate synthase from *Bacillus subtilis* bound to ThDP - crystal form II
Authors : Sommer, B.; von Moeller, H.; Haack, M.; Qoura, F.; Langner, C.; Bourenkov, G.; Garbe, D.; Brueck, T.; Loll, B.
Deposited on : 2014-10-09
Resolution : 2.34 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

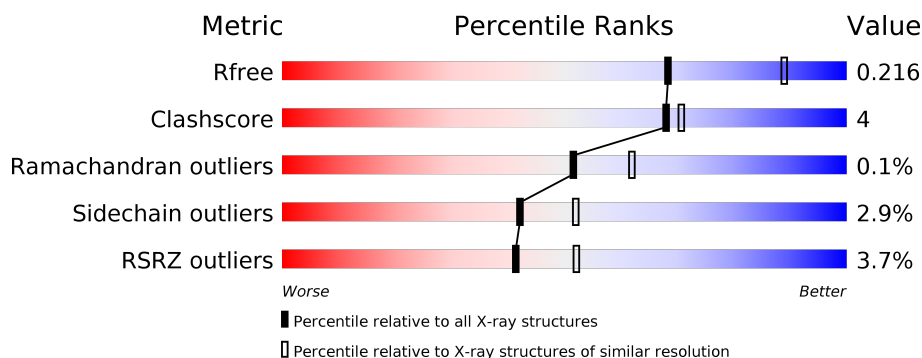
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	571	<div> <div>4%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
1	B	571	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
1	C	571	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	D	571	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
1	E	571	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
1	F	571	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	571	
1	H	571	

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	PG4	E	603	-	-	X	-

2 Entry composition

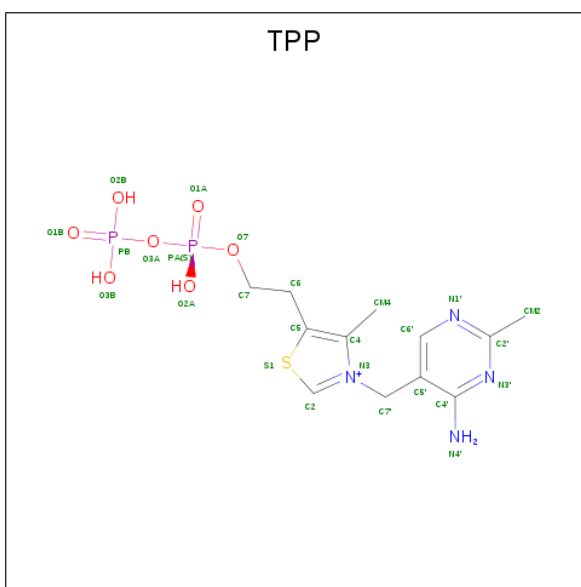
There are 6 unique types of molecules in this entry. The entry contains 36626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetolactate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	2	0
			4261	2704	732	813	12			
1	B	553	Total	C	N	O	S	0	3	0
			4250	2697	729	812	12			
1	C	553	Total	C	N	O	S	0	5	0
			4259	2702	730	814	13			
1	D	553	Total	C	N	O	S	0	9	0
			4276	2723	729	812	12			
1	E	555	Total	C	N	O	S	0	5	0
			4281	2722	734	813	12			
1	F	553	Total	C	N	O	S	0	1	0
			4241	2692	728	809	12			
1	G	554	Total	C	N	O	S	0	1	0
			4250	2696	730	812	12			
1	H	553	Total	C	N	O	S	0	2	0
			4248	2695	729	812	12			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

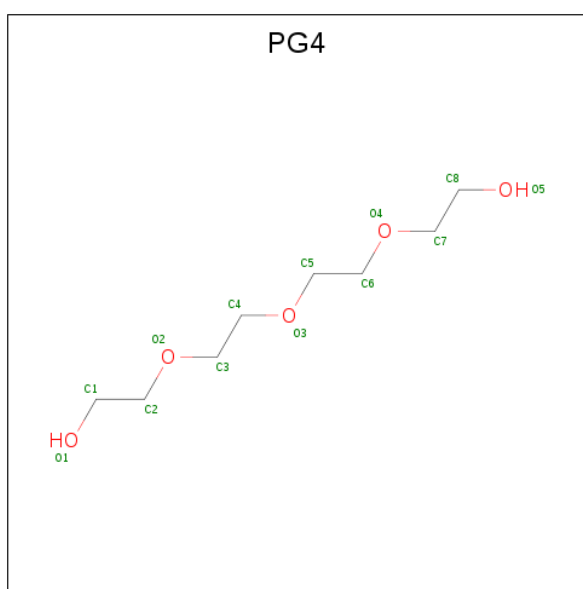
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

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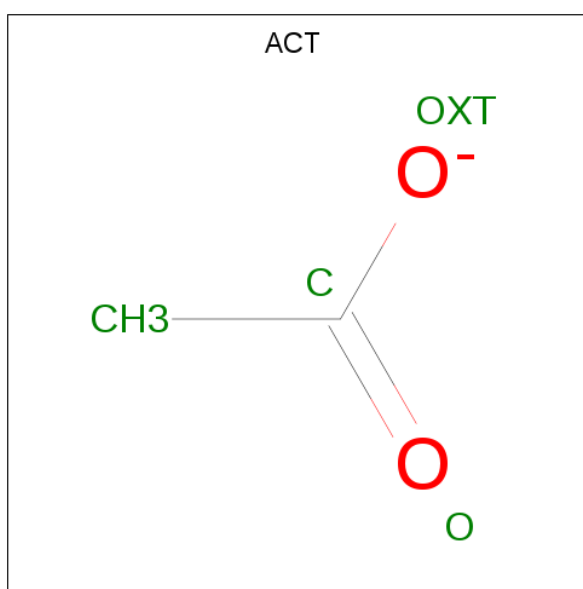
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			11	7	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			8	5	3		
4	H	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	215	Total	O	0	0
			215	215		
6	B	259	Total	O	0	2
			259	259		
6	C	277	Total	O	0	2
			277	277		
6	D	245	Total	O	0	0
			245	245		

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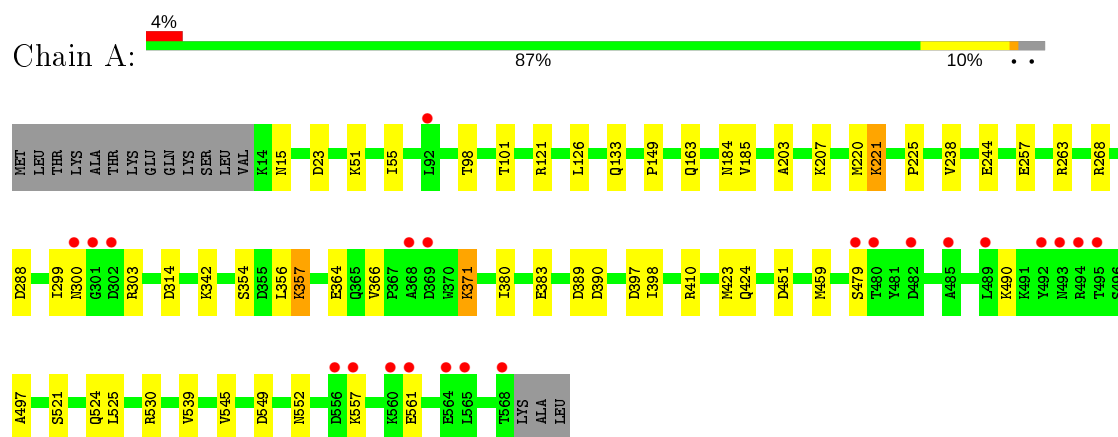
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	260	Total 260	O 260	0	1
6	F	264	Total 264	O 264	0	0
6	G	232	Total 232	O 232	0	0
6	H	203	Total 203	O 203	0	2

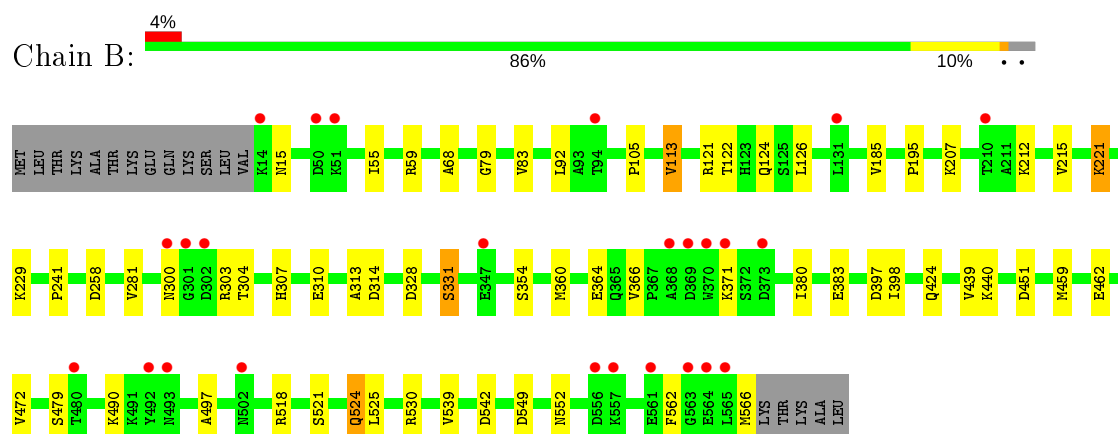
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

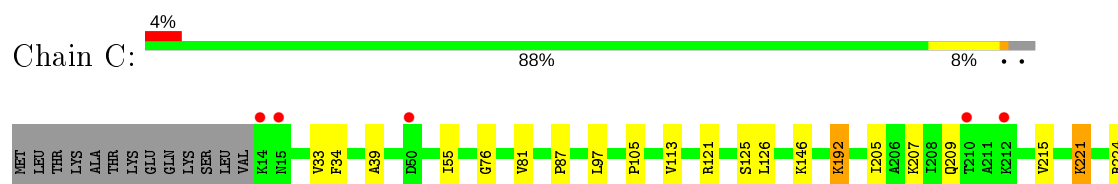
• Molecule 1: Acetolactate synthase

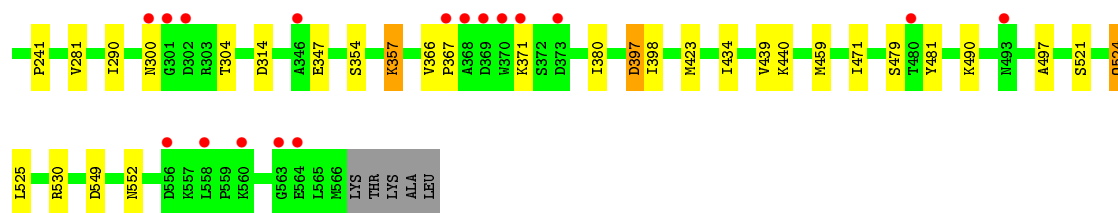


• Molecule 1: Acetolactate synthase

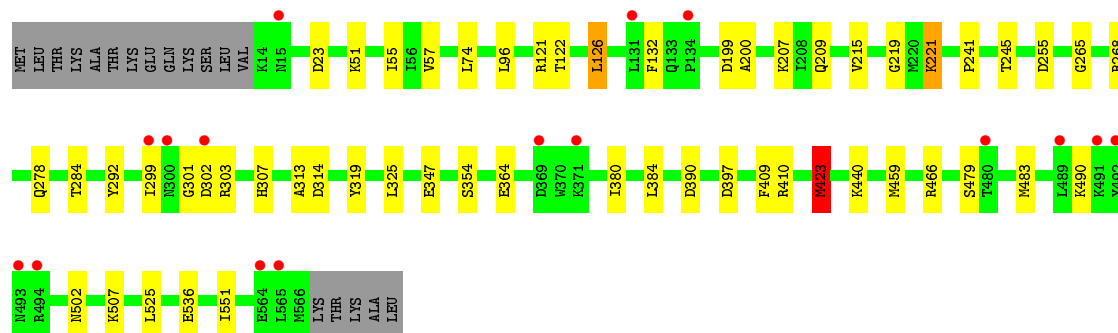
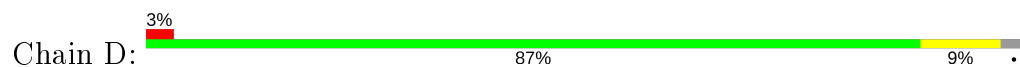


• Molecule 1: Acetolactate synthase

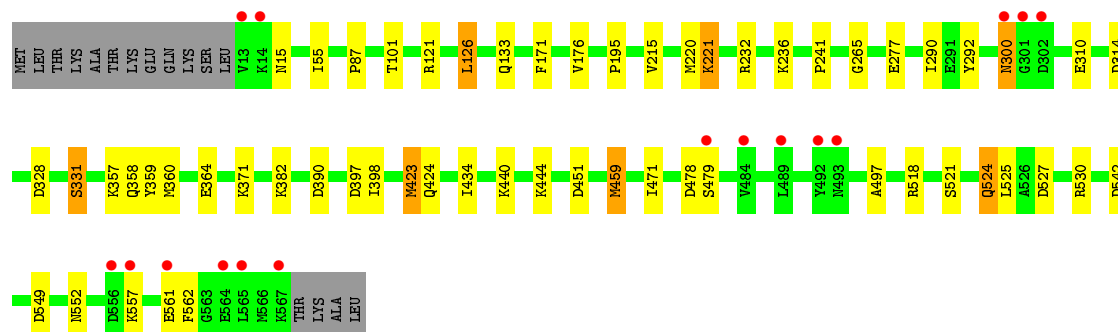
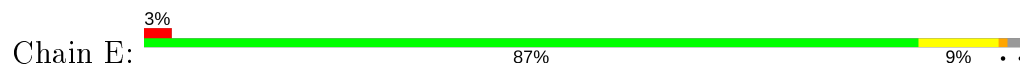




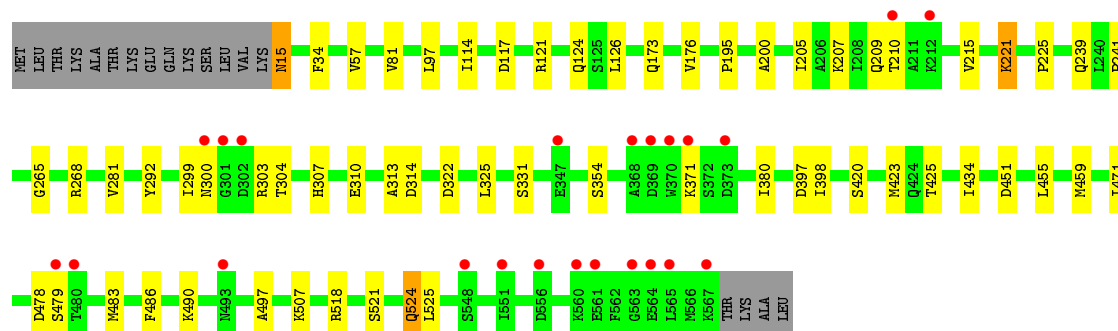
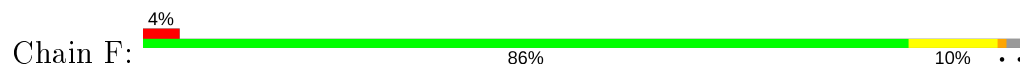
• Molecule 1: Acetolactate synthase



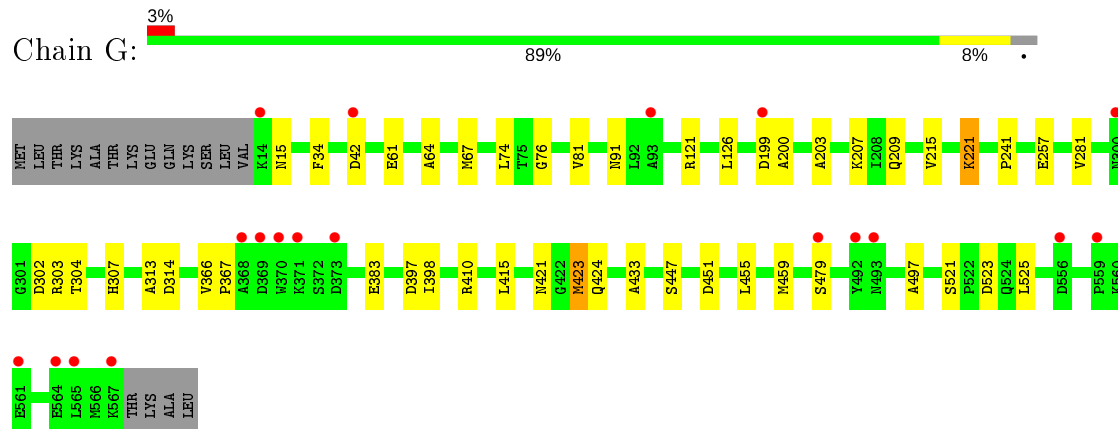
• Molecule 1: Acetolactate synthase



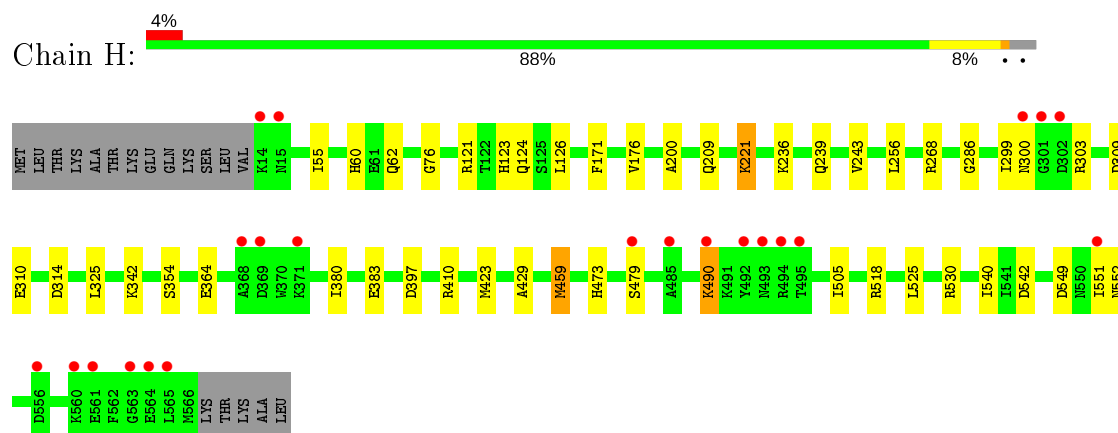
• Molecule 1: Acetolactate synthase



- Molecule 1: Acetolactate synthase



- Molecule 1: Acetolactate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.67Å 170.00Å 339.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.34 48.44 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.34) 98.5 (48.44-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.172 , 0.216 0.171 , 0.216	Depositor DCC
R_{free} test set	13402 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36626	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 25.76 % 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 2.9849e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, TPP, MG, ACT

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	0.44	0/4348	0.58	0/5912
1	B	0.44	0/4340	0.58	0/5902
1	C	0.46	0/4354	0.59	0/5920
1	D	0.45	0/4385	0.59	1/5965 (0.0%)
1	E	0.45	0/4377	0.58	0/5951
1	F	0.45	0/4325	0.58	0/5881
1	G	0.44	0/4334	0.59	0/5892
1	H	0.43	0/4335	0.57	0/5894
All	All	0.45	0/34798	0.58	1/47317 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	423	MET	CG-SD-CE	-5.52	91.36	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4261	0	4280	48	0
1	B	4250	0	4264	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4259	0	4273	32	0
1	D	4276	0	4318	36	0
1	E	4281	0	4319	40	0
1	F	4241	0	4256	37	0
1	G	4250	0	4262	26	0
1	H	4248	0	4259	27	0
2	A	26	0	16	0	0
2	B	26	0	16	1	0
2	C	26	0	16	2	0
2	D	26	0	16	3	0
2	E	26	0	16	0	0
2	F	26	0	16	0	0
2	G	26	0	16	0	0
2	H	26	0	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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	46	0	62	5	0
4	B	46	0	62	7	0
4	C	49	0	67	9	0
4	D	62	0	85	9	0
4	E	65	0	90	17	0
4	F	36	0	49	5	0
4	G	45	0	58	2	0
4	H	36	0	49	2	0
5	D	4	0	3	0	0
6	A	215	0	0	3	0
6	B	259	0	0	0	0
6	C	277	0	0	2	0
6	D	245	0	0	4	0
6	E	260	0	0	3	0
6	F	264	0	0	2	0
6	G	232	0	0	1	0
6	H	203	0	0	2	0
All	All	36626	0	34884	264	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 4.

The worst 5 of 264 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:A:101:THR:HG22	4:A:605:PG4:H82	1.61	0.83
1:D:390:ASP:H	4:D:603:PG4:H12	1.44	0.83
1:E:390:ASP:H	4:E:603:PG4:H71	1.44	0.82
1:F:398:ILE:HD11	1:F:420:SER:HB3	1.61	0.82
1:H:60:HIS:HD1	1:H:62:GLN:H	1.27	0.81

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	555/571 (97%)	544 (98%)	11 (2%)	0	100	100
1	B	554/571 (97%)	540 (98%)	13 (2%)	1 (0%)	47	55
1	C	556/571 (97%)	544 (98%)	11 (2%)	1 (0%)	47	55
1	D	560/571 (98%)	549 (98%)	10 (2%)	1 (0%)	47	55
1	E	558/571 (98%)	546 (98%)	11 (2%)	1 (0%)	47	55
1	F	552/571 (97%)	538 (98%)	13 (2%)	1 (0%)	47	55
1	G	553/571 (97%)	544 (98%)	9 (2%)	0	100	100
1	H	553/571 (97%)	542 (98%)	10 (2%)	1 (0%)	47	55
All	All	4441/4568 (97%)	4347 (98%)	88 (2%)	6 (0%)	51	62

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	302	ASP
1	E	300	ASN
1	B	300	ASN

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Mol	Chain	Res	Type
1	H	300	ASN
1	C	300	ASN

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	456/468 (97%)	443 (97%)	13 (3%)	42	52
1	B	455/468 (97%)	438 (96%)	17 (4%)	34	43
1	C	457/468 (98%)	442 (97%)	15 (3%)	38	46
1	D	461/468 (98%)	449 (97%)	12 (3%)	46	56
1	E	459/468 (98%)	445 (97%)	14 (3%)	40	49
1	F	453/468 (97%)	439 (97%)	14 (3%)	40	49
1	G	454/468 (97%)	444 (98%)	10 (2%)	52	63
1	H	454/468 (97%)	443 (98%)	11 (2%)	49	59
All	All	3649/3744 (98%)	3543 (97%)	106 (3%)	42	52

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	221	LYS
1	E	221	LYS
1	H	243	VAL
1	D	303	ARG
1	D	423	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	534	ASN
1	H	123	HIS
1	F	124	GLN

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Mol	Chain	Res	Type
1	D	124	GLN
1	E	124	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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	$\# Z > 2$
4	PG4	G	603	-	12,12,12	0.59	0	11,11,11	0.99	0
4	PG4	H	603	-	12,12,12	0.46	0	11,11,11	1.03	1 (9%)
4	PG4	C	606	-	9,9,12	0.47	0	8,8,11	0.96	1 (12%)
4	PG4	B	606	-	9,9,12	0.48	0	8,8,11	1.04	1 (12%)
5	ACT	D	608	-	1,3,3	2.15	1 (100%)	0,3,3	0.00	-
2	TPP	C	601	3	22,27,27	2.31	7 (31%)	29,40,40	2.07	10 (34%)
2	TPP	B	601	3	22,27,27	2.39	6 (27%)	29,40,40	1.81	10 (34%)
4	PG4	C	604	-	12,12,12	0.55	0	11,11,11	0.88	0
4	PG4	D	605	-	12,12,12	0.61	0	11,11,11	0.85	0
4	PG4	E	606	-	12,12,12	0.53	0	11,11,11	1.22	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG4	D	607	-	9,9,12	0.61	0	8,8,11	0.80	0
2	TPP	H	601	3	22,27,27	2.43	9 (40%)	29,40,40	1.81	7 (24%)
2	TPP	D	601	3	22,27,27	2.35	9 (40%)	29,40,40	2.02	10 (34%)
2	TPP	G	601	3	22,27,27	2.49	6 (27%)	29,40,40	1.75	10 (34%)
4	PG4	H	604	-	9,9,12	0.57	0	8,8,11	0.96	1 (12%)
4	PG4	B	604	-	12,12,12	0.58	0	11,11,11	0.96	0
4	PG4	C	603	-	12,12,12	0.55	0	11,11,11	0.86	0
2	TPP	E	601	3	22,27,27	2.53	8 (36%)	29,40,40	2.02	11 (37%)
4	PG4	D	606	-	12,12,12	0.58	0	11,11,11	0.89	0
4	PG4	C	605	-	12,12,12	0.63	0	11,11,11	0.68	0
4	PG4	G	605	-	10,10,12	0.49	0	9,9,11	0.85	0
2	TPP	A	601	3	22,27,27	2.62	10 (45%)	29,40,40	1.73	8 (27%)
4	PG4	A	604	-	12,12,12	0.56	0	11,11,11	0.95	1 (9%)
4	PG4	D	604	-	12,12,12	0.56	0	11,11,11	0.83	0
4	PG4	E	607	-	12,12,12	0.61	0	11,11,11	0.85	0
4	PG4	F	605	-	9,9,12	0.60	0	8,8,11	0.79	0
4	PG4	E	603	-	12,12,12	0.69	0	11,11,11	0.99	0
4	PG4	G	606	-	7,7,12	0.51	0	6,6,11	0.92	0
4	PG4	A	606	-	9,9,12	0.62	0	8,8,11	0.96	1 (12%)
4	PG4	G	604	-	12,12,12	0.55	0	11,11,11	0.92	0
4	PG4	B	603	-	9,9,12	0.70	0	8,8,11	0.95	0
4	PG4	E	605	-	12,12,12	0.60	0	11,11,11	0.85	0
4	PG4	D	603	-	12,12,12	0.65	0	11,11,11	0.83	0
4	PG4	F	604	-	12,12,12	0.64	0	11,11,11	0.92	1 (9%)
4	PG4	E	604	-	12,12,12	0.56	0	11,11,11	0.95	0
2	TPP	F	601	3	22,27,27	2.79	9 (40%)	29,40,40	1.85	8 (27%)
4	PG4	H	605	-	12,12,12	0.57	0	11,11,11	1.01	1 (9%)
4	PG4	A	603	-	9,9,12	0.63	0	8,8,11	0.80	0
4	PG4	F	603	-	12,12,12	0.62	0	11,11,11	0.95	0
4	PG4	B	605	-	12,12,12	0.58	0	11,11,11	1.02	0
4	PG4	A	605	-	12,12,12	0.48	0	11,11,11	1.01	1 (9%)

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
4	PG4	G	603	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	H	603	-	-	5/10/10/10	-
4	PG4	C	606	-	-	5/7/7/10	-
4	PG4	B	606	-	-	4/7/7/10	-
2	TPP	C	601	3	-	1/16/17/17	0/2/2/2
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
4	PG4	C	604	-	-	3/10/10/10	-
4	PG4	D	605	-	-	7/10/10/10	-
4	PG4	E	606	-	-	5/10/10/10	-
4	PG4	D	607	-	-	4/7/7/10	-
2	TPP	H	601	3	-	1/16/17/17	0/2/2/2
2	TPP	D	601	3	-	2/16/17/17	0/2/2/2
2	TPP	G	601	3	-	2/16/17/17	0/2/2/2
4	PG4	H	604	-	-	2/7/7/10	-
4	PG4	B	604	-	-	6/10/10/10	-
4	PG4	C	603	-	-	1/10/10/10	-
2	TPP	E	601	3	-	1/16/17/17	0/2/2/2
4	PG4	D	606	-	-	7/10/10/10	-
4	PG4	C	605	-	-	4/10/10/10	-
4	PG4	G	605	-	-	5/8/8/10	-
2	TPP	A	601	3	-	2/16/17/17	0/2/2/2
4	PG4	A	604	-	-	7/10/10/10	-
4	PG4	D	604	-	-	3/10/10/10	-
4	PG4	E	607	-	-	6/10/10/10	-
4	PG4	F	605	-	-	5/7/7/10	-
4	PG4	E	603	-	-	7/10/10/10	-
4	PG4	G	606	-	-	2/5/5/10	-
4	PG4	A	606	-	-	1/7/7/10	-
4	PG4	G	604	-	-	1/10/10/10	-
4	PG4	B	603	-	-	5/7/7/10	-
4	PG4	E	605	-	-	5/10/10/10	-
4	PG4	D	603	-	-	7/10/10/10	-
4	PG4	F	604	-	-	2/10/10/10	-
4	PG4	E	604	-	-	5/10/10/10	-
2	TPP	F	601	3	-	2/16/17/17	0/2/2/2
4	PG4	H	605	-	-	8/10/10/10	-
4	PG4	A	603	-	-	1/7/7/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	F	603	-	-	7/10/10/10	-
4	PG4	B	605	-	-	6/10/10/10	-
4	PG4	A	605	-	-	5/10/10/10	-

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	TPP	C6-C5	9.20	1.55	1.50
2	A	601	TPP	C6-C5	7.98	1.54	1.50
2	E	601	TPP	C6-C5	7.33	1.54	1.50
2	G	601	TPP	C6-C5	7.04	1.54	1.50
2	H	601	TPP	C6-C5	6.53	1.53	1.50

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	TPP	CM2-C2'-N1'	5.54	123.23	117.14
2	C	601	TPP	CM2-C2'-N1'	5.41	123.09	117.14
2	D	601	TPP	CM2-C2'-N1'	4.69	122.30	117.14
2	C	601	TPP	N1'-C2'-N3'	-4.22	118.28	125.54
2	D	601	TPP	N1'-C2'-N3'	-3.75	119.09	125.54

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	TPP	C4-C5-C6-C7
2	F	601	TPP	C4-C5-C6-C7
2	H	601	TPP	PB-O3A-PA-O7
2	D	601	TPP	C4-C5-C6-C7
2	G	601	TPP	C4-C5-C6-C7

There are no ring outliers.

26 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	603	PG4	2	0
4	C	606	PG4	2	0
4	B	606	PG4	1	0
2	C	601	TPP	2	0

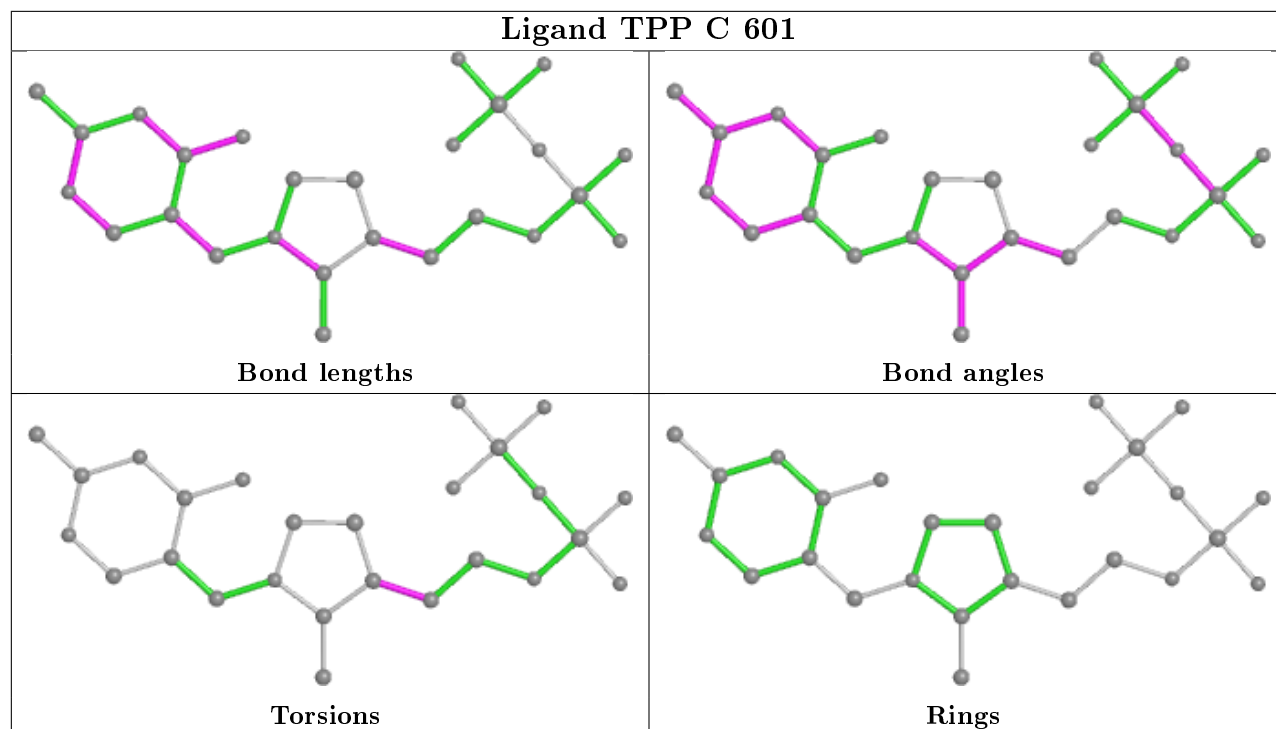
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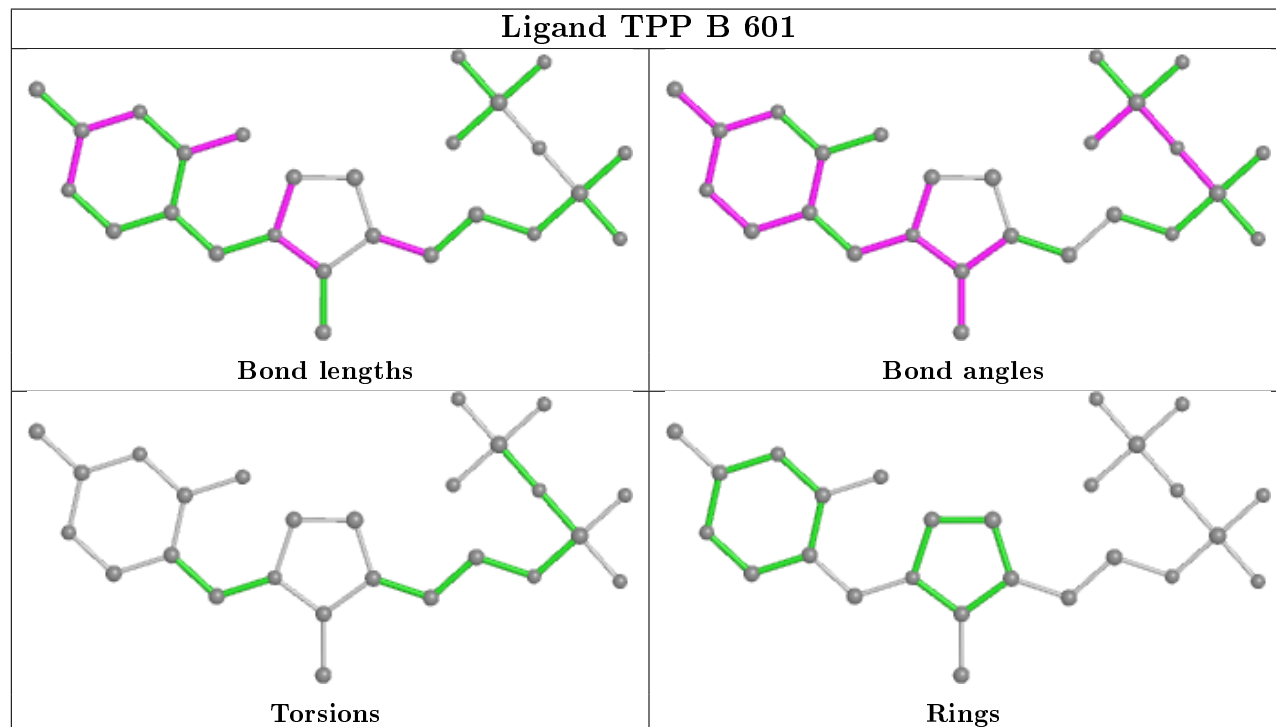
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	TPP	1	0
4	C	604	PG4	2	0
4	D	605	PG4	2	0
4	E	606	PG4	6	0
4	D	607	PG4	2	0
2	H	601	TPP	1	0
2	D	601	TPP	3	0
4	C	603	PG4	1	0
4	D	606	PG4	3	0
4	C	605	PG4	4	0
4	A	604	PG4	3	0
4	D	604	PG4	1	0
4	E	607	PG4	2	0
4	E	603	PG4	9	0
4	B	603	PG4	2	0
4	D	603	PG4	1	0
4	F	604	PG4	1	0
4	H	605	PG4	2	0
4	A	603	PG4	1	0
4	F	603	PG4	4	0
4	B	605	PG4	4	0
4	A	605	PG4	1	0

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

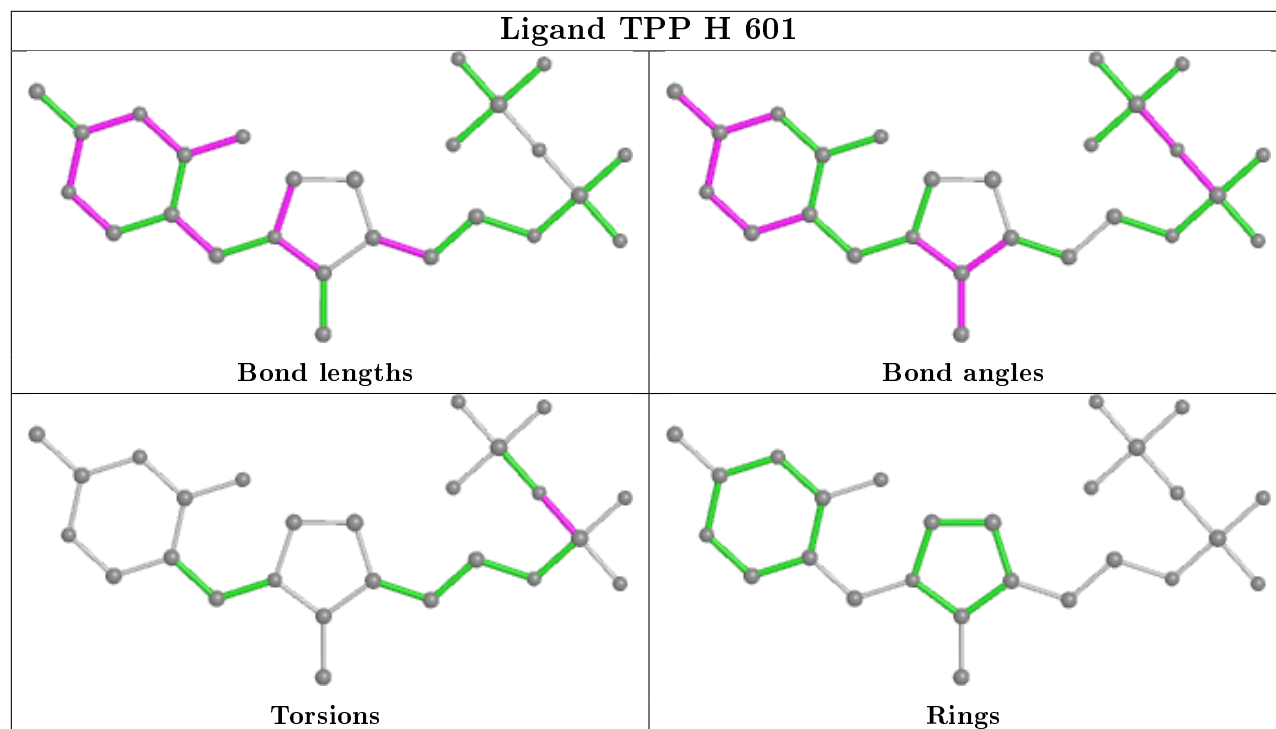
Ligand TPP C 601



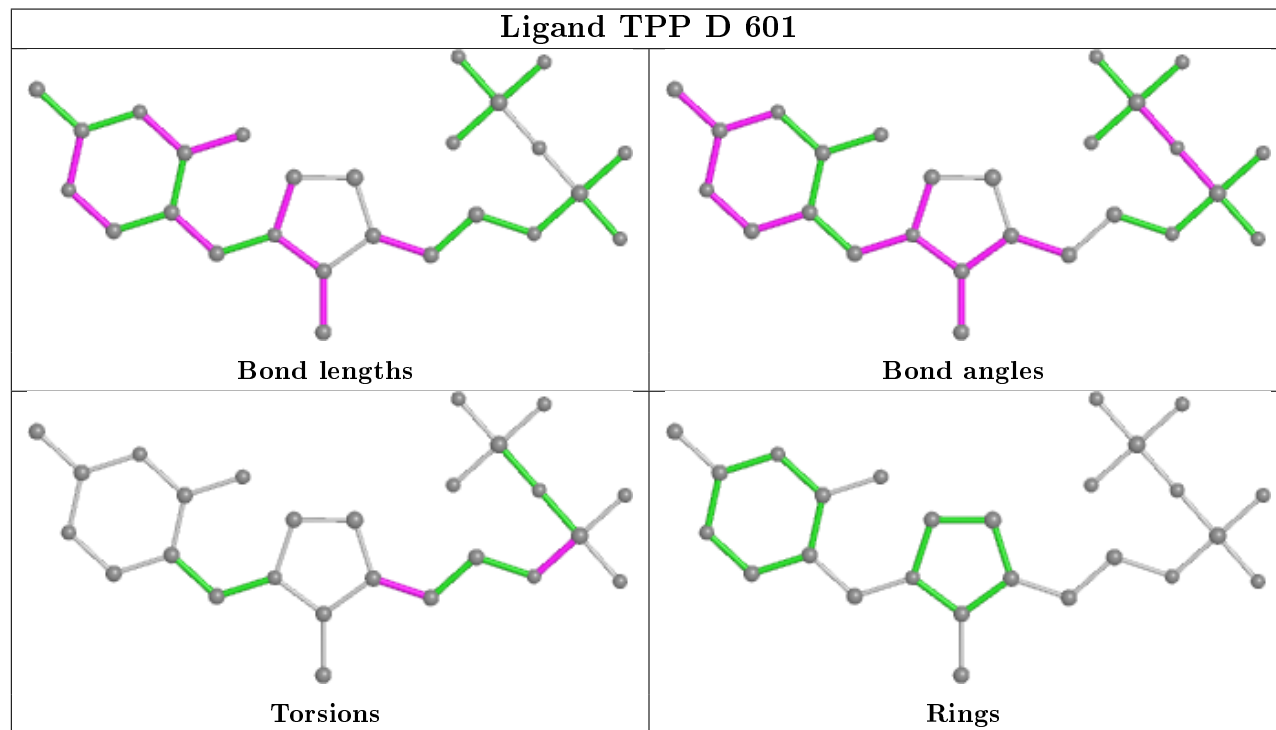
Ligand TPP B 601



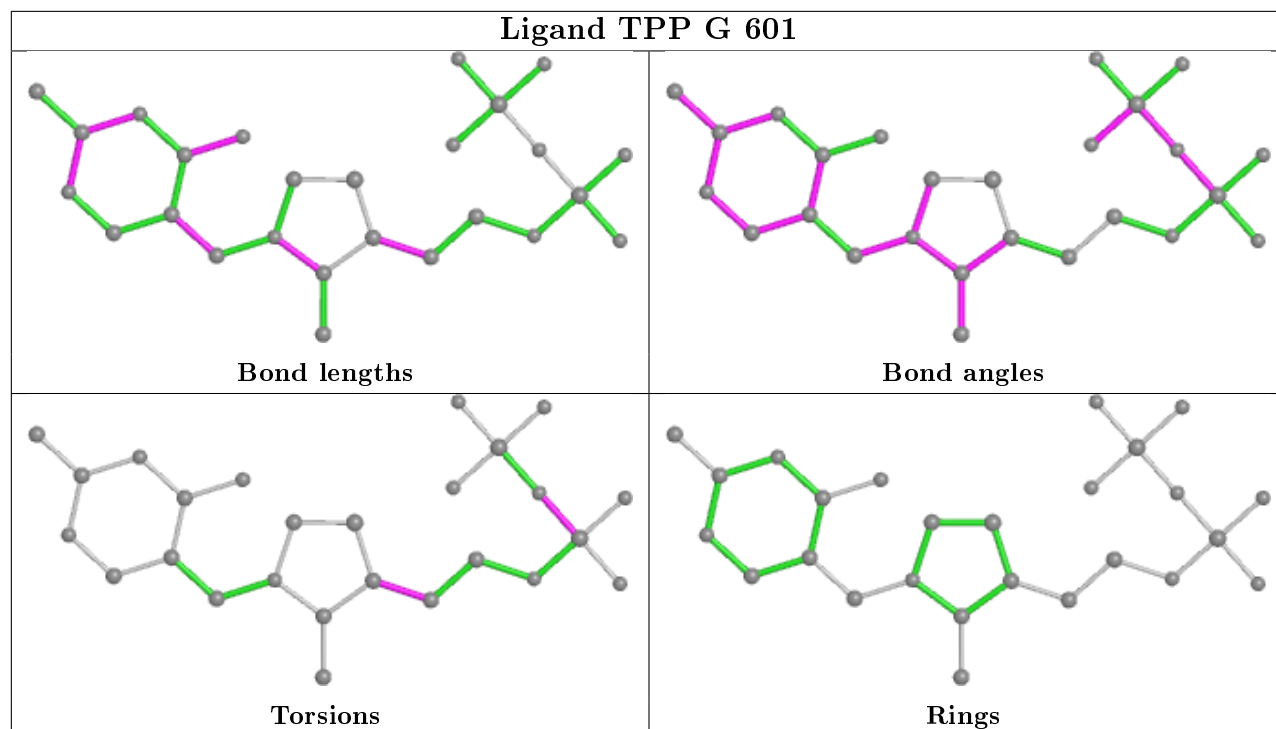
Ligand TPP H 601



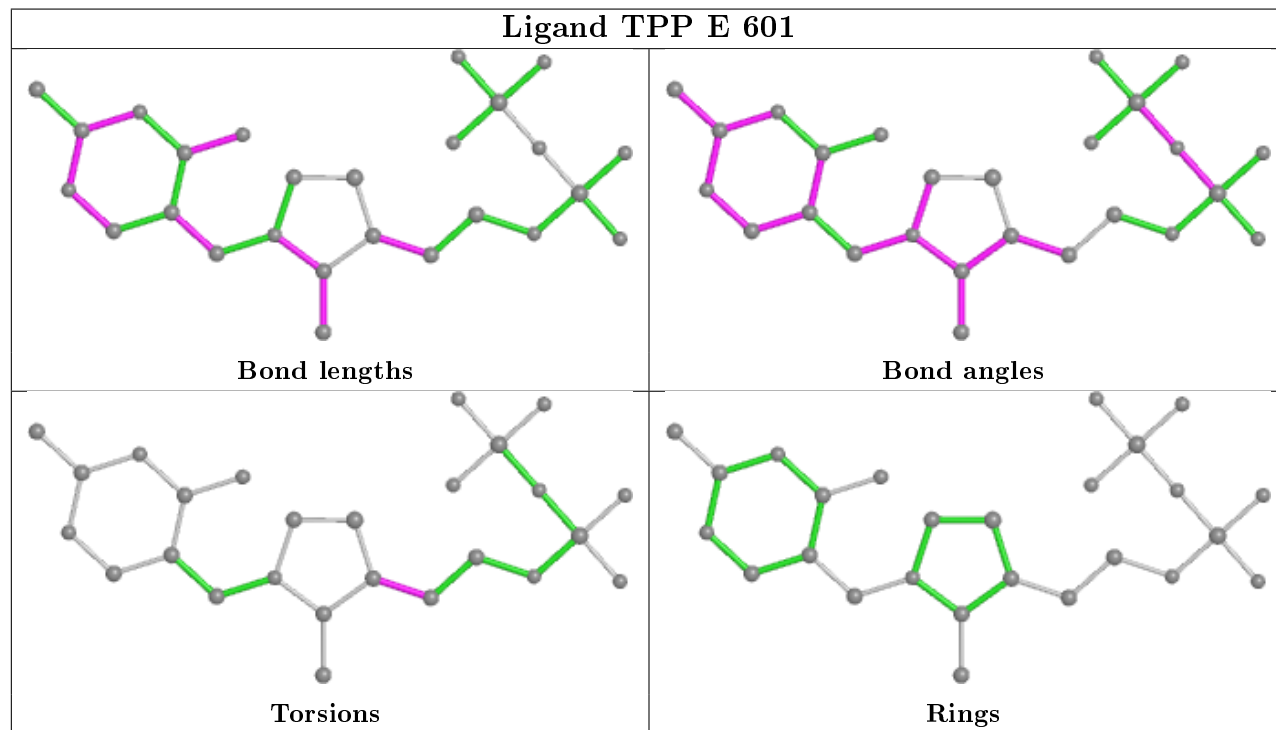
Ligand TPP D 601

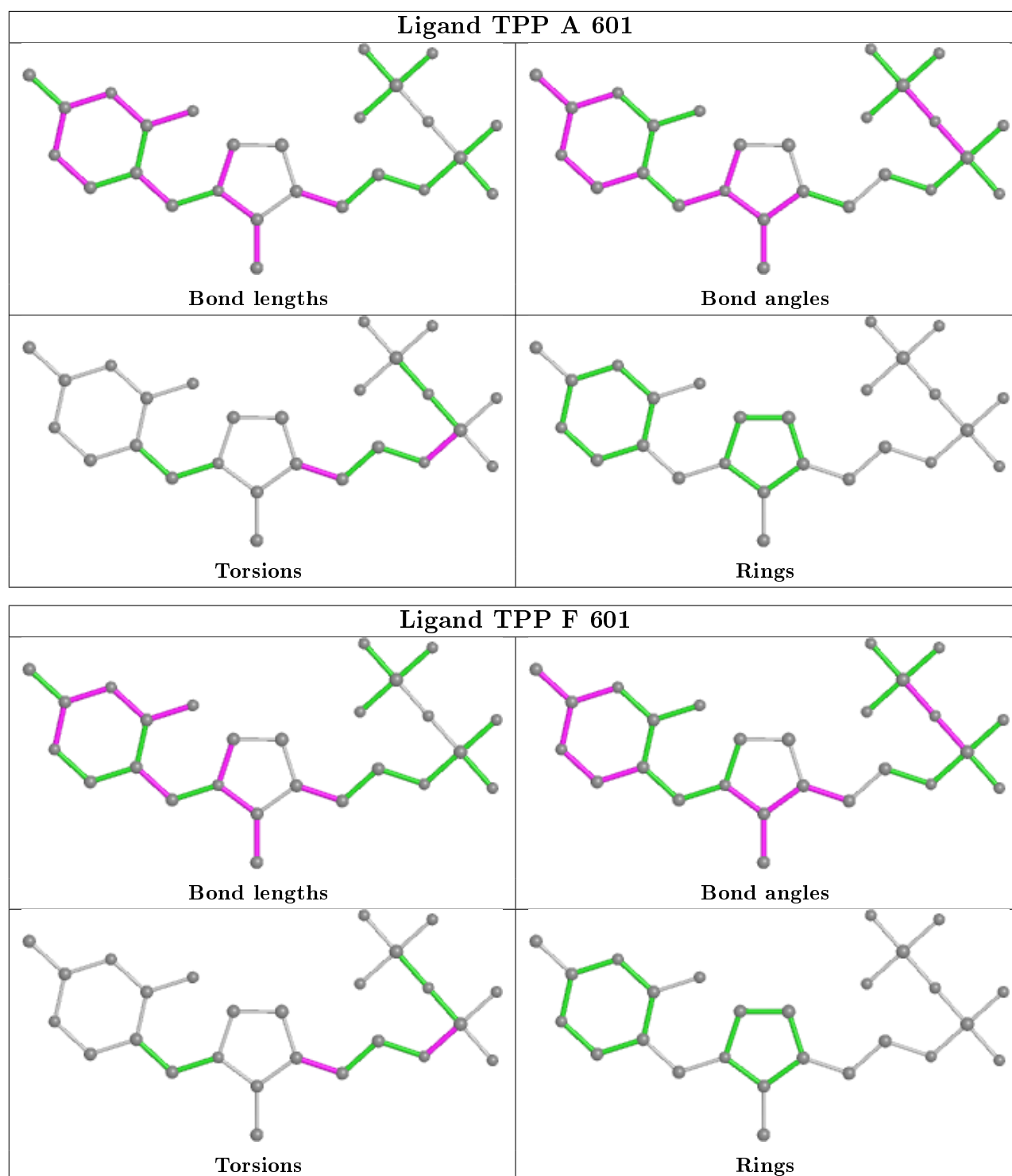


Ligand TPP G 601



Ligand TPP E 601





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 ⓘ

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, 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	555/571 (97%)	-0.16	22 (3%)	38	49	11, 23, 45, 79	0
1	B	553/571 (96%)	-0.01	25 (4%)	33	44	9, 20, 44, 72	0
1	C	553/571 (96%)	-0.03	22 (3%)	38	49	11, 19, 40, 71	0
1	D	553/571 (96%)	-0.22	16 (2%)	51	61	10, 20, 43, 70	0
1	E	555/571 (97%)	-0.24	16 (2%)	51	61	9, 19, 42, 71	0
1	F	553/571 (96%)	-0.05	23 (4%)	36	47	11, 20, 42, 68	0
1	G	554/571 (97%)	-0.04	19 (3%)	45	55	11, 21, 43, 76	0
1	H	553/571 (96%)	-0.15	22 (3%)	38	49	13, 24, 47, 71	0
All	All	4429/4568 (96%)	-0.11	165 (3%)	41	52	9, 21, 44, 79	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	THR	7.8
1	E	300	ASN	6.8
1	D	564	GLU	4.4
1	A	493	ASN	4.3
1	A	492	TYR	4.2

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 carbohydrates 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, 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.

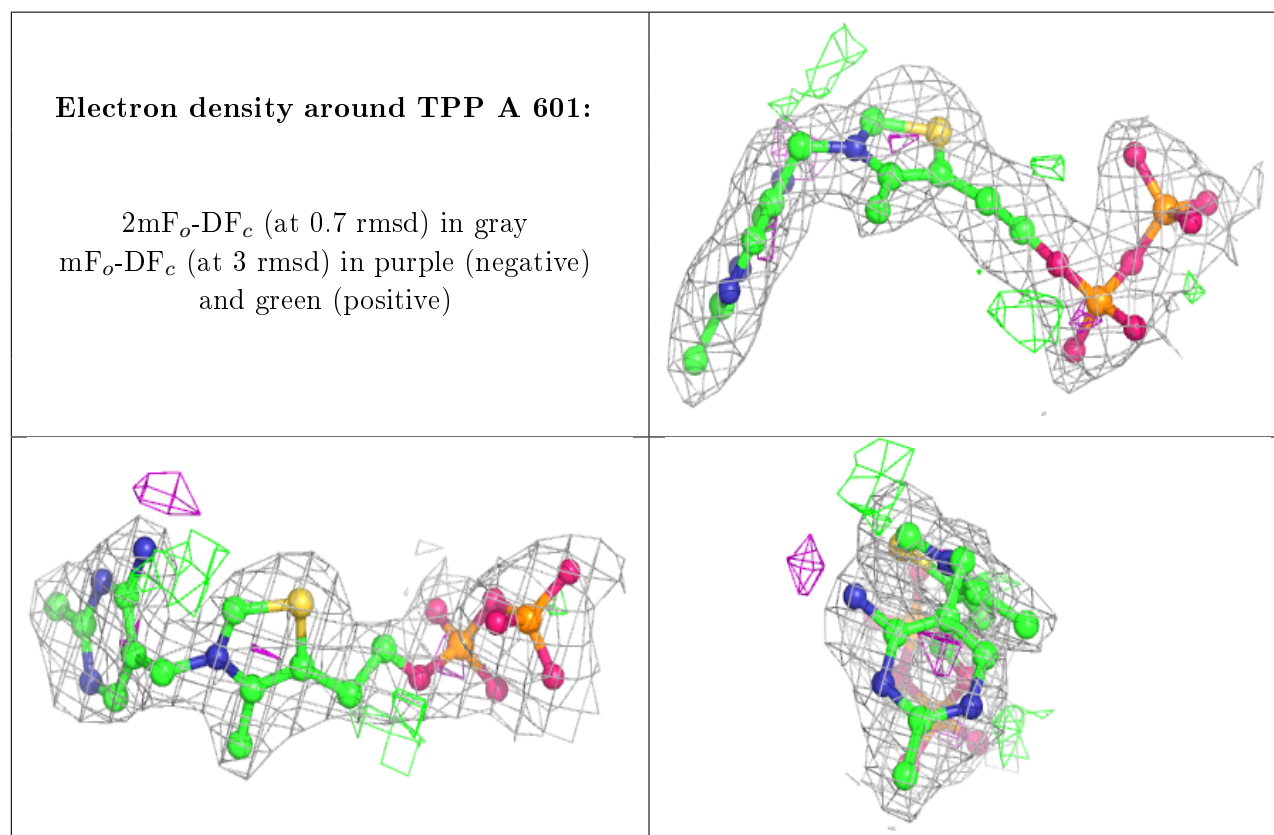
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PG4	H	603	13/13	0.79	0.21	28,40,48,50	0
4	PG4	G	606	8/13	0.83	0.19	41,46,52,53	0
4	PG4	B	606	10/13	0.84	0.22	33,45,50,58	0
5	ACT	D	608	4/4	0.84	0.16	30,32,34,37	0
4	PG4	C	606	10/13	0.84	0.21	36,48,52,55	0
4	PG4	E	606	13/13	0.85	0.24	18,31,41,42	0
4	PG4	E	605	13/13	0.85	0.19	33,46,53,58	0
4	PG4	A	605	13/13	0.85	0.17	28,37,48,48	0
4	PG4	E	604	13/13	0.86	0.17	37,49,60,74	0
4	PG4	G	605	11/13	0.86	0.15	31,39,47,52	0
4	PG4	H	605	13/13	0.87	0.20	26,37,46,50	0
4	PG4	D	603	13/13	0.88	0.19	20,27,37,42	0
4	PG4	F	605	10/13	0.89	0.13	34,40,43,48	0
4	PG4	H	604	10/13	0.89	0.15	36,42,48,52	0
4	PG4	G	603	13/13	0.90	0.15	17,31,49,49	0
4	PG4	C	604	13/13	0.91	0.13	32,37,47,49	0
4	PG4	B	604	13/13	0.91	0.15	37,42,51,59	0
4	PG4	E	603	13/13	0.91	0.19	24,30,36,40	0
4	PG4	D	607	10/13	0.91	0.12	31,39,47,49	0
4	PG4	D	604	13/13	0.92	0.17	23,32,42,46	0
4	PG4	E	607	13/13	0.92	0.19	37,47,58,59	0
4	PG4	A	604	13/13	0.92	0.13	27,35,47,47	0
2	TPP	A	601	26/26	0.93	0.14	19,30,38,38	0
4	PG4	G	604	13/13	0.93	0.19	22,29,41,41	0
4	PG4	B	605	13/13	0.93	0.20	24,29,39,44	0
4	PG4	F	603	13/13	0.94	0.24	25,31,38,40	0
3	MG	C	602	1/1	0.94	0.04	28,28,28,28	0
4	PG4	C	605	13/13	0.94	0.15	16,28,41,41	0
4	PG4	F	604	13/13	0.94	0.13	19,29,41,42	0
2	TPP	H	601	26/26	0.94	0.13	17,28,36,39	0
2	TPP	F	601	26/26	0.94	0.13	17,27,33,34	0
4	PG4	A	606	10/13	0.94	0.10	36,41,45,47	0
4	PG4	D	605	13/13	0.95	0.18	22,30,49,52	0
4	PG4	D	606	13/13	0.95	0.17	26,33,38,43	0
4	PG4	B	603	10/13	0.95	0.13	13,24,31,42	0
2	TPP	D	601	26/26	0.95	0.14	15,27,35,41	0
2	TPP	C	601	26/26	0.95	0.12	13,27,33,34	0

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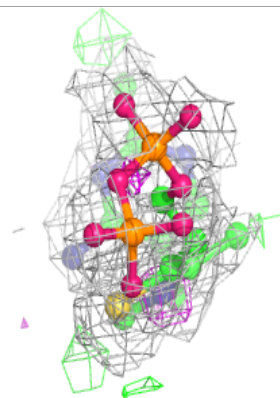
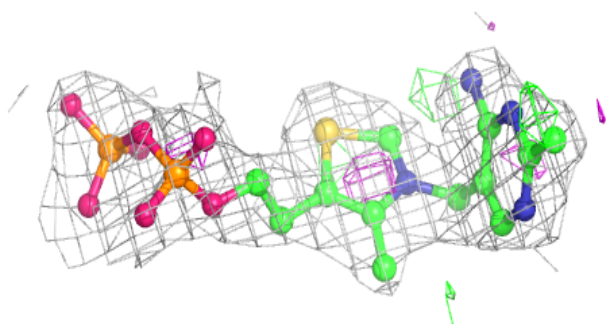
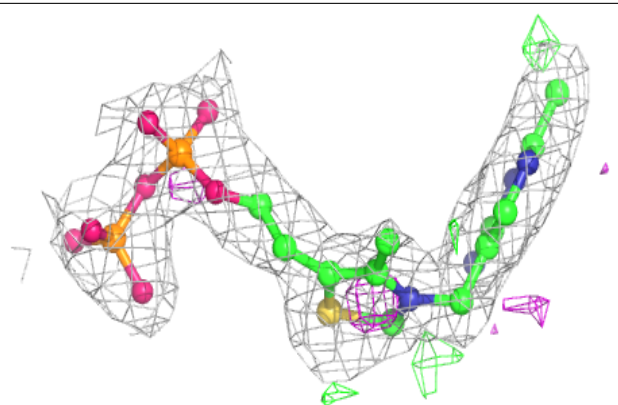
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	602	1/1	0.96	0.06	29,29,29,29	0
4	PG4	C	603	13/13	0.96	0.17	21,27,34,36	0
2	TPP	E	601	26/26	0.96	0.13	15,24,35,35	0
2	TPP	G	601	26/26	0.96	0.12	17,25,32,35	0
2	TPP	B	601	26/26	0.96	0.11	17,29,33,36	0
4	PG4	A	603	10/13	0.96	0.14	21,29,38,40	0
3	MG	H	602	1/1	0.96	0.15	36,36,36,36	0
3	MG	E	602	1/1	0.97	0.11	30,30,30,30	0
3	MG	G	602	1/1	0.97	0.05	21,21,21,21	0
3	MG	A	602	1/1	0.98	0.05	29,29,29,29	0
3	MG	F	602	1/1	0.98	0.10	24,24,24,24	0
3	MG	D	602	1/1	0.98	0.06	25,25,25,25	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.

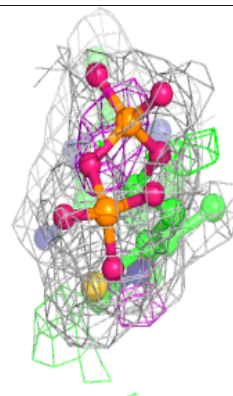
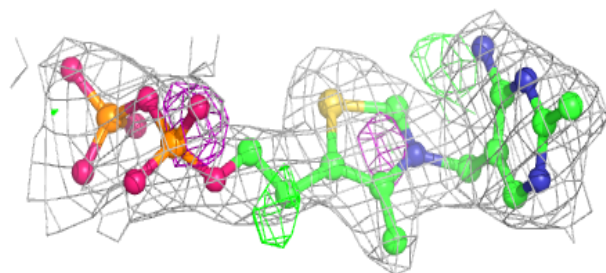
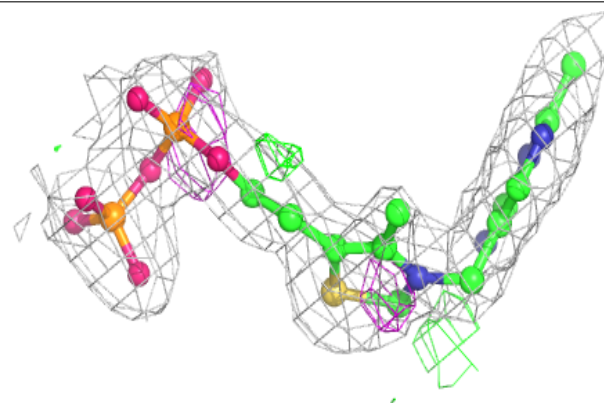


Electron density around TPP H 601:

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

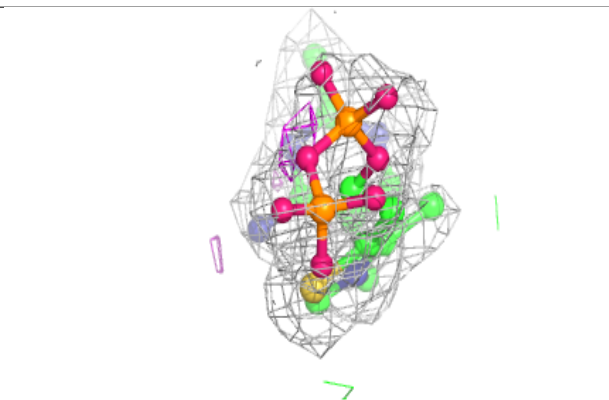
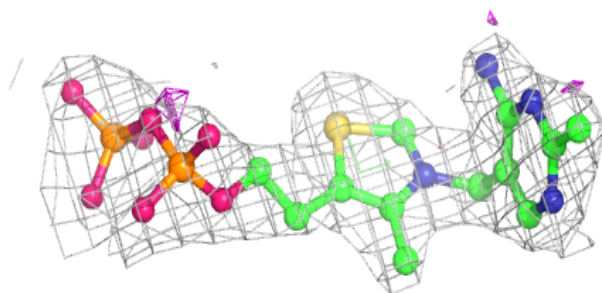
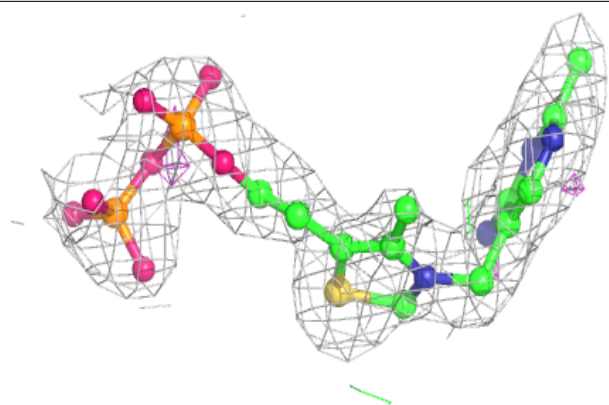
**Electron density around TPP F 601:**

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

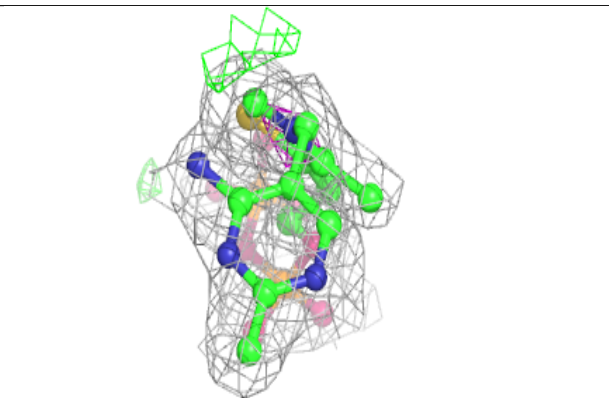
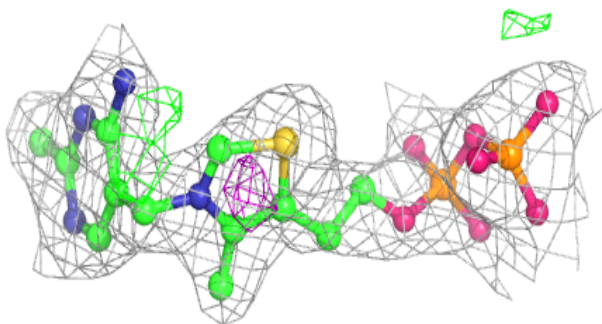
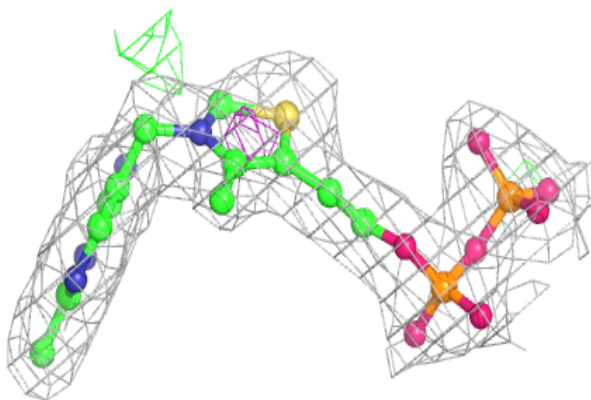


Electron density around TPP D 601:

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

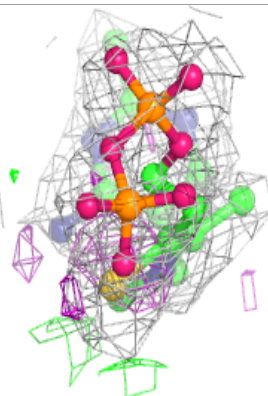
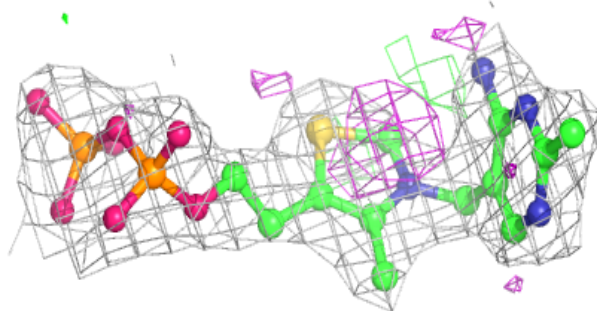
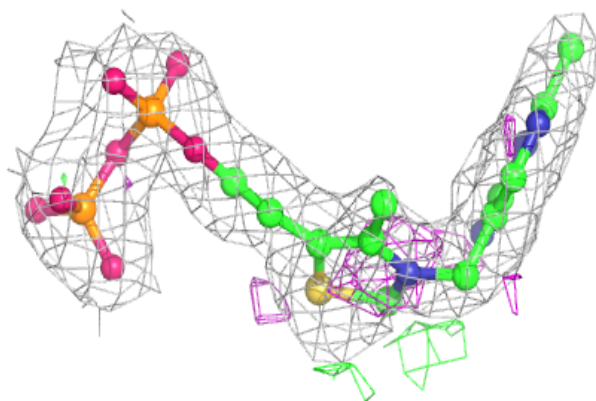
**Electron density around TPP C 601:**

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

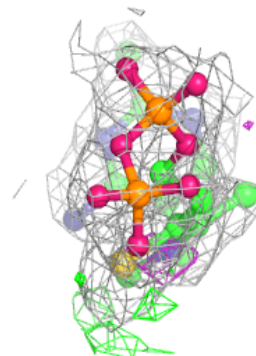
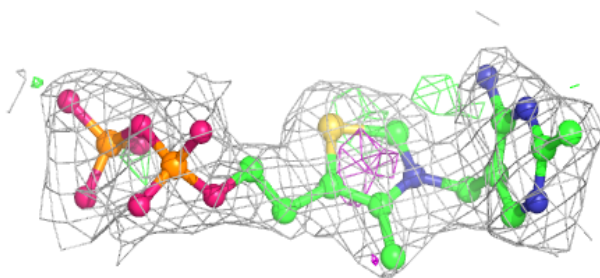
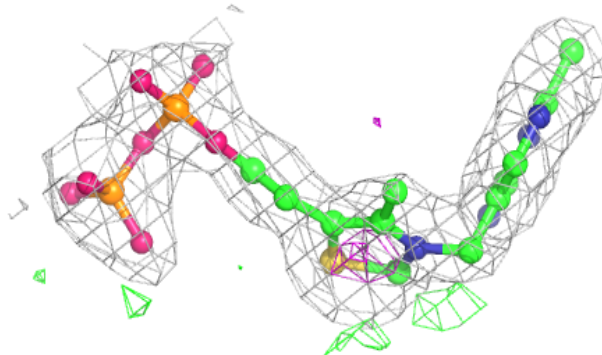


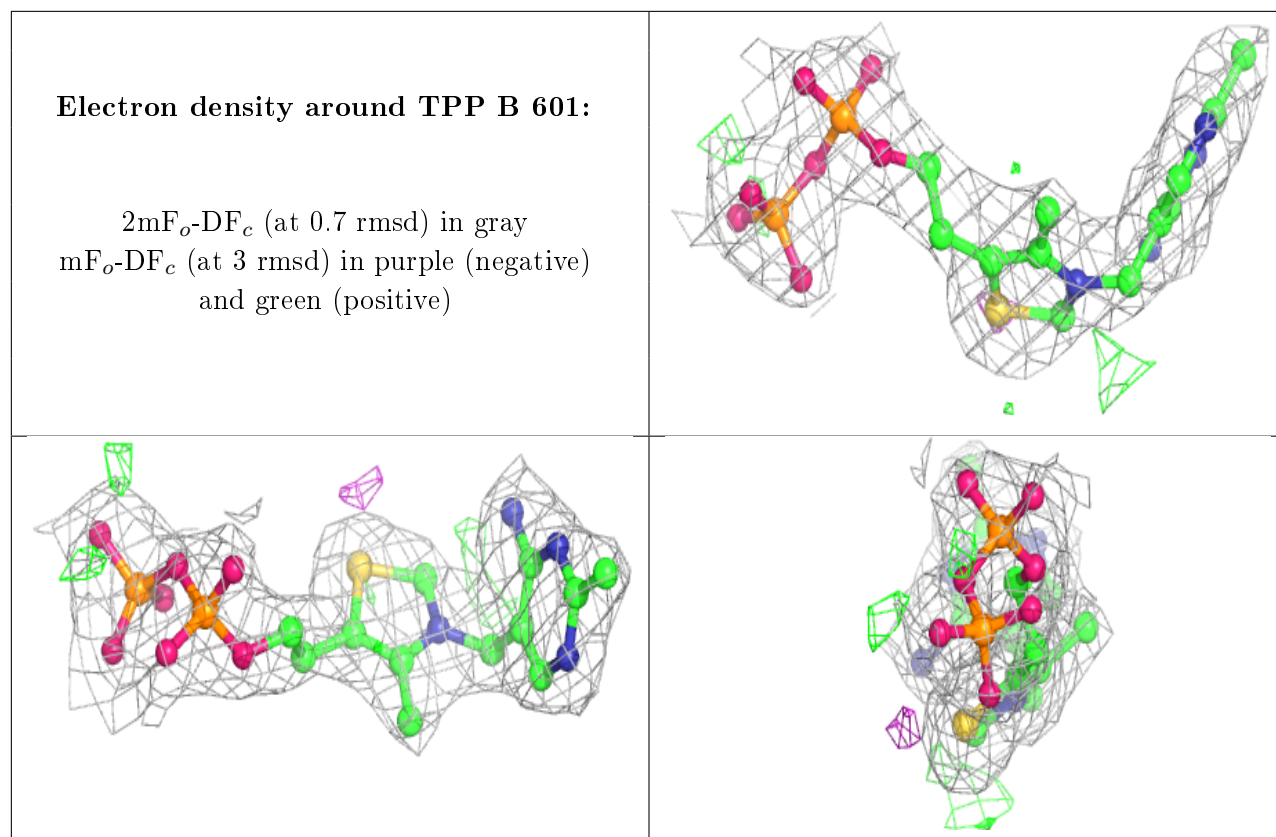
Electron density around TPP E 601:

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

**Electron density around TPP G 601:**

$2mF_o-DF_c$ (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.