



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 10:24 AM BST

PDB ID : 4RJK
Title : Acetolactate synthase from *Bacillus subtilis* bound to LThDP - 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 : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 2.13
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) : 2.13

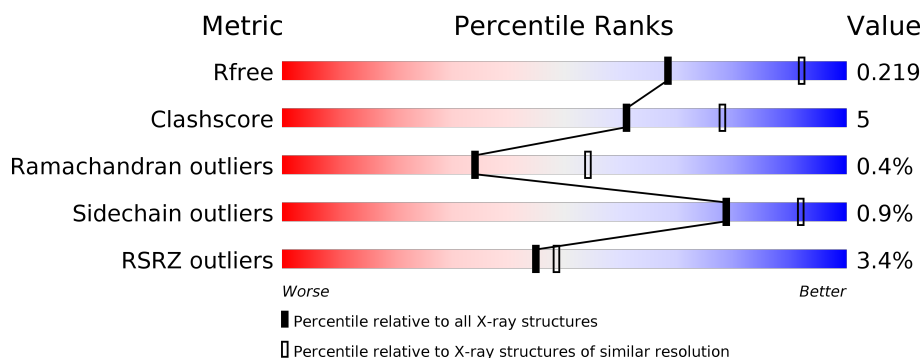
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	571	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
1	C	571	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	D	571	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
1	E	571	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>••</div> </div> </div>
1	F	571	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	571	<div><div></div><div>3%</div><div>87%</div><div>9%</div><div></div></div>
1	H	571	<div><div></div><div>4%</div><div>82%</div><div>13%</div><div></div></div>

2 Entry composition

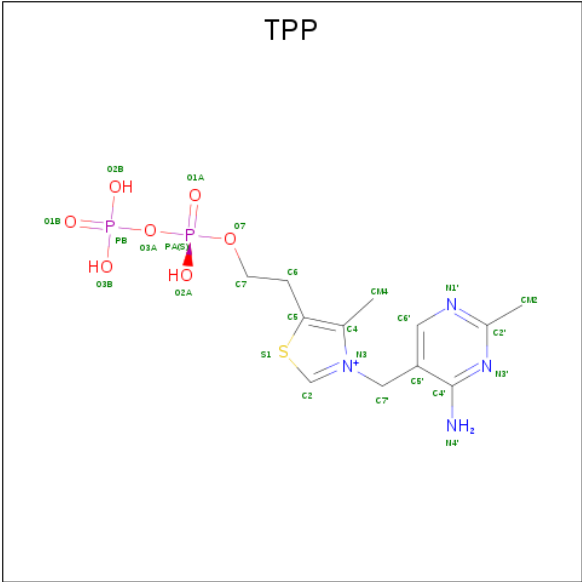
There are 7 unique types of molecules in this entry. The entry contains 35447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	552	Total	C	N	O	S	0	2	0
			4236	2688	727	809	12			
1	B	550	Total	C	N	O	S	0	4	0
			4231	2685	724	810	12			
1	C	553	Total	C	N	O	S	0	4	0
			4257	2702	730	812	13			
1	D	550	Total	C	N	O	S	0	7	0
			4246	2702	724	808	12			
1	E	552	Total	C	N	O	S	0	4	0
			4247	2699	726	810	12			
1	F	552	Total	C	N	O	S	0	2	0
			4239	2689	729	809	12			
1	G	553	Total	C	N	O	S	0	4	0
			4252	2697	730	813	12			
1	H	548	Total	C	N	O	S	0	1	0
			4201	2665	723	802	11			

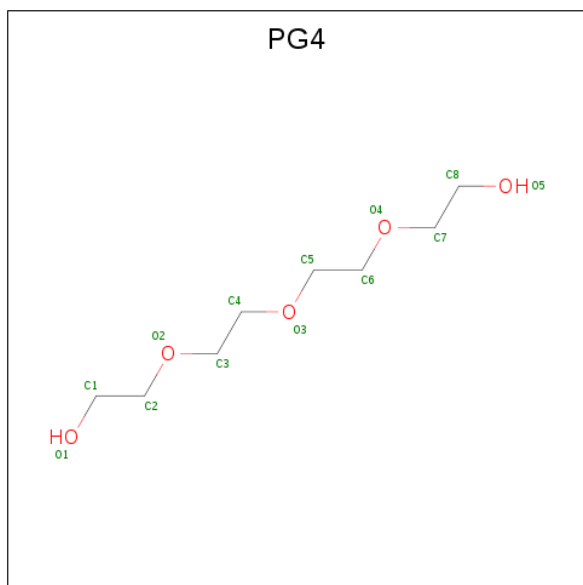
- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
			10	6	4		
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
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

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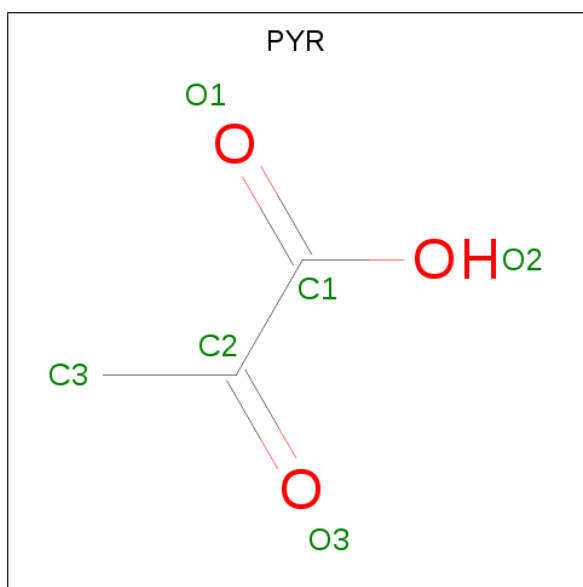
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			11	7	4		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	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
			8	5	3		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			8	5	3		
4	E	1	Total	C	O	0	0
			10	6	4		

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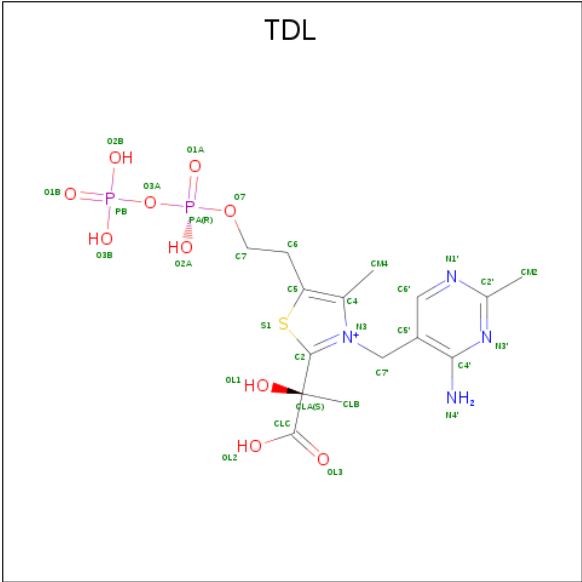
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			11	7	4		
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
			13	8	5		

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula: C₁₅H₂₃N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	H	1	Total	C	N	O	P	S	0	0
			32	15	4	10	2	1		

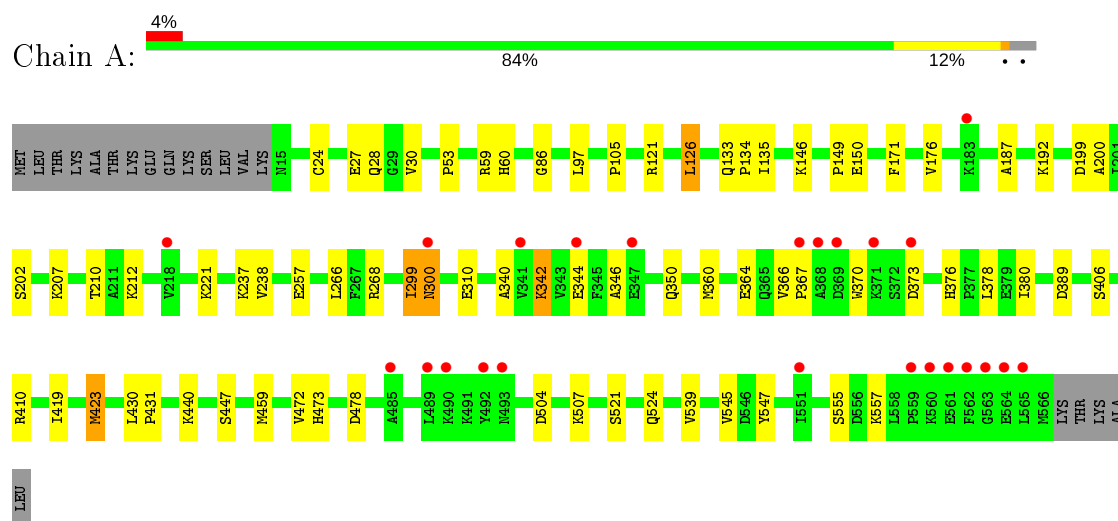
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total	O	0	0
			91	91		
7	B	112	Total	O	0	0
			112	112		
7	C	117	Total	O	0	0
			117	117		
7	D	109	Total	O	0	1
			109	109		
7	E	133	Total	O	0	0
			133	133		
7	F	119	Total	O	0	0
			119	119		
7	G	96	Total	O	0	0
			96	96		
7	H	60	Total	O	0	0
			60	60		

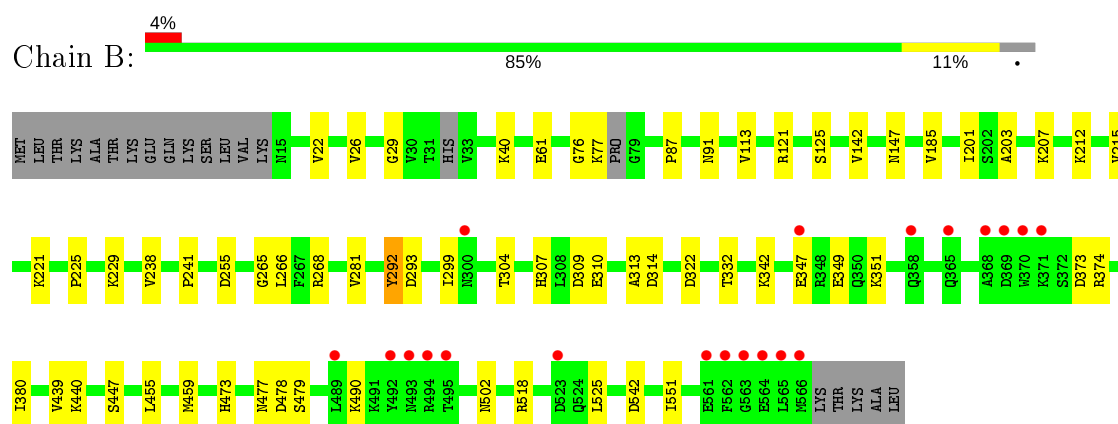
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

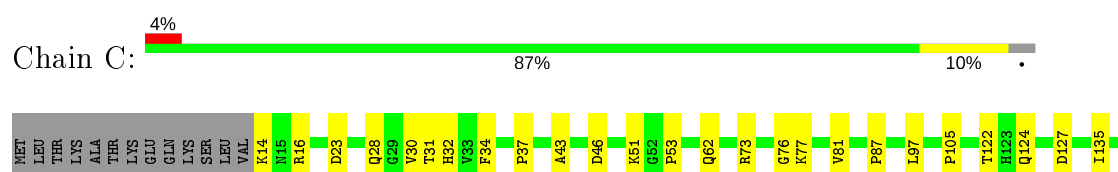
• Molecule 1: Acetolactate synthase

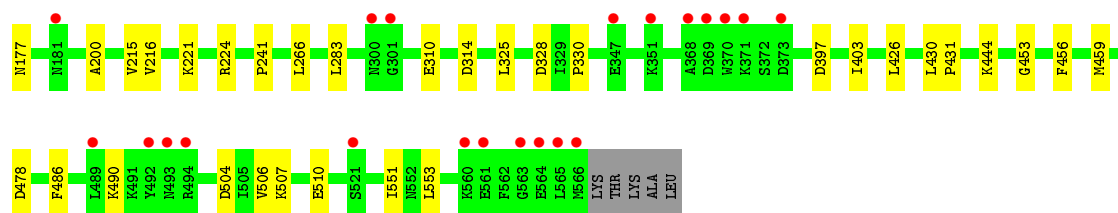


• Molecule 1: Acetolactate synthase

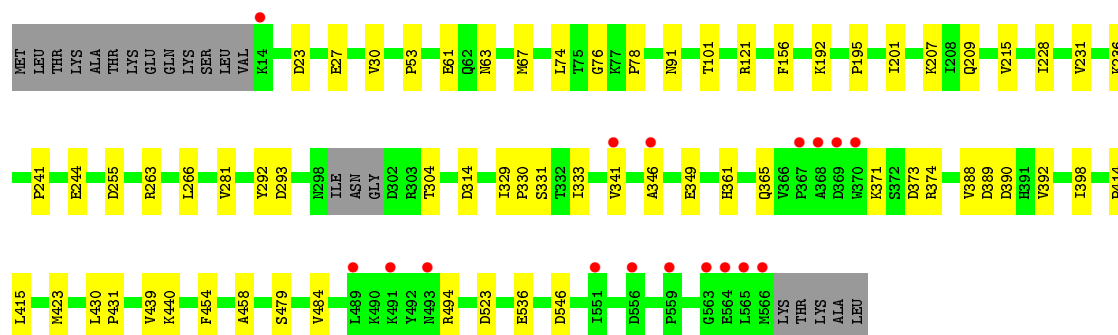
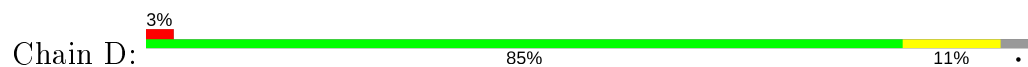


• Molecule 1: Acetolactate synthase

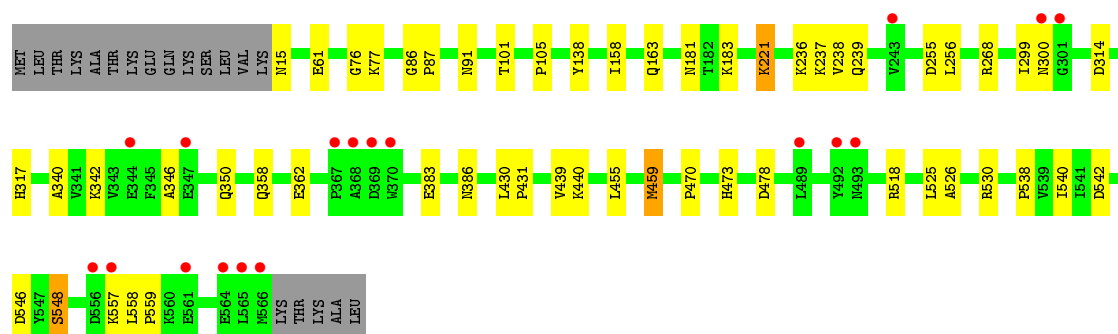
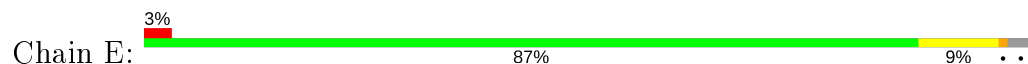




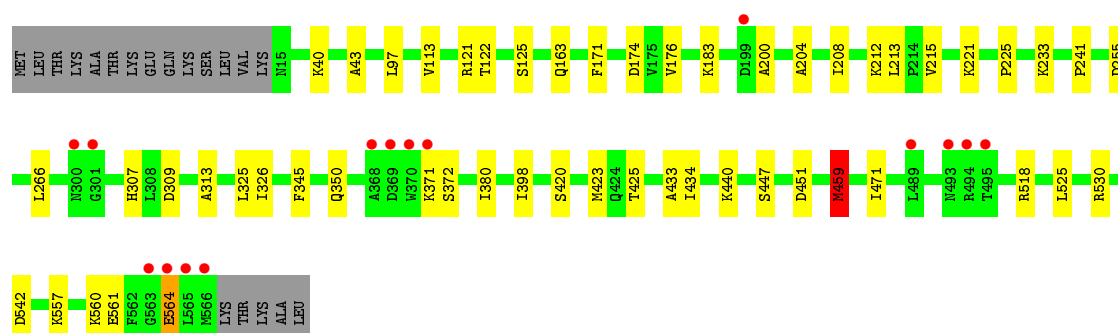
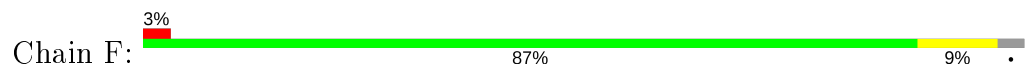
• Molecule 1: Acetolactate synthase



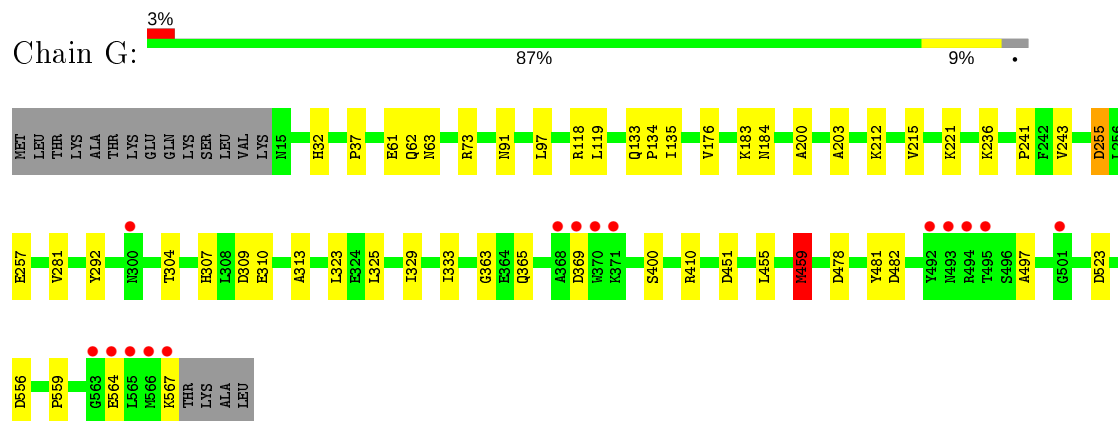
• Molecule 1: Acetolactate synthase



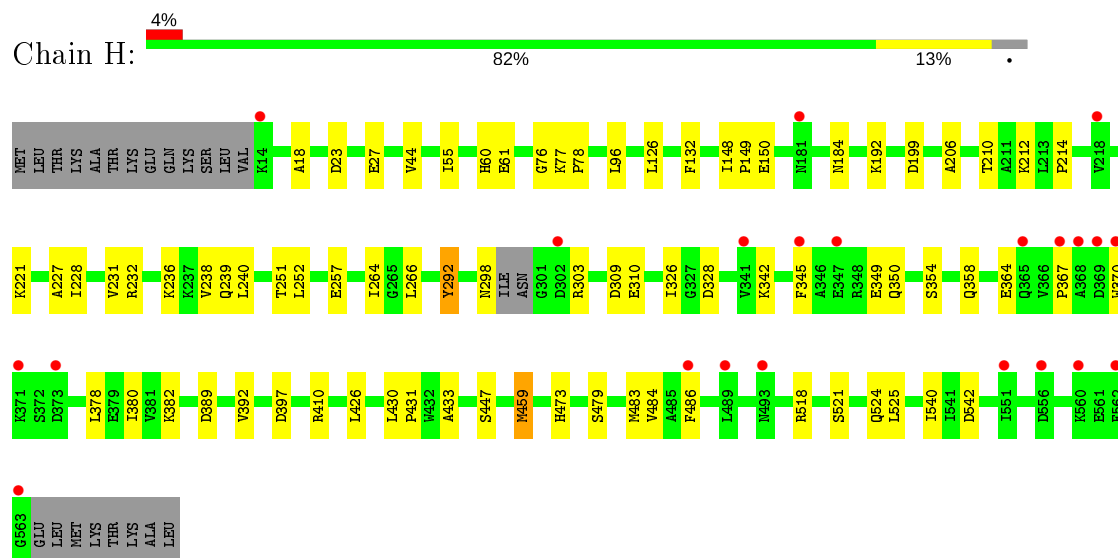
• Molecule 1: Acetolactate synthase



- 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	111.51Å 170.75Å 342.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.50) 99.9 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.166 , 0.217 0.172 , 0.219	Depositor DCC
R_{free} test set	11235 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35447	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.75 % 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 3.6146e-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, MG, TPP, PYR, TDL

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	0.43	0/4323	0.58	1/5880 (0.0%)
1	B	0.42	0/4321	0.57	0/5873
1	C	0.43	0/4347	0.56	1/5911 (0.0%)
1	D	0.44	0/4347	0.58	0/5911
1	E	0.44	0/4340	0.58	2/5903 (0.0%)
1	F	0.44	0/4327	0.58	1/5885 (0.0%)
1	G	0.42	0/4345	0.57	1/5908 (0.0%)
1	H	0.42	0/4284	0.57	1/5824 (0.0%)
All	All	0.43	0/34634	0.57	7/47095 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	459	MET	CG-SD-CE	-7.11	88.83	100.20
1	A	423	MET	CG-SD-CE	-6.46	89.86	100.20
1	E	459	MET	CA-CB-CG	-6.29	102.61	113.30
1	F	459	MET	CA-CB-CG	-5.96	103.16	113.30
1	C	459	MET	CA-CB-CG	-5.92	103.24	113.30

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	4236	0	4247	48	0
1	B	4231	0	4240	39	0
1	C	4257	0	4275	32	0
1	D	4246	0	4282	45	0
1	E	4247	0	4269	37	0
1	F	4239	0	4245	38	0
1	G	4252	0	4267	40	0
1	H	4201	0	4209	44	0
2	A	26	0	16	0	0
2	B	26	0	16	0	0
2	C	26	0	16	3	0
2	D	26	0	16	2	0
2	E	26	0	16	0	0
2	F	26	0	16	1	0
2	G	26	0	16	2	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	66	0	88	7	0
4	B	56	0	75	8	0
4	C	53	0	71	4	0
4	D	71	0	93	9	0
4	E	72	0	92	7	0
4	F	63	0	84	6	0
4	G	42	0	53	0	0
4	H	26	0	36	1	0
5	F	12	0	6	0	0
5	G	12	0	6	2	0
5	H	6	0	3	0	0
6	H	32	0	19	3	0
7	A	91	0	0	1	0
7	B	112	0	0	1	0
7	C	117	0	0	1	0
7	D	109	0	0	1	0
7	E	133	0	0	5	0
7	F	119	0	0	0	0
7	G	96	0	0	2	0
7	H	60	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35447	0	34772	315	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 5.

The worst 5 of 315 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:D:76:GLY:HA2	4:D:607:PG4:H31	1.52	0.88
1:B:76:GLY:HA2	4:B:603:PG4:H51	1.53	0.87
1:C:28:GLN:O	1:C:77:LYS:NZ	2.09	0.85
1:F:398:ILE:HD11	1:F:420:SER:HB3	1.63	0.81
1:H:367:PRO:HG2	1:H:370:TRP:HB2	1.63	0.80

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	552/571 (97%)	537 (97%)	12 (2%)	3 (0%)	29	48
1	B	548/571 (96%)	530 (97%)	16 (3%)	2 (0%)	34	54
1	C	555/571 (97%)	534 (96%)	19 (3%)	2 (0%)	34	54
1	D	553/571 (97%)	534 (97%)	16 (3%)	3 (0%)	29	48
1	E	554/571 (97%)	538 (97%)	15 (3%)	1 (0%)	47	68
1	F	552/571 (97%)	534 (97%)	16 (3%)	2 (0%)	34	54
1	G	555/571 (97%)	535 (96%)	19 (3%)	1 (0%)	47	68
1	H	545/571 (95%)	531 (97%)	11 (2%)	3 (1%)	25	43
All	All	4414/4568 (97%)	4273 (97%)	124 (3%)	17 (0%)	34	54

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	D	479	SER
1	A	300	ASN
1	E	300	ASN
1	F	564	GLU

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	453/468 (97%)	448 (99%)	5 (1%)	73	89
1	B	453/468 (97%)	448 (99%)	5 (1%)	73	89
1	C	456/468 (97%)	453 (99%)	3 (1%)	84	94
1	D	457/468 (98%)	455 (100%)	2 (0%)	91	97
1	E	455/468 (97%)	448 (98%)	7 (2%)	65	85
1	F	453/468 (97%)	451 (100%)	2 (0%)	91	97
1	G	456/468 (97%)	451 (99%)	5 (1%)	73	89
1	H	448/468 (96%)	445 (99%)	3 (1%)	84	94
All	All	3631/3744 (97%)	3599 (99%)	32 (1%)	78	92

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	314	ASP
1	E	221	LYS
1	H	397	ASP
1	E	181	ASN
1	E	239	GLN

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	F	15	ASN
1	H	534	ASN
1	G	63	ASN
1	D	209	GLN
1	G	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 8 are monoatomic - leaving 55 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	$\# Z > 2$
5	PYR	G	608	-	2,5,5	2.08	1 (50%)	2,6,6	0.33	0
2	TPP	A	601	3	22,27,27	1.48	5 (22%)	29,40,40	1.82	11 (37%)
2	TPP	B	601	3	22,27,27	1.52	6 (27%)	29,40,40	1.70	7 (24%)
2	TPP	C	601	3	22,27,27	1.54	6 (27%)	29,40,40	1.95	11 (37%)
2	TPP	D	601	3	22,27,27	1.50	5 (22%)	29,40,40	1.75	9 (31%)
4	PG4	D	604	-	10,10,12	0.63	0	9,9,11	0.92	0
4	PG4	D	609	-	6,6,12	0.62	0	5,5,11	0.67	0
4	PG4	D	603	-	12,12,12	0.81	0	11,11,11	0.89	0
4	PG4	D	608	-	6,6,12	0.59	0	5,5,11	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PYR	H	605	-	2,5,5	2.00	1 (50%)	2,6,6	0.10	0
4	PG4	G	605	-	10,10,12	0.58	0	9,9,11	0.88	0
5	PYR	F	610	-	2,5,5	2.09	1 (50%)	2,6,6	0.38	0
4	PG4	H	603	-	12,12,12	0.51	0	11,11,11	1.10	1 (9%)
4	PG4	C	606	-	9,9,12	0.62	0	8,8,11	0.96	0
4	PG4	B	605	-	9,9,12	0.52	0	8,8,11	0.88	0
4	PG4	G	606	-	7,7,12	0.56	0	6,6,11	0.84	0
4	PG4	A	607	-	12,12,12	0.51	0	11,11,11	1.03	0
4	PG4	G	604	-	12,12,12	0.65	0	11,11,11	0.63	0
2	TPP	G	601	3	22,27,27	1.59	5 (22%)	29,40,40	1.79	8 (27%)
4	PG4	H	604	-	12,12,12	0.68	0	11,11,11	0.76	0
4	PG4	D	605	-	12,12,12	0.64	0	11,11,11	0.86	0
4	PG4	D	607	-	9,9,12	0.67	0	8,8,11	0.76	0
4	PG4	B	607	-	12,12,12	0.65	0	11,11,11	0.69	0
4	PG4	B	604	-	9,9,12	0.51	0	8,8,11	0.77	0
4	PG4	F	606	-	9,9,12	0.64	0	8,8,11	0.89	0
4	PG4	E	603	-	9,9,12	0.80	0	8,8,11	1.09	0
5	PYR	G	607	-	2,5,5	2.12	1 (50%)	2,6,6	0.09	0
4	PG4	A	603	-	9,9,12	0.63	0	8,8,11	0.63	0
4	PG4	C	604	-	12,12,12	0.64	0	11,11,11	0.71	0
2	TPP	F	601	3	22,27,27	1.61	5 (22%)	29,40,40	1.77	7 (24%)
4	PG4	C	605	-	9,9,12	0.65	0	8,8,11	0.68	0
4	PG4	E	605	-	7,7,12	0.59	0	6,6,11	0.71	0
4	PG4	F	603	-	12,12,12	0.68	0	11,11,11	1.00	0
4	PG4	A	606	-	9,9,12	0.62	0	8,8,11	0.74	0
4	PG4	B	603	-	9,9,12	0.77	0	8,8,11	0.85	0
4	PG4	C	607	-	6,6,12	0.57	0	5,5,11	0.77	0
4	PG4	F	605	-	9,9,12	0.52	0	8,8,11	0.85	0
4	PG4	C	603	-	12,12,12	0.63	0	11,11,11	0.68	0
4	PG4	E	608	-	9,9,12	0.54	0	8,8,11	1.09	2 (25%)
4	PG4	E	607	-	7,7,12	0.56	0	6,6,11	0.84	0
4	PG4	E	609	-	9,9,12	0.66	0	8,8,11	0.74	0
4	PG4	A	608	-	9,9,12	0.68	0	8,8,11	0.84	0
2	TPP	E	601	3	22,27,27	1.45	5 (22%)	29,40,40	1.81	10 (34%)
4	PG4	A	604	-	12,12,12	0.59	0	11,11,11	1.09	1 (9%)
4	PG4	F	604	-	6,6,12	0.49	0	5,5,11	0.79	0
5	PYR	F	609	-	2,5,5	2.16	1 (50%)	2,6,6	0.54	0
4	PG4	A	605	-	9,9,12	0.58	0	8,8,11	0.95	0
4	PG4	E	604	-	12,12,12	0.69	0	11,11,11	0.94	1 (9%)
4	PG4	F	608	-	12,12,12	0.62	0	11,11,11	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TDL	H	601	3	24,33,33	3.60	6 (25%)	28,51,51	1.77	8 (28%)
4	PG4	B	606	-	12,12,12	0.60	0	11,11,11	0.90	0
4	PG4	F	607	-	9,9,12	0.47	0	8,8,11	1.16	1 (12%)
4	PG4	E	606	-	12,12,12	0.54	0	11,11,11	0.94	1 (9%)
4	PG4	D	606	-	9,9,12	0.54	0	8,8,11	0.96	1 (12%)
4	PG4	G	603	-	9,9,12	0.69	0	8,8,11	1.09	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
5	PYR	G	608	-	-	0/0/4/4	-
2	TPP	A	601	3	-	3/16/17/17	0/2/2/2
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
2	TPP	C	601	3	-	2/16/17/17	0/2/2/2
2	TPP	D	601	3	-	0/16/17/17	0/2/2/2
4	PG4	D	604	-	-	2/8/8/10	-
4	PG4	D	609	-	-	1/4/4/10	-
4	PG4	D	603	-	-	8/10/10/10	-
4	PG4	D	608	-	-	2/4/4/10	-
5	PYR	H	605	-	-	0/0/4/4	-
4	PG4	G	605	-	-	3/8/8/10	-
5	PYR	F	610	-	-	0/0/4/4	-
4	PG4	H	603	-	-	7/10/10/10	-
4	PG4	C	606	-	-	3/7/7/10	-
4	PG4	B	605	-	-	4/7/7/10	-
4	PG4	G	606	-	-	3/5/5/10	-
4	PG4	A	607	-	-	8/10/10/10	-
4	PG4	G	604	-	-	1/10/10/10	-
2	TPP	G	601	3	-	2/16/17/17	0/2/2/2
4	PG4	H	604	-	-	5/10/10/10	-
4	PG4	D	605	-	-	5/10/10/10	-
4	PG4	D	607	-	-	3/7/7/10	-
4	PG4	B	607	-	-	5/10/10/10	-
4	PG4	B	604	-	-	4/7/7/10	-
4	PG4	F	606	-	-	4/7/7/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	E	603	-	-	3/7/7/10	-
5	PYR	G	607	-	-	0/0/4/4	-
4	PG4	A	603	-	-	3/7/7/10	-
4	PG4	C	604	-	-	1/10/10/10	-
2	TPP	F	601	3	-	2/16/17/17	0/2/2/2
4	PG4	C	605	-	-	1/7/7/10	-
4	PG4	E	605	-	-	3/5/5/10	-
4	PG4	F	603	-	-	5/10/10/10	-
4	PG4	A	606	-	-	4/7/7/10	-
4	PG4	B	603	-	-	3/7/7/10	-
4	PG4	C	607	-	-	2/4/4/10	-
4	PG4	F	605	-	-	3/7/7/10	-
4	PG4	C	603	-	-	0/10/10/10	-
4	PG4	E	608	-	-	2/7/7/10	-
4	PG4	E	607	-	-	0/5/5/10	-
4	PG4	E	609	-	-	2/7/7/10	-
4	PG4	A	608	-	-	4/7/7/10	-
2	TPP	E	601	3	-	0/16/17/17	0/2/2/2
4	PG4	A	604	-	-	4/10/10/10	-
4	PG4	F	604	-	-	3/4/4/10	-
5	PYR	F	609	-	-	0/0/4/4	-
4	PG4	A	605	-	-	4/7/7/10	-
4	PG4	E	604	-	-	7/10/10/10	-
4	PG4	F	608	-	-	3/10/10/10	-
6	TDL	H	601	3	-	4/16/29/29	0/2/2/2
4	PG4	B	606	-	-	7/10/10/10	-
4	PG4	F	607	-	-	4/7/7/10	-
4	PG4	E	606	-	-	6/10/10/10	-
4	PG4	D	606	-	-	6/7/7/10	-
4	PG4	G	603	-	-	3/7/7/10	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	601	TDL	C5-S1	-10.47	1.54	1.74
6	H	601	TDL	C4-N3	8.75	1.58	1.39
6	H	601	TDL	C6-C5	8.58	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	601	TDL	C2-N3	4.81	1.46	1.35
2	F	601	TPP	C4-N3	-3.75	1.36	1.39

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TPP	CM4-C4-N3	4.45	128.21	122.53
2	E	601	TPP	CM2-C2'-N1'	4.44	122.02	117.14
2	F	601	TPP	C6-C5-C4	4.25	130.84	127.43
2	G	601	TPP	CM2-C2'-N1'	4.14	121.70	117.14
2	B	601	TPP	C6-C5-C4	4.08	130.71	127.43

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TPP	PB-O3A-PA-O7
2	F	601	TPP	PA-O3A-PB-O2B
6	H	601	TDL	PB-O3A-PA-O7
6	H	601	TDL	C7-O7-PA-O1A
4	G	603	PG4	C3-C4-O3-C5

There are no ring outliers.

30 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	608	PYR	2	0
2	C	601	TPP	3	0
2	D	601	TPP	2	0
4	D	604	PG4	1	0
4	D	603	PG4	3	0
4	C	606	PG4	1	0
2	G	601	TPP	2	0
4	H	604	PG4	1	0
4	D	605	PG4	1	0
4	D	607	PG4	2	0
4	B	607	PG4	3	0
4	F	606	PG4	2	0
4	E	603	PG4	1	0
4	A	603	PG4	1	0
2	F	601	TPP	1	0

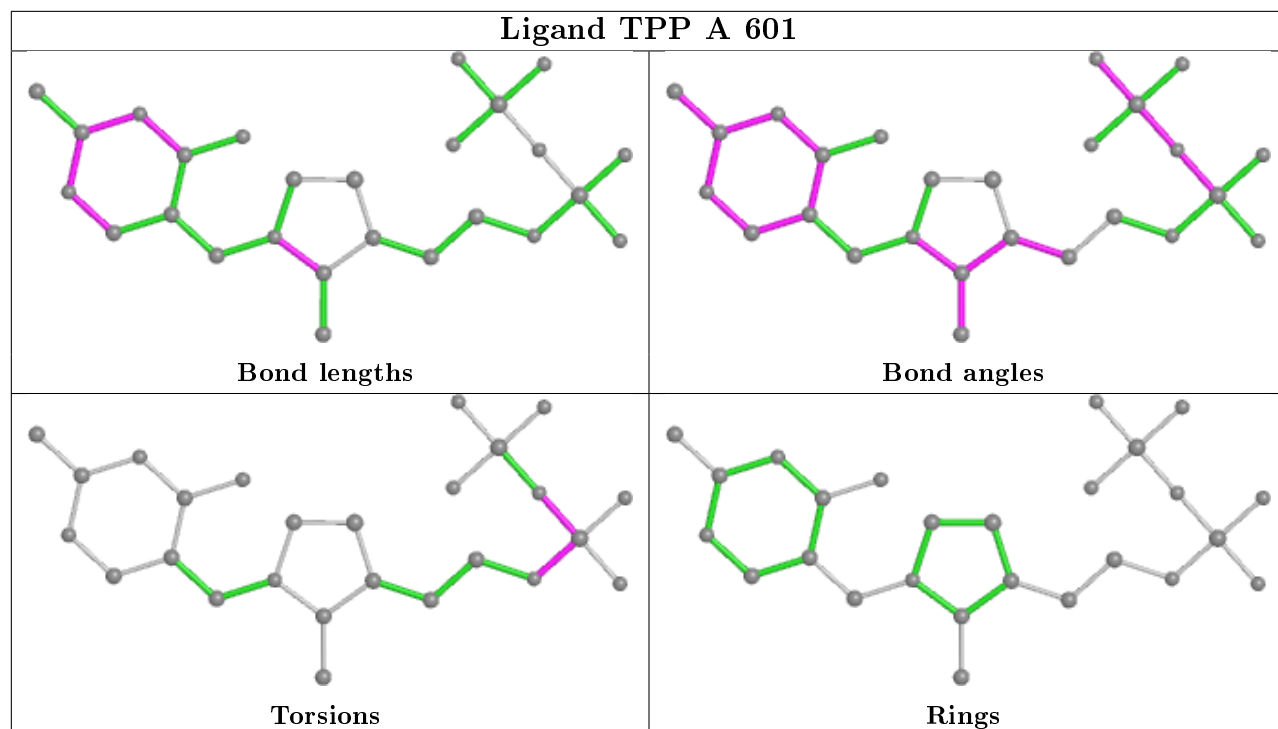
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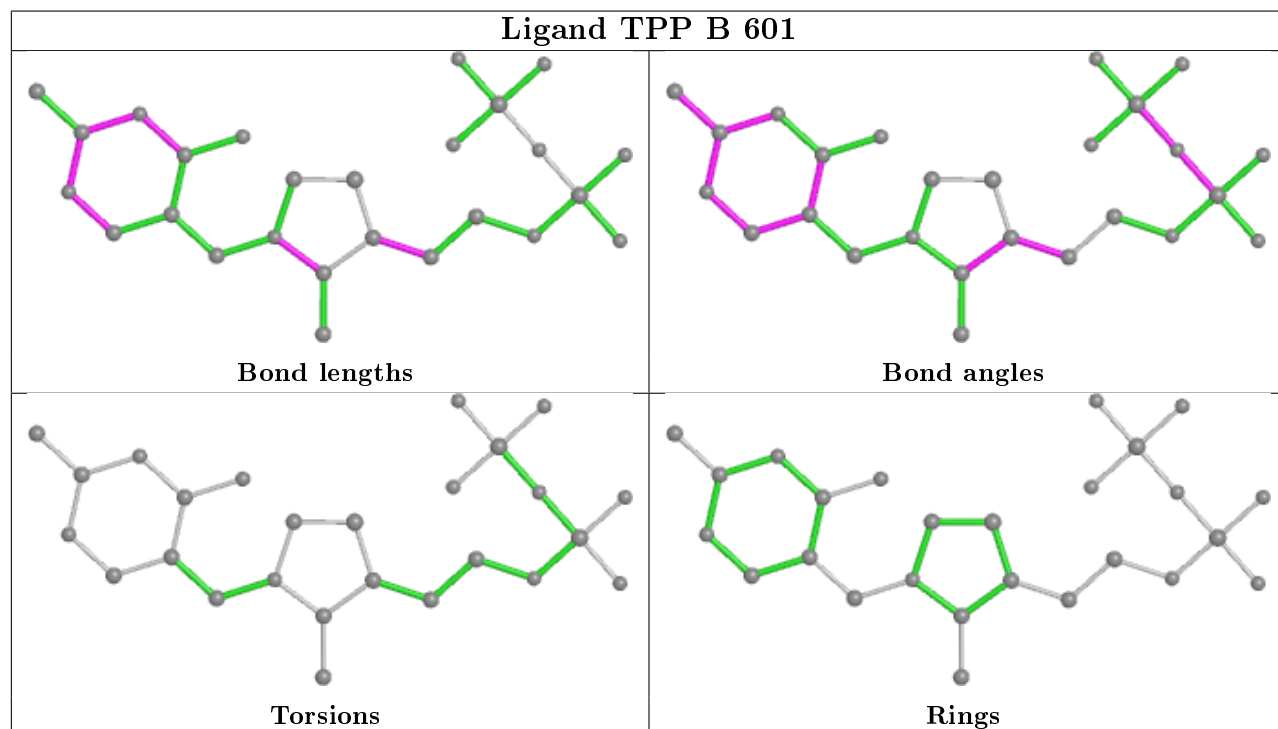
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	605	PG4	3	0
4	F	603	PG4	1	0
4	A	606	PG4	2	0
4	B	603	PG4	3	0
4	F	605	PG4	1	0
4	E	609	PG4	3	0
4	A	608	PG4	2	0
4	A	604	PG4	1	0
4	F	604	PG4	2	0
4	A	605	PG4	2	0
4	E	604	PG4	1	0
6	H	601	TDL	3	0
4	B	606	PG4	2	0
4	E	606	PG4	2	0
4	D	606	PG4	2	0

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.

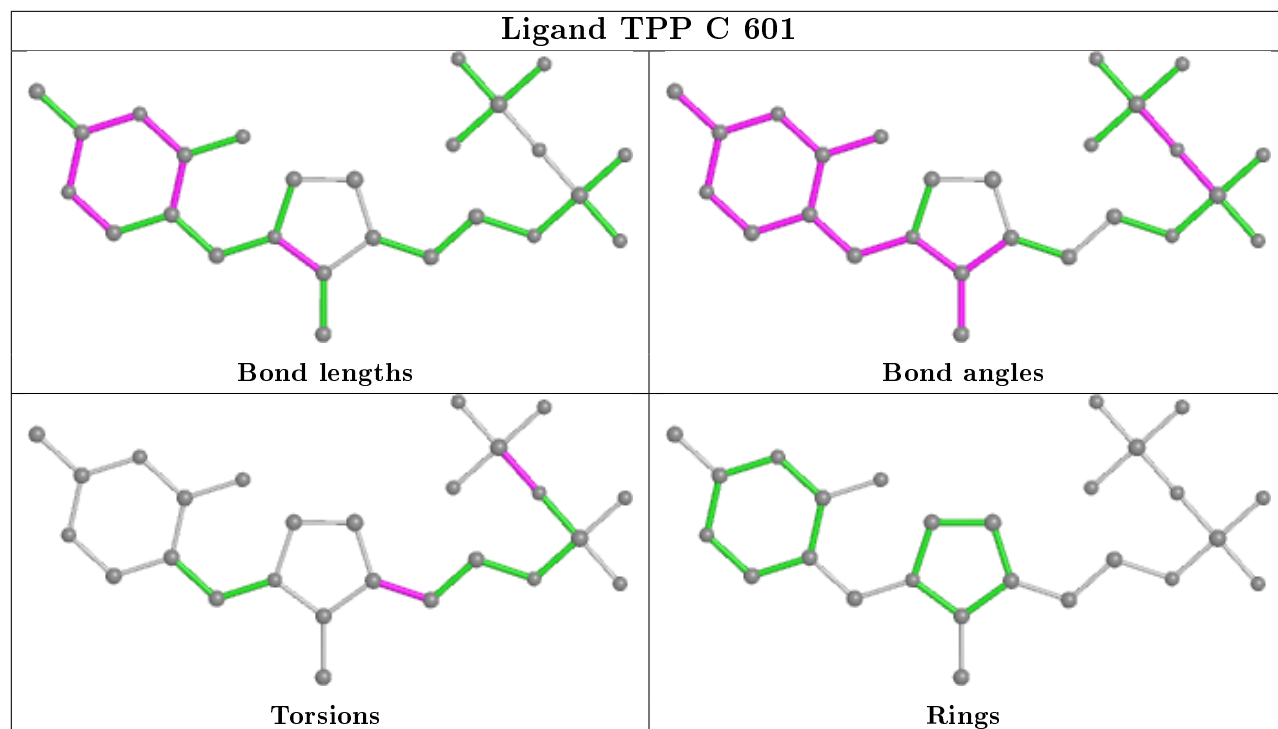
Ligand TPP A 601



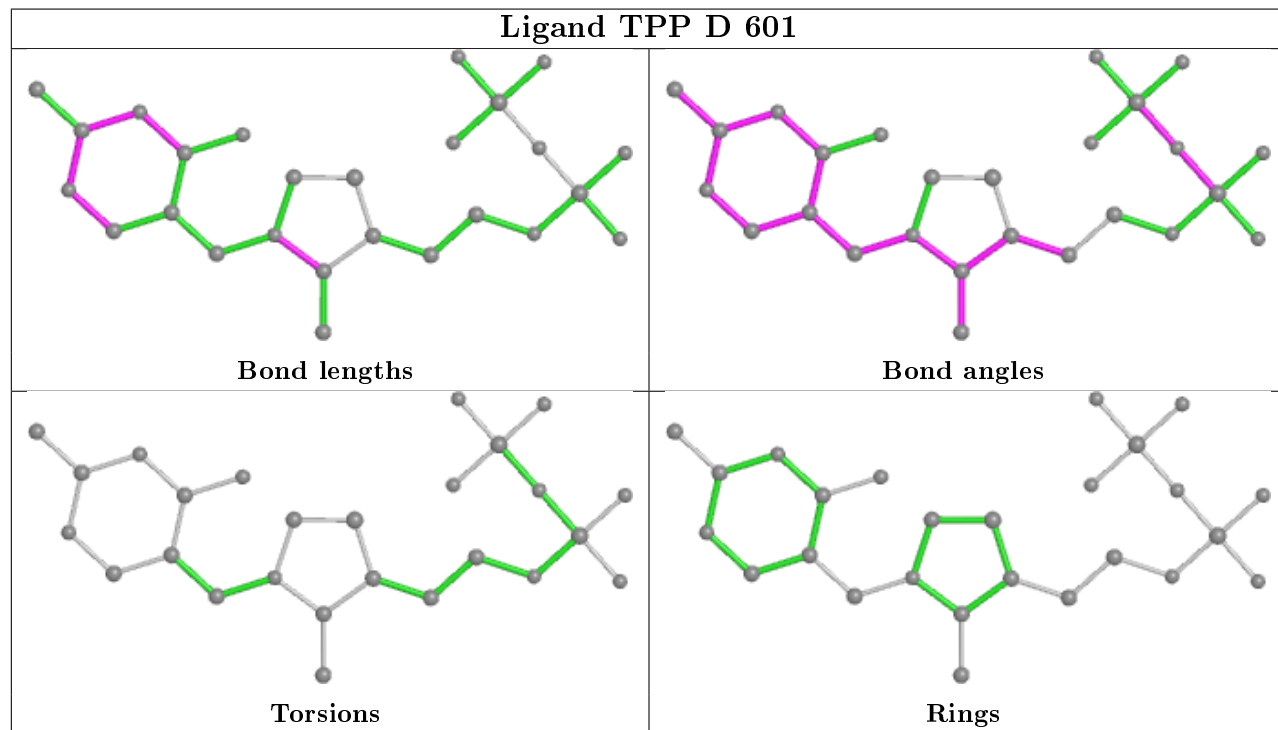
Ligand TPP B 601



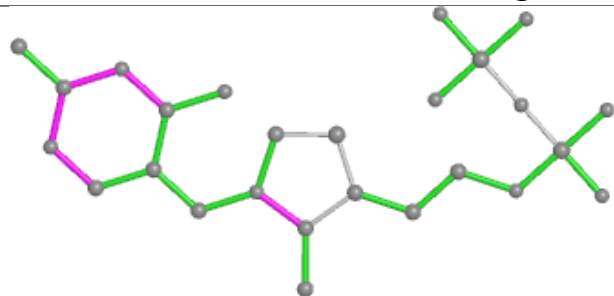
Ligand TPP C 601



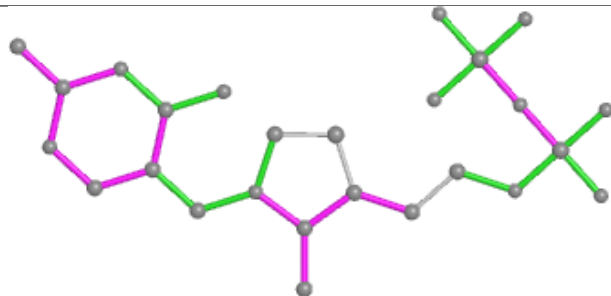
Ligand TPP D 601



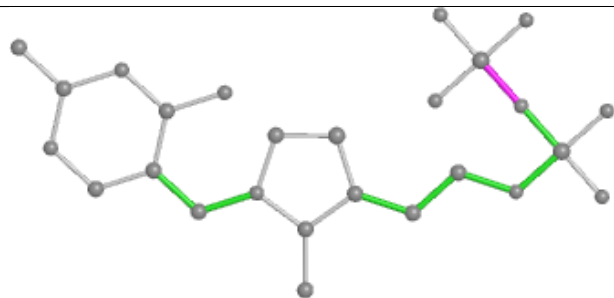
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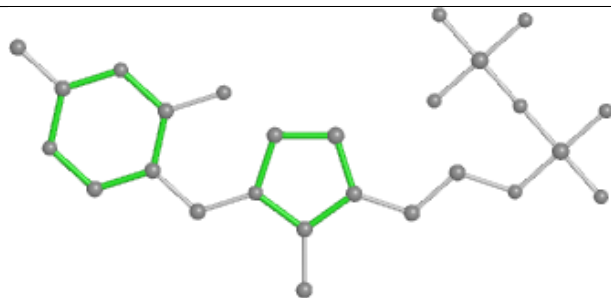
Bond lengths



Bond angles

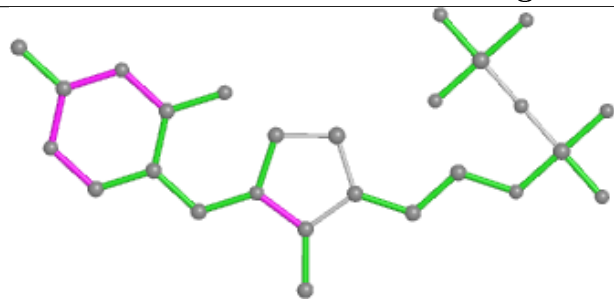


Torsions

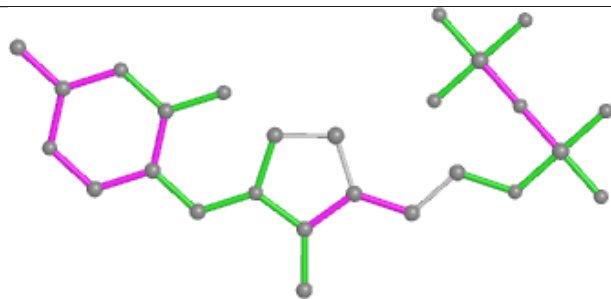


Rings

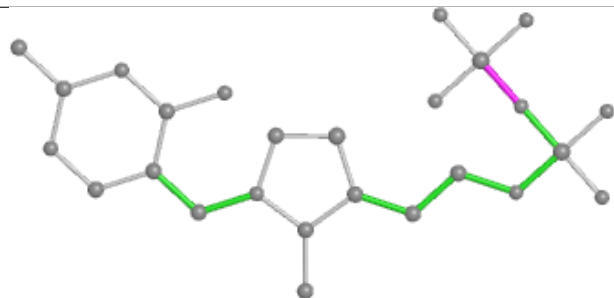
Ligand TPP F 601



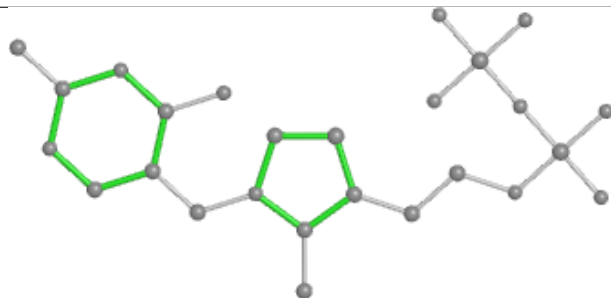
Bond lengths



Bond angles

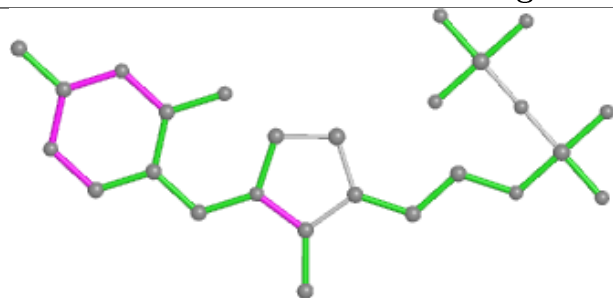


Torsions

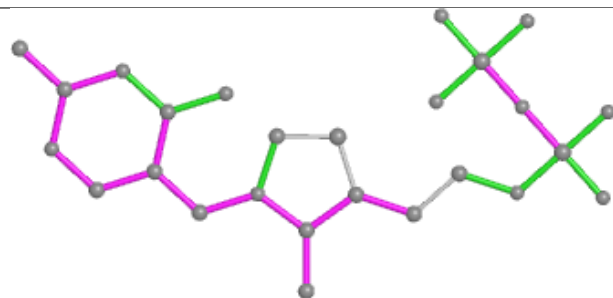


Rings

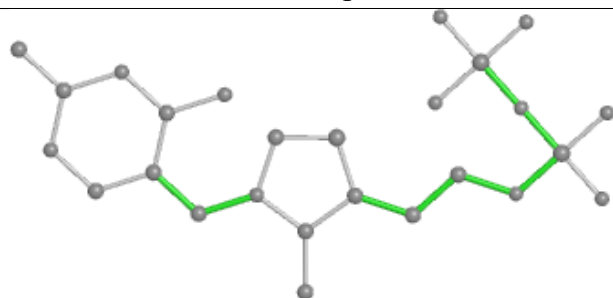
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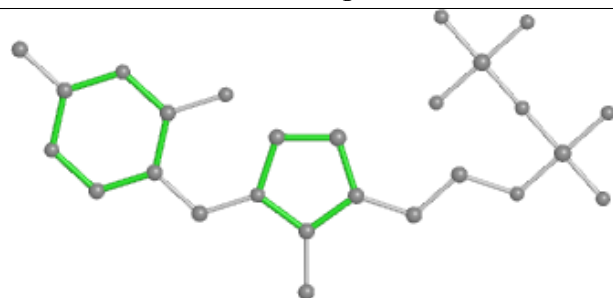
Bond lengths



Bond angles

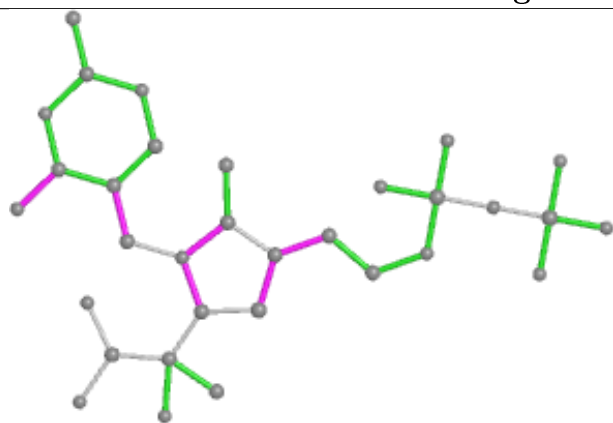


Torsions

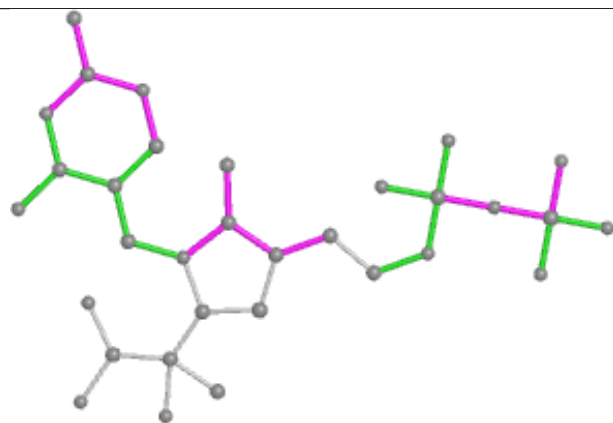


Rings

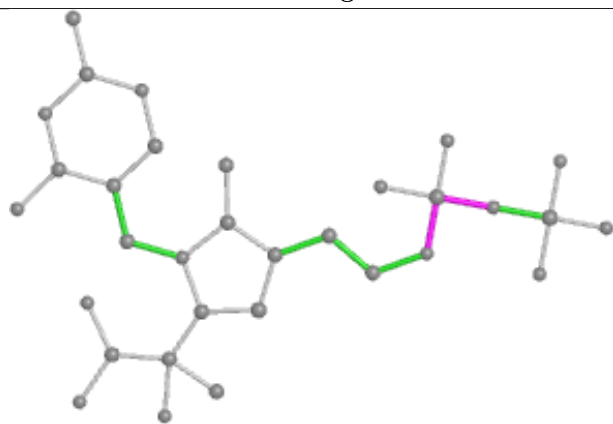
Ligand TDL H 601



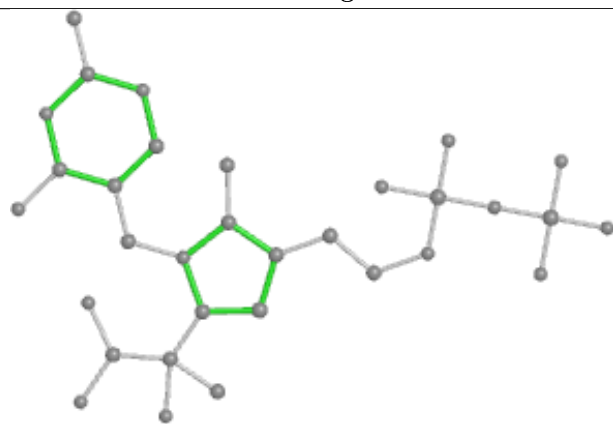
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	552/571 (96%)	-0.15	24 (4%)	35	38	34, 49, 73, 104	0
1	B	550/571 (96%)	-0.20	20 (3%)	42	46	34, 47, 73, 101	0
1	C	553/571 (96%)	-0.24	21 (3%)	40	43	32, 46, 70, 96	0
1	D	550/571 (96%)	-0.23	17 (3%)	49	52	32, 45, 70, 101	0
1	E	552/571 (96%)	-0.26	18 (3%)	46	50	33, 44, 69, 98	0
1	F	552/571 (96%)	-0.26	15 (2%)	54	58	32, 46, 72, 104	0
1	G	553/571 (96%)	-0.28	15 (2%)	54	58	34, 46, 72, 96	0
1	H	548/571 (95%)	-0.15	22 (4%)	38	41	36, 49, 73, 100	0
All	All	4410/4568 (96%)	-0.22	152 (3%)	45	48	32, 47, 72, 104	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	LEU	5.7
1	B	368	ALA	5.6
1	F	564	GLU	5.4
1	D	565	LEU	5.1
1	G	368	ALA	4.9

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 monosaccharides 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
5	PYR	F	609	6/6	0.71	0.40	63,67,72,75	0
4	PG4	B	605	10/13	0.77	0.23	58,64,73,74	0
4	PG4	F	607	10/13	0.80	0.22	51,61,64,66	0
4	PG4	B	606	13/13	0.82	0.37	55,66,74,74	0
4	PG4	A	606	10/13	0.83	0.29	59,69,76,77	0
4	PG4	H	603	13/13	0.84	0.19	42,62,69,69	0
4	PG4	F	604	7/13	0.85	0.16	55,60,64,64	0
4	PG4	A	605	10/13	0.87	0.22	56,63,70,72	0
4	PG4	E	605	8/13	0.87	0.36	59,66,74,78	0
4	PG4	F	606	10/13	0.87	0.26	52,65,69,78	0
4	PG4	G	605	11/13	0.88	0.26	64,69,78,78	0
5	PYR	F	610	6/6	0.88	0.30	54,65,75,76	0
4	PG4	F	603	13/13	0.88	0.17	38,50,66,70	0
4	PG4	E	606	13/13	0.88	0.18	40,57,64,66	0
4	PG4	E	608	10/13	0.89	0.19	55,61,67,75	0
4	PG4	D	606	10/13	0.89	0.35	64,71,75,77	0
4	PG4	G	606	8/13	0.90	0.27	68,78,81,82	0
4	PG4	A	607	13/13	0.91	0.12	50,56,67,67	0
5	PYR	G	607	6/6	0.91	0.24	53,70,72,72	0
4	PG4	E	607	8/13	0.91	0.17	62,70,72,73	0
4	PG4	E	604	13/13	0.91	0.21	40,53,74,74	0
4	PG4	B	604	10/13	0.92	0.15	54,57,65,66	0
4	PG4	C	603	13/13	0.92	0.19	52,58,63,65	0
4	PG4	D	608	7/13	0.92	0.14	46,48,56,58	0
5	PYR	H	605	6/6	0.92	0.39	75,83,84,85	0
4	PG4	D	609	7/13	0.92	0.23	50,52,67,71	0
4	PG4	D	603	13/13	0.92	0.17	43,52,63,66	0
4	PG4	C	606	10/13	0.93	0.15	55,59,63,66	0
4	PG4	F	605	10/13	0.93	0.14	48,53,60,63	0
4	PG4	D	604	11/13	0.93	0.17	47,50,64,65	0
4	PG4	C	604	13/13	0.93	0.29	56,63,71,74	0
4	PG4	H	604	13/13	0.93	0.24	48,53,65,73	0
4	PG4	A	608	10/13	0.93	0.22	45,62,72,73	0
4	PG4	B	607	13/13	0.93	0.26	50,57,63,65	0
4	PG4	F	608	13/13	0.94	0.16	48,55,60,64	0
4	PG4	D	605	13/13	0.94	0.16	54,65,70,74	0
4	PG4	A	604	13/13	0.94	0.13	52,59,64,66	0

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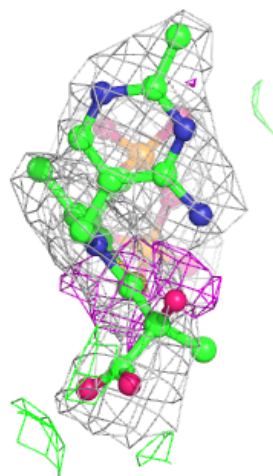
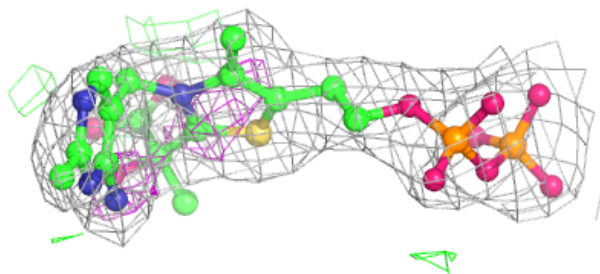
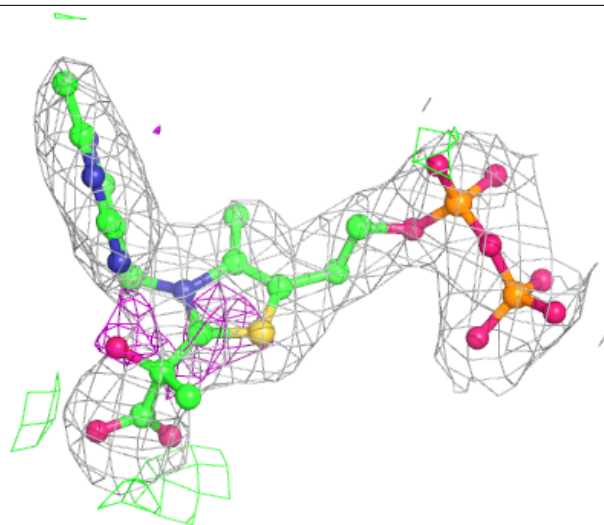
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PG4	A	603	10/13	0.94	0.19	46,56,59,59	0
3	MG	A	602	1/1	0.94	0.05	56,56,56,56	0
4	PG4	G	604	13/13	0.95	0.24	41,57,65,71	0
6	TDL	H	601	32/32	0.95	0.15	38,57,69,72	0
4	PG4	C	605	10/13	0.95	0.13	35,48,55,56	0
2	TPP	A	601	26/26	0.95	0.13	42,56,63,66	0
4	PG4	E	603	10/13	0.95	0.15	45,52,58,60	0
3	MG	E	602	1/1	0.95	0.03	59,59,59,59	0
5	PYR	G	608	6/6	0.96	0.11	65,72,75,77	0
4	PG4	E	609	10/13	0.96	0.17	43,49,54,64	0
4	PG4	C	607	7/13	0.96	0.10	46,52,62,62	0
2	TPP	D	601	26/26	0.96	0.13	29,52,62,64	0
4	PG4	G	603	10/13	0.96	0.13	36,46,55,66	0
2	TPP	F	601	26/26	0.97	0.12	42,51,59,60	0
3	MG	C	602	1/1	0.97	0.12	54,54,54,54	0
2	TPP	B	601	26/26	0.97	0.12	42,55,64,66	0
4	PG4	D	607	10/13	0.97	0.10	42,47,53,58	0
3	MG	B	602	1/1	0.97	0.10	57,57,57,57	0
2	TPP	G	601	26/26	0.97	0.12	37,49,60,63	0
2	TPP	E	601	26/26	0.97	0.13	39,54,59,62	0
2	TPP	C	601	26/26	0.97	0.12	38,50,59,60	0
3	MG	G	602	1/1	0.97	0.09	49,49,49,49	0
4	PG4	B	603	10/13	0.97	0.12	43,46,60,63	0
3	MG	H	602	1/1	0.98	0.08	55,55,55,55	0
3	MG	D	602	1/1	0.99	0.11	50,50,50,50	0
3	MG	F	602	1/1	0.99	0.07	53,53,53,53	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.

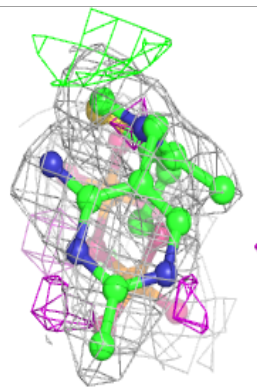
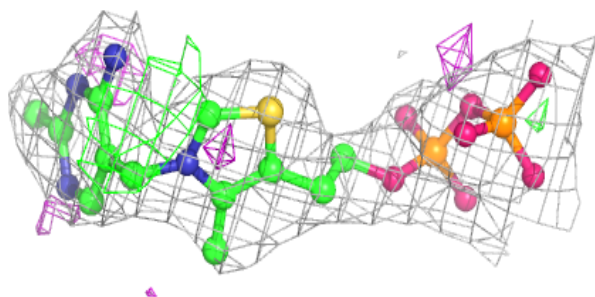
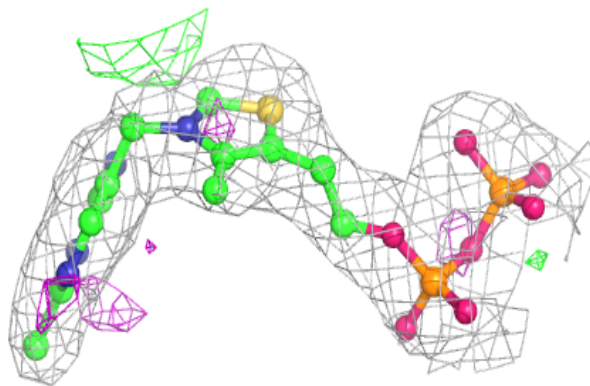
Electron density around TDL H 601:

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

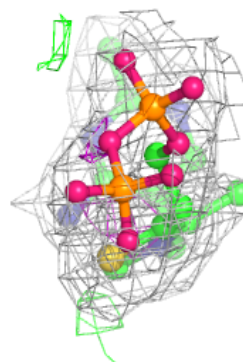
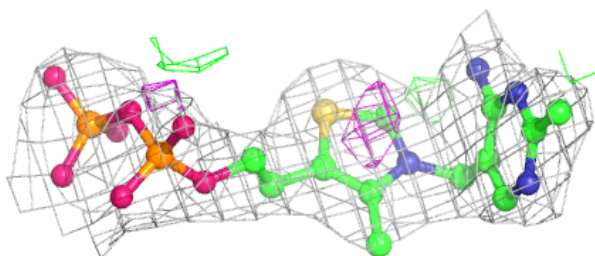
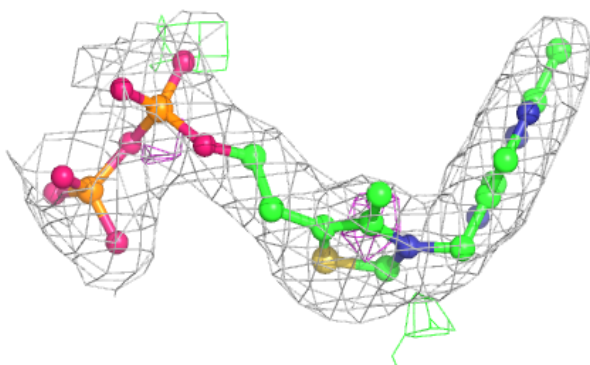


Electron density around TPP A 601:

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

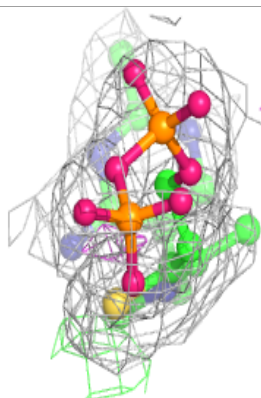
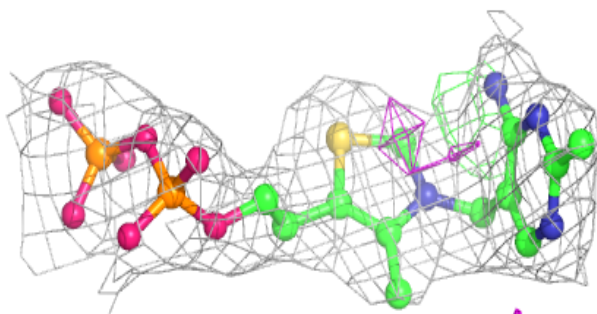
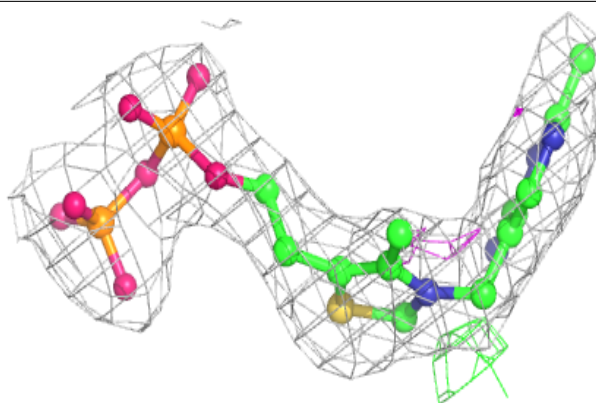
**Electron density around TPP D 601:**

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

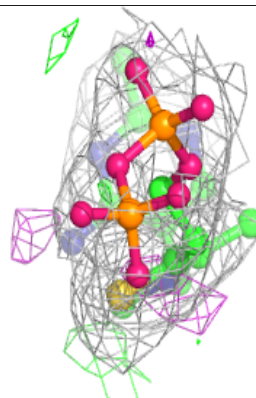
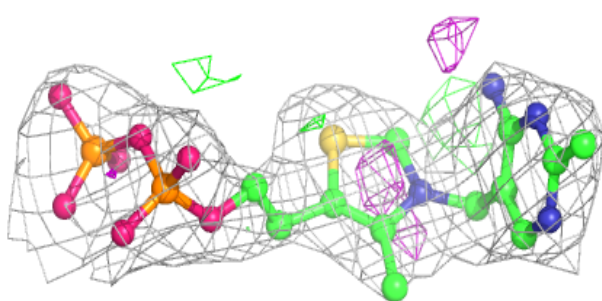
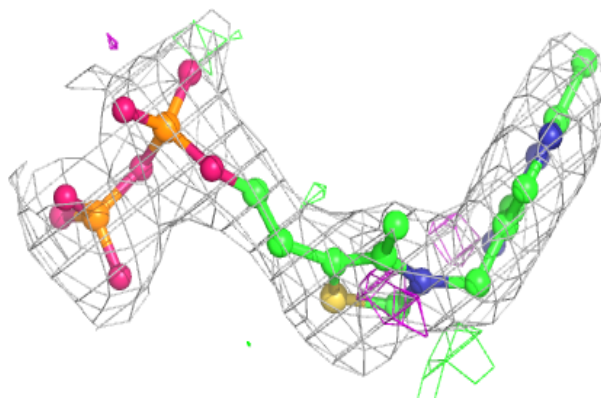


Electron density around TPP F 601:

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

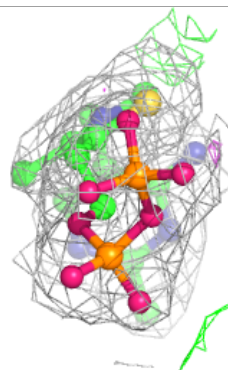
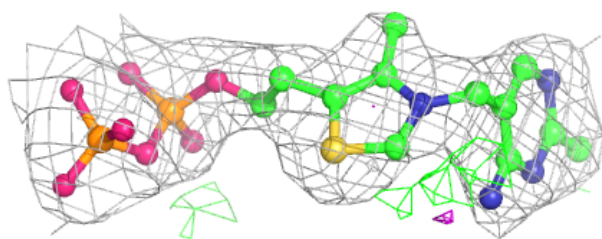
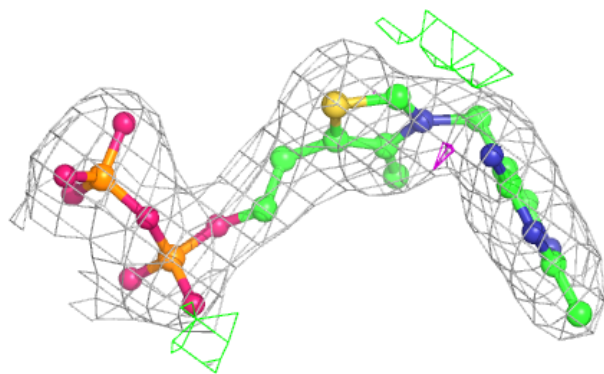
**Electron density around TPP B 601:**

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

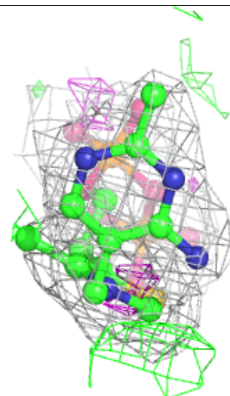
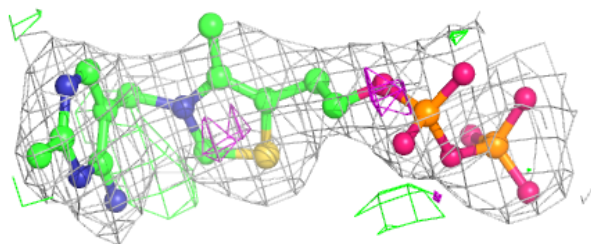
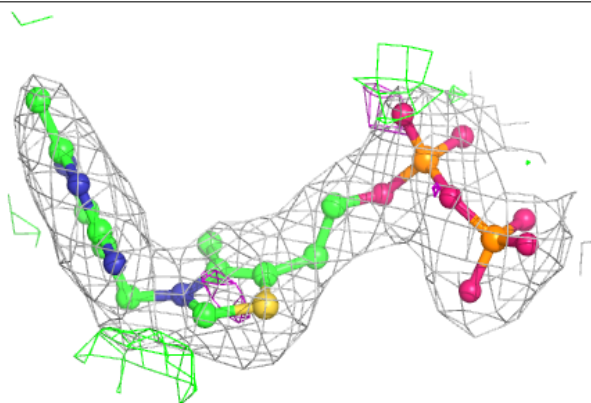


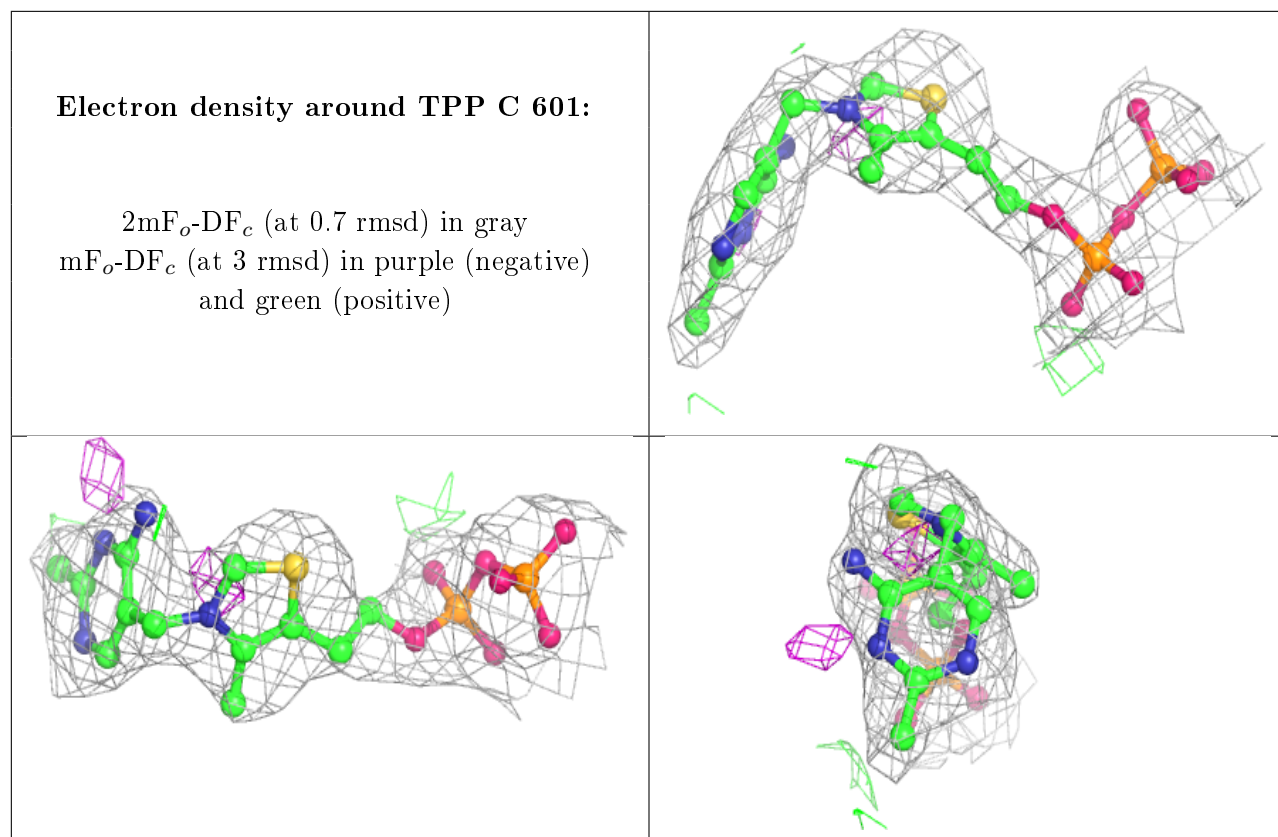
Electron density around TPP G 601:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.