wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2023 – 09:32 pm GMT

PDB ID	:	8CI0
Title	:	Maize Transketolase in complex with TPP and hydrolyzed (+)-Cornexistin
Authors	:	Freigang, J.
Deposited on	:	2023-02-08
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

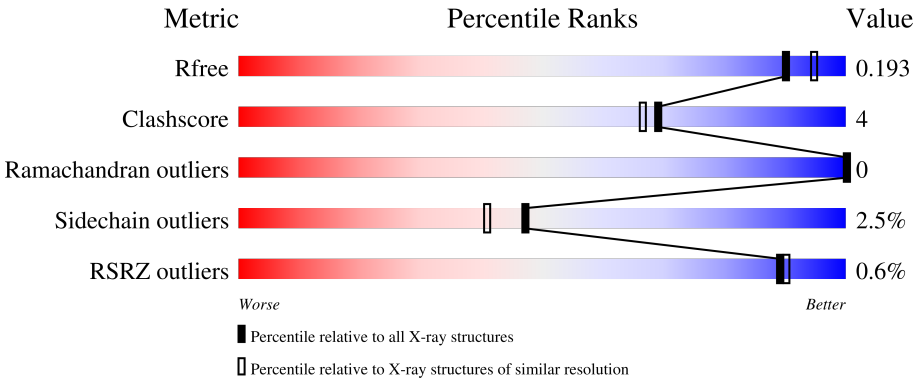
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	688	89% 7%
1	BBB	688	% 89% 8%
1	CCC	688	90% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17364 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, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	666	Total	C	N	O	S	46	0	0
			5082	3216	868	977	21			
1	BBB	666	Total	C	N	O	S	46	0	0
			5082	3216	868	977	21			
1	CCC	666	Total	C	N	O	S	12	0	0
			5082	3216	868	977	21			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-12	MET	-	initiating methionine	UNP Q7SIC9
AAA	-11	HIS	-	expression tag	UNP Q7SIC9
AAA	-10	HIS	-	expression tag	UNP Q7SIC9
AAA	-9	HIS	-	expression tag	UNP Q7SIC9
AAA	-8	HIS	-	expression tag	UNP Q7SIC9
AAA	-7	HIS	-	expression tag	UNP Q7SIC9
AAA	-6	HIS	-	expression tag	UNP Q7SIC9
AAA	-5	GLU	-	expression tag	UNP Q7SIC9
AAA	-4	ASN	-	expression tag	UNP Q7SIC9
AAA	-3	LEU	-	expression tag	UNP Q7SIC9
AAA	-2	TYR	-	expression tag	UNP Q7SIC9
AAA	-1	PHE	-	expression tag	UNP Q7SIC9
AAA	0	GLN	-	expression tag	UNP Q7SIC9
BBB	-12	MET	-	initiating methionine	UNP Q7SIC9
BBB	-11	HIS	-	expression tag	UNP Q7SIC9
BBB	-10	HIS	-	expression tag	UNP Q7SIC9
BBB	-9	HIS	-	expression tag	UNP Q7SIC9
BBB	-8	HIS	-	expression tag	UNP Q7SIC9
BBB	-7	HIS	-	expression tag	UNP Q7SIC9
BBB	-6	HIS	-	expression tag	UNP Q7SIC9
BBB	-5	GLU	-	expression tag	UNP Q7SIC9
BBB	-4	ASN	-	expression tag	UNP Q7SIC9
BBB	-3	LEU	-	expression tag	UNP Q7SIC9

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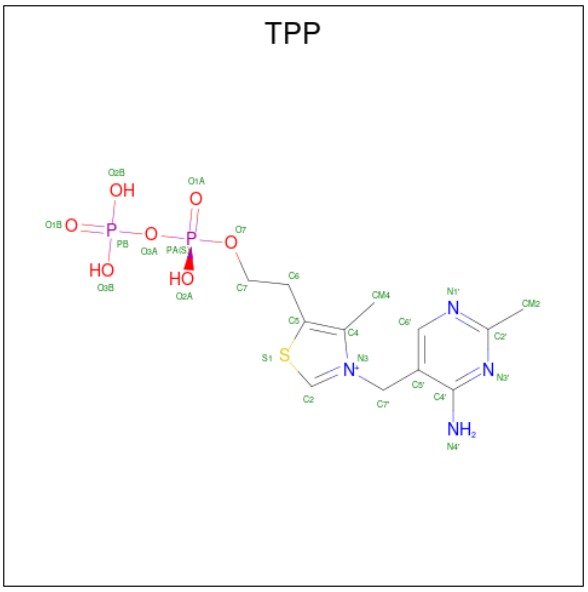
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-2	TYR	-	expression tag	UNP Q7SIC9
BBB	-1	PHE	-	expression tag	UNP Q7SIC9
BBB	0	GLN	-	expression tag	UNP Q7SIC9
CCC	-12	MET	-	initiating methionine	UNP Q7SIC9
CCC	-11	HIS	-	expression tag	UNP Q7SIC9
CCC	-10	HIS	-	expression tag	UNP Q7SIC9
CCC	-9	HIS	-	expression tag	UNP Q7SIC9
CCC	-8	HIS	-	expression tag	UNP Q7SIC9
CCC	-7	HIS	-	expression tag	UNP Q7SIC9
CCC	-6	HIS	-	expression tag	UNP Q7SIC9
CCC	-5	GLU	-	expression tag	UNP Q7SIC9
CCC	-4	ASN	-	expression tag	UNP Q7SIC9
CCC	-3	LEU	-	expression tag	UNP Q7SIC9
CCC	-2	TYR	-	expression tag	UNP Q7SIC9
CCC	-1	PHE	-	expression tag	UNP Q7SIC9
CCC	0	GLN	-	expression tag	UNP Q7SIC9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

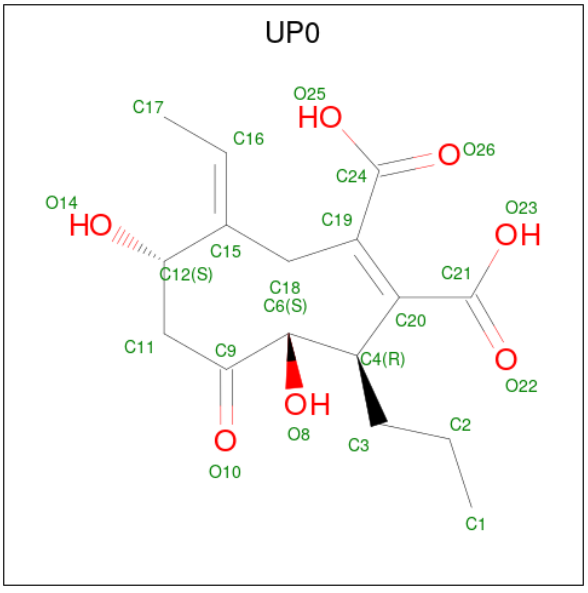
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Mg 1 1	0	0
2	BBB	1	Total Mg 1 1	0	0
2	CCC	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



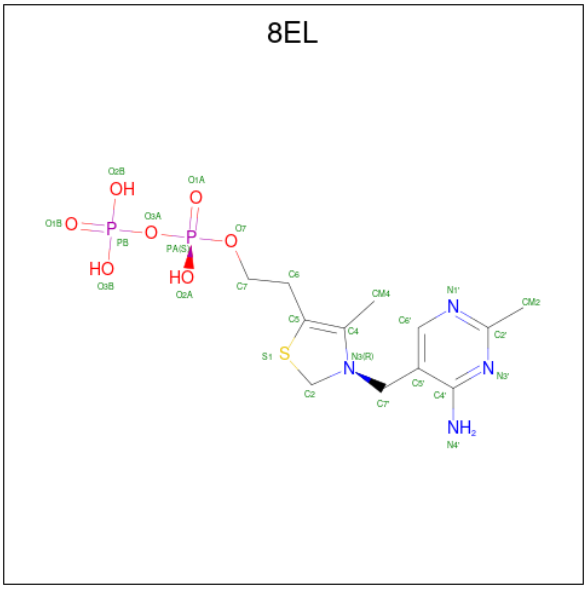
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	BBB	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is (1 {Z},3 {R},4 {S},7 {S},8 {Z})-8-ethylidene-4,7-bis(oxidanyl)-5-oxidanylidene-3-propyl-cyclononene-1,2-dicarboxylic acid (three-letter code: UP0) (formula: $C_{16}H_{22}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	CCC	1	Total	C	O		0	0
			23	16	7			

- Molecule 5 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2H-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: 8EL) (formula: $C_{12}H_{20}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	CCC	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is water.

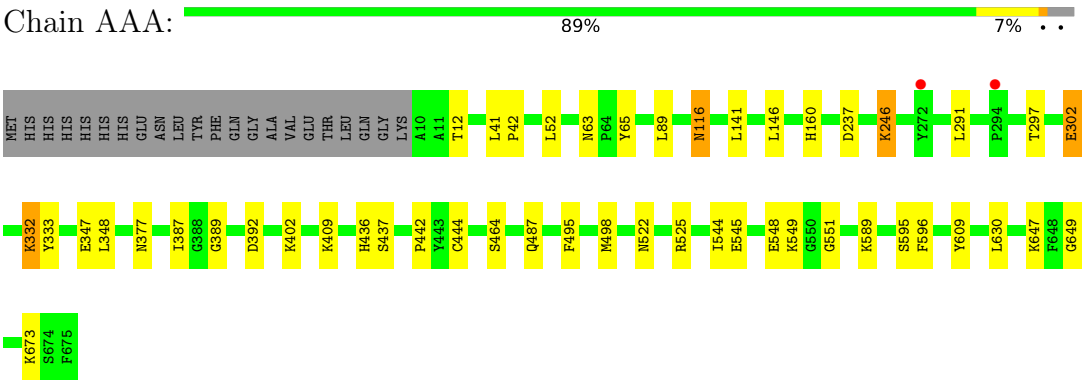
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	698	Total	O	0	0
			698	698		
6	BBB	705	Total	O	0	0
			705	705		
6	CCC	611	Total	O	0	0
			611	611		

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.

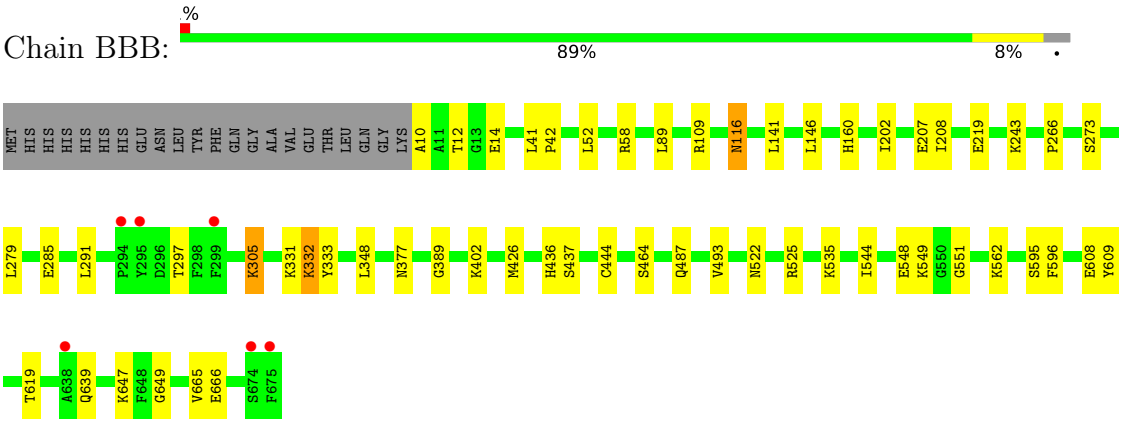
• Molecule 1: Transketolase, chloroplastic

Chain AAA:



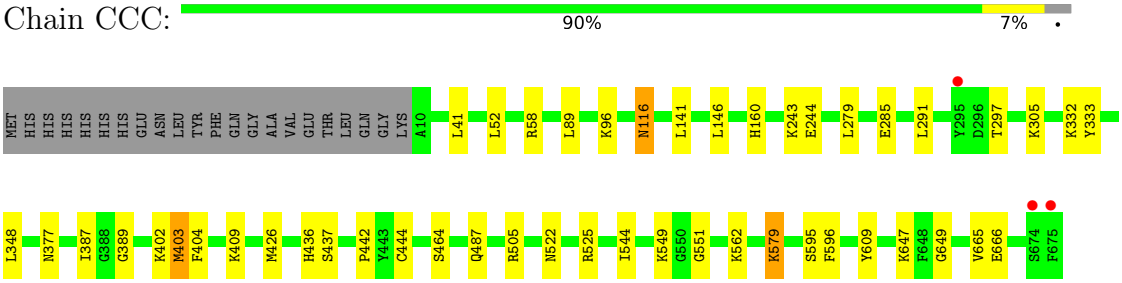
• Molecule 1: Transketolase, chloroplastic

Chain BBB:



• Molecule 1: Transketolase, chloroplastic

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.31Å 135.31Å 201.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.73 – 1.90 23.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (23.73-1.90) 94.3 (23.72-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.153 , 0.184 0.165 , 0.193	Depositor DCC
R_{free} test set	7754 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17364	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, 8EL, UP0

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	AAA	0.89	4/5202 (0.1%)	0.80	1/7060 (0.0%)
1	BBB	0.81	6/5202 (0.1%)	0.81	2/7060 (0.0%)
1	CCC	0.77	2/5202 (0.0%)	0.79	1/7060 (0.0%)
All	All	0.82	12/15606 (0.1%)	0.80	4/21180 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	302	GLU	CG-CD	-29.09	1.08	1.51
1	BBB	14	GLU	CG-CD	-10.25	1.36	1.51
1	BBB	273	SER	CB-OG	-10.15	1.29	1.42
1	CCC	285	GLU	CG-CD	-10.00	1.36	1.51
1	AAA	347	GLU	CG-CD	-8.36	1.39	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	331	LYS	CG-CD-CE	7.28	133.74	111.90
1	AAA	647	LYS	CG-CD-CE	6.01	129.94	111.90
1	CCC	505	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	BBB	109	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	AAA	5082	0	4957	39	0
1	BBB	5082	0	4957	40	0
1	CCC	5082	0	4957	33	1
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
3	AAA	26	0	16	0	0
3	BBB	26	0	16	0	0
4	CCC	23	0	0	0	0
5	CCC	26	0	0	0	0
6	AAA	698	0	0	16	0
6	BBB	705	0	0	19	0
6	CCC	611	0	0	11	3
All	All	17364	0	14903	111	3

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 111 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:BBB:219:GLU:HG2	6:BBB:1521:HOH:O	1.46	1.14
1:CCC:305:LYS:CE	6:CCC:1363:HOH:O	2.03	1.06
1:BBB:10:ALA:N	6:BBB:1101:HOH:O	1.88	1.04
1:CCC:647:LYS:HD2	6:CCC:1128:HOH:O	1.57	1.04
1:BBB:305:LYS:HE3	6:BBB:1479:HOH:O	1.64	0.96

All (3) 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)
6:CCC:1132:HOH:O	6:CCC:1391:HOH:O[4_556]	1.62	0.58
1:CCC:96:LYS:CE	6:CCC:1127:HOH:O[5_675]	2.07	0.13
6:CCC:1557:HOH:O	6:CCC:1595:HOH:O[5_675]	2.14	0.06

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	AAA	664/688 (96%)	645 (97%)	19 (3%)	0	100	100
1	BBB	664/688 (96%)	645 (97%)	19 (3%)	0	100	100
1	CCC	664/688 (96%)	642 (97%)	22 (3%)	0	100	100
All	All	1992/2064 (96%)	1932 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	528/547 (96%)	515 (98%)	13 (2%)	47	41
1	BBB	528/547 (96%)	514 (97%)	14 (3%)	44	38
1	CCC	528/547 (96%)	515 (98%)	13 (2%)	47	41
All	All	1584/1641 (96%)	1544 (98%)	40 (2%)	47	41

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	89	LEU
1	CCC	409	LYS
1	CCC	116	ASN
1	CCC	291	LEU
1	CCC	579	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	UP0	CCC	1000	-	21,23,23	1.83	4 (19%)	13,32,32	1.51	3 (23%)
5	8EL	CCC	1002	2	24,27,27	1.24	1 (4%)	30,40,40	0.90	1 (3%)
3	TPP	AAA	1002	2	22,27,27	0.75	0	29,40,40	0.95	1 (3%)
3	TPP	BBB	1002	2	22,27,27	0.54	0	29,40,40	0.96	1 (3%)

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	UP0	CCC	1000	-	-	0/12/41/41	0/0/1/1
5	8EL	CCC	1002	2	-	1/17/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	AAA	1002	2	-	1/16/17/17	0/2/2/2
3	TPP	BBB	1002	2	-	2/16/17/17	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CCC	1000	UP0	O26-C24	4.93	1.35	1.22
5	CCC	1002	8EL	C2-N3	-4.30	1.32	1.45
4	CCC	1000	UP0	C18-C15	4.09	1.55	1.51
4	CCC	1000	UP0	O25-C24	-2.73	1.22	1.30
4	CCC	1000	UP0	C18-C19	2.20	1.54	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	CCC	1002	8EL	CM4-C4-N3	3.65	123.57	120.04
3	AAA	1002	TPP	C7'-N3-C2	-2.73	120.42	125.35
4	CCC	1000	UP0	O25-C24-C19	2.53	123.58	115.92
3	BBB	1002	TPP	C5-C4-N3	2.18	111.94	107.57
4	CCC	1000	UP0	C18-C15-C16	-2.18	117.71	121.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1002	TPP	C4-C5-C6-C7
3	BBB	1002	TPP	C4-C5-C6-C7
3	BBB	1002	TPP	C5-C6-C7-O7
5	CCC	1002	8EL	C5-C6-C7-O7

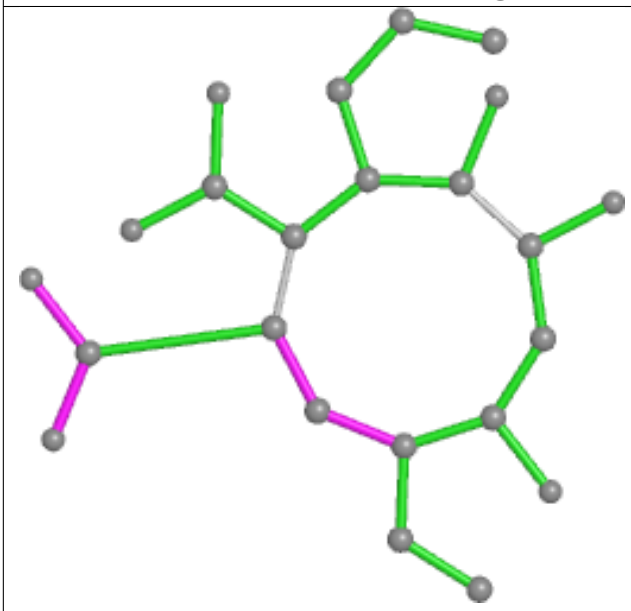
There are no ring outliers.

No monomer is involved in short contacts.

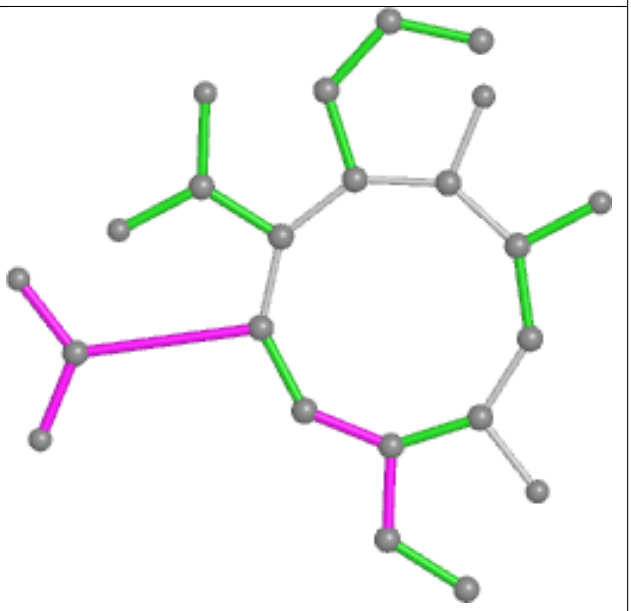
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

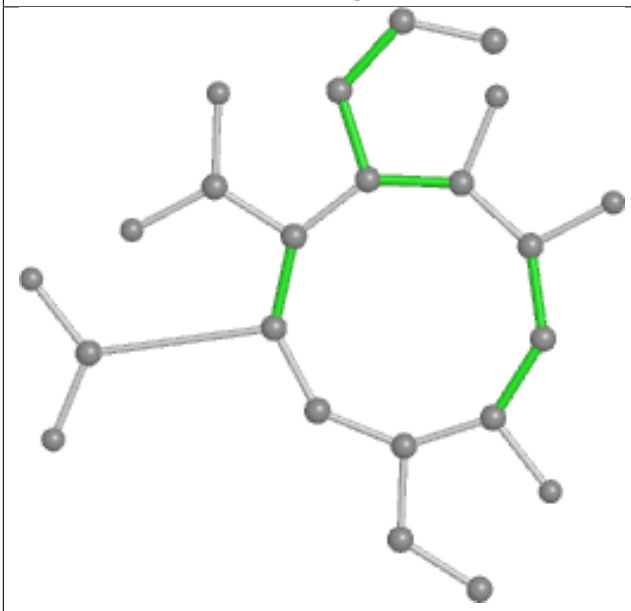
Ligand UP0 CCC 1000



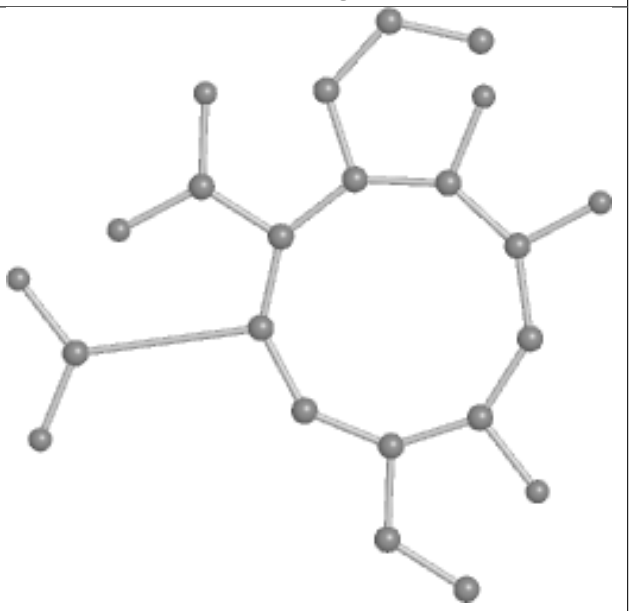
Bond lengths



Bond angles

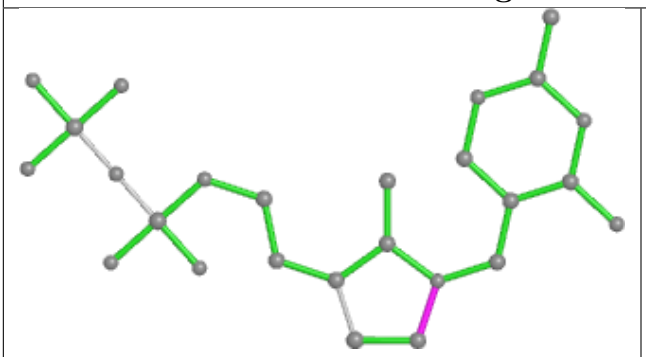


Torsions

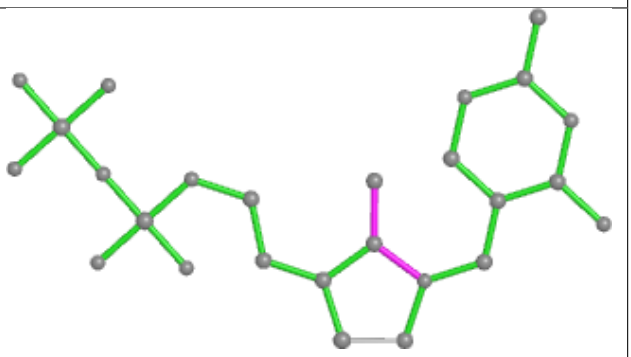


Rings

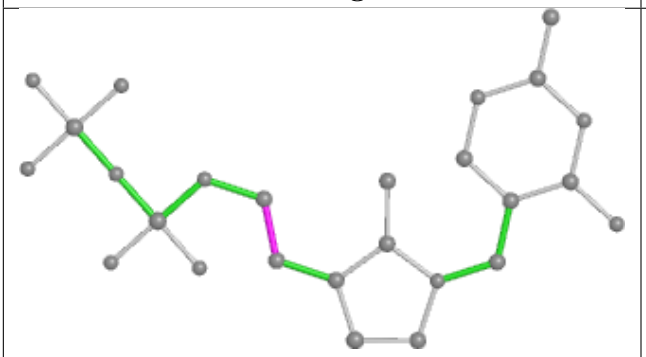
Ligand 8EL CCC 1002



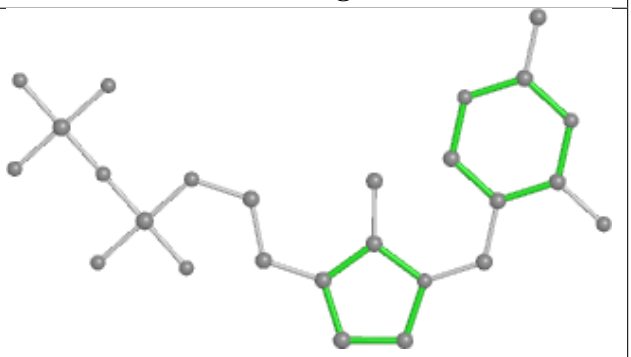
Bond lengths



Bond angles

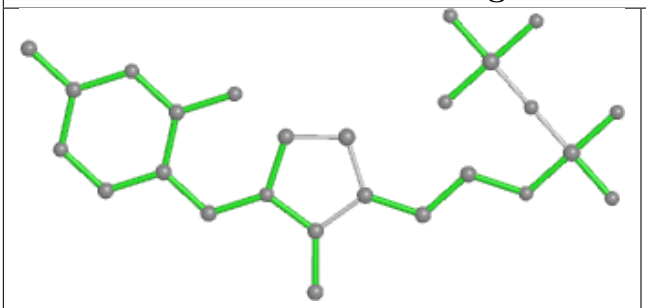


Torsions

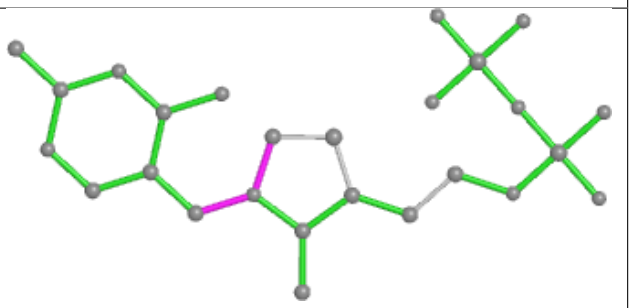


Rings

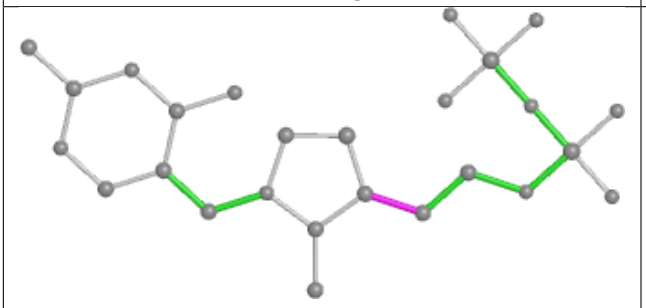
Ligand TPP AAA 1002



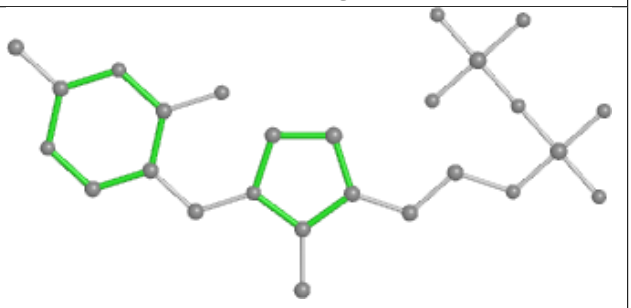
Bond lengths



Bond angles

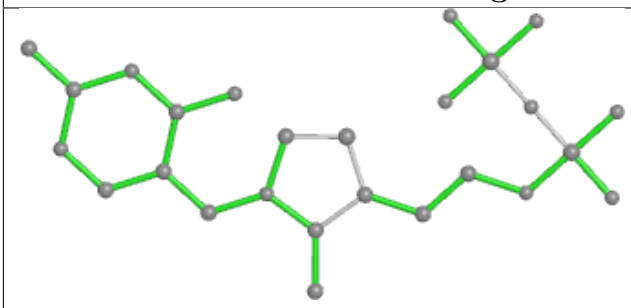


Torsions

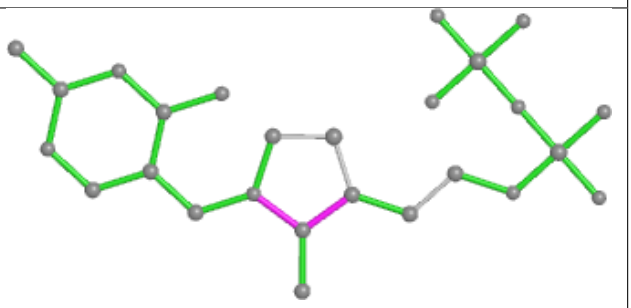


Rings

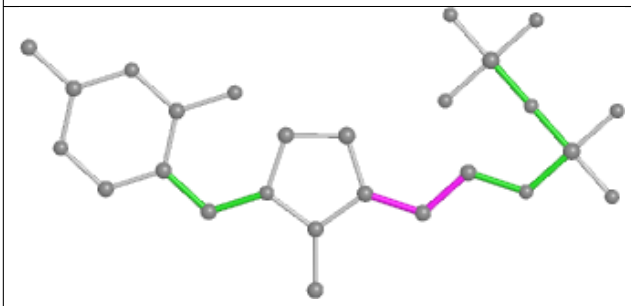
Ligand TPP BBB 1002



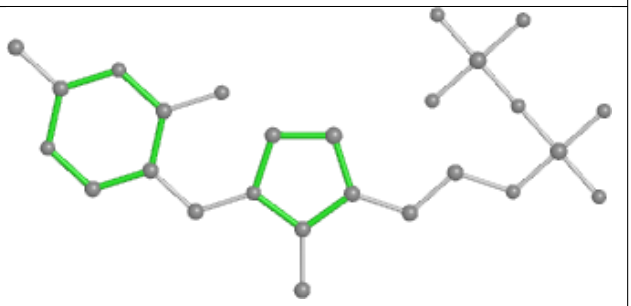
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	666/688 (96%)	-0.43	2 (0%)	94	94	6, 11, 21, 37	15 (2%)
1	BBB	666/688 (96%)	-0.37	6 (0%)	84	85	6, 11, 23, 42	14 (2%)
1	CCC	666/688 (96%)	-0.48	3 (0%)	91	92	5, 9, 20, 39	4 (0%)
All	All	1998/2064 (96%)	-0.43	11 (0%)	89	90	5, 10, 22, 42	33 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	295	TYR	2.6
1	BBB	674	SER	2.6
1	BBB	295	TYR	2.5
1	BBB	638	ALA	2.4
1	CCC	674	SER	2.3

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

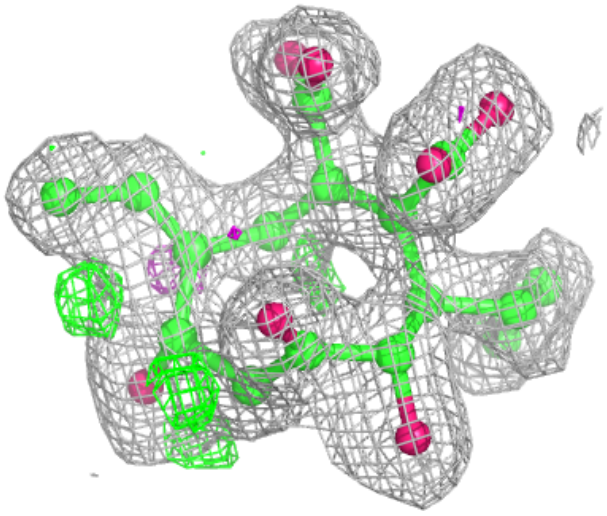
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

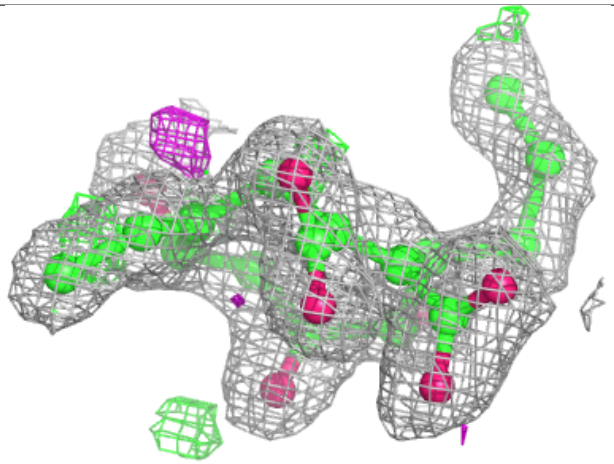
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UP0	CCC	1000	23/23	0.87	0.15	13,15,17,17	23
3	TPP	AAA	1002	26/26	0.98	0.07	8,11,14,14	0
5	8EL	CCC	1002	26/26	0.98	0.06	6,9,11,12	0
2	MG	CCC	1001	1/1	0.99	0.03	8,8,8,8	0
3	TPP	BBB	1002	26/26	0.99	0.06	7,10,13,13	0
2	MG	BBB	1001	1/1	1.00	0.04	9,9,9,9	0
2	MG	AAA	1001	1/1	1.00	0.03	11,11,11,11	0

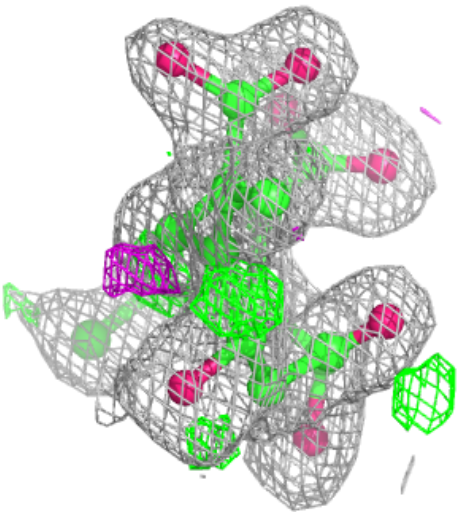
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UP0 CCC 1000:

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

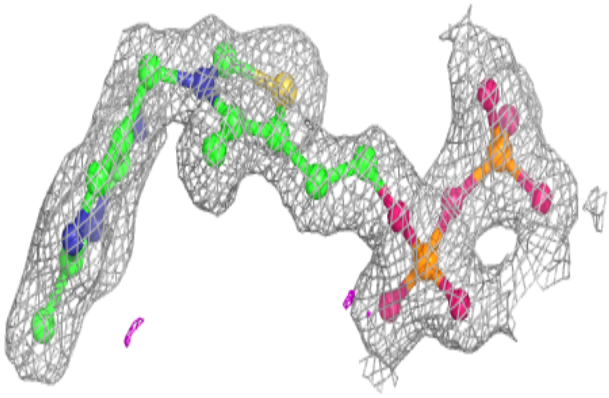


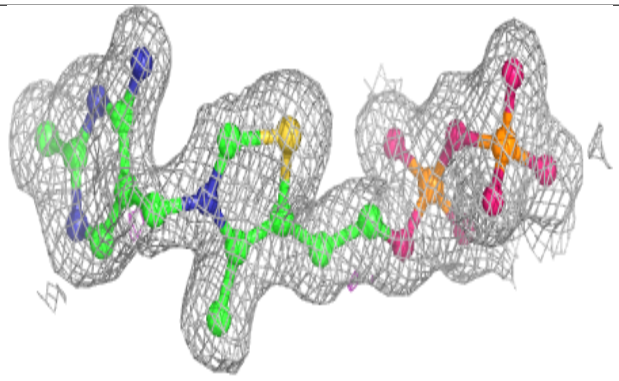


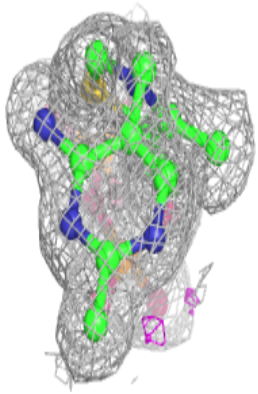


Electron density around TPP AAA 1002:

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

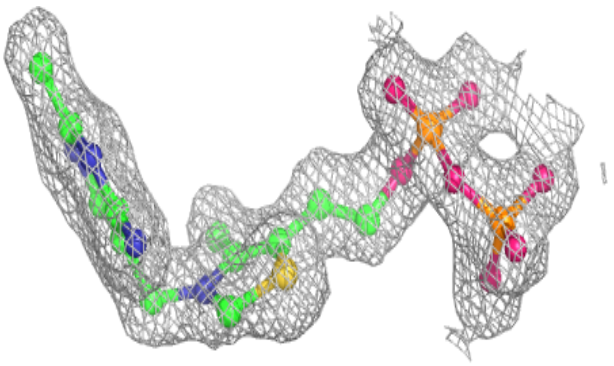


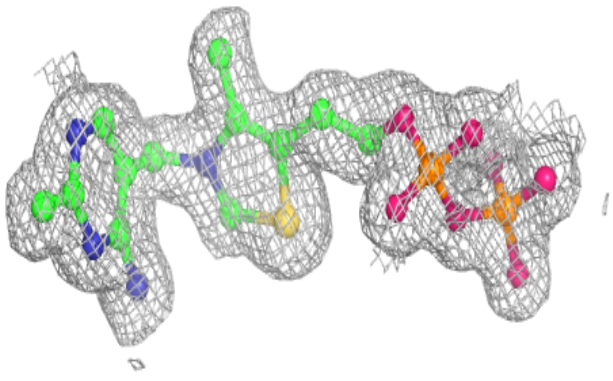


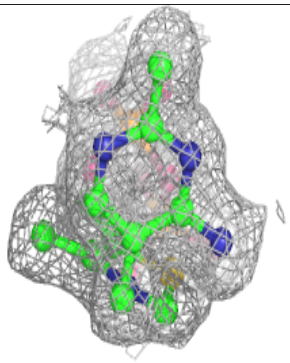


Electron density around 8EL CCC 1002:

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

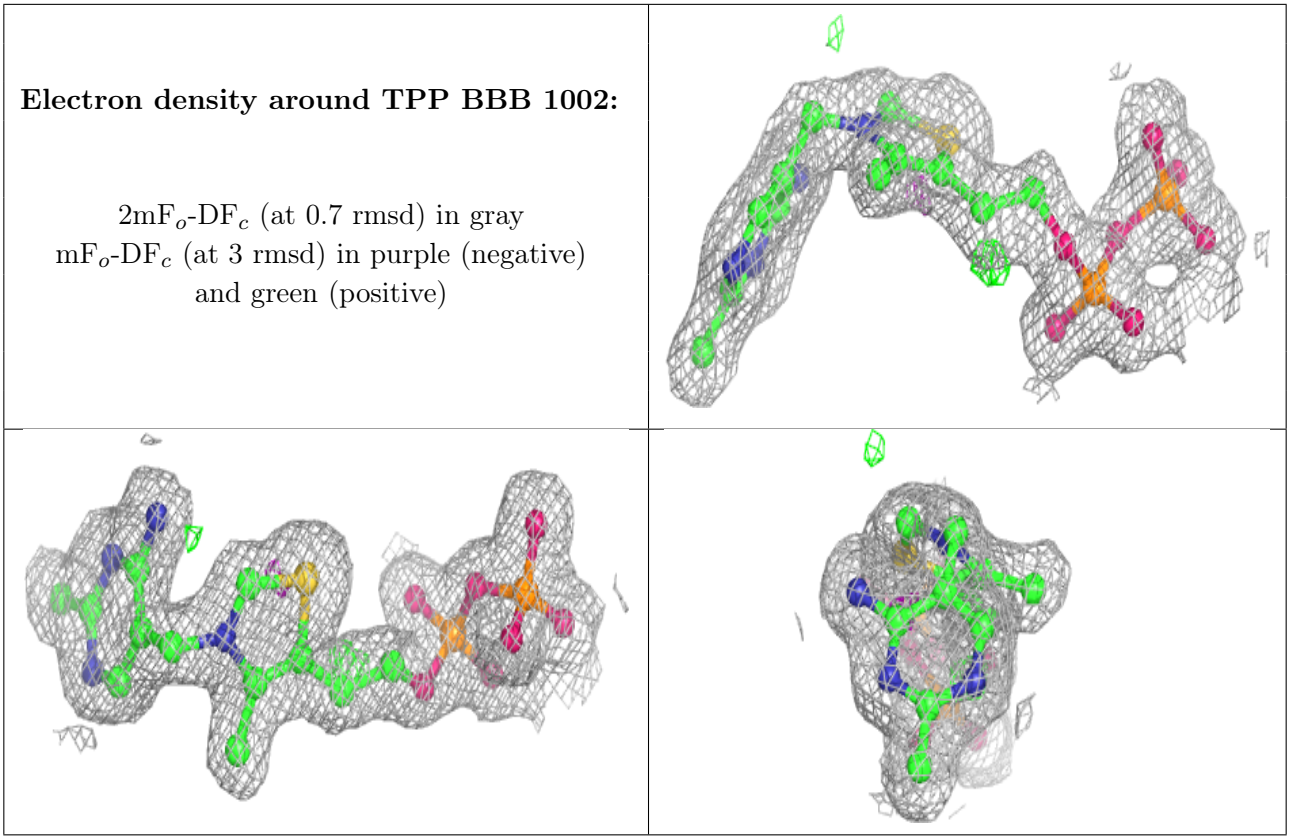






Electron density around TPP BBB 1002:

$2mF_o$-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.