wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 06:31 pm GMT

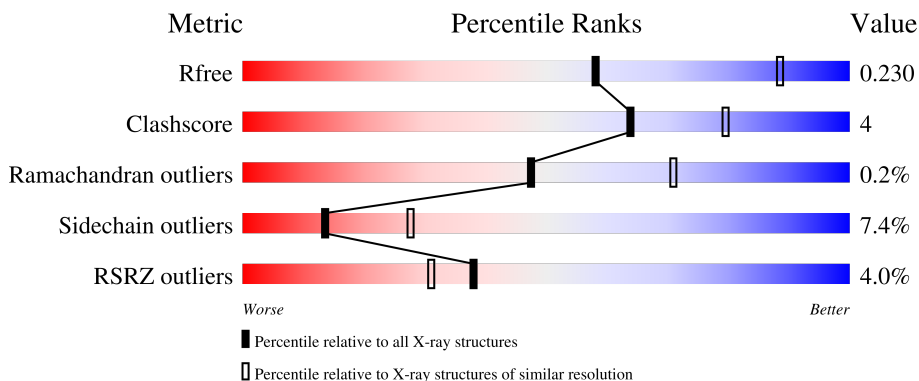|		
PDB ID	:	7ORX
Title	:	Rhodococcus jostii RHA1 thiamine diphosphate-dependent 4-hydroxybenzoyl formate decarboxylase
Authors	:	Wilkinson, R.C.; Fulop, V.
Deposited on	:	2021-06-06
Resolution	:	2.60 Å(reported)

1   Overall quality at a glance   ⓘ

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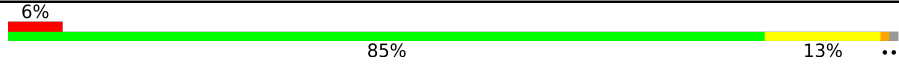*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		7.4%
RSRZ outliers		4.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	531	6% / 85% / 13% / ••
1	BBB	531	5% / 85% / 13% / ••
1	CCC	531	2% / 87% / 12% / •
1	DDD	531	2% / 86% / 12% / ••

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15727 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 Probable benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	527	Total	C	N	O	P	S	0	0	0
			3881	2456	653	762	1	9			
1	BBB	527	Total	C	N	O	P	S	0	0	0
			3881	2456	653	762	1	9			
1	CCC	531	Total	C	N	O	P	S	0	0	0
			3913	2477	658	767	1	10			
1	DDD	527	Total	C	N	O	P	S	0	0	0
			3881	2456	653	762	1	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	PHE	-	expression tag	UNP Q0SCE8
AAA	-1	GLN	-	expression tag	UNP Q0SCE8
AAA	0	GLY	-	expression tag	UNP Q0SCE8
BBB	-2	PHE	-	expression tag	UNP Q0SCE8
BBB	-1	GLN	-	expression tag	UNP Q0SCE8
BBB	0	GLY	-	expression tag	UNP Q0SCE8
CCC	-2	PHE	-	expression tag	UNP Q0SCE8
CCC	-1	GLN	-	expression tag	UNP Q0SCE8
CCC	0	GLY	-	expression tag	UNP Q0SCE8
DDD	-2	PHE	-	expression tag	UNP Q0SCE8
DDD	-1	GLN	-	expression tag	UNP Q0SCE8
DDD	0	GLY	-	expression tag	UNP Q0SCE8

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).

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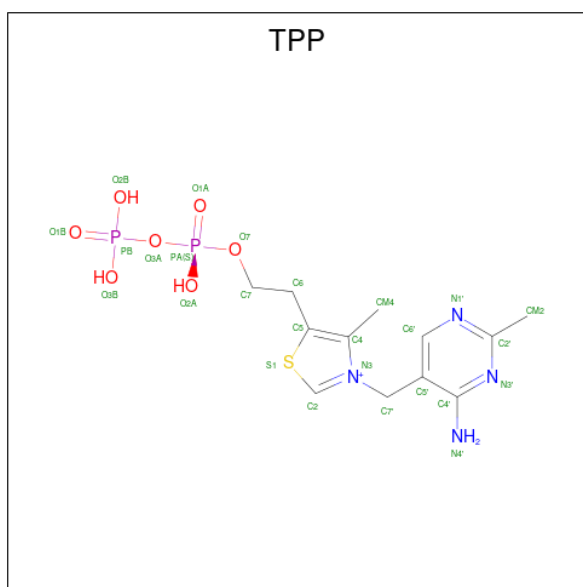
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	BBB	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	CCC	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	DDD	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Na	0	0
			1	1		
3	BBB	1	Total	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		
3	DDD	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	17	Total 17	O 17	0	0
4	CCC	15	Total 15	O 15	0	0
4	DDD	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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.

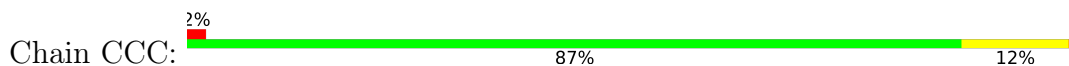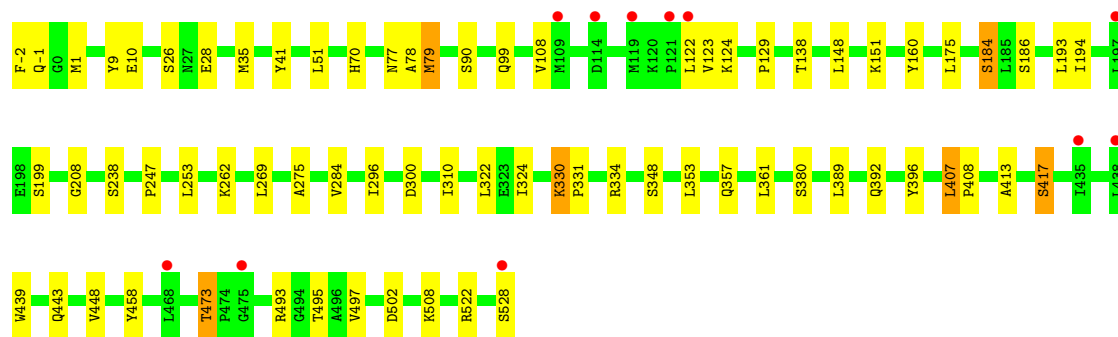• Molecule 1: Probable benzoylformate decarboxylase
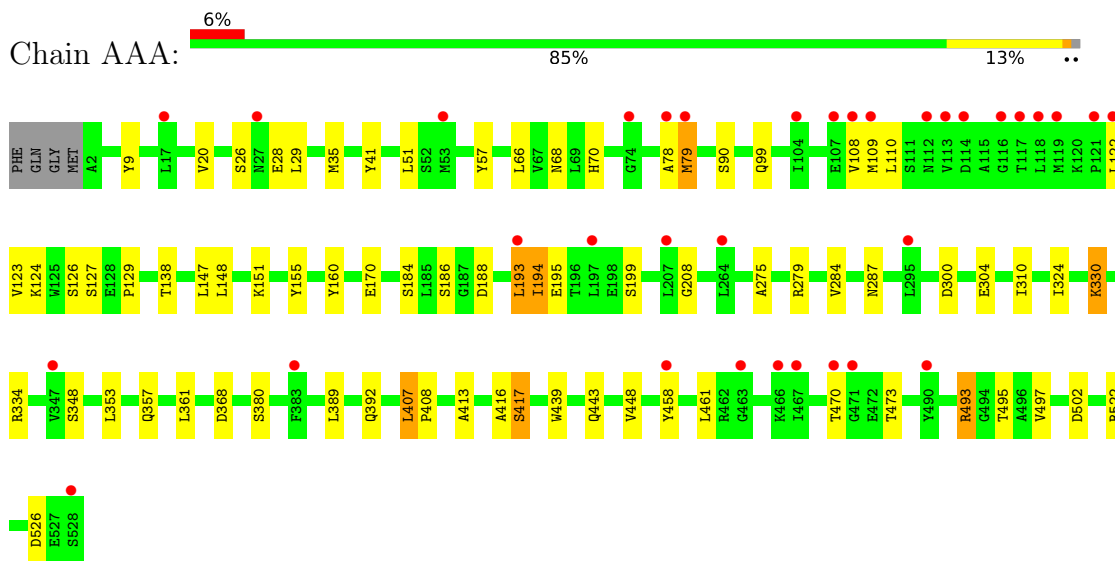
Chain AAA:

• Molecule 1: Probable benzoylformate decarboxylase
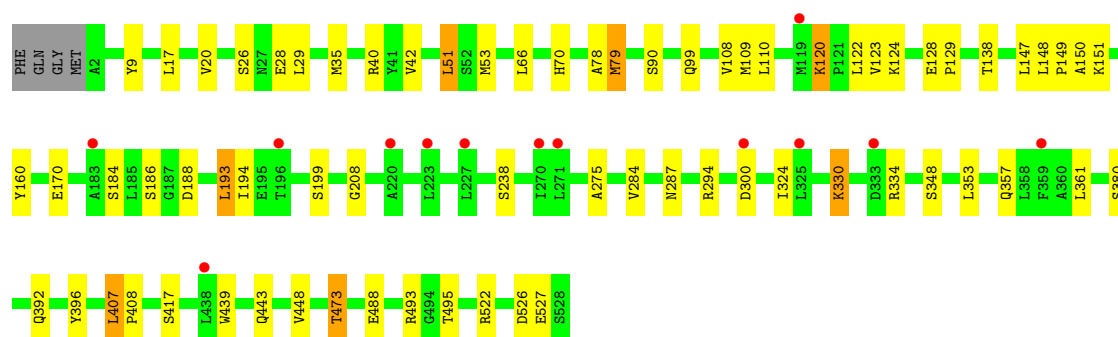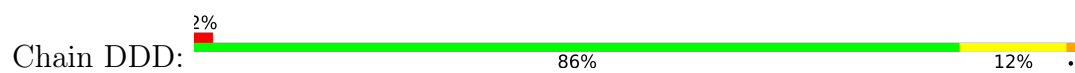
Chain BBB:

• Molecule 1: Probable benzoylformate decarboxylase

Chain CCC:
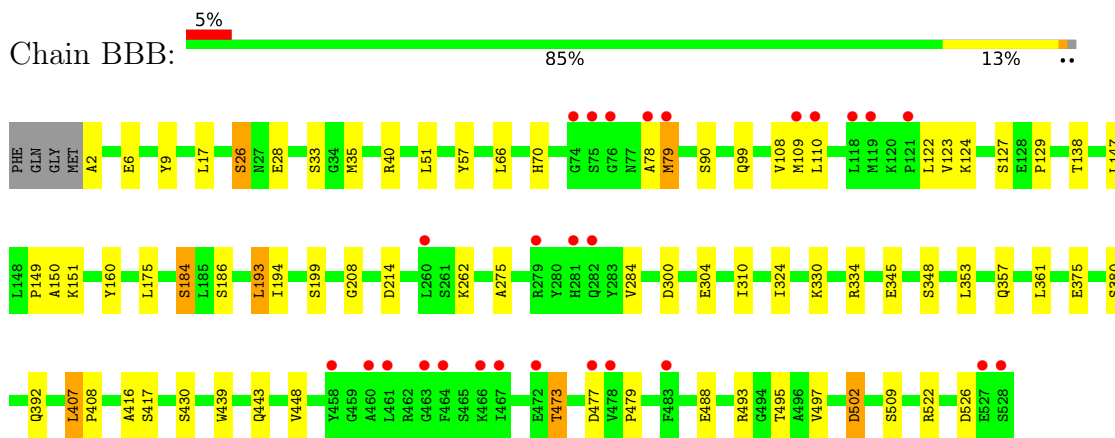
• Molecule 1: Probable benzoylformate decarboxylase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.50Å 132.24Å 138.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.42 – 2.60 90.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.42-2.60) 100.0 (90.26-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.233 0.192 , 0.230	Depositor DCC
R_{free} test set	2975 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15727	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

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

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	0.77	1/3962 (0.0%)	0.92	2/5425 (0.0%)
1	BBB	0.84	3/3962 (0.1%)	0.97	4/5425 (0.1%)
1	CCC	0.82	0/3995	0.96	1/5468 (0.0%)
1	DDD	0.80	2/3962 (0.1%)	0.94	2/5425 (0.0%)
All	All	0.81	6/15881 (0.0%)	0.95	9/21743 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1
1	BBB	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	128	GLU	CD-OE2	7.77	1.34	1.25
1	BBB	304	GLU	CD-OE1	6.30	1.32	1.25
1	AAA	304	GLU	CD-OE2	5.83	1.32	1.25
1	BBB	345	GLU	CD-OE2	5.72	1.31	1.25
1	BBB	488	GLU	CD-OE1	5.65	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	40	ARG	CG-CD-NE	7.47	127.48	111.80
1	DDD	124	LYS	CB-CA-C	-7.06	96.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	124	LYS	CB-CA-C	-6.83	96.75	110.40
1	CCC	124	LYS	CB-CA-C	-6.74	96.91	110.40
1	BBB	40	ARG	CG-CD-NE	6.73	125.93	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	127	SER	Peptide
1	BBB	127	SER	Peptide

5.2   Too-close contacts   ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3881	0	3802	39	0
1	BBB	3881	0	3802	31	0
1	CCC	3913	0	3834	32	0
1	DDD	3881	0	3802	32	0
2	AAA	26	0	16	4	0
2	BBB	26	0	16	0	0
2	CCC	26	0	16	1	0
2	DDD	26	0	16	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	12	0	0	1	0
4	BBB	17	0	0	0	0
4	CCC	15	0	0	1	0
4	DDD	19	0	0	1	0
All	All	15727	0	15304	130	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 130 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:DDD:79:MET:HE2	1:DDD:122:LEU:HD12	1.60	0.83
1:BBB:79:MET:HE2	1:BBB:122:LEU:HD12	1.64	0.78
1:CCC:79:MET:HE2	1:CCC:122:LEU:HD12	1.68	0.75
1:AAA:79:MET:HE2	1:AAA:122:LEU:HD12	1.69	0.73
2:AAA:601:TPP:HN42	2:AAA:601:TPP:H2	1.54	0.71

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	524/531 (99%)	502 (96%)	21 (4%)	1 (0%)	47	71
1	BBB	524/531 (99%)	501 (96%)	22 (4%)	1 (0%)	47	71
1	CCC	528/531 (99%)	505 (96%)	22 (4%)	1 (0%)	47	71
1	DDD	524/531 (99%)	502 (96%)	21 (4%)	1 (0%)	47	71
All	All	2100/2124 (99%)	2010 (96%)	86 (4%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	123	VAL
1	AAA	123	VAL
1	DDD	123	VAL
1	CCC	123	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	406/409 (99%)	378 (93%)	28 (7%)	15	31
1	BBB	406/409 (99%)	377 (93%)	29 (7%)	14	29
1	CCC	409/409 (100%)	375 (92%)	34 (8%)	11	22
1	DDD	406/409 (99%)	377 (93%)	29 (7%)	14	29
All	All	1627/1636 (99%)	1507 (93%)	120 (7%)	13	28

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	-2	PHE
1	DDD	380	SER
1	CCC	262	LYS
1	DDD	361	LEU
1	DDD	526	ASP

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

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#|Z| > 2$
1	SEP	DDD	26	1	8,9,10	2.22	3 (37%)	8,12,14	3.19	3 (37%)
1	SEP	CCC	26	1	8,9,10	2.39	3 (37%)	8,12,14	3.18	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	SEP	BBB	26	1	8,9,10	2.42	3 (37%)	8,12,14	3.18	3 (37%)
1	SEP	AAA	26	1	8,9,10	2.07	3 (37%)	8,12,14	3.07	2 (25%)

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
1	SEP	DDD	26	1	-	2/5/8/10	-
1	SEP	CCC	26	1	-	2/5/8/10	-
1	SEP	BBB	26	1	-	2/5/8/10	-
1	SEP	AAA	26	1	-	2/5/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	26	SEP	P-OG	5.57	1.78	1.60
1	CCC	26	SEP	P-OG	5.33	1.77	1.60
1	DDD	26	SEP	P-OG	4.49	1.74	1.60
1	AAA	26	SEP	P-OG	4.39	1.74	1.60
1	BBB	26	SEP	CB-CA	2.91	1.60	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	26	SEP	OG-CB-CA	8.18	116.10	108.14
1	CCC	26	SEP	OG-CB-CA	8.18	116.10	108.14
1	AAA	26	SEP	OG-CB-CA	7.93	115.86	108.14
1	BBB	26	SEP	OG-CB-CA	7.75	115.69	108.14
1	CCC	26	SEP	P-OG-CB	3.38	127.60	118.30

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	26	SEP	N-CA-CB-OG
1	AAA	26	SEP	CA-CB-OG-P
1	BBB	26	SEP	N-CA-CB-OG
1	BBB	26	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
1	CCC	26	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	26	SEP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	TPP	BBB	601	3	22,27,27	0.57	0	29,40,40	0.85	1 (3%)
2	TPP	DDD	601	3	22,27,27	0.63	0	29,40,40	0.79	1 (3%)
2	TPP	CCC	601	3	22,27,27	0.49	0	29,40,40	0.89	1 (3%)
2	TPP	AAA	601	3	22,27,27	0.66	0	29,40,40	1.08	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
2	TPP	BBB	601	3	-	2/16/17/17	0/2/2/2
2	TPP	DDD	601	3	-	2/16/17/17	0/2/2/2
2	TPP	CCC	601	3	-	4/16/17/17	0/2/2/2

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	AAA	601	3	-	6/16/17/17	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	601	TPP	C7'-N3-C2	-2.72	120.44	125.35
2	CCC	601	TPP	O7-PA-O1A	2.31	118.11	109.07
2	DDD	601	TPP	O2A-PA-O1A	2.20	123.11	112.24
2	BBB	601	TPP	C7'-N3-C2	-2.07	121.61	125.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	TPP	C4'-C5'-C7'-N3
2	AAA	601	TPP	C5-C6-C7-O7
2	AAA	601	TPP	C7-O7-PA-O1A
2	AAA	601	TPP	C7-O7-PA-O2A
2	AAA	601	TPP	PB-O3A-PA-O7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	601	TPP	1	0
2	CCC	601	TPP	1	0
2	AAA	601	TPP	4	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 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 TPP BBB 601

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP DDD 601

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP CCC 601

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP AAA 601

Bond lengths

Bond angles

Torsions

Rings
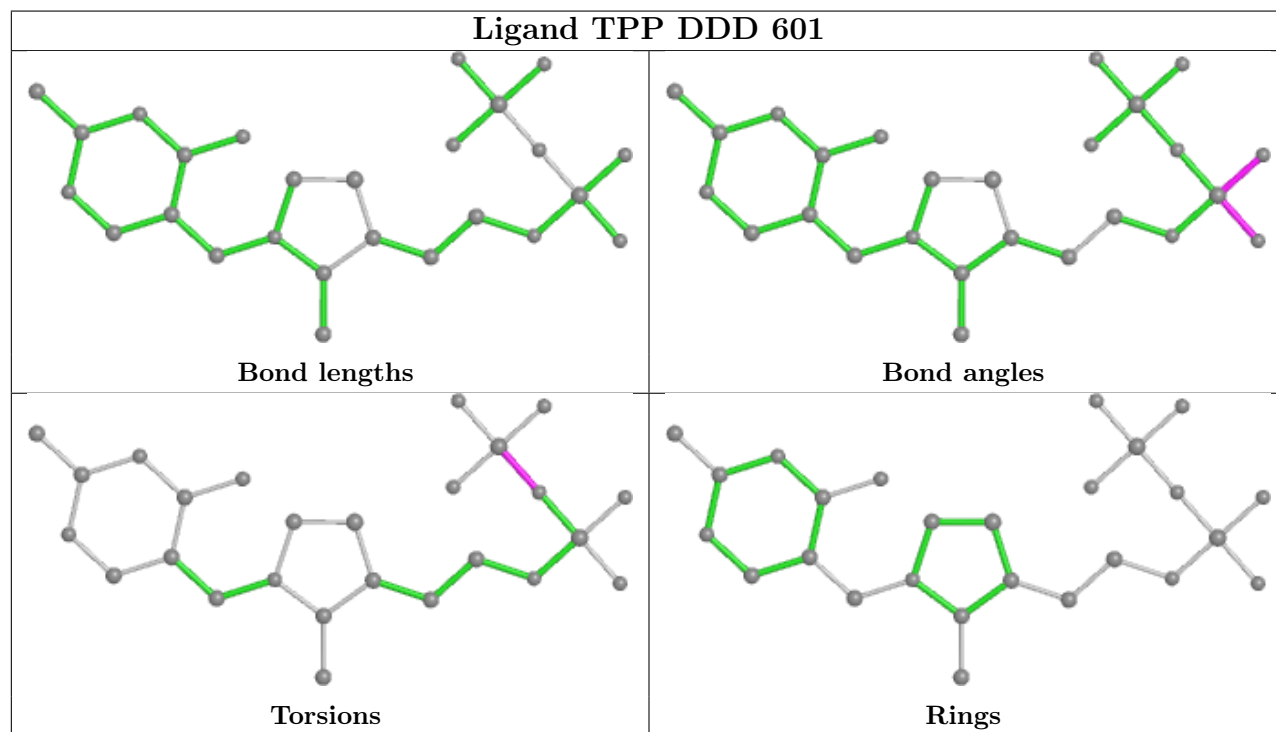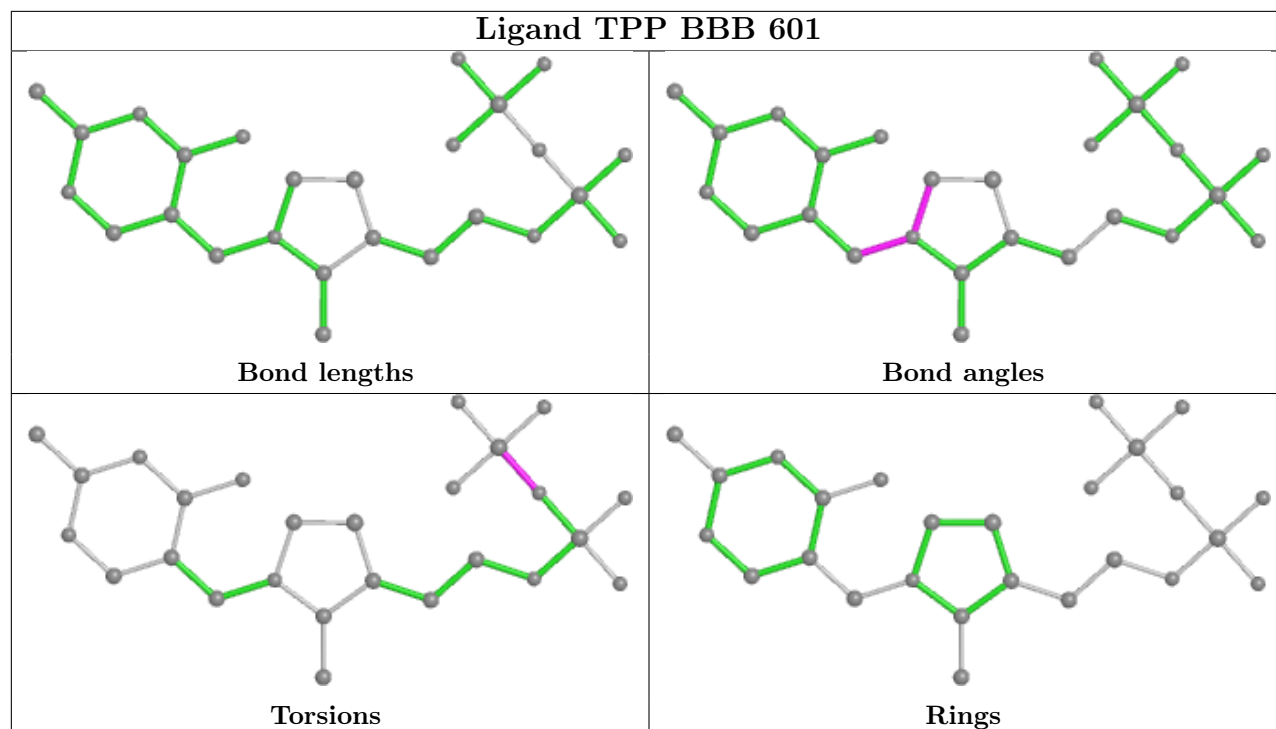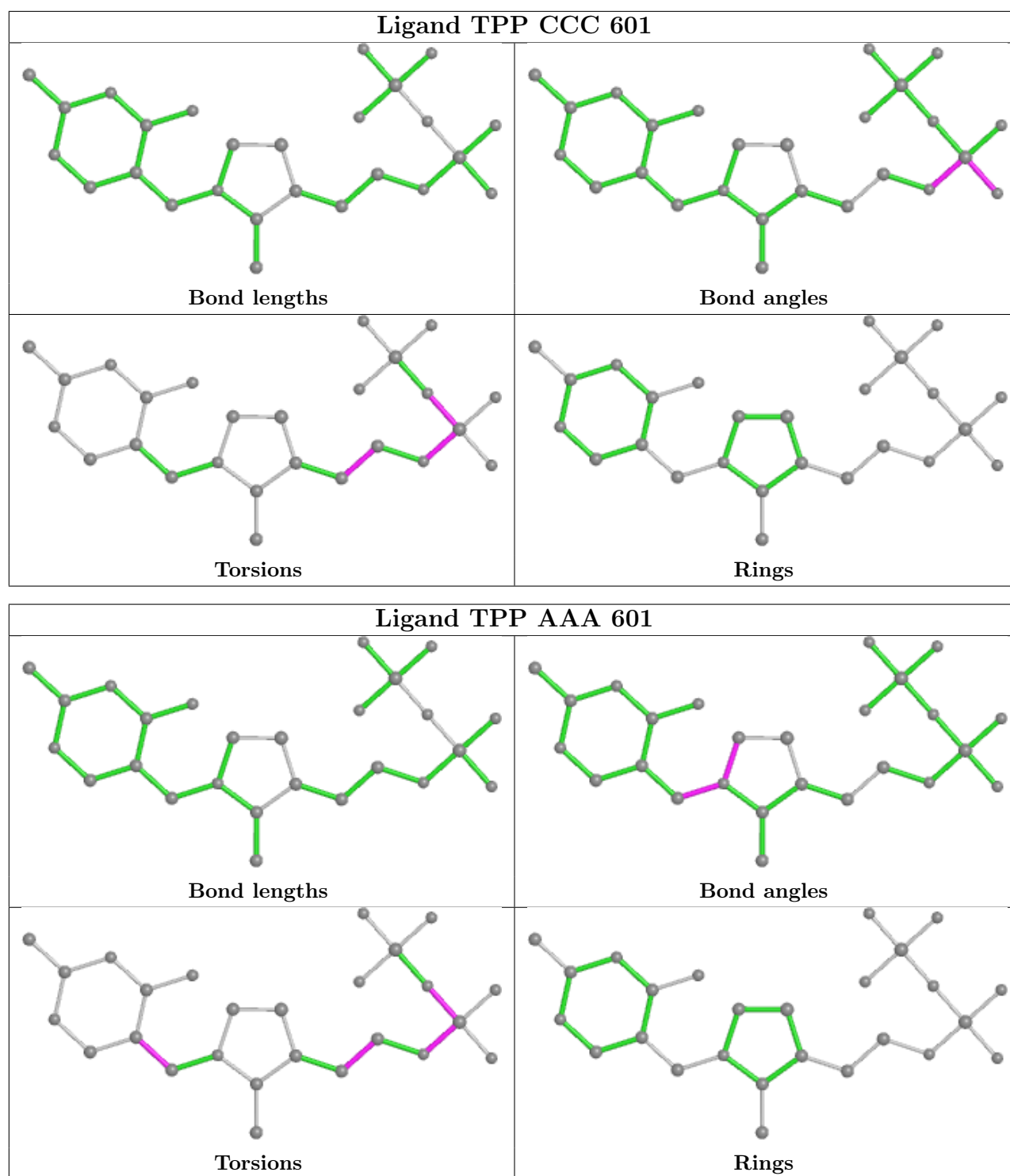
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	AAA	526/531 (99%)	0.26	34 (6%)	18	14	70, 93, 133, 159	0
1	BBB	526/531 (99%)	0.23	27 (5%)	28	22	57, 80, 122, 174	0
1	CCC	530/531 (99%)	0.07	11 (2%)	63	58	59, 79, 108, 150	0
1	DDD	526/531 (99%)	0.15	13 (2%)	57	51	63, 87, 131, 160	0
All	All	2108/2124 (99%)	0.18	85 (4%)	38	31	57, 85, 127, 174	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	528	SER	9.9
1	AAA	119	MET	5.7
1	CCC	528	SER	5.6
1	BBB	75	SER	5.5
1	BBB	467	ILE	4.9

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

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(Å²)	Q<0.9
1	SEP	CCC	26	10/11	0.88	0.17	88,90,95,100	0
1	SEP	BBB	26	10/11	0.91	0.21	87,95,102,104	0
1	SEP	AAA	26	10/11	0.93	0.20	116,123,132,135	0
1	SEP	DDD	26	10/11	0.93	0.17	85,95,106,109	0

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, 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
3	NA	BBB	602	1/1	0.90	0.04	83,83,83,83	0
3	NA	DDD	602	1/1	0.95	0.10	67,67,67,67	0
2	TPP	CCC	601	26/26	0.96	0.19	64,83,90,109	0
3	NA	AAA	602	1/1	0.96	0.06	84,84,84,84	0
2	TPP	AAA	601	26/26	0.96	0.25	76,96,106,108	0
3	NA	CCC	602	1/1	0.96	0.10	66,66,66,66	0
2	TPP	BBB	601	26/26	0.96	0.27	90,112,126,132	0
2	TPP	DDD	601	26/26	0.97	0.18	69,80,99,104	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.

WORLDWIDE wwPDB PROTEIN DATA BANK

Electron density around TPP CCC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
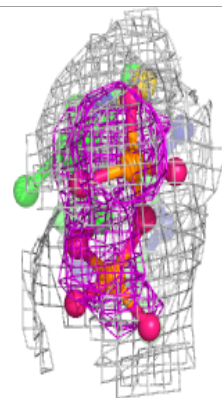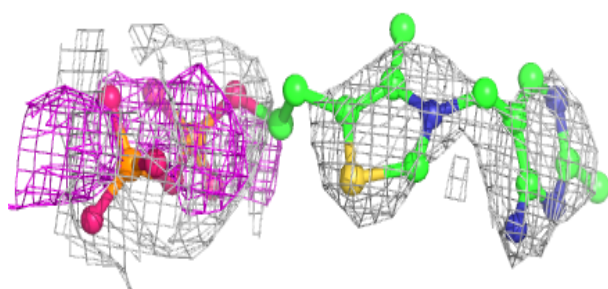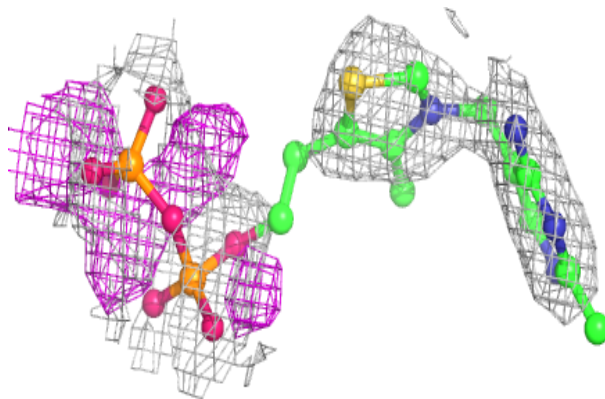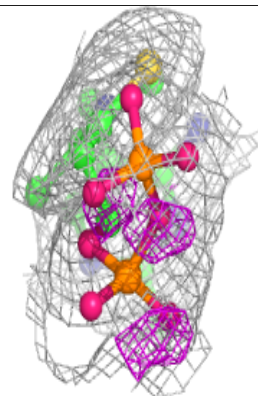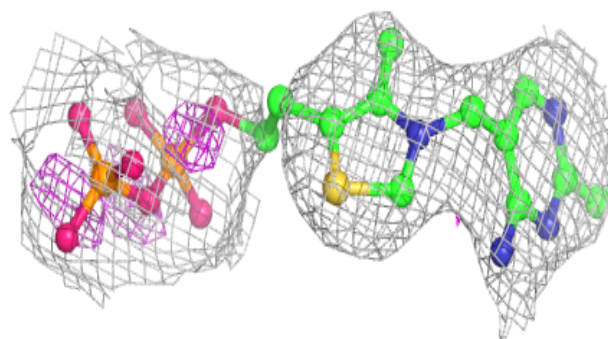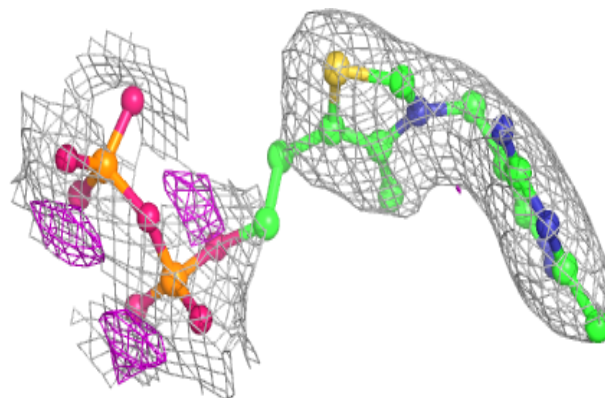mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
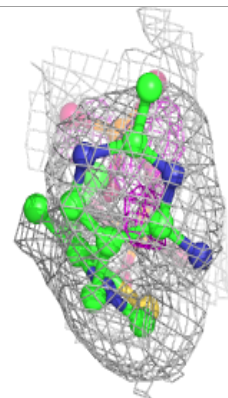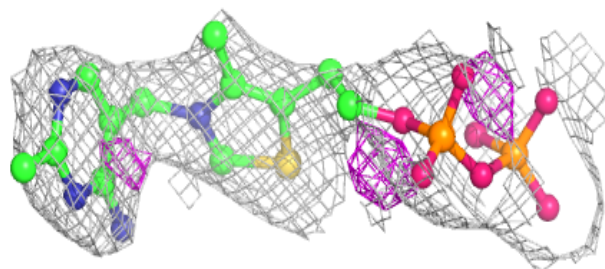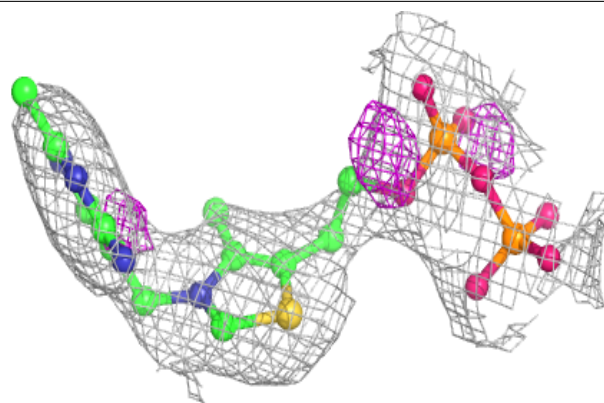
Electron density around TPP AAA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
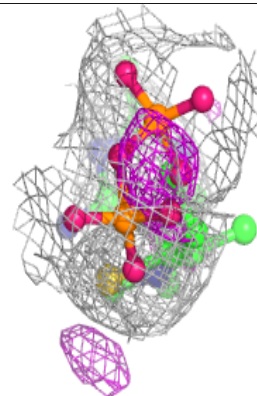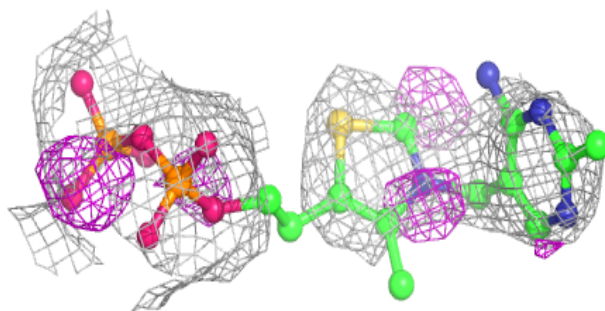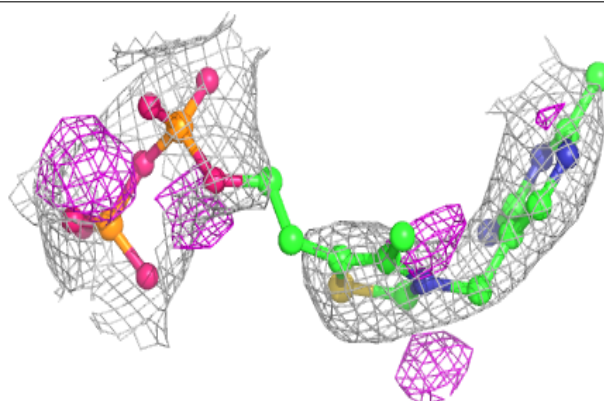
Electron density around TPP BBB 601:

$2mF_o$-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 DDD 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 ⓘ

There are no such residues in this entry.