wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2024 – 04:09 PM EDT

PDB ID	:	8VZI
Title	:	Crystal Structure of 2-Hydroxyacyl-CoA Lyase/Synthase CcHACS from Conidiobolus coronatus in the Complex with THDP and ADP
Authors	:	Kim, Y.; Gade, P.; Endres, M.; Lee, S.; Yoshikuni, Y.; Gonzalez, R.; Michalska, K.; Joachimiak, A.
Deposited on	:	2024-02-11
Resolution	:	1.85 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:

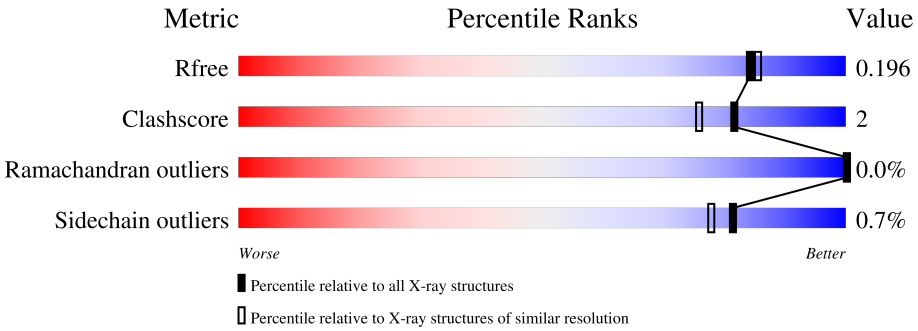
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)

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%

Mol	Chain	Length	Quality of chain
1	A	563	89% 6% ·
1	B	563	90% 6% ·
1	C	563	89% 6% ·
1	D	563	90% 6% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GLY	B	605	-	X	-	-

2 Entry composition

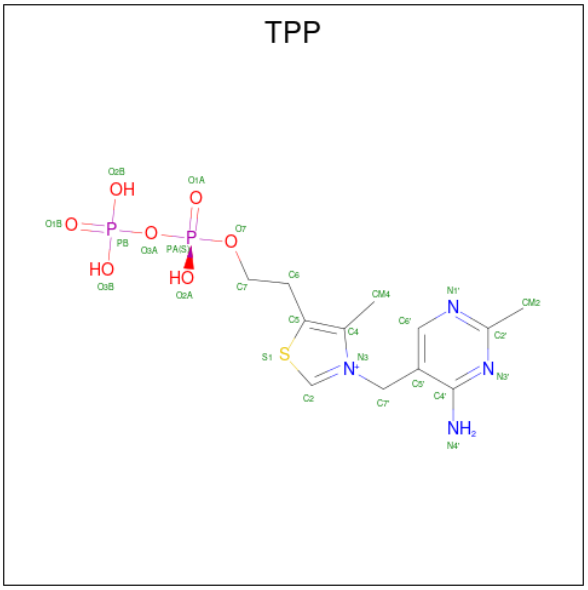
There are 11 unique types of molecules in this entry. The entry contains 18554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-hydroxyacyl-CoA lyase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	10	0
			4197	2676	722	775	24			
1	B	538	Total	C	N	O	S	0	11	0
			4215	2685	729	777	24			
1	C	539	Total	C	N	O	S	0	9	0
			4205	2679	725	777	24			
1	D	540	Total	C	N	O	S	0	10	0
			4215	2685	726	780	24			

- 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).



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

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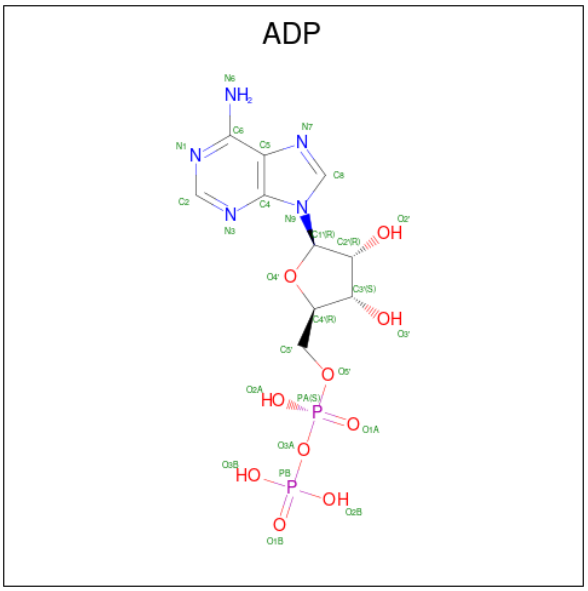
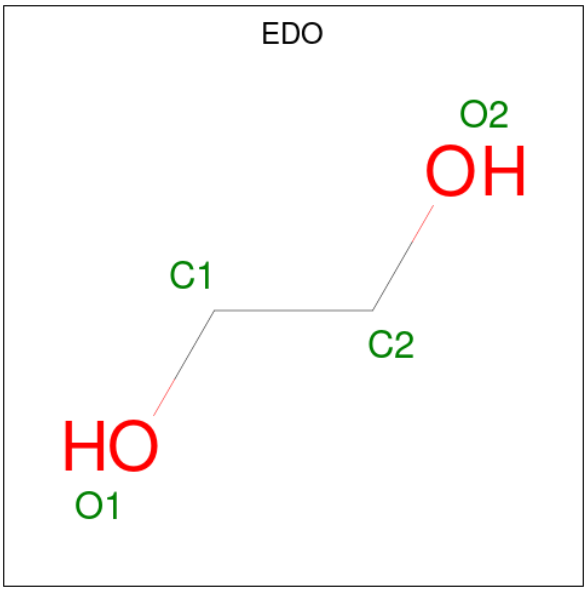
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



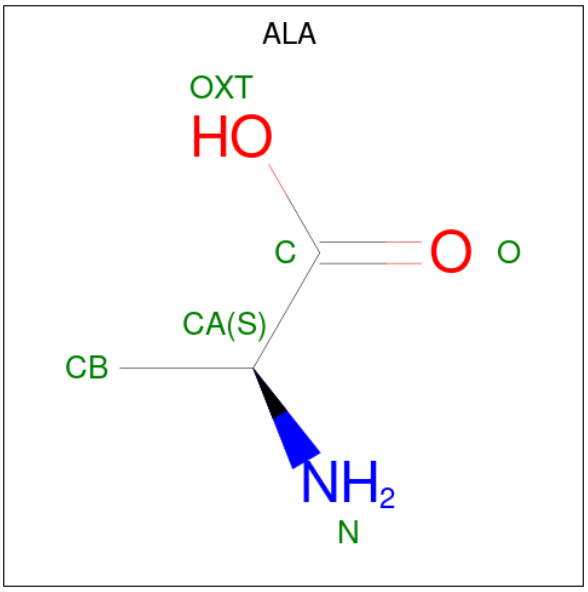
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



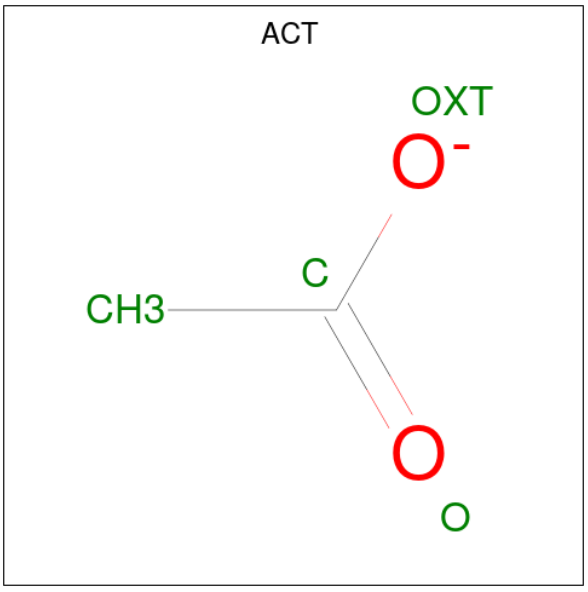
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 6 3 1 2	0	0
5	A	1	Total C N O 6 3 1 2	0	0
5	A	1	Total C N O 6 3 1 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

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

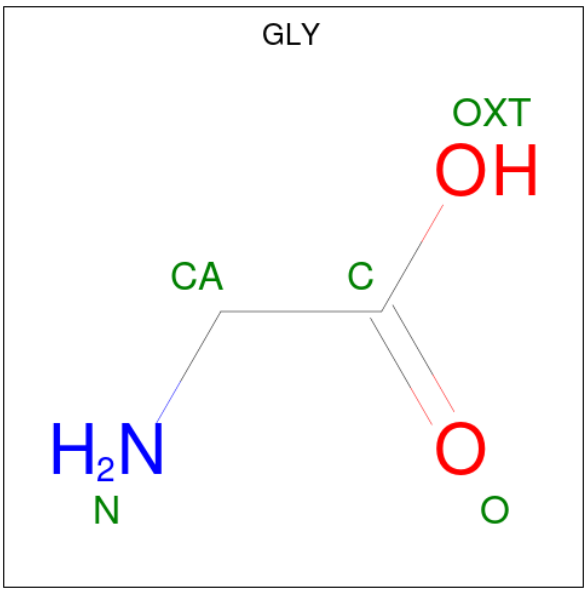
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

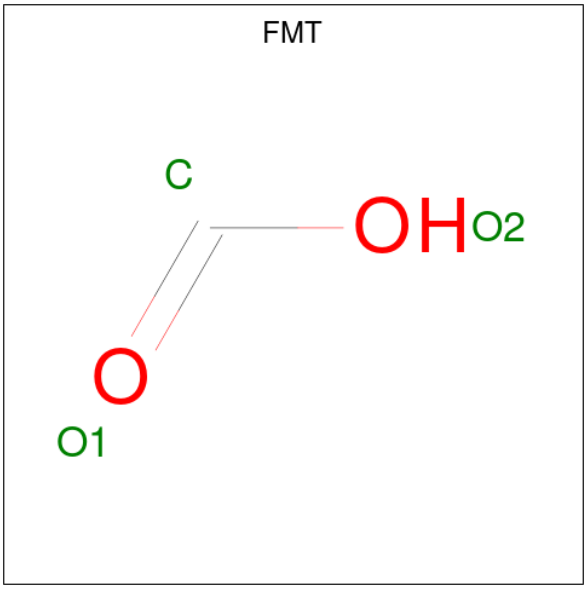
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 5 2 1 2	0	0

- Molecule 10 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 3 1 2	0	0
10	B	1	Total C O 3 1 2	0	0
10	B	1	Total C O 3 1 2	0	0
10	C	1	Total C O 3 1 2	0	0
10	C	1	Total C O 3 1 2	0	0
10	C	1	Total C O 3 1 2	0	0
10	C	1	Total C O 3 1 2	0	0
10	D	1	Total C O 3 1 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	340	Total O 340 340	0	0

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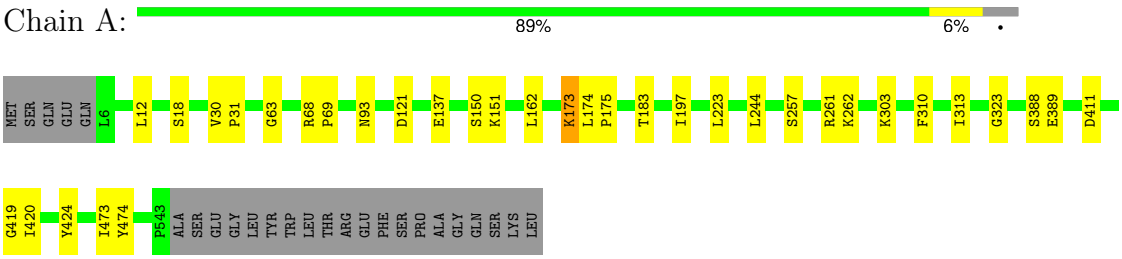
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	353	Total O 353 353	0	0
11	C	366	Total O 366 366	0	0
11	D	346	Total O 346 346	0	0

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. 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. 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.

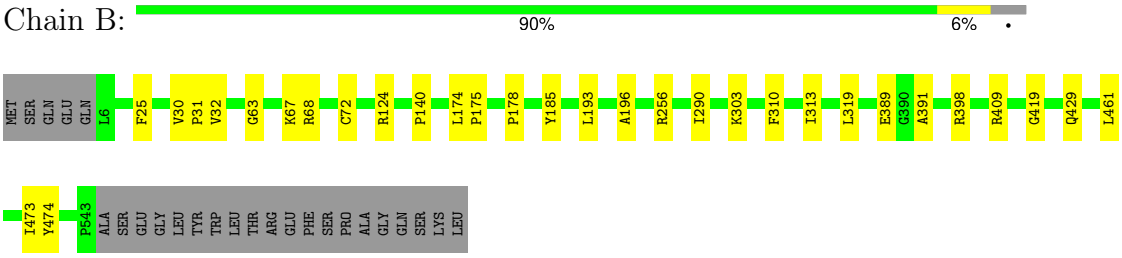
• Molecule 1: 2-hydroxyacyl-CoA lyase-like protein 1

Chain A:



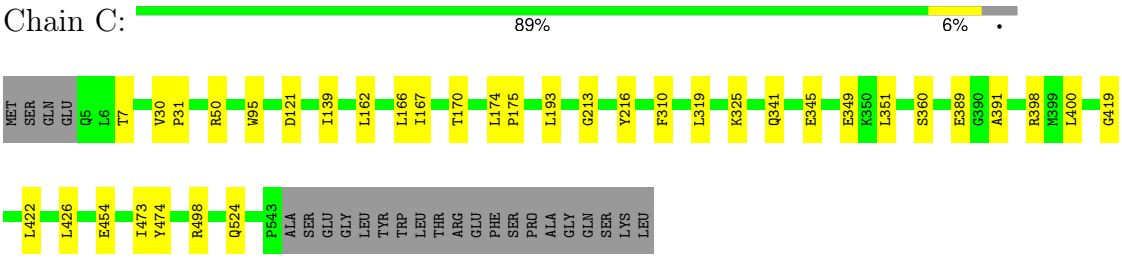
• Molecule 1: 2-hydroxyacyl-CoA lyase-like protein 1

Chain B:



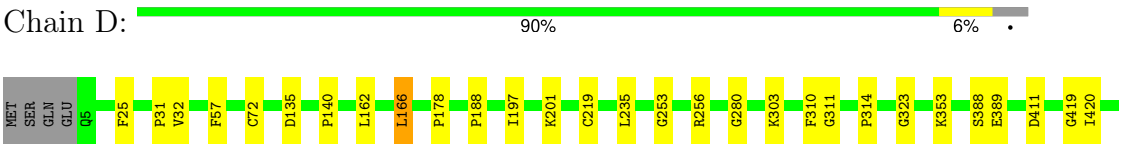
• Molecule 1: 2-hydroxyacyl-CoA lyase-like protein 1

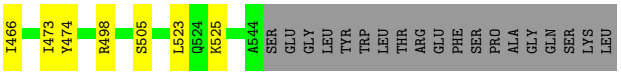
Chain C:



• Molecule 1: 2-hydroxyacyl-CoA lyase-like protein 1

Chain D:




I466
I473
Y474
R498
S505
L523
Q524
K525
A544
SER
GLU
GLY
LEU
TYR
TRP
LEU
THR
ARG
GLU
PHE
SER
PRO
ALA
GLY
GLN
SER
LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.74Å 179.29Å 96.83Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	44.82 – 1.85 44.82 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.9 (44.82-1.85) 94.0 (44.82-1.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.156 , 0.196 0.156 , 0.196	Depositor DCC
R_{free} test set	8861 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18554	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/4281	0.55	0/5802
1	B	0.34	0/4299	0.56	0/5827
1	C	0.35	0/4289	0.56	0/5814
1	D	0.35	0/4299	0.56	0/5827
All	All	0.34	0/17168	0.56	0/23270

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4197	0	4279	21	0
1	B	4215	0	4296	20	0
1	C	4205	0	4281	22	0
1	D	4215	0	4287	21	0
2	A	26	0	16	0	0
2	B	26	0	16	2	0
2	C	26	0	16	1	0
2	D	26	0	16	1	0
3	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	12	0	18	2	0
4	B	8	0	12	2	0
4	C	8	0	12	3	0
4	D	12	0	18	0	0
5	A	18	0	12	0	0
6	A	4	0	3	0	0
6	C	8	0	6	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	5	0	2	1	0
10	B	9	0	3	0	0
10	C	12	0	4	0	0
10	D	3	0	1	0	0
11	A	340	0	0	2	0
11	B	353	0	0	1	0
11	C	366	0	0	2	0
11	D	346	0	0	3	0
All	All	18554	0	17346	83	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 2.

The worst 5 of 83 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:C:30[B]:VAL:HB	1:C:31[B]:PRO:HD3	1.76	0.66
1:B:389:GLU:OE2	1:B:419:GLY:N	2.32	0.63
1:B:256:ARG:HD3	4:B:604:EDO:H21	1.83	0.61
1:D:389:GLU:OE2	1:D:419:GLY:N	2.29	0.58
1:A:303[A]:LYS:NZ	11:A:703:HOH:O	2.37	0.58

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	546/563 (97%)	535 (98%)	11 (2%)	0	100 100
1	B	547/563 (97%)	536 (98%)	11 (2%)	0	100 100
1	C	546/563 (97%)	529 (97%)	16 (3%)	1 (0%)	44 32
1	D	548/563 (97%)	540 (98%)	8 (2%)	0	100 100
All	All	2187/2252 (97%)	2140 (98%)	46 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	360	SER

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	A	462/474 (98%)	458 (99%)	4 (1%)	75 70
1	B	464/474 (98%)	462 (100%)	2 (0%)	89 88
1	C	463/474 (98%)	461 (100%)	2 (0%)	89 88
1	D	463/474 (98%)	459 (99%)	4 (1%)	75 70
All	All	1852/1896 (98%)	1840 (99%)	12 (1%)	81 81

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	325	LYS
1	D	162	LEU
1	D	353	LYS
1	D	166	LEU
1	A	310	PHE

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
6	ACT	C	610	-	3,3,3	1.53	1 (33%)	3,3,3	1.32	0
4	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.37	0
5	ALA	A	607	-	5,5,5	1.05	1 (20%)	6,6,6	1.60	2 (33%)
4	EDO	B	603	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	D	605	-	3,3,3	0.43	0	2,2,2	0.50	0
4	EDO	D	606	-	3,3,3	0.42	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TPP	D	601	7	23,27,27	0.54	0	30,40,40	0.71	0
4	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.37	0
2	TPP	C	601	7	23,27,27	0.49	0	30,40,40	0.70	0
10	FMT	B	608	-	2,2,2	0.68	0	1,1,1	0.24	0
3	ADP	A	602	-	24,29,29	1.05	2 (8%)	29,45,45	1.38	4 (13%)
10	FMT	B	606	-	2,2,2	0.72	0	1,1,1	0.26	0
10	FMT	C	605	-	2,2,2	0.68	0	1,1,1	0.18	0
4	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.37	0
2	TPP	A	601	7	23,27,27	0.98	1 (4%)	30,40,40	0.78	2 (6%)
4	EDO	C	604	-	3,3,3	0.45	0	2,2,2	0.41	0
6	ACT	A	608	-	3,3,3	1.49	1 (33%)	3,3,3	1.30	0
5	ALA	A	605	-	5,5,5	1.14	1 (20%)	6,6,6	1.58	1 (16%)
10	FMT	C	609	-	2,2,2	0.68	0	1,1,1	0.22	0
3	ADP	C	602	-	24,29,29	1.06	2 (8%)	29,45,45	1.35	3 (10%)
2	TPP	B	601	7	23,27,27	0.79	1 (4%)	30,40,40	0.69	1 (3%)
3	ADP	B	602	-	24,29,29	1.00	1 (4%)	29,45,45	1.47	5 (17%)
4	EDO	C	603	-	3,3,3	0.39	0	2,2,2	0.17	0
10	FMT	C	606	-	2,2,2	0.70	0	1,1,1	0.25	0
10	FMT	D	604	-	2,2,2	0.69	0	1,1,1	0.26	0
4	EDO	D	603	-	3,3,3	0.54	0	2,2,2	0.19	0
6	ACT	C	608	-	3,3,3	1.51	1 (33%)	3,3,3	1.33	0
5	ALA	A	606	-	5,5,5	0.98	0	6,6,6	1.47	2 (33%)
10	FMT	B	607	-	2,2,2	0.74	0	1,1,1	0.30	0
4	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.41	0
10	FMT	C	607	-	2,2,2	0.68	0	1,1,1	0.20	0
3	ADP	D	602	-	24,29,29	1.13	3 (12%)	29,45,45	1.41	3 (10%)
9	GLY	B	605	-	4,4,4	1.14	1 (25%)	3,4,4	1.66	1 (33%)

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	EDO	A	609	-	-	1/1/1/1	-
5	ALA	A	607	-	-	2/4/4/4	-
4	EDO	B	603	-	-	0/1/1/1	-
4	EDO	D	605	-	-	0/1/1/1	-
4	EDO	D	606	-	-	0/1/1/1	-
2	TPP	D	601	7	-	2/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	604	-	-	0/1/1/1	-
2	TPP	C	601	7	-	3/16/17/17	0/2/2/2
3	ADP	A	602	-	-	2/12/32/32	0/3/3/3
4	EDO	A	604	-	-	0/1/1/1	-
2	TPP	A	601	7	-	4/16/17/17	0/2/2/2
4	EDO	C	604	-	-	1/1/1/1	-
5	ALA	A	605	-	-	2/4/4/4	-
3	ADP	C	602	-	-	2/12/32/32	0/3/3/3
2	TPP	B	601	7	-	4/16/17/17	0/2/2/2
3	ADP	B	602	-	-	3/12/32/32	0/3/3/3
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	D	603	-	-	0/1/1/1	-
5	ALA	A	606	-	-	2/4/4/4	-
4	EDO	A	603	-	-	1/1/1/1	-
3	ADP	D	602	-	-	2/12/32/32	0/3/3/3
9	GLY	B	605	-	-	2/2/2/2	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	PA-O3A	-3.78	1.55	1.59
3	D	602	ADP	PA-O3A	3.32	1.63	1.59
3	C	602	ADP	PA-O3A	2.91	1.62	1.59
2	B	601	TPP	PA-O3A	-2.91	1.56	1.59
3	B	602	ADP	C2-N3	2.72	1.36	1.32

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	602	ADP	N3-C2-N1	-4.21	122.96	128.67
3	B	602	ADP	N3-C2-N1	-4.00	123.24	128.67
3	A	602	ADP	N3-C2-N1	-3.95	123.31	128.67
3	C	602	ADP	N3-C2-N1	-3.81	123.50	128.67
5	A	605	ALA	OXT-C-O	-3.19	116.85	124.08

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TPP	C4-C5-C6-C7
2	B	601	TPP	C4-C5-C6-C7
2	C	601	TPP	C4-C5-C6-C7
2	D	601	TPP	C4-C5-C6-C7
3	B	602	ADP	C5'-O5'-PA-O1A

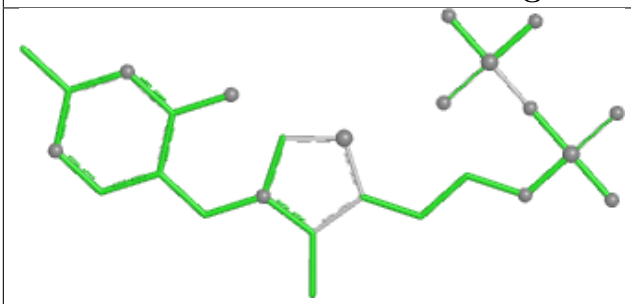
There are no ring outliers.

11 monomers are involved in 14 short contacts:

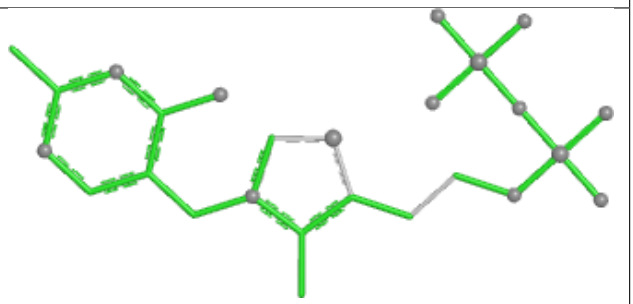
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	610	ACT	1	0
4	A	609	EDO	1	0
2	D	601	TPP	1	0
4	B	604	EDO	2	0
2	C	601	TPP	1	0
3	A	602	ADP	1	0
2	B	601	TPP	2	0
3	B	602	ADP	1	0
4	C	603	EDO	3	0
4	A	603	EDO	1	0
9	B	605	GLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

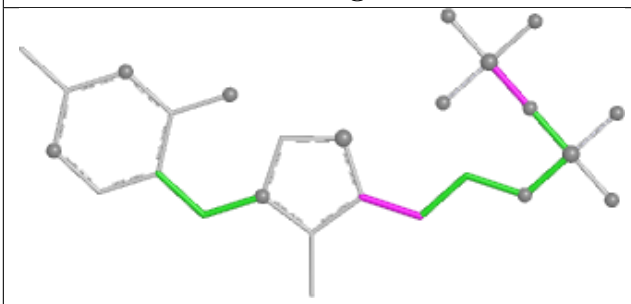
Ligand TPP D 601



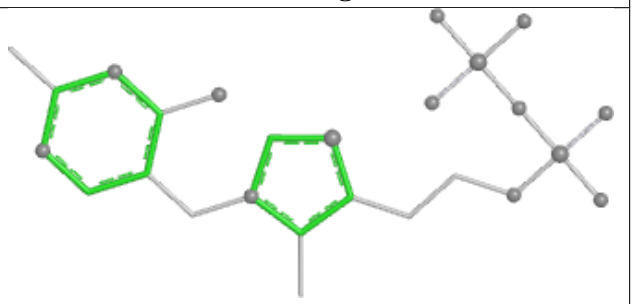
Bond lengths



Bond angles

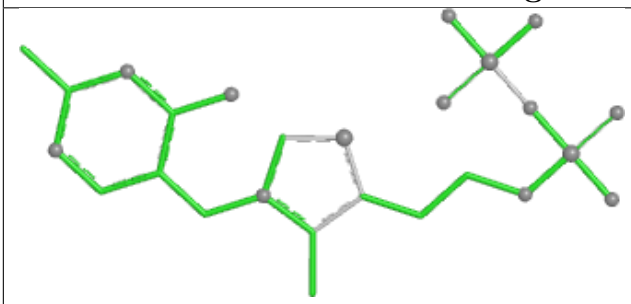


Torsions

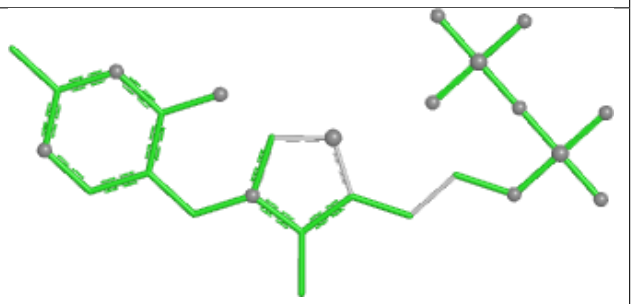


Rings

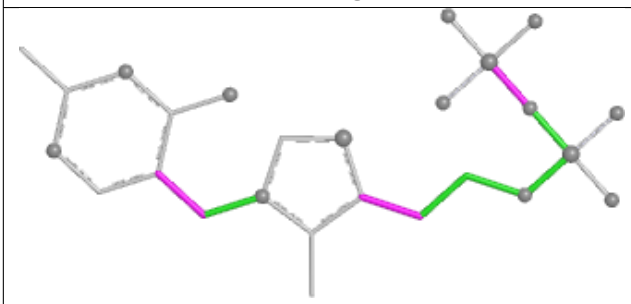
Ligand TPP C 601



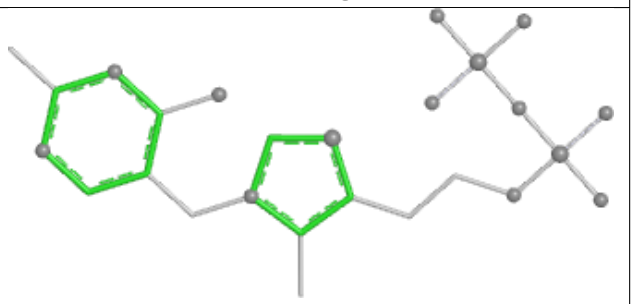
Bond lengths



Bond angles

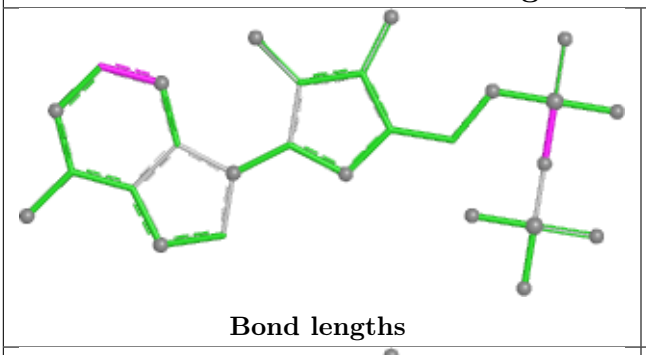


Torsions

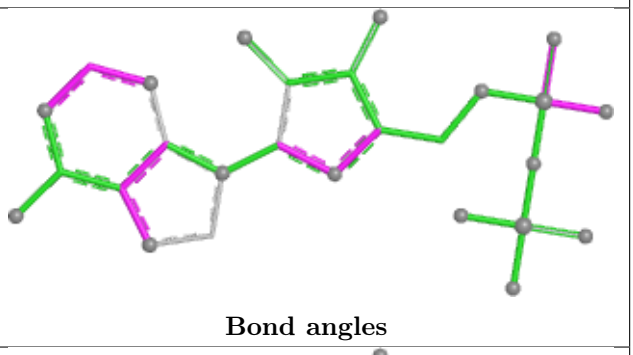


Rings

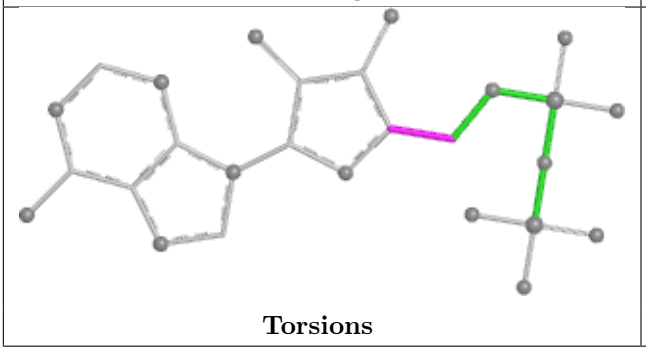
Ligand ADP A 602



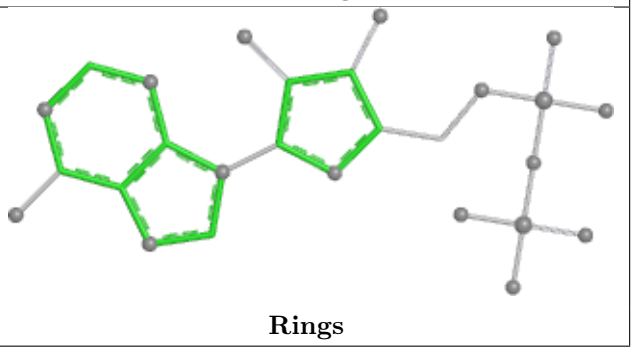
Bond lengths



Bond angles

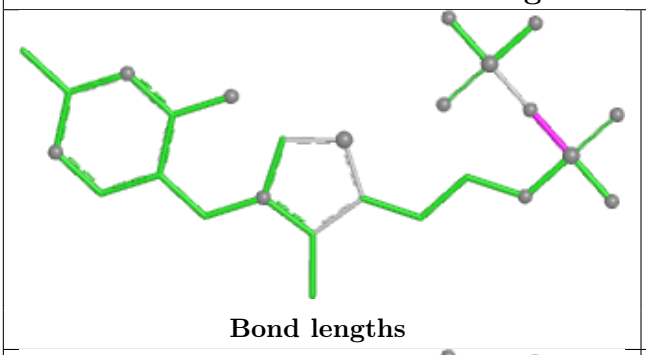


Torsions

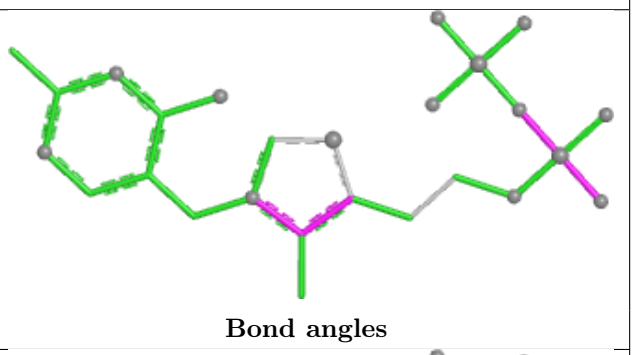


Rings

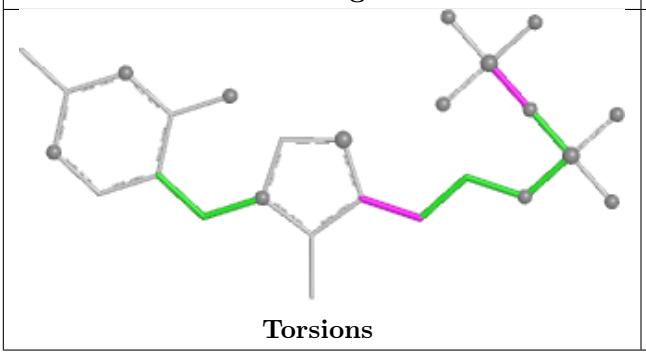
Ligand TPP A 601



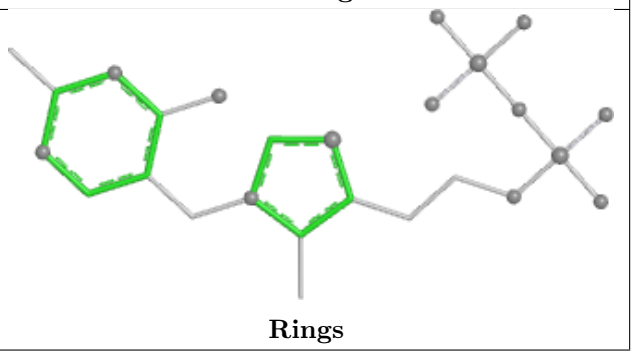
Bond lengths



Bond angles

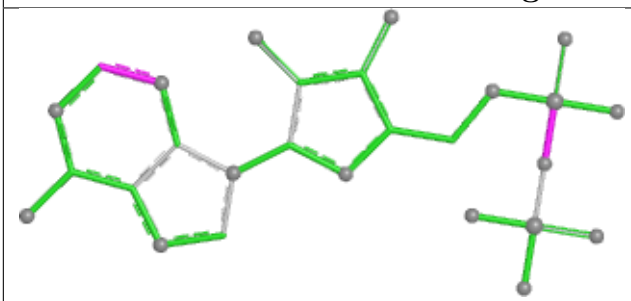


Torsions

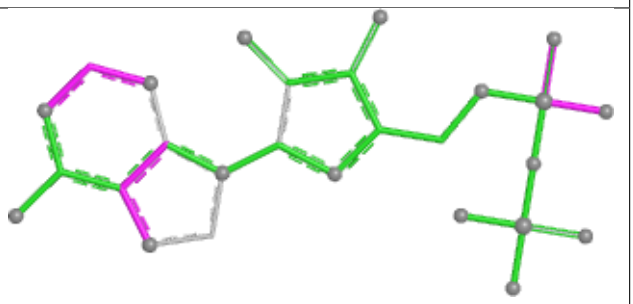


Rings

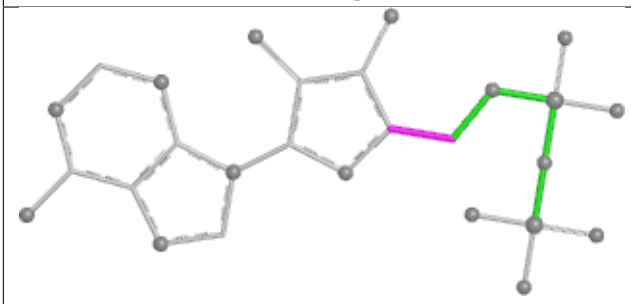
Ligand ADP C 602



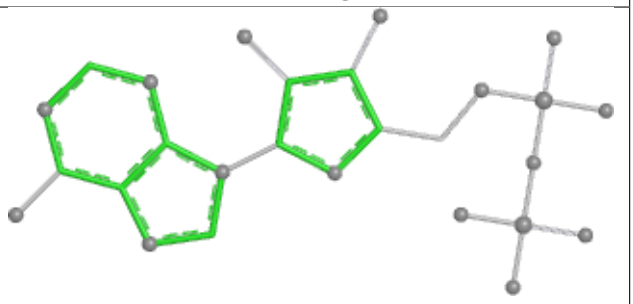
Bond lengths



Bond angles

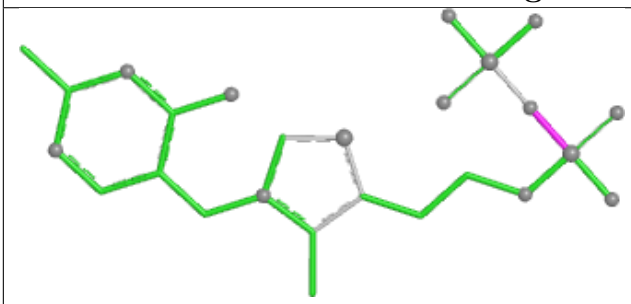


Torsions

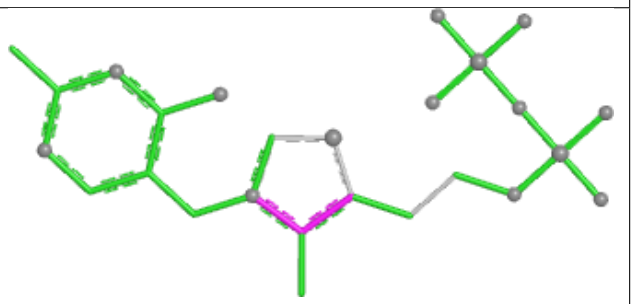


Rings

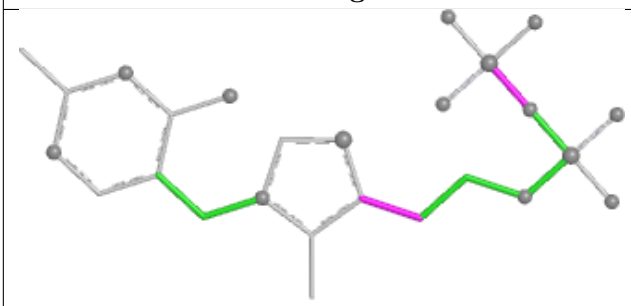
Ligand TPP B 601



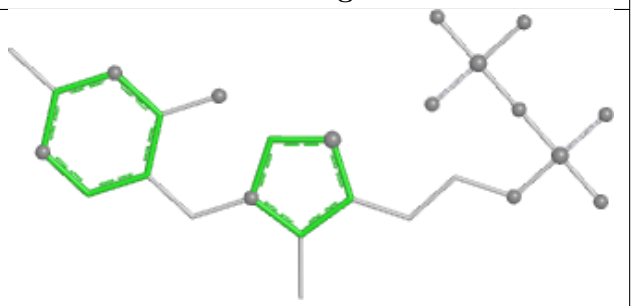
Bond lengths



Bond angles

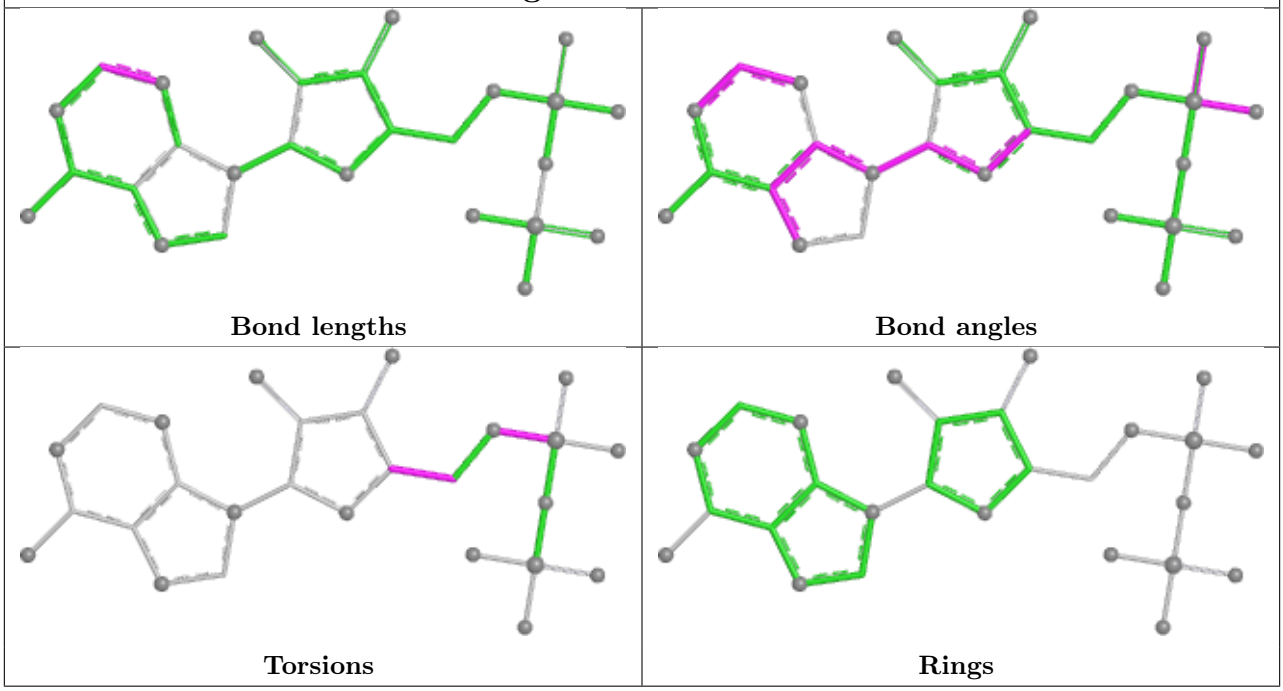


Torsions

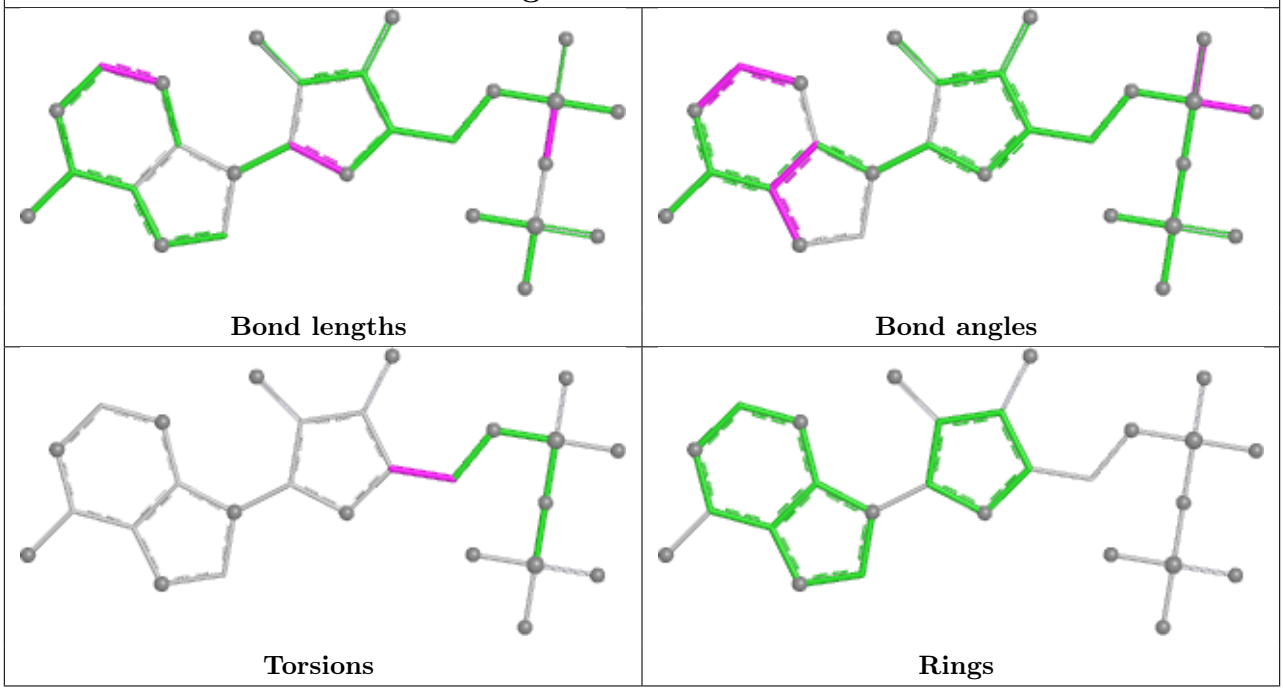


Rings

Ligand ADP B 602



Ligand ADP D 602



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

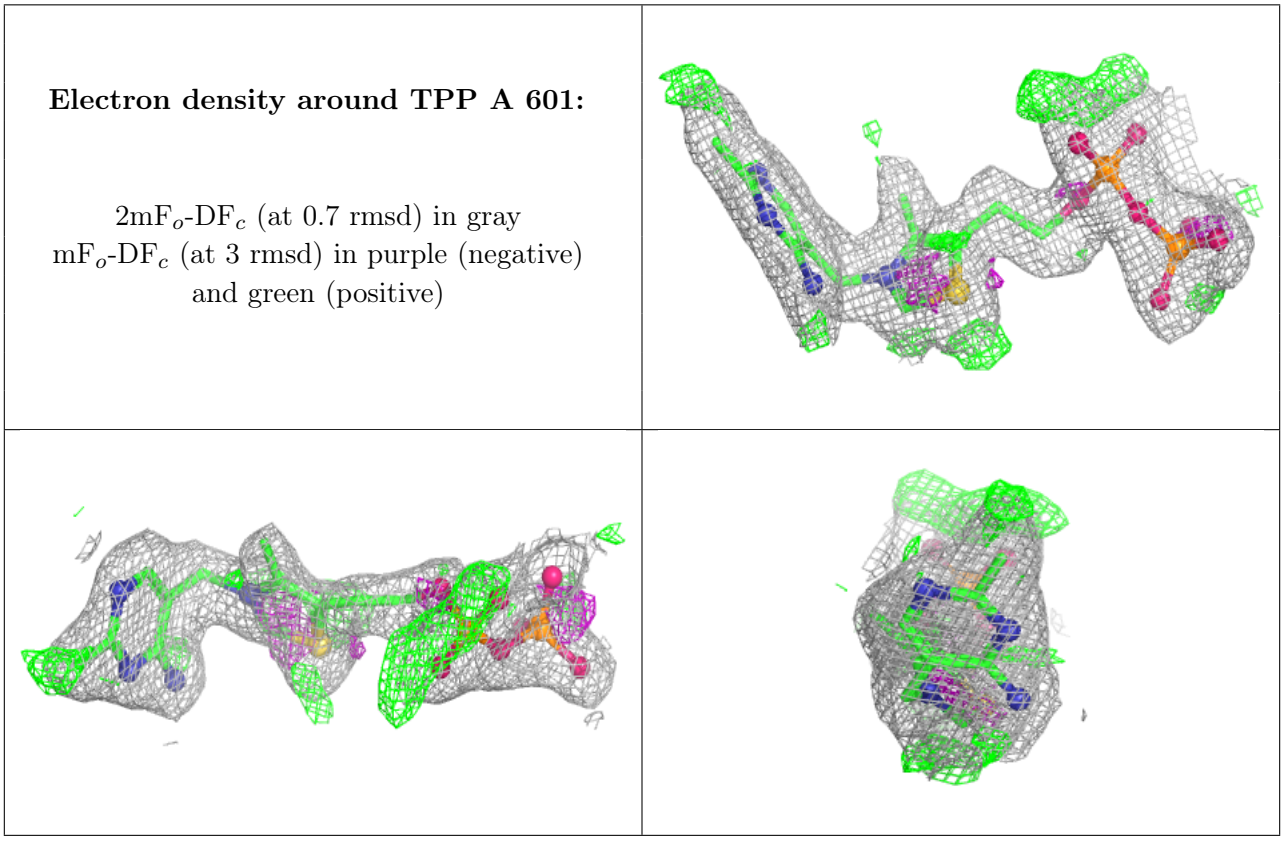
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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

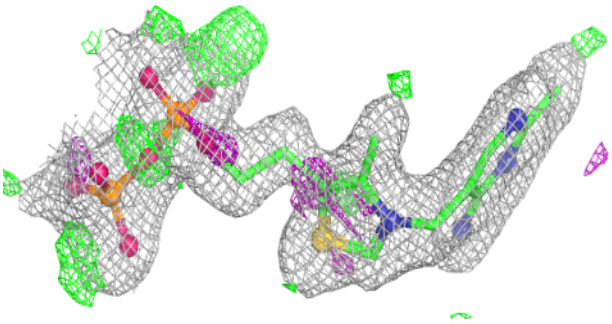
Electron density around TPP A 601:

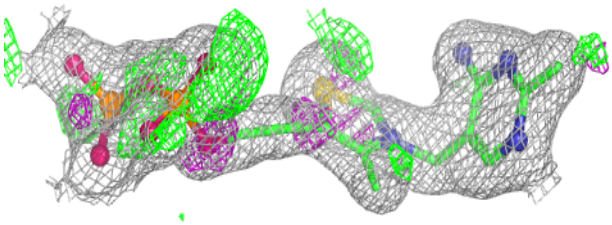
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

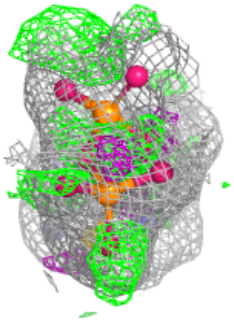


Electron density around TPP B 601:

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

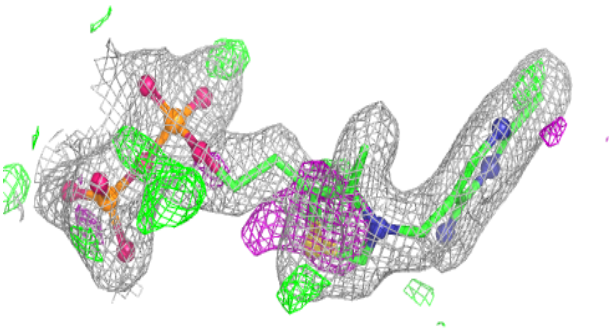


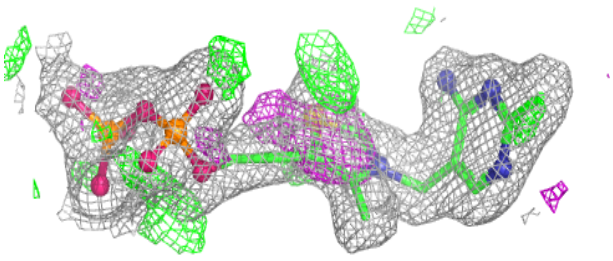


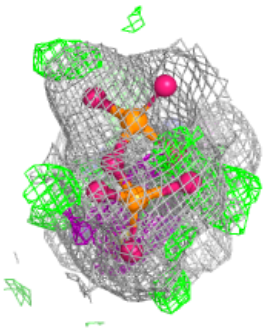


Electron density around TPP C 601:

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

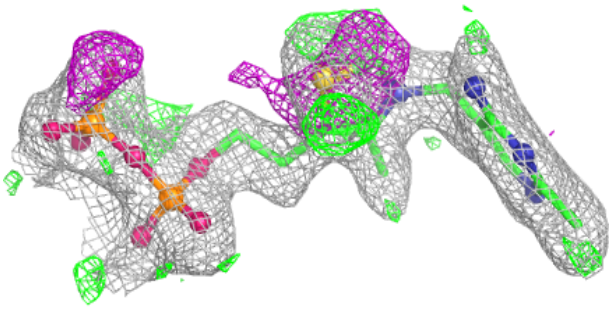


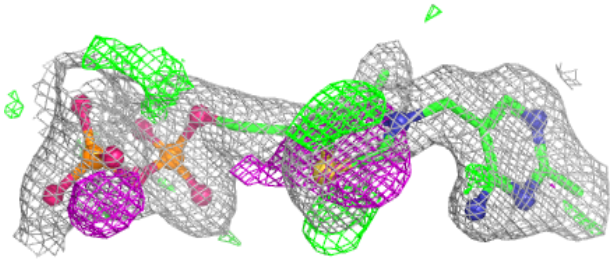


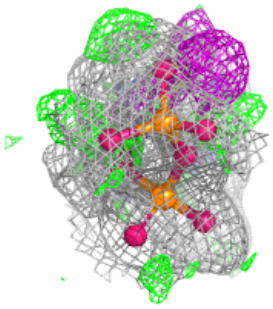


Electron density around TPP D 601:

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







Electron density around ADP A 602:

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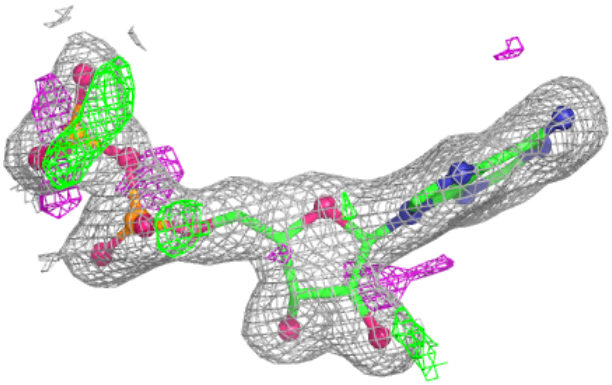
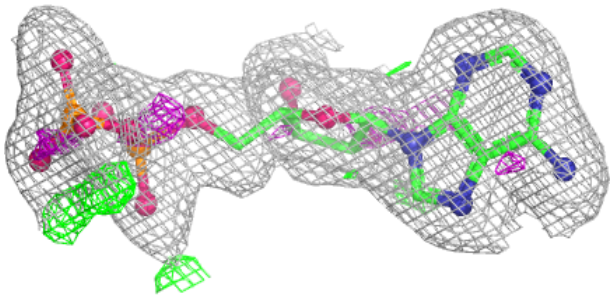
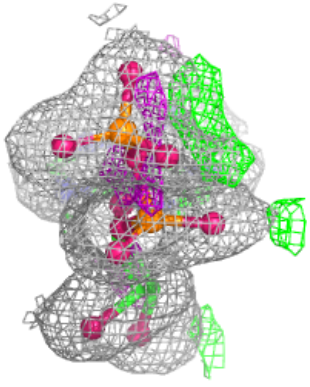
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

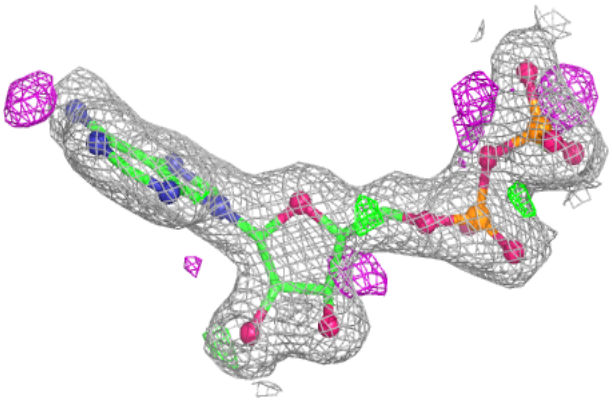


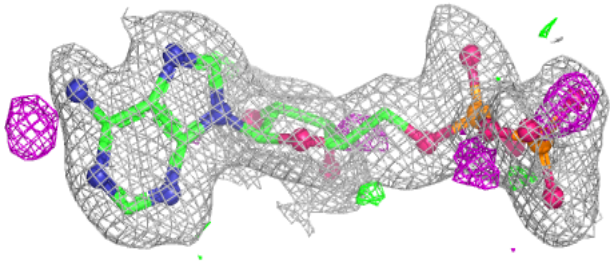


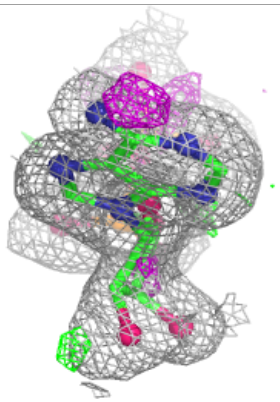


Electron density around ADP B 602:

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

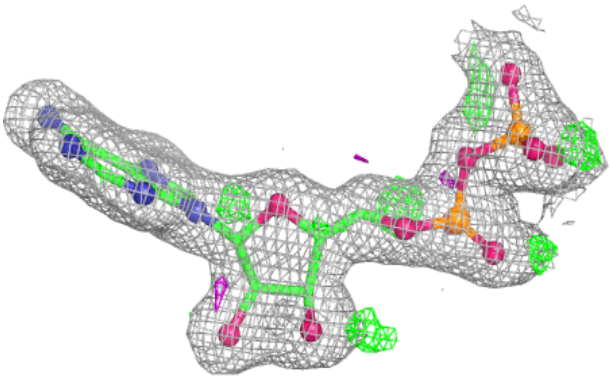


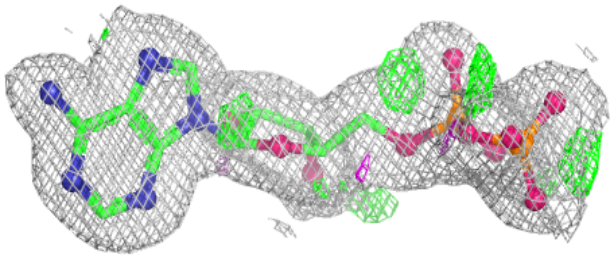


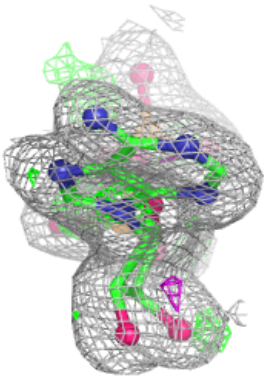


Electron density around ADP C 602:

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

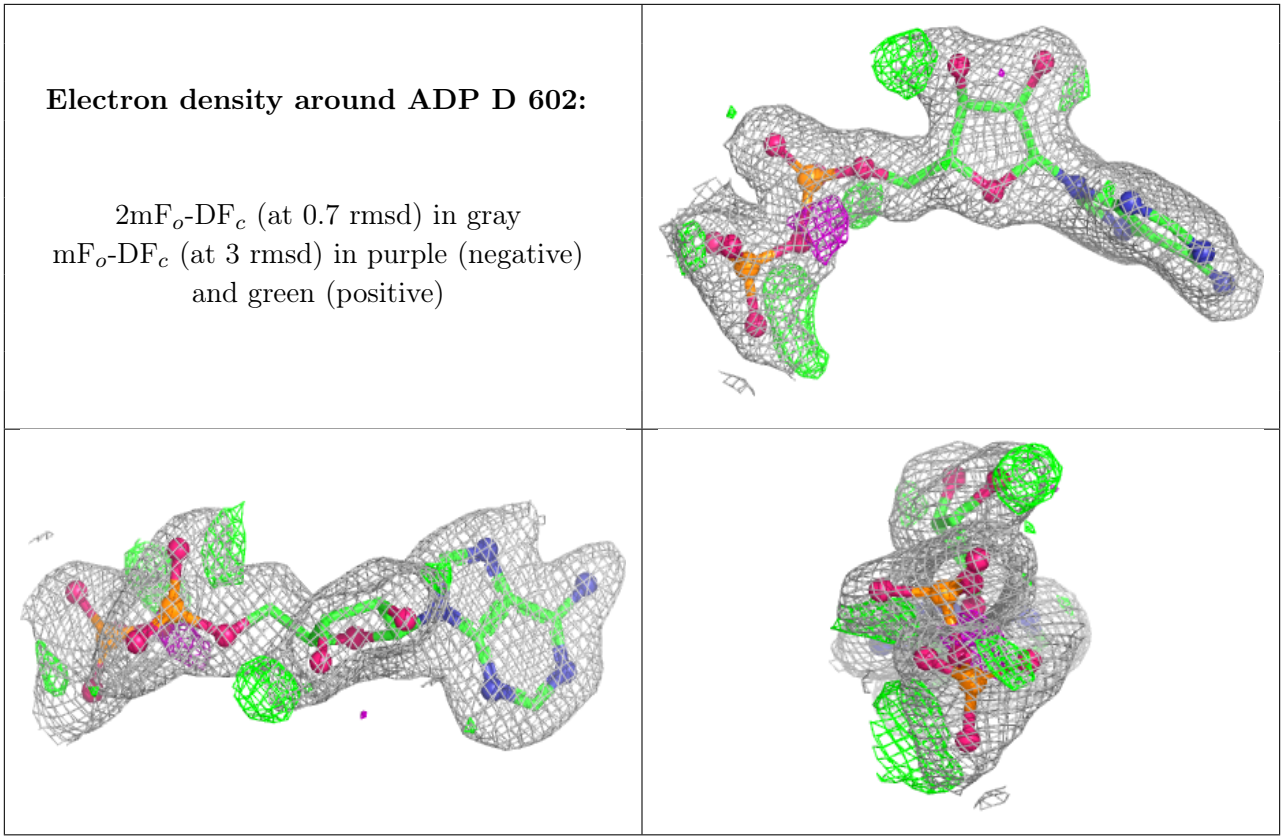






Electron density around ADP D 602:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.