wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 09:58 AM EDT

PDB ID	:	5W3Y
Title	:	Crystal structure of PopP2 C321A in complex with IP6 and AcCoA
Authors	:	Zhang, Z.M.; Gao, L.; Song, J.
Deposited on	:	2017-06-08
Resolution	:	2.20 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:

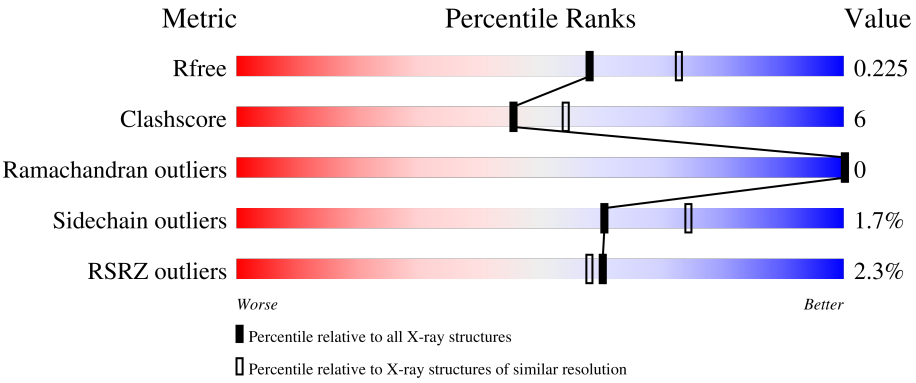
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	352	83% 12% • 5%
1	B	352	6% 78% 14% • 7%
1	C	352	85% 10% 5%
1	D	352	82% 13% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10739 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 PopP2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2538	1570	475	481	12			
1	B	327	Total	C	N	O	S	0	0	0
			2401	1486	451	454	10			
1	C	335	Total	C	N	O	S	0	0	0
			2536	1567	474	483	12			
1	D	334	Total	C	N	O	S	0	0	0
			2536	1569	472	483	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	-	expression tag	UNP A0A0S4VB05
A	138	GLU	-	expression tag	UNP A0A0S4VB05
A	139	PHE	-	expression tag	UNP A0A0S4VB05
A	140	GLU	-	expression tag	UNP A0A0S4VB05
A	141	LEU	-	expression tag	UNP A0A0S4VB05
A	142	GLY	-	expression tag	UNP A0A0S4VB05
A	143	ALA	-	expression tag	UNP A0A0S4VB05
A	144	PRO	-	expression tag	UNP A0A0S4VB05
A	145	ALA	-	expression tag	UNP A0A0S4VB05
A	146	GLY	-	expression tag	UNP A0A0S4VB05
A	147	ARG	-	expression tag	UNP A0A0S4VB05
A	148	GLN	-	expression tag	UNP A0A0S4VB05
A	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
B	137	SER	-	expression tag	UNP A0A0S4VB05
B	138	GLU	-	expression tag	UNP A0A0S4VB05
B	139	PHE	-	expression tag	UNP A0A0S4VB05
B	140	GLU	-	expression tag	UNP A0A0S4VB05
B	141	LEU	-	expression tag	UNP A0A0S4VB05
B	142	GLY	-	expression tag	UNP A0A0S4VB05
B	143	ALA	-	expression tag	UNP A0A0S4VB05
B	144	PRO	-	expression tag	UNP A0A0S4VB05

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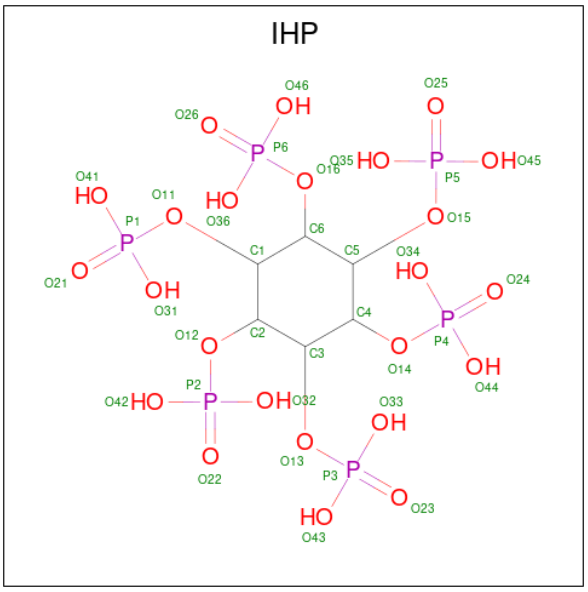
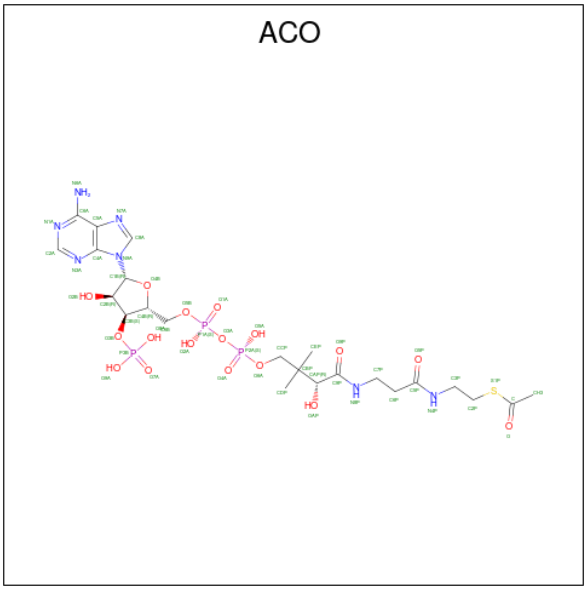
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	-	expression tag	UNP A0A0S4VB05
B	146	GLY	-	expression tag	UNP A0A0S4VB05
B	147	ARG	-	expression tag	UNP A0A0S4VB05
B	148	GLN	-	expression tag	UNP A0A0S4VB05
B	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
C	137	SER	-	expression tag	UNP A0A0S4VB05
C	138	GLU	-	expression tag	UNP A0A0S4VB05
C	139	PHE	-	expression tag	UNP A0A0S4VB05
C	140	GLU	-	expression tag	UNP A0A0S4VB05
C	141	LEU	-	expression tag	UNP A0A0S4VB05
C	142	GLY	-	expression tag	UNP A0A0S4VB05
C	143	ALA	-	expression tag	UNP A0A0S4VB05
C	144	PRO	-	expression tag	UNP A0A0S4VB05
C	145	ALA	-	expression tag	UNP A0A0S4VB05
C	146	GLY	-	expression tag	UNP A0A0S4VB05
C	147	ARG	-	expression tag	UNP A0A0S4VB05
C	148	GLN	-	expression tag	UNP A0A0S4VB05
C	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05
D	137	SER	-	expression tag	UNP A0A0S4VB05
D	138	GLU	-	expression tag	UNP A0A0S4VB05
D	139	PHE	-	expression tag	UNP A0A0S4VB05
D	140	GLU	-	expression tag	UNP A0A0S4VB05
D	141	LEU	-	expression tag	UNP A0A0S4VB05
D	142	GLY	-	expression tag	UNP A0A0S4VB05
D	143	ALA	-	expression tag	UNP A0A0S4VB05
D	144	PRO	-	expression tag	UNP A0A0S4VB05
D	145	ALA	-	expression tag	UNP A0A0S4VB05
D	146	GLY	-	expression tag	UNP A0A0S4VB05
D	147	ARG	-	expression tag	UNP A0A0S4VB05
D	148	GLN	-	expression tag	UNP A0A0S4VB05
D	321	ALA	CYS	engineered mutation	UNP A0A0S4VB05

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 36 6 24 6	0	0
2	B	1	Total C O P 36 6 24 6	0	0
2	C	1	Total C O P 36 6 24 6	0	0
2	D	1	Total C O P 36 6 24 6	0	0

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

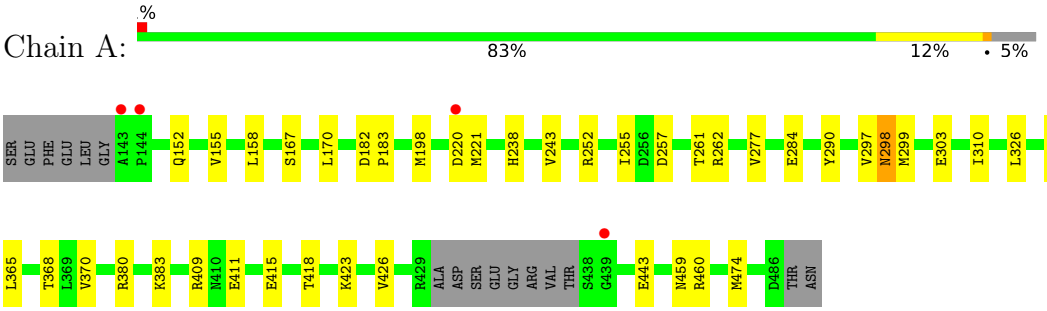
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	92	Total	O	0	0
			92	92		
4	C	119	Total	O	0	0
			119	119		
4	D	143	Total	O	0	0
			143	143		

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.

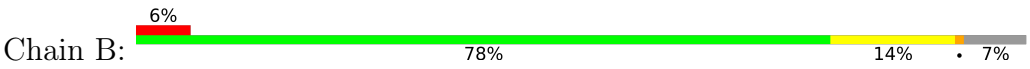
• Molecule 1: PopP2 protein

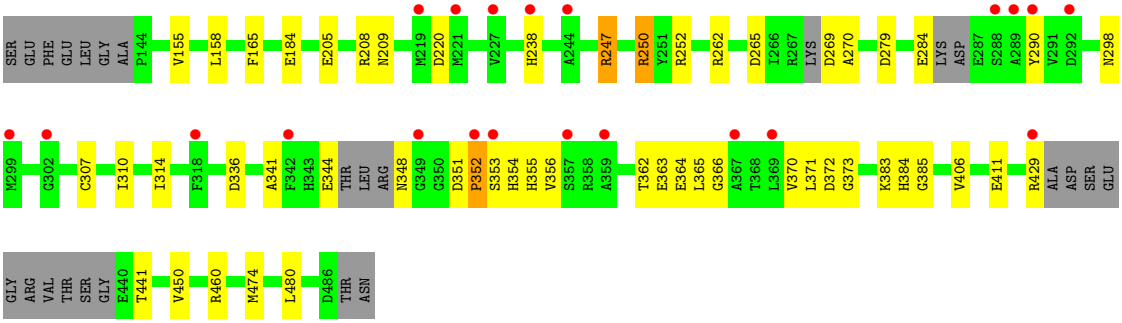
Chain A:



• Molecule 1: PopP2 protein

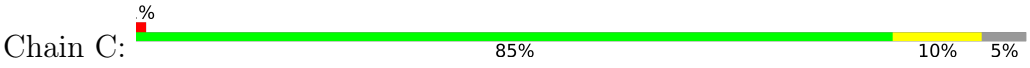
Chain B:

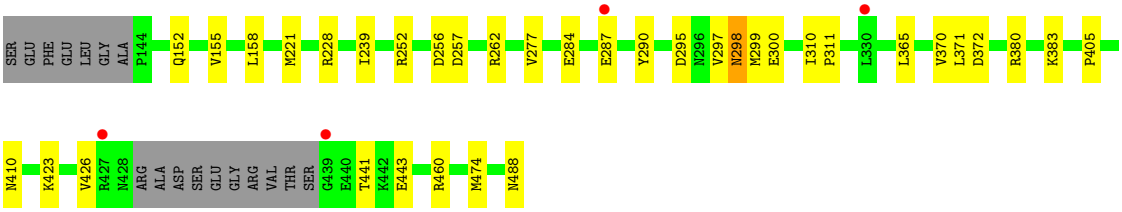




• Molecule 1: PopP2 protein

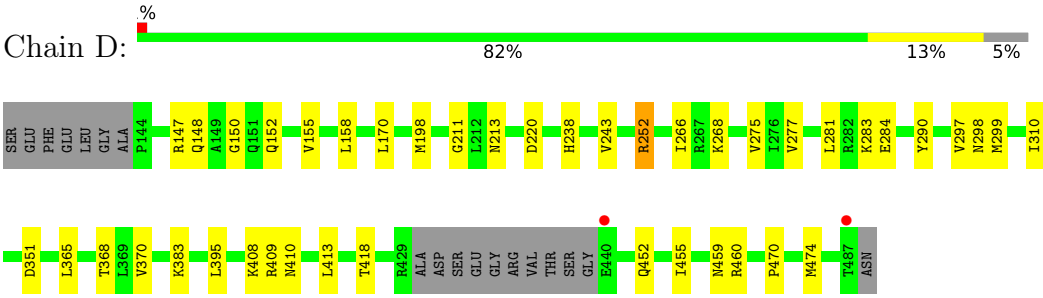
Chain C:





• Molecule 1: PopP2 protein

Chain D:


%
82%
13%
5%
SER GLU PHE GLU LEU GLY ALA P144 R147 Q148 A149 G150 Q151 Q152 V155 L158 L170 M198 G211 L212 N213 D220 H238 V243 R252 I266 R267 K268 V275 I276 V277 L281 R282 K283 E284 Y290 V297 N298 M299 I310 R322 L326
D351 L365 T368 L369 V370 K383 L395 K408 R409 N410 L413 T418 R429 ALA ASP SER GLU GLY ARG VAL THR SER GLY E440 Q452 I455 N459 R460 P470 M474 T487 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.39Å 79.88Å 77.75Å 112.33° 111.65° 103.39°	Depositor
Resolution (Å)	39.09 – 2.20 39.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.09-2.20) 97.8 (39.08-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.225 0.185 , 0.225	Depositor DCC
R_{free} test set	1900 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.186 for -l,h+k+l,-k 0.186 for h+k+l,-l,-h 0.016 for l,-h-k-l,h 0.012 for -h-k-l,l,k 0.126 for k,h,-h-k-l 0.013 for -k,-h,-l 0.010 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10739	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: IHP, ACO

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	0.33	0/2579	0.53	0/3493
1	B	0.32	0/2436	0.54	0/3301
1	C	0.34	0/2576	0.52	0/3487
1	D	0.35	0/2577	0.55	0/3488
All	All	0.33	0/10168	0.53	0/13769

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	352	PRO	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	A	2538	0	2492	30	0
1	B	2401	0	2310	40	0
1	C	2536	0	2502	26	0
1	D	2536	0	2495	33	0
2	A	36	0	6	3	0
2	B	36	0	6	3	0
2	C	36	0	6	2	0
2	D	36	0	6	4	0
3	A	31	0	11	0	0
3	B	31	0	11	1	0
3	C	31	0	11	0	0
3	D	31	0	11	1	0
4	A	106	0	0	7	0
4	B	92	0	0	5	1
4	C	119	0	0	3	1
4	D	143	0	0	8	0
All	All	10739	0	9867	129	1

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 6.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:O	4:A:601:HOH:O	1.93	0.86
1:C:256:ASP:OD2	4:C:601:HOH:O	1.92	0.86
1:D:252:ARG:NH2	4:D:602:HOH:O	2.09	0.85
1:D:452:GLN:NE2	4:D:603:HOH:O	2.13	0.81
1:B:269:ASP:OD1	1:B:270:ALA:N	2.15	0.77

All (1) 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)
4:B:624:HOH:O	4:C:699:HOH:O[1_454]	2.13	0.07

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	332/352 (94%)	325 (98%)	7 (2%)	0	100	100
1	B	317/352 (90%)	310 (98%)	7 (2%)	0	100	100
1	C	331/352 (94%)	323 (98%)	8 (2%)	0	100	100
1	D	330/352 (94%)	324 (98%)	6 (2%)	0	100	100
All	All	1310/1408 (93%)	1282 (98%)	28 (2%)	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	A	262/290 (90%)	257 (98%)	5 (2%)	57	71
1	B	238/290 (82%)	232 (98%)	6 (2%)	47	60
1	C	265/290 (91%)	261 (98%)	4 (2%)	65	78
1	D	264/290 (91%)	262 (99%)	2 (1%)	81	90
All	All	1029/1160 (89%)	1012 (98%)	17 (2%)	60	74

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	441	THR
1	D	298	ASN
1	B	252	ARG

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Mol	Chain	Res	Type
1	B	298	ASN
1	B	307	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	HIS

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)

8 ligands 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	$\#\|Z\| > 2$
3	ACO	D	502	-	28,33,53	2.99	4 (14%)	35,52,79	1.96	8 (22%)
3	ACO	A	502	-	28,33,53	3.10	5 (17%)	35,52,79	1.88	7 (20%)
2	IHP	A	501	-	36,36,36	2.59	14 (38%)	54,60,60	1.80	8 (14%)
2	IHP	C	501	-	36,36,36	2.59	14 (38%)	54,60,60	1.42	5 (9%)
2	IHP	D	501	-	36,36,36	2.53	14 (38%)	54,60,60	1.46	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACO	C	502	-	28,33,53	3.35	5 (17%)	35,52,79	1.96	8 (22%)
3	ACO	B	502	-	28,33,53	3.13	5 (17%)	35,52,79	2.00	11 (31%)
2	IHP	B	501	-	36,36,36	2.77	16 (44%)	54,60,60	1.70	10 (18%)

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
3	ACO	D	502	-	-	4/17/37/67	0/3/3/3
3	ACO	A	502	-	-	6/17/37/67	0/3/3/3
2	IHP	A	501	-	-	4/30/54/54	0/1/1/1
2	IHP	C	501	-	-	3/30/54/54	0/1/1/1
2	IHP	D	501	-	-	3/30/54/54	0/1/1/1
3	ACO	C	502	-	-	4/17/37/67	0/3/3/3
3	ACO	B	502	-	-	7/17/37/67	0/3/3/3
2	IHP	B	501	-	-	5/30/54/54	0/1/1/1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	ACO	P3B-O3B	15.57	1.88	1.59
3	B	502	ACO	P3B-O3B	14.33	1.86	1.59
3	A	502	ACO	P3B-O3B	14.16	1.86	1.59
3	D	502	ACO	P3B-O3B	13.46	1.84	1.59
2	A	501	IHP	P5-O15	8.15	1.74	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	ACO	P1A-O3A-P2A	-7.49	107.13	132.83
3	B	502	ACO	P1A-O3A-P2A	-7.19	108.15	132.83
3	C	502	ACO	P1A-O3A-P2A	-7.14	108.32	132.83
3	A	502	ACO	P1A-O3A-P2A	-6.39	110.89	132.83
2	C	501	IHP	C5-C6-C1	5.45	122.34	110.41

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	IHP	C4-O14-P4-O34
3	A	502	ACO	C5B-O5B-P1A-O1A
3	A	502	ACO	C5B-O5B-P1A-O2A
3	B	502	ACO	C3B-O3B-P3B-O9A
3	B	502	ACO	C3B-C4B-C5B-O5B

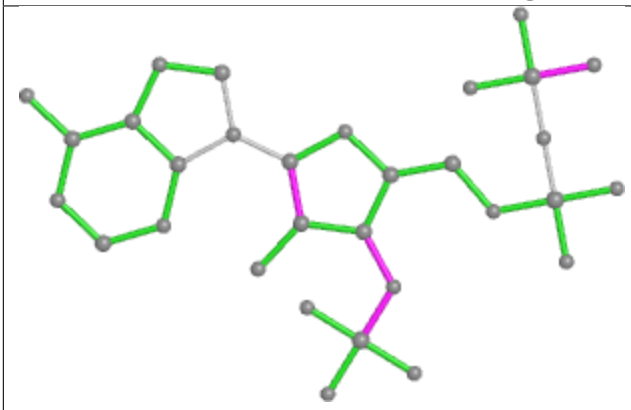
There are no ring outliers.

6 monomers are involved in 14 short contacts:

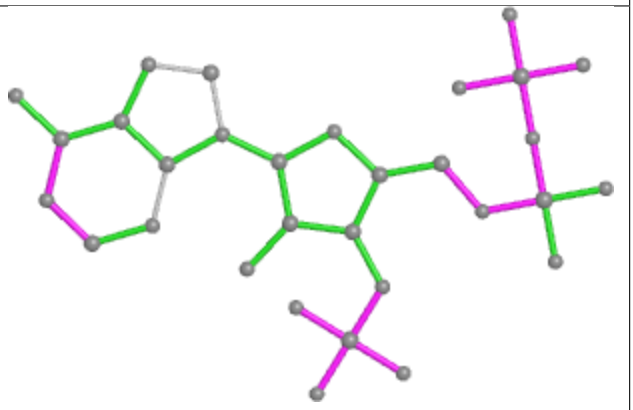
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	ACO	1	0
2	A	501	IHP	3	0
2	C	501	IHP	2	0
2	D	501	IHP	4	0
3	B	502	ACO	1	0
2	B	501	IHP	3	0

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.

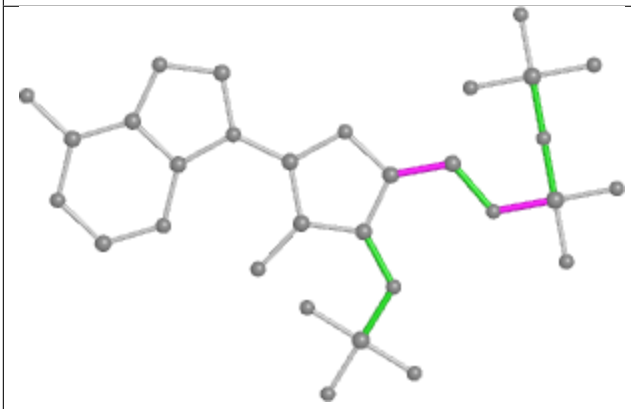
Ligand ACO D 502



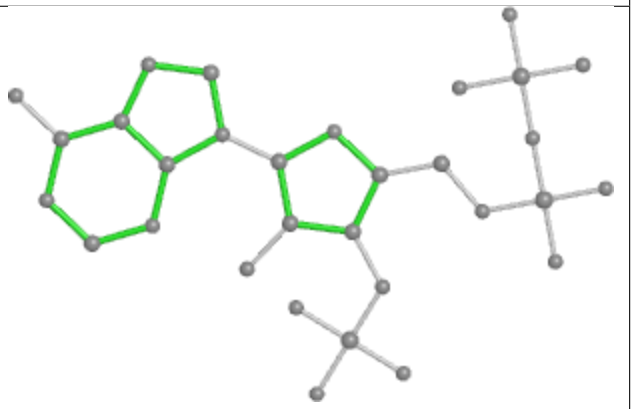
Bond lengths



Bond angles

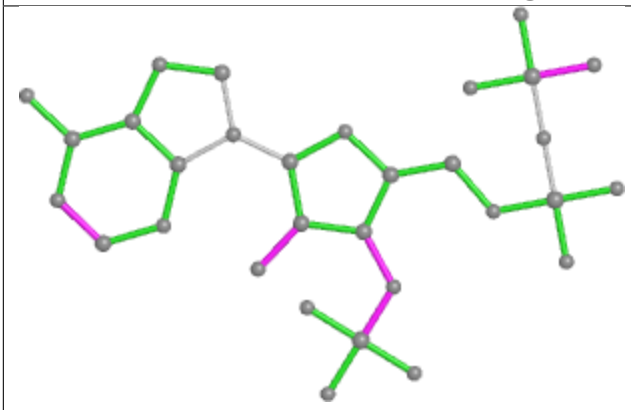


Torsions

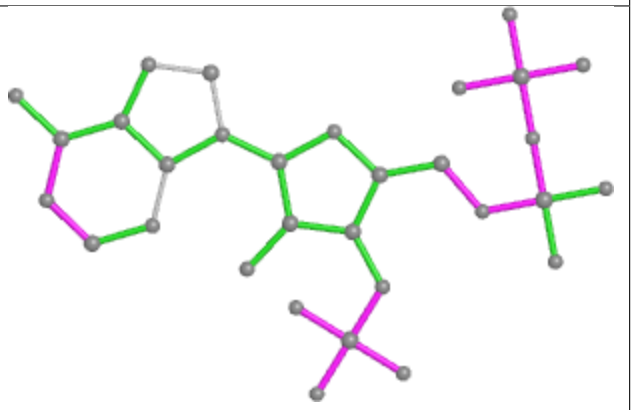


Rings

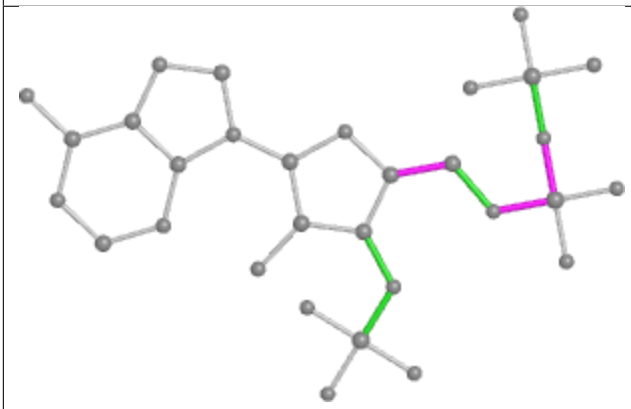
Ligand ACO A 502



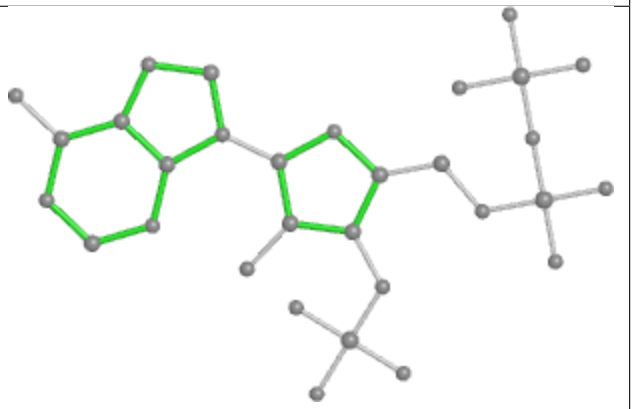
Bond lengths



Bond angles

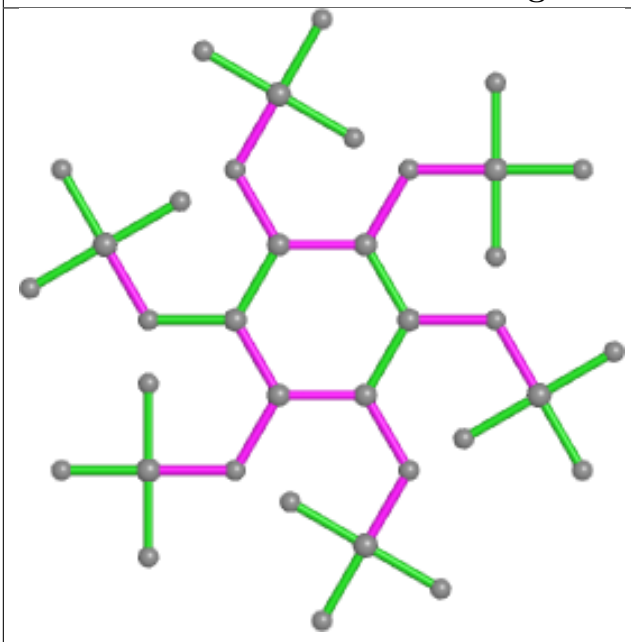


Torsions

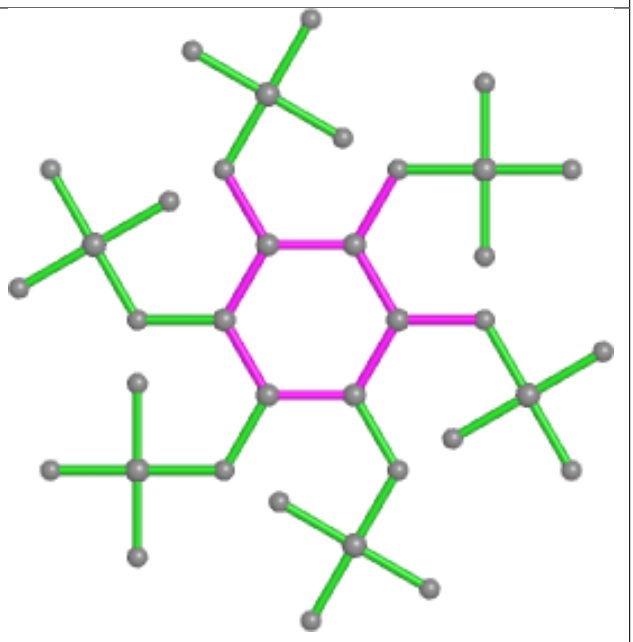


Rings

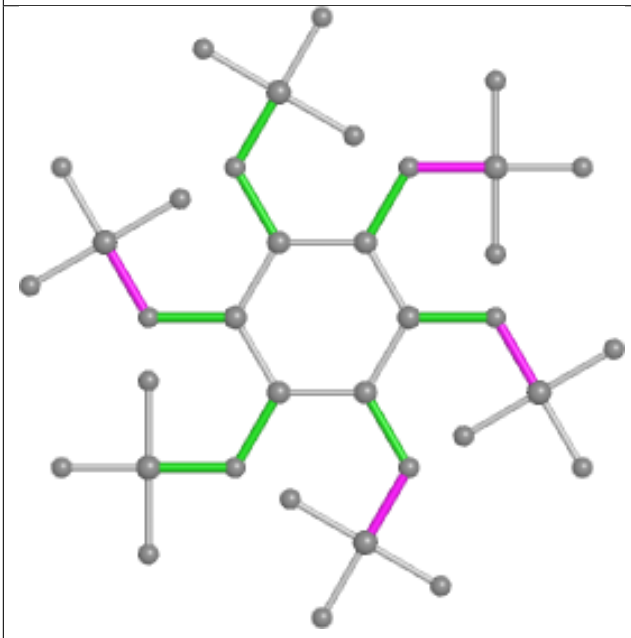
Ligand IHP A 501



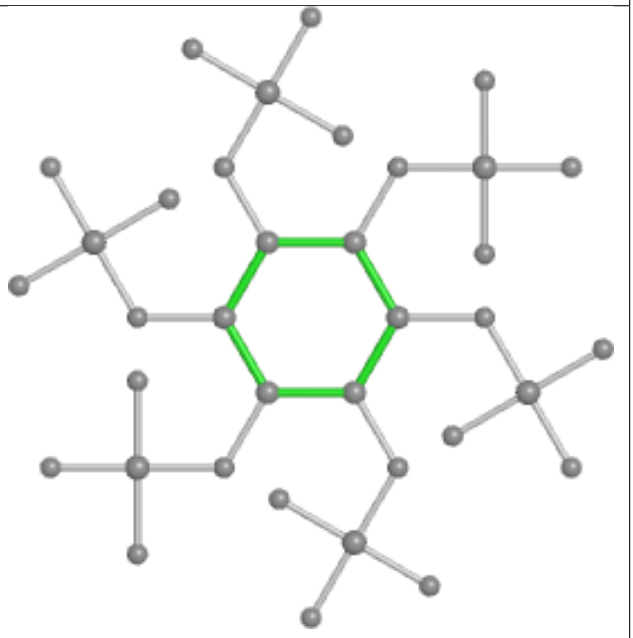
Bond lengths



Bond angles

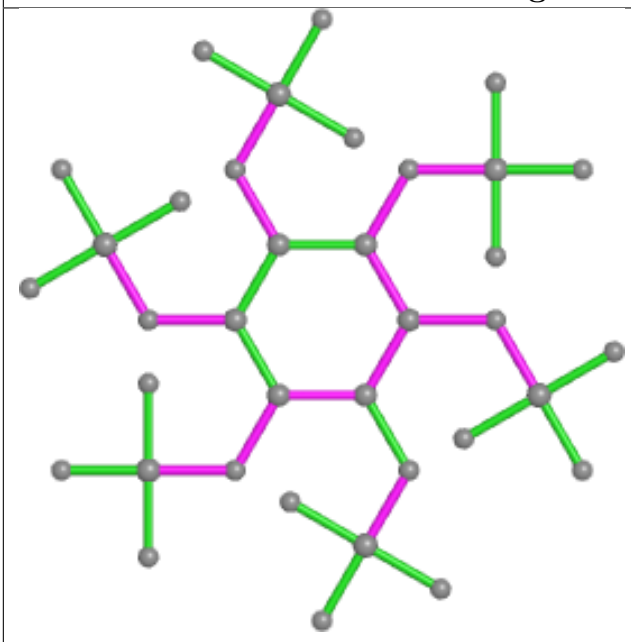


Torsions

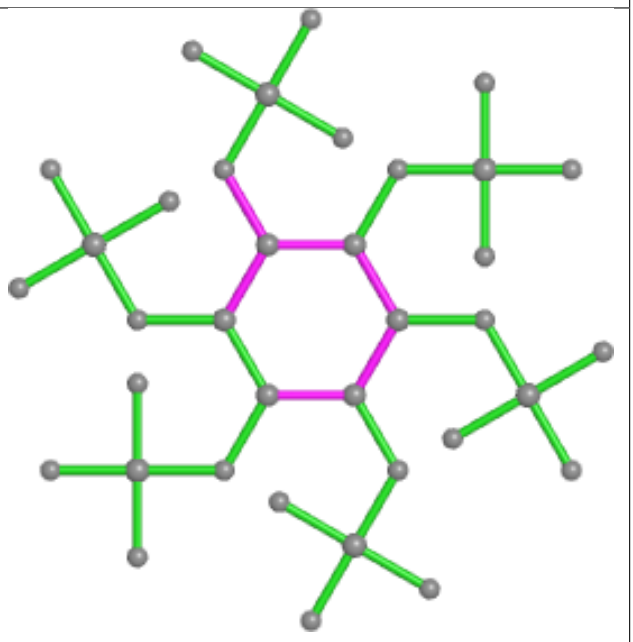


Rings

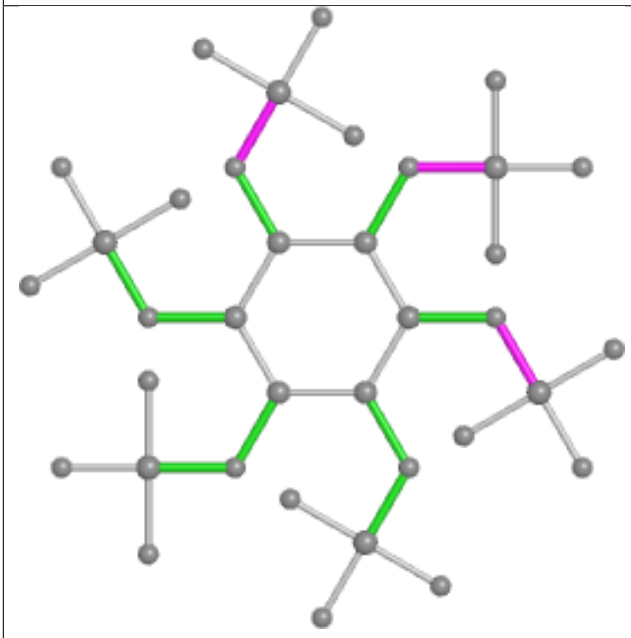
Ligand IHP C 501



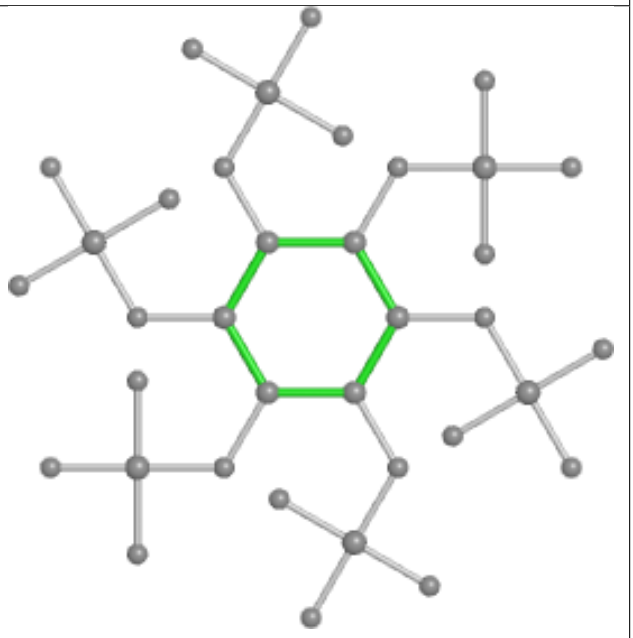
Bond lengths



Bond angles

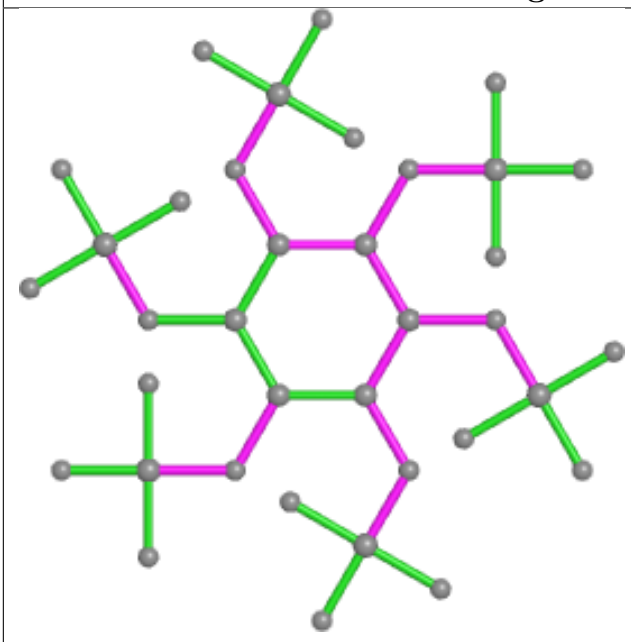


Torsions

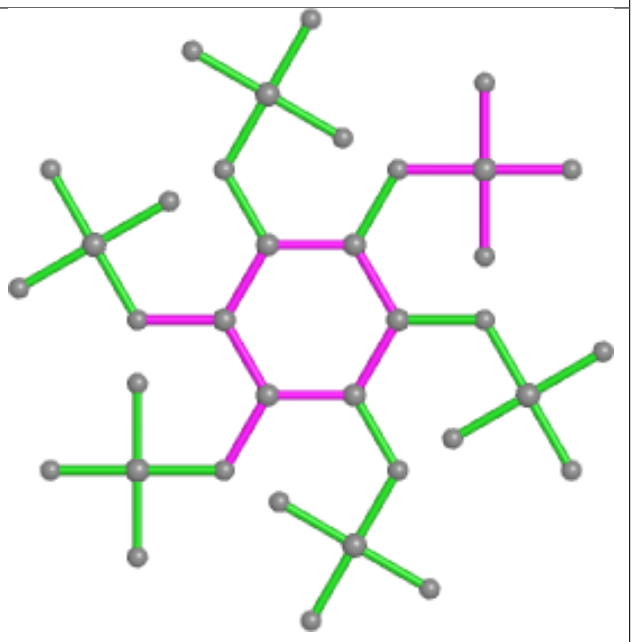


Rings

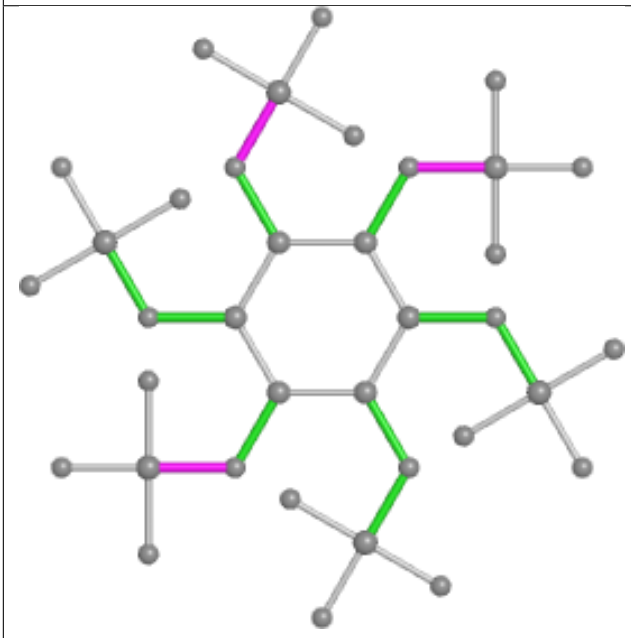
Ligand IHP D 501



Bond lengths



Bond angles



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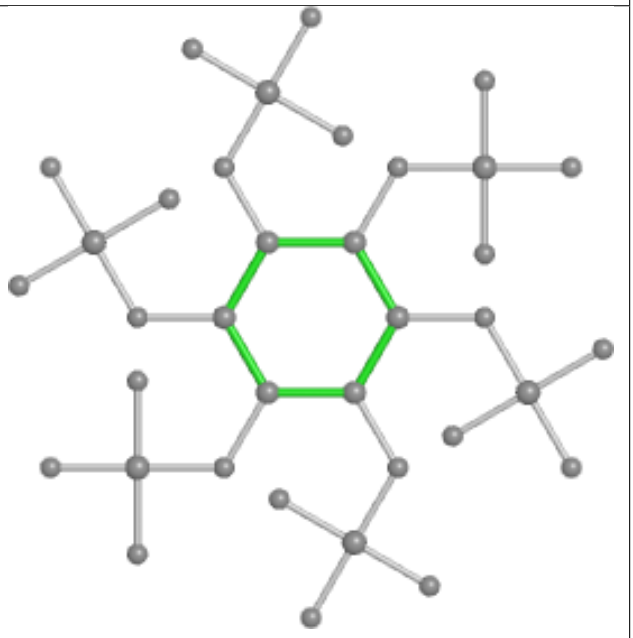
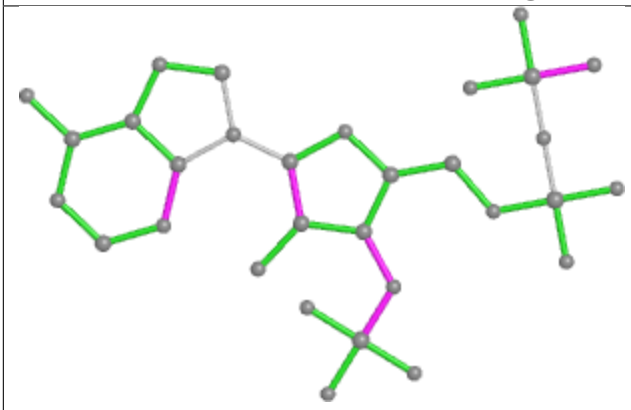


Rings

Ligand ACO C 502



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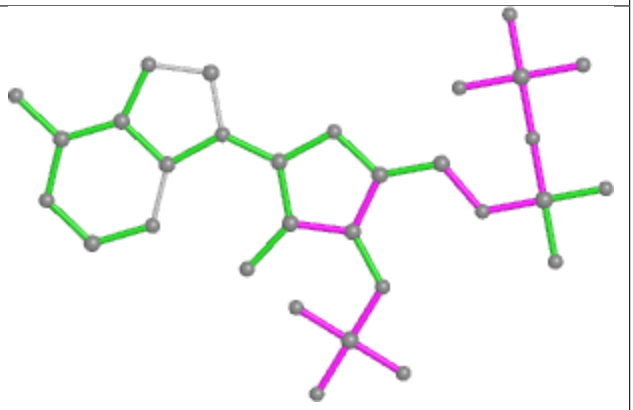
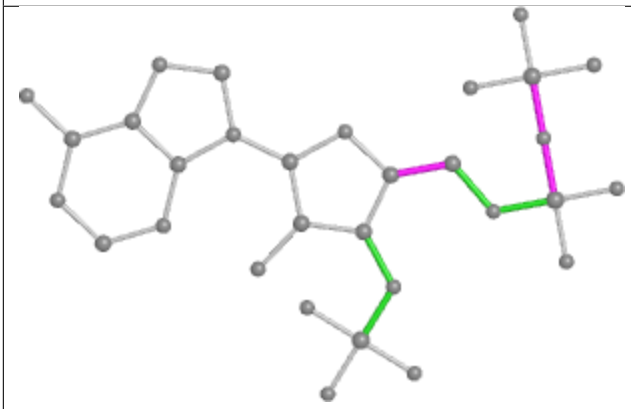


Bond angles



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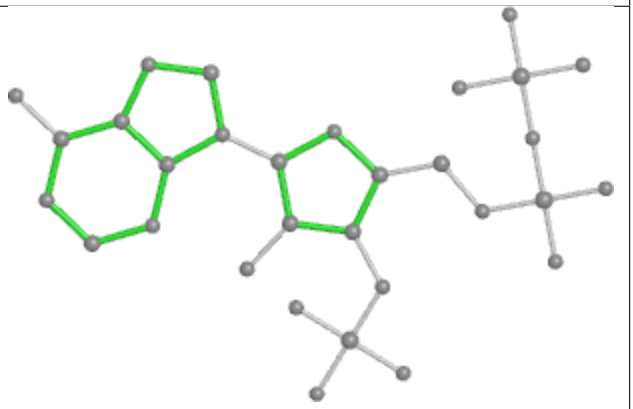
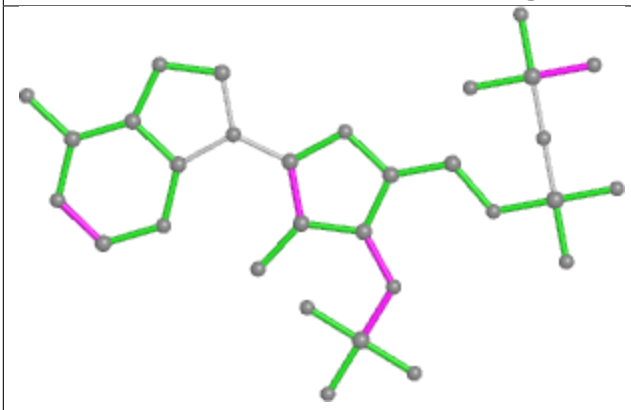
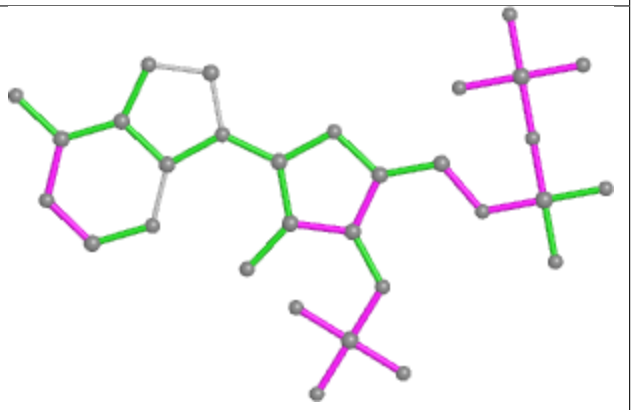


Rings

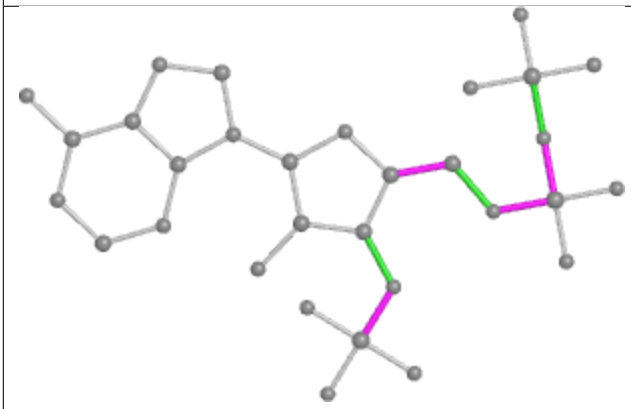
Ligand ACO B 502



Bond lengths



Bond angles



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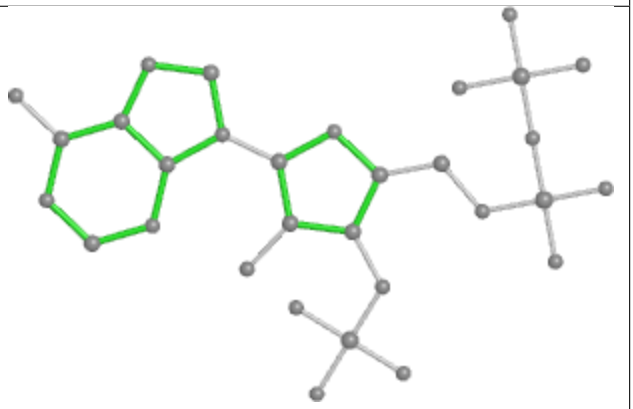
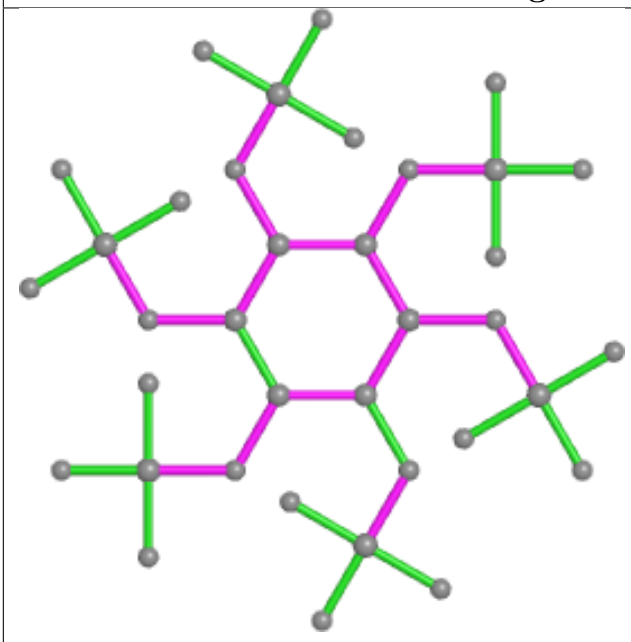
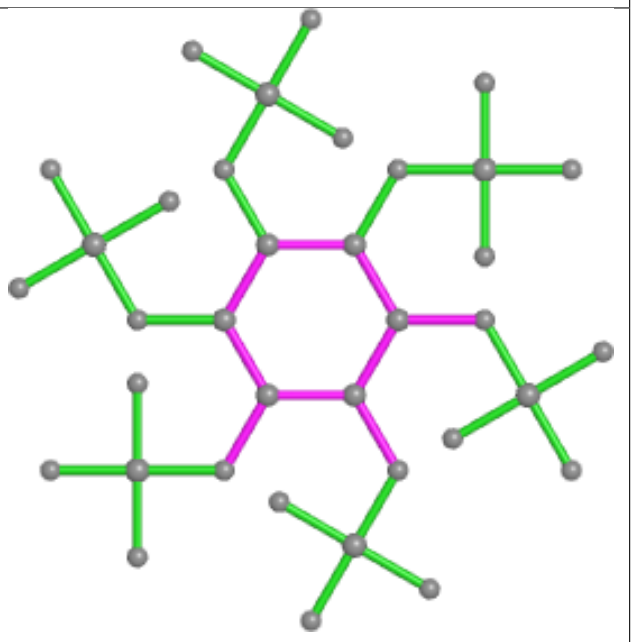


Rings

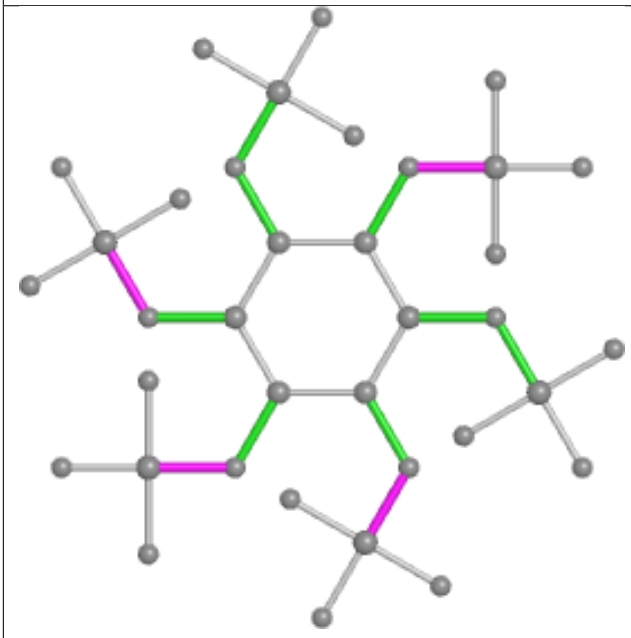
Ligand IHP B 501



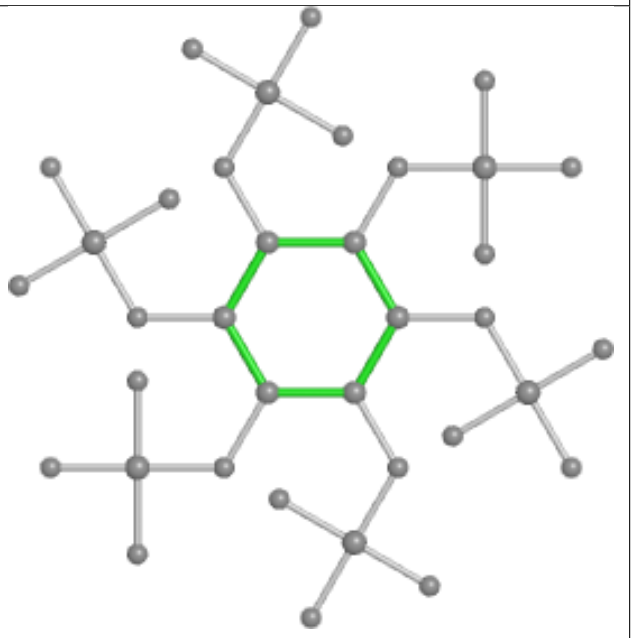
Bond lengths



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	A	336/352 (95%)	-0.20	4 (1%)	79	77	33, 52, 87, 116	0
1	B	327/352 (92%)	0.06	21 (6%)	19	18	34, 63, 112, 127	0
1	C	335/352 (95%)	-0.24	4 (1%)	79	77	31, 52, 88, 104	0
1	D	334/352 (94%)	-0.35	2 (0%)	89	88	32, 48, 80, 101	0
All	All	1332/1408 (94%)	-0.18	31 (2%)	60	58	31, 52, 98, 127	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	9.4
1	B	302	GLY	8.0
1	B	429	ARG	4.5
1	B	299	MET	3.1
1	B	369	LEU	3.0

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

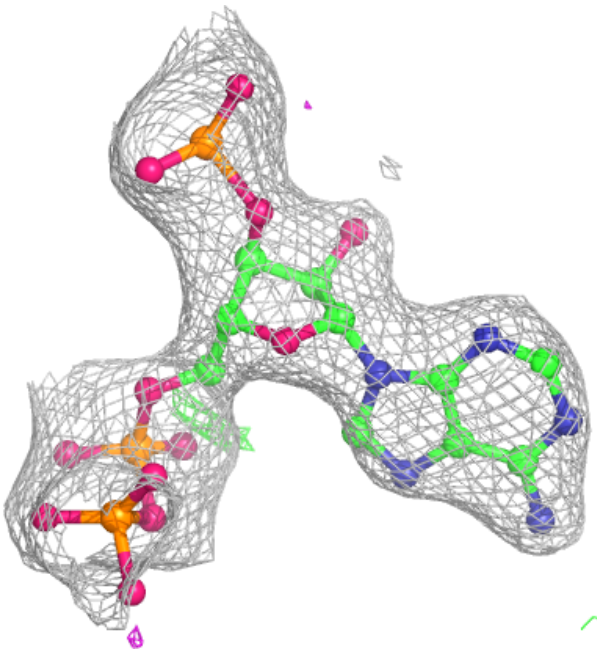
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

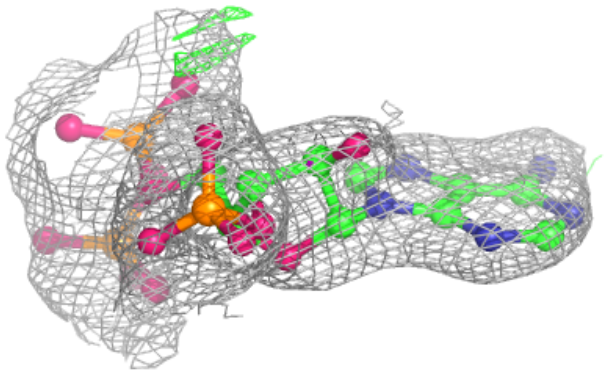
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACO	B	502	31/51	0.91	0.13	57,72,145,150	0
3	ACO	A	502	31/51	0.94	0.11	47,59,118,119	0
3	ACO	D	502	31/51	0.95	0.12	40,46,131,135	0
2	IHP	B	501	36/36	0.96	0.17	32,53,124,132	0
3	ACO	C	502	31/51	0.96	0.10	41,62,173,174	0
2	IHP	A	501	36/36	0.96	0.17	35,54,94,95	0
2	IHP	C	501	36/36	0.97	0.18	30,52,77,87	0
2	IHP	D	501	36/36	0.98	0.14	31,53,75,87	0

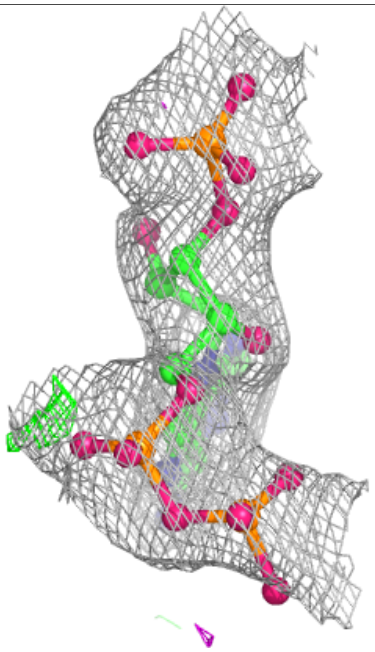
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO B 502:

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

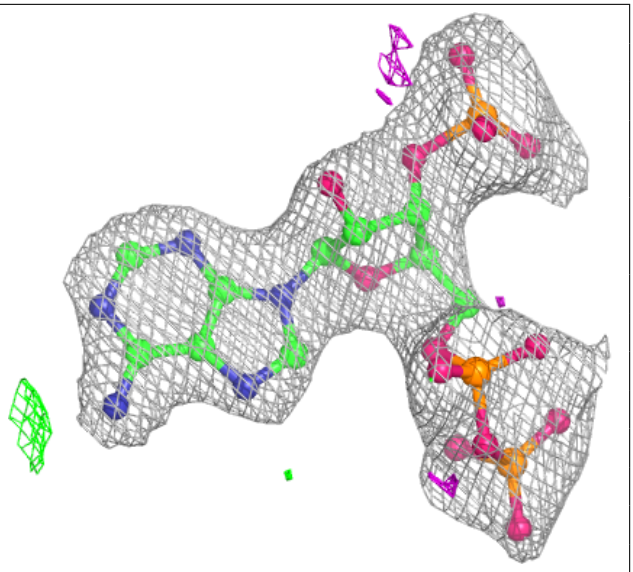


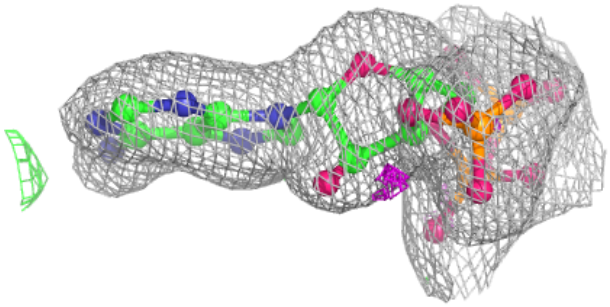


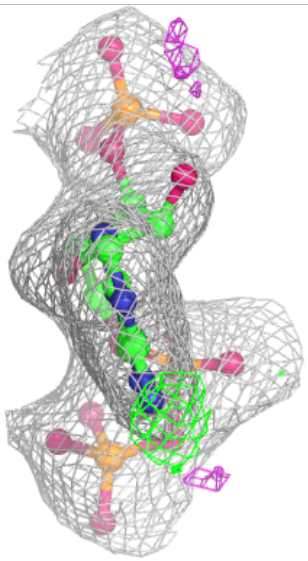


Electron density around ACO A 502:

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

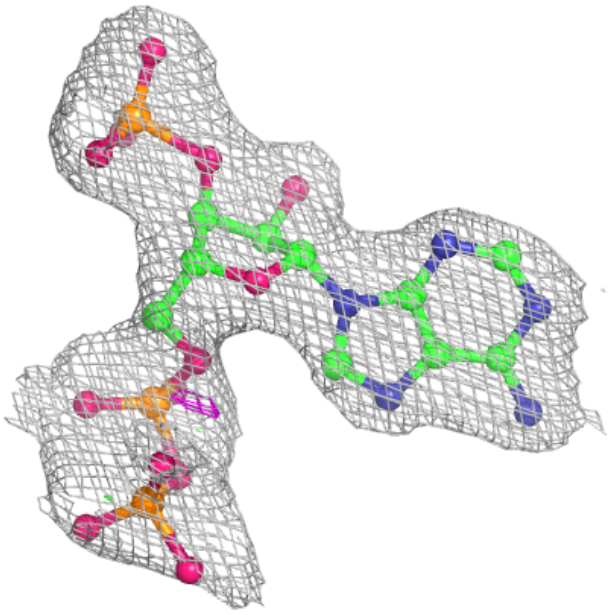


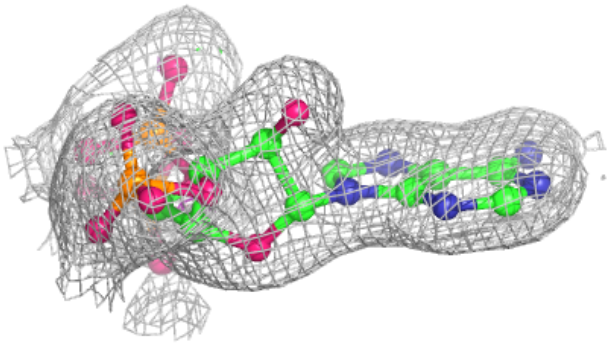


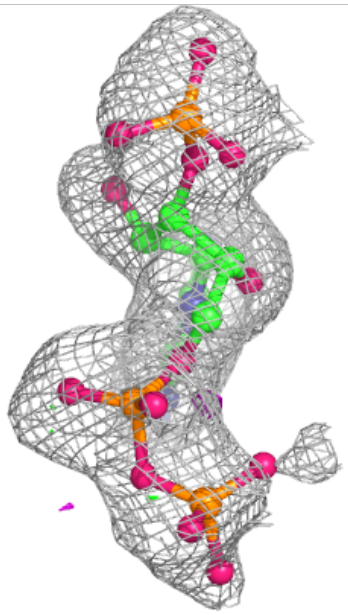


Electron density around ACO D 502:

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

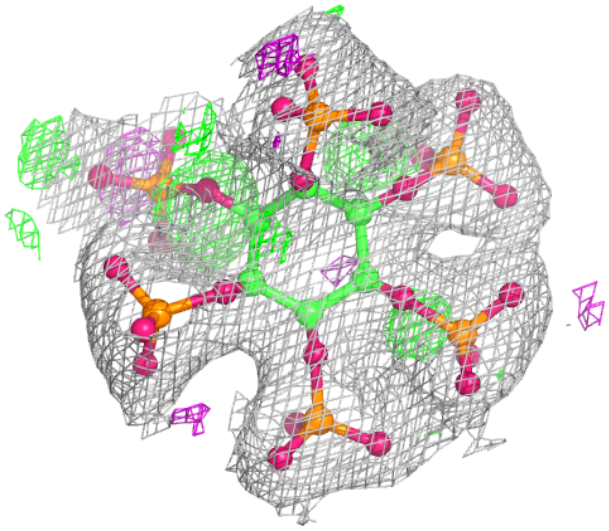


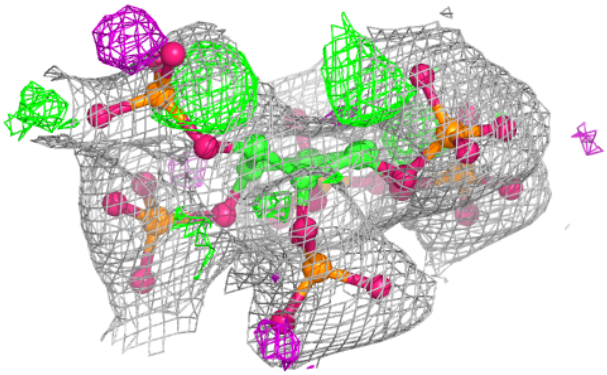


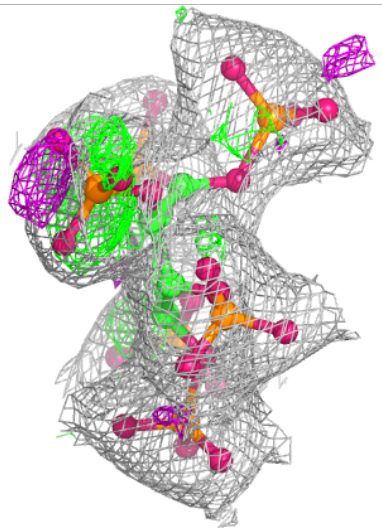


Electron density around IHP B 501:

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

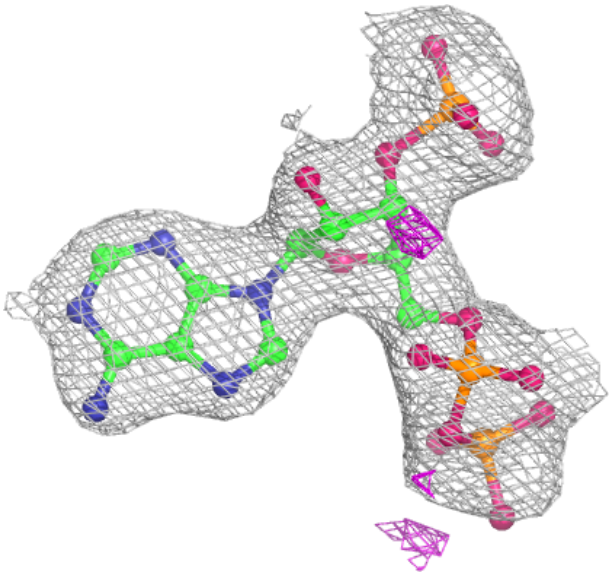


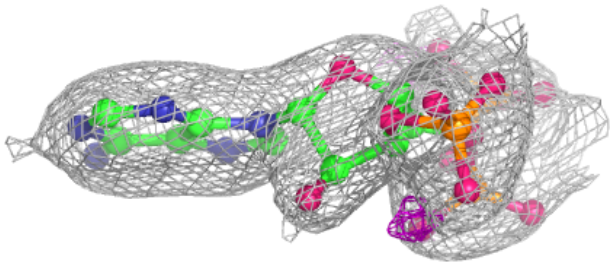


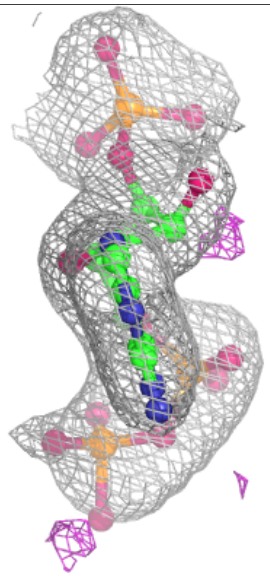


Electron density around ACO C 502:

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

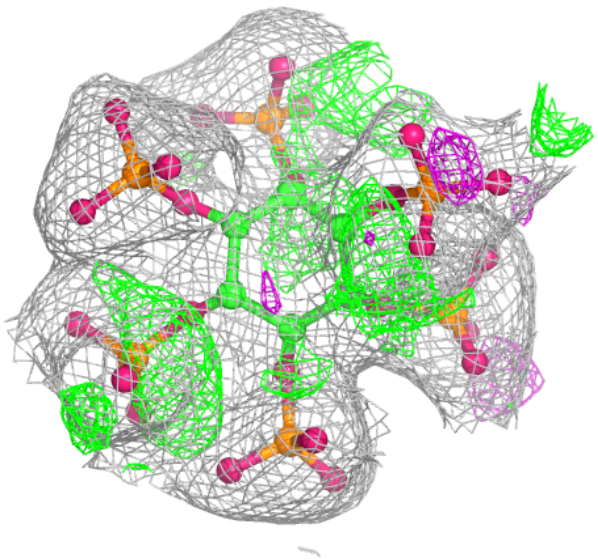


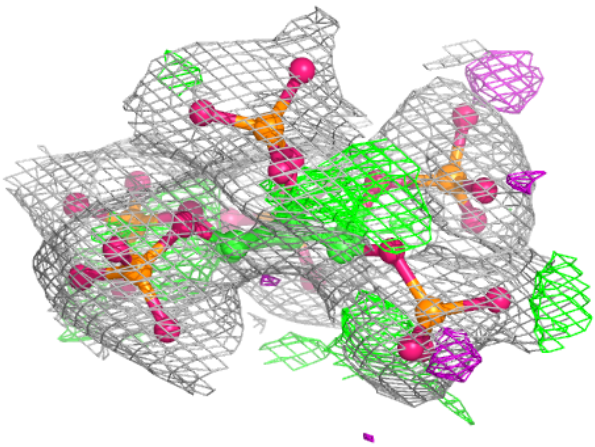


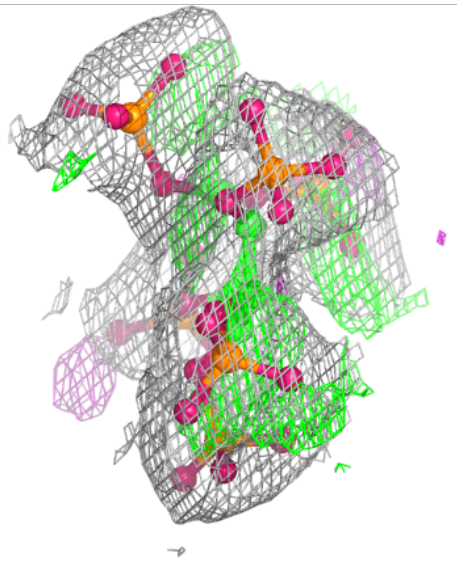


Electron density around IHP A 501:

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

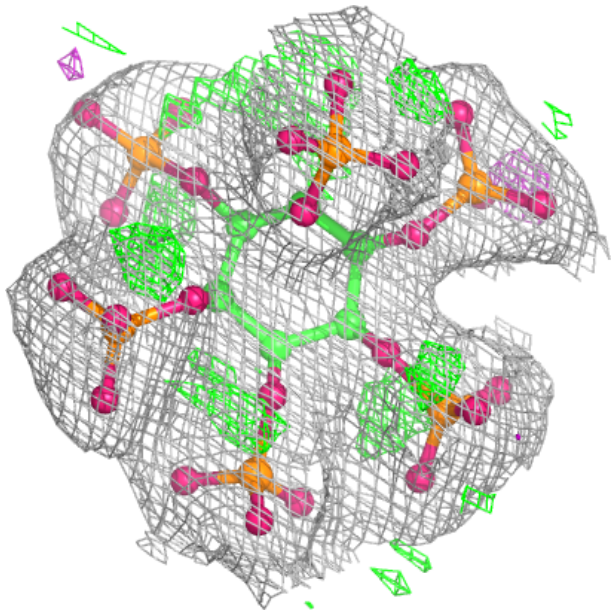


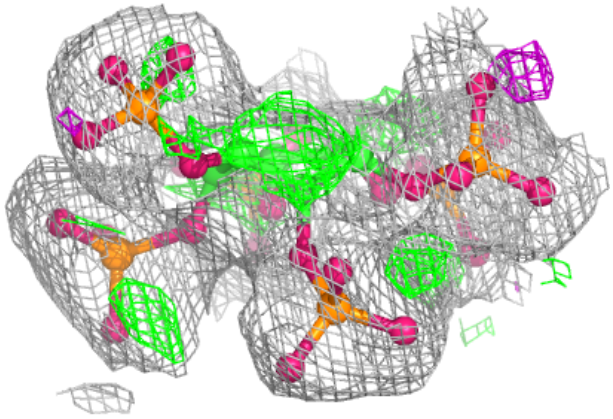


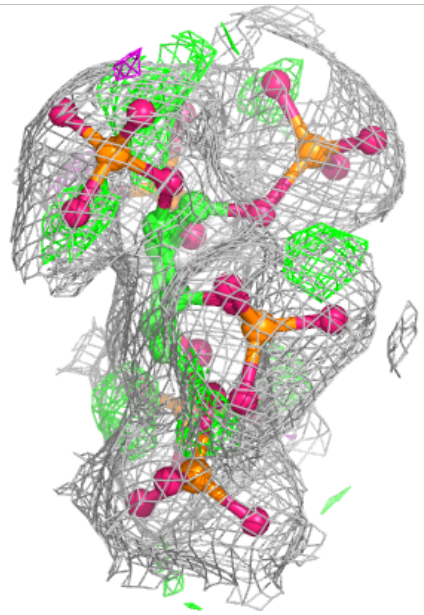


Electron density around IHP C 501:

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

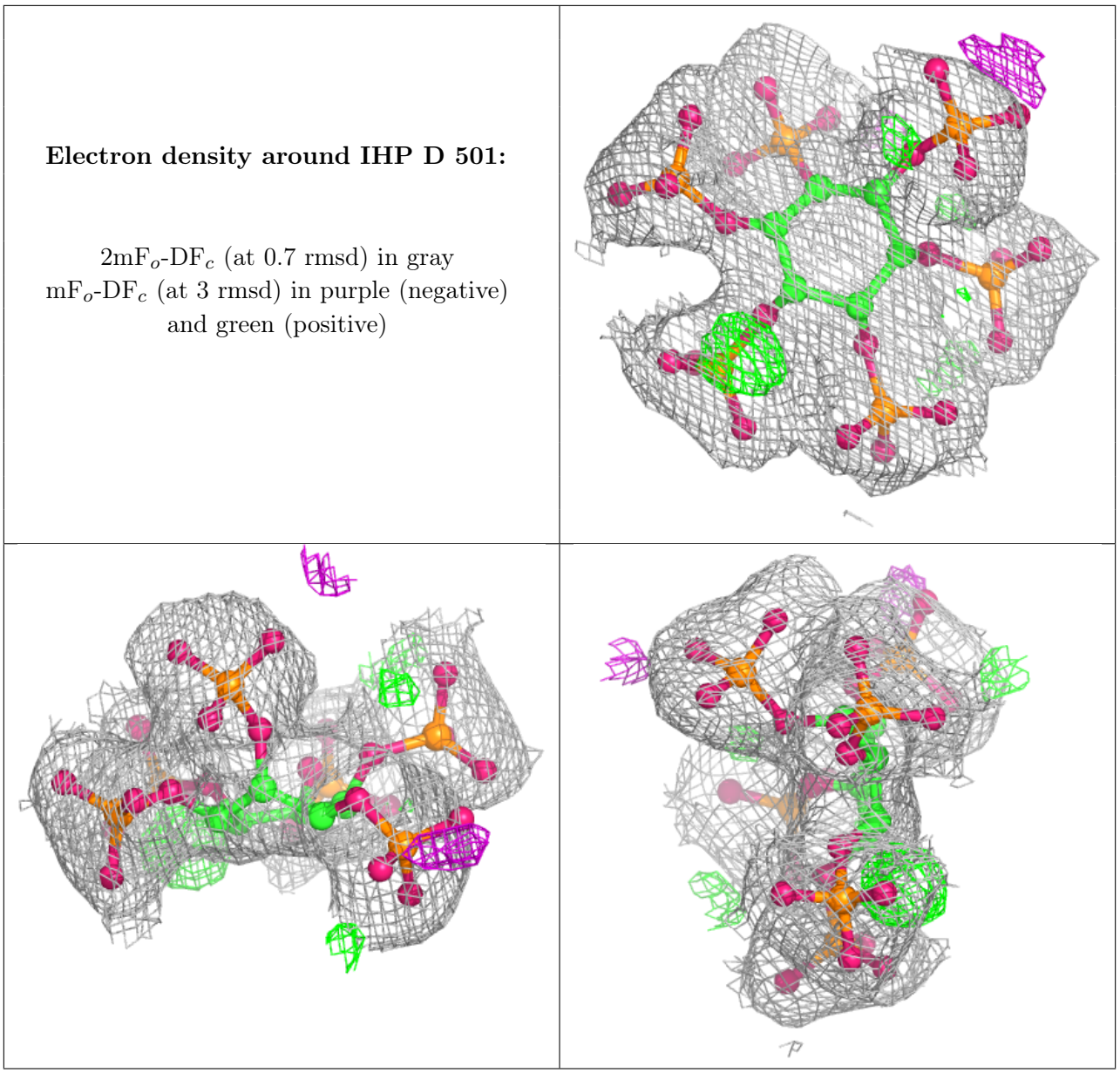






Electron density around IHP D 501:

$2mF_o$-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.