wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 02:19 AM EDT

PDB ID	:	5W40
Title	:	Crystal structure of PopP2 F318S in complex with IP6 and AcCoA
Authors	:	Zhang, Z.M.; Gao, L.; Song, J.
Deposited on	:	2017-06-08
Resolution	:	2.53 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:

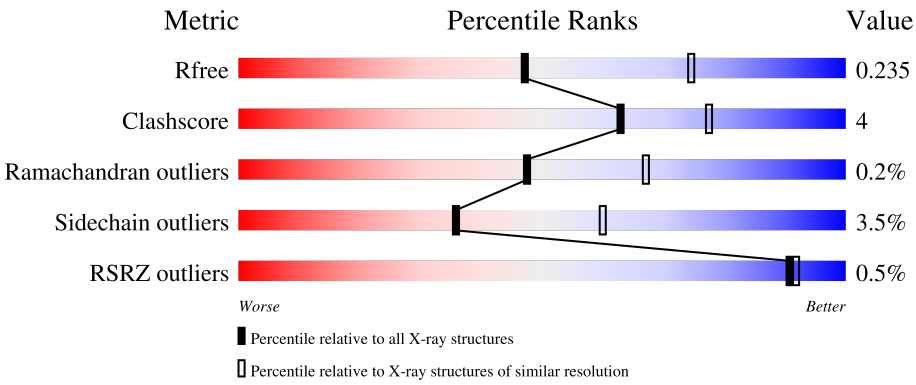
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	86% 9% • 5%
1	B	352	80% 14% • 5%
1	C	352	85% 9% • 5%
1	D	352	2% 82% 11% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10487 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
			Total	C	N	O	S			
1	A	336	2527	1559	473	483	12	0	0	0
1	B	333	2520	1557	471	479	13	0	0	0
1	C	333	2534	1564	476	481	13	0	0	0
1	D	327	2400	1483	452	454	11	0	0	0

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	318	SER	PHE	conflict	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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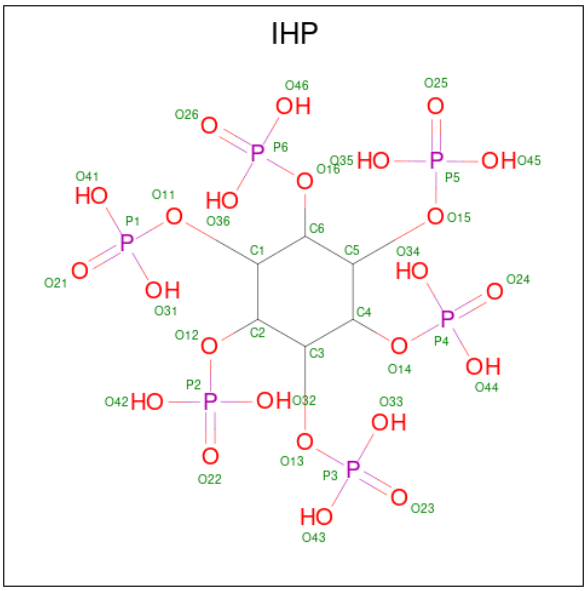
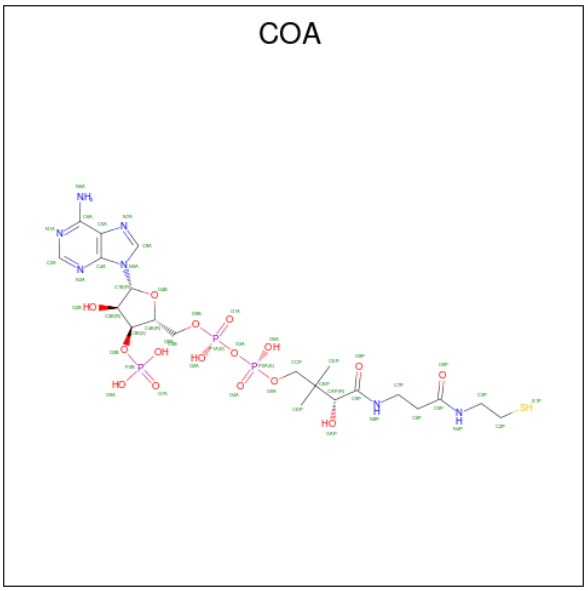
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	-	expression tag	UNP A0A0S4VB05
B	146	GLY	-	expression tag	UNP A0A0S4VB05
B	147	ARG	-	expression tag	UNP A0A0S4VB05
B	148	GLN	-	expression tag	UNP A0A0S4VB05
B	318	SER	PHE	conflict	UNP A0A0S4VB05
C	137	SER	-	expression tag	UNP A0A0S4VB05
C	138	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	318	SER	PHE	conflict	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	318	SER	PHE	conflict	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
			Total	C	O	P		
2	A	1	36	6	24	6	0	0
			Total	C	O	P		
2	B	1	36	6	24	6	0	0
			Total	C	O	P		
2	C	1	36	6	24	6	0	0
			Total	C	O	P		
2	D	1	36	6	24	6	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	45	19	7	16	3	0	0
			Total	C	N	O	P		
3	B	1	40	16	6	15	3	0	0
			Total	C	N	O	P		
3	C	1	36	15	5	13	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	5	13	3	0	0

- Molecule 4 is water.

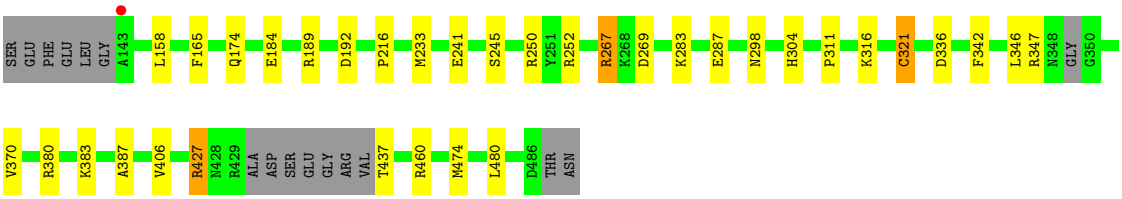
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	53	53	53	0	0
			Total	O		
4	B	73	73	73	0	0
			Total	O		
4	C	49	49	49	0	0
			Total	O		
4	D	35	35	35	0	0

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 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.

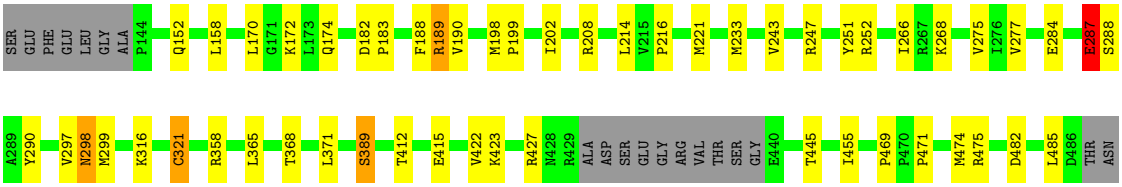
• Molecule 1: PopP2 protein

Chain A:



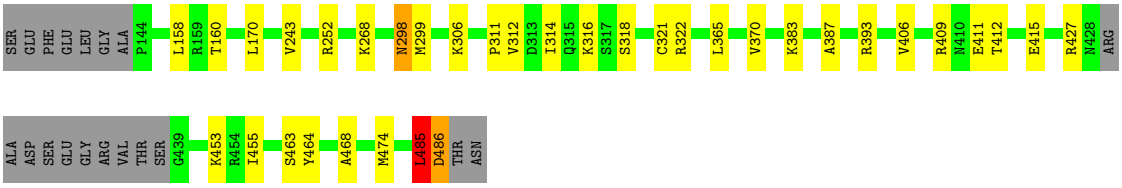
• Molecule 1: PopP2 protein

Chain B:



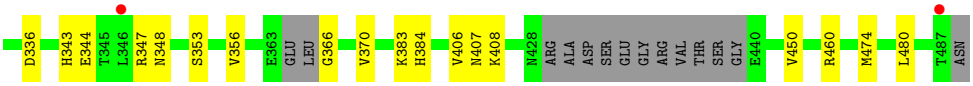
• Molecule 1: PopP2 protein

Chain C:



• Molecule 1: PopP2 protein

Chain D:


D336
H343
E344
T345
L346
R347
N348
S353
V356
E363
GLU
LEU
G366
V370
K383
H384
V406
N407
K408
N428
ARG
ALA
ASP
SER
GLU
GLY
ARG
VAL
THR
SER
GLY
E440
V450
R460
M474
L480
T487
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.78Å 78.64Å 79.85Å 103.00° 112.43° 111.85°	Depositor
Resolution (Å)	39.26 – 2.53 39.26 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.26-2.53) 98.7 (39.26-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.235 0.191 , 0.235	Depositor DCC
R_{free} test set	1923 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.149 for -l,-h,h+k+l 0.149 for -k,h+k+l,-h 0.021 for k,h,-h-k-l 0.016 for l,-h-k-l,h 0.179 for -h-k-l,l,k 0.015 for -h,-l,-k 0.013 for h+k+l,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10487	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SCY, IHP, COA

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	0.29	0/2555	0.54	0/3460
1	B	0.30	0/2550	0.55	0/3450
1	C	0.29	0/2564	0.53	1/3466 (0.0%)
1	D	0.29	0/2425	0.53	0/3289
All	All	0.29	0/10094	0.54	1/13665 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	485	LEU	CA-CB-CG	6.62	130.52	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	SCY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2527	0	2476	15	0
1	B	2520	0	2487	28	0
1	C	2534	0	2513	20	0
1	D	2400	0	2303	22	0
2	A	36	0	6	1	0
2	B	36	0	6	0	0
2	C	36	0	6	1	0
2	D	36	0	6	5	0
3	A	45	0	26	0	0
3	B	40	0	21	2	0
3	C	36	0	19	0	0
3	D	31	0	11	0	0
4	A	53	0	0	1	0
4	B	73	0	0	2	0
4	C	49	0	0	3	0
4	D	35	0	0	3	0
All	All	10487	0	9880	86	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 86 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:158:LEU:HD12	1:C:474:MET:HE1	1.55	0.86
1:A:158:LEU:HD12	1:A:474:MET:HE1	1.55	0.85
1:D:347:ARG:NH1	4:D:601:HOH:O	1.96	0.83
1:C:318:SER:OG	1:C:427:ARG:NH1	2.12	0.83
1:B:158:LEU:HD12	1:B:474:MET:HE1	1.68	0.75

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	329/352 (94%)	324 (98%)	4 (1%)	1 (0%)	41	59
1	B	328/352 (93%)	323 (98%)	4 (1%)	1 (0%)	41	59
1	C	328/352 (93%)	322 (98%)	6 (2%)	0	100	100
1	D	318/352 (90%)	312 (98%)	5 (2%)	1 (0%)	41	59
All	All	1303/1408 (92%)	1281 (98%)	19 (2%)	3 (0%)	47	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	GLU
1	A	287	GLU
1	D	225	GLU

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	261/290 (90%)	251 (96%)	10 (4%)	33	56
1	B	263/290 (91%)	249 (95%)	14 (5%)	22	40
1	C	266/290 (92%)	260 (98%)	6 (2%)	50	74
1	D	237/290 (82%)	231 (98%)	6 (2%)	47	72
All	All	1027/1160 (88%)	991 (96%)	36 (4%)	36	60

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	485	LEU
1	D	298	ASN
1	C	486	ASP
1	D	241	GLU
1	B	190	VAL

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

Mol	Chain	Res	Type
1	C	304	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)

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	SCY	A	321	1	7,8,9	1.75	2 (28%)	3,9,11	0.77	0
1	SCY	B	321	1	7,8,9	1.99	3 (42%)	3,9,11	0.65	0
1	SCY	C	321	1	7,8,9	1.96	3 (42%)	3,9,11	0.87	0
1	SCY	D	321	1	7,8,9	2.05	4 (57%)	3,9,11	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	A	321	1	-	0/5/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	B	321	1	-	2/5/7/9	-
1	SCY	C	321	1	-	0/5/7/9	-
1	SCY	D	321	1	-	2/5/7/9	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	SCY	CB-SG	-3.32	1.73	1.81
1	D	321	SCY	CB-SG	-3.30	1.73	1.81
1	B	321	SCY	CB-SG	-3.26	1.73	1.81
1	C	321	SCY	CB-SG	-3.19	1.74	1.81
1	D	321	SCY	O-C	2.64	1.30	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	321	SCY	OCD-CD-SG-CB
1	D	321	SCY	CE-CD-SG-CB
1	B	321	SCY	OCD-CD-SG-CB
1	B	321	SCY	CE-CD-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	SCY	1	0

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	COA	C	502	-	33,38,50	4.08	8 (24%)	40,60,75	1.48	5 (12%)
3	COA	B	502	-	35,42,50	3.95	10 (28%)	45,66,75	1.71	8 (17%)
2	IHP	D	501	-	36,36,36	3.18	13 (36%)	54,60,60	1.62	10 (18%)
2	IHP	C	501	-	36,36,36	3.28	13 (36%)	54,60,60	1.71	10 (18%)
3	COA	D	502	-	28,33,50	4.41	8 (28%)	35,52,75	1.72	7 (20%)
2	IHP	B	501	-	36,36,36	3.18	16 (44%)	54,60,60	1.66	8 (14%)
3	COA	A	502	-	39,47,50	3.84	11 (28%)	49,72,75	1.48	6 (12%)
2	IHP	A	501	-	36,36,36	3.30	16 (44%)	54,60,60	1.66	9 (16%)

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	COA	C	502	-	-	10/24/44/64	0/3/3/3
3	COA	B	502	-	-	14/33/54/64	0/3/3/3
2	IHP	D	501	-	-	8/30/54/54	0/1/1/1
2	IHP	C	501	-	-	12/30/54/54	0/1/1/1
3	COA	D	502	-	-	7/17/37/64	0/3/3/3
2	IHP	B	501	-	-	4/30/54/54	0/1/1/1
3	COA	A	502	-	-	8/40/60/64	0/3/3/3
2	IHP	A	501	-	-	5/30/54/54	0/1/1/1

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	COA	C2B-C1B	-14.66	1.31	1.53
3	D	502	COA	C2B-C1B	-14.54	1.31	1.53
3	A	502	COA	O4B-C1B	14.48	1.61	1.41
3	C	502	COA	O4B-C1B	14.37	1.61	1.41
3	D	502	COA	O4B-C1B	14.32	1.61	1.41

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	COA	N3A-C2A-N1A	-5.70	119.77	128.68
3	D	502	COA	N3A-C2A-N1A	-5.47	120.12	128.68
3	A	502	COA	N3A-C2A-N1A	-5.42	120.21	128.68
3	C	502	COA	N3A-C2A-N1A	-5.37	120.28	128.68
3	D	502	COA	C5A-C6A-N6A	5.14	128.16	120.35

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	IHP	C5-O15-P5-O45
2	C	501	IHP	C1-C2-O12-P2
2	C	501	IHP	C3-C2-O12-P2
2	C	501	IHP	C6-O16-P6-O26
2	D	501	IHP	C4-O14-P4-O34

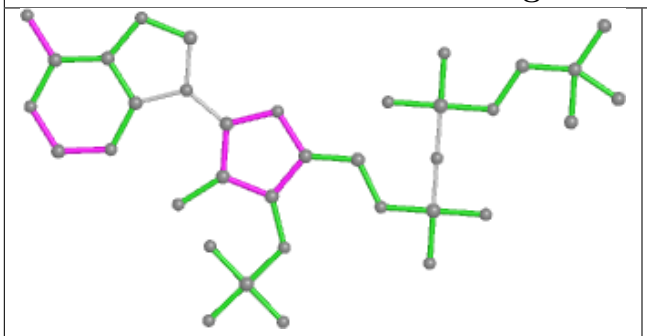
There are no ring outliers.

4 monomers are involved in 9 short contacts:

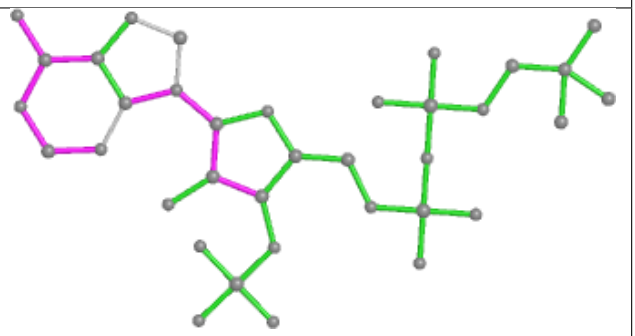
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	COA	2	0
2	D	501	IHP	5	0
2	C	501	IHP	1	0
2	A	501	IHP	1	0

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.

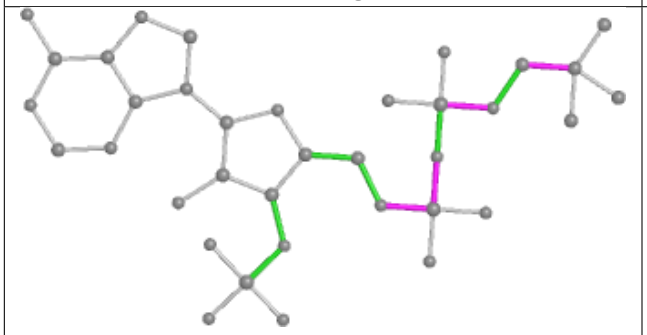
Ligand COA C 502



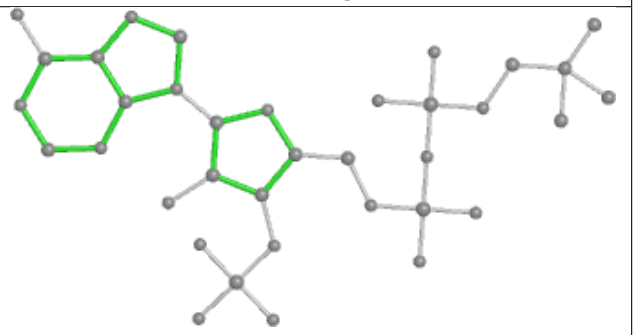
Bond lengths



Bond angles

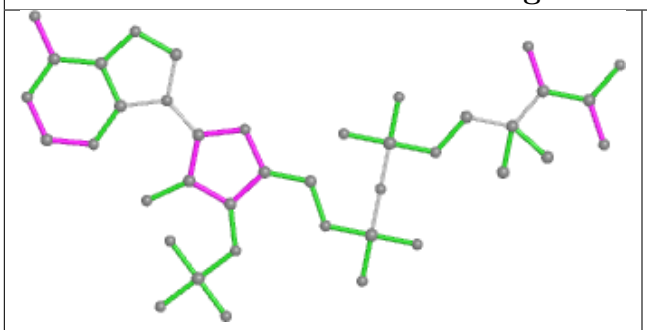


Torsions

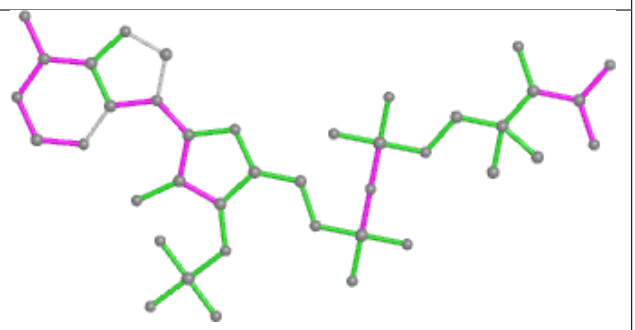


Rings

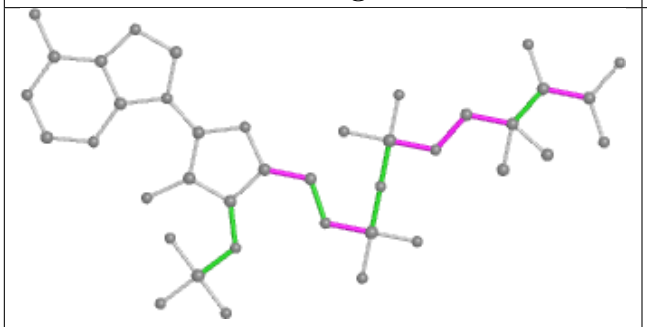
Ligand COA B 502



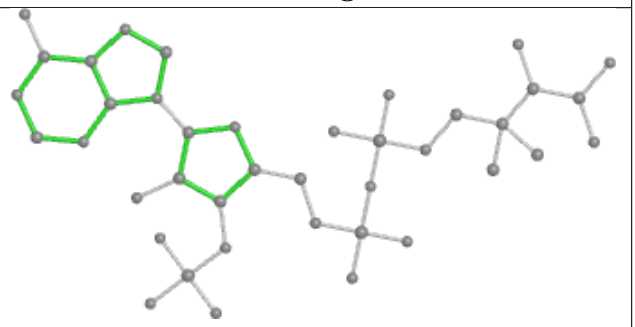
Bond lengths



Bond angles

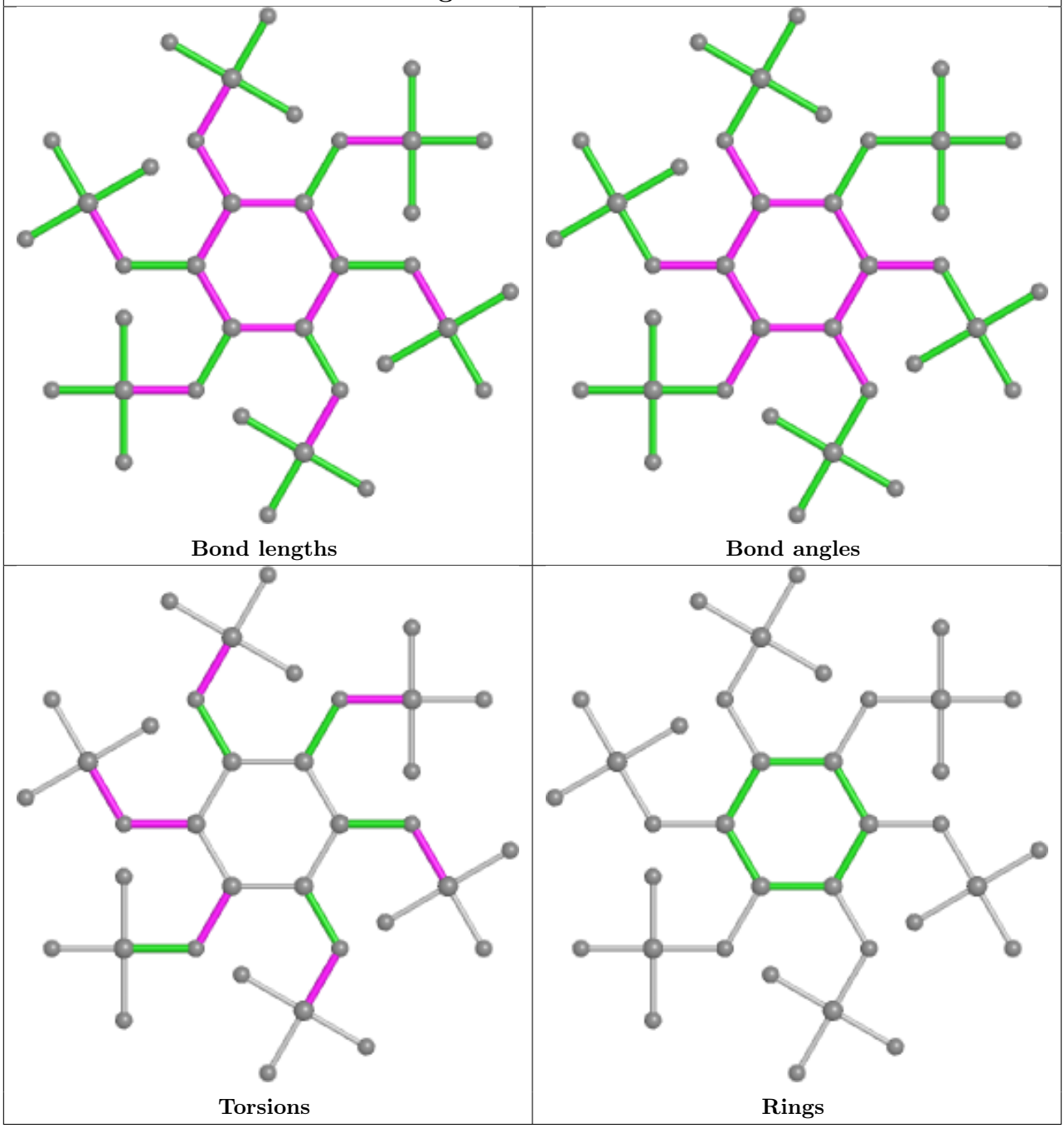


Torsions

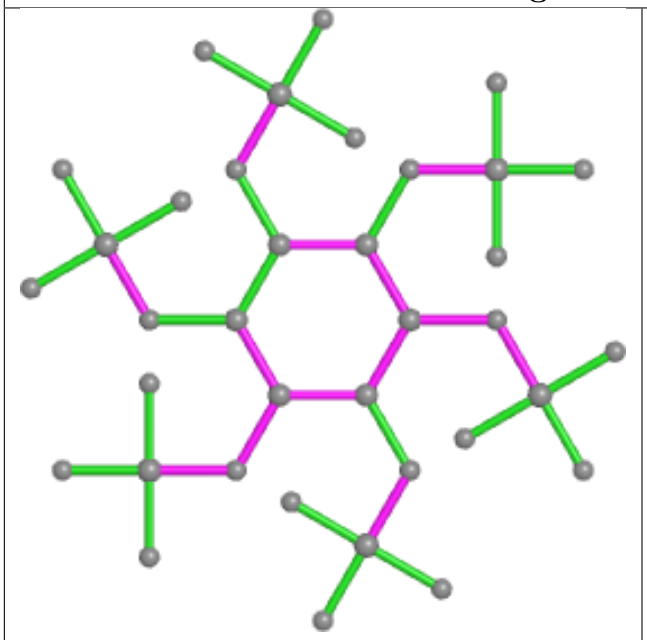


Rings

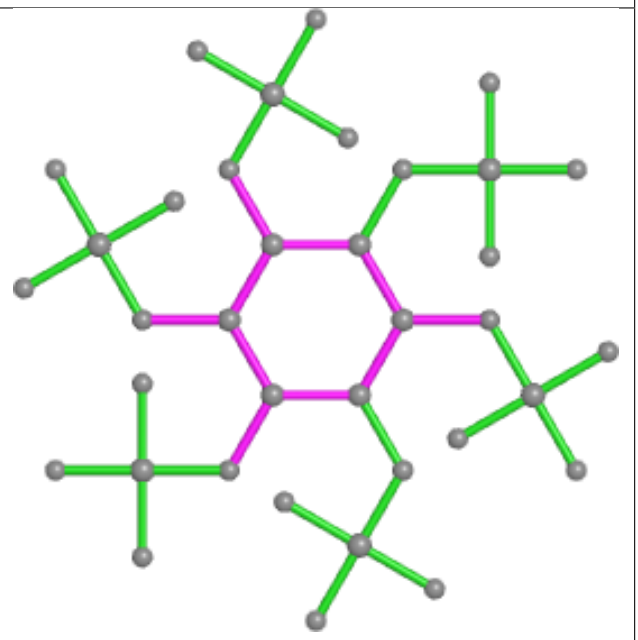
Ligand IHP D 501



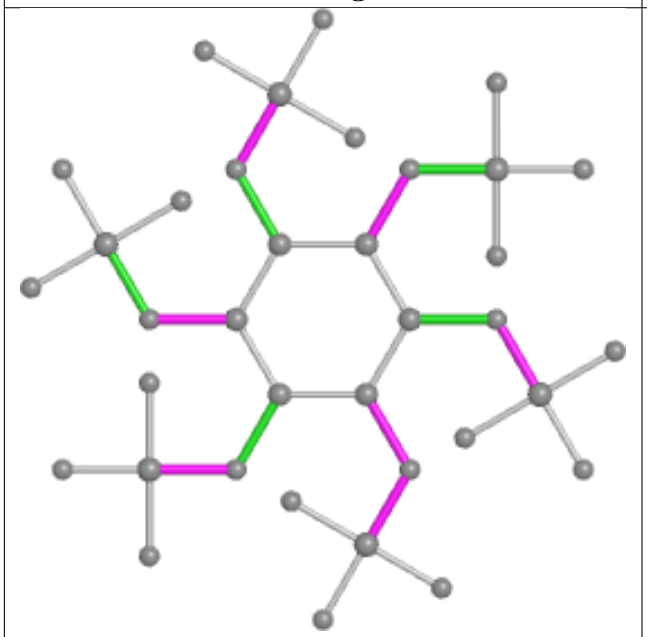
Ligand IHP C 501



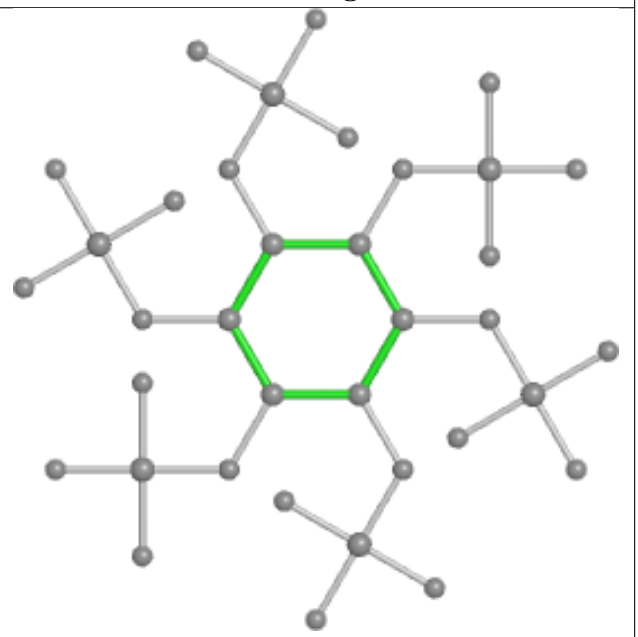
Bond lengths



Bond angles

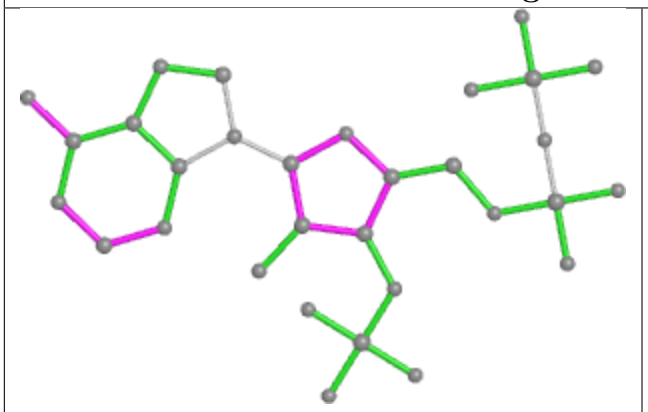


Torsions

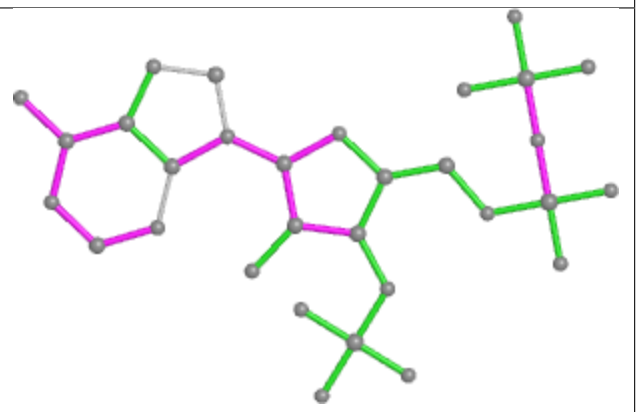


Rings

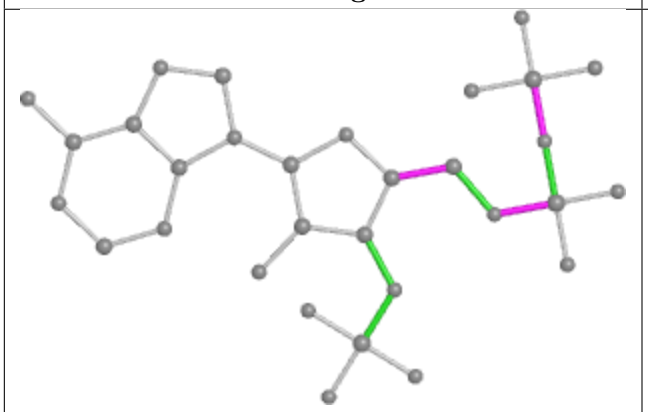
Ligand COA D 502



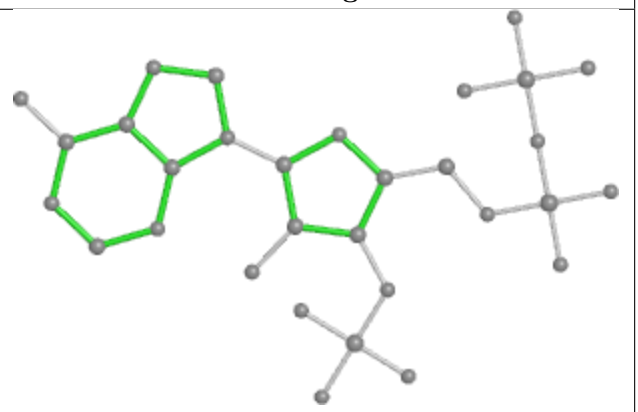
Bond lengths



Bond angles

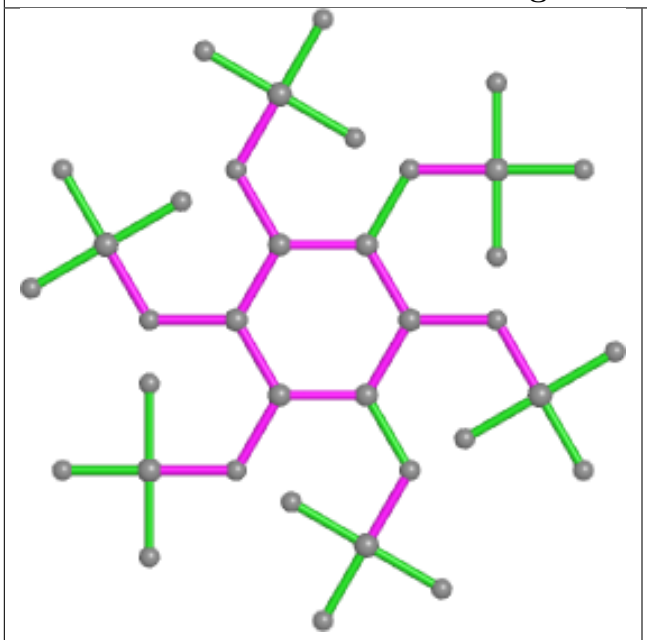


Torsions

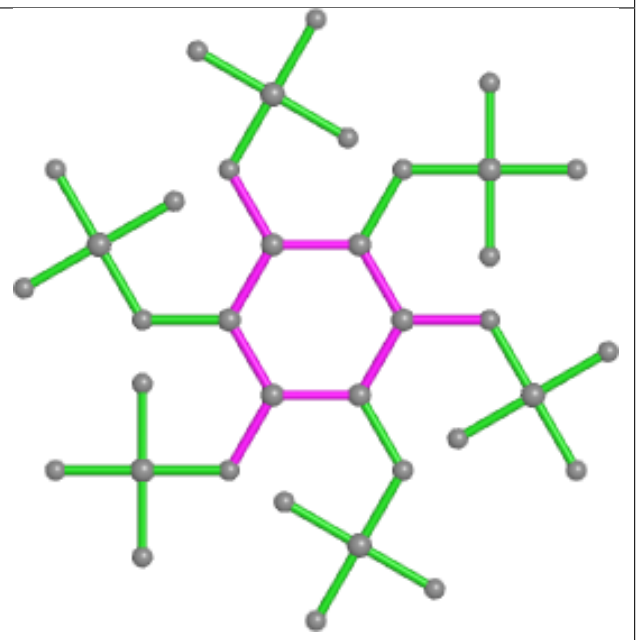


Rings

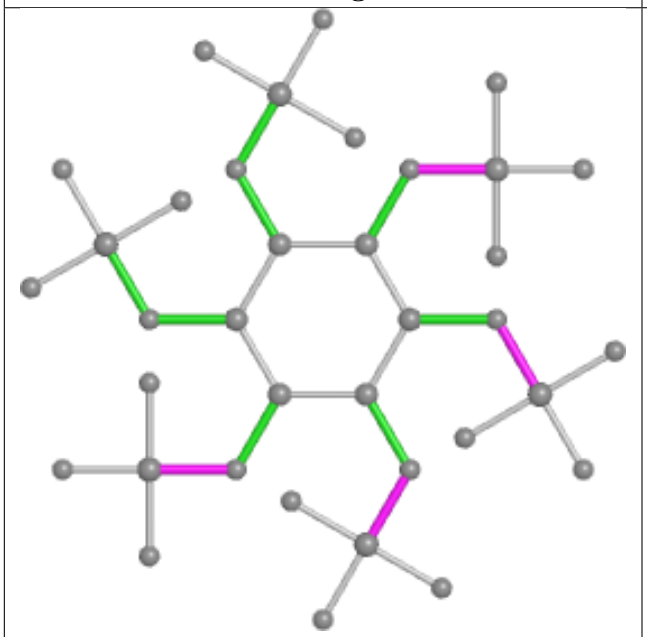
Ligand IHP B 501



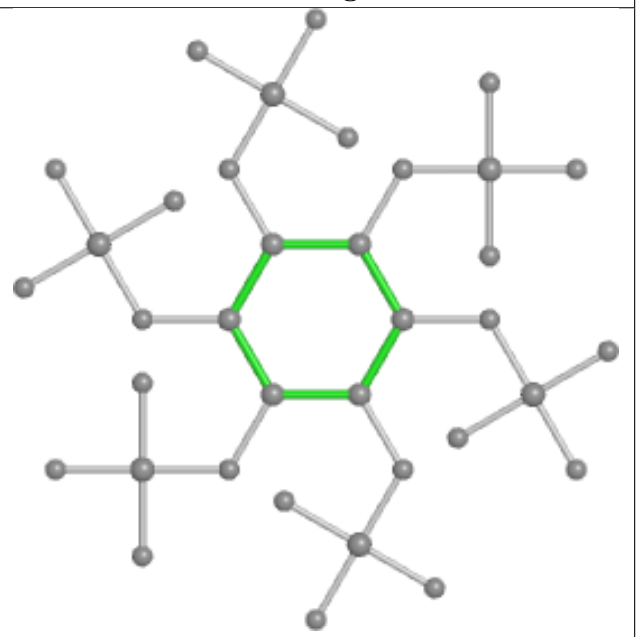
Bond lengths



Bond angles

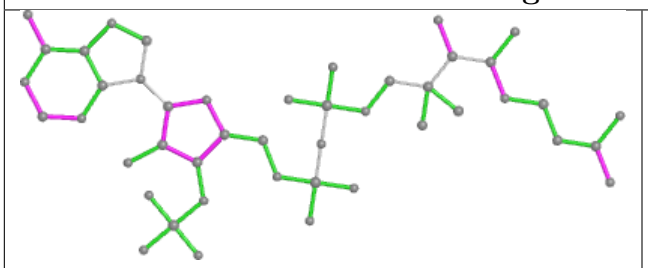


Torsions

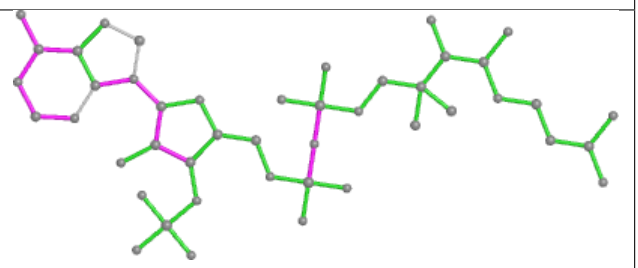


Rings

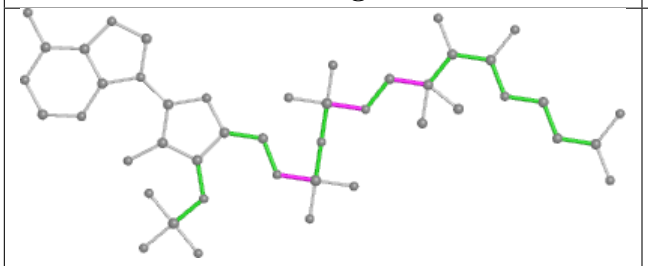
Ligand COA A 502



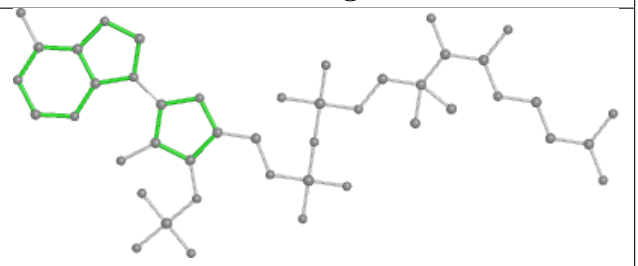
Bond lengths



Bond angles

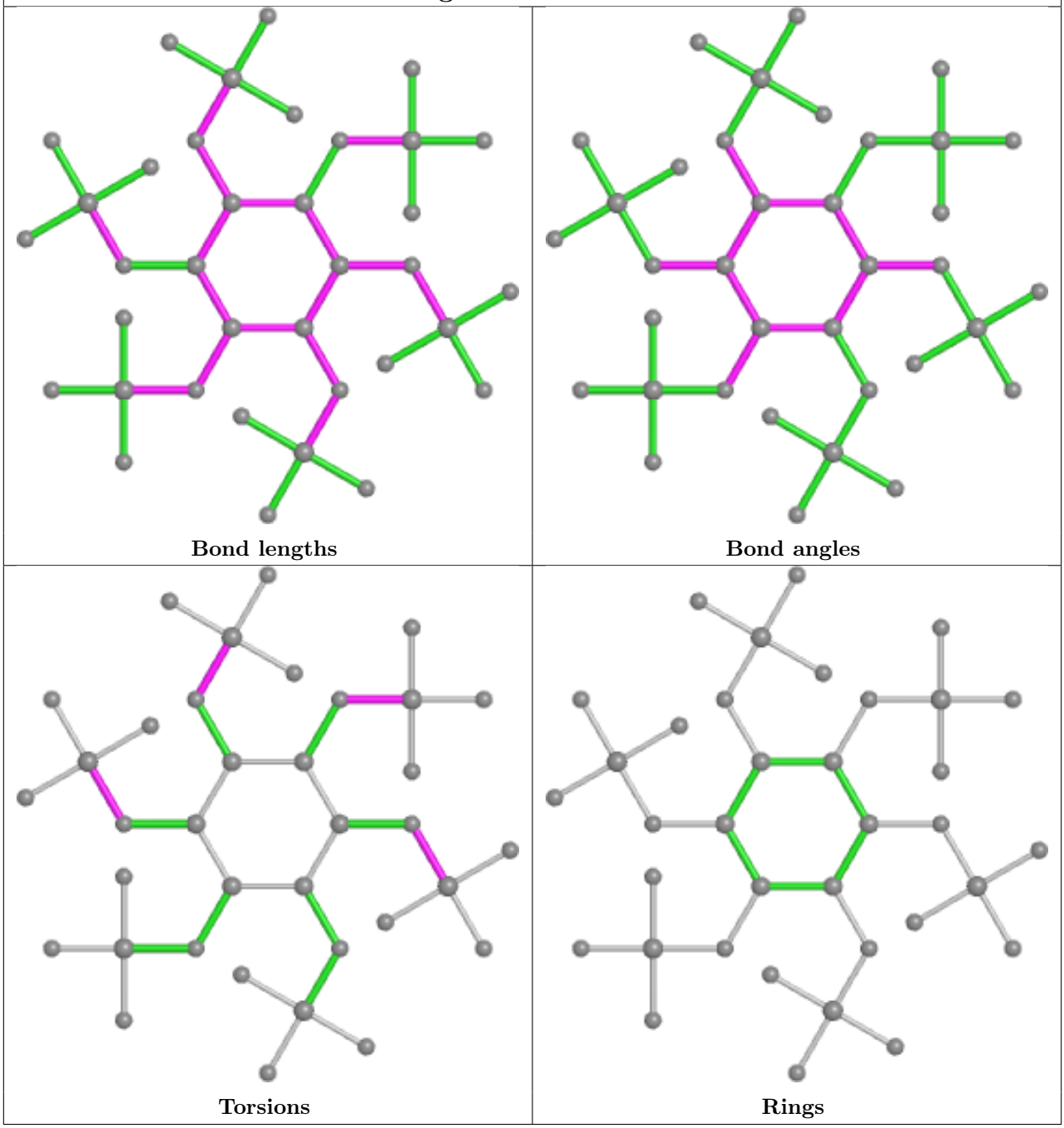


Torsions



Rings

Ligand IHP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/352 (95%)	-0.31	1 (0%) 94 94	31, 57, 94, 124	0
1	B	332/352 (94%)	-0.57	0 100 100	32, 48, 79, 105	0
1	C	332/352 (94%)	-0.49	0 100 100	31, 51, 83, 111	0
1	D	326/352 (92%)	-0.24	6 (1%) 68 71	35, 63, 106, 126	0
All	All	1325/1408 (94%)	-0.40	7 (0%) 91 92	31, 54, 97, 126	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	4.3
1	D	346	LEU	3.7
1	D	289	ALA	3.1
1	D	487	THR	2.6
1	D	302	GLY	2.3

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

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
1	SCY	D	321	9/10	0.95	0.11	47,57,75,76	0
1	SCY	C	321	9/10	0.96	0.11	31,39,50,52	0
1	SCY	A	321	9/10	0.96	0.13	34,42,51,52	0
1	SCY	B	321	9/10	0.97	0.12	26,35,77,77	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

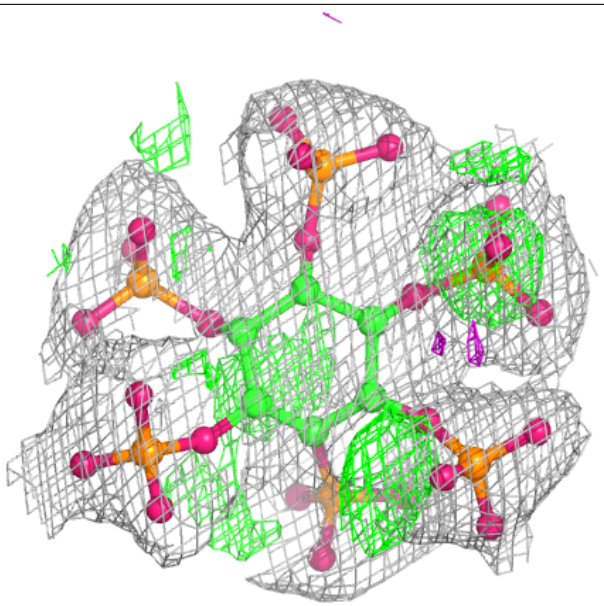
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

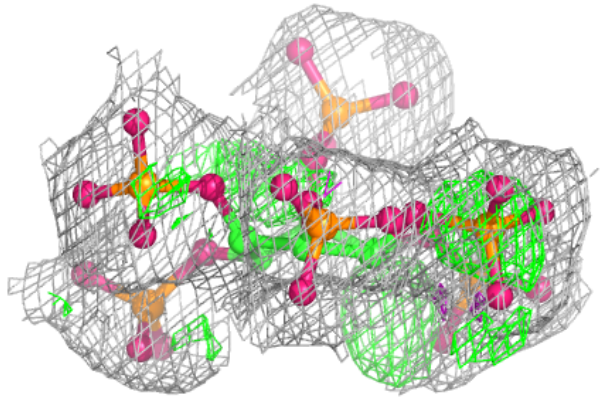
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IHP	A	501	36/36	0.93	0.21	36,57,109,116	0
3	COA	D	502	31/48	0.94	0.14	52,70,183,183	0
2	IHP	C	501	36/36	0.95	0.18	39,57,90,95	0
2	IHP	D	501	36/36	0.95	0.18	36,62,91,108	0
3	COA	A	502	45/48	0.95	0.17	43,79,135,144	0
3	COA	B	502	40/48	0.95	0.13	38,54,118,168	0
3	COA	C	502	36/48	0.95	0.12	41,63,144,159	0
2	IHP	B	501	36/36	0.95	0.18	29,54,115,122	0

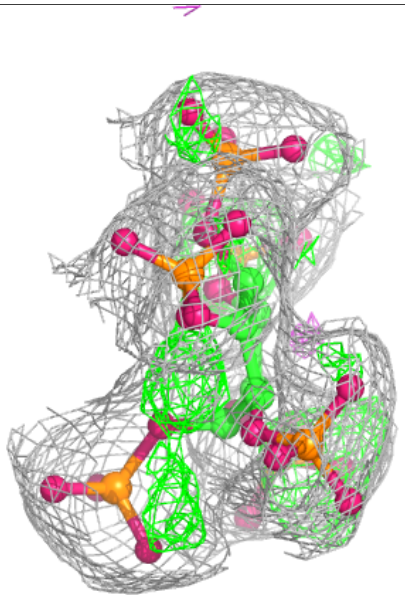
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

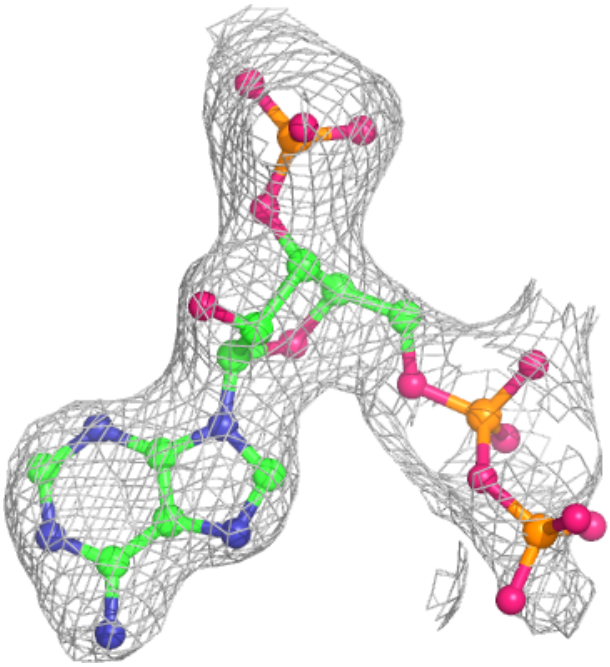


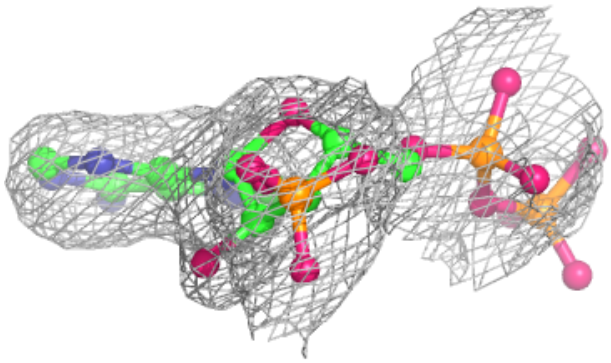


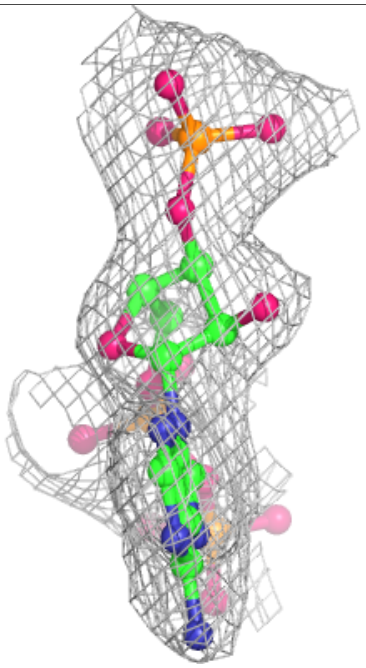


Electron density around COA D 502:

$2mF_o$-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 C 501:

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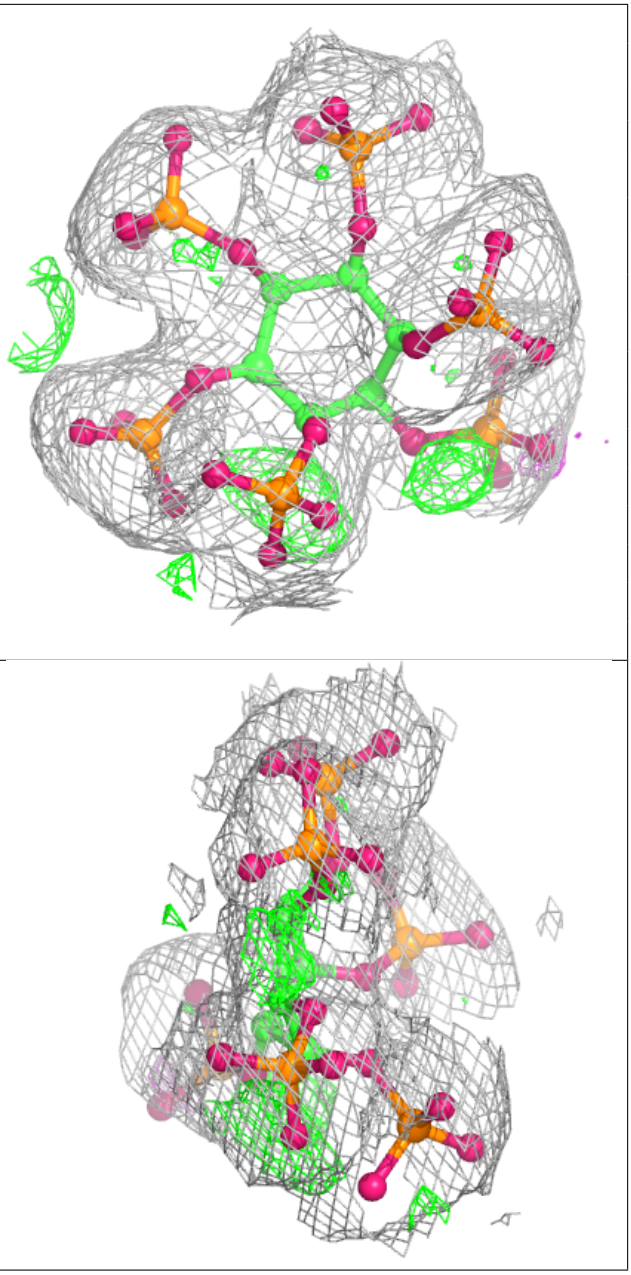
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IHP D 501:

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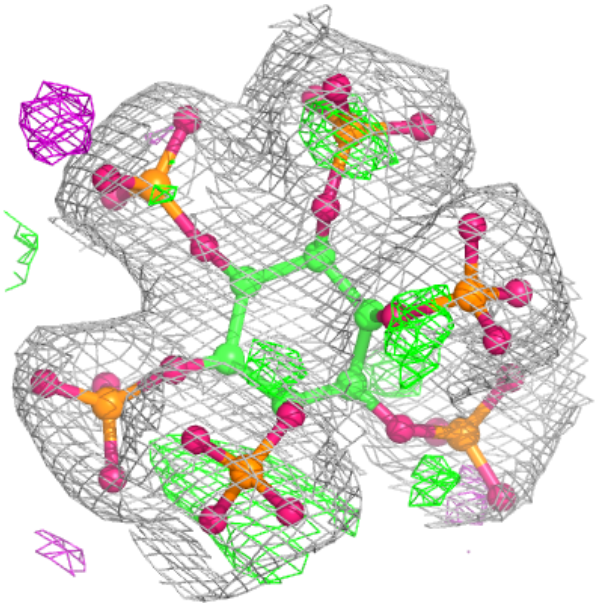
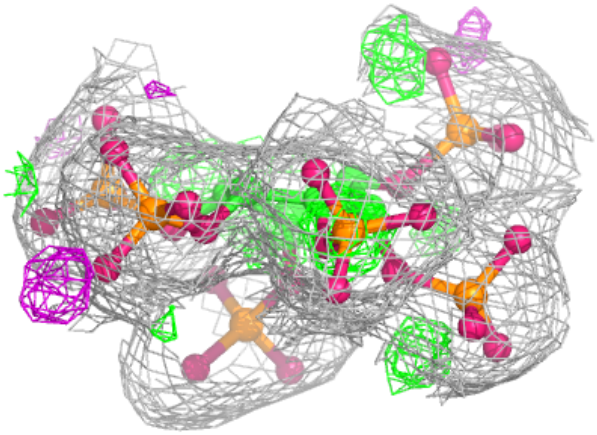
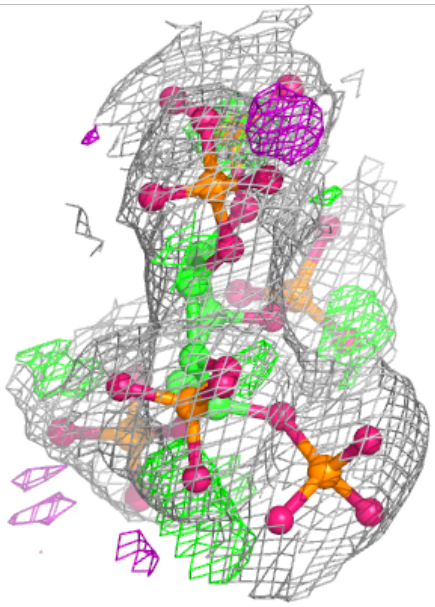
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

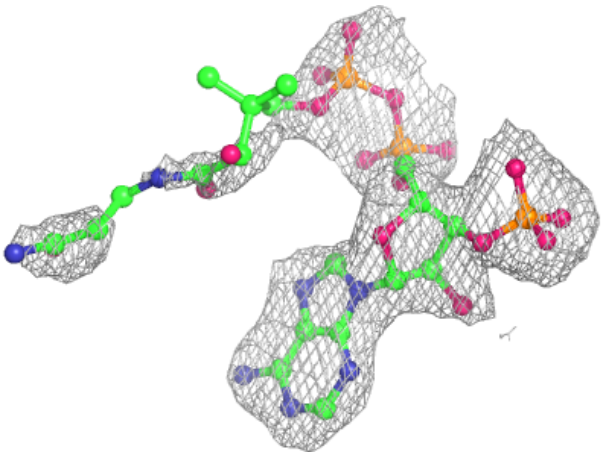


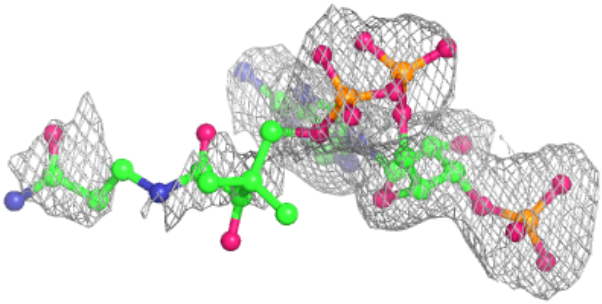


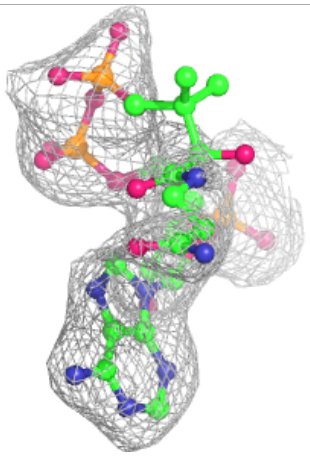


Electron density around COA A 502:

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

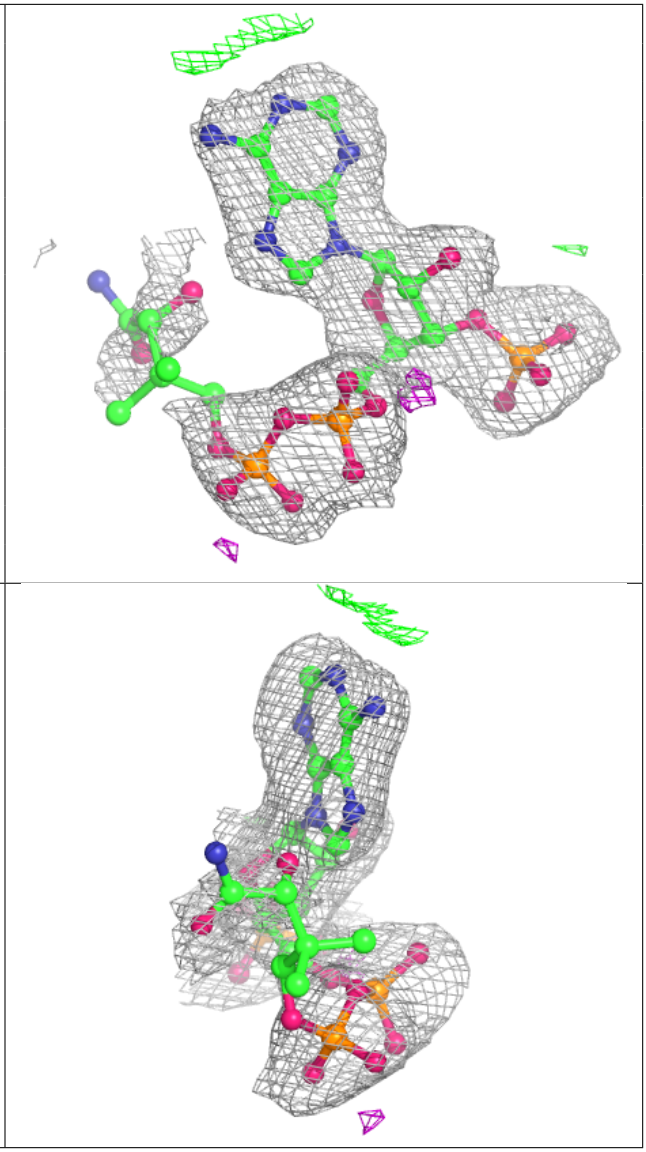






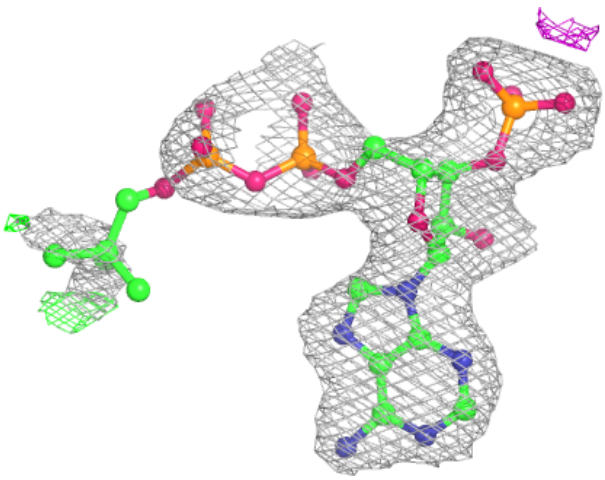
Electron density around COA B 502:

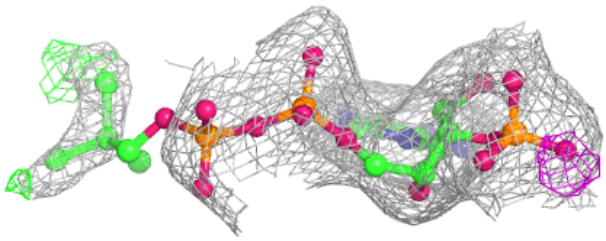
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

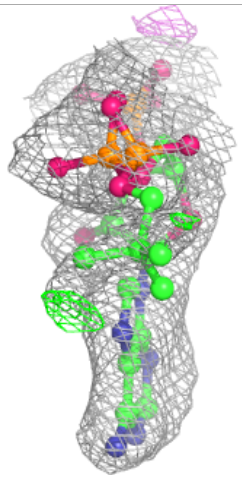


Electron density around COA C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

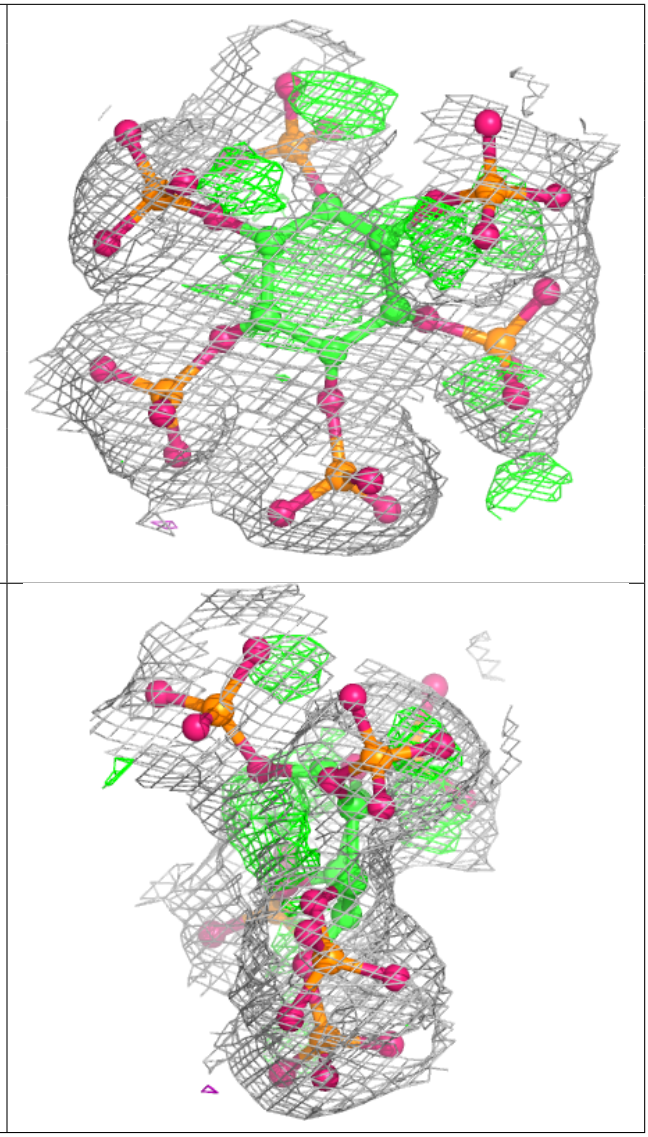






Electron density around IHP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.