



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 04:38 pm BST

PDB ID : 6IHI  
Title : Crystal structure of RasADH 3B3/I91V from Ralstonia.sp in complex with NADPH and A6O  
Authors : Zhang, H.L.; Chen, X.; Liu, W.D.; Wu, Q.Q.; Zhu, D.M.  
Deposited on : 2018-09-30  
Resolution : 1.78 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

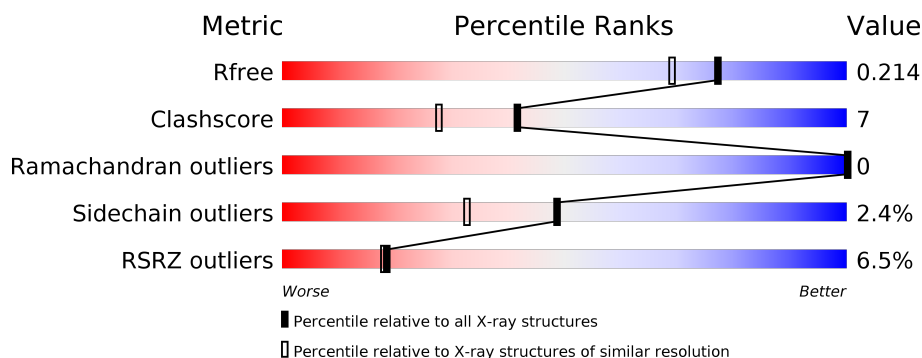
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	249	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	B	249	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	249	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	D	249	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8124 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.

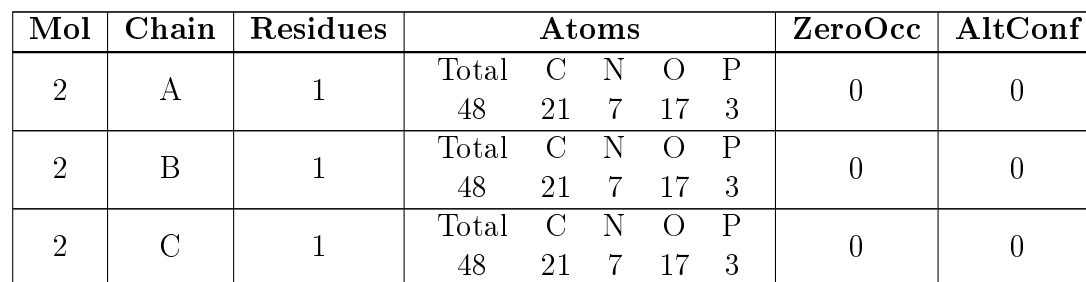
- Molecule 1 is a protein called Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O		0	0	0
			1868	1168	335	365				
1	B	235	Total	C	N	O	S	0	0	0
			1765	1108	319	337	1			
1	C	239	Total	C	N	O	S	0	0	0
			1798	1129	323	345	1			
1	D	236	Total	C	N	O	S	0	0	0
			1773	1114	320	338	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	VAL	ILE	engineered mutation	UNP C0IR58
A	187	SER	ILE	engineered mutation	UNP C0IR58
A	188	LEU	ILE	engineered mutation	UNP C0IR58
A	205	ALA	PHE	engineered mutation	UNP C0IR58
B	91	VAL	ILE	engineered mutation	UNP C0IR58
B	187	SER	ILE	engineered mutation	UNP C0IR58
B	188	LEU	ILE	engineered mutation	UNP C0IR58
B	205	ALA	PHE	engineered mutation	UNP C0IR58
C	91	VAL	ILE	engineered mutation	UNP C0IR58
C	187	SER	ILE	engineered mutation	UNP C0IR58
C	188	LEU	ILE	engineered mutation	UNP C0IR58
C	205	ALA	PHE	engineered mutation	UNP C0IR58
D	91	VAL	ILE	engineered mutation	UNP C0IR58
D	187	SER	ILE	engineered mutation	UNP C0IR58
D	188	LEU	ILE	engineered mutation	UNP C0IR58
D	205	ALA	PHE	engineered mutation	UNP C0IR58

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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- ORTEP diagram of compound A60. The structure shows a bicyclic system consisting of a benzene ring fused to a cyclohexene ring. The benzene ring is substituted with a methoxy group (C16, O17, C18) and a hydroxyl group (C05, O06). The cyclohexene ring is substituted with a carboxylate group (C01, O01) and a hydroxyl group (C05, O06). The molecule is labeled A60.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	20	3		
3	C	1	Total	C	O	0	0
			23	20	3		

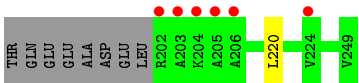
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	196	Total	O	0	0
			196	196		
4	C	167	Total	O	0	0
			167	167		
4	D	178	Total	O	0	0
			178	178		



- Molecule 1: Alcohol dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.08 Å 69.08 Å 388.99 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.71 – 1.78 24.71 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.71-1.78) 99.9 (24.71-1.78)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.78 Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.185 , 0.214 0.186 , 0.214	Depositor DCC
$R_{free}$ test set	2007 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.082 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NAP, A6O

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	0/1890	0.50	0/2561
1	B	0.29	0/1786	0.51	0/2417
1	C	0.30	0/1819	0.50	0/2462
1	D	0.33	0/1794	0.52	0/2428
All	All	0.30	0/7289	0.51	0/9868

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 [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	1868	0	1902	18	0
1	B	1765	0	1815	20	0
1	C	1798	0	1847	28	0
1	D	1773	0	1826	34	0
2	A	48	0	23	4	0
2	B	48	0	23	4	0
2	C	48	0	25	3	0
3	A	23	0	0	6	0
3	C	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	189	0	0	3	0
4	B	196	0	0	2	0
4	C	167	0	0	3	0
4	D	178	0	0	2	0
All	All	8124	0	7461	104	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 7.

The worst 5 of 104 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)
2:B:301:NAP:C1D	2:B:301:NAP:O4D	1.63	1.10
1:D:1:MET:H3	1:D:5:LEU:HD13	1.14	1.08
1:D:1:MET:N	1:D:5:LEU:HD13	1.72	1.05
1:C:15:ASN:ND2	1:C:42:GLU:HG2	1.82	0.94
1:B:202:ARG:HG2	1:B:203:ALA:H	1.31	0.94

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	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
1	B	231/249 (93%)	225 (97%)	6 (3%)	0	100	100
1	C	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
1	D	232/249 (93%)	228 (98%)	4 (2%)	0	100	100
All	All	944/996 (95%)	920 (98%)	24 (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	193/194 (100%)	188 (97%)	5 (3%)	46	29
1	B	181/194 (93%)	176 (97%)	5 (3%)	43	27
1	C	185/194 (95%)	181 (98%)	4 (2%)	52	36
1	D	182/194 (94%)	178 (98%)	4 (2%)	52	36
All	All	741/776 (96%)	723 (98%)	18 (2%)	49	33

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	ARG
1	B	204	LYS
1	D	1	MET
1	B	148	ASP
1	B	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	C	15	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	A6O	C	302	-	25,25,25	4.17	13 (52%)	28,36,36	1.78	5 (17%)
2	NAP	B	301	-	45,52,52	4.53	15 (33%)	56,80,80	2.04	9 (16%)
2	NAP	A	301	-	45,52,52	4.50	14 (31%)	56,80,80	2.07	9 (16%)
2	NAP	C	301	-	45,52,52	0.83	1 (2%)	56,80,80	1.09	3 (5%)
3	A6O	A	302	-	25,25,25	4.16	15 (60%)	28,36,36	1.69	4 (14%)

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	A6O	C	302	-	-	6/11/38/38	0/3/3/3
2	NAP	B	301	-	-	11/31/67/67	0/5/5/5
2	NAP	A	301	-	-	7/31/67/67	0/5/5/5
2	NAP	C	301	-	-	7/31/67/67	0/5/5/5
3	A6O	A	302	-	-	8/11/38/38	0/3/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	O4D-C1D	16.35	1.63	1.41
2	B	301	NAP	O4B-C1B	15.45	1.62	1.41
2	A	301	NAP	C2D-C1D	-15.26	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	O4B-C1B	15.23	1.62	1.41
2	A	301	NAP	O4D-C1D	15.14	1.62	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	C5A-C6A-N6A	10.08	135.67	120.35
2	B	301	NAP	C5A-C6A-N6A	9.65	135.02	120.35
2	A	301	NAP	N6A-C6A-N1A	-7.08	103.88	118.57
2	B	301	NAP	N6A-C6A-N1A	-6.57	104.95	118.57
3	A	302	A6O	C03-C02-C07	-6.24	103.86	109.25

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	A6O	C10-C11-C12-C13
3	C	302	A6O	C10-C11-C12-C23
3	C	302	A6O	C02-C07-C08-C09
2	B	301	NAP	C5B-O5B-PA-O1A
2	B	301	NAP	C5B-O5B-PA-O2A

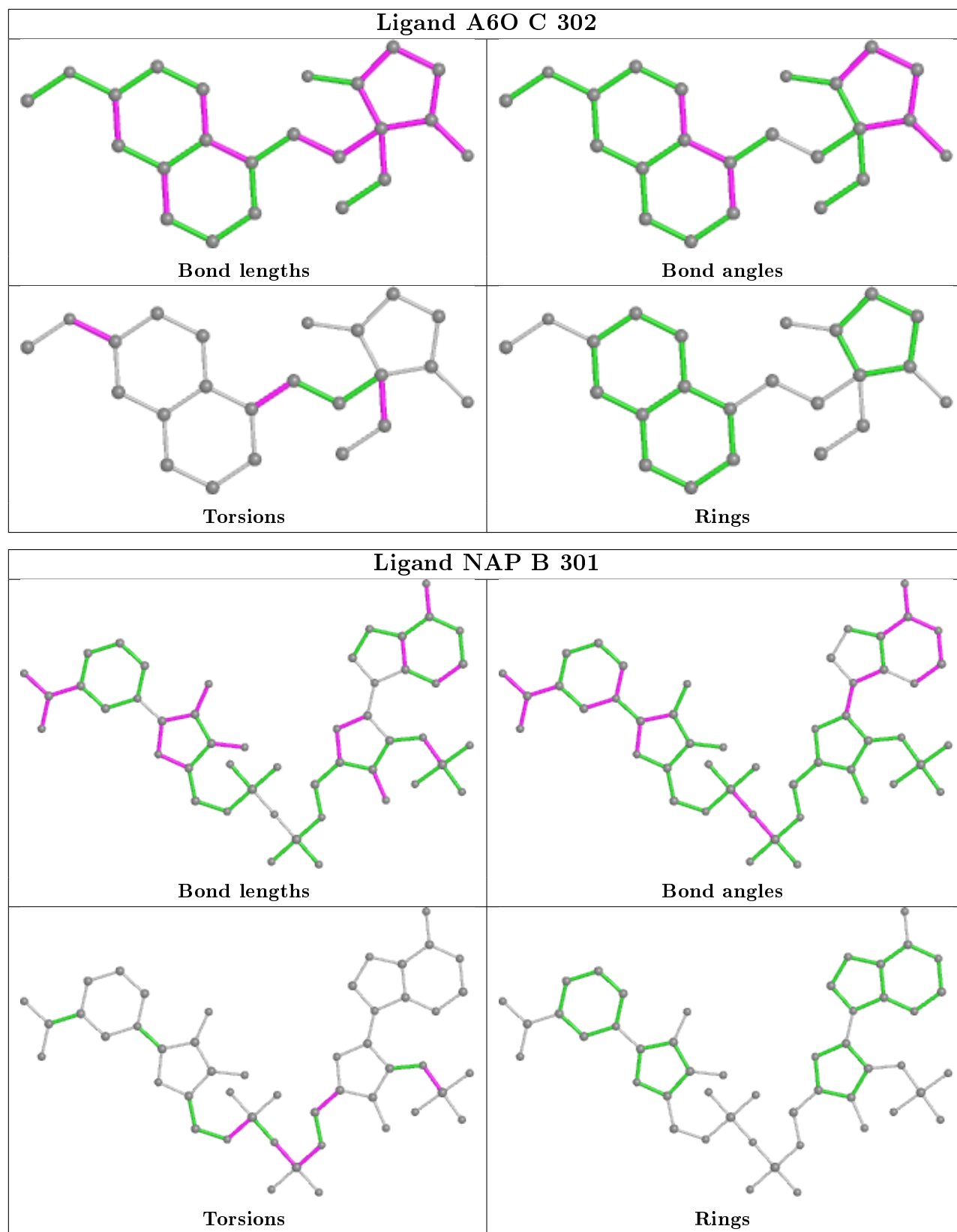
There are no ring outliers.

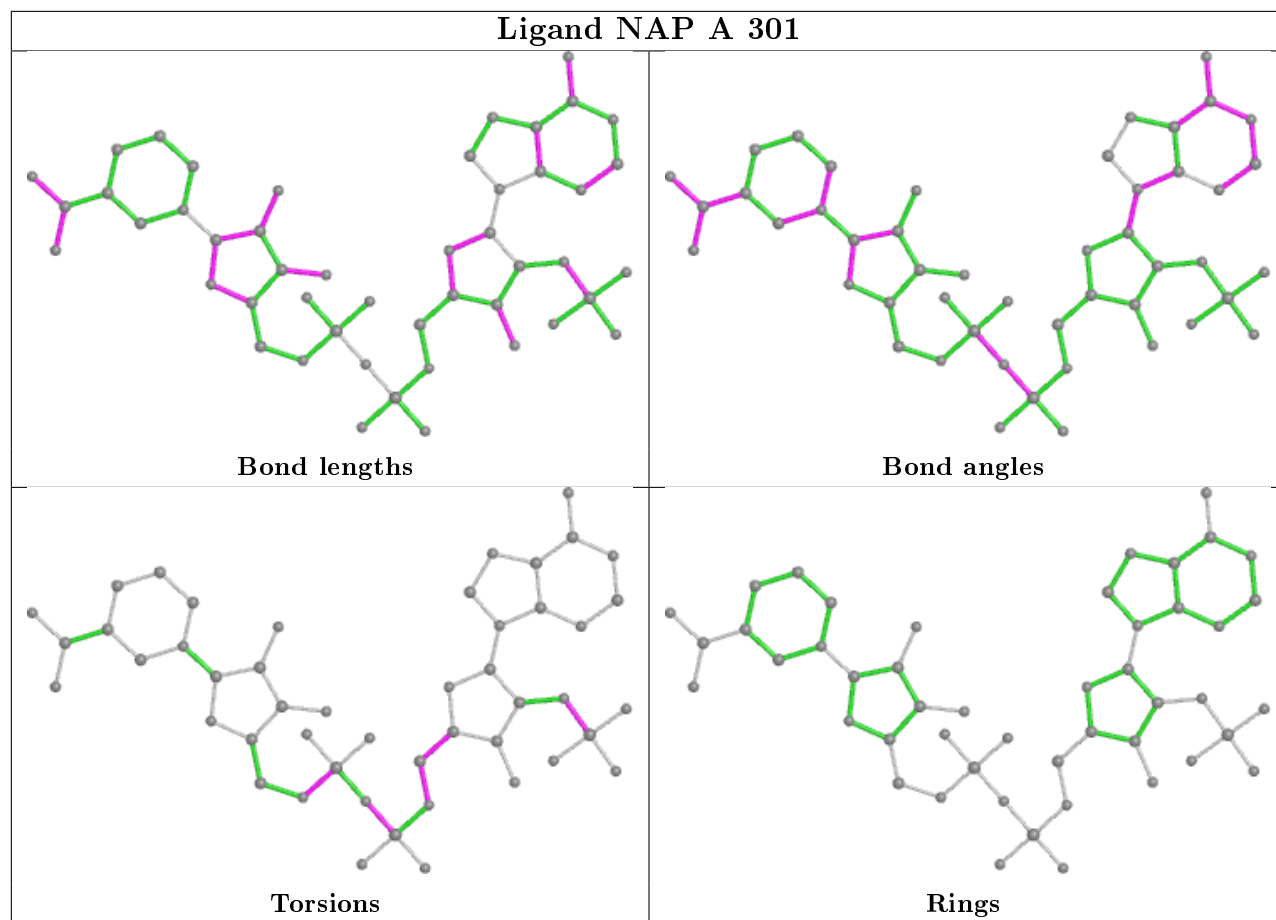
4 monomers are involved in 17 short contacts:

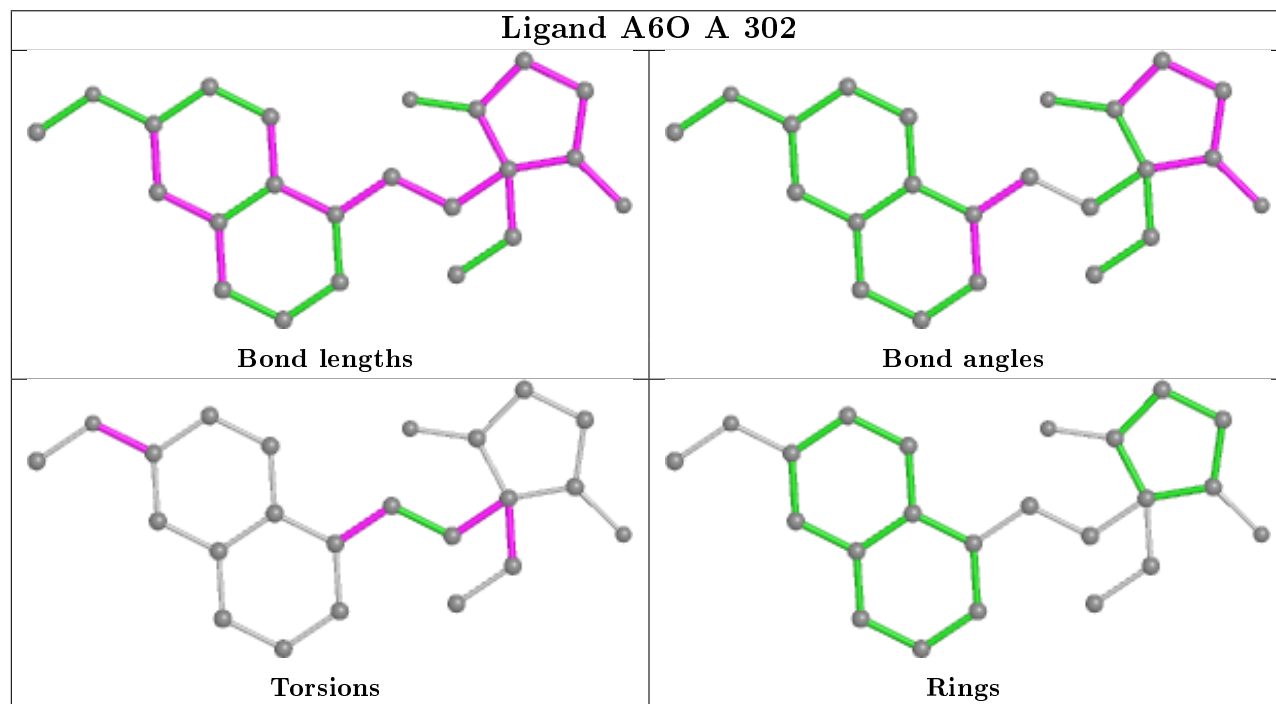
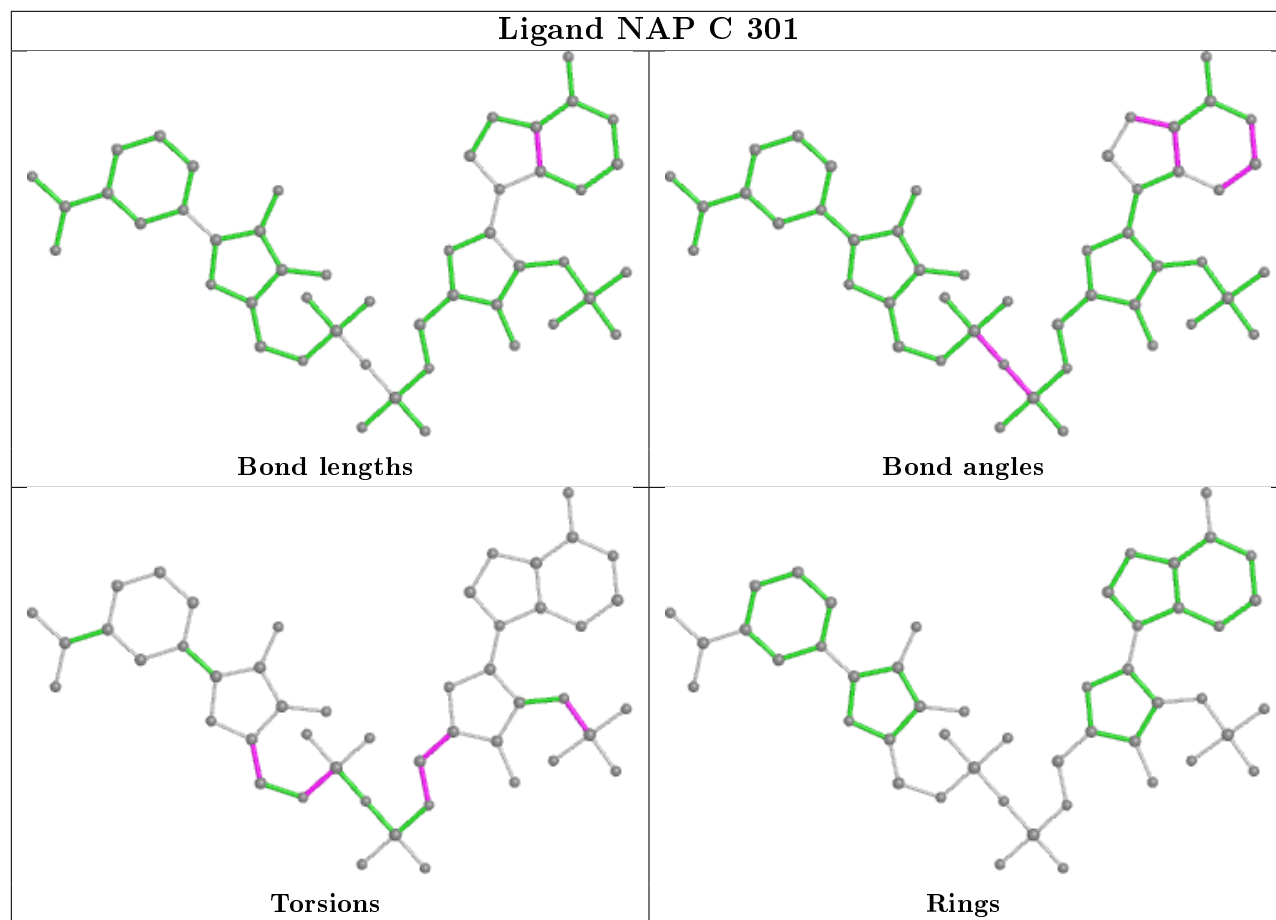
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	4	0
2	A	301	NAP	4	0
2	C	301	NAP	3	0
3	A	302	A6O	6	0

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 than 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.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	248/249 (99%)	0.14	20 (8%) 12 11	18, 27, 62, 80	0
1	B	235/249 (94%)	0.05	8 (3%) 45 44	18, 26, 44, 77	0
1	C	239/249 (95%)	0.29	14 (5%) 22 21	18, 30, 53, 98	0
1	D	236/249 (94%)	0.31	20 (8%) 10 10	20, 31, 54, 81	0
All	All	958/996 (96%)	0.20	62 (6%) 18 18	18, 28, 54, 98	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186	PRO	9.8
1	D	1	MET	9.4
1	C	188	LEU	9.1
1	C	186	PRO	9.0
1	D	188	LEU	8.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

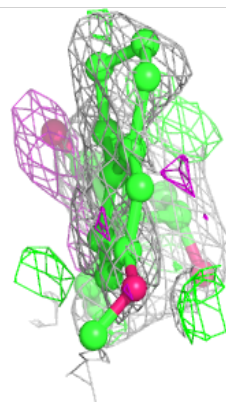
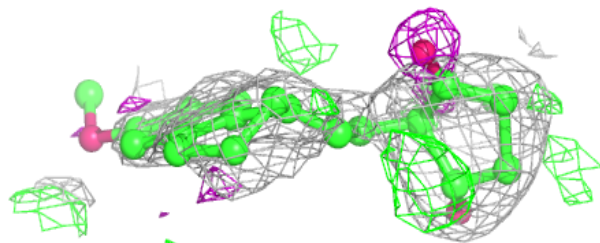
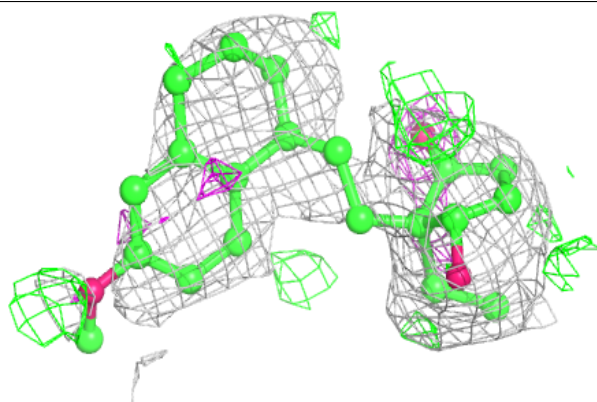
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A6O	A	302	23/23	0.47	0.31	53,68,72,89	0
3	A6O	C	302	23/23	0.49	0.29	61,77,86,92	0
2	NAP	C	301	48/48	0.75	0.22	42,59,77,92	0
2	NAP	B	301	48/48	0.85	0.16	33,47,76,92	0
2	NAP	A	301	48/48	0.87	0.17	39,56,81,89	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.

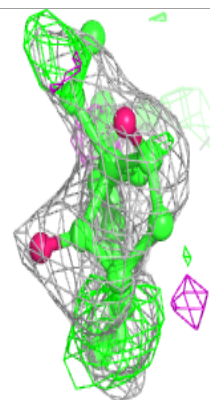
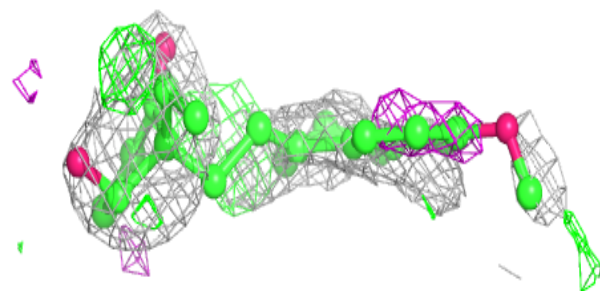
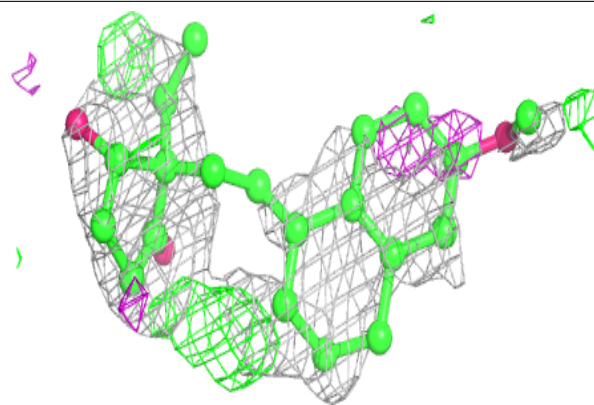
**Electron density around A6O A 302:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

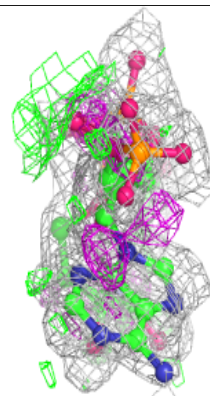
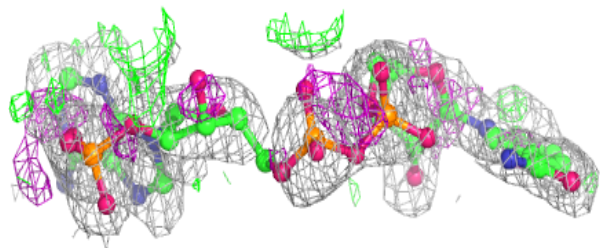
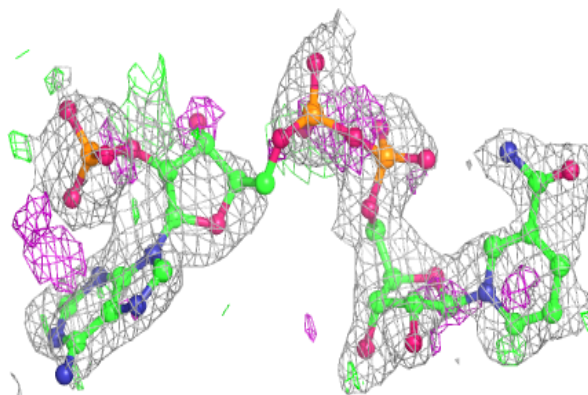


**Electron density around A6O C 302:**

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

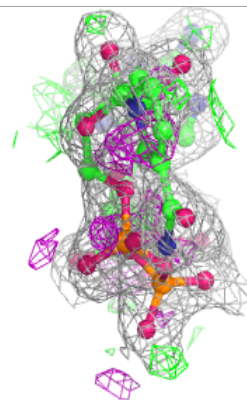
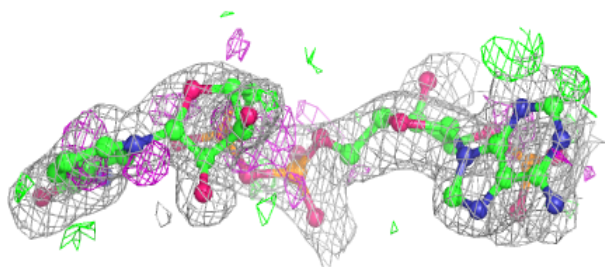
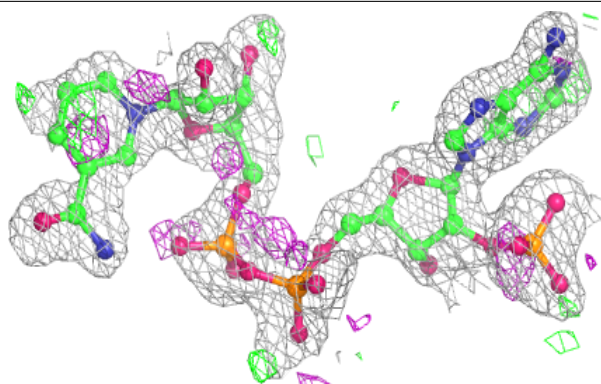
**Electron density around NAP C 301:**

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

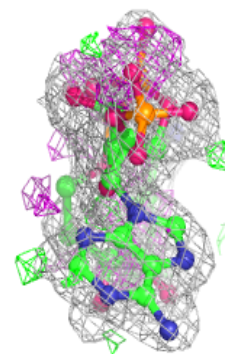
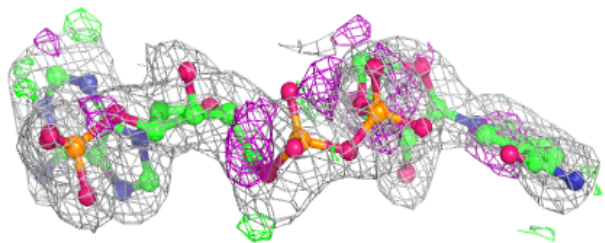
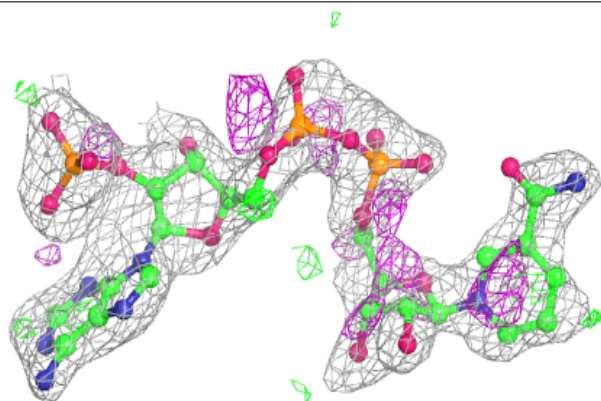


**Electron density around NAP B 301:**

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

**Electron density around NAP A 301:**

$2mF_o-DF_c$  (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.