



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 03:33 pm BST

PDB ID : 2GN6  
Title : Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADP and UDP-GlcNAc  
Authors : Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.  
Deposited on : 2006-04-09  
Resolution : 2.70 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

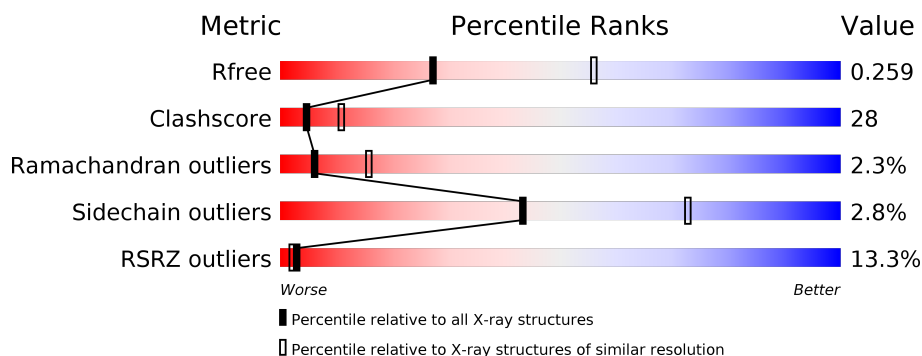
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	344	<div> <div>15%</div> <div>51%</div> <div>42%</div> <div>• •</div> </div>
1	B	344	<div> <div>10%</div> <div>56%</div> <div>36%</div> <div>• 5%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	B	336	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5517 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 UDP-GlcNAc C6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2590	1656	440	479	15			
1	B	327	Total	C	N	O	S	0	0	0
			2573	1647	436	475	15			

There are 22 discrepancies between the modelled and reference sequences:

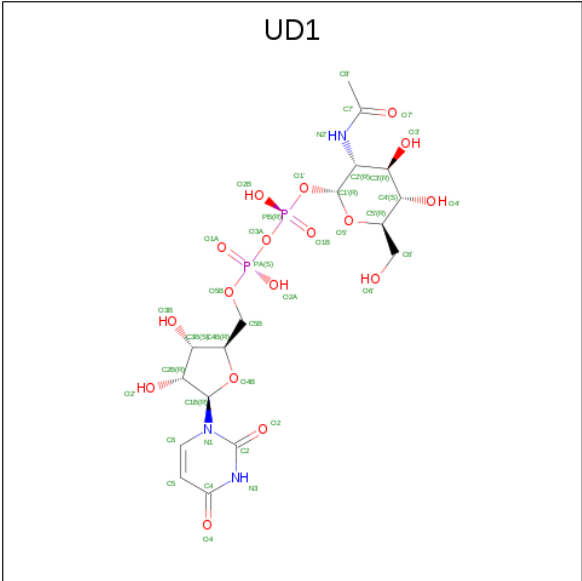
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP O25511
A	-9	HIS	-	EXPRESSION TAG	UNP O25511
A	-8	HIS	-	EXPRESSION TAG	UNP O25511
A	-7	HIS	-	EXPRESSION TAG	UNP O25511
A	-6	HIS	-	EXPRESSION TAG	UNP O25511
A	-5	HIS	-	EXPRESSION TAG	UNP O25511
A	-4	HIS	-	EXPRESSION TAG	UNP O25511
A	-3	GLY	-	cloning artifact	UNP O25511
A	-2	SER	-	cloning artifact	UNP O25511
A	-1	MET	-	cloning artifact	UNP O25511
A	0	SER	-	cloning artifact	UNP O25511
B	-10	MET	-	cloning artifact	UNP O25511
B	-9	HIS	-	EXPRESSION TAG	UNP O25511
B	-8	HIS	-	EXPRESSION TAG	UNP O25511
B	-7	HIS	-	EXPRESSION TAG	UNP O25511
B	-6	HIS	-	EXPRESSION TAG	UNP O25511
B	-5	HIS	-	EXPRESSION TAG	UNP O25511
B	-4	HIS	-	EXPRESSION TAG	UNP O25511
B	-3	GLY	-	cloning artifact	UNP O25511
B	-2	SER	-	cloning artifact	UNP O25511
B	-1	MET	-	cloning artifact	UNP O25511
B	0	SER	-	cloning artifact	UNP O25511

- 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>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>17</sub>P<sub>2</sub>).



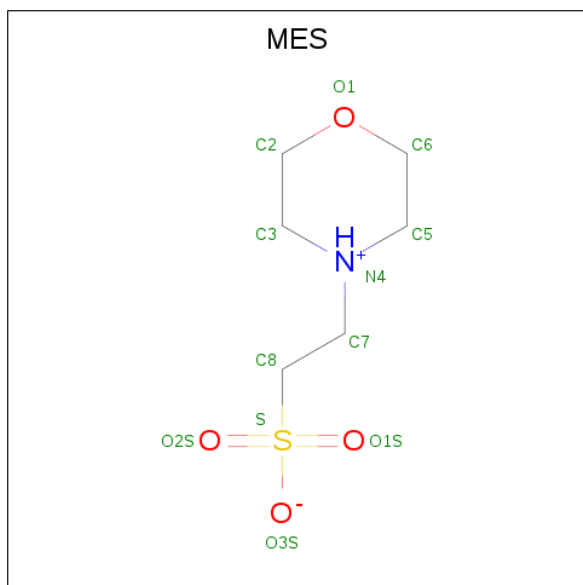
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	14	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	14	0
			39	17	3	17	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	91	Total	O	0	0
			91	91		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

15% 51% 42%

Chain A is a sequence of 100 amino acids, represented by three-letter codes. The sequence is: MET, HIS, HIS, HIS, HIS, HIS, HIS, GLY, SER, SER, MET, MET, PRO, ASN, HIS, G5, N6, K7, L8, L14, I15, T16, G17, S21, F22, G23, V27, V30, L31, T34, K35, K36, K37, K38, I39, D45, E46, L47, K48, E51, E52, E55, F56, R62, R68, N75, L78, H85, A88, A89, I90, K91, H92, N93, P94, I95, Y98, N99, P100, L101, T104, K105, I108, A117, Q125, V126, I127, S130, T131, D132, K133, A134, A135, N136, P137, L140, N156, I157, F158, K159, G160, S161, S162, V168, Y169, R170, Y171, G172, N173, V174, Y175, G176, S177, L178, G179, S180, H181, V182, F183, F184, K186, K187, L188, Y189, Q190, N191, K192, A193, S194, E195, I196, P197, I198, T199, D200, I201, R202, M203, T204, R205, F206, W207, L210, D211, F216, V217, L218, L221, K222, R223, E228, I229, F230, V231, P232, K233, I234, P235, S236, M237, K238, M239, T240, D241, L242, A243, K244, A245, W246, G247, L248, S249, T250, D251, T252, K253, I254, I255, G256, I257, R258, H264, W267, I268, P269, H274, L275, F279, E280, D281, F282, I285, T288, Q292, T293, P294, Y297, T298, L299, T300, K301, L302, H303, E304, K308, V309, A310, P311, D312, F313, S314, Y315, S316, S317, H318, N319, N320, N321, Q322, W323, L324, P325, E326, D327, D328, L329, L330, K331, L332, L333.

Chain B:

10% 56% 36% 5%

Label	Value
Q256	10%
Q257	10%
Q258	10%
Q259	10%
Q260	10%
Q261	10%
Q264	10%
Q269	10%
Q286	10%
Q292	10%
Q293	10%
Q294	10%
Q295	10%
Q296	10%
Q297	10%
Q298	10%
Q299	10%
Q300	10%
Q301	10%
Q307	10%
S316	10%
S317	10%
H318	10%
N319	10%
L324	10%
E325	10%
P326	10%
D327	10%
D328	10%
L329	10%
L330	10%
L331	10%
L332	10%
L333	10%
R178	10%
G179	10%
S180	10%
H181	10%
V182	10%
P183	10%
F184	10%
F185	10%
K186	10%
K187	10%
L188	10%
V189	10%
Q190	10%
N191	10%
E192	10%
F193	10%
A194	10%
S195	10%
E196	10%
I197	10%
P198	10%
T199	10%
D200	10%
L201	10%
R202	10%
M203	10%
T204	10%
R205	10%
F206	10%
M207	10%
L210	10%
V214	10%
M224	10%
E228	10%
L234	10%
M237	10%
K238	10%
M239	10%
T240	10%
D241	10%
L242	10%
A243	10%
P244	10%
A245	10%
L246	10%
A247	10%
P248	10%
N249	10%
T250	10%
P251	10%
T252	10%
K253	10%
L254	10%
T255	10%
C84	10%
I85	10%
H86	10%
A87	10%
H82	10%
V93	10%
P94	10%
I95	10%
A96	10%
S97	10%
P100	10%
L101	10%
K105	10%
T106	10%
M109	10%
G110	10%
L119	10%
K120	10%
N121	10%
A122	10%
I123	10%
S124	10%
Q125	10%
V126	10%
L129	10%
S130	10%
T131	10%
D132	10%
N136	10%
P137	10%
I138	10%
N139	10%
L140	10%
T144	10%
F158	10%
K159	10%
G160	10%
S161	10%
S162	10%
Q163	10%
T164	10%
V168	10%
I171	10%
G172	10%
M173	10%
V174	10%
V175	10%
G176	10%
H82	10%
I82	10%
L82	10%
P82	10%
T82	10%
A82	10%
S82	10%
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V82	10%
F82	10%
P82	10%
T82	10%
A82	10%
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K82	10%
V82	10%
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V82	10%
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V82	10%
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S82	10%
M82	10%
I82	10%
G82	10%
K82	10%
V82	10%
F82	10%
P82	10%
T82	10%
A82	10%
S82	10%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.85Å 109.85Å 107.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.70) 97.7 (48.95-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.43 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.269 0.196 , 0.259	Depositor DCC
$R_{free}$ test set	2005 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5517	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 5.07% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, UD1, MES

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	0.35	0/2641	0.62	0/3568
1	B	0.36	0/2624	0.63	0/3545
All	All	0.36	0/5265	0.62	0/7113

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2590	0	2641	165	0
1	B	2573	0	2627	134	0
2	A	48	0	25	5	0
2	B	48	0	25	3	0
3	A	39	0	25	1	0
3	B	39	0	25	0	0
4	B	12	0	13	0	0
5	A	77	0	0	4	0
5	B	91	0	0	0	0
All	All	5517	0	5381	299	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 28.

The worst 5 of 299 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:198:ILE:HG22	1:A:199:THR:H	1.31	0.92
1:A:223:ARG:HA	1:A:301:LYS:HB2	1.56	0.88
1:A:176:GLY:HA2	1:A:183:PRO:HD3	1.54	0.87
1:B:8:LEU:HD22	1:B:13:ILE:HD11	1.56	0.86
1:A:186:LYS:HG2	1:A:246:LEU:HD22	1.58	0.84

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	327/344 (95%)	283 (86%)	36 (11%)	8 (2%)	6	15
1	B	325/344 (94%)	298 (92%)	20 (6%)	7 (2%)	6	17
All	All	652/688 (95%)	581 (89%)	56 (9%)	15 (2%)	6	16

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	178	ARG
1	A	247	ALA
1	A	308	LYS
1	B	254	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/304 (95%)	282 (97%)	8 (3%)	43	73
1	B	288/304 (95%)	280 (97%)	8 (3%)	43	73
All	All	578/608 (95%)	562 (97%)	16 (3%)	43	73

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	LEU
1	B	10	ASN
1	B	203	MET
1	A	244	LYS
1	B	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	B	35	ASN
1	B	286	GLN
1	A	322	GLN
1	B	10	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	UD1	A	335	-	34,41,41	1.30	3 (8%)	45,62,62	1.51	3 (6%)
3	UD1	B	335	-	34,41,41	1.36	3 (8%)	45,62,62	1.52	3 (6%)
4	MES	B	336	-	12,12,12	0.93	1 (8%)	14,16,16	1.03	0
2	NAP	A	334	-	45,52,52	1.70	12 (26%)	56,80,80	1.66	8 (14%)
2	NAP	B	334	-	45,52,52	1.74	11 (24%)	56,80,80	1.64	8 (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	UD1	A	335	-	-	11/24/63/63	0/3/3/3
3	UD1	B	335	-	-	9/24/63/63	0/3/3/3
4	MES	B	336	-	-	2/6/14/14	0/1/1/1
2	NAP	A	334	-	-	4/31/67/67	0/5/5/5
2	NAP	B	334	-	-	2/31/67/67	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	NAP	C2N-N1N	4.23	1.40	1.35
3	B	335	UD1	C4-N3	4.18	1.40	1.33
3	A	335	UD1	C4-N3	3.98	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAP	C2N-N1N	3.89	1.39	1.35
2	B	334	NAP	P2B-O1X	3.58	1.62	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	335	UD1	O5'-C1'-O1'	-6.69	102.61	111.36
3	A	335	UD1	O5'-C1'-O1'	-6.53	102.83	111.36
2	A	334	NAP	C6N-N1N-C2N	6.35	127.76	121.97
2	B	334	NAP	C6N-N1N-C2N	6.18	127.61	121.97
2	B	334	NAP	C3N-C2N-N1N	-4.93	115.61	120.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

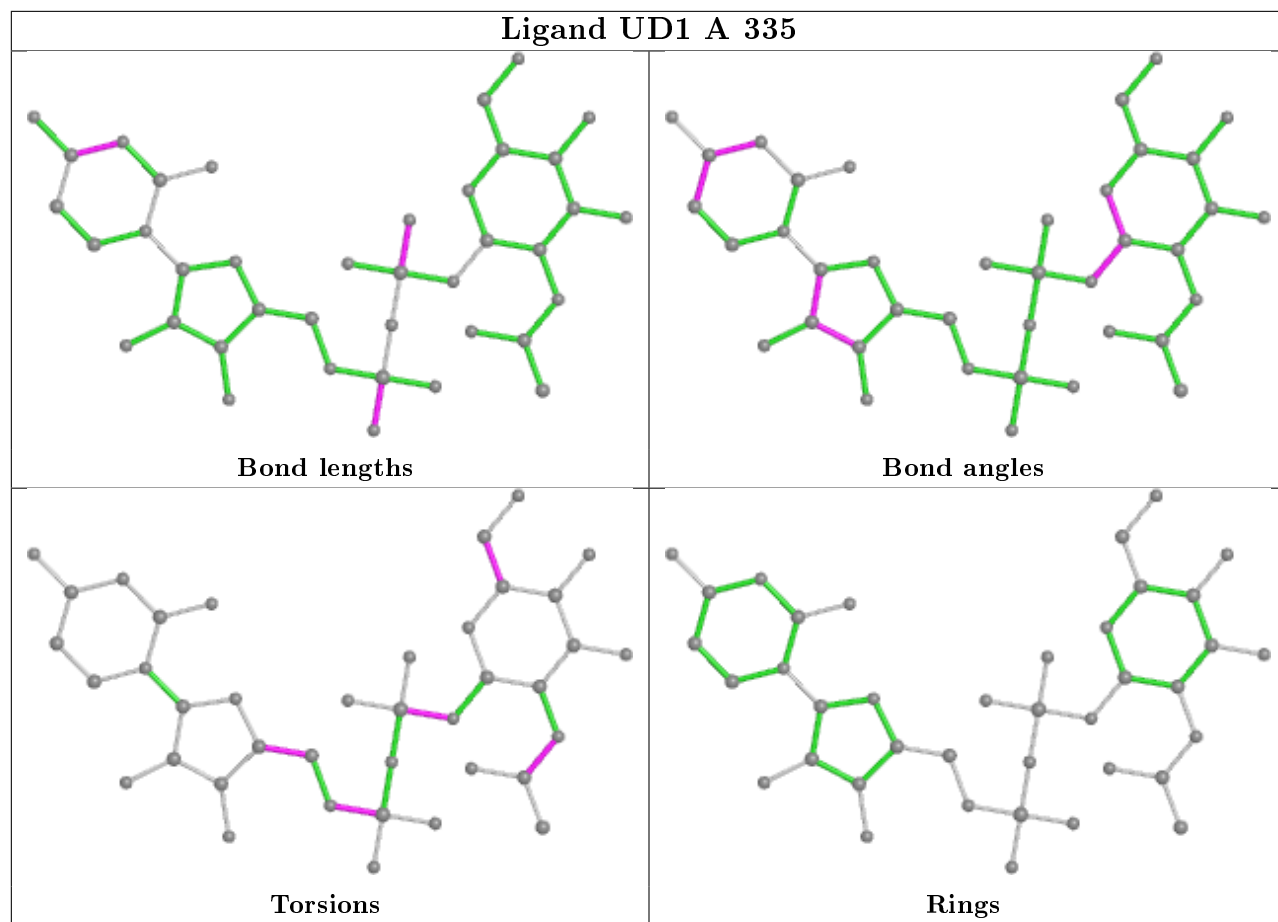
Mol	Chain	Res	Type	Atoms
3	A	335	UD1	C8'-C7'-N2'-C2'
3	A	335	UD1	O7'-C7'-N2'-C2'
3	A	335	UD1	C1'-O1'-PB-O3A
3	A	335	UD1	O4B-C4B-C5B-O5B
3	A	335	UD1	C5B-O5B-PA-O1A

There are no ring outliers.

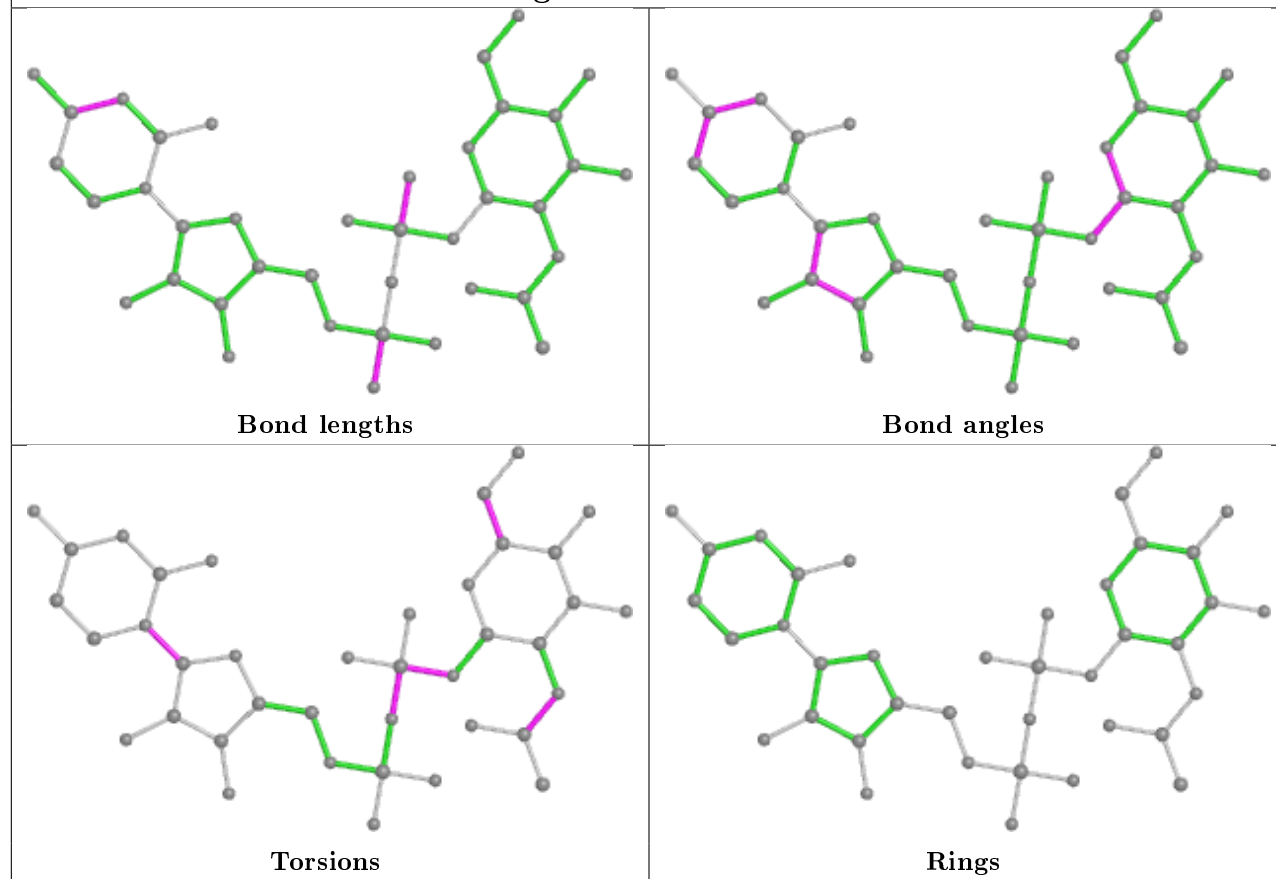
3 monomers are involved in 9 short contacts:

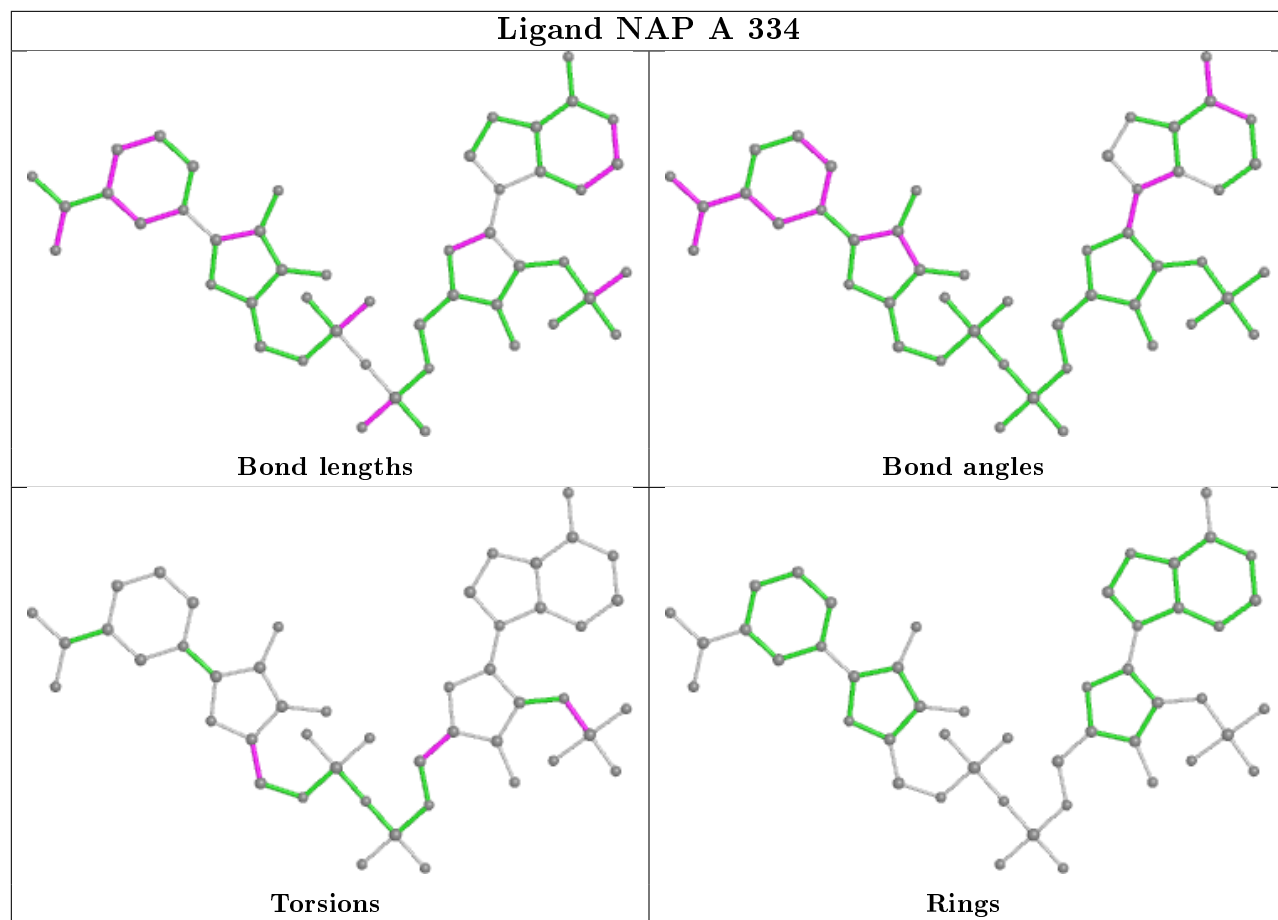
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	335	UD1	1	0
2	A	334	NAP	5	0
2	B	334	NAP	3	0

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 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.

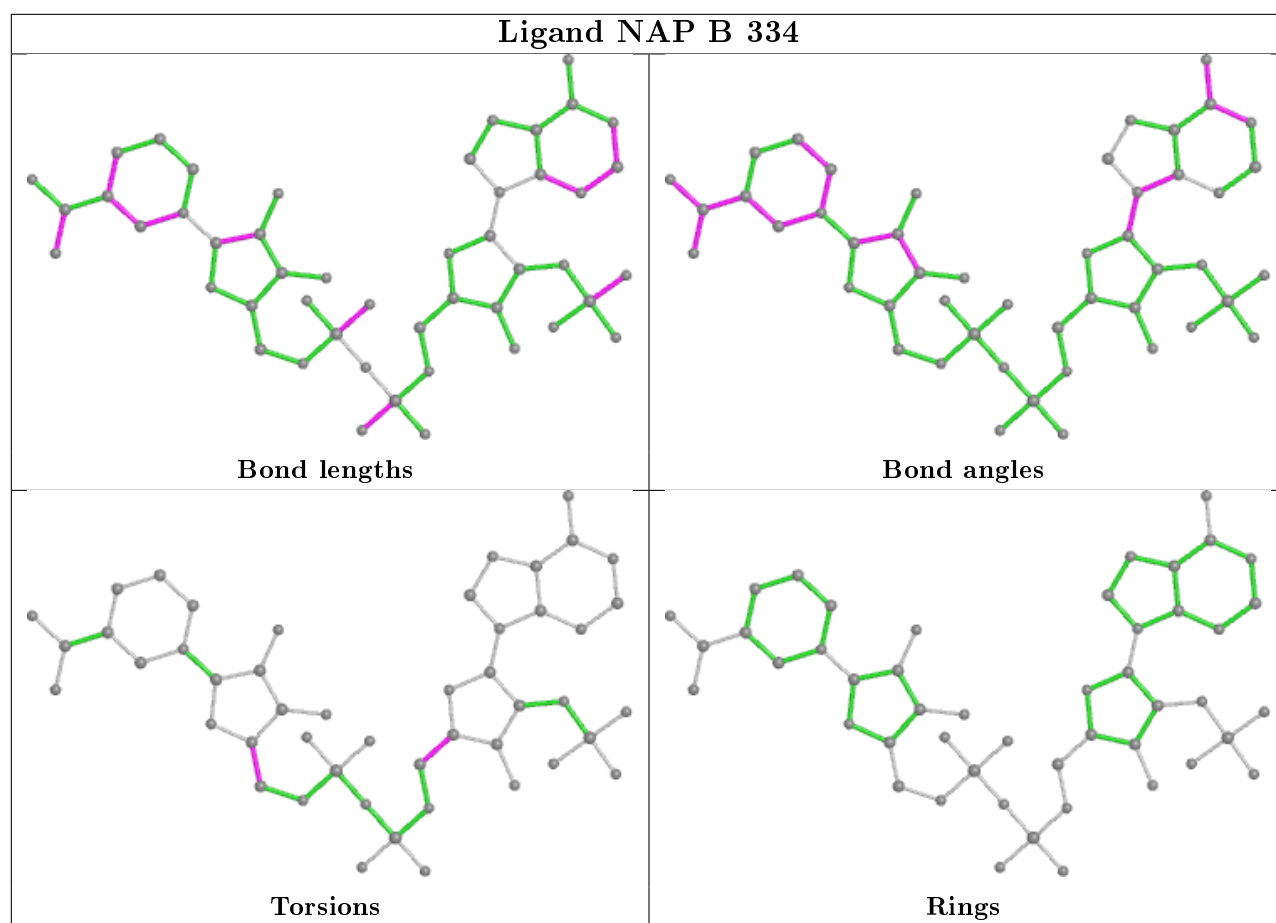


## Ligand UD1 B 335









## 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	329/344 (95%)	0.53	52 (15%) 2 1	5, 26, 80, 80	0
1	B	327/344 (95%)	0.23	35 (10%) 6 4	5, 22, 76, 80	0
All	All	656/688 (95%)	0.38	87 (13%) 3 2	5, 24, 80, 80	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	11.3
1	A	161	SER	8.2
1	A	247	ALA	8.1
1	A	243	ALA	8.0
1	A	248	PRO	7.9

### 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](#)

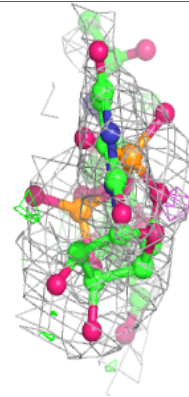
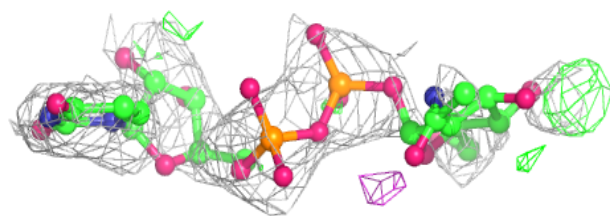
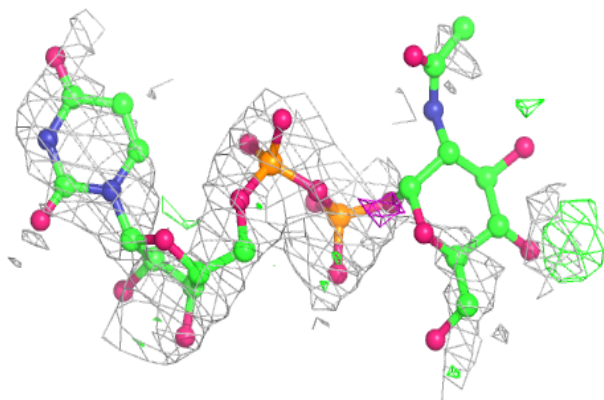
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
4	MES	B	336	12/12	0.66	0.46	78,80,80,80	0
3	UD1	A	335	39/39	0.81	0.27	75,79,80,80	14
3	UD1	B	335	39/39	0.86	0.21	56,61,72,72	14
2	NAP	B	334	48/48	0.96	0.17	13,24,49,51	0
2	NAP	A	334	48/48	0.97	0.16	7,22,40,42	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.

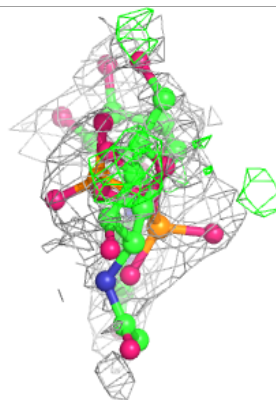
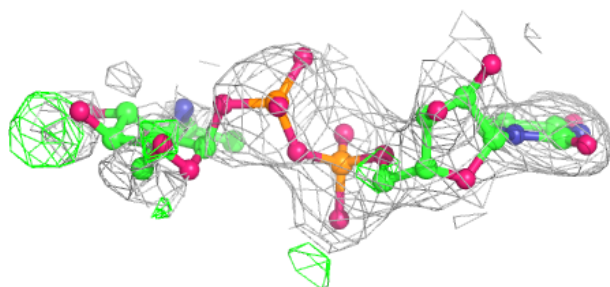
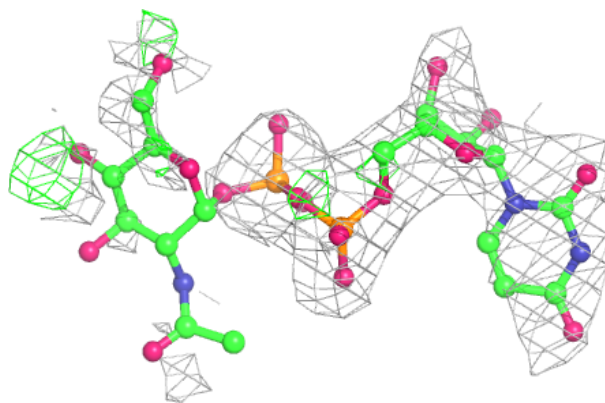
**Electron density around UD1 A 335:**

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)

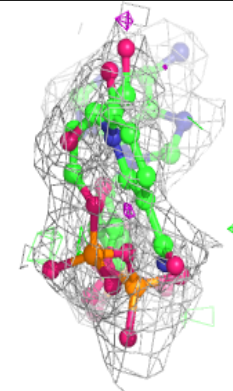
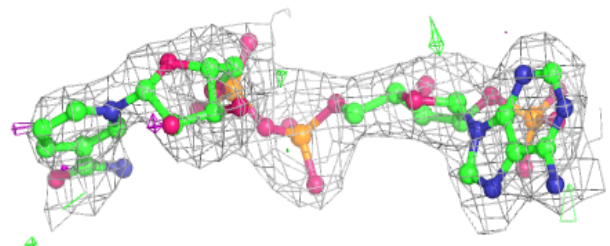
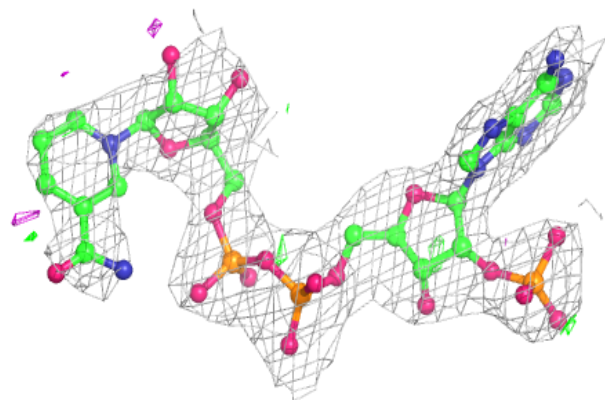


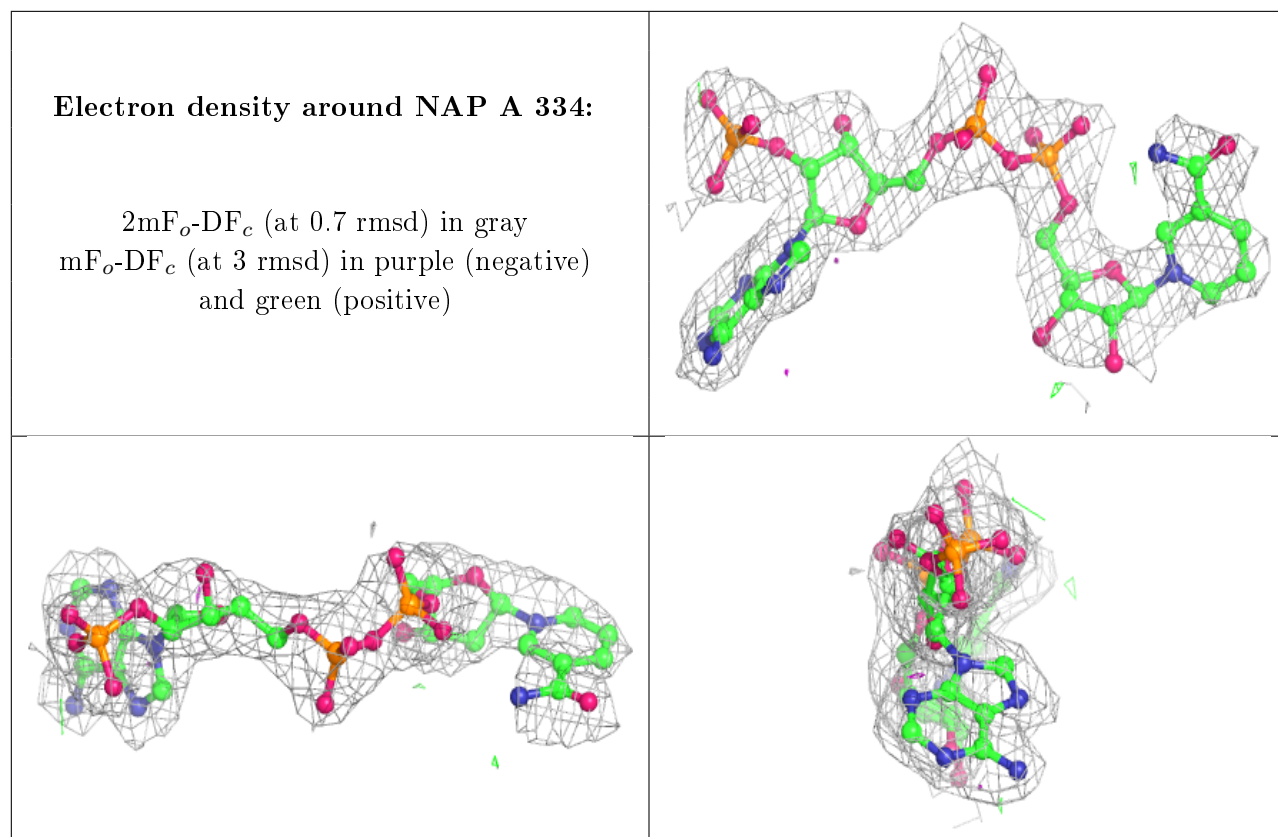
**Electron density around UD1 B 335:**

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

**Electron density around NAP B 334:**

$2mF_o-DF_c$  (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.