Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:41 am BST

PDB ID	:	6R0P
Title	:	Getah virus macro domain in complex with ADPr in double open conformation
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Deposited on	:	2019-03-13
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

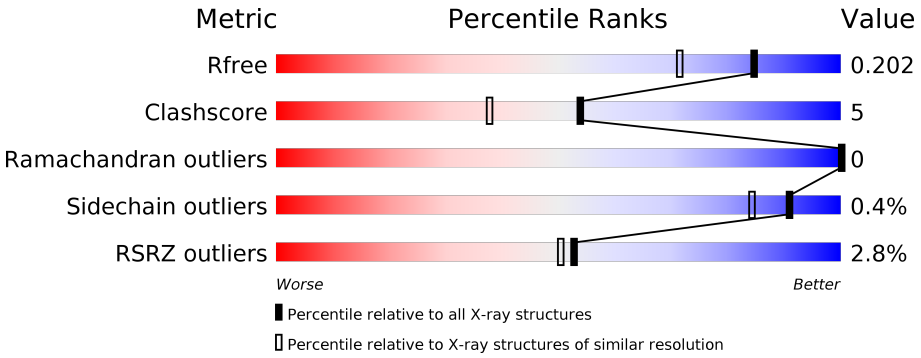
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 >=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	168	2% 88% 7% 5%
1	B	168	3% 88% 8% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2870 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.

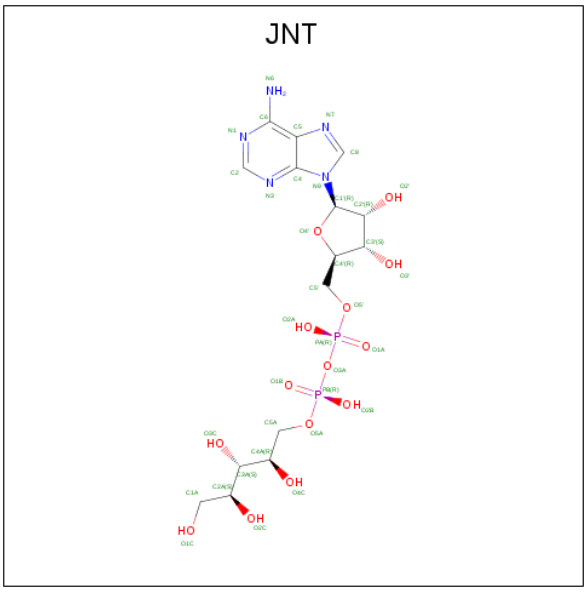
- Molecule 1 is a protein called Non-structural polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	9	0
			1218	760	220	231	7			
1	B	161	Total	C	N	O	S	0	6	0
			1221	758	222	235	6			

There are 16 discrepancies between the modelled and reference sequences:

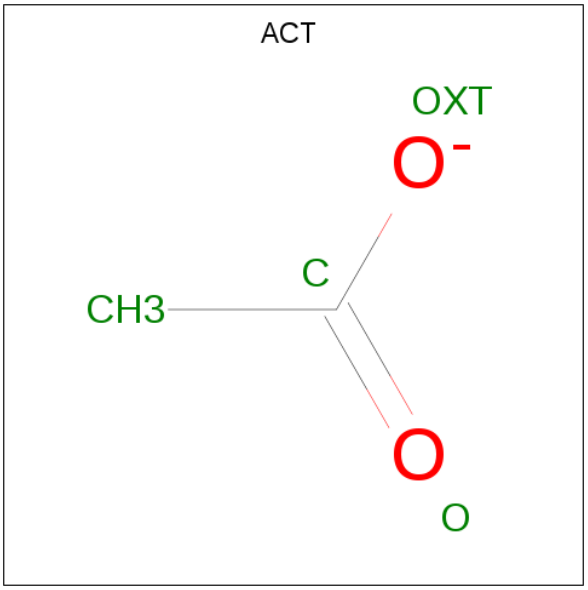
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP A0A143SL92
A	0	LYS	-	expression tag	UNP A0A143SL92
A	161	HIS	-	expression tag	UNP A0A143SL92
A	162	HIS	-	expression tag	UNP A0A143SL92
A	163	HIS	-	expression tag	UNP A0A143SL92
A	164	HIS	-	expression tag	UNP A0A143SL92
A	165	HIS	-	expression tag	UNP A0A143SL92
A	166	HIS	-	expression tag	UNP A0A143SL92
B	-1	MET	-	initiating methionine	UNP A0A143SL92
B	0	LYS	-	expression tag	UNP A0A143SL92
B	161	HIS	-	expression tag	UNP A0A143SL92
B	162	HIS	-	expression tag	UNP A0A143SL92
B	163	HIS	-	expression tag	UNP A0A143SL92
B	164	HIS	-	expression tag	UNP A0A143SL92
B	165	HIS	-	expression tag	UNP A0A143SL92
B	166	HIS	-	expression tag	UNP A0A143SL92

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {S})-2,3,4,5-tetrakis(oxidanyl)pentyl] hydrogen phosphate (three-letter code: JNT) (formula: $C_{15}H_{25}N_5O_{14}P_2$).



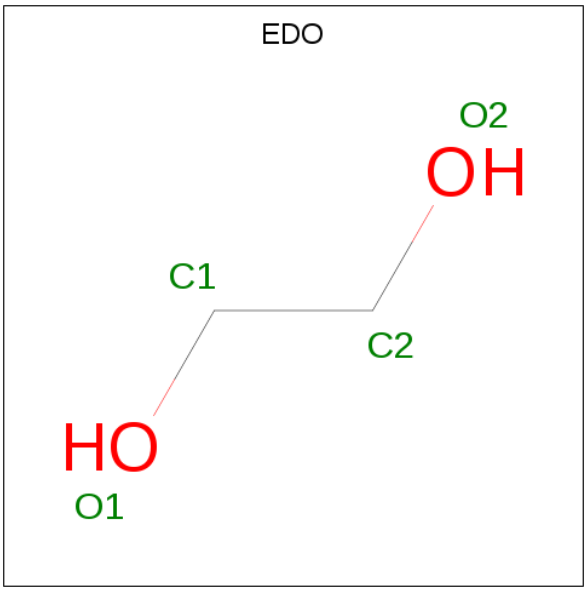
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			72	30	10	28	4		
2	B	1	Total	C	N	O	P	0	1
			72	30	10	28	4		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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



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

- Molecule 5 is water.

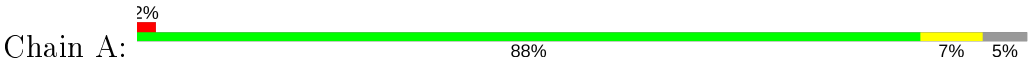
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	151	Total O 151 151	0	0
5	B	128	Total O 128 128	0	0

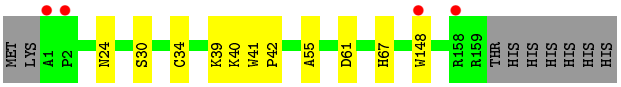
3 Residue-property plots (i)

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 (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: Non-structural polyprotein

Chain A:





- Molecule 1: Non-structural polyprotein

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.70Å 71.45Å 99.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.41 – 1.60 36.38 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (36.41-1.60) 98.8 (36.38-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.169 , 0.194 0.175 , 0.202	Depositor DCC
R_{free} test set	2576 reflections (5.83%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2870	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: ACT, EDO, JNT

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	0.65	0/1257	0.70	0/1700
1	B	0.65	0/1254	0.70	0/1697
All	All	0.65	0/2511	0.70	0/3397

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	1218	0	1251	15	0
1	B	1221	0	1243	11	0
2	A	72	0	0	9	0
2	B	72	0	0	4	0
3	A	4	0	3	1	0
4	A	4	0	6	0	0
5	A	151	0	0	2	0
5	B	128	0	0	1	0
All	All	2870	0	2503	27	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 5.

All (27) 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:34[B]:CYS:SG	2:A:201[B]:JNT:O2C	2.11	1.07
1:B:34[B]:CYS:SG	2:B:201[B]:JNT:O2C	2.43	0.76
1:A:148:TRP:CZ3	2:A:201[B]:JNT:O3'	2.47	0.67
1:A:34[B]:CYS:HG	2:A:201[B]:JNT:C2A	2.06	0.66
2:A:201[B]:JNT:C1A	2:A:201[B]:JNT:O4C	2.50	0.60
1:A:34[B]:CYS:SG	2:A:201[B]:JNT:C2A	2.91	0.56
2:B:201[B]:JNT:C1A	2:B:201[B]:JNT:O4C	2.55	0.54
1:B:132[B]:LEU:HD23	1:B:139:VAL:CG2	2.39	0.53
1:A:30:SER:OG	2:A:201[A]:JNT:C2A	2.59	0.51
1:A:30:SER:O	1:A:34[B]:CYS:SG	2.70	0.50
1:B:132[B]:LEU:HD23	1:B:139:VAL:HG21	1.94	0.50
1:A:39[B]:LYS:HG3	5:A:405:HOH:O	2.11	0.49
1:A:34[B]:CYS:SG	2:A:201[B]:JNT:C1A	3.01	0.49
1:A:148:TRP:HZ3	2:A:201[B]:JNT:O3'	1.92	0.48
1:A:40:LYS:HG2	1:A:41:TRP:CZ2	2.49	0.47
1:A:24:ASN:HB3	2:A:201[A]:JNT:O2C	2.13	0.47
1:B:118:LYS:NZ	5:B:303:HOH:O	2.48	0.47
1:B:30:SER:O	1:B:34[B]:CYS:SG	2.74	0.46
1:B:30:SER:OG	2:B:201[A]:JNT:C2A	2.64	0.45
1:B:121:VAL:HG21	1:B:148:TRP:CE2	2.53	0.44
1:B:55:ALA:HA	1:B:67:HIS:O	2.18	0.44
1:A:61:ASP:HA	3:A:202:ACT:H3	2.00	0.43
1:A:30:SER:HB2	5:A:372:HOH:O	2.18	0.43
1:A:42:PRO:HB2	1:B:127:HIS:CE1	2.54	0.43
1:A:55:ALA:HA	1:A:67:HIS:O	2.20	0.42
1:B:34[B]:CYS:SG	2:B:201[B]:JNT:C1A	3.08	0.41
1:B:43[B]:SER:OG	1:B:60:ALA:HB1	2.21	0.40

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	164/168 (98%)	163 (99%)	1 (1%)	0	100	100
1	B	164/168 (98%)	164 (100%)	0	0	100	100
All	All	328/336 (98%)	327 (100%)	1 (0%)	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	130/132 (98%)	130 (100%)	0	100	100
1	B	130/132 (98%)	129 (99%)	1 (1%)	81	70
All	All	260/264 (98%)	259 (100%)	1 (0%)	91	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	EDO	A	203	-	3,3,3	0.05	0	2,2,2	0.25	0
3	ACT	A	202	-	1,3,3	4.00	1 (100%)	0,3,3	0.00	-
2	JNT	B	201[B]	-	33,38,38	1.18	3 (9%)	38,57,57	1.42	6 (15%)
2	JNT	A	201[B]	-	33,38,38	1.17	4 (12%)	38,57,57	1.50	5 (13%)
2	JNT	A	201[A]	-	33,38,38	1.17	2 (6%)	38,57,57	1.50	6 (15%)
2	JNT	B	201[A]	-	33,38,38	1.18	2 (6%)	38,57,57	1.42	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	203	-	-	0/1/1/1	-
2	JNT	B	201[B]	-	-	14/28/48/48	0/3/3/3
2	JNT	B	201[A]	-	-	12/28/48/48	0/3/3/3
2	JNT	A	201[B]	-	-	14/28/48/48	0/3/3/3
2	JNT	A	201[A]	-	-	16/28/48/48	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	JNT	O1C-C1A	-5.01	1.21	1.42
2	B	201[A]	JNT	O1C-C1A	-4.87	1.21	1.42
2	A	201[B]	JNT	O1C-C1A	-4.71	1.22	1.42
2	B	201[B]	JNT	O1C-C1A	-4.67	1.22	1.42
3	A	202	ACT	CH3-C	4.00	1.53	1.48
2	B	201[B]	JNT	C5-C4	2.36	1.47	1.40
2	B	201[A]	JNT	C5-C4	2.35	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	JNT	C5-C4	2.14	1.46	1.40
2	A	201[B]	JNT	C5-C4	2.06	1.46	1.40
2	A	201[B]	JNT	O4'-C1'	2.01	1.43	1.41
2	A	201[B]	JNT	C2-N3	2.01	1.35	1.32
2	B	201[B]	JNT	O4'-C1'	2.01	1.43	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201[B]	JNT	O1C-C1A-C2A	5.38	122.79	111.07
2	B	201[B]	JNT	O1C-C1A-C2A	4.75	121.41	111.07
2	A	201[A]	JNT	O1C-C1A-C2A	4.05	119.90	111.07
2	B	201[A]	JNT	O1C-C1A-C2A	3.73	119.19	111.07
2	A	201[B]	JNT	N3-C2-N1	-3.57	123.11	128.68
2	A	201[A]	JNT	N3-C2-N1	-3.56	123.11	128.68
2	B	201[B]	JNT	N3-C2-N1	-3.38	123.40	128.68
2	B	201[A]	JNT	N3-C2-N1	-3.38	123.40	128.68
2	B	201[A]	JNT	C3'-C2'-C1'	2.89	105.33	100.98
2	A	201[A]	JNT	C3'-C2'-C1'	2.84	105.25	100.98
2	B	201[B]	JNT	C1'-N9-C4	-2.66	121.97	126.64
2	B	201[A]	JNT	C4-C5-N7	-2.53	106.76	109.40
2	B	201[B]	JNT	C4-C5-N7	-2.38	106.92	109.40
2	B	201[A]	JNT	C5'-C4'-C3'	-2.22	106.88	115.18
2	A	201[A]	JNT	C4-C5-N7	-2.19	107.11	109.40
2	A	201[B]	JNT	C4A-C3A-C2A	2.16	117.86	113.36
2	A	201[A]	JNT	C2'-C3'-C4'	2.11	106.75	102.64
2	A	201[B]	JNT	C1'-N9-C4	-2.10	122.94	126.64
2	A	201[A]	JNT	O2C-C2A-C1A	-2.07	104.28	109.14
2	B	201[B]	JNT	C4A-C3A-C2A	2.06	117.65	113.36
2	B	201[B]	JNT	C1A-C2A-C3A	2.01	116.77	112.41
2	A	201[B]	JNT	N6-C6-N1	2.00	122.73	118.57

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201[B]	JNT	C5'-O5'-PA-O3A
2	B	201[B]	JNT	C5'-O5'-PA-O1A
2	B	201[B]	JNT	C5'-O5'-PA-O2A
2	B	201[B]	JNT	O1C-C1A-C2A-C3A
2	B	201[B]	JNT	C1A-C2A-C3A-C4A
2	B	201[B]	JNT	O2C-C2A-C3A-O3C

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Mol	Chain	Res	Type	Atoms
2	B	201[B]	JNT	O2C-C2A-C3A-C4A
2	A	201[B]	JNT	C5'-O5'-PA-O3A
2	A	201[B]	JNT	O1C-C1A-C2A-C3A
2	A	201[B]	JNT	C1A-C2A-C3A-C4A
2	A	201[B]	JNT	O2C-C2A-C3A-O3C
2	A	201[B]	JNT	O2C-C2A-C3A-C4A
2	A	201[A]	JNT	C5'-O5'-PA-O3A
2	A	201[A]	JNT	C5'-O5'-PA-O1A
2	A	201[A]	JNT	C5'-O5'-PA-O2A
2	A	201[A]	JNT	O1C-C1A-C2A-C3A
2	A	201[A]	JNT	C1A-C2A-C3A-C4A
2	A	201[A]	JNT	O2C-C2A-C3A-O3C
2	A	201[A]	JNT	O2C-C2A-C3A-C4A
2	B	201[A]	JNT	C5'-O5'-PA-O3A
2	B	201[A]	JNT	C5'-O5'-PA-O1A
2	B	201[A]	JNT	C5'-O5'-PA-O2A
2	B	201[A]	JNT	O1C-C1A-C2A-O2C
2	B	201[A]	JNT	C1A-C2A-C3A-C4A
2	B	201[A]	JNT	O2C-C2A-C3A-O3C
2	B	201[A]	JNT	O2C-C2A-C3A-C4A
2	B	201[B]	JNT	O1C-C1A-C2A-O2C
2	A	201[B]	JNT	O1C-C1A-C2A-O2C
2	A	201[A]	JNT	O1C-C1A-C2A-O2C
2	B	201[A]	JNT	O1C-C1A-C2A-C3A
2	A	201[A]	JNT	O3C-C3A-C4A-O4C
2	A	201[A]	JNT	C2A-C3A-C4A-O4C
2	B	201[B]	JNT	C1A-C2A-C3A-O3C
2	A	201[B]	JNT	C1A-C2A-C3A-O3C
2	A	201[A]	JNT	C1A-C2A-C3A-O3C
2	B	201[A]	JNT	C1A-C2A-C3A-O3C
2	A	201[A]	JNT	O3C-C3A-C4A-C5A
2	A	201[A]	JNT	C2A-C3A-C4A-C5A
2	B	201[B]	JNT	O3C-C3A-C4A-C5A
2	A	201[B]	JNT	O3C-C3A-C4A-C5A
2	A	201[B]	JNT	O3C-C3A-C4A-O4C
2	B	201[B]	JNT	O3C-C3A-C4A-O4C
2	B	201[B]	JNT	C2A-C3A-C4A-C5A
2	A	201[B]	JNT	C2A-C3A-C4A-C5A
2	B	201[B]	JNT	PA-O3A-PB-O5A
2	A	201[B]	JNT	PA-O3A-PB-O5A
2	A	201[A]	JNT	PA-O3A-PB-O5A
2	A	201[B]	JNT	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	201[B]	JNT	C5'-O5'-PA-O2A
2	B	201[B]	JNT	C2A-C3A-C4A-O4C
2	A	201[B]	JNT	C2A-C3A-C4A-O4C
2	B	201[A]	JNT	C2A-C3A-C4A-O4C
2	A	201[A]	JNT	O4'-C4'-C5'-O5'
2	A	201[A]	JNT	C3'-C4'-C5'-O5'
2	B	201[A]	JNT	O3C-C3A-C4A-C5A
2	B	201[A]	JNT	O3C-C3A-C4A-O4C

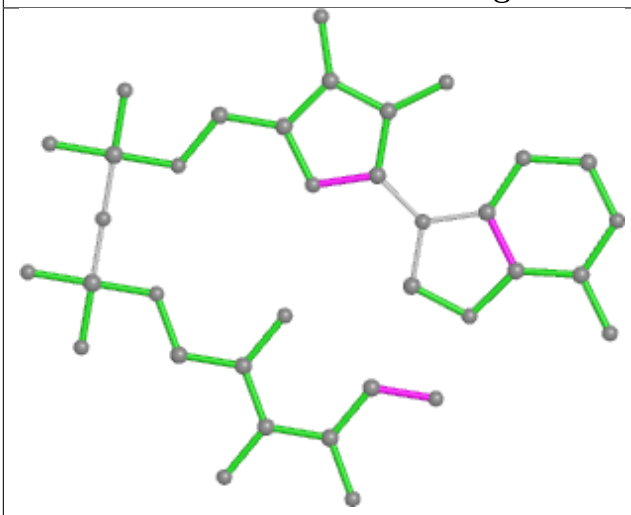
There are no ring outliers.

5 monomers are involved in 14 short contacts:

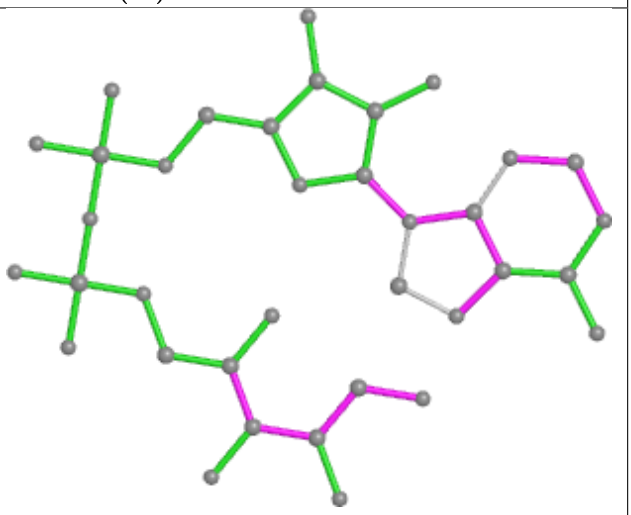
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	ACT	1	0
2	B	201[B]	JNT	3	0
2	A	201[B]	JNT	7	0
2	A	201[A]	JNT	2	0
2	B	201[A]	JNT	1	0

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.

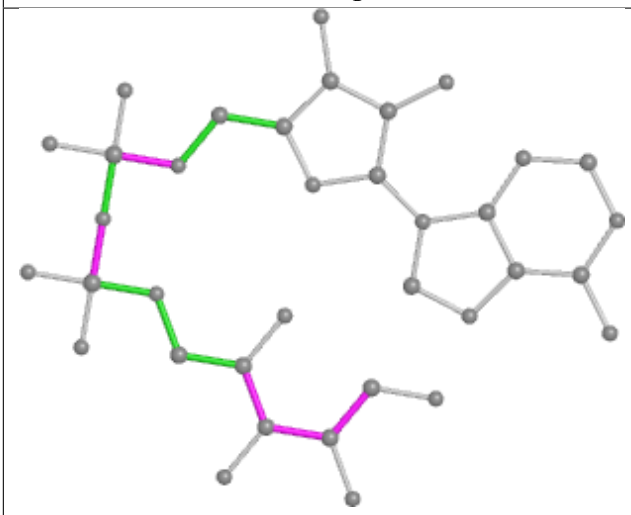
Ligand JNT B 201 (B)



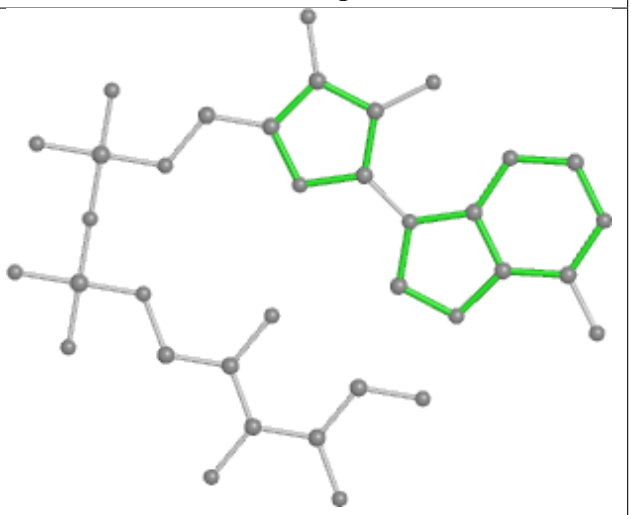
Bond lengths



Bond angles

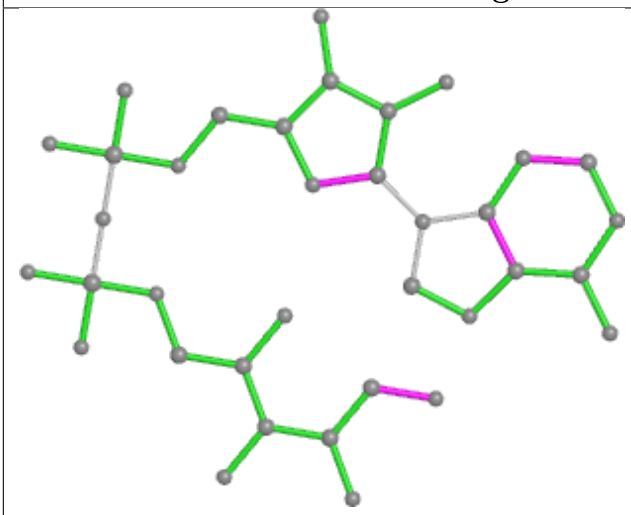


Torsions

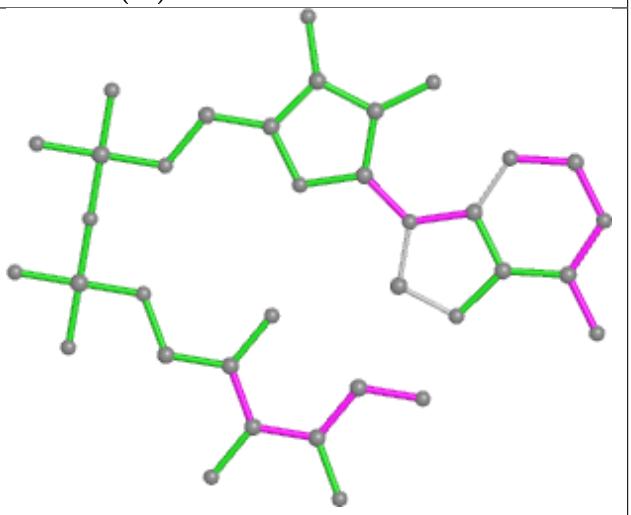


Rings

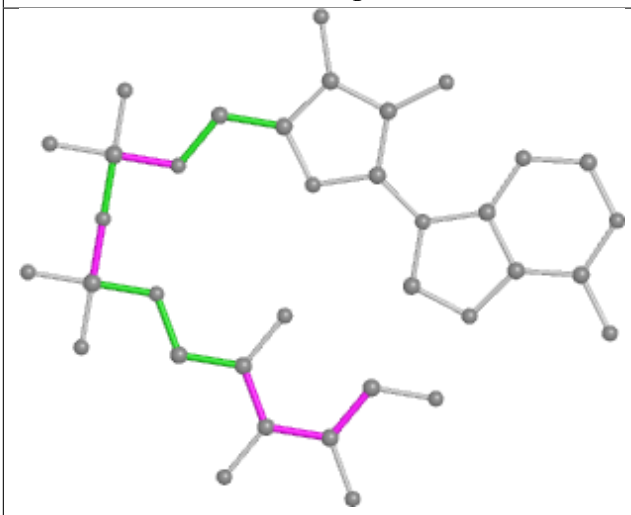
Ligand JNT A 201 (B)



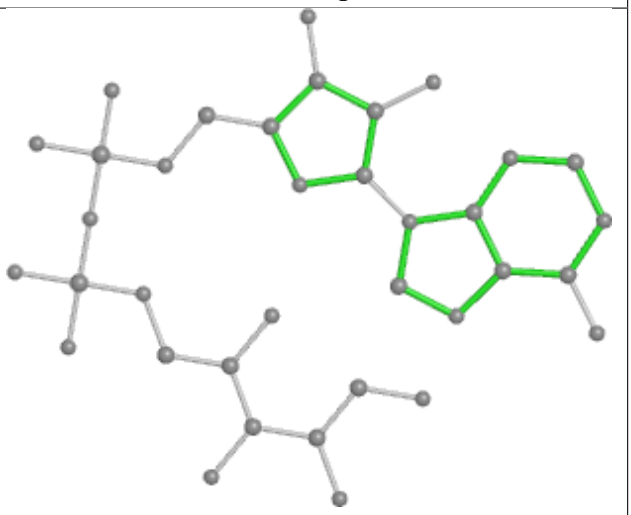
Bond lengths



Bond angles

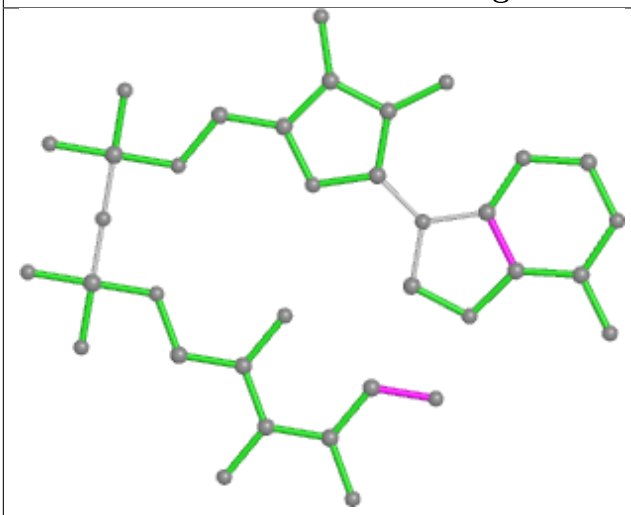


Torsions

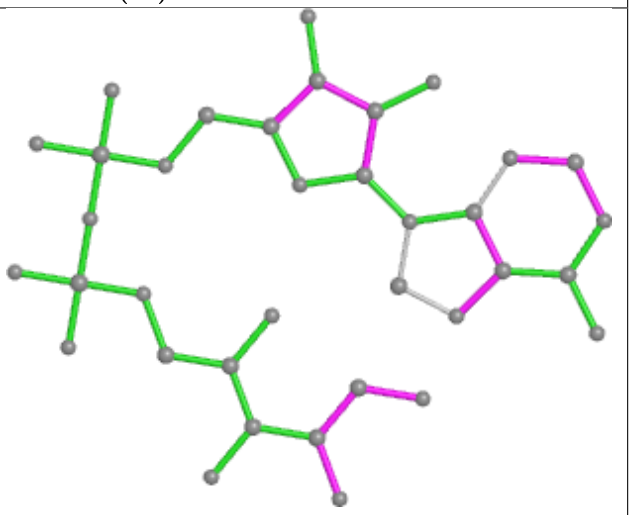


Rings

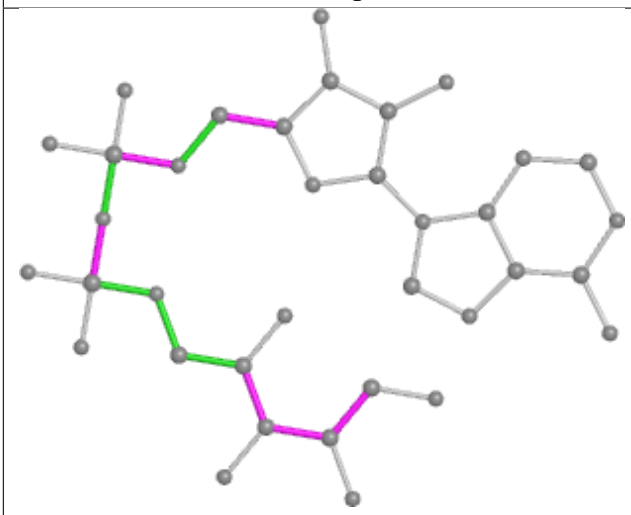
Ligand JNT A 201 (A)



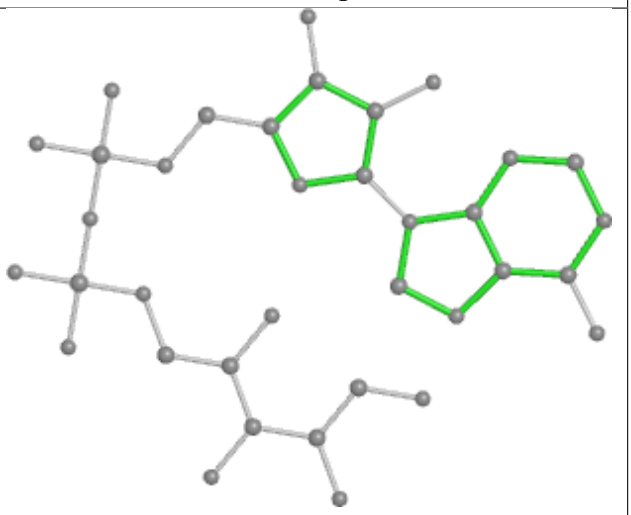
Bond lengths



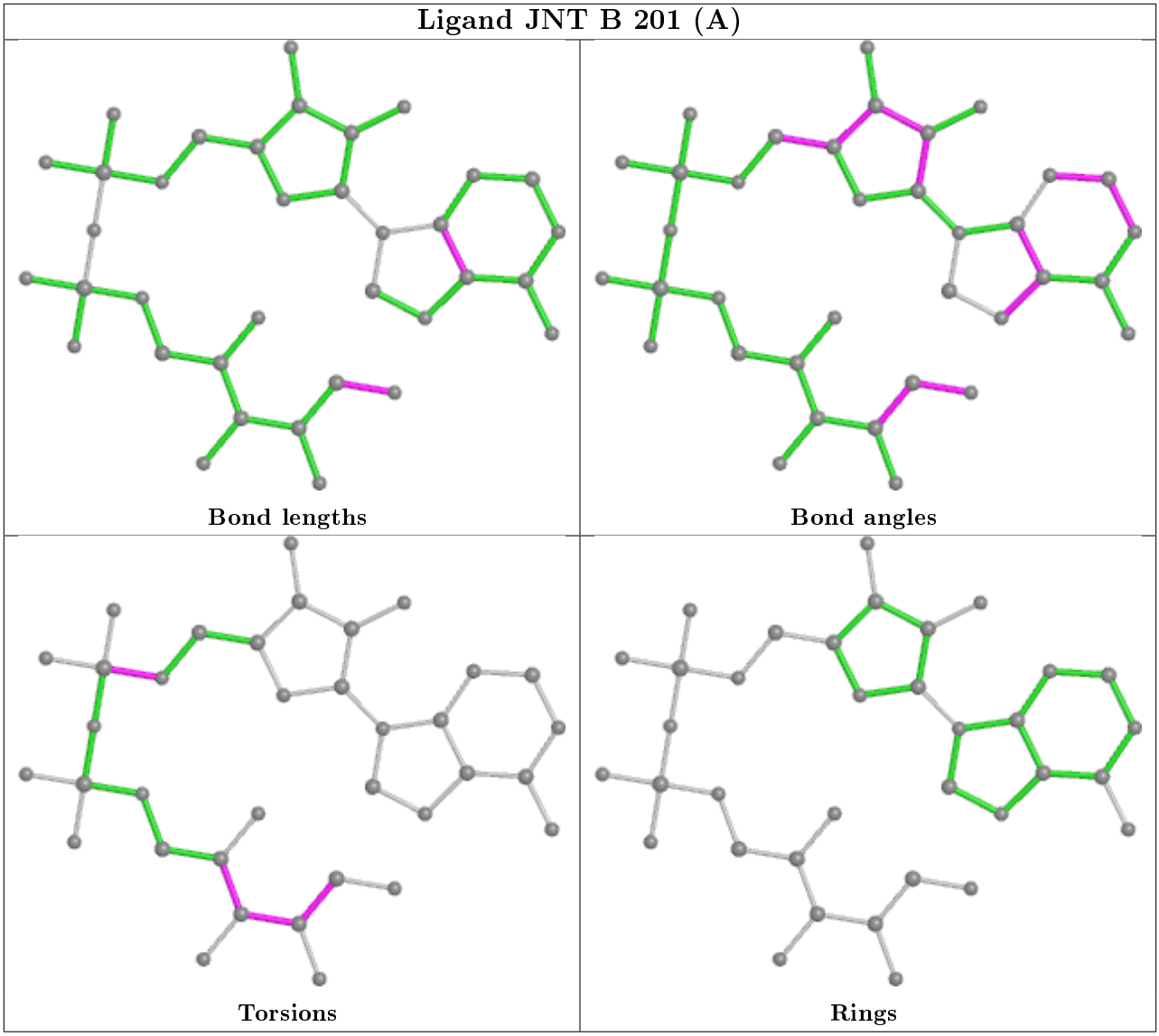
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	159/168 (94%)	0.18	4 (2%)	57	55	14, 19, 49, 88	0
1	B	161/168 (95%)	0.17	5 (3%)	49	46	14, 22, 50, 65	0
All	All	320/336 (95%)	0.18	9 (2%)	53	50	14, 21, 50, 88	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	TRP	5.4
1	A	1	ALA	4.1
1	B	160	THR	3.7
1	B	145[A]	ASP	3.1
1	A	158	ARG	3.0
1	A	2	PRO	2.8
1	B	1	ALA	2.7
1	B	148	TRP	2.6
1	B	31	ASP	2.2

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 carbohydrates 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,

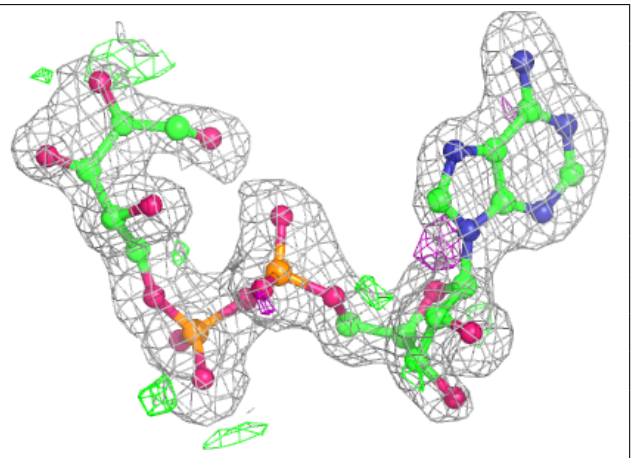
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

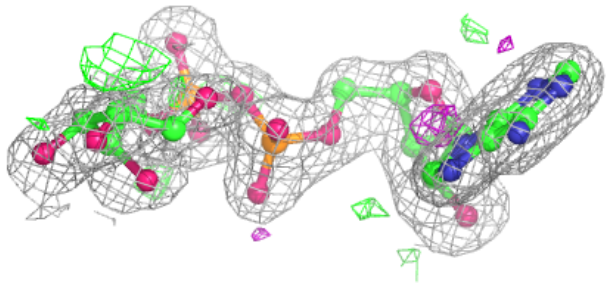
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	A	202	4/4	0.56	0.23	33,38,44,54	0
4	EDO	A	203	4/4	0.86	0.17	33,34,40,40	0
2	JNT	B	201[B]	36/36	0.95	0.13	20,28,33,43	36
2	JNT	A	201[B]	36/36	0.95	0.12	17,22,31,34	36
2	JNT	A	201[A]	36/36	0.95	0.12	16,23,35,43	36
2	JNT	B	201[A]	36/36	0.95	0.13	19,30,36,41	36

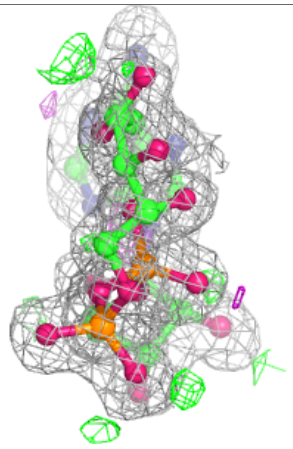
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JNT B 201 (B):

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

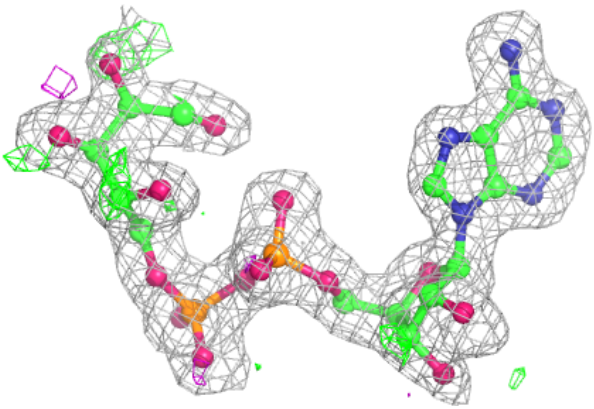


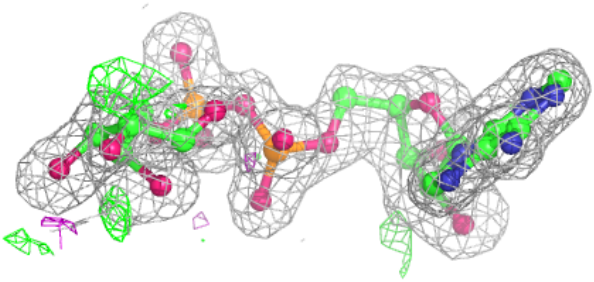


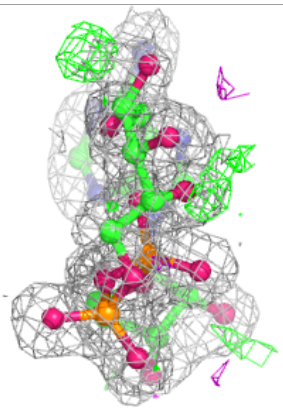


Electron density around JNT A 201 (B):

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

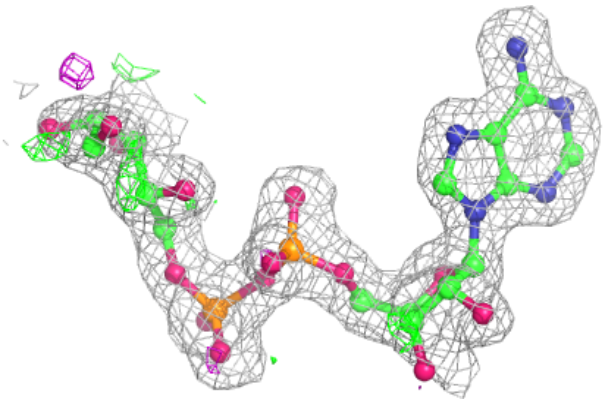


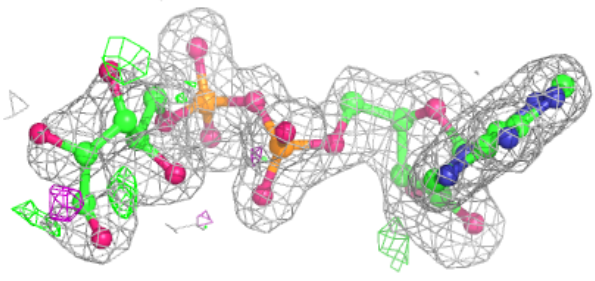


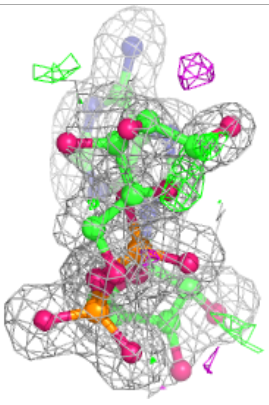


Electron density around JNT A 201 (A):

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

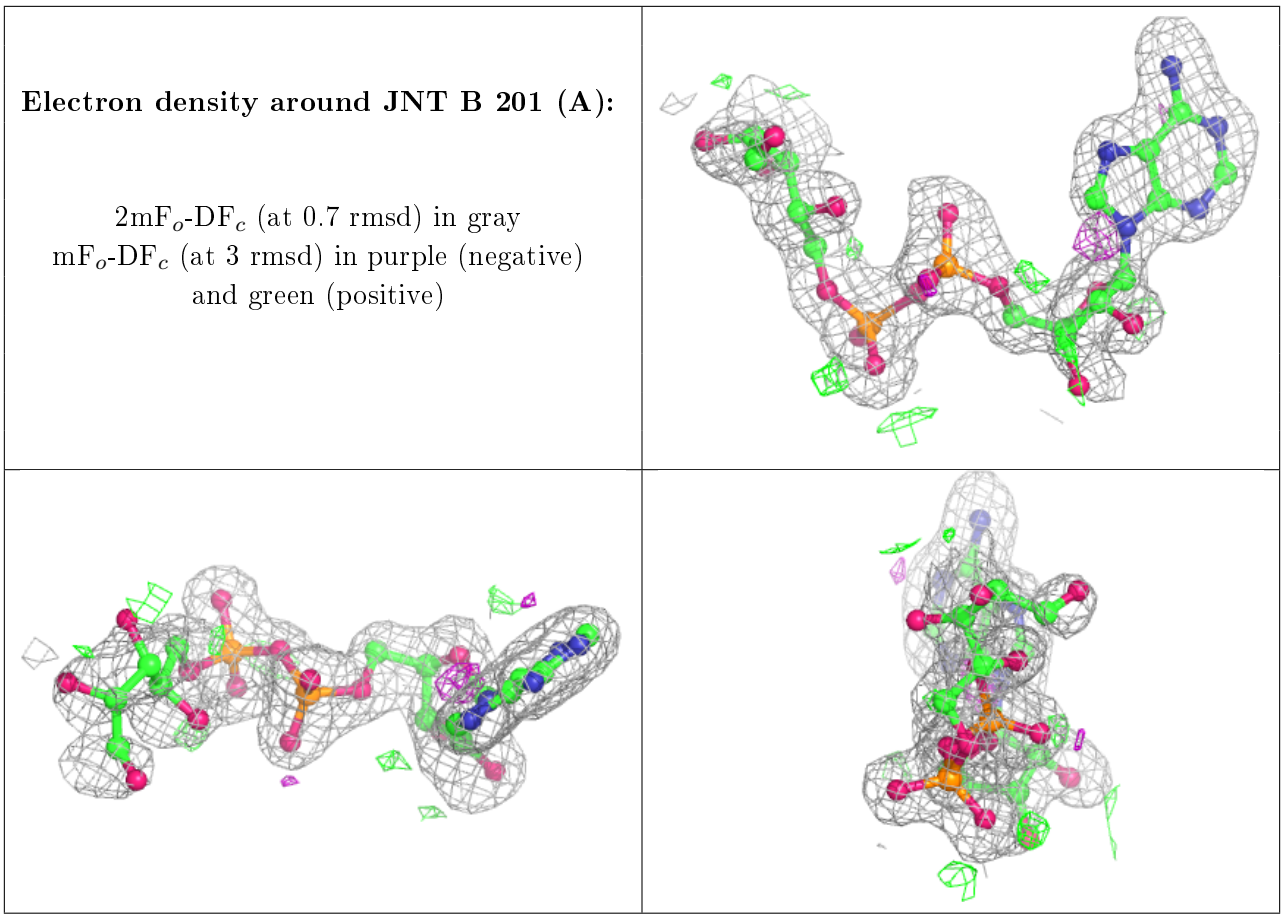






Electron density around JNT B 201 (A):

$2mF_o$-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

There are no such residues in this entry.