



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:44 am BST

PDB ID : 4WVF  
Title : Crystal structure of KPT276 in complex with CRM1-Ran-RanBP1  
Authors : Sun, Q.; Chook, Y.  
Deposited on : 2014-11-05  
Resolution : 1.80 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](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

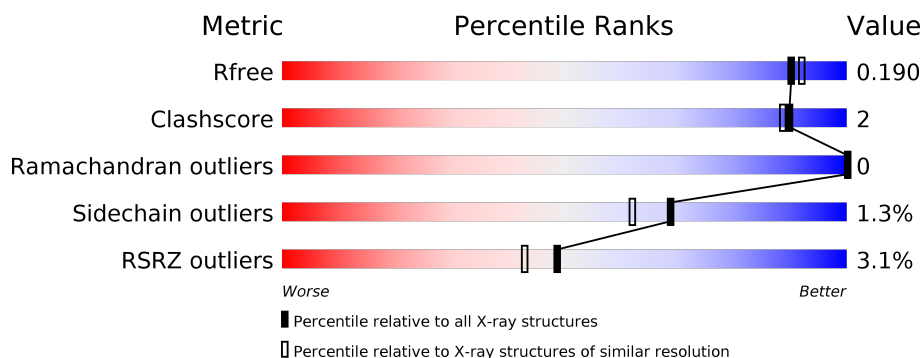
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	216	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div></div> </div>
2	B	140	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> <div></div> </div>
3	C	1024	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> <div></div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12622 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	5	0
			1714	1105	294	308	7			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	1	0
			1075	683	186	201	5			

- Molecule 3 is a protein called Crm1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1017	Total	C	N	O	S	0	27	0
			8367	5386	1361	1577	43			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP W7PTE1
C	-1	GLY	-	expression tag	UNP W7PTE1
C	0	SER	-	expression tag	UNP W7PTE1
C	?	-	VAL	deletion	UNP W7PTE1
C	?	-	GLN	deletion	UNP W7PTE1
C	?	-	ARG	deletion	UNP W7PTE1
C	?	-	LEU	deletion	UNP W7PTE1
C	?	-	PRO	deletion	UNP W7PTE1
C	?	-	ALA	deletion	UNP W7PTE1
C	?	-	THR	deletion	UNP W7PTE1
C	?	-	GLU	deletion	UNP W7PTE1
C	?	-	MET	deletion	UNP W7PTE1
C	?	-	SER	deletion	UNP W7PTE1
C	?	-	PRO	deletion	UNP W7PTE1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP W7PTE1
C	?	-	ILE	deletion	UNP W7PTE1
C	?	-	GLN	deletion	UNP W7PTE1
C	?	-	LEU	deletion	UNP W7PTE1
C	?	-	SER	deletion	UNP W7PTE1
C	?	-	VAL	deletion	UNP W7PTE1
C	?	-	GLY	deletion	UNP W7PTE1
C	?	-	SER	deletion	UNP W7PTE1
C	?	-	GLN	deletion	UNP W7PTE1
C	?	-	ALA	deletion	UNP W7PTE1
C	?	-	ILE	deletion	UNP W7PTE1
C	?	-	SER	deletion	UNP W7PTE1
C	?	-	THR	deletion	UNP W7PTE1
C	?	-	GLY	deletion	UNP W7PTE1
C	?	-	SER	deletion	UNP W7PTE1
C	?	-	GLY	deletion	UNP W7PTE1
C	?	-	ALA	deletion	UNP W7PTE1
C	?	-	LEU	deletion	UNP W7PTE1
C	?	-	ASN	deletion	UNP W7PTE1
C	?	-	PRO	deletion	UNP W7PTE1
C	?	-	GLU	deletion	UNP W7PTE1
C	?	-	TYR	deletion	UNP W7PTE1
C	?	-	MET	deletion	UNP W7PTE1
C	?	-	LYS	deletion	UNP W7PTE1
C	?	-	ARG	deletion	UNP W7PTE1
C	?	-	PHE	deletion	UNP W7PTE1
C	539	CYS	THR	engineered mutation	UNP W7PTE1
C	1022	CYS	TYR	cloning artifact	UNP W7PTE1

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

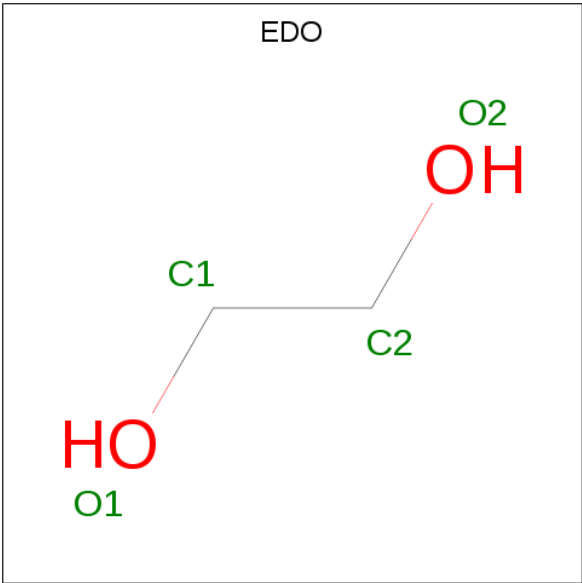


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



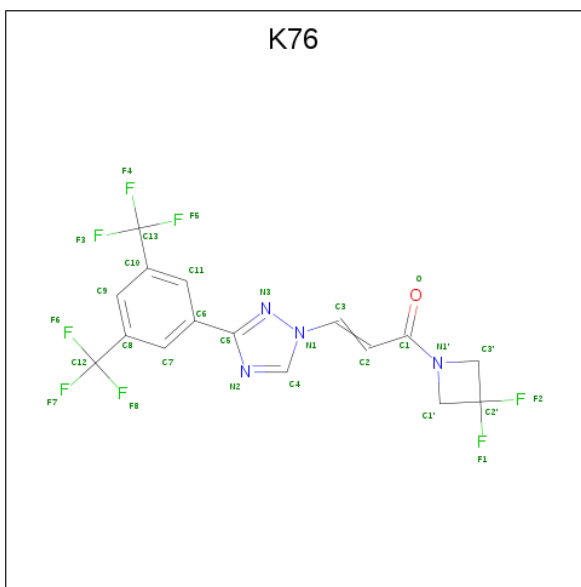
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is (2E)-3-{3-[3,5-bis(trifluoromethyl)phenyl]-1H-1,2,4-triazol-1-yl}-1-(3,3-difluorooazetidin-1-yl)prop-2-en-1-one (three-letter code: K76) (formula:  $C_{16}H_{10}F_8N_4O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	F	N	O	0	0
			29	16	8	4	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	3	Total	Cl	0	0
			3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	220	Total	O	0	0
			220	220		
10	B	74	Total	O	0	0
			74	74		
10	C	1075	Total	O	0	0
			1075	1075		

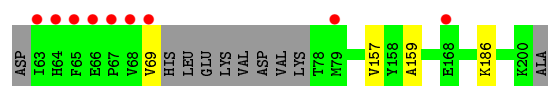
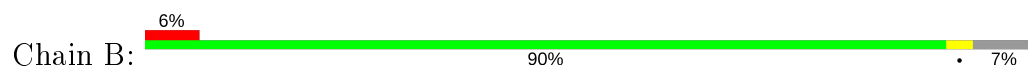
### 3 Residue-property plots [i](#)

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.

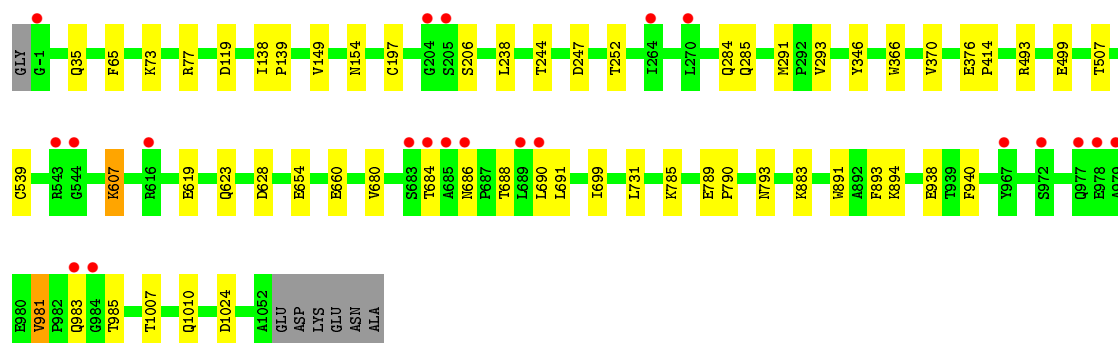
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Crm1p





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.91Å 105.91Å 305.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 46.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.80) 99.1 (46.80-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.137 , 0.183 0.145 , 0.190	Depositor DCC
$R_{free}$ test set	7989 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: GOL, GNP, CL, MG, EDO, K76

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	0.41	0/1764	0.61	0/2388
2	B	0.37	0/1094	0.59	0/1462
3	C	0.40	1/8595 (0.0%)	0.55	2/11645 (0.0%)
All	All	0.40	1/11453 (0.0%)	0.56	2/15495 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	414	PRO	N-CD	5.28	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	376	GLU	C-N-CD	5.28	139.49	128.40
3	C	893	PHE	CB-CA-C	-5.18	100.03	110.40

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	1714	0	1724	11	0
2	B	1075	0	1070	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8367	0	8492	30	0
4	A	32	0	13	0	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
6	C	4	0	6	0	0
7	A	6	0	8	0	0
7	C	18	0	24	1	0
8	C	29	0	9	0	0
9	C	3	0	0	0	0
10	A	220	0	0	1	0
10	B	74	0	0	1	0
10	C	1075	0	0	7	0
All	All	12622	0	11352	41	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 2.

All (41) 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:8:GLN:HG2	1:A:9:VAL:H	1.49	0.77
3:C:686:ASN:HB3	3:C:688:THR:HG22	1.70	0.73
3:C:293[B]:VAL:HG12	3:C:346:TYR:CE2	2.35	0.62
1:A:8:GLN:CG	1:A:9:VAL:H	2.13	0.60
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.50	0.59
3:C:688:THR:HA	3:C:691:LEU:HD23	1.88	0.54
3:C:247:ASP:HB3	10:C:1323:HOH:O	2.09	0.53
1:A:95:ARG:O	1:A:99[B]:LYS:HE2	2.09	0.53
3:C:660[B]:GLU:OE1	3:C:660[B]:GLU:N	2.42	0.52
3:C:894:LYS:NZ	3:C:938:GLU:OE1	2.36	0.51
3:C:891:TRP:CE3	7:C:1103:GOL:H12	2.46	0.51
3:C:197[A]:CYS:SG	10:C:2269:HOH:O	2.60	0.49
1:A:99[B]:LYS:NZ	10:A:401:HOH:O	2.46	0.48
3:C:493:ARG:HE	3:C:499:GLU:CD	2.18	0.48
3:C:238:LEU:O	3:C:252:THR:HG21	2.15	0.47
1:A:95:ARG:O	1:A:99[B]:LYS:CE	2.62	0.47
3:C:507[B]:THR:HG23	10:C:2228:HOH:O	2.15	0.47
3:C:619:GLU:OE2	3:C:623:GLN:NE2	2.45	0.47
3:C:149:VAL:HG12	10:C:2264:HOH:O	2.15	0.46
1:A:99[B]:LYS:N	1:A:99[B]:LYS:HE2	2.30	0.46
3:C:366:TRP:O	3:C:370:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:284[B]:GLN:HG3	10:C:2155:HOH:O	2.15	0.45
3:C:1024:ASP:HB2	10:C:2046:HOH:O	2.18	0.44
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.99	0.43
3:C:789[B]:GLU:HB2	3:C:790:PRO:HD3	1.99	0.43
3:C:73:LYS:HE3	3:C:77:ARG:HD3	2.01	0.43
1:A:118:VAL:HG22	1:A:163:TRP:CE3	2.55	0.42
3:C:1007:THR:H	3:C:1010:GLN:NE2	2.15	0.42
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.50	0.42
3:C:793:ASN:HB3	10:C:1865:HOH:O	2.20	0.42
3:C:981:VAL:HG11	3:C:985:THR:HG21	2.01	0.42
1:A:8:GLN:CG	1:A:9:VAL:N	2.81	0.42
2:B:69:VAL:CG2	10:B:304:HOH:O	2.68	0.42
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.54	0.41
3:C:607:LYS:HG3	3:C:654:GLU:CG	2.50	0.41
3:C:138:ILE:HB	3:C:139:PRO:HD3	2.01	0.41
1:A:197:TYR:HE1	2:B:159:ALA:HB3	1.86	0.41
1:A:117:ILE:HB	1:A:144:LEU:HD22	2.03	0.41
3:C:244:THR:HG22	3:C:285:GLN:OE1	2.20	0.40
3:C:680:VAL:O	3:C:684:THR:HG23	2.21	0.40
3:C:789[A]:GLU:HB3	3:C:790:PRO:HD3	2.04	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	212/216 (98%)	206 (97%)	6 (3%)	0	100	100
2	B	127/140 (91%)	117 (92%)	10 (8%)	0	100	100
3	C	1043/1024 (102%)	1029 (99%)	14 (1%)	0	100	100
All	All	1382/1380 (100%)	1352 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	186/185 (100%)	184 (99%)	2 (1%)	73	68
2	B	113/121 (93%)	111 (98%)	2 (2%)	59	48
3	C	957/934 (102%)	944 (99%)	13 (1%)	67	59
All	All	1256/1240 (101%)	1239 (99%)	17 (1%)	69	59

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	179	MET
2	B	157	VAL
2	B	186	LYS
3	C	35	GLN
3	C	206	SER
3	C	291	MET
3	C	539	CYS
3	C	607	LYS
3	C	628	ASP
3	C	690	LEU
3	C	785[A]	LYS
3	C	785[B]	LYS
3	C	883	LYS
3	C	940	PHE
3	C	981	VAL
3	C	983	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	196	GLN
3	C	203	GLN
3	C	434	ASN
3	C	983	GLN
3	C	1010	GLN

### 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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
7	GOL	C	1102	-	5,5,5	0.44	0	5,5,5	0.36	0
8	K76	C	1101	3	29,31,31	1.89	4 (13%)	32,49,49	1.77	4 (12%)
6	EDO	C	1104	-	3,3,3	0.69	0	2,2,2	0.27	0
4	GNP	A	301	5	28,34,34	2.75	7 (25%)	30,54,54	1.51	4 (13%)
6	EDO	A	303	-	3,3,3	0.51	0	2,2,2	0.18	0
7	GOL	C	1103	-	5,5,5	0.29	0	5,5,5	0.10	0
7	GOL	A	304	-	5,5,5	0.87	0	5,5,5	1.01	0
7	GOL	C	1108	-	5,5,5	0.27	0	5,5,5	0.30	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
7	GOL	C	1102	-	-	2/4/4/4	-
8	K76	C	1101	3	-	3/21/35/35	0/3/3/3
6	EDO	C	1104	-	-	1/1/1/1	-
4	GNP	A	301	5	-	4/17/38/38	0/3/3/3
6	EDO	A	303	-	-	0/1/1/1	-
7	GOL	C	1103	-	-	2/4/4/4	-
7	GOL	A	304	-	-	3/4/4/4	-
7	GOL	C	1108	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	C4-N9	-12.17	1.31	1.47
8	C	1101	K76	C3-C2	8.30	1.52	1.32
4	A	301	GNP	PG-N3B	3.22	1.71	1.63
8	C	1101	K76	F2-C2'	-3.22	1.32	1.38
8	C	1101	K76	F1-C2'	-3.10	1.32	1.38
4	A	301	GNP	PB-N3B	2.97	1.71	1.63
4	A	301	GNP	C5-C6	-2.72	1.48	1.52
4	A	301	GNP	C8-N9	-2.70	1.36	1.45
4	A	301	GNP	PG-O1G	2.50	1.50	1.46
4	A	301	GNP	C2-N1	-2.39	1.34	1.44
8	C	1101	K76	C2-C1	2.05	1.51	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1101	K76	N3-C5-N2	-7.12	108.81	114.72
4	A	301	GNP	O1G-PG-N3B	-4.91	104.54	111.77
4	A	301	GNP	C4-C5-N7	3.45	107.03	102.46
8	C	1101	K76	F1-C2'-F2	2.93	113.50	107.49
4	A	301	GNP	PA-O3A-PB	-2.91	122.38	132.62
4	A	301	GNP	O2B-PB-O1B	2.40	114.96	109.92
8	C	1101	K76	F8-C12-C8	-2.29	107.90	112.93
8	C	1101	K76	F5-C13-C10	-2.09	108.34	112.93

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1101	K76	C1-C2-C3-N1
7	A	304	GOL	C1-C2-C3-O3
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	PA-O3A-PB-O1B
4	A	301	GNP	PA-O3A-PB-O2B
4	A	301	GNP	C2'-C1'-N9-C4
7	C	1103	GOL	C1-C2-C3-O3
7	C	1108	GOL	C1-C2-C3-O3
6	C	1104	EDO	O1-C1-C2-O2
8	C	1101	K76	O-C1-C2-C3
7	A	304	GOL	O2-C2-C3-O3
7	C	1103	GOL	O2-C2-C3-O3
7	C	1108	GOL	O2-C2-C3-O3
8	C	1101	K76	N1'-C1-C2-C3
7	C	1102	GOL	O2-C2-C3-O3
7	A	304	GOL	O1-C1-C2-O2
7	C	1102	GOL	C1-C2-C3-O3

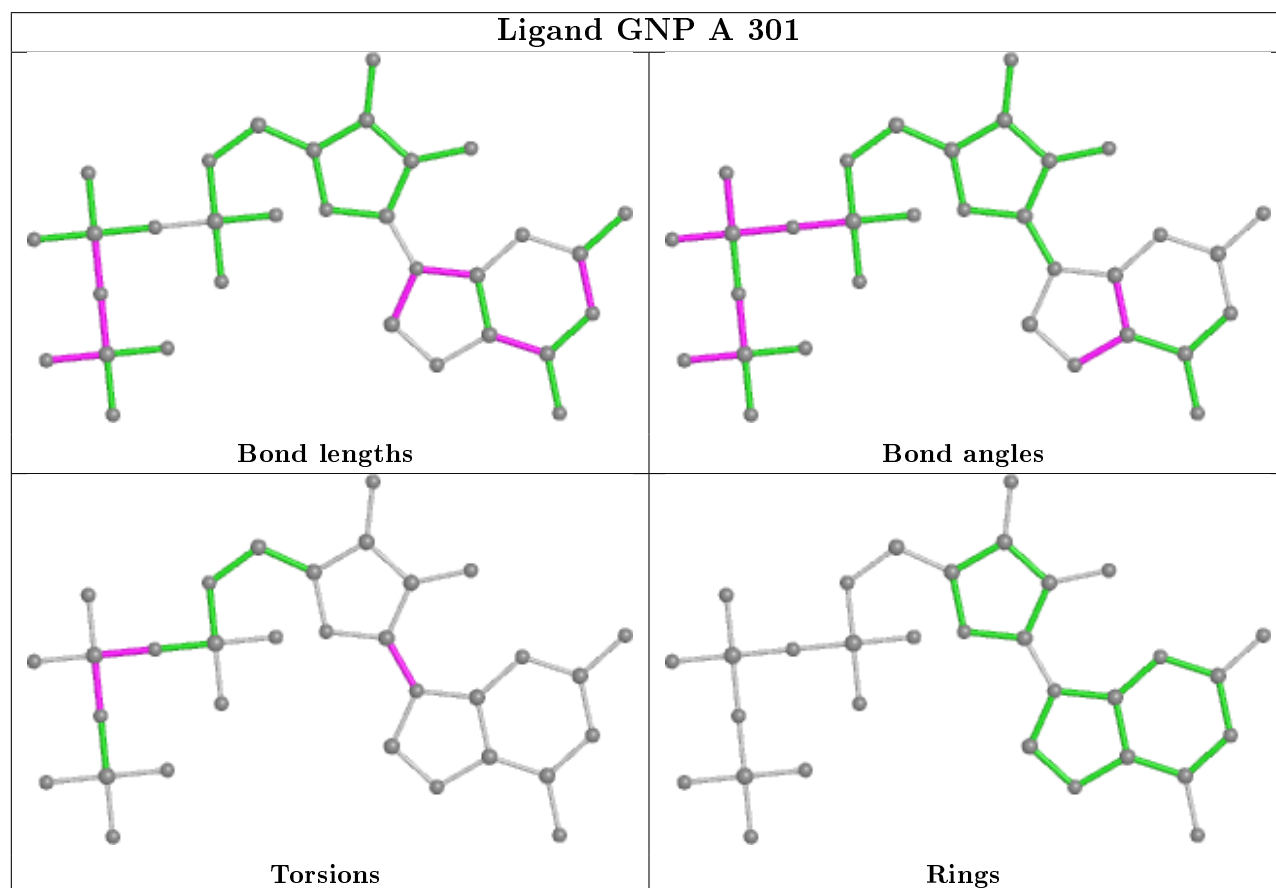
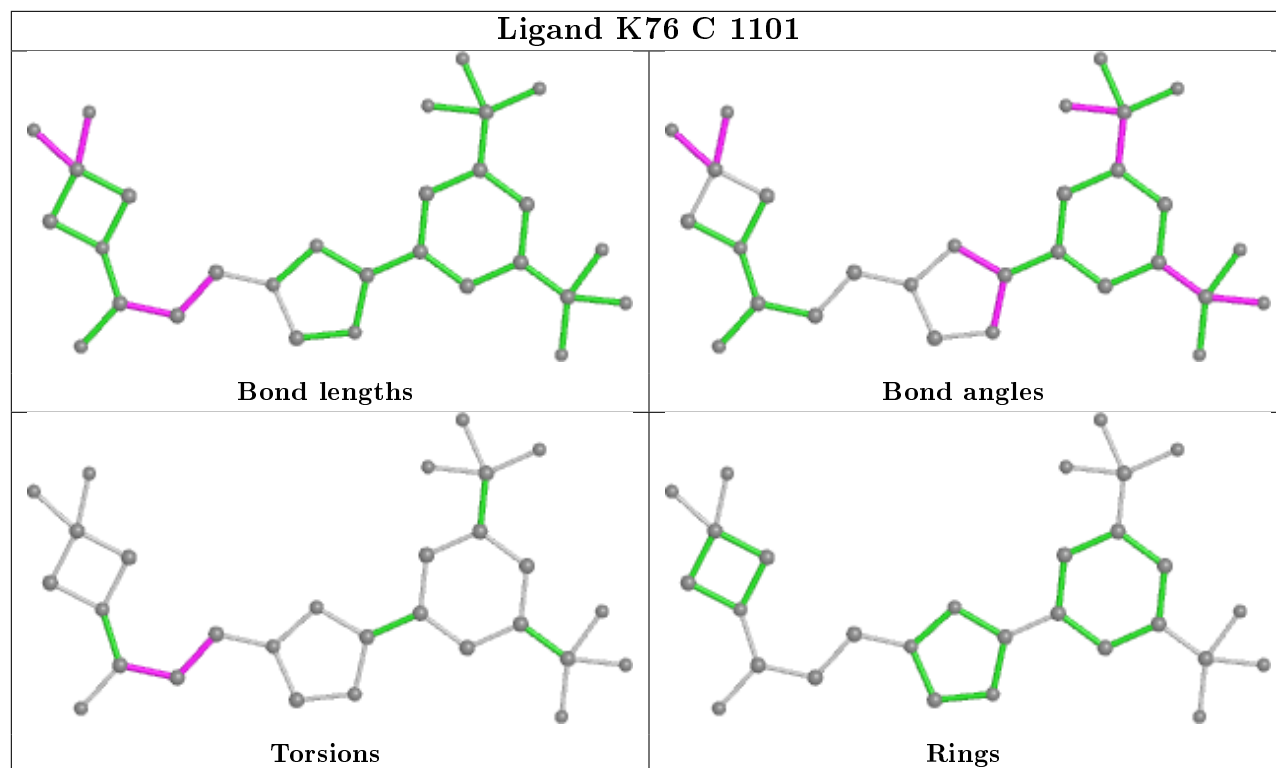
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1103	GOL	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 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

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<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	209/216 (96%)	-0.23	12 (5%)	23 19	27, 38, 89, 101	0
2	B	130/140 (92%)	-0.32	9 (6%)	16 13	39, 50, 85, 98	0
3	C	1017/1024 (99%)	-0.54	21 (2%)	63 59	27, 40, 71, 138	0
All	All	1356/1380 (98%)	-0.47	42 (3%)	49 43	27, 42, 75, 138	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	ILE	6.7
1	A	197	TYR	6.1
2	B	79	MET	6.0
2	B	64	HIS	6.0
2	B	69	VAL	5.9
3	C	689	LEU	5.7
3	C	205	SER	5.1
2	B	66	GLU	4.7
1	A	192	ALA	4.6
2	B	65	PHE	4.3
1	A	193	LEU	4.2
1	A	191	PRO	4.2
2	B	67	PRO	4.2
2	B	68	VAL	4.0
3	C	979	ALA	3.8
1	A	190	ASP	3.8
3	C	983	GLN	3.8
1	A	195	ALA	3.5
1	A	189	MET	3.5
1	A	187	VAL	3.3
3	C	978	GLU	3.0
1	A	194	ALA	3.0
1	A	9	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	690	LEU	2.9
3	C	967	TYR	2.9
3	C	684	THR	2.7
3	C	543	ARG	2.7
3	C	616	ARG	2.6
1	A	196	GLN	2.6
1	A	199	HIS	2.6
3	C	977	GLN	2.5
3	C	686	ASN	2.5
3	C	683	SER	2.4
3	C	270	LEU	2.3
2	B	168[A]	GLU	2.3
3	C	204	GLY	2.2
3	C	-1	GLY	2.2
3	C	264	ILE	2.1
3	C	685	ALA	2.1
3	C	972	SER	2.1
3	C	544	GLY	2.1
3	C	984	GLY	2.0

## 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.

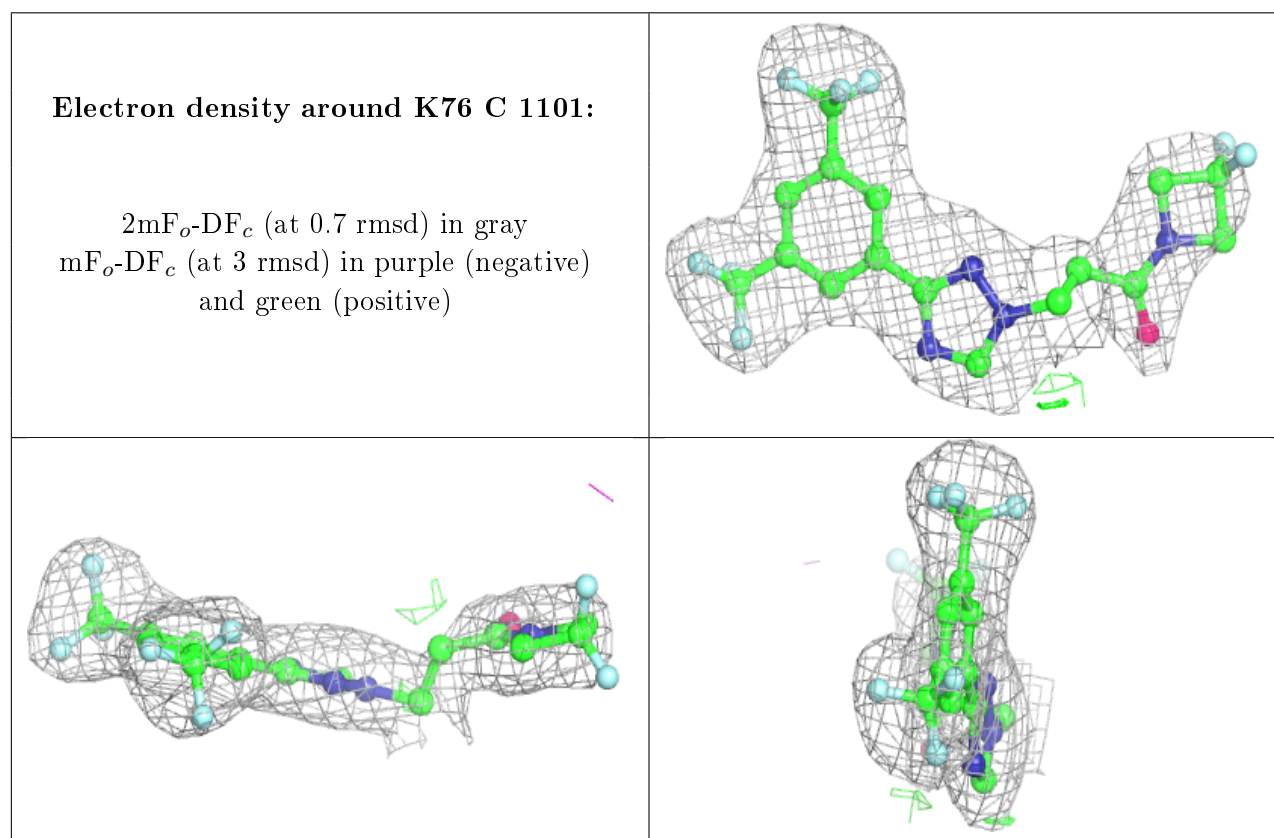
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	C	1104	4/4	0.83	0.20	58,73,81,87	0
7	GOL	C	1102	6/6	0.84	0.25	74,83,92,109	0
7	GOL	A	304	6/6	0.88	0.22	41,47,51,52	0
7	GOL	C	1108	6/6	0.95	0.27	53,54,54,60	0

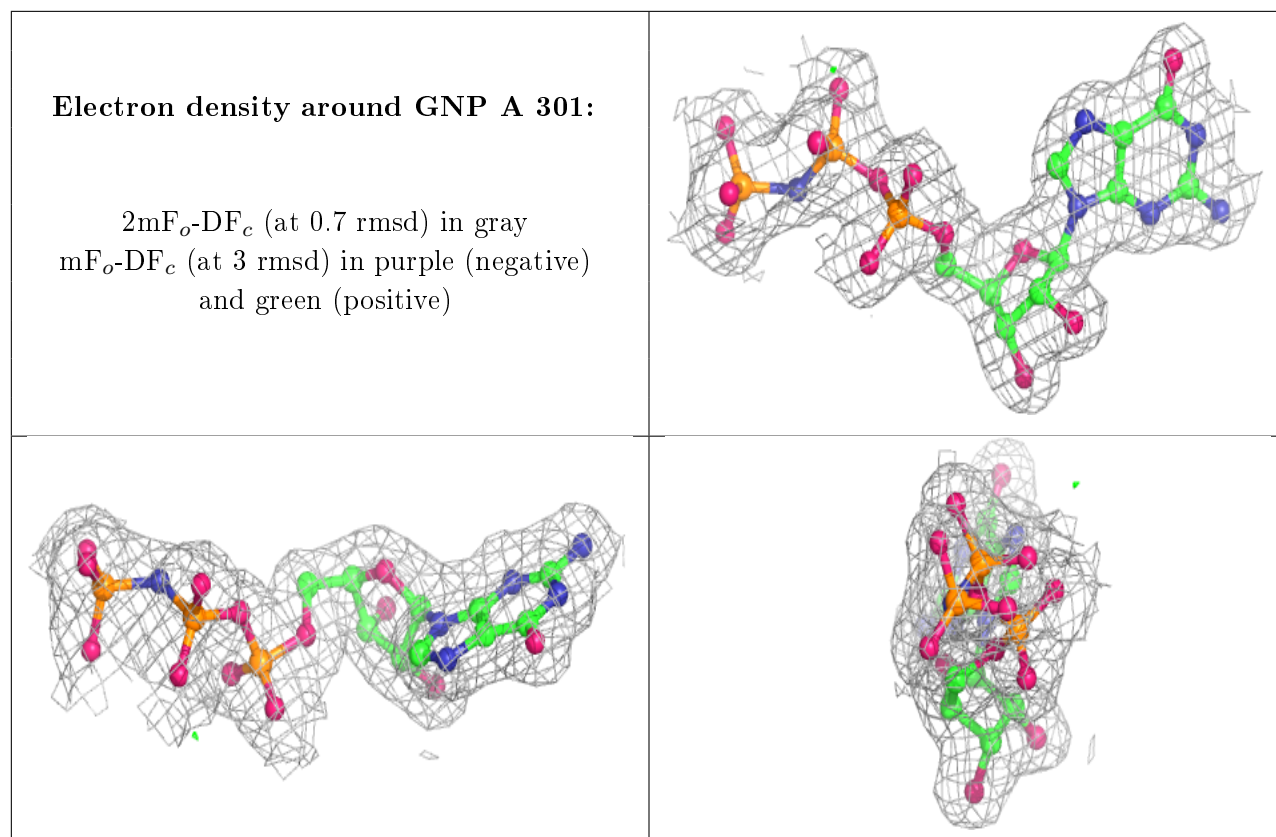
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	303	4/4	0.95	0.22	56,60,66,72	0
7	GOL	C	1103	6/6	0.96	0.08	49,55,65,71	0
9	CL	C	1105	1/1	0.97	0.03	74,74,74,74	0
8	K76	C	1101	29/29	0.97	0.14	42,55,105,123	0
9	CL	C	1107	1/1	0.98	0.06	81,81,81,81	0
4	GNP	A	301	32/32	0.99	0.06	29,34,37,40	0
9	CL	C	1106	1/1	0.99	0.06	63,63,63,63	0
5	MG	A	302	1/1	0.99	0.04	33,33,33,33	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.