



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 04:07 PM EDT

PDB ID : 7MNW
Title : Crystal Structure of Nup358/RanBP2 Ran-binding domain 1 in complex with Ran-GPPNHP
Authors : Bley, C.J.; Nie, S.; Mobbs, G.W.; Petrovic, S.; Gres, A.T.; Liu, X.; Mukherjee, S.; Harvey, S.; Huber, F.M.; Lin, D.H.; Brown, B.; Tang, A.W.; Rundlet, E.J.; Correia, A.R.; Chen, S.; Regmi, S.G.; Stevens, T.A.; Jette, C.A.; Dasso, M.; Patke, A.; Palazzo, A.F.; Kossiakoff, A.A.; Hoelz, A.
Deposited on : 2021-05-01
Resolution : 2.40 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 : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

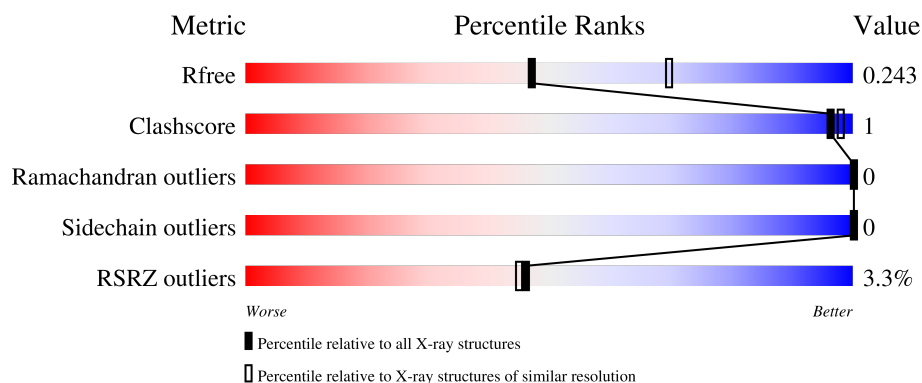
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

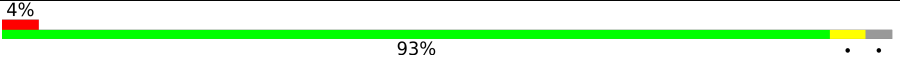
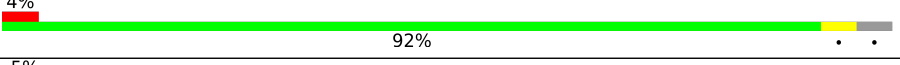
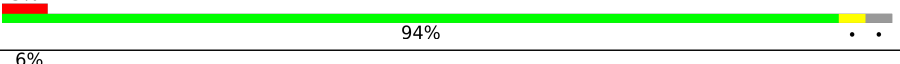
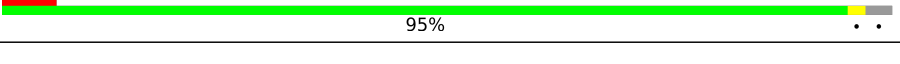
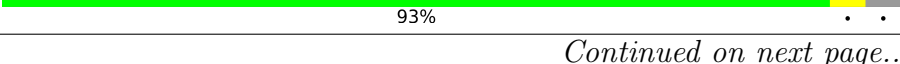
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	217	 4% 93%
1	C	217	 4% 92%
1	E	217	 5% 94%
1	G	217	 6% 95%
2	B	140	 93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	140	<div><div>%</div><div><div></div><div>95%</div><div></div></div><div></div></div>
2	F	140	<div><div></div><div><div></div><div>95%</div><div></div></div><div></div></div>
2	H	140	<div><div>2%</div><div><div></div><div>95%</div><div></div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22967 atoms, of which 11256 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	210	Total	C	H	N	O	S	0	0	0
			3369	1086	1685	288	304	6			
1	C	209	Total	C	H	N	O	S	0	0	0
			3354	1081	1677	287	303	6			
1	E	210	Total	C	H	N	O	S	0	0	0
			3369	1086	1685	288	304	6			
1	G	210	Total	C	H	N	O	S	0	0	0
			3369	1086	1685	288	304	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P62826
C	0	SER	-	expression tag	UNP P62826
E	0	SER	-	expression tag	UNP P62826
G	0	SER	-	expression tag	UNP P62826

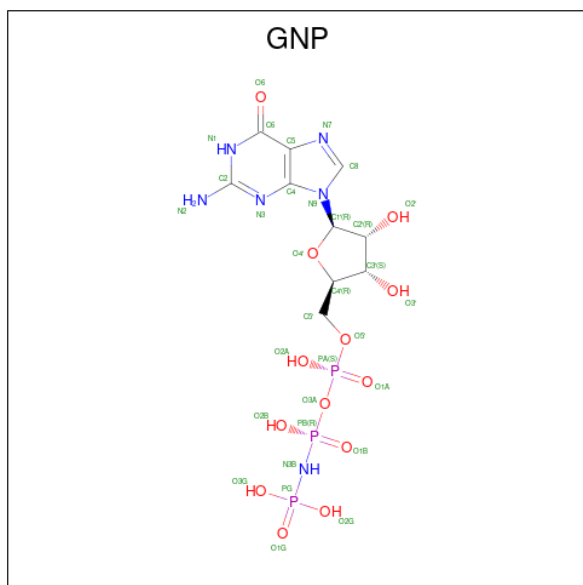
- Molecule 2 is a protein called E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	135	Total	C	H	N	O	S	0	0	0
			2231	712	1119	192	203	5			
2	D	135	Total	C	H	N	O	S	0	0	0
			2231	712	1119	192	203	5			
2	F	135	Total	C	H	N	O	S	0	0	0
			2231	712	1119	192	203	5			
2	H	135	Total	C	H	N	O	S	0	0	0
			2231	712	1119	192	203	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1167	GLY	-	expression tag	UNP P49792
B	1168	PRO	-	expression tag	UNP P49792
B	1169	GLY	-	expression tag	UNP P49792
B	1170	SER	-	expression tag	UNP P49792
D	1167	GLY	-	expression tag	UNP P49792
D	1168	PRO	-	expression tag	UNP P49792
D	1169	GLY	-	expression tag	UNP P49792
D	1170	SER	-	expression tag	UNP P49792
F	1167	GLY	-	expression tag	UNP P49792
F	1168	PRO	-	expression tag	UNP P49792
F	1169	GLY	-	expression tag	UNP P49792
F	1170	SER	-	expression tag	UNP P49792
H	1167	GLY	-	expression tag	UNP P49792
H	1168	PRO	-	expression tag	UNP P49792
H	1169	GLY	-	expression tag	UNP P49792
H	1170	SER	-	expression tag	UNP P49792

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	0
3	C	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	0
3	E	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	
									0
									0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg		
			1	1	0	0
4	C	1	Total	Mg		
			1	1	0	0
4	E	1	Total	Mg		
			1	1	0	0
4	G	1	Total	Mg		
			1	1	0	0

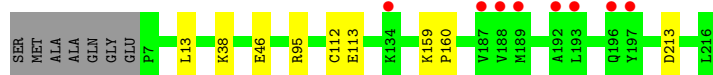
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O		
			79	79	0	0
5	B	70	Total	O		
			70	70	0	0
5	C	49	Total	O		
			49	49	0	0
5	D	38	Total	O		
			38	38	0	0
5	E	25	Total	O		
			25	25	0	0
5	F	63	Total	O		
			63	63	0	0
5	G	44	Total	O		
			44	44	0	0
5	H	34	Total	O		
			34	34	0	0

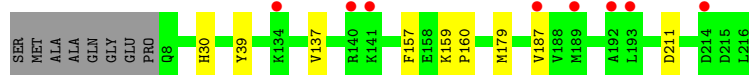
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

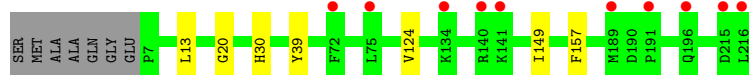
- Molecule 1: GTP-binding nuclear protein Ran



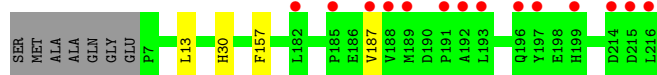
- Molecule 1: GTP-binding nuclear protein Ran



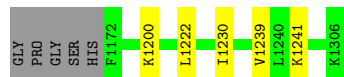
- Molecule 1: GTP-binding nuclear protein Ran



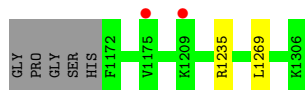
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.37Å 137.83Å 172.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.96 – 2.40 28.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.96-2.40) 99.7 (28.96-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.200 , 0.242 0.199 , 0.243	Depositor DCC
R_{free} test set	3186 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.125 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22967	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9540e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GNP, MG

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	0.25	0/1726	0.42	0/2340
1	C	0.25	0/1718	0.42	0/2329
1	E	0.25	0/1726	0.42	0/2340
1	G	0.25	0/1726	0.43	0/2340
2	B	0.25	0/1137	0.41	0/1526
2	D	0.25	0/1137	0.41	0/1526
2	F	0.25	0/1137	0.41	0/1526
2	H	0.25	0/1137	0.41	0/1526
All	All	0.25	0/11444	0.42	0/15453

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	1684	1685	1685	7	0
1	C	1677	1677	1677	7	0
1	E	1684	1685	1685	4	0
1	G	1684	1685	1685	3	0
2	B	1112	1119	1119	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1112	1119	1119	2	0
2	F	1112	1119	1119	1	0
2	H	1112	1119	1119	1	0
3	A	32	12	13	0	0
3	C	32	12	13	0	0
3	E	32	12	13	0	0
3	G	32	12	13	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	79	0	0	1	0
5	B	70	0	0	0	0
5	C	49	0	0	0	0
5	D	38	0	0	0	0
5	E	25	0	0	0	0
5	F	63	0	0	0	0
5	G	44	0	0	0	0
5	H	34	0	0	0	0
All	All	11711	11256	11260	23	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 1.

All (23) 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:95:ARG:NH1	1:C:211:ASP:OD2	2.32	0.62
1:C:187:VAL:HG21	2:D:1269:LEU:HD22	1.85	0.58
1:A:213:ASP:OD2	2:B:1200:LYS:NZ	2.35	0.56
1:C:137:VAL:O	1:C:137:VAL:HG22	2.12	0.51
1:C:30:HIS:NE2	1:C:157:PHE:O	2.46	0.46
1:G:30:HIS:NE2	1:G:157:PHE:O	2.48	0.45
2:H:1237:GLU:O	2:H:1239:VAL:N	2.50	0.45
1:A:38:LYS:HG2	1:C:39:TYR:CE2	2.52	0.44
1:A:46:GLU:OE2	5:A:401:HOH:O	2.21	0.44
1:C:179:MET:O	2:D:1235:ARG:NH1	2.41	0.43
2:B:1239:VAL:HG23	2:B:1241:LYS:H	1.84	0.42
1:A:159:LYS:N	1:A:160:PRO:CD	2.83	0.42
1:E:20:GLY:HA2	1:E:39:TYR:CE2	2.53	0.42
1:E:13:LEU:HD23	1:E:13:LEU:C	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:HIS:NE2	1:E:157:PHE:O	2.52	0.42
1:A:13:LEU:C	1:A:13:LEU:HD23	2.40	0.41
1:G:13:LEU:C	1:G:13:LEU:HD23	2.39	0.41
1:G:187:VAL:HG13	1:G:187:VAL:O	2.20	0.41
2:B:1222:LEU:O	2:B:1230:ILE:HA	2.20	0.41
1:A:112:CYS:O	1:A:113:GLU:HB2	2.21	0.40
1:C:159:LYS:N	1:C:160:PRO:CD	2.84	0.40
1:E:124:VAL:HG22	1:E:149:ILE:O	2.21	0.40
2:F:1201:LEU:HD12	2:F:1282:ALA:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	208/217 (96%)	201 (97%)	7 (3%)	0	100	100
1	C	207/217 (95%)	204 (99%)	3 (1%)	0	100	100
1	E	208/217 (96%)	205 (99%)	3 (1%)	0	100	100
1	G	208/217 (96%)	206 (99%)	2 (1%)	0	100	100
2	B	133/140 (95%)	130 (98%)	3 (2%)	0	100	100
2	D	133/140 (95%)	129 (97%)	4 (3%)	0	100	100
2	F	133/140 (95%)	130 (98%)	3 (2%)	0	100	100
2	H	133/140 (95%)	132 (99%)	1 (1%)	0	100	100
All	All	1363/1428 (95%)	1337 (98%)	26 (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	182/186 (98%)	182 (100%)	0	100	100
1	C	181/186 (97%)	181 (100%)	0	100	100
1	E	182/186 (98%)	182 (100%)	0	100	100
1	G	182/186 (98%)	182 (100%)	0	100	100
2	B	121/124 (98%)	121 (100%)	0	100	100
2	D	121/124 (98%)	121 (100%)	0	100	100
2	F	121/124 (98%)	121 (100%)	0	100	100
2	H	121/124 (98%)	121 (100%)	0	100	100
All	All	1211/1240 (98%)	1211 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	GNP	C	301	4	28,34,34	2.41	10 (35%)	30,54,54	1.95	5 (16%)
3	GNP	G	301	4	28,34,34	2.39	9 (32%)	30,54,54	2.03	5 (16%)
3	GNP	E	301	4	28,34,34	2.37	10 (35%)	30,54,54	2.02	5 (16%)
3	GNP	A	301	4	28,34,34	2.41	10 (35%)	30,54,54	1.97	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	C	301	4	-	3/17/38/38	0/3/3/3
3	GNP	G	301	4	-	6/17/38/38	0/3/3/3
3	GNP	E	301	4	-	4/17/38/38	0/3/3/3
3	GNP	A	301	4	-	4/17/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	GNP	C4-N9	-7.48	1.37	1.47
3	A	301	GNP	C4-N9	-7.48	1.37	1.47
3	G	301	GNP	C4-N9	-7.36	1.37	1.47
3	E	301	GNP	C4-N9	-7.30	1.38	1.47
3	C	301	GNP	C5-C6	-6.23	1.42	1.52
3	G	301	GNP	C5-C6	-6.17	1.42	1.52
3	A	301	GNP	C5-C6	-6.16	1.42	1.52
3	E	301	GNP	C5-C6	-6.06	1.42	1.52
3	A	301	GNP	C6-N1	4.22	1.40	1.33
3	C	301	GNP	C6-N1	4.21	1.40	1.33
3	G	301	GNP	C6-N1	4.14	1.40	1.33
3	E	301	GNP	C6-N1	4.07	1.39	1.33
3	E	301	GNP	PG-O1G	3.29	1.51	1.46
3	C	301	GNP	PG-O1G	3.25	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	GNP	PG-O1G	3.24	1.51	1.46
3	A	301	GNP	PG-O1G	3.20	1.51	1.46
3	E	301	GNP	PB-O1B	2.78	1.50	1.46
3	A	301	GNP	PB-O1B	2.77	1.50	1.46
3	G	301	GNP	PB-O1B	2.76	1.50	1.46
3	C	301	GNP	PB-O1B	2.73	1.50	1.46
3	E	301	GNP	C5-C4	-2.38	1.38	1.53
3	G	301	GNP	C5-C4	-2.38	1.38	1.53
3	A	301	GNP	C5-C4	-2.38	1.38	1.53
3	C	301	GNP	C5-C4	-2.37	1.38	1.53
3	G	301	GNP	PB-O2B	-2.34	1.50	1.56
3	A	301	GNP	C8-N9	-2.33	1.37	1.45
3	A	301	GNP	PB-O2B	-2.32	1.50	1.56
3	C	301	GNP	C8-N9	-2.32	1.37	1.45
3	E	301	GNP	C8-N9	-2.30	1.37	1.45
3	G	301	GNP	C8-N9	-2.30	1.37	1.45
3	E	301	GNP	PB-O2B	-2.26	1.50	1.56
3	C	301	GNP	PB-O2B	-2.25	1.50	1.56
3	A	301	GNP	PG-O3G	-2.19	1.50	1.56
3	E	301	GNP	PG-O3G	-2.17	1.50	1.56
3	G	301	GNP	PG-O3G	-2.14	1.51	1.56
3	C	301	GNP	PG-O2G	-2.11	1.51	1.56
3	E	301	GNP	PG-O2G	-2.08	1.51	1.56
3	C	301	GNP	PG-O3G	-2.07	1.51	1.56
3	A	301	GNP	PG-O2G	-2.05	1.51	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	GNP	C4-C5-N7	6.16	110.62	102.46
3	C	301	GNP	C4-C5-N7	6.13	110.59	102.46
3	E	301	GNP	C4-C5-N7	6.12	110.58	102.46
3	A	301	GNP	C4-C5-N7	6.07	110.51	102.46
3	A	301	GNP	C5-C6-N1	-5.50	111.41	118.19
3	C	301	GNP	C5-C6-N1	-5.48	111.43	118.19
3	G	301	GNP	C5-C6-N1	-5.38	111.56	118.19
3	E	301	GNP	C5-C6-N1	-5.34	111.61	118.19
3	G	301	GNP	O2B-PB-O1B	4.35	119.04	109.92
3	E	301	GNP	O2B-PB-O1B	4.27	118.88	109.92
3	E	301	GNP	O6-C6-C5	4.20	128.44	119.86
3	G	301	GNP	O6-C6-C5	4.13	128.29	119.86
3	A	301	GNP	O6-C6-C5	4.08	128.19	119.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	GNP	O6-C6-C5	4.04	128.10	119.86
3	A	301	GNP	O2B-PB-O1B	3.87	118.03	109.92
3	C	301	GNP	O2B-PB-O1B	3.67	117.61	109.92
3	G	301	GNP	O3G-PG-O1G	-2.35	107.54	113.45
3	C	301	GNP	O3G-PG-O1G	-2.12	108.12	113.45
3	E	301	GNP	O6-C6-N1	-2.03	119.96	122.69
3	A	301	GNP	O3G-PG-O1G	-2.00	108.42	113.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

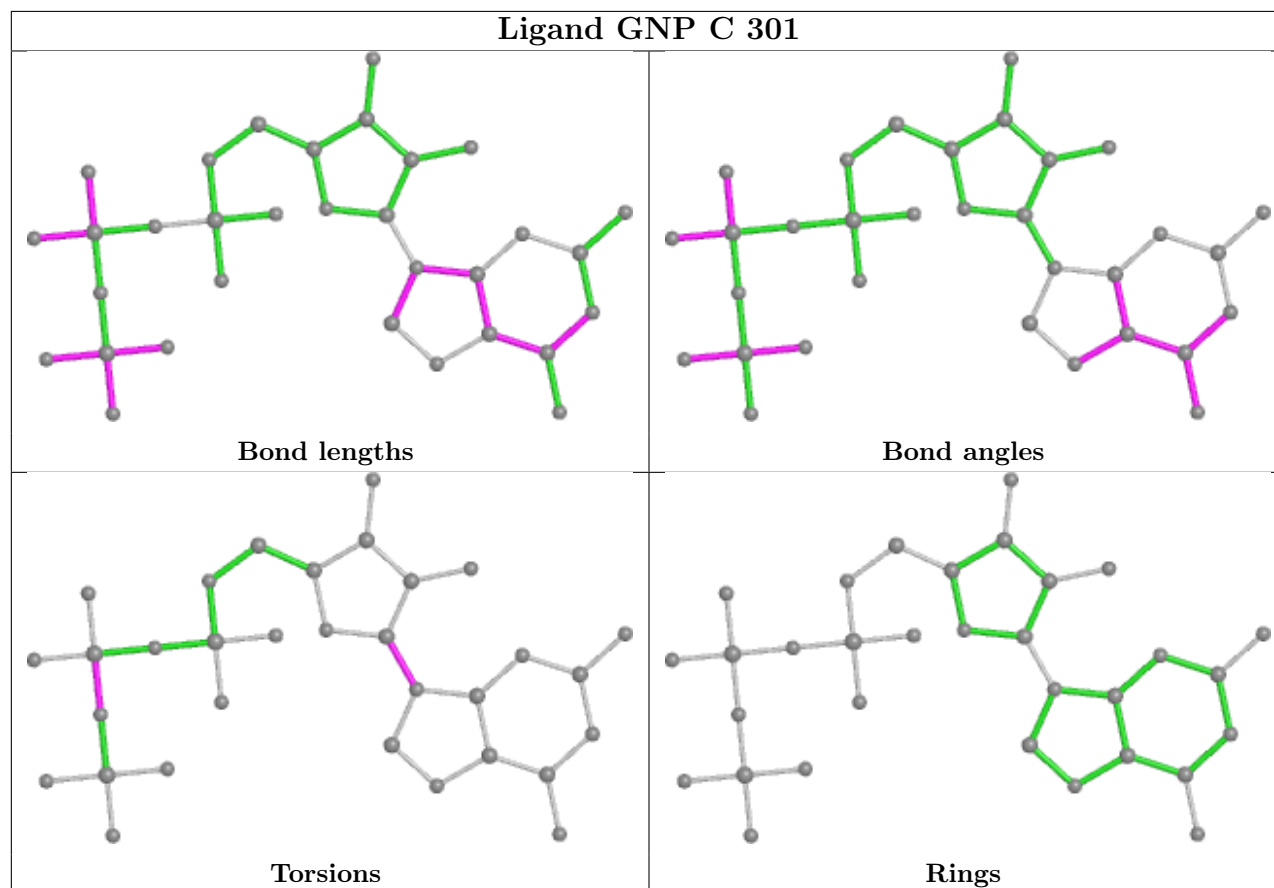
Mol	Chain	Res	Type	Atoms
3	A	301	GNP	PG-N3B-PB-O1B
3	A	301	GNP	PA-O3A-PB-O1B
3	A	301	GNP	PA-O3A-PB-O2B
3	A	301	GNP	C2'-C1'-N9-C4
3	C	301	GNP	PG-N3B-PB-O1B
3	C	301	GNP	C2'-C1'-N9-C4
3	E	301	GNP	PG-N3B-PB-O1B
3	E	301	GNP	PA-O3A-PB-O1B
3	E	301	GNP	PA-O3A-PB-O2B
3	E	301	GNP	C2'-C1'-N9-C4
3	G	301	GNP	PB-N3B-PG-O1G
3	G	301	GNP	PG-N3B-PB-O1B
3	G	301	GNP	PA-O3A-PB-O1B
3	G	301	GNP	PA-O3A-PB-O2B
3	G	301	GNP	C2'-C1'-N9-C4
3	C	301	GNP	PG-N3B-PB-O3A
3	G	301	GNP	PG-N3B-PB-O3A

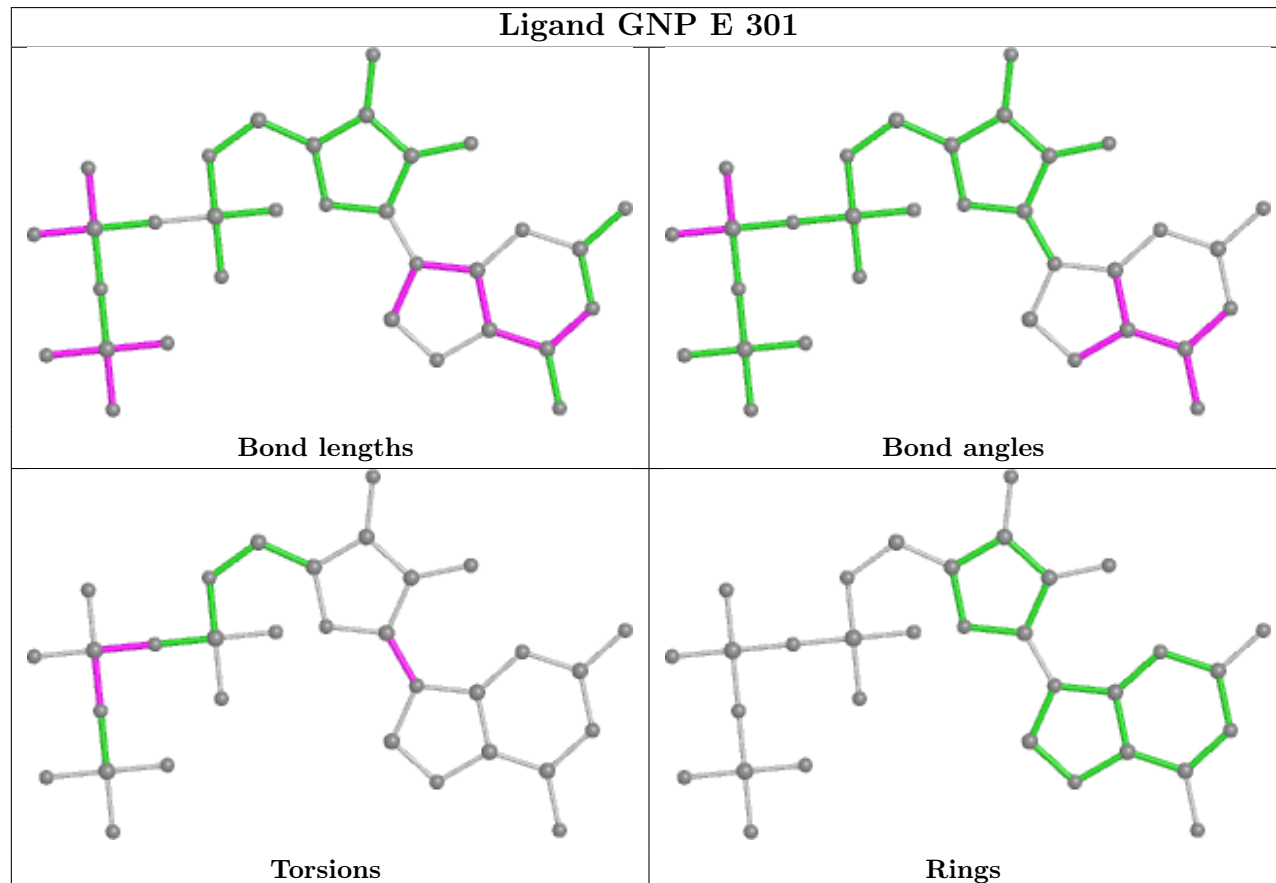
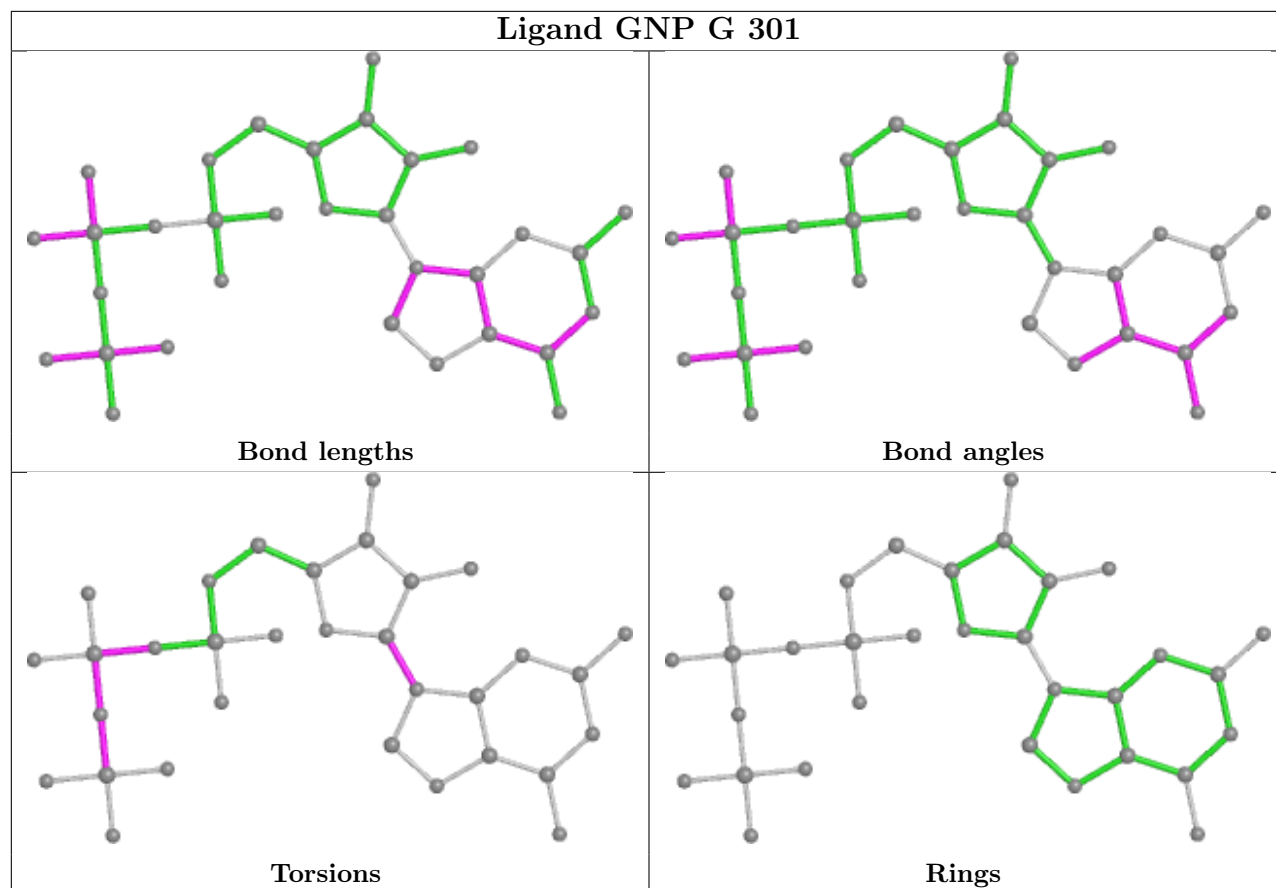
There are no ring outliers.

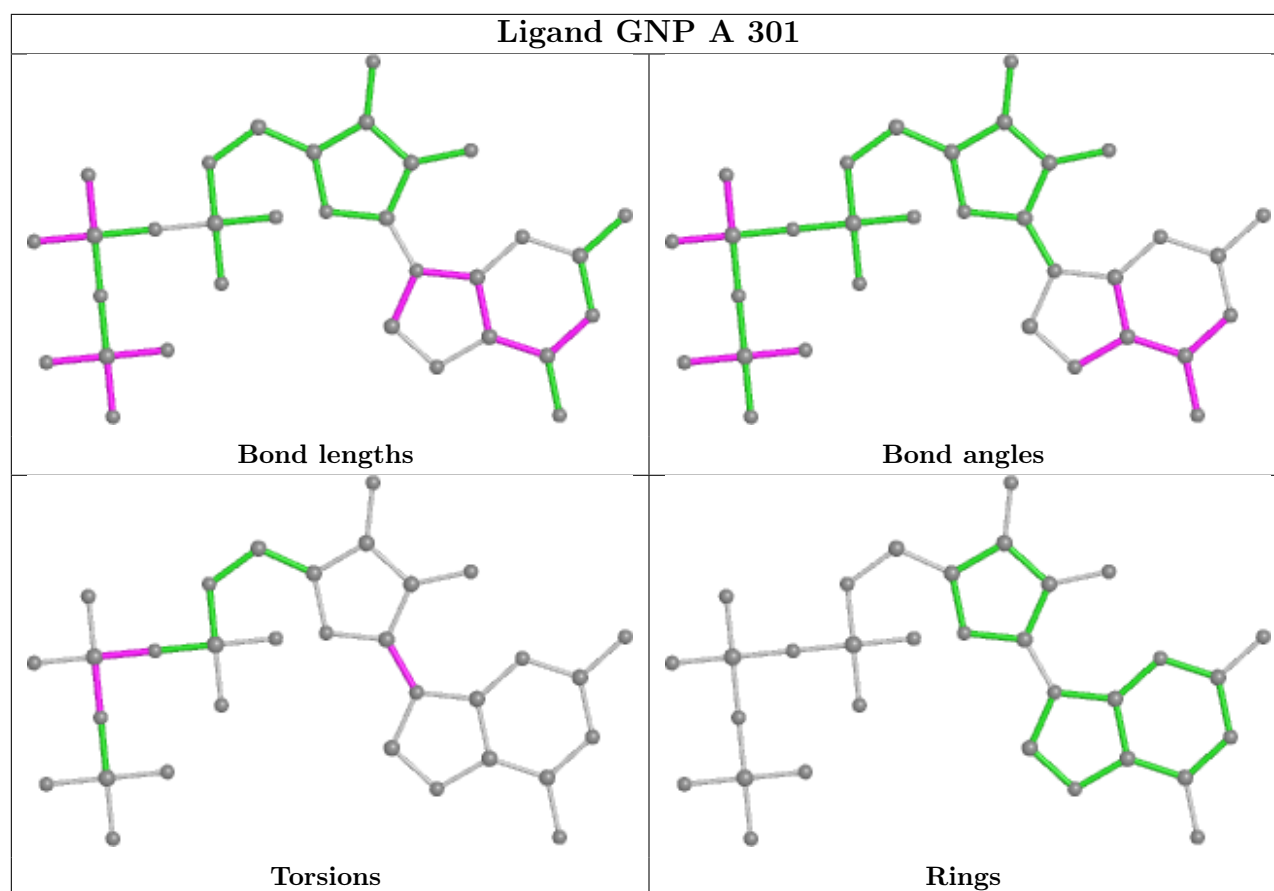
No monomer is involved in short contacts.

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	210/217 (96%)	-0.10	8 (3%)	40	39	29, 41, 108, 133	0
1	C	209/217 (96%)	0.03	8 (3%)	40	39	30, 47, 106, 132	0
1	E	210/217 (96%)	0.14	10 (4%)	30	29	34, 63, 107, 147	0
1	G	210/217 (96%)	0.12	14 (6%)	17	16	32, 52, 117, 156	0
2	B	135/140 (96%)	-0.37	0	100	100	27, 40, 64, 97	0
2	D	135/140 (96%)	-0.29	2 (1%)	73	72	31, 47, 78, 111	0
2	F	135/140 (96%)	-0.31	0	100	100	28, 42, 73, 112	0
2	H	135/140 (96%)	-0.17	3 (2%)	62	60	29, 51, 85, 124	0
All	All	1379/1428 (96%)	-0.08	45 (3%)	46	45	27, 48, 102, 156	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	192	ALA	12.3
1	G	189	MET	7.9
1	C	192	ALA	6.3
1	E	134	LYS	6.2
1	G	197	TYR	5.2
1	G	188	VAL	4.9
1	G	216	LEU	4.4
1	A	189	MET	4.4
1	E	216	LEU	4.3
1	C	134	LYS	4.2
2	H	1306	LYS	4.1
1	A	193	LEU	4.0
1	G	187	VAL	4.0
1	E	191	PRO	4.0
1	C	214	ASP	3.8
1	G	193	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	75	LEU	3.8
1	C	187	VAL	3.7
1	A	196	GLN	3.7
1	A	192	ALA	3.5
1	G	199	HIS	3.4
1	G	196	GLN	3.4
1	C	141	LYS	3.0
2	H	1305	LEU	3.0
1	E	141	LYS	2.9
1	A	187	VAL	2.9
1	A	197	TYR	2.8
1	G	214	ASP	2.8
1	C	189	MET	2.7
1	E	189	MET	2.7
1	E	140	ARG	2.6
1	A	188	VAL	2.6
2	D	1175	VAL	2.5
1	G	182	LEU	2.5
2	H	1209	LYS	2.4
1	G	215	ASP	2.3
1	C	140	ARG	2.3
1	G	191	PRO	2.2
2	D	1209	LYS	2.1
1	G	185	PRO	2.1
1	E	215	ASP	2.1
1	A	134	LYS	2.1
1	C	193	LEU	2.1
1	E	72	PHE	2.1
1	E	196	GLN	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](#)

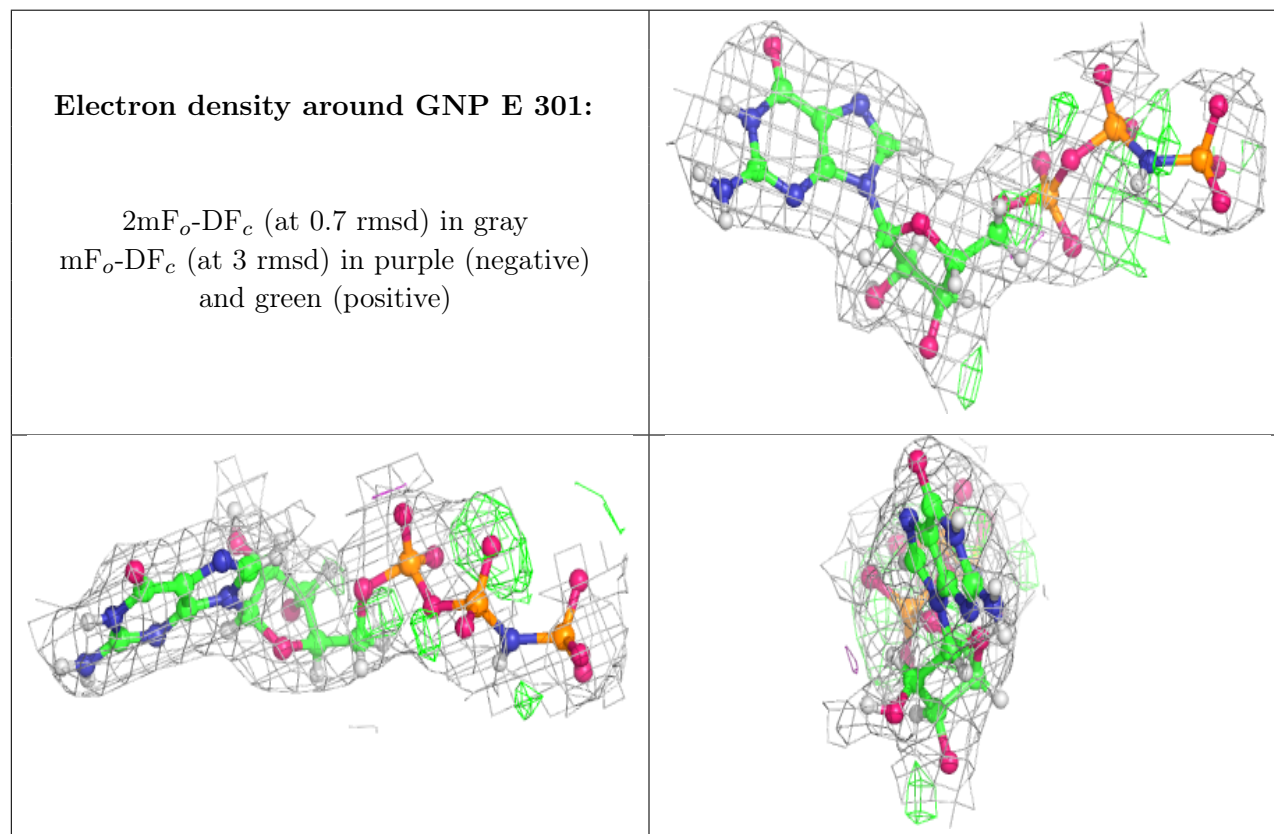
There are no monosaccharides in this entry.

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

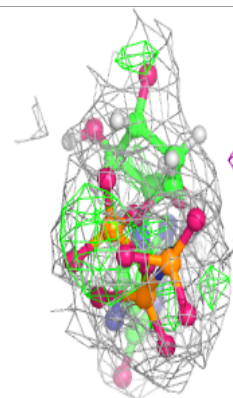
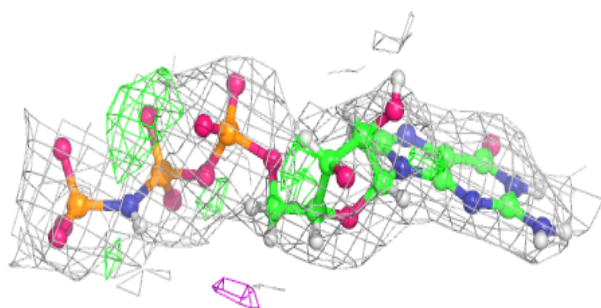
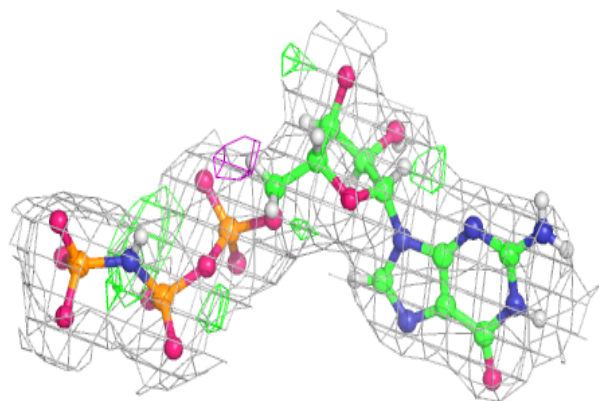
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	E	302	1/1	0.77	0.17	54,54,54,54	0
3	GNP	E	301	32/32	0.95	0.13	48,57,73,77	0
4	MG	G	302	1/1	0.96	0.18	45,45,45,45	0
3	GNP	G	301	32/32	0.97	0.14	38,51,68,70	0
4	MG	C	302	1/1	0.97	0.17	34,34,34,34	0
3	GNP	C	301	32/32	0.98	0.13	32,41,52,55	0
3	GNP	A	301	32/32	0.98	0.14	27,34,41,46	0
4	MG	A	302	1/1	0.99	0.18	32,32,32,32	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.

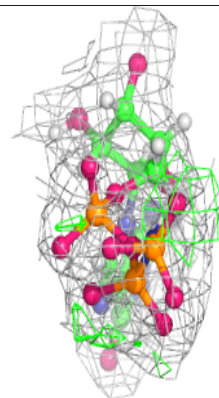
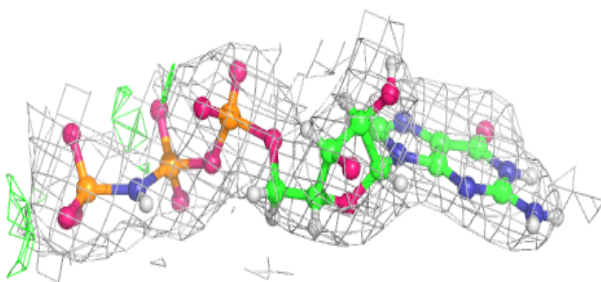
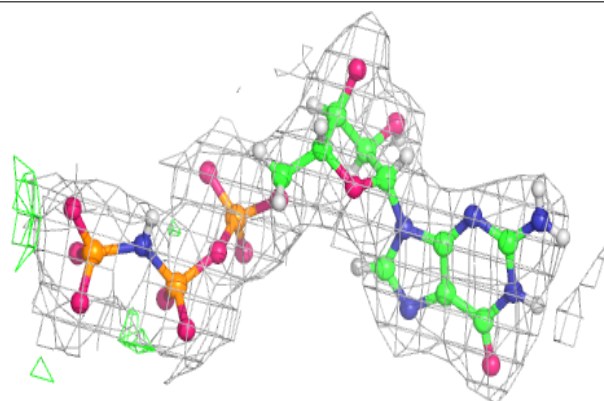


Electron density around GNP G 301:

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

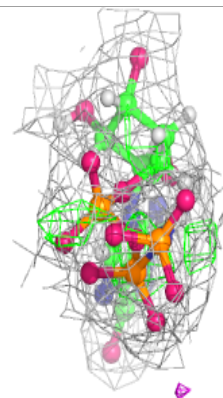
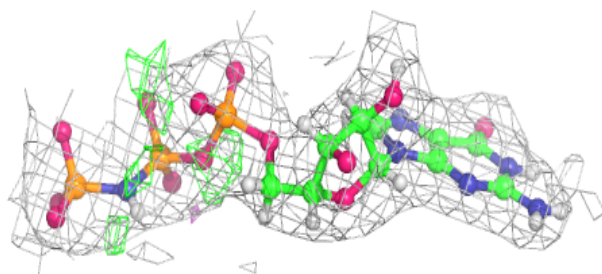
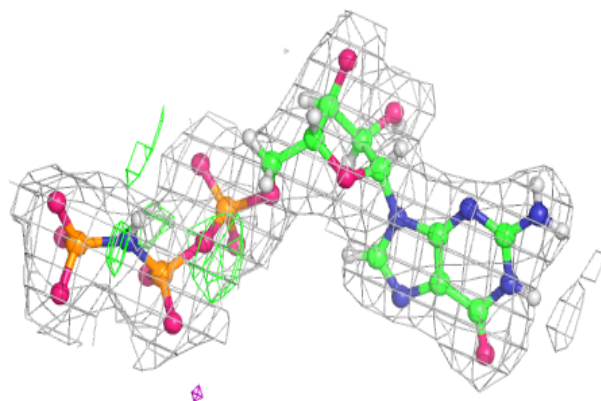
**Electron density around GNP C 301:**

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



Electron density around GNP 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.