



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 04:07 PM EDT

PDB ID : 7MNX
Title : Crystal Structure of Nup358/RanBP2 Ran-binding domain 2 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

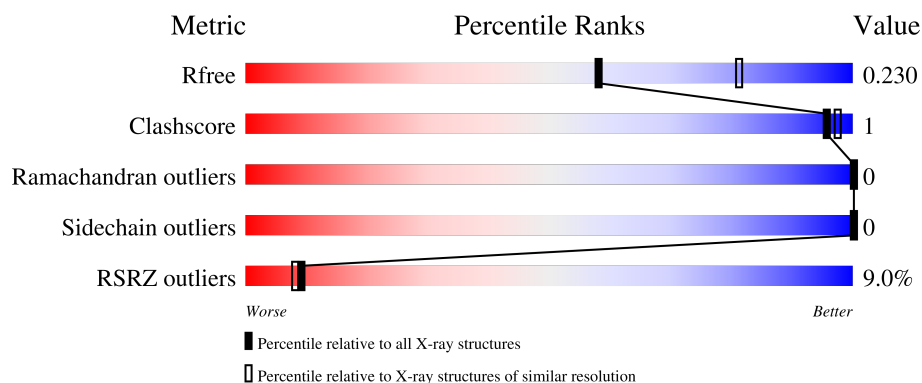
1 Overall quality at a glance

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	<div> <div>10%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	C	217	<div> <div>8%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	E	217	<div> <div>12%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	G	217	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	I	217	<div> <div>11%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	217	<div><div></div><div>12%</div><div>94%</div><div>5%</div></div>
2	B	141	<div><div></div><div>%</div><div>91%</div><div>8%</div></div>
2	D	141	<div><div></div><div>5%</div><div>90%</div><div>7%</div></div>
2	F	141	<div><div></div><div>12%</div><div>89%</div><div>7%</div></div>
2	H	141	<div><div></div><div>4%</div><div>89%</div><div>9%</div></div>
2	J	141	<div><div></div><div>6%</div><div>91%</div><div>7%</div></div>
2	L	141	<div><div></div><div>8%</div><div>93%</div><div>7%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33570 atoms, of which 16591 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	207	Total	C	H	N	O	S	0	0	0
			3325	1072	1666	285	296	6			
1	C	205	Total	C	H	N	O	S	0	0	0
			3298	1063	1654	283	292	6			
1	E	204	Total	C	H	N	O	S	0	0	0
			3283	1058	1648	282	289	6			
1	G	207	Total	C	H	N	O	S	0	0	0
			3322	1071	1662	285	298	6			
1	I	207	Total	C	H	N	O	S	0	0	0
			3322	1071	1662	285	298	6			
1	K	206	Total	C	H	N	O	S	0	0	0
			3313	1068	1662	284	293	6			

There are 6 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
I	0	SER	-	expression tag	UNP P62826
K	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	130	Total	C	H	N	O	S	0	0	0
			2150	678	1082	185	198	7			
2	D	131	Total	C	H	N	O	S	0	3	0
			2214	698	1110	191	208	7			
2	F	131	Total	C	H	N	O	S	0	0	0
			2167	683	1090	187	200	7			

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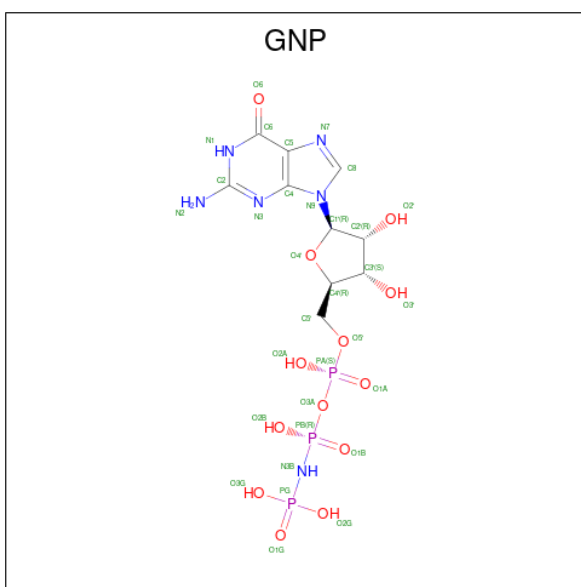
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	129	Total	C	H	N	O	S	0	2	0
			2167	684	1090	186	200	7			
2	J	131	Total	C	H	N	O	S	0	1	0
			2188	688	1103	190	200	7			
2	L	131	Total	C	H	N	O	S	0	0	0
			2167	683	1090	187	200	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2008	GLY	-	expression tag	UNP P49792
B	2009	PRO	-	expression tag	UNP P49792
B	2010	GLY	-	expression tag	UNP P49792
B	2011	SER	-	expression tag	UNP P49792
D	2008	GLY	-	expression tag	UNP P49792
D	2009	PRO	-	expression tag	UNP P49792
D	2010	GLY	-	expression tag	UNP P49792
D	2011	SER	-	expression tag	UNP P49792
F	2008	GLY	-	expression tag	UNP P49792
F	2009	PRO	-	expression tag	UNP P49792
F	2010	GLY	-	expression tag	UNP P49792
F	2011	SER	-	expression tag	UNP P49792
H	2008	GLY	-	expression tag	UNP P49792
H	2009	PRO	-	expression tag	UNP P49792
H	2010	GLY	-	expression tag	UNP P49792
H	2011	SER	-	expression tag	UNP P49792
J	2008	GLY	-	expression tag	UNP P49792
J	2009	PRO	-	expression tag	UNP P49792
J	2010	GLY	-	expression tag	UNP P49792
J	2011	SER	-	expression tag	UNP P49792
L	2008	GLY	-	expression tag	UNP P49792
L	2009	PRO	-	expression tag	UNP P49792
L	2010	GLY	-	expression tag	UNP P49792
L	2011	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
3	G	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	0
3	I	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	0
3	K	1	Total	C	H	N	O	P	
			44	10	12	6	13	3	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
4	I	1	Total	Mg		
			1	1	0	0
4	K	1	Total	Mg		
			1	1	0	0

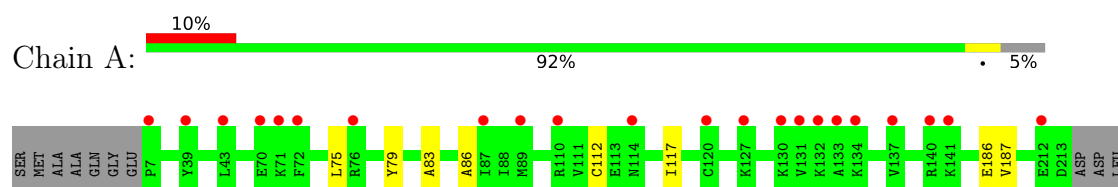
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total 23	O 23	0	0
5	B	48	Total 48	O 48	0	0
5	C	45	Total 45	O 45	0	0
5	D	27	Total 27	O 27	0	0
5	E	27	Total 27	O 27	0	0
5	F	4	Total 4	O 4	0	0
5	G	39	Total 39	O 39	0	0
5	H	31	Total 31	O 31	0	0
5	I	38	Total 38	O 38	0	0
5	J	30	Total 30	O 30	0	0
5	K	31	Total 31	O 31	0	0
5	L	41	Total 41	O 41	0	0

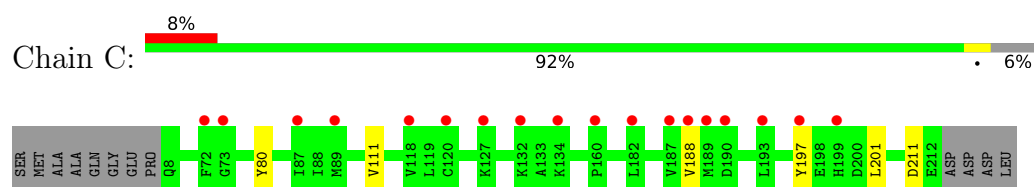
3 Residue-property plots [i](#)

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.

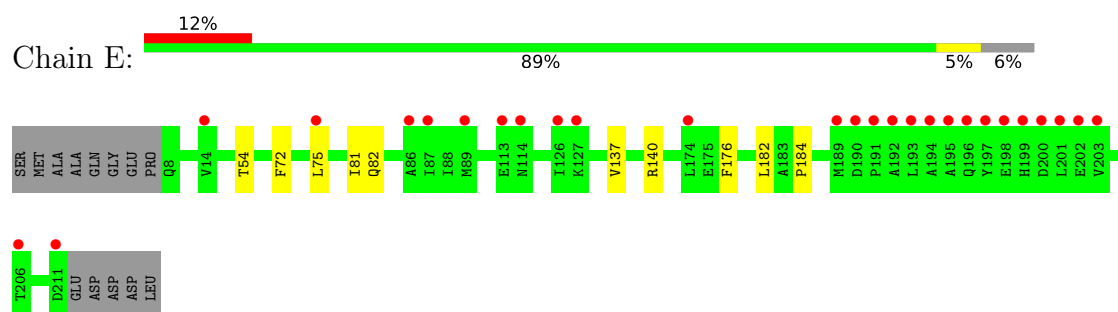
- Molecule 1: GTP-binding nuclear protein Ran



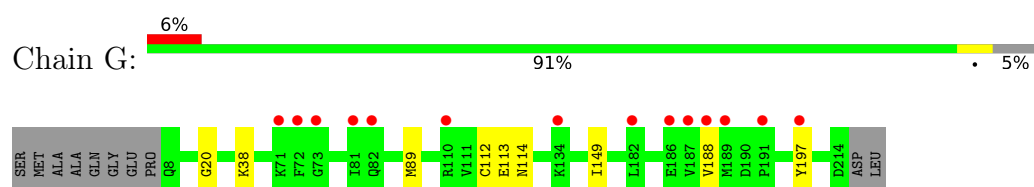
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 1: GTP-binding nuclear protein Ran

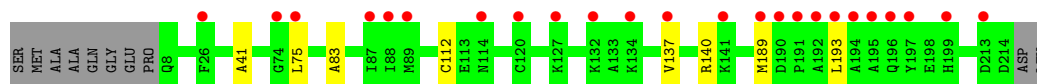


- Molecule 1: GTP-binding nuclear protein Ran

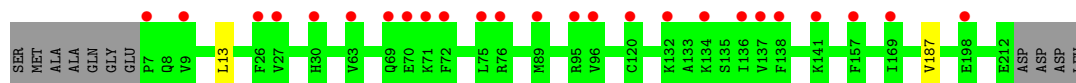
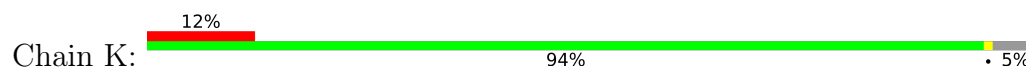


- Molecule 1: GTP-binding nuclear protein Ran

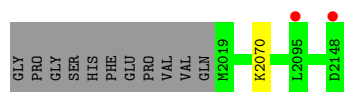
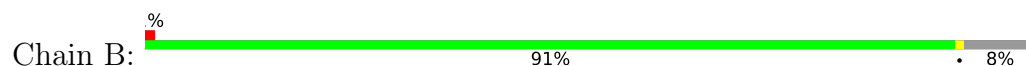




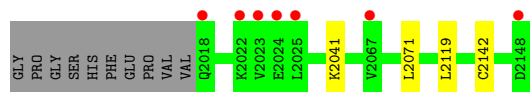
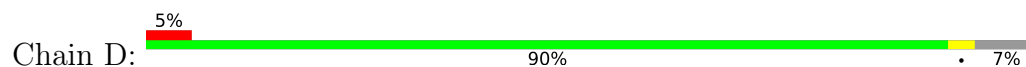
- Molecule 1: GTP-binding nuclear protein Ran



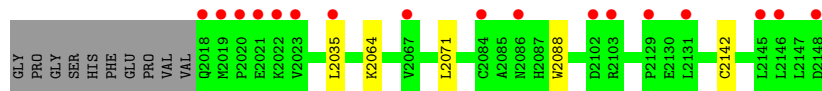
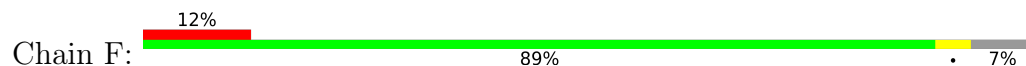
- Molecule 2: E3 SUMO-protein ligase RanBP2



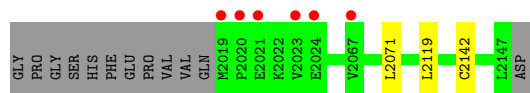
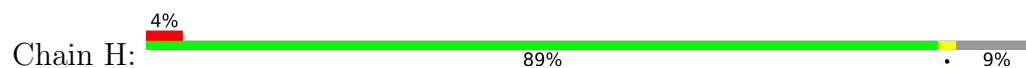
- Molecule 2: E3 SUMO-protein ligase RanBP2



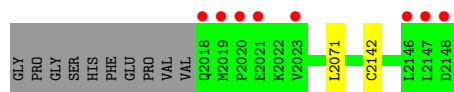
- Molecule 2: E3 SUMO-protein ligase RanBP2



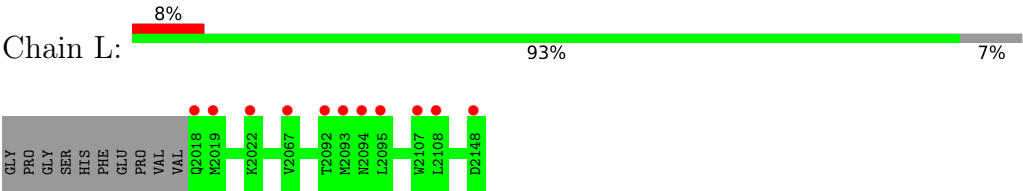
- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.17Å 133.97Å 182.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.40 29.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.82-2.40) 90.4 (29.82-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.192 , 0.230 0.192 , 0.230	Depositor DCC
R_{free} test set	2357 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33570	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, GNP

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	0.26	0/1701	0.45	0/2307
1	C	0.27	0/1685	0.45	0/2285
1	E	0.27	0/1676	0.46	0/2273
1	G	0.27	0/1701	0.45	0/2307
1	I	0.27	0/1701	0.44	0/2307
1	K	0.27	0/1693	0.45	0/2296
2	B	0.27	0/1086	0.46	0/1454
2	D	0.27	0/1122	0.44	0/1502
2	F	0.25	0/1095	0.43	0/1466
2	H	0.26	0/1095	0.44	0/1467
2	J	0.26	0/1106	0.46	0/1480
2	L	0.25	0/1095	0.45	0/1466
All	All	0.27	0/16756	0.45	0/22610

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	1659	1666	1666	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1644	1654	1654	5	0
1	E	1635	1648	1648	7	0
1	G	1660	1662	1662	8	0
1	I	1660	1662	1662	5	0
1	K	1651	1662	1662	2	0
2	B	1068	1082	1082	1	0
2	D	1104	1110	1107	3	0
2	F	1077	1090	1090	3	0
2	H	1077	1090	1088	2	0
2	J	1085	1103	1103	1	0
2	L	1077	1090	1090	0	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	1	0
3	I	32	12	13	0	0
3	K	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
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	23	0	0	0	0
5	B	48	0	0	0	0
5	C	45	0	0	0	0
5	D	27	0	0	0	0
5	E	27	0	0	0	0
5	F	4	0	0	0	0
5	G	39	0	0	0	0
5	H	31	0	0	0	0
5	I	38	0	0	0	0
5	J	30	0	0	0	0
5	K	31	0	0	0	0
5	L	41	0	0	0	0
All	All	16979	16591	16592	35	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 (35) 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:I:189:MET:HG3	1:I:193:LEU:HD23	1.78	0.66
1:G:197:TYR:CD2	2:H:2119:LEU:HD23	2.36	0.61
1:G:112:CYS:O	1:G:113:GLU:HG2	2.05	0.57
1:C:188:VAL:HG22	1:C:188:VAL:O	2.05	0.56
1:A:186:GLU:OE2	2:B:2070:LYS:NZ	2.37	0.56
1:A:83:ALA:HB3	1:A:112:CYS:SG	2.47	0.55
2:F:2071:LEU:HD13	2:F:2142:CYS:HB3	1.90	0.53
1:G:38:LYS:HD2	1:I:41:ALA:HB2	1.90	0.53
2:H:2071:LEU:HD13	2:H:2142:CYS:HB3	1.92	0.51
2:D:2071:LEU:HD13	2:D:2142:CYS:HB3	1.95	0.48
1:A:75:LEU:O	1:E:182:LEU:HD21	2.13	0.48
1:A:86:ALA:HB3	1:A:117:ILE:HG12	1.97	0.47
1:E:137:VAL:HG12	1:E:140:ARG:HH12	1.78	0.47
1:G:188:VAL:HG22	1:G:188:VAL:O	2.14	0.47
1:E:81:ILE:HG22	1:E:82:GLN:HG3	1.96	0.47
1:E:184:PRO:O	2:F:2088:TRP:NE1	2.48	0.46
1:G:112:CYS:O	1:G:113:GLU:CG	2.64	0.45
1:I:83:ALA:HB3	1:I:112:CYS:SG	2.56	0.45
1:I:137:VAL:HG12	1:I:140:ARG:HH12	1.81	0.45
1:A:79:TYR:CE2	1:E:182:LEU:HD23	2.51	0.45
1:K:187:VAL:O	1:K:187:VAL:HG13	2.16	0.44
1:C:197:TYR:CD2	2:D:2119:LEU:HD23	2.52	0.44
1:E:72:PHE:HB3	1:E:75:LEU:HD11	1.99	0.44
1:A:187:VAL:HG13	1:A:187:VAL:O	2.18	0.43
2:F:2035:LEU:HD11	2:F:2064:LYS:HB2	2.01	0.43
1:E:54:THR:HG22	1:E:176:PHE:HD1	1.85	0.42
1:C:211:ASP:OD2	2:D:2041:LYS:CD	2.68	0.42
1:C:197:TYR:O	1:C:201:LEU:N	2.52	0.42
1:G:89:MET:CE	1:G:149:ILE:HD11	2.50	0.42
1:G:113:GLU:HG3	1:G:114:ASN:N	2.35	0.41
1:C:80:TYR:HB2	1:C:111:VAL:HG11	2.03	0.41
1:I:75:LEU:C	1:I:75:LEU:HD12	2.41	0.41
1:G:20:GLY:H	3:G:301:GNP:HNB3	1.69	0.41
1:K:13:LEU:HD23	1:K:13:LEU:C	2.42	0.41
2:J:2071:LEU:HD13	2:J:2142:CYS:HB3	2.03	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	205/217 (94%)	201 (98%)	4 (2%)	0	100	100
1	C	203/217 (94%)	200 (98%)	3 (2%)	0	100	100
1	E	202/217 (93%)	199 (98%)	3 (2%)	0	100	100
1	G	205/217 (94%)	202 (98%)	3 (2%)	0	100	100
1	I	205/217 (94%)	203 (99%)	2 (1%)	0	100	100
1	K	204/217 (94%)	198 (97%)	6 (3%)	0	100	100
2	B	128/141 (91%)	125 (98%)	3 (2%)	0	100	100
2	D	132/141 (94%)	129 (98%)	3 (2%)	0	100	100
2	F	129/141 (92%)	126 (98%)	3 (2%)	0	100	100
2	H	129/141 (92%)	126 (98%)	3 (2%)	0	100	100
2	J	130/141 (92%)	125 (96%)	5 (4%)	0	100	100
2	L	129/141 (92%)	126 (98%)	3 (2%)	0	100	100
All	All	2001/2148 (93%)	1960 (98%)	41 (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	179/186 (96%)	179 (100%)	0	100	100
1	C	177/186 (95%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	176/186 (95%)	176 (100%)	0	100	100
1	G	179/186 (96%)	179 (100%)	0	100	100
1	I	179/186 (96%)	179 (100%)	0	100	100
1	K	178/186 (96%)	178 (100%)	0	100	100
2	B	116/125 (93%)	116 (100%)	0	100	100
2	D	120/125 (96%)	120 (100%)	0	100	100
2	F	117/125 (94%)	117 (100%)	0	100	100
2	H	117/125 (94%)	117 (100%)	0	100	100
2	J	118/125 (94%)	118 (100%)	0	100	100
2	L	117/125 (94%)	117 (100%)	0	100	100
All	All	1773/1866 (95%)	1773 (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 ⓘ

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	E	301	4	28,34,34	2.46	10 (35%)	30,54,54	2.27	7 (23%)
3	GNP	I	301	4	28,34,34	2.43	8 (28%)	30,54,54	2.29	6 (20%)
3	GNP	K	301	4	28,34,34	2.44	8 (28%)	30,54,54	2.51	8 (26%)
3	GNP	C	301	4	28,34,34	2.43	10 (35%)	30,54,54	2.32	7 (23%)
3	GNP	G	301	4	28,34,34	2.47	10 (35%)	30,54,54	2.37	8 (26%)
3	GNP	A	301	4	28,34,34	2.46	9 (32%)	30,54,54	2.44	8 (26%)

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	E	301	4	-	4/17/38/38	0/3/3/3
3	GNP	I	301	4	-	5/17/38/38	0/3/3/3
3	GNP	K	301	4	-	5/17/38/38	0/3/3/3
3	GNP	C	301	4	-	5/17/38/38	0/3/3/3
3	GNP	G	301	4	-	4/17/38/38	0/3/3/3
3	GNP	A	301	4	-	5/17/38/38	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	301	GNP	C4-N9	-7.39	1.37	1.47
3	A	301	GNP	C4-N9	-7.36	1.37	1.47
3	E	301	GNP	C4-N9	-7.35	1.37	1.47
3	I	301	GNP	C4-N9	-7.30	1.38	1.47
3	G	301	GNP	C4-N9	-7.30	1.38	1.47
3	C	301	GNP	C4-N9	-7.24	1.38	1.47
3	A	301	GNP	C5-C6	-6.25	1.42	1.52
3	G	301	GNP	C5-C6	-6.19	1.42	1.52
3	K	301	GNP	C5-C6	-6.15	1.42	1.52
3	C	301	GNP	C5-C6	-6.12	1.42	1.52
3	I	301	GNP	C5-C6	-6.11	1.42	1.52
3	E	301	GNP	C5-C6	-6.09	1.42	1.52
3	E	301	GNP	PG-O1G	4.26	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	GNP	PG-O1G	4.20	1.52	1.46
3	I	301	GNP	PG-O1G	4.13	1.52	1.46
3	C	301	GNP	C6-N1	4.09	1.39	1.33
3	A	301	GNP	PG-O1G	4.06	1.52	1.46
3	A	301	GNP	C6-N1	4.06	1.39	1.33
3	G	301	GNP	PG-O1G	4.04	1.52	1.46
3	K	301	GNP	PG-O1G	4.03	1.52	1.46
3	G	301	GNP	C6-N1	3.96	1.39	1.33
3	K	301	GNP	C6-N1	3.95	1.39	1.33
3	E	301	GNP	C6-N1	3.93	1.39	1.33
3	I	301	GNP	C6-N1	3.89	1.39	1.33
3	A	301	GNP	PB-O1B	3.46	1.51	1.46
3	K	301	GNP	PB-O1B	3.32	1.51	1.46
3	G	301	GNP	PB-O1B	3.16	1.51	1.46
3	E	301	GNP	PB-O1B	3.13	1.51	1.46
3	I	301	GNP	PB-O1B	3.05	1.51	1.46
3	G	301	GNP	PB-O3A	2.72	1.62	1.59
3	C	301	GNP	PB-O1B	2.49	1.50	1.46
3	C	301	GNP	PB-O2B	-2.36	1.50	1.56
3	C	301	GNP	C8-N9	-2.35	1.37	1.45
3	E	301	GNP	C8-N9	-2.35	1.37	1.45
3	E	301	GNP	C5-C4	-2.32	1.38	1.53
3	G	301	GNP	C5-C4	-2.31	1.38	1.53
3	I	301	GNP	C5-C4	-2.30	1.38	1.53
3	C	301	GNP	C5-C4	-2.30	1.38	1.53
3	I	301	GNP	C8-N9	-2.29	1.37	1.45
3	K	301	GNP	C5-C4	-2.29	1.38	1.53
3	K	301	GNP	C8-N9	-2.26	1.37	1.45
3	E	301	GNP	PB-O3A	2.26	1.61	1.59
3	A	301	GNP	C8-N9	-2.25	1.37	1.45
3	G	301	GNP	C8-N9	-2.24	1.38	1.45
3	A	301	GNP	C5-C4	-2.24	1.39	1.53
3	C	301	GNP	PG-O2G	-2.22	1.50	1.56
3	E	301	GNP	PG-O2G	-2.19	1.50	1.56
3	I	301	GNP	PB-O2B	-2.18	1.50	1.56
3	E	301	GNP	PB-O2B	-2.15	1.51	1.56
3	G	301	GNP	PB-O2B	-2.15	1.51	1.56
3	K	301	GNP	PG-O2G	-2.13	1.51	1.56
3	C	301	GNP	PB-O3A	2.03	1.61	1.59
3	G	301	GNP	PG-O3G	-2.01	1.51	1.56
3	A	301	GNP	PG-O2G	-2.01	1.51	1.56
3	A	301	GNP	PB-O3A	2.00	1.61	1.59

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	GNP	C4-C5-N7	6.39	110.93	102.46
3	A	301	GNP	C5-C6-N1	-6.28	110.44	118.19
3	G	301	GNP	C4-C5-N7	6.28	110.78	102.46
3	K	301	GNP	C5-C6-N1	-6.28	110.45	118.19
3	I	301	GNP	C5-C6-N1	-6.28	110.45	118.19
3	C	301	GNP	C4-C5-N7	6.20	110.68	102.46
3	I	301	GNP	C4-C5-N7	6.17	110.64	102.46
3	E	301	GNP	C4-C5-N7	6.09	110.53	102.46
3	K	301	GNP	C4-C5-N7	6.09	110.53	102.46
3	C	301	GNP	C5-C6-N1	-6.04	110.74	118.19
3	E	301	GNP	C5-C6-N1	-5.95	110.85	118.19
3	G	301	GNP	C5-C6-N1	-5.85	110.97	118.19
3	K	301	GNP	O1B-PB-N3B	5.27	119.53	111.77
3	K	301	GNP	O6-C6-C5	4.80	129.65	119.86
3	I	301	GNP	O6-C6-C5	4.71	129.48	119.86
3	E	301	GNP	O2G-PG-O1G	-4.69	101.65	113.45
3	E	301	GNP	O6-C6-C5	4.68	129.41	119.86
3	G	301	GNP	O6-C6-C5	4.63	129.30	119.86
3	K	301	GNP	O2G-PG-O1G	-4.63	101.83	113.45
3	A	301	GNP	O6-C6-C5	4.45	128.94	119.86
3	C	301	GNP	O6-C6-C5	4.40	128.84	119.86
3	A	301	GNP	O2G-PG-O1G	-4.33	102.56	113.45
3	A	301	GNP	O1B-PB-N3B	4.29	118.08	111.77
3	G	301	GNP	O2G-PG-O1G	-4.22	102.84	113.45
3	C	301	GNP	O2G-PG-O1G	-4.13	103.08	113.45
3	C	301	GNP	O1B-PB-N3B	3.90	117.51	111.77
3	G	301	GNP	O2B-PB-O1B	3.90	118.09	109.92
3	I	301	GNP	O2G-PG-O1G	-3.88	103.69	113.45
3	I	301	GNP	O1B-PB-N3B	3.75	117.29	111.77
3	G	301	GNP	O1B-PB-N3B	3.74	117.28	111.77
3	C	301	GNP	O2B-PB-O1B	3.71	117.69	109.92
3	K	301	GNP	O2B-PB-O1B	3.55	117.36	109.92
3	A	301	GNP	O2B-PB-O1B	3.47	117.19	109.92
3	E	301	GNP	O1B-PB-N3B	3.29	116.61	111.77
3	I	301	GNP	O2B-PB-O1B	3.20	116.64	109.92
3	E	301	GNP	O2B-PB-O1B	3.08	116.37	109.92
3	A	301	GNP	O4'-C1'-N9	-2.73	104.97	109.04
3	K	301	GNP	O2B-PB-O3A	2.46	112.84	104.64
3	G	301	GNP	O2B-PB-O3A	2.27	112.21	104.64
3	A	301	GNP	O2B-PB-O3A	2.22	112.06	104.64
3	G	301	GNP	O6-C6-N1	-2.20	119.73	122.69
3	E	301	GNP	O6-C6-N1	-2.19	119.74	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	301	GNP	O6-C6-N1	-2.08	119.90	122.69
3	C	301	GNP	O2B-PB-O3A	2.02	111.38	104.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

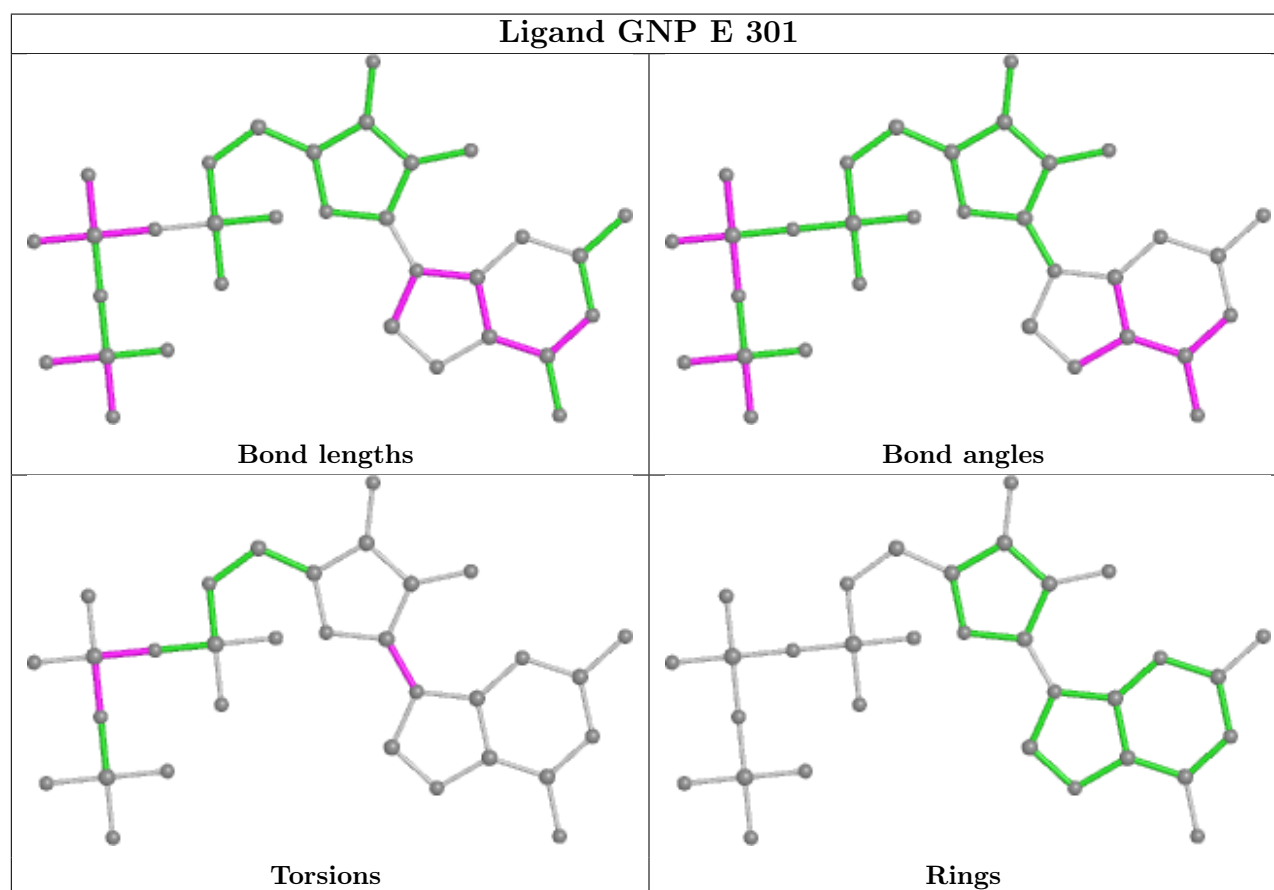
Mol	Chain	Res	Type	Atoms
3	A	301	GNP	PG-N3B-PB-O1B
3	A	301	GNP	PA-O3A-PB-O1B
3	A	301	GNP	C2'-C1'-N9-C4
3	C	301	GNP	PG-N3B-PB-O1B
3	C	301	GNP	PA-O3A-PB-O1B
3	C	301	GNP	PA-O3A-PB-O2B
3	C	301	GNP	C2'-C1'-N9-C4
3	E	301	GNP	PG-N3B-PB-O1B
3	E	301	GNP	PA-O3A-PB-O1B
3	E	301	GNP	PA-O3A-PB-O2B
3	E	301	GNP	C2'-C1'-N9-C4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

There are no ring outliers.

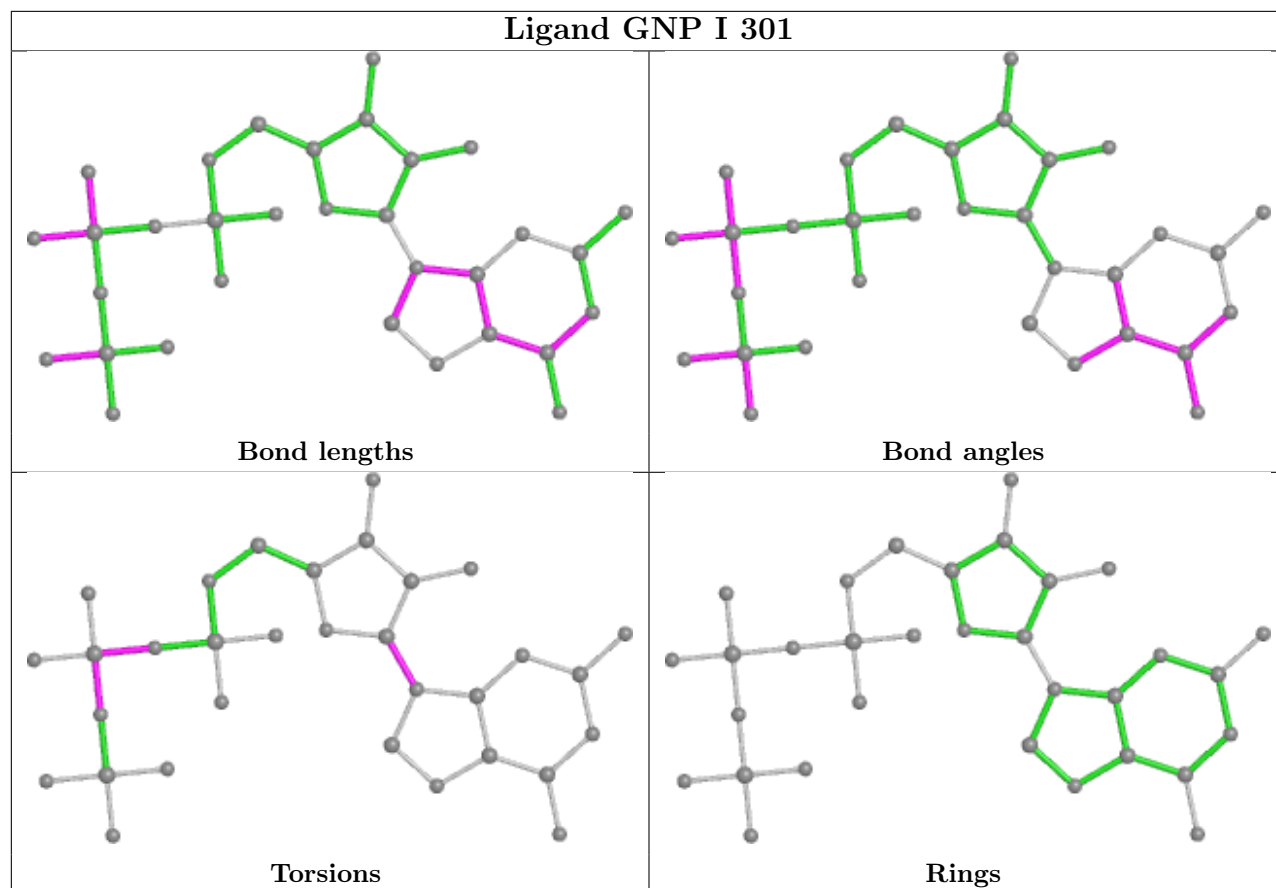
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	GNP	1	0

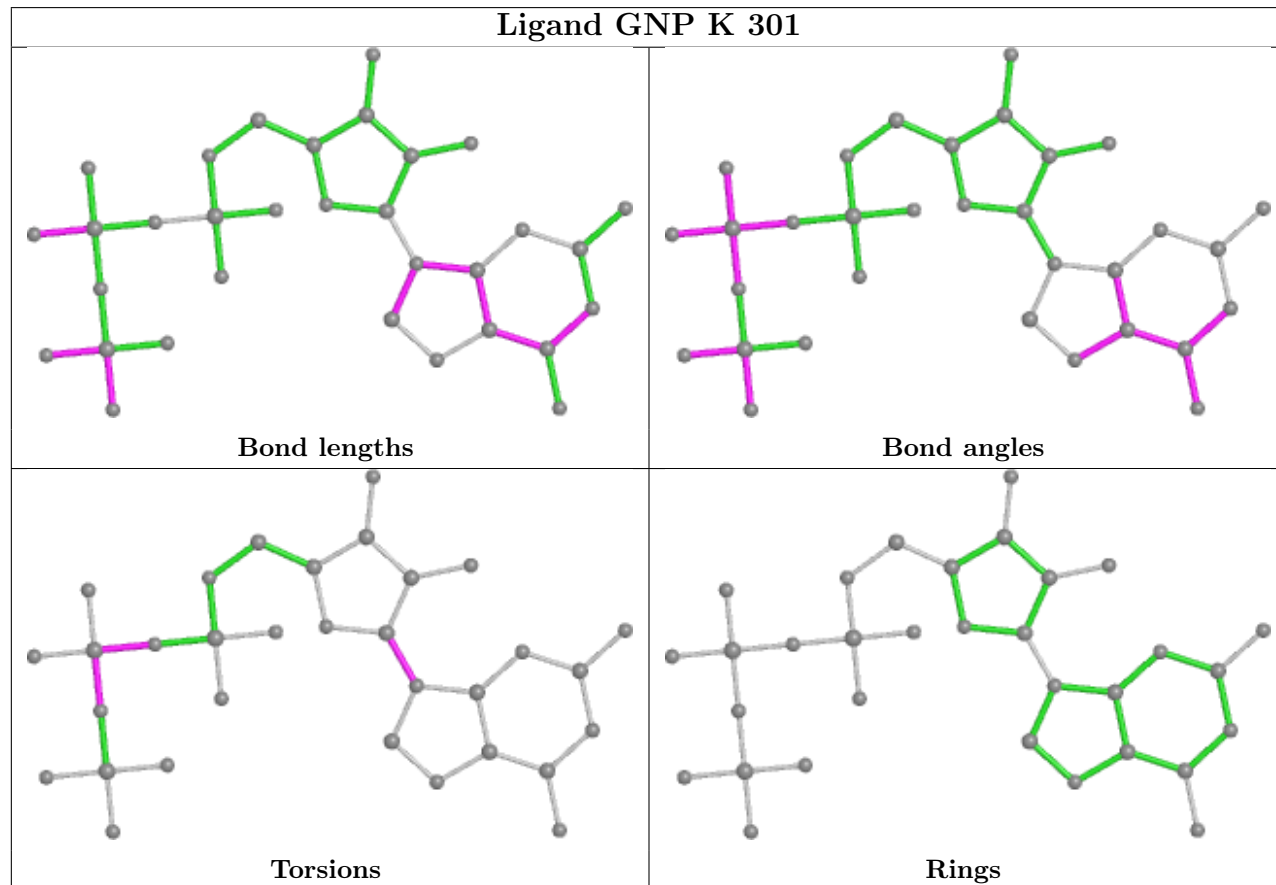
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



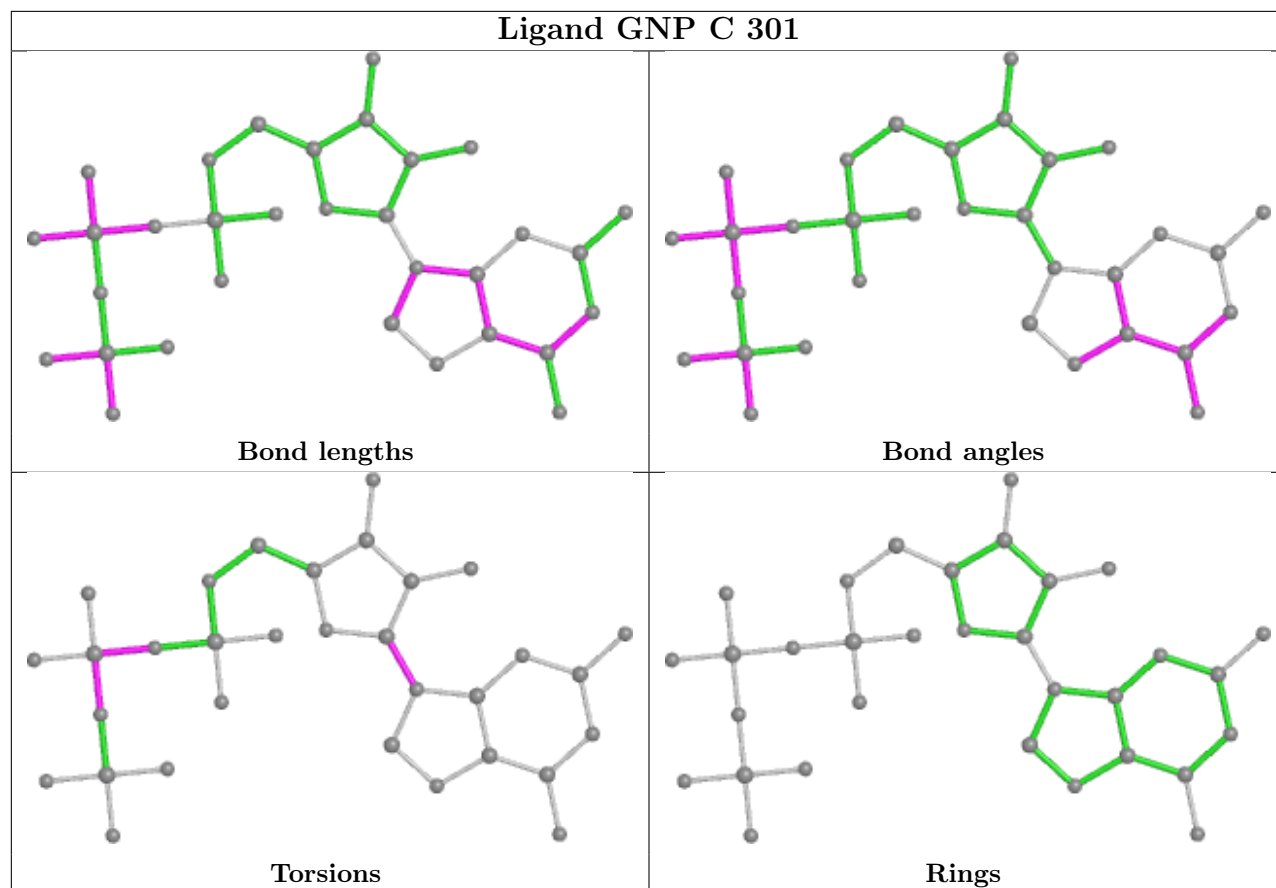
Ligand GNP I 301



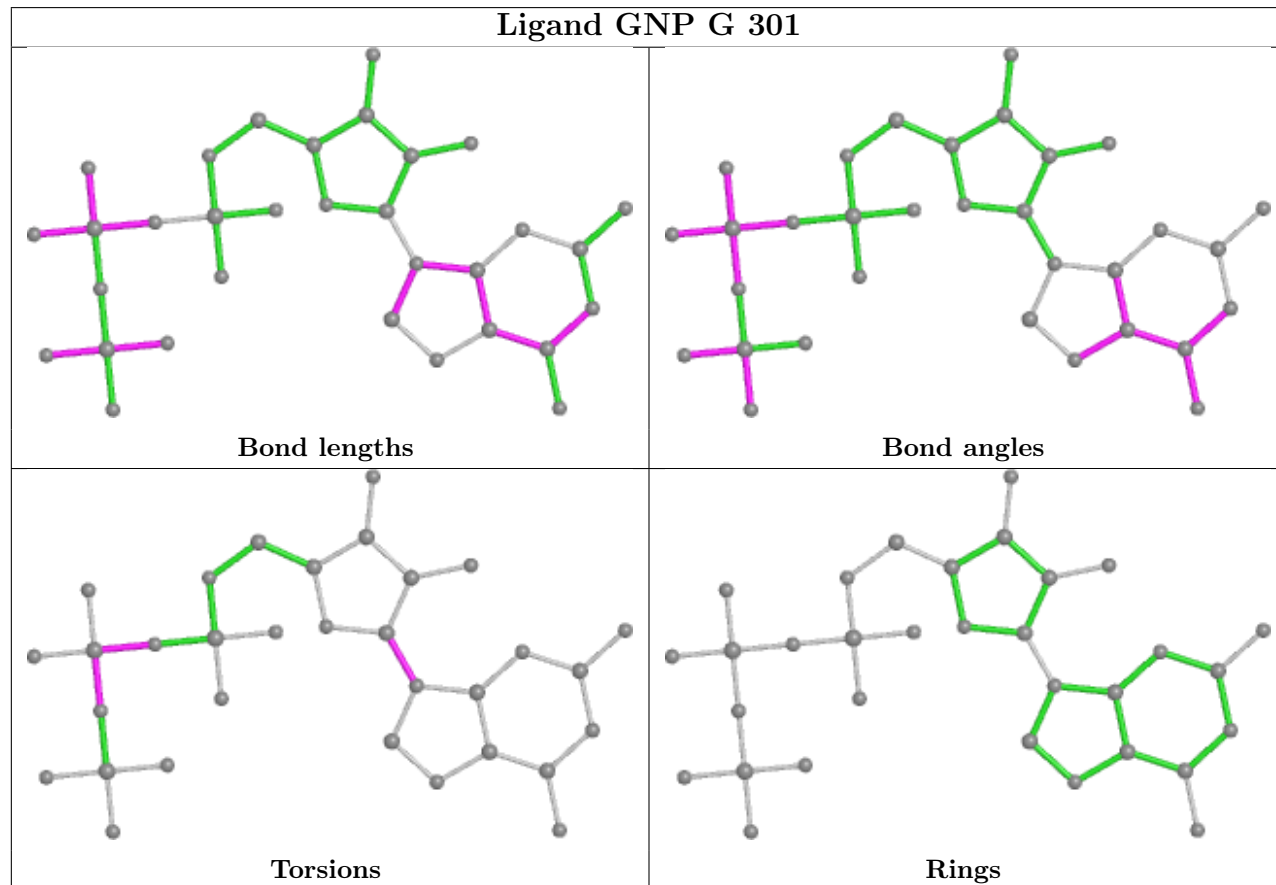
Ligand GNP K 301

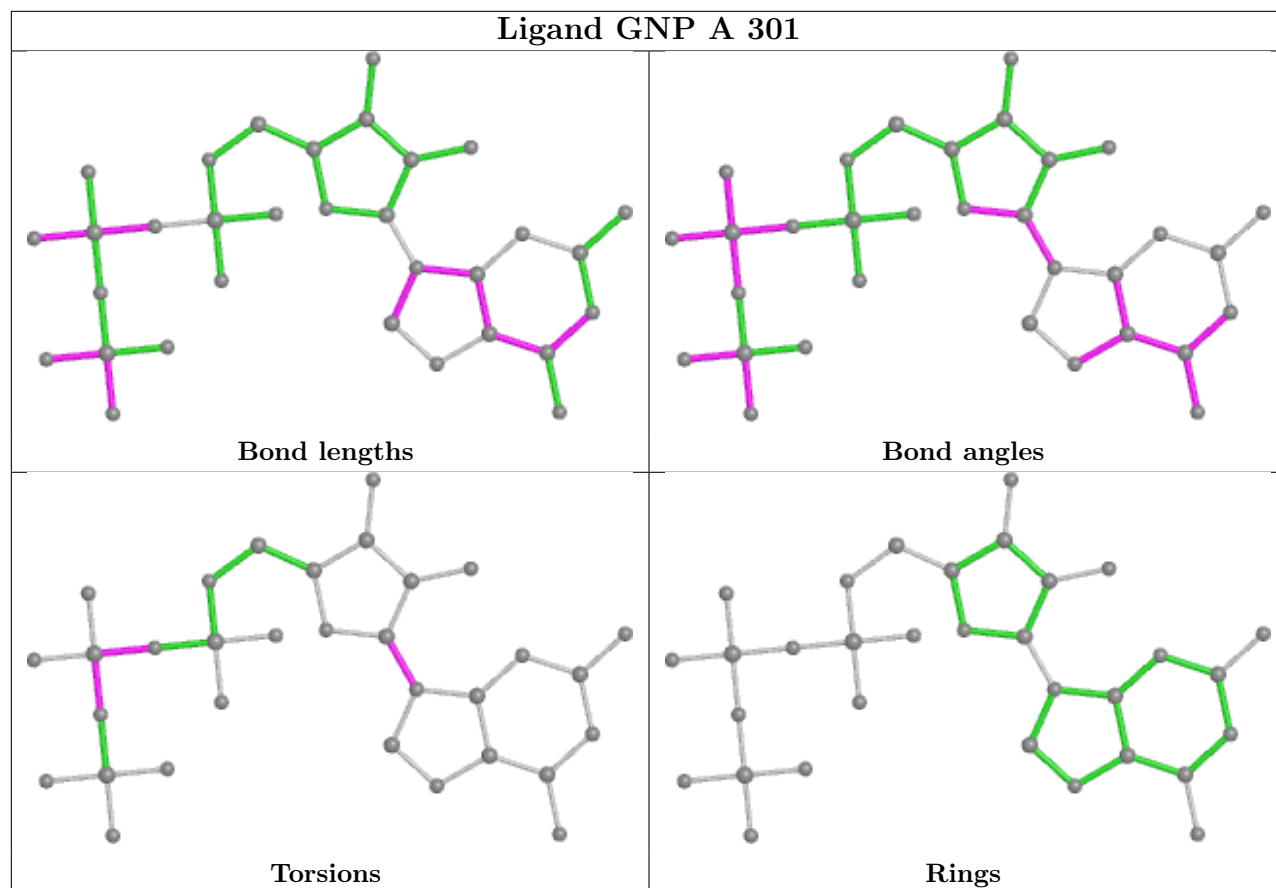


Ligand GNP C 301



Ligand GNP G 301





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	207/217 (95%)	0.45	22 (10%) 6 5	44, 69, 120, 156	0
1	C	205/217 (94%)	0.35	18 (8%) 10 9	40, 59, 122, 176	0
1	E	204/217 (94%)	0.63	27 (13%) 3 3	44, 63, 149, 181	0
1	G	207/217 (95%)	0.38	14 (6%) 17 15	37, 64, 124, 198	0
1	I	207/217 (95%)	0.56	24 (11%) 4 4	39, 61, 127, 153	0
1	K	206/217 (94%)	0.62	25 (12%) 4 3	44, 64, 118, 146	0
2	B	130/141 (92%)	0.11	2 (1%) 73 72	40, 55, 84, 116	0
2	D	131/141 (92%)	0.15	7 (5%) 26 25	41, 59, 99, 122	0
2	F	131/141 (92%)	0.79	17 (12%) 3 3	53, 80, 125, 155	0
2	H	129/141 (91%)	0.23	6 (4%) 31 30	39, 58, 104, 135	0
2	J	131/141 (92%)	0.08	8 (6%) 21 20	40, 57, 110, 156	0
2	L	131/141 (92%)	0.21	11 (8%) 11 10	41, 56, 87, 129	0
All	All	2019/2148 (93%)	0.41	181 (8%) 9 8	37, 63, 122, 198	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	TYR	9.0
1	I	192	ALA	7.8
1	E	75	LEU	7.5
1	E	196	GLN	7.2
1	I	197	TYR	6.8
1	G	72	PHE	6.0
1	K	70	GLU	6.0
2	J	2019	MET	5.9
1	I	191	PRO	5.4
1	I	194	ALA	5.4
1	I	75	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	I	195	ALA	5.3
1	G	81	ILE	5.0
1	E	192	ALA	4.9
2	F	2148	ASP	4.9
1	A	212	GLU	4.9
1	G	188	VAL	4.9
1	A	7	PRO	4.8
1	E	194	ALA	4.8
2	F	2019	MET	4.7
1	E	190	ASP	4.6
1	E	193	LEU	4.5
2	J	2018	GLN	4.5
2	H	2019	MET	4.5
1	A	134	LYS	4.3
2	H	2024	GLU	4.3
1	I	213	ASP	4.2
1	E	191	PRO	4.1
1	C	188	VAL	4.0
1	E	195	ALA	4.0
1	C	197	TYR	3.9
1	E	199	HIS	3.9
2	L	2019	MET	3.9
1	E	113	GLU	3.9
2	D	2018	GLN	3.9
1	K	26	PHE	3.8
1	A	72	PHE	3.7
2	L	2018	GLN	3.7
2	L	2094	ASN	3.7
1	C	120	CYS	3.6
1	G	187	VAL	3.6
1	A	132	LYS	3.6
1	A	71	LYS	3.5
1	A	89	MET	3.5
2	F	2023	VAL	3.5
1	K	7	PRO	3.5
1	E	189	MET	3.5
1	I	89	MET	3.5
1	C	190	ASP	3.4
2	L	2148	ASP	3.4
1	G	191	PRO	3.4
1	I	137	VAL	3.4
1	C	189	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	134	LYS	3.4
1	K	132	LYS	3.3
1	G	71	LYS	3.3
2	F	2020	PRO	3.3
2	J	2147	LEU	3.3
1	G	73	GLY	3.2
1	A	140	ARG	3.2
1	K	134	LYS	3.2
1	G	182	LEU	3.2
2	D	2148	ASP	3.1
2	F	2103	ARG	3.1
2	F	2018	GLN	3.1
1	E	206	THR	3.1
2	F	2129	PRO	3.0
1	A	114	ASN	3.0
2	F	2022	LYS	3.0
2	F	2021	GLU	3.0
1	I	190	ASP	3.0
1	A	70	GLU	2.9
1	I	193	LEU	2.9
2	H	2023	VAL	2.9
1	A	120	CYS	2.9
1	I	189	MET	2.9
1	C	72	PHE	2.9
1	G	189	MET	2.9
1	I	114	ASN	2.9
2	D	2067	VAL	2.9
1	C	87	ILE	2.8
1	I	134	LYS	2.8
1	K	136	ILE	2.8
1	E	198	GLU	2.8
1	A	127	LYS	2.8
1	E	174	LEU	2.8
1	A	131	VAL	2.8
1	K	72	PHE	2.8
2	H	2021	GLU	2.8
1	I	74	GLY	2.8
2	F	2145	LEU	2.8
1	C	132	LYS	2.7
1	K	69	GLN	2.7
1	E	203	VAL	2.7
2	L	2108	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	130	LYS	2.7
1	C	127	LYS	2.7
2	J	2020	PRO	2.7
1	C	187	VAL	2.7
1	K	9	VAL	2.7
1	K	95	ARG	2.7
1	I	87	ILE	2.7
1	C	73	GLY	2.6
1	E	202	GLU	2.6
1	E	211	ASP	2.6
1	G	186	GLU	2.6
2	L	2093	MET	2.6
2	D	2024	GLU	2.6
1	K	27	VAL	2.6
2	J	2148	ASP	2.6
1	K	89	MET	2.6
2	F	2084	CYS	2.6
2	F	2131	LEU	2.6
1	I	196	GLN	2.6
1	K	75	LEU	2.5
2	L	2092	THR	2.5
1	I	132	LYS	2.5
2	F	2102	ASP	2.5
2	D	2023	VAL	2.5
1	K	198	GLU	2.5
1	I	88	ILE	2.5
1	C	89	MET	2.5
2	J	2021	GLU	2.5
1	K	30	HIS	2.4
1	E	86	ALA	2.4
1	A	43	LEU	2.4
1	G	197	TYR	2.4
1	A	87	ILE	2.4
2	J	2023	VAL	2.4
1	K	120	CYS	2.4
2	F	2086	ASN	2.4
1	C	160	PRO	2.4
1	I	199	HIS	2.4
1	I	120	CYS	2.4
2	B	2148	ASP	2.4
2	H	2020	PRO	2.4
1	C	193	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	89	MET	2.3
1	K	76	ARG	2.3
1	A	133	ALA	2.3
1	K	141	LYS	2.3
1	G	82	GLN	2.3
1	A	39	TYR	2.3
1	K	138	PHE	2.3
1	A	110	ARG	2.3
2	D	2022	LYS	2.3
1	K	137	VAL	2.3
1	E	127	LYS	2.3
1	I	26	PHE	2.3
2	F	2067	VAL	2.3
1	E	114	ASN	2.3
2	F	2146	LEU	2.3
1	E	201	LEU	2.2
1	K	63	VAL	2.2
1	C	118	VAL	2.2
2	L	2067	VAL	2.2
1	K	157	PHE	2.2
1	C	182	LEU	2.2
1	C	199	HIS	2.1
1	A	76	ARG	2.1
2	F	2035	LEU	2.1
2	J	2146	LEU	2.1
1	K	96	VAL	2.1
2	H	2067	VAL	2.1
1	K	169	ILE	2.1
1	I	127	LYS	2.1
2	B	2095	LEU	2.1
1	A	141	LYS	2.1
1	E	87	ILE	2.1
2	L	2095	LEU	2.1
2	L	2107	TRP	2.1
1	C	134	LYS	2.1
1	A	137	VAL	2.0
1	I	141	LYS	2.0
1	E	200	ASP	2.0
1	K	71	LYS	2.0
1	E	14	VAL	2.0
1	G	110	ARG	2.0
1	E	126	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	2025	LEU	2.0
2	L	2022	LYS	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 [i](#)

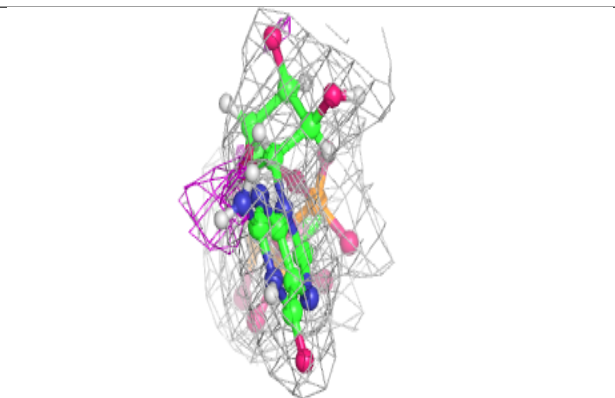
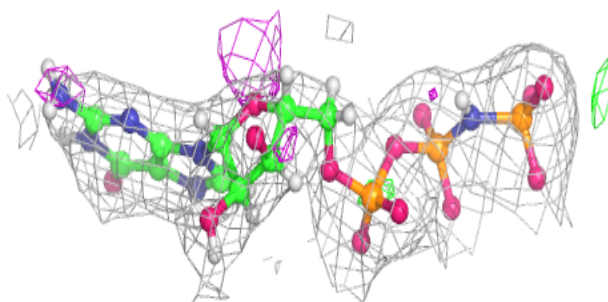
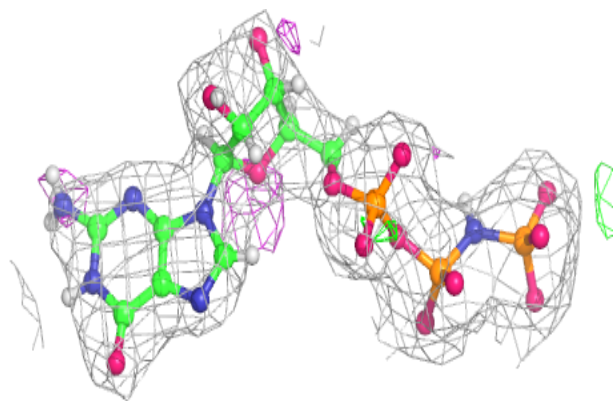
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.88	0.16	47,47,47,47	0
3	GNP	I	301	32/32	0.95	0.19	35,46,58,62	0
4	MG	G	302	1/1	0.95	0.10	43,43,43,43	0
4	MG	K	302	1/1	0.96	0.15	48,48,48,48	0
3	GNP	K	301	32/32	0.97	0.15	41,52,70,82	0
4	MG	A	302	1/1	0.97	0.11	49,49,49,49	0
3	GNP	E	301	32/32	0.97	0.16	37,48,62,74	0
3	GNP	G	301	32/32	0.97	0.14	37,42,58,77	0
3	GNP	C	301	32/32	0.97	0.15	35,42,62,71	0
4	MG	C	302	1/1	0.98	0.15	43,43,43,43	0
3	GNP	A	301	32/32	0.98	0.10	44,56,70,79	0
4	MG	I	302	1/1	0.99	0.22	42,42,42,42	0

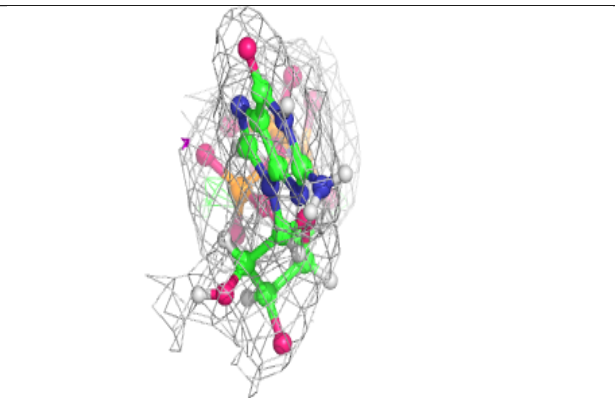
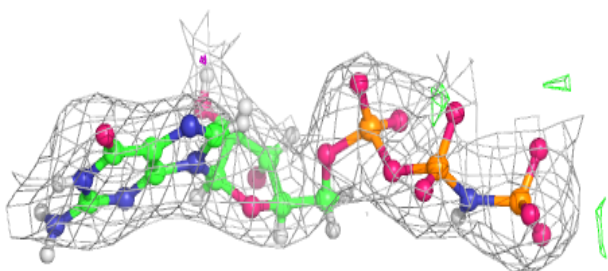
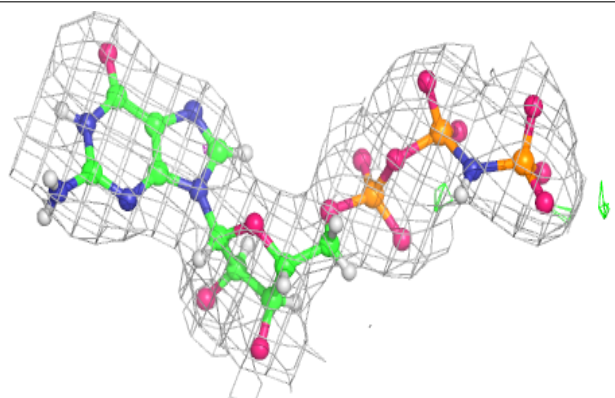
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP I 301:

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

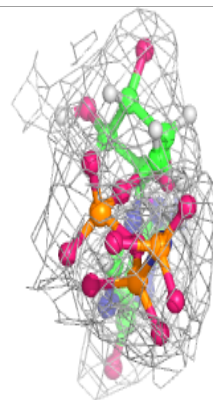
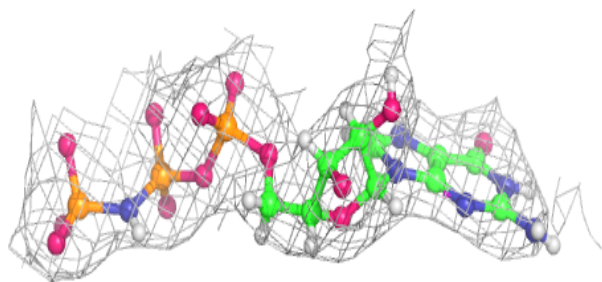
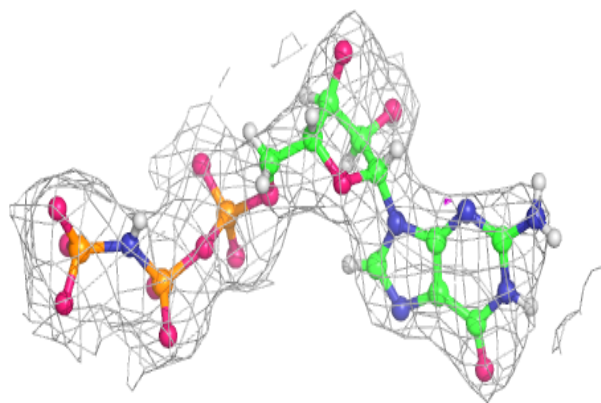
**Electron density around GNP K 301:**

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

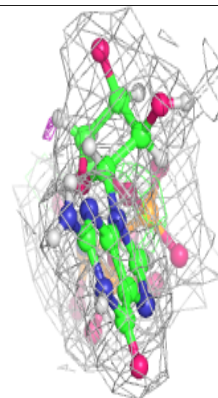
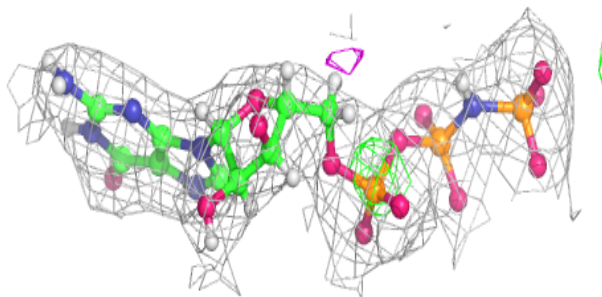
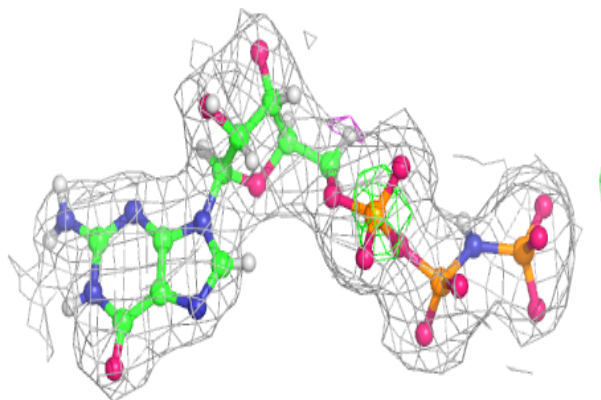


Electron density around GNP E 301:

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

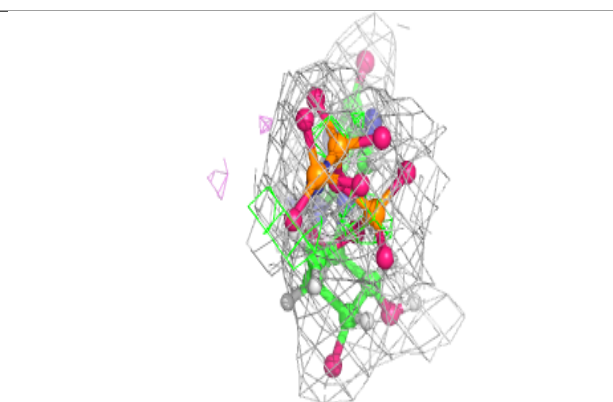
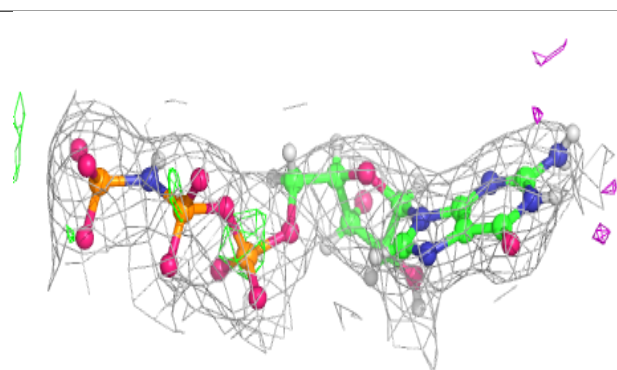
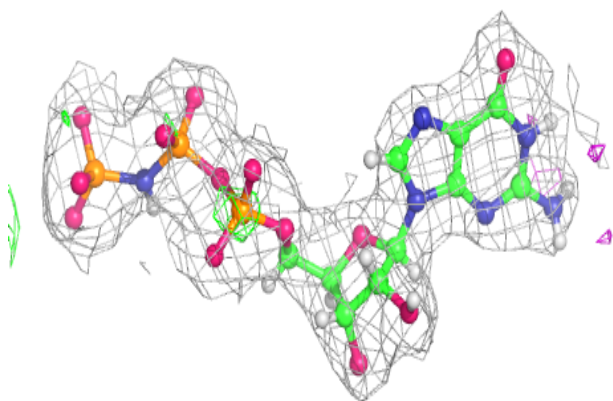
**Electron density around GNP G 301:**

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

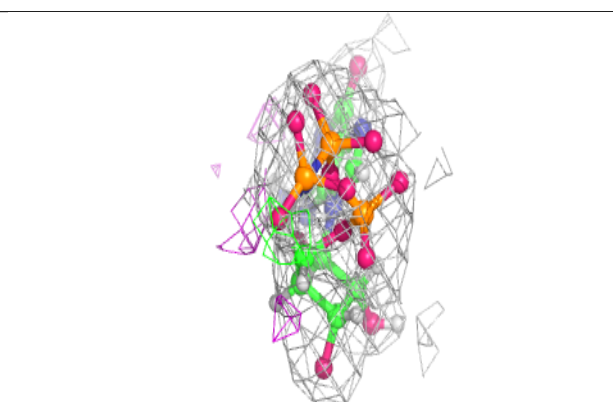
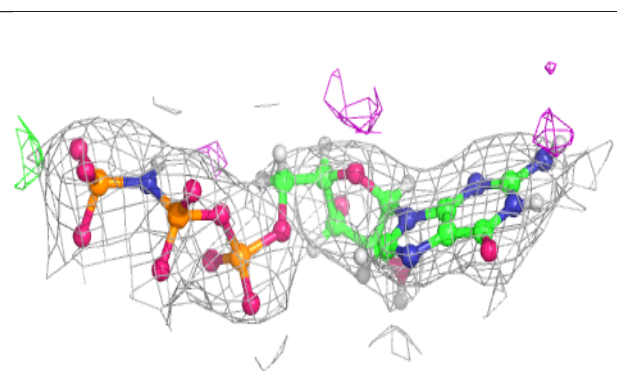
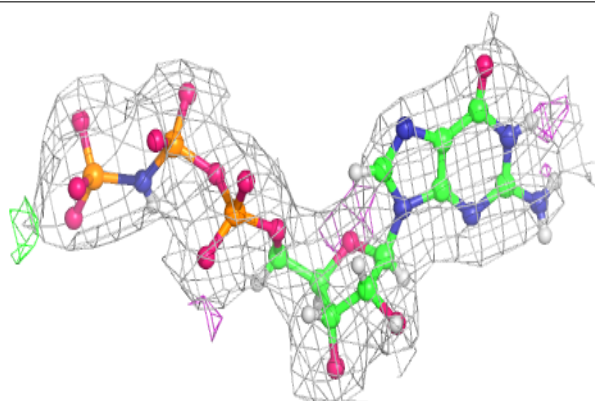


Electron density around GNP C 301:

$2mF_o-DF_c$ (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.