Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 04:08 PM EDT

PDB ID	:	1JPN
Title	:	GMPPNP Complex of SRP GTPase NG Domain
Authors	:	Padmanabhan, S.; Freymann, D.M.
Deposited on	:	2001-08-02
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

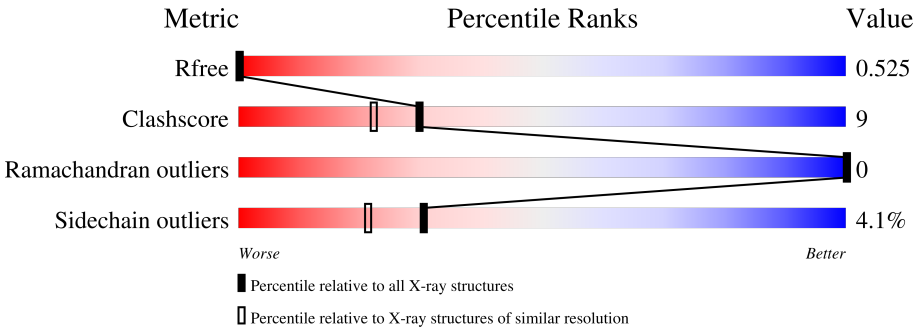
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	296	81% 18% .
1	B	296	77% 21% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	A	952	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5117 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.

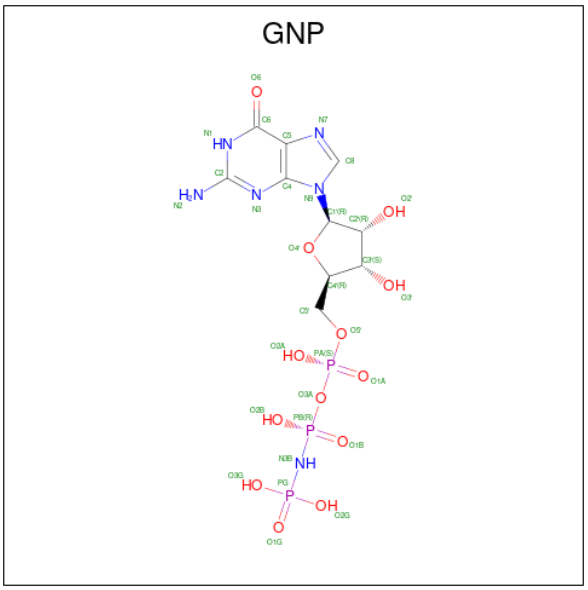
- Molecule 1 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	295	Total	C	N	O	S	0	6	0
			2318	1454	423	434	7			
1	A	296	Total	C	N	O	S	0	1	0
			2286	1435	416	428	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

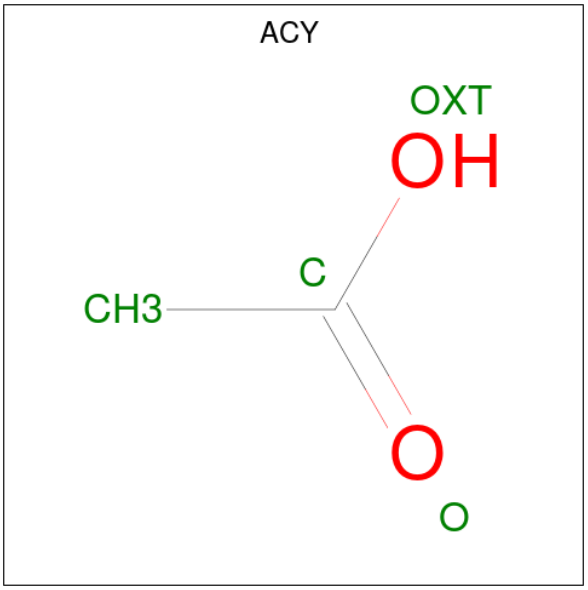
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- 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	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

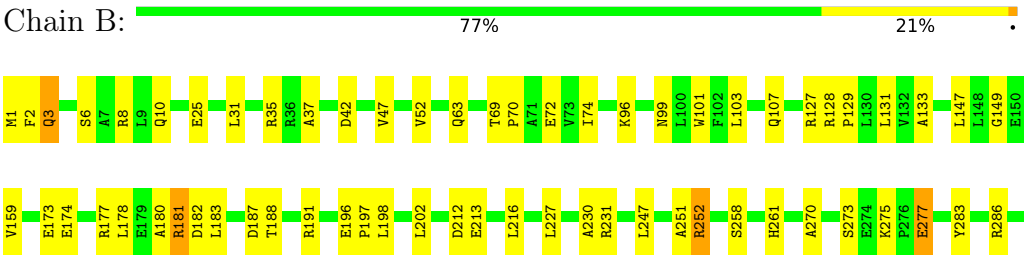
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	180	Total	O	0	0
			180	180		
5	A	251	Total	O	0	0
			251	251		

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. 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. 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.

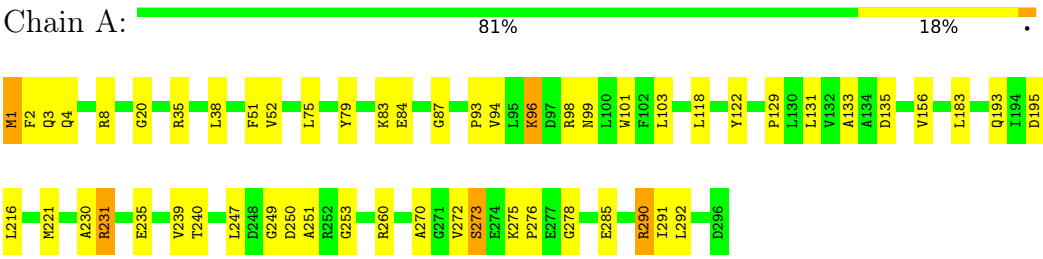
• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain B:



• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.81Å 54.53Å 99.08Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 17.84 – 0.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.90) 7.5 (17.84-0.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.241 0.522 , 0.525	Depositor DCC
R_{free} test set	4875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.01 , -2.0	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.43	EDS
Total number of atoms	5117	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, GNP, CA

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	0.23	0/2311	0.46	0/3112
1	B	0.23	0/2343	0.45	0/3155
All	All	0.23	0/4654	0.45	0/6267

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2286	0	2385	37	0
1	B	2318	0	2416	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	1	0
4	A	8	0	6	3	0
4	B	8	0	6	1	0
5	A	251	0	0	4	3
5	B	180	0	0	2	3
All	All	5117	0	4839	90	4

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 9.

All (90) 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:B:96:LYS:H	1:B:99:ASN:HD21	1.06	0.93
1:A:96:LYS:H	1:A:99:ASN:HD21	1.13	0.92
1:B:35:ARG:HB2	1:B:52[A]:VAL:HG21	1.68	0.76
1:B:69:THR:HB	1:B:72:GLU:HG3	1.69	0.73
1:A:1:MET:HA	1:A:3:GLN:HE22	1.51	0.73
1:B:96:LYS:H	1:B:99:ASN:ND2	1.85	0.71
1:B:96:LYS:N	1:B:99:ASN:HD21	1.86	0.70
1:B:283:TYR:HB3	1:B:286:ARG:HG3	1.73	0.68
1:A:231:ARG:O	1:A:235:GLU:HG2	1.94	0.68
1:B:247:LEU:HD12	1:B:270:ALA:HB1	1.76	0.67
1:B:128:ARG:NH1	1:B:180:ALA:HB3	2.11	0.66
1:A:20:GLY:HA2	5:A:1476:HOH:O	1.96	0.64
1:A:247:LEU:HD12	1:A:270:ALA:HB1	1.80	0.63
1:B:275:LYS:HG3	1:B:277:GLU:HG2	1.83	0.60
1:B:283:TYR:CB	1:B:286:ARG:HG3	2.32	0.59
1:B:227:LEU:HD11	1:B:258:SER:HB2	1.85	0.58
1:B:273:SER:OG	1:B:275:LYS:HG2	2.04	0.58
1:A:195:ASP:HB3	1:A:198:LEU:HB3	1.84	0.58
1:B:128:ARG:HH12	1:B:180:ALA:HB3	1.69	0.58
1:A:272:VAL:HG22	1:A:278:GLY:O	2.05	0.57
1:A:1:MET:HG2	1:A:247:LEU:O	2.04	0.57
1:B:174:GLU:HG3	1:B:177:ARG:HH22	1.69	0.57
1:A:1:MET:SD	1:A:251:ALA:HB3	2.45	0.56
1:B:1:MET:N	1:B:3:GLN:HE22	2.04	0.55
1:A:1:MET:HA	1:A:3:GLN:NE2	2.19	0.55
1:A:35:ARG:HB2	1:A:52:VAL:HG21	1.88	0.54
1:B:42:ASP:HB2	1:B:252:ARG:HD3	1.88	0.54
1:B:196:GLU:HB3	1:B:197:PRO:HD3	1.89	0.54
1:A:290:ARG:HG3	1:A:291:ILE:N	2.23	0.53
1:B:8[A]:ARG:HG2	1:B:37:ALA:HB2	1.90	0.53
1:A:216:LEU:CD2	1:A:230:ALA:HA	2.39	0.53
1:B:25:GLU:HB2	5:B:1334:HOH:O	2.08	0.53
1:A:133:ALA:HB1	4:A:952:ACY:H2	1.90	0.52
1:A:87:GLY:HA2	1:A:260:ARG:HD2	1.91	0.52
1:B:191:ARG:HG2	1:B:198:LEU:HD13	1.91	0.51
1:B:47:VAL:HG22	1:B:261:HIS:CG	2.45	0.51
1:B:31:LEU:HD22	1:B:52[A]:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:HB2	1:B:252:ARG:HH11	1.76	0.50
1:B:216:LEU:CD2	1:B:230:ALA:HA	2.42	0.49
1:B:273:SER:OG	1:B:275:LYS:HE3	2.13	0.48
1:B:31:LEU:HB3	1:B:52[B]:VAL:CG2	2.43	0.48
1:B:216:LEU:HD21	1:B:230:ALA:HA	1.97	0.47
1:A:38:LEU:HD11	1:A:51:PHE:CD1	2.50	0.47
1:A:118:LEU:HD22	1:A:122:TYR:HE2	1.80	0.47
1:A:216:LEU:HD21	1:A:230:ALA:HA	1.96	0.47
1:B:35:ARG:HG2	1:B:35:ARG:HH11	1.80	0.47
1:B:127:ARG:HH21	1:B:182:ASP:HB2	1.79	0.47
1:B:129:PRO:HA	1:B:183:LEU:O	2.16	0.46
1:B:1:MET:H1	1:B:3:GLN:HE22	1.63	0.46
1:B:131:LEU:HB2	1:B:156:VAL:HG22	1.97	0.46
1:A:129:PRO:HA	1:A:183:LEU:O	2.16	0.46
1:A:84:GLU:HG3	5:A:1452:HOH:O	2.15	0.45
1:B:133:ALA:O	1:B:159:VAL:HG22	2.17	0.45
1:B:1:MET:O	1:B:2:PHE:HB2	2.17	0.45
1:B:174:GLU:O	1:B:178:LEU:HG	2.17	0.45
1:A:193:GLN:HG2	5:A:1443:HOH:O	2.16	0.45
1:B:149:GLY:O	1:B:152:VAL:HG22	2.17	0.44
1:A:275:LYS:HB2	1:A:276:PRO:HD2	1.99	0.44
1:A:273:SER:OG	1:A:275:LYS:HG2	2.17	0.44
1:B:107:GLN:HA	3:B:910:GNP:O2G	2.17	0.44
1:B:128:ARG:NH2	1:B:181:ARG:HH21	2.15	0.44
1:B:188:THR:HB	1:B:202:LEU:HD21	2.00	0.44
1:A:93:PRO:HB2	1:A:101:TRP:CH2	2.53	0.44
1:A:135:ASP:HB2	4:A:952:ACY:H1	1.99	0.43
1:B:273:SER:HG	1:B:275:LYS:HE3	1.82	0.43
1:A:1:MET:O	1:A:2:PHE:HB2	2.18	0.43
1:A:1:MET:HE3	1:A:253:GLY:HA2	1.99	0.43
1:A:131:LEU:HB2	1:A:156:VAL:HG22	1.99	0.43
1:B:6[B]:SER:O	1:B:10:GLN:HG3	2.18	0.43
1:B:101:TRP:CD1	1:B:213:GLU:HB2	2.54	0.43
1:A:135:ASP:CB	4:A:952:ACY:H1	2.49	0.43
1:B:1:MET:N	1:B:3:GLN:NE2	2.66	0.42
1:A:195:ASP:CG	1:A:197:PRO:HD2	2.39	0.42
1:B:2:PHE:HE1	1:B:247:LEU:HD22	1.85	0.42
1:B:6[A]:SER:O	1:B:10:GLN:HG3	2.19	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.91	0.42
1:A:94:VAL:HG23	5:A:1252:HOH:O	2.20	0.42
1:B:187:ASP:OD2	4:B:950:ACY:H2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD12	1:A:292:LEU:HD13	2.01	0.42
1:A:8:ARG:HA	1:A:8:ARG:HD3	1.87	0.42
1:A:239:VAL:HG12	1:A:240:THR:N	2.35	0.42
1:B:1:MET:HG3	1:B:251:ALA:O	2.20	0.41
1:B:70:PRO:O	1:B:74:ILE:HG12	2.20	0.41
1:B:1:MET:HG2	1:B:2:PHE:CD1	2.55	0.41
1:A:221:MET:SD	1:A:249:GLY:HA3	2.61	0.41
1:B:31:LEU:HB3	1:B:52[A]:VAL:CG1	2.49	0.41
1:B:261:HIS:HB2	5:B:1266:HOH:O	2.20	0.41
1:A:79:TYR:OH	1:A:285:GLU:HG3	2.21	0.41
1:B:147:LEU:O	1:B:151:LYS:HB2	2.21	0.41
1:A:3:GLN:HE21	1:A:3:GLN:HB2	1.76	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1121:HOH:O	5:B:1407:HOH:O[2_656]	1.93	0.27
5:B:1299:HOH:O	5:A:1385:HOH:O[3_445]	2.02	0.18
5:A:1180:HOH:O	5:A:1321:HOH:O[2_655]	2.04	0.16
5:B:1158:HOH:O	5:A:1050:HOH:O[4_546]	2.11	0.09

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	295/296 (100%)	289 (98%)	6 (2%)	0	100	100
1	B	299/296 (101%)	295 (99%)	4 (1%)	0	100	100
All	All	594/592 (100%)	584 (98%)	10 (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	235/234 (100%)	225 (96%)	10 (4%)	29	19
1	B	239/234 (102%)	230 (96%)	9 (4%)	33	24
All	All	474/468 (101%)	455 (96%)	19 (4%)	30	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	63	GLN
1	B	103	LEU
1	B	173	GLU
1	B	181	ARG
1	B	212	ASP
1	B	231	ARG
1	B	252	ARG
1	B	277	GLU
1	A	1	MET
1	A	4	GLN
1	A	83	LYS
1	A	96	LYS
1	A	98	ARG
1	A	103	LEU
1	A	231	ARG
1	A	250	ASP
1	A	273	SER
1	A	290	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	99	ASN
1	B	144	GLN

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	261	HIS
1	A	44	ASN
1	A	99	ASN
1	A	224	GLN
1	A	261	HIS

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 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	ACY	A	952	-	3,3,3	1.25	0	3,3,3	1.34	0
3	GNP	A	911	-	29,34,34	1.95	12 (41%)	33,54,54	2.26	7 (21%)
3	GNP	B	910	-	29,34,34	1.93	12 (41%)	33,54,54	2.28	9 (27%)
4	ACY	B	950	-	3,3,3	1.37	0	3,3,3	1.26	0
4	ACY	B	951	-	3,3,3	1.36	0	3,3,3	1.27	0
4	ACY	A	953	-	3,3,3	1.34	0	3,3,3	1.27	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
3	GNP	A	911	-	-	1/14/38/38	0/3/3/3
3	GNP	B	910	-	-	2/14/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	911	GNP	C6-N1	4.49	1.40	1.33
3	B	910	GNP	C6-N1	4.43	1.40	1.33
3	A	911	GNP	C5-C6	3.25	1.47	1.41
3	A	911	GNP	PB-N3B	3.19	1.71	1.63
3	B	910	GNP	C5-C6	3.16	1.46	1.41
3	A	911	GNP	PG-N3B	3.12	1.71	1.63
3	B	910	GNP	PB-N3B	2.96	1.71	1.63
3	B	910	GNP	PG-N3B	2.94	1.71	1.63
3	B	910	GNP	C8-N7	-2.81	1.29	1.34
3	A	911	GNP	C8-N7	-2.80	1.29	1.34
3	B	910	GNP	PB-O1B	2.77	1.50	1.46
3	A	911	GNP	PB-O1B	2.75	1.50	1.46
3	A	911	GNP	C2-N1	2.62	1.40	1.35
3	B	910	GNP	C2-N1	2.59	1.40	1.35
3	A	911	GNP	PG-O1G	2.52	1.50	1.46
3	B	910	GNP	PG-O2G	-2.48	1.50	1.56
3	A	911	GNP	PG-O3G	-2.47	1.50	1.56
3	B	910	GNP	PG-O1G	2.47	1.50	1.46
3	B	910	GNP	PB-O2B	-2.36	1.50	1.56
3	A	911	GNP	PG-O2G	-2.35	1.50	1.56
3	A	911	GNP	PB-O2B	-2.33	1.50	1.56
3	B	910	GNP	PG-O3G	-2.29	1.50	1.56
3	B	910	GNP	C4-N3	2.10	1.38	1.35
3	A	911	GNP	C4-N3	2.02	1.38	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	911	GNP	C5-C6-N1	-7.94	112.57	123.43
3	B	910	GNP	C5-C6-N1	-7.90	112.62	123.43
3	B	910	GNP	C2-N1-C6	6.09	125.61	115.93
3	A	911	GNP	C2-N1-C6	6.06	125.56	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	911	GNP	O2B-PB-O1B	4.26	118.85	109.92
3	B	910	GNP	O2B-PB-O1B	4.25	118.83	109.92
3	B	910	GNP	N3-C2-N1	-3.85	122.08	127.22
3	A	911	GNP	N3-C2-N1	-3.82	122.12	127.22
3	A	911	GNP	C4-C5-C6	-2.48	118.43	120.80
3	B	910	GNP	C4-C5-C6	-2.44	118.47	120.80
3	B	910	GNP	O1G-PG-N3B	-2.25	108.46	111.77
3	A	911	GNP	O3A-PB-N3B	-2.15	100.64	106.59
3	A	911	GNP	O1B-PB-N3B	-2.14	108.62	111.77
3	B	910	GNP	O1B-PB-N3B	-2.11	108.66	111.77
3	B	910	GNP	O4'-C1'-C2'	-2.07	103.91	106.93
3	B	910	GNP	O3A-PB-N3B	-2.04	100.94	106.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	910	GNP	PB-N3B-PG-O1G
3	A	911	GNP	PG-N3B-PB-O1B
3	B	910	GNP	PB-O3A-PA-O1A

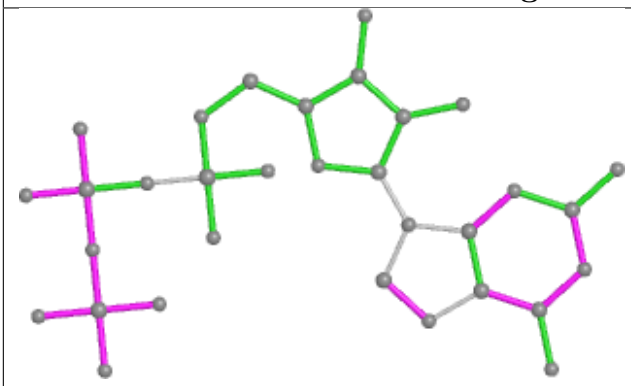
There are no ring outliers.

3 monomers are involved in 5 short contacts:

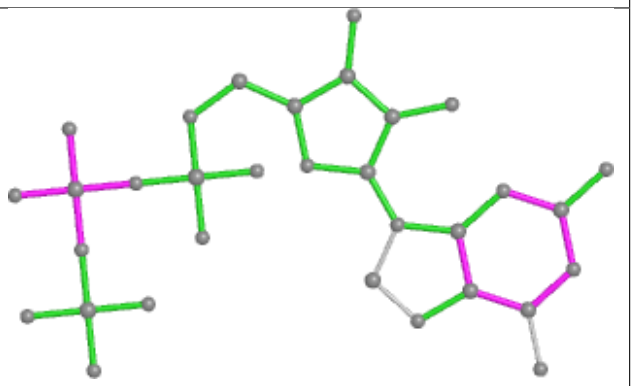
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	952	ACY	3	0
3	B	910	GNP	1	0
4	B	950	ACY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

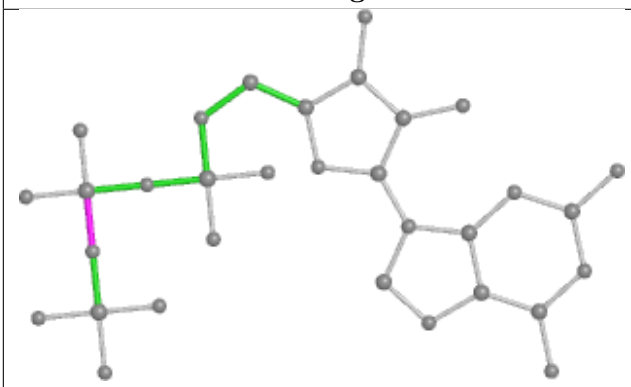
Ligand GNP A 911



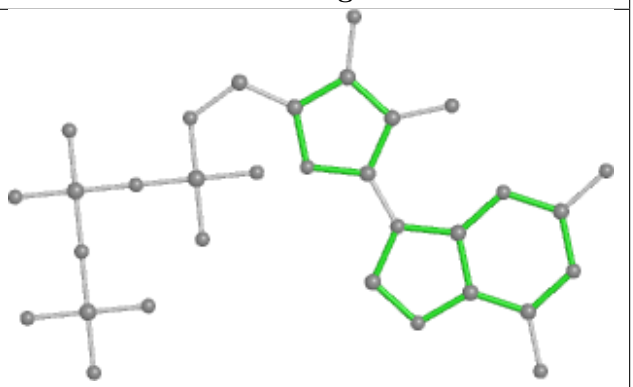
Bond lengths



Bond angles

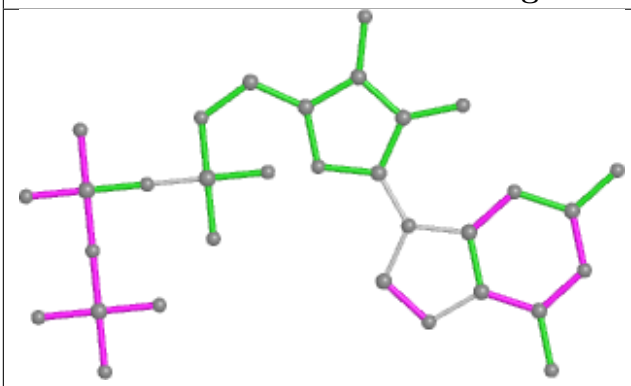


Torsions

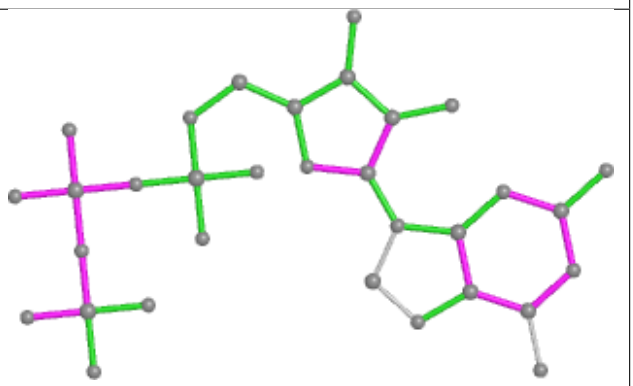


Rings

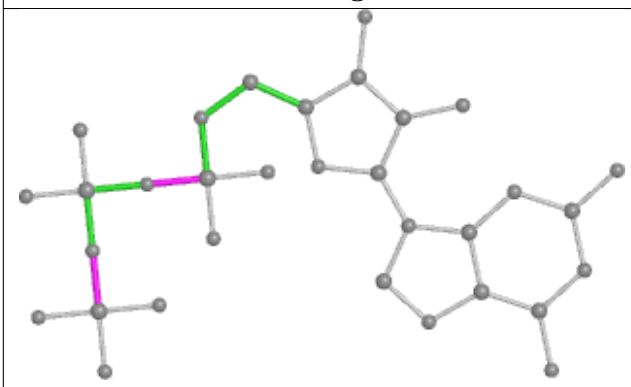
Ligand GNP B 910



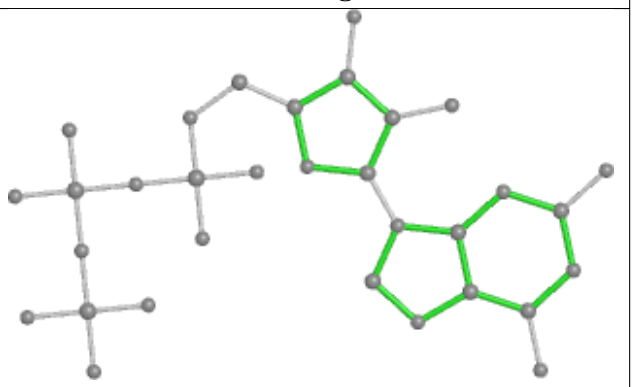
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

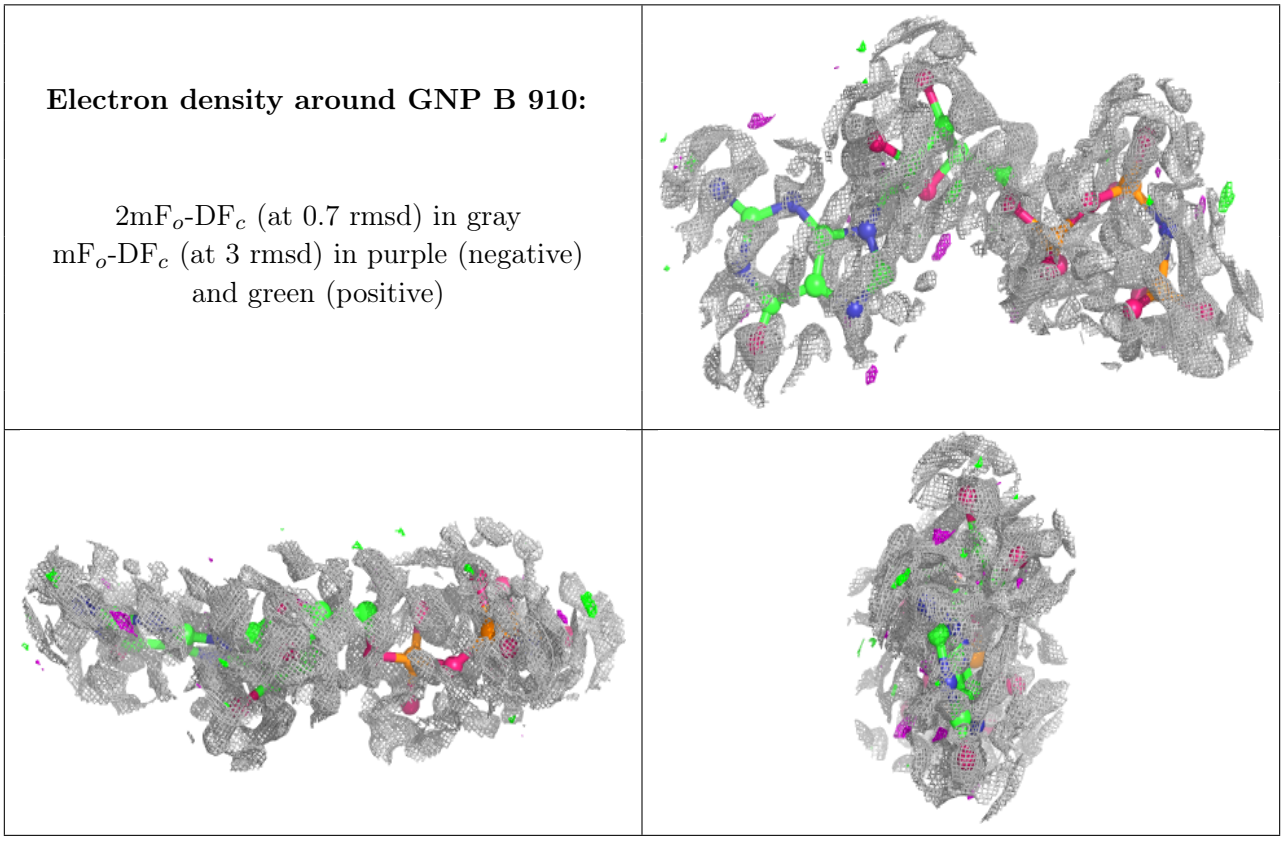
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

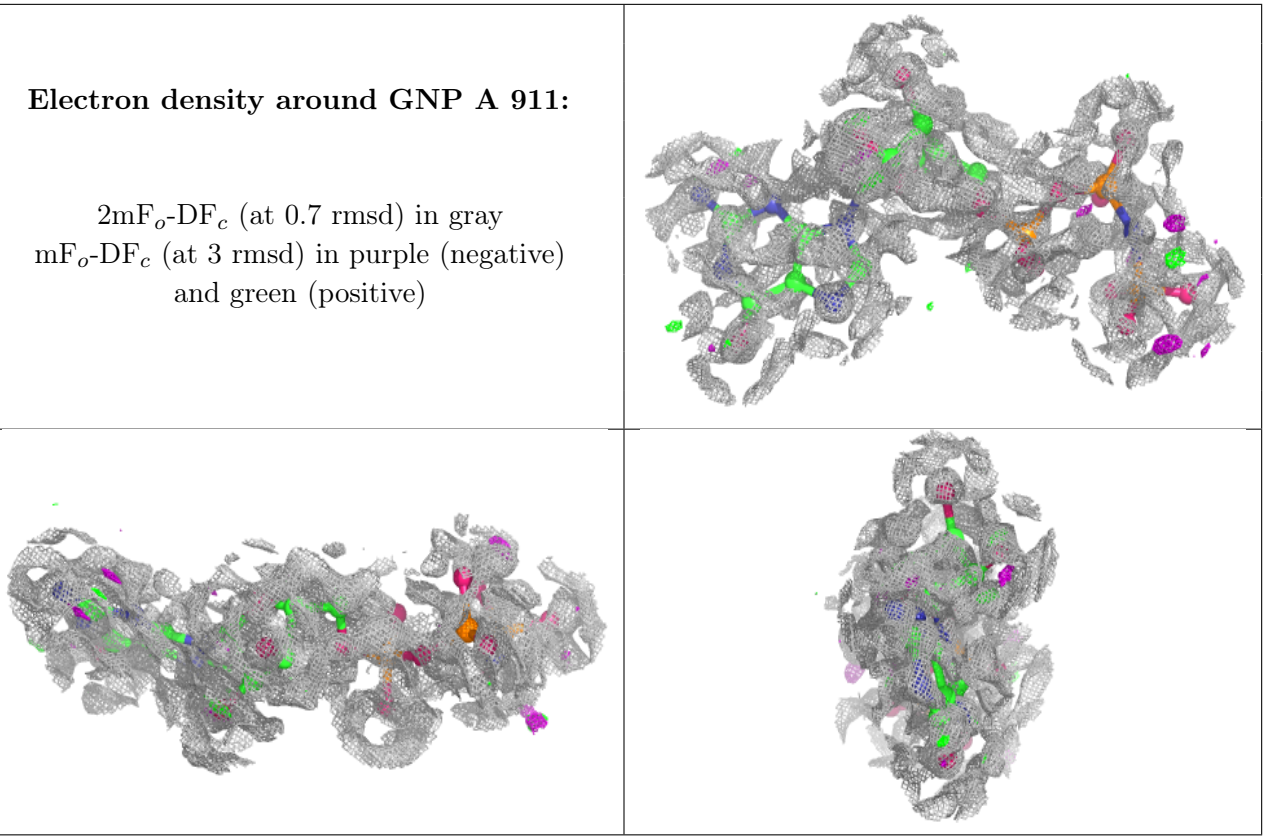
Electron density around GNP B 910:

$2mF_o$-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 911:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.