wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2020 – 02:43 PM BST

PDB ID	:	3V11
Title	:	Structure of the ternary initiation complex AIF2:GDPNP:methionylated initiator TRNA
Authors	:	Mechulam, Y.; Schmitt, E.
Deposited on	:	2011-12-09
Resolution	:	5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

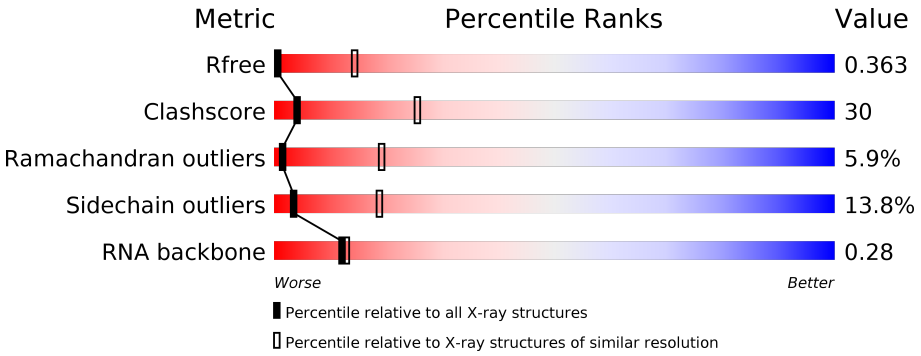
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 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	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RNA backbone	3102	1068 (7.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	414	42% 46% 9% • •
2	B	266	36% 48% 11% • 5%
3	C	138	6% 5% • 88%
4	D	77	10% 35% 38% 16% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6975 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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3131	2004	533	582	12			

- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			2033	1301	346	384	2			

- Molecule 3 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	17	Total	C	N	O	S	0	0	0
			146	94	22	29	1			

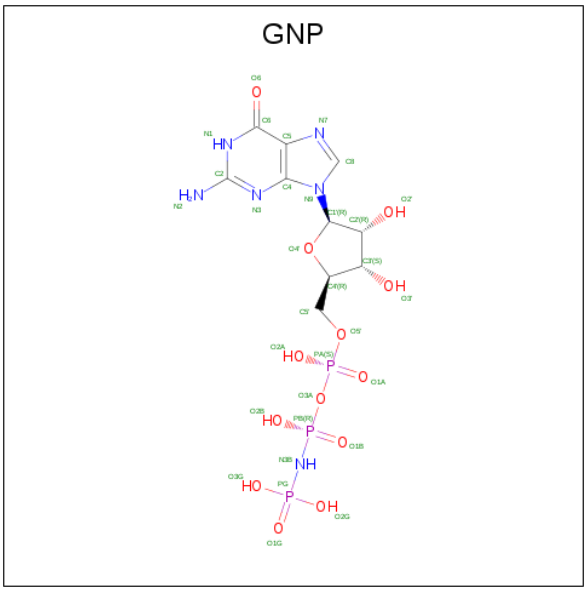
- Molecule 4 is a RNA chain called Initiator tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	76	Total	C	N	O	P	S	0	0	0
			1624	725	294	528	76	1			

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

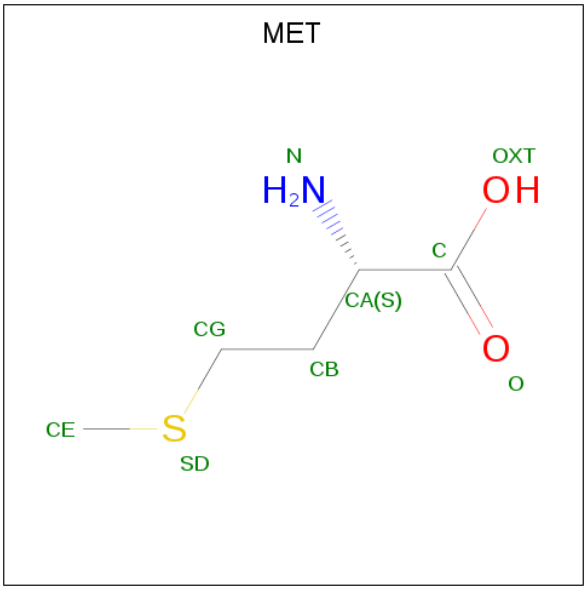
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 7 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



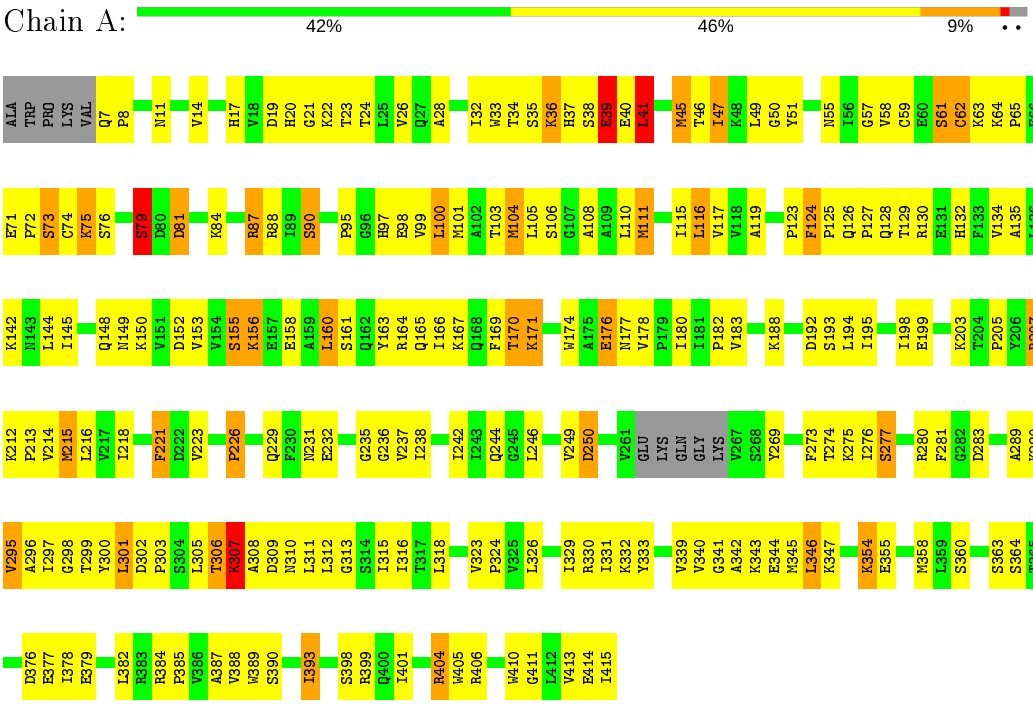
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

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.

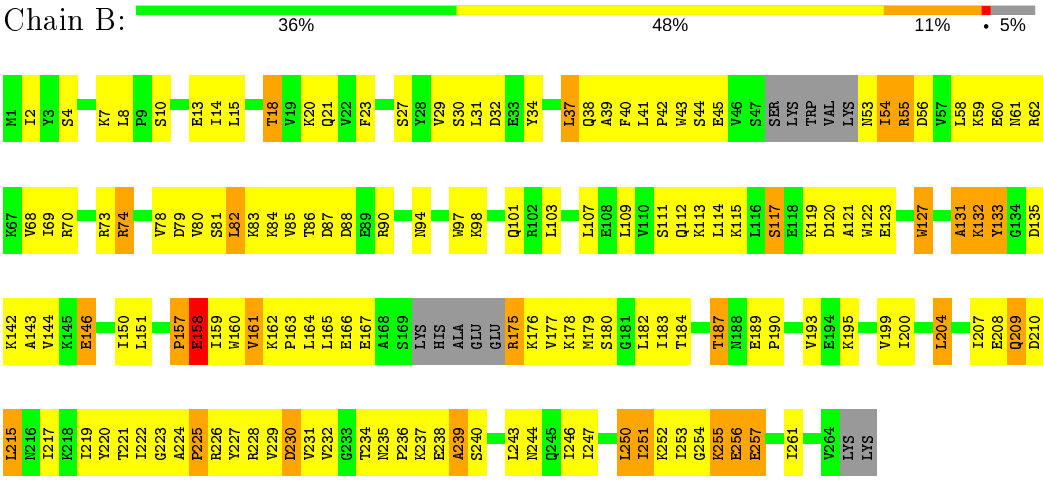
- Molecule 1: Translation initiation factor 2 subunit gamma

Chain A:



- Molecule 2: Translation initiation factor 2 subunit alpha

Chain B:

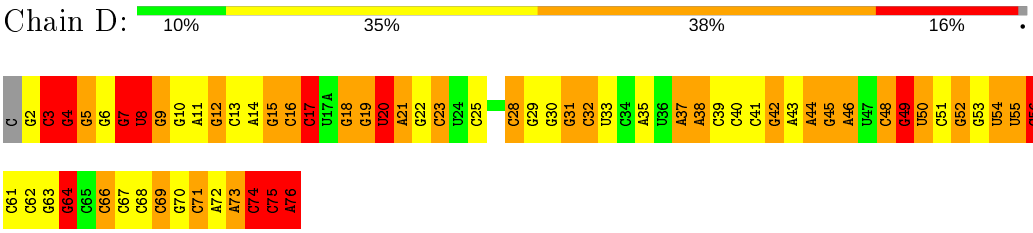


- Molecule 3: Translation initiation factor 2 subunit beta

Chain C:

- Molecule 4: Initiator tRNA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.00Å 133.00Å 167.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.43 – 5.00 47.43 – 5.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.43-5.00) 98.8 (47.43-5.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 5.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.262 , 0.344 0.289 , 0.363	Depositor DCC
R_{free} test set	360 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	341.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 390.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.071 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å^2)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, GNP, H2U, MG, 4SU, PSU

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	0.51	0/3186	0.79	1/4313 (0.0%)
2	B	0.52	0/2058	0.76	1/2770 (0.0%)
3	C	0.65	0/148	1.10	2/197 (1.0%)
4	D	0.99	4/1702 (0.2%)	1.76	46/2653 (1.7%)
All	All	0.66	4/7094 (0.1%)	1.13	50/9933 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	76	A	N3-C4	16.59	1.44	1.34
4	D	76	A	C8-N7	12.46	1.40	1.31
4	D	76	A	C5-C4	6.94	1.43	1.38
4	D	76	A	C6-N1	5.21	1.39	1.35

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	76	A	C2-N3-C4	18.67	119.94	110.60
4	D	76	A	C8-N9-C4	18.01	113.00	105.80
4	D	76	A	N7-C8-N9	-15.89	105.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	76	A	N1-C2-N3	-15.02	121.79	129.30
4	D	56	C	C6-N1-C2	-13.76	114.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	SER	Peptide
2	B	212	GLU	Peptide

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	3131	0	3248	194	0
2	B	2033	0	2145	119	0
3	C	146	0	146	6	0
4	D	1624	0	830	97	0
5	A	1	0	0	0	0
6	A	32	0	13	2	0
7	D	8	0	8	5	0
All	All	6975	0	6390	393	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 30.

The worst 5 of 393 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:294:LEU:HB3	7:D:101:MET:HG2	1.48	0.94
2:B:18:THR:HB	2:B:63:LYS:HG2	1.52	0.91
1:A:37:HIS:HB2	4:D:74:C:C4	2.08	0.88
2:B:240:SER:HA	2:B:243:LEU:HB3	1.55	0.88
1:A:62:CYS:SG	1:A:63:LYS:N	2.45	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	400/414 (97%)	314 (78%)	64 (16%)	22 (6%)	2 21
2	B	248/266 (93%)	183 (74%)	48 (19%)	17 (7%)	1 16
3	C	15/138 (11%)	9 (60%)	6 (40%)	0	100 100
All	All	663/818 (81%)	506 (76%)	118 (18%)	39 (6%)	1 19

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	75	LYS
1	A	124	PHE
1	A	176	GLU
1	A	307	LYS

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	348/356 (98%)	296 (85%)	52 (15%)	3 16
2	B	227/239 (95%)	199 (88%)	28 (12%)	4 21
3	C	17/125 (14%)	16 (94%)	1 (6%)	19 46
All	All	592/720 (82%)	511 (86%)	81 (14%)	3 19

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	VAL
1	A	347	LYS
2	B	215	LEU
1	A	301	LEU
1	A	326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	177	ASN
1	A	400	GLN
2	B	61	ASN
2	B	245	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	75/77 (97%)	34 (45%)	2 (2%)

5 of 34 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	C
4	D	4	G
4	D	5	G
4	D	7	G
4	D	8	4SU

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	73	A
4	D	74	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	4SU	D	8	4	14,21,22	3.38	3 (21%)	15,30,33	2.13	2 (13%)
4	OMC	D	32	4	15,22,23	2.25	4 (26%)	17,31,34	1.47	2 (11%)
4	PSU	D	55	4	17,21,22	1.10	2 (11%)	20,30,33	4.26	8 (40%)
4	H2U	D	20	4	18,21,22	1.28	2 (11%)	21,30,33	2.95	6 (28%)
4	5MU	D	54	4	15,22,23	2.06	3 (20%)	16,32,35	2.87	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4SU	D	8	4	-	2/5/25/26	0/2/2/2
4	OMC	D	32	4	-	2/7/27/28	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	H2U	D	20	4	-	3/7/38/39	0/2/2/2
4	5MU	D	54	4	-	0/5/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	4SU	C5-C4	9.03	1.48	1.38
4	D	8	4SU	C6-N1	8.39	1.46	1.35
4	D	54	5MU	C4-N3	5.76	1.43	1.33
4	D	32	OMC	C6-N1	5.02	1.42	1.35
4	D	32	OMC	C5-C4	4.69	1.52	1.41

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	55	PSU	N1-C2-N3	-14.43	116.96	128.43
4	D	54	5MU	C4-N3-C2	10.84	124.29	115.14
4	D	20	H2U	O2-C2-N1	8.03	133.19	123.11
4	D	55	PSU	C4-N3-C2	7.92	121.83	115.14
4	D	8	4SU	C2-N3-C4	6.78	124.98	115.15

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	20	H2U	C4'-C5'-O5'-P
4	D	20	H2U	O4'-C1'-N1-C2
4	D	20	H2U	O4'-C1'-N1-C6
4	D	8	4SU	O4'-C4'-C5'-O5'
4	D	32	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	8	4SU	5	0
4	D	55	PSU	2	0
4	D	20	H2U	1	0
4	D	54	5MU	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MET	D	101	4	6,7,8	1.30	1 (16%)	2,7,9	1.76	1 (50%)
6	GNP	A	502	5	28,34,34	2.73	11 (39%)	30,54,54	2.19	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
7	MET	D	101	4	-	1/5/6/8	-
6	GNP	A	502	5	-	8/17/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	502	GNP	PB-O3A	-7.41	1.49	1.59
6	A	502	GNP	C5-C6	-6.53	1.41	1.52
6	A	502	GNP	C4-N9	-6.12	1.39	1.47
6	A	502	GNP	C6-N1	3.96	1.39	1.33
6	A	502	GNP	PB-O2B	-3.61	1.47	1.56

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	502	GNP	C4-C5-N7	6.58	111.18	102.46
6	A	502	GNP	C5-C6-N1	-5.31	111.64	118.19
6	A	502	GNP	O6-C6-C5	3.70	127.41	119.86
6	A	502	GNP	O3G-PG-O1G	-3.60	104.41	113.45
6	A	502	GNP	PA-O3A-PB	-3.42	120.56	132.62

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	101	MET	N-CA-CB-CG
6	A	502	GNP	PG-N3B-PB-O1B
6	A	502	GNP	PG-N3B-PB-O3A
6	A	502	GNP	C5'-O5'-PA-O3A
6	A	502	GNP	O4'-C1'-N9-C4

There are no ring outliers.

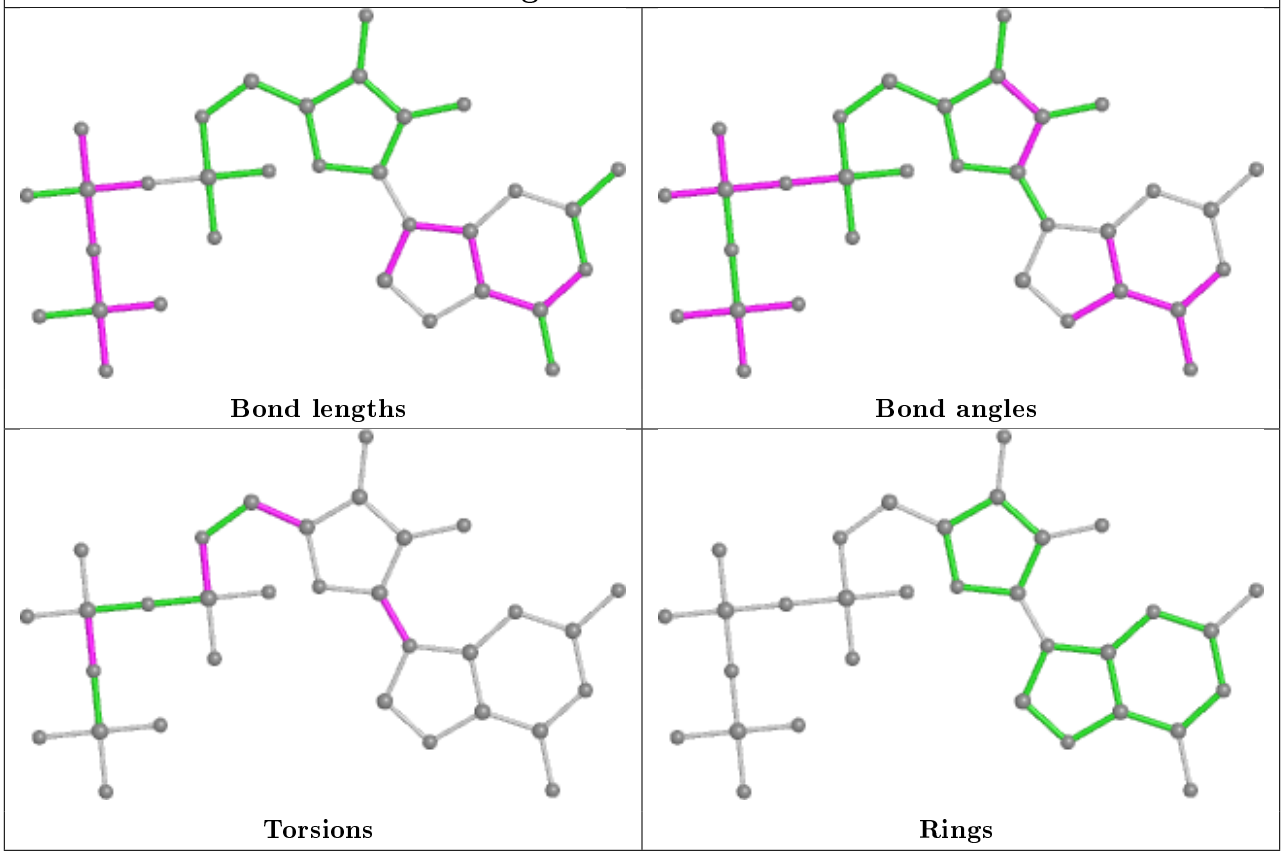
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	101	MET	5	0
6	A	502	GNP	2	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 502



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.

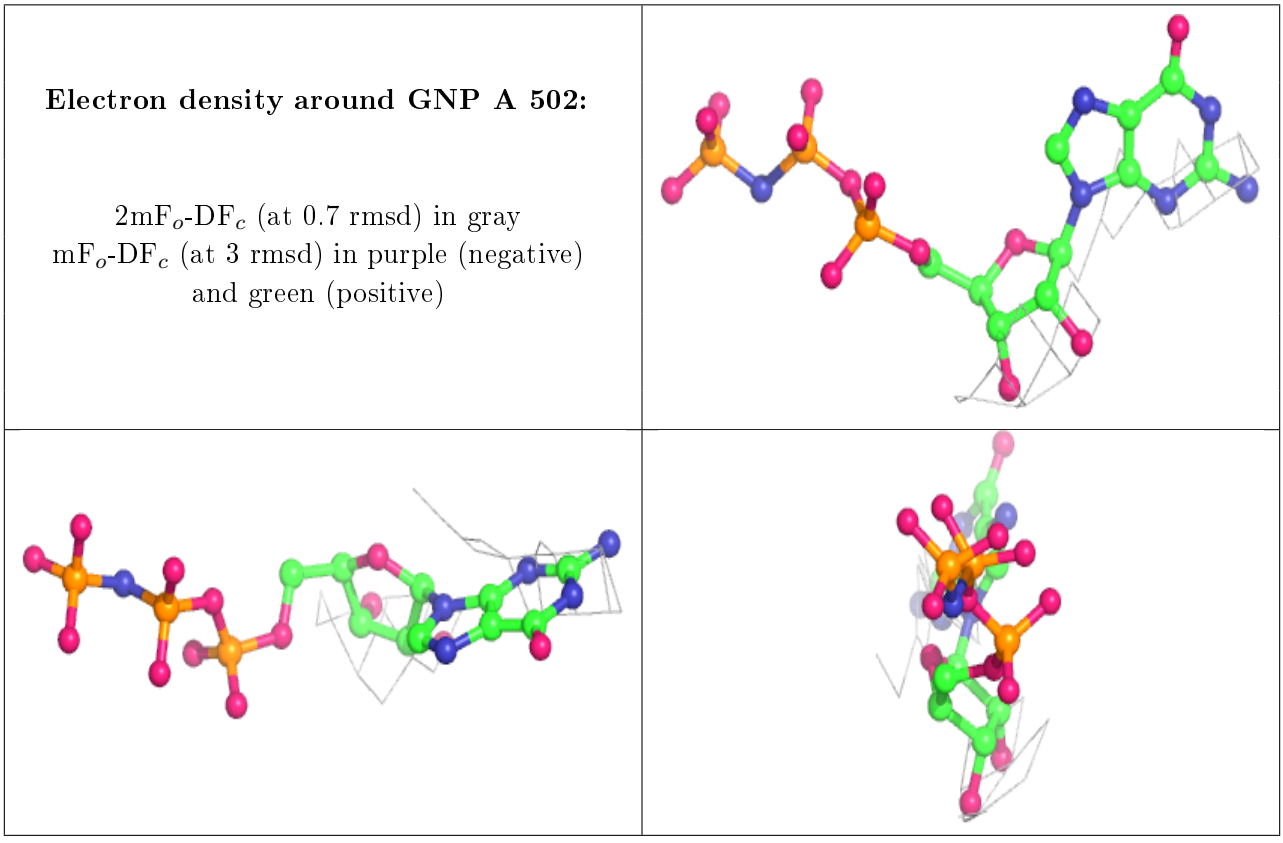
6.4 Ligands

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 A 502:

$2mF_o$-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.