



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2025 – 11:18 AM EDT

PDB ID : 7I2I
Title : Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z1262628644 (DNV2_NS5A-x0472)
Authors : Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on : 2025-03-06
Resolution : 1.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

<https://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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

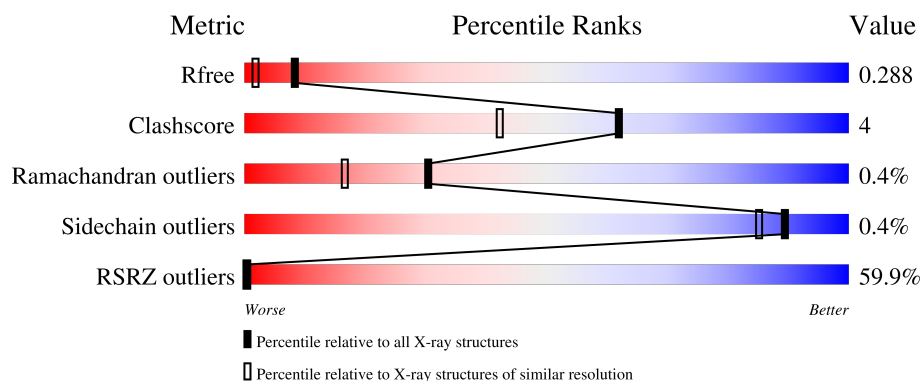
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.74 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}	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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	637	

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1006	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5127 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 NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	5	0
			4687	2951	840	862	34			

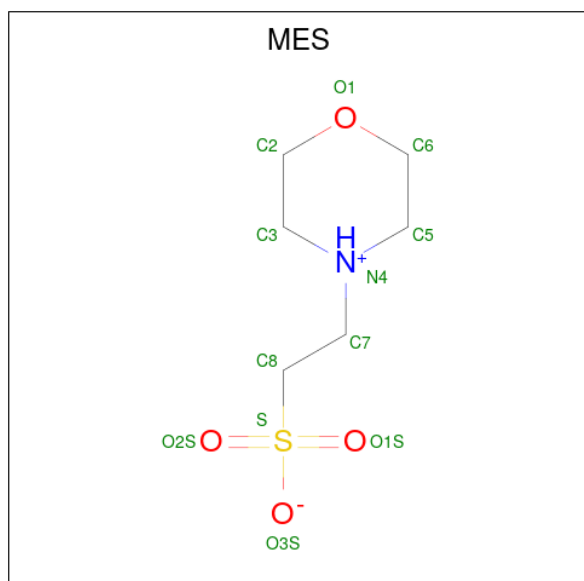
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



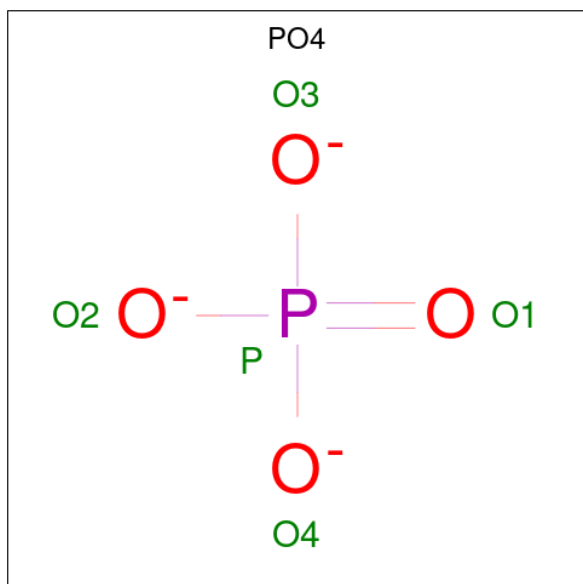
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

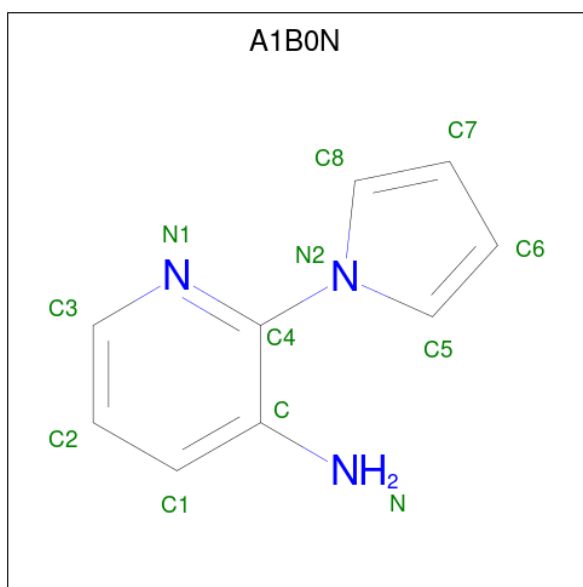


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 2-(1H-pyrrol-1-yl)pyridin-3-amine (three-letter code: A1B0N) (formula: C₉H₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			12	9	3		
8	A	1	Total	C	N	0	0
			12	9	3		

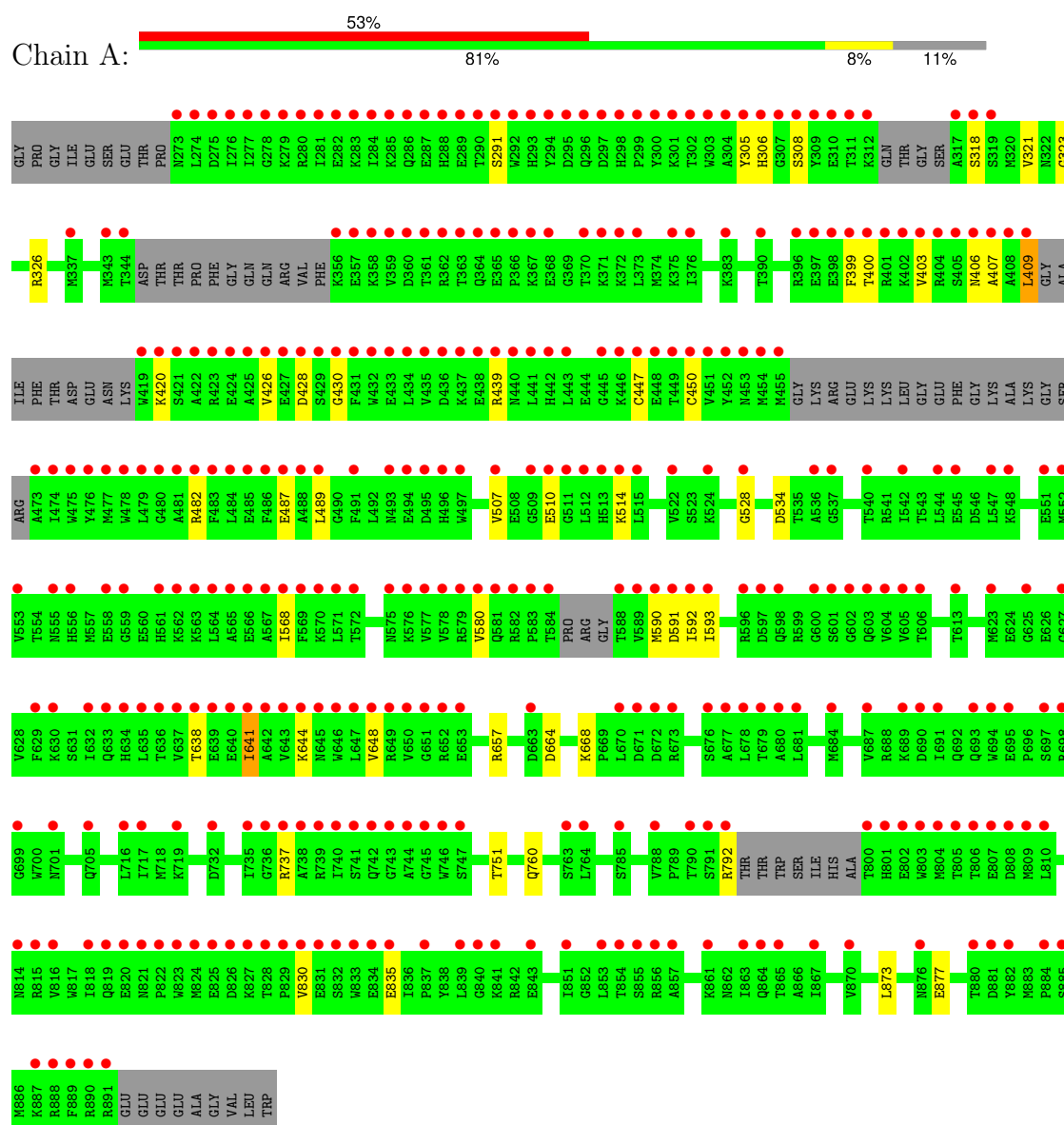
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	364	Total	O	0	0
			364	364		

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: NS5 RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 116.59Å 148.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.77 – 1.74 91.77 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.8 (91.77-1.74) 97.8 (91.77-1.74)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.239 0.268 , 0.288	Depositor DCC
R_{free} test set	3770 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 161.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5127	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: A1B0N, DMS, ZN, CL, MES, PO4, PEG

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	0.79	3/4791 (0.1%)	0.85	1/6459 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	751	THR	C-O	5.65	1.34	1.23
1	A	760	GLN	C-O	5.49	1.33	1.23
1	A	877	GLU	CD-OE2	-5.07	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	CG-CD-NE	-6.20	98.78	111.80

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	4687	0	4591	37	0
2	A	2	0	0	0	0
3	A	24	0	26	4	0
4	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	24	0	0	2	0
9	A	364	0	0	2	1
All	All	5127	0	4639	38	1

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 4.

The worst 5 of 38 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:638:THR:O	1:A:641:ILE:HG22	1.71	0.90
1:A:323:GLY:HA3	3:A:1003[B]:MES:H71	1.58	0.86
1:A:534:ASP:OD1	5:A:1006:PO4:O2	1.97	0.82
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.70	0.71
1:A:305:TYR:HE1	1:A:591:ASP:OD1	1.73	0.71

All (1) 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)
9:A:1130:HOH:O	9:A:1130:HOH:O[2_445]	1.74	0.46

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	559/637 (88%)	532 (95%)	25 (4%)	2 (0%)	30 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	SER
1	A	420	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	504/554 (91%)	502 (100%)	2 (0%)	89 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LEU
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	556	HIS
1	A	645	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
6	PEG	A	1008	-	6,6,6	0.16	0	5,5,5	0.09	0
4	DMS	A	1004	-	3,3,3	0.19	0	3,3,3	0.17	0
3	MES	A	1003[B]	-	12,12,12	0.77	0	15,16,16	0.59	0
3	MES	A	1003[A]	-	12,12,12	0.71	0	15,16,16	0.28	0
8	A1B0N	A	1010	-	12,13,13	0.78	1 (8%)	14,17,17	0.58	0
4	DMS	A	1005	-	3,3,3	0.23	0	3,3,3	0.08	0
5	PO4	A	1007	-	4,4,4	0.59	0	6,6,6	0.46	0
5	PO4	A	1006	-	4,4,4	1.43	1 (25%)	6,6,6	0.60	0
8	A1B0N	A	1011	-	12,13,13	0.91	1 (8%)	14,17,17	0.54	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
6	PEG	A	1008	-	-	0/4/4/4	-
3	MES	A	1003[B]	-	-	0/6/14/14	0/1/1/1
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
8	A1B0N	A	1010	-	-	0/2/4/4	0/2/2/2
8	A1B0N	A	1011	-	-	1/2/4/4	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1011	A1B0N	C4-N2	-2.75	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	2.61	1.56	1.50
8	A	1010	A1B0N	C4-N2	-2.26	1.42	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1011	A1B0N	N1-C4-N2-C5

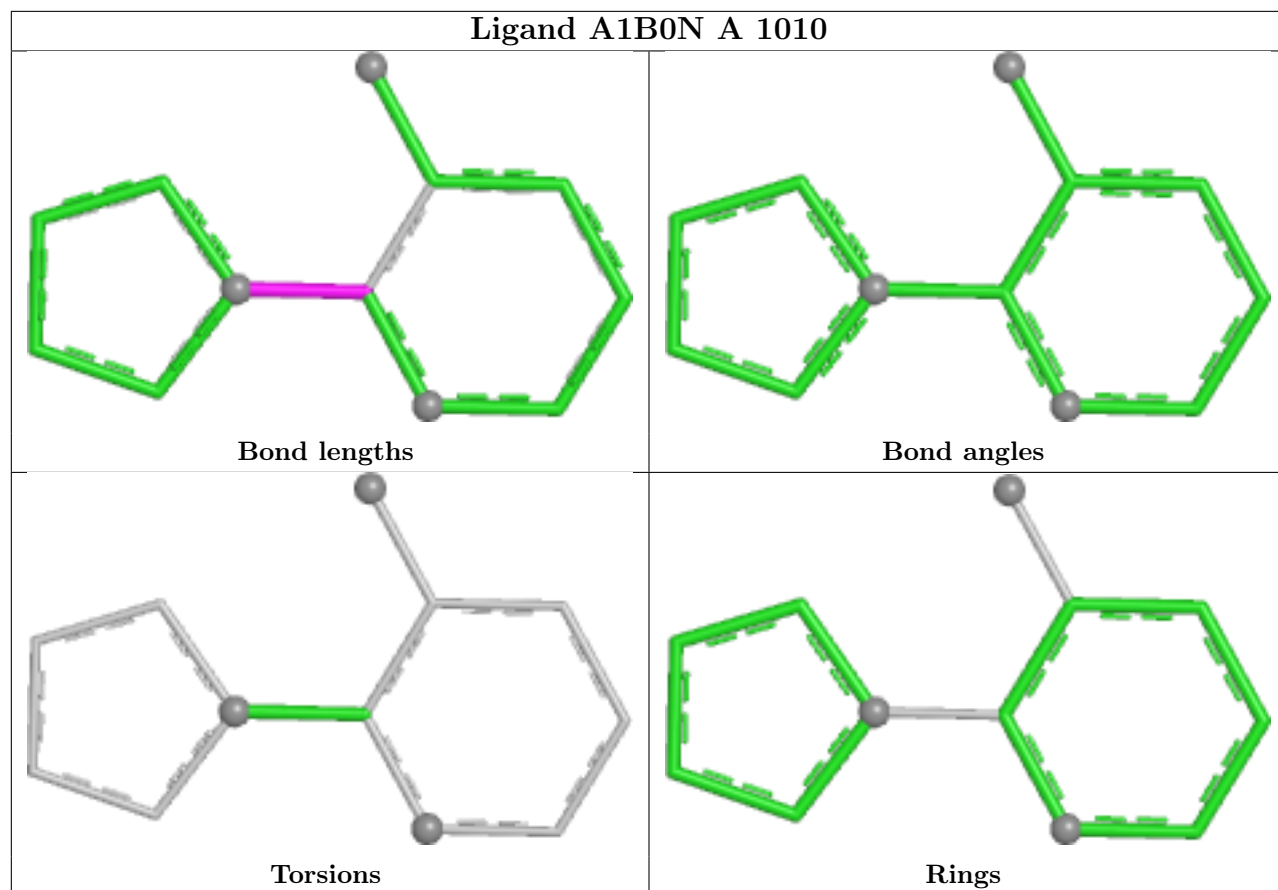
There are no ring outliers.

4 monomers are involved in 9 short contacts:

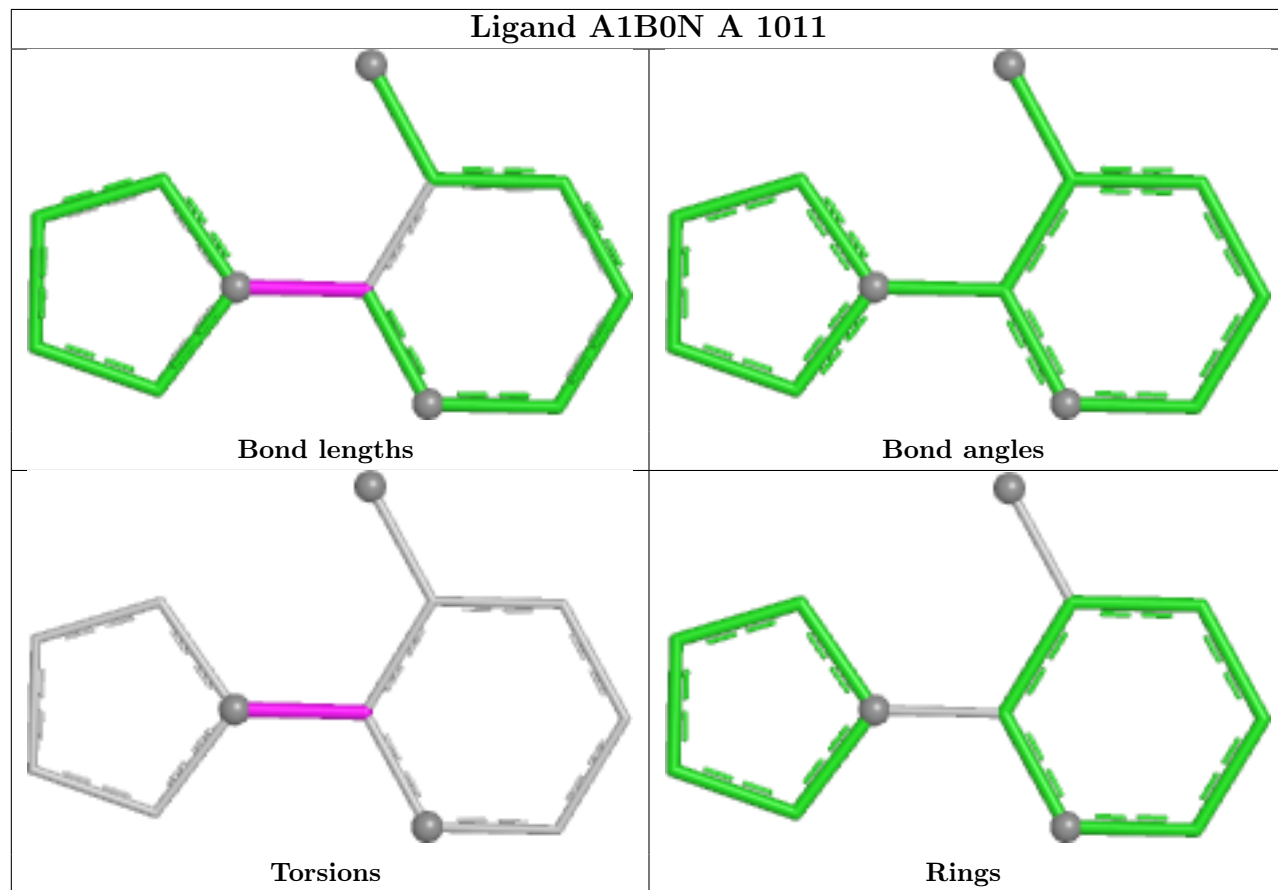
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	3	0
3	A	1003[A]	MES	1	0
5	A	1006	PO4	3	0
8	A	1011	A1B0N	2	0

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 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 A1B0N A 1010



Ligand A1B0N A 1011



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	568/637 (89%)	4.13	340 (59%) 0 0	6, 38, 92, 135	181 (31%)

The worst 5 of 340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	LEU	14.8
1	A	589	VAL	13.6
1	A	851	ILE	13.4
1	A	483	PHE	12.9
1	A	304	ALA	12.7

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
8	A1B0N	A	1011	12/12	0.28	0.38	59,65,67,67	12
5	PO4	A	1006	5/5	0.54	0.38	36,44,47,48	5

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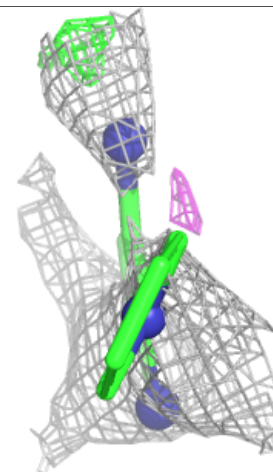
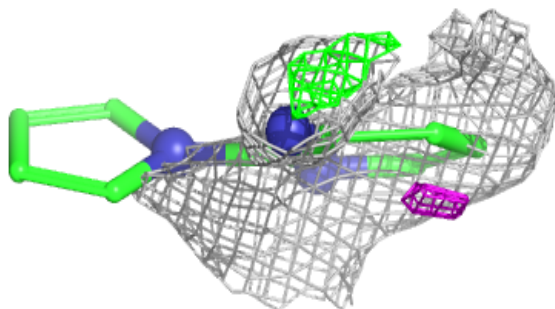
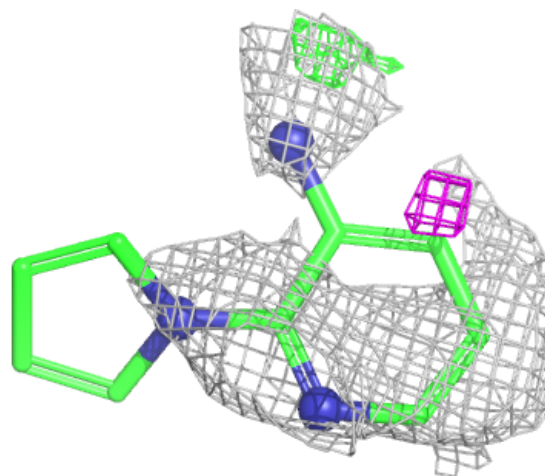
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	A1B0N	A	1010	12/12	0.58	0.32	45,52,54,56	12
5	PO4	A	1007	5/5	0.58	0.21	66,70,79,79	5
6	PEG	A	1008	7/7	0.81	0.44	59,64,70,71	7
4	DMS	A	1005	4/4	0.83	0.32	68,73,76,79	4
4	DMS	A	1004	4/4	0.88	0.51	75,80,83,84	4
3	MES	A	1003[B]	12/12	0.94	0.24	29,32,33,34	12
3	MES	A	1003[A]	12/12	0.94	0.24	652,666,752,764	12
2	ZN	A	1002	1/1	0.96	0.29	60,60,60,60	1
7	CL	A	1009	1/1	0.97	0.11	45,45,45,45	0
2	ZN	A	1001	1/1	0.99	0.03	27,27,27,27	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.

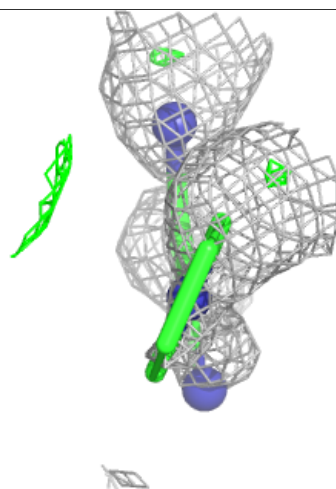
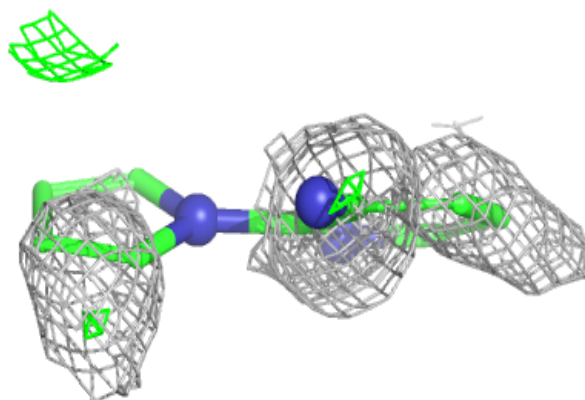
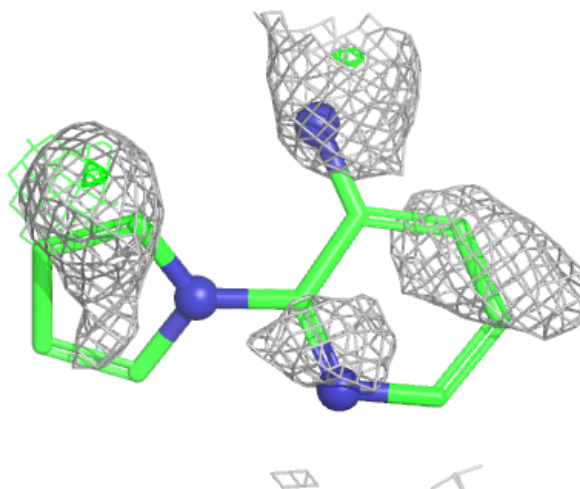
Electron density around A1B0N A 1011:

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 A1B0N A 1010:

$2mF_o-DF_c$ (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.