



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:53 PM UTC

PDB ID : 7I2I / pdb_00007i2i
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)
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Deposited on : 2025-03-06
Resolution : 1.74 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	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

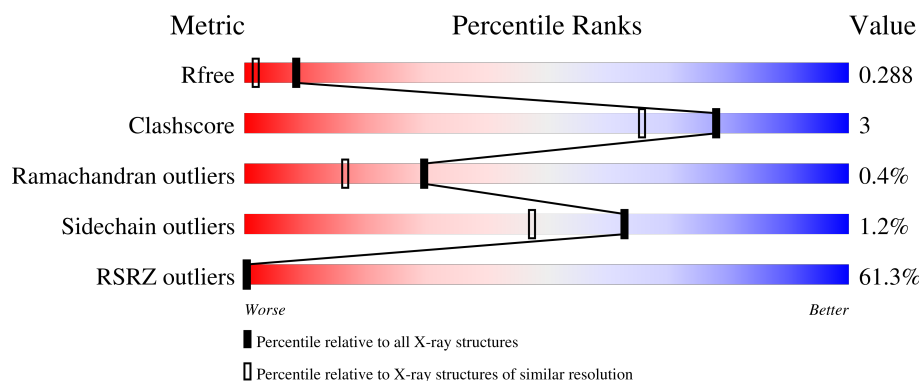
1 Overall quality at a glance

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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (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) : 2.49

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			

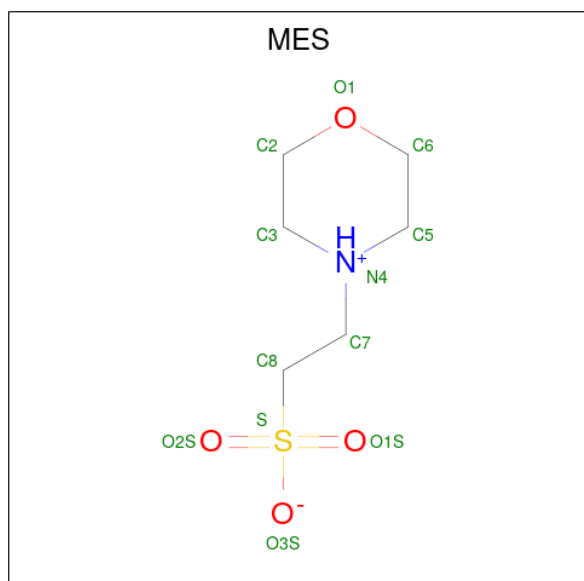
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: MES) (formula: C₆H₁₃NO₄S).



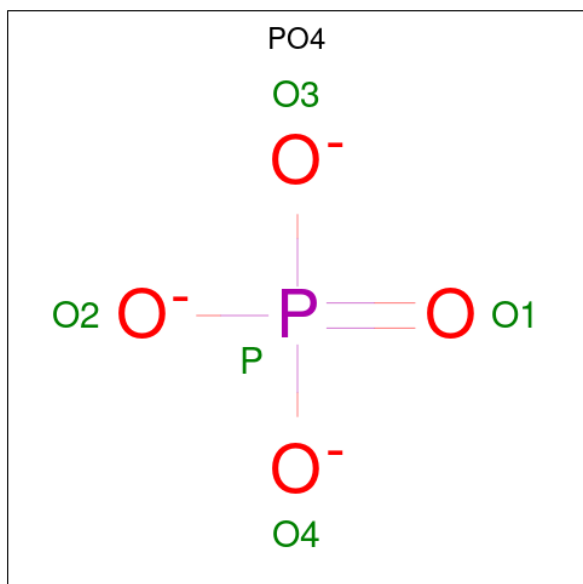
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: 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 (CCD ID: 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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

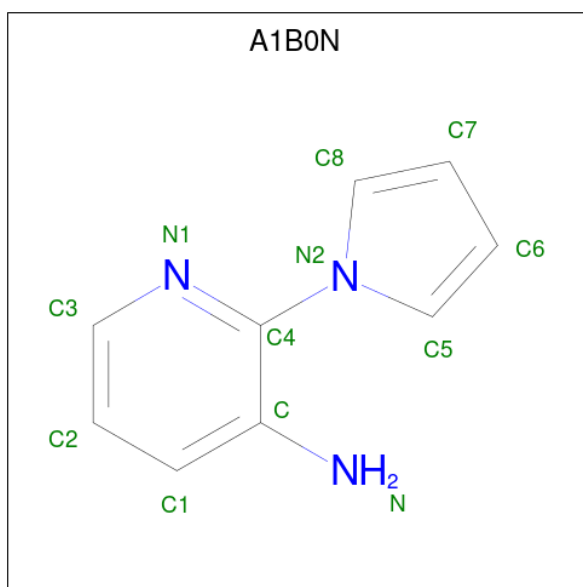


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (CCD ID: 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 (CCD ID: A1B0N) (formula: $C_9H_9N_3$) (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		

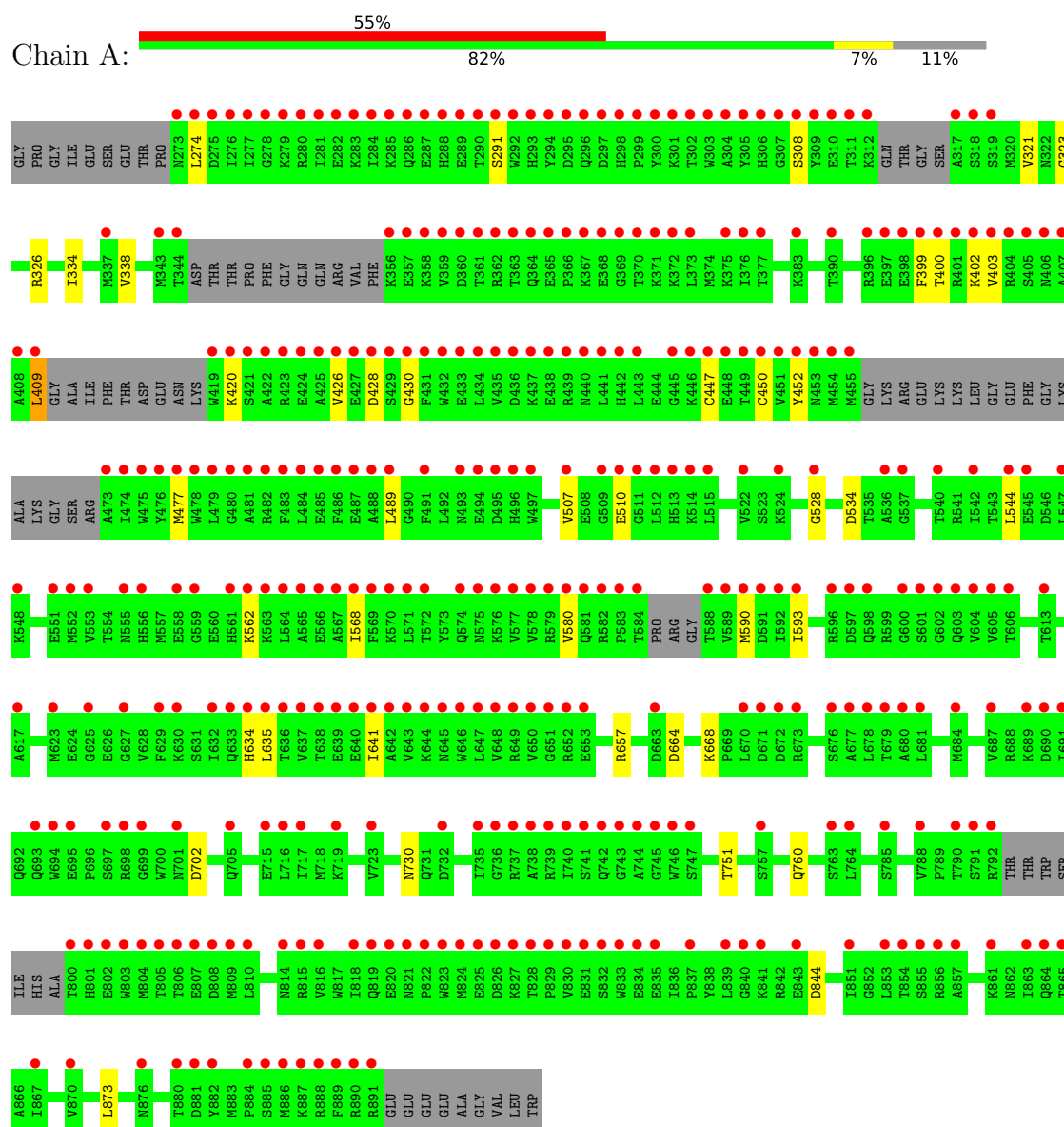
- Molecule 9 is water.

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

3 Residue-property plots

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PEG, ZN, PO4, A1B0N, MES, DMS

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	1.14	3/4791 (0.1%)	1.38	7/6459 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	751	THR	C-O	8.69	1.34	1.24
1	A	760	GLN	C-O	7.70	1.33	1.24
1	A	338	VAL	C-O	-6.28	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	844	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	657	ARG	CG-CD-NE	-6.01	98.78	112.00
1	A	702	ASP	CB-CA-C	5.50	118.60	110.14
1	A	544	LEU	N-CA-C	-5.31	106.06	112.54
1	A	730	ASN	CA-CB-CG	-5.27	107.33	112.60
1	A	334	ILE	N-CA-C	-5.24	107.61	112.43

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	4687	0	4591	25	0
2	A	2	0	0	0	0
3	A	24	0	26	4	0
4	A	8	0	12	1	0
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	0	0
9	A	364	0	0	2	1
All	All	5127	0	4639	26	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 3.

All (26) 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: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:664:ASP:OD1	5:A:1006:PO4:O2	2.11	0.67
1:A:403:VAL:HG12	1:A:409:LEU:HD22	1.80	0.63
1:A:403:VAL:HG12	1:A:409:LEU:CD2	2.31	0.60
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
4:A:1004:DMS:H12	9:A:1279:HOH:O	2.07	0.54
1:A:323:GLY:CA	3:A:1003[B]:MES:H71	2.36	0.51
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.70	0.50
1:A:873:LEU:HD13	3:A:1003[B]:MES:H62	1.92	0.50
1:A:528:GLY:O	1:A:668:LYS:HE3	2.15	0.47
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.97	0.47
1:A:308:SER:HA	1:A:590:MET:O	2.15	0.47
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.97	0.47
1:A:562:LYS:NZ	9:A:1109:HOH:O	2.48	0.46
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.96	0.46
1:A:507:VAL:C	1:A:510:GLU:HG2	2.41	0.45
1:A:403:VAL:HA	1:A:409:LEU:HD21	2.00	0.43
1:A:489:LEU:CD1	1:A:568:ILE:HG21	2.49	0.42
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.48	0.42
1:A:428:ASP:OD1	1:A:430:GLY:N	2.52	0.42
1:A:452:TYR:CE1	1:A:477:MET:HE3	2.56	0.41
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.45	0.41
1:A:507:VAL:O	1:A:510:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PHE:O	1:A:403:VAL:HG13	2.21	0.40

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%)	498 (99%)	6 (1%)	63 47

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	402	LYS
1	A	409	LEU
1	A	634	HIS
1	A	635	LEU
1	A	641	ILE

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

Mol	Chain	Res	Type
1	A	406	ASN
1	A	493	ASN
1	A	556	HIS
1	A	705	GLN
1	A	786	HIS

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
4	DMS	A	1005	-	3,3,3	0.23	0	3,3,3	0.08	0
3	MES	A	1003[B]	-	12,12,12	0.77	0	15,16,16	0.59	0
4	DMS	A	1004	-	3,3,3	0.19	0	3,3,3	0.17	0
6	PEG	A	1008	-	6,6,6	0.16	0	5,5,5	0.09	0
8	A1B0N	A	1011	-	13,13,13	0.26	0	15,17,17	0.45	0
5	PO4	A	1007	-	4,4,4	0.59	0	6,6,6	0.46	0
8	A1B0N	A	1010	-	13,13,13	0.19	0	15,17,17	0.46	0
3	MES	A	1003[A]	-	12,12,12	0.71	0	15,16,16	0.28	0
5	PO4	A	1006	-	4,4,4	1.43	1 (25%)	6,6,6	0.60	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	MES	A	1003[B]	-	-	0/6/14/14	0/1/1/1
6	PEG	A	1008	-	-	0/4/4/4	-
8	A1B0N	A	1011	-	-	0/4/4/4	0/2/2/2
8	A1B0N	A	1010	-	-	0/4/4/4	0/2/2/2
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	2.61	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

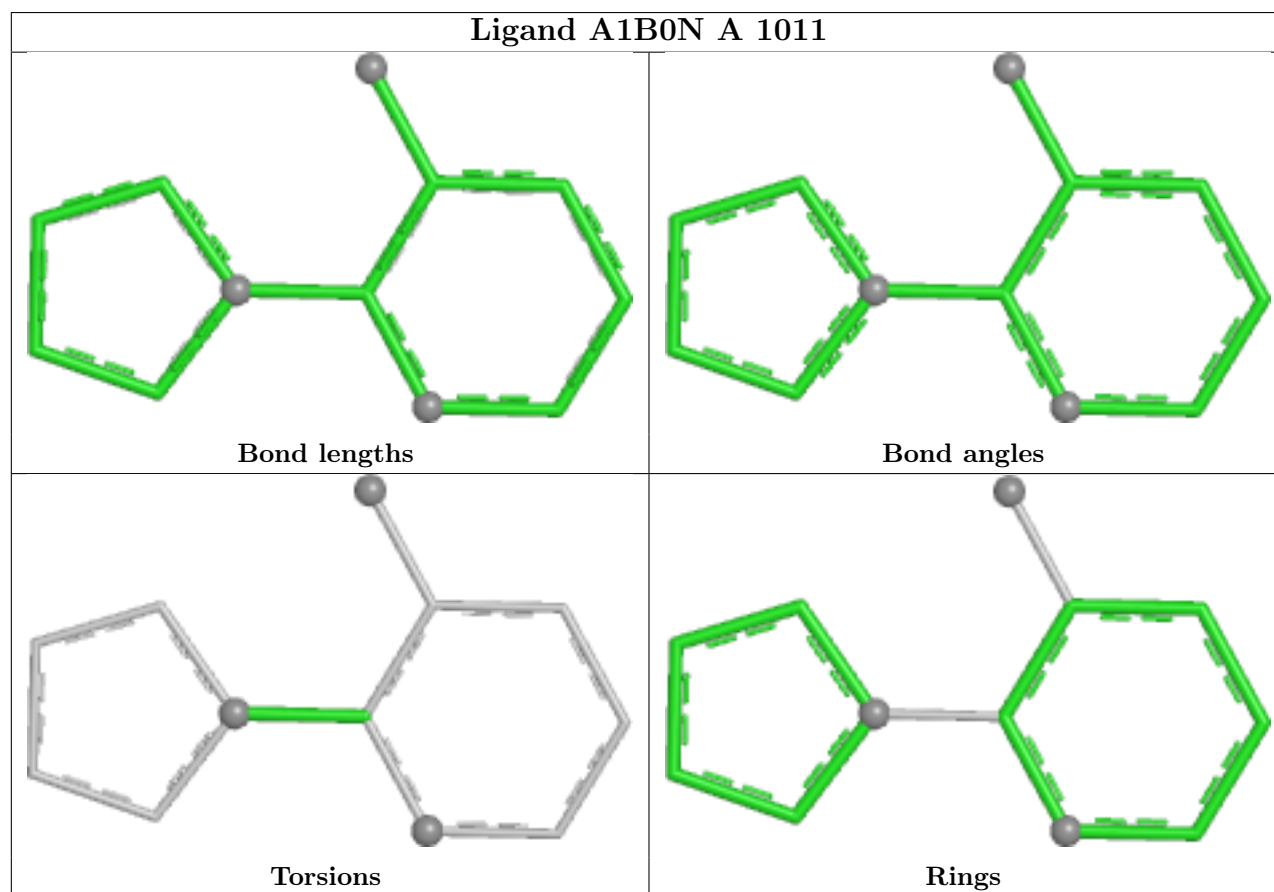
There are no ring outliers.

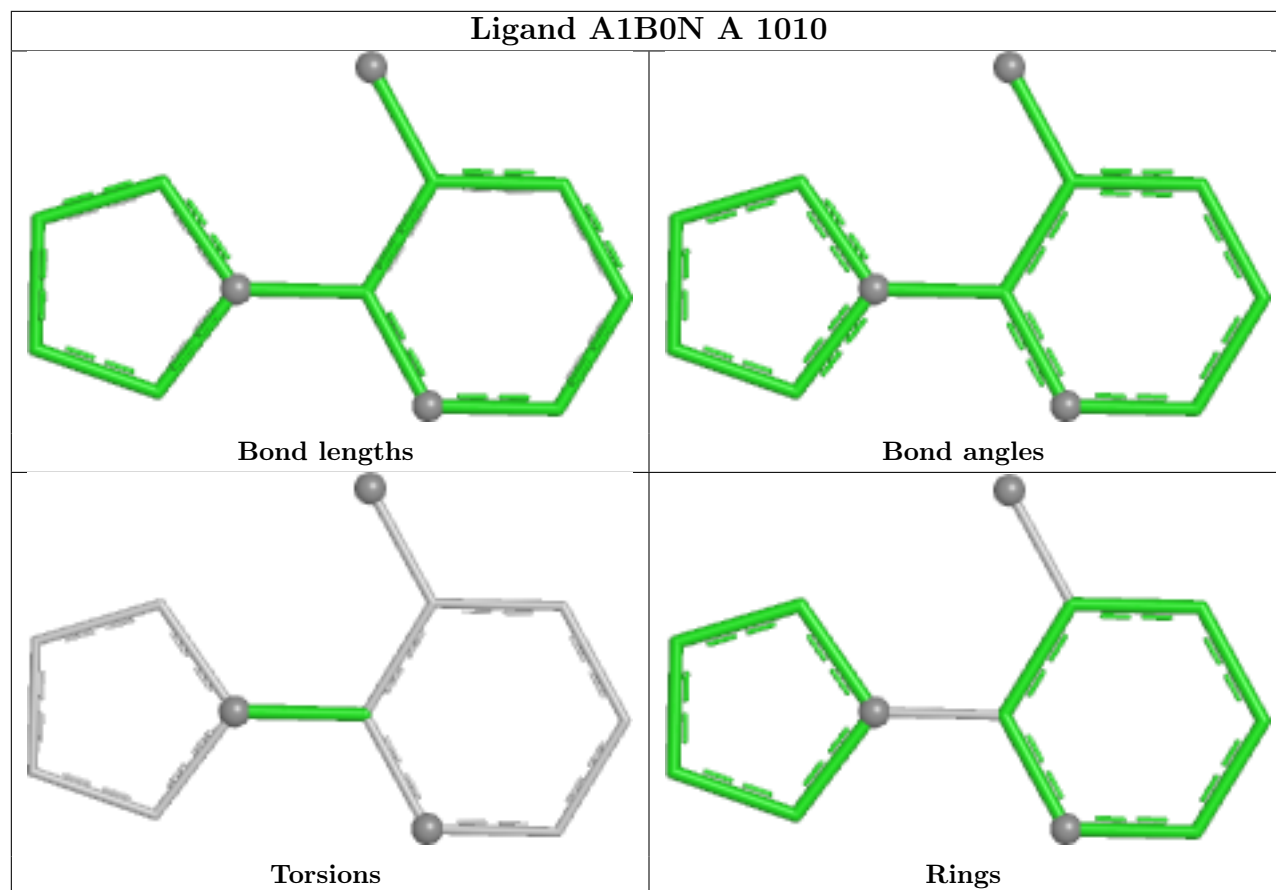
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	3	0
4	A	1004	DMS	1	0
3	A	1003[A]	MES	1	0
5	A	1006	PO4	3	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.





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	568/637 (89%)	4.25	348 (61%) 0 0	6, 38, 92, 135	181 (31%)

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	LEU	15.1
1	A	589	VAL	14.0
1	A	851	ILE	13.7
1	A	304	ALA	13.1
1	A	483	PHE	13.1
1	A	359	VAL	13.1
1	A	830	VAL	12.9
1	A	419	TRP	12.8
1	A	305	TYR	12.8
1	A	512	LEU	12.8
1	A	839	LEU	12.8
1	A	281	ILE	12.6
1	A	853	LEU	12.3
1	A	735	ILE	12.3
1	A	889	PHE	12.2
1	A	592	ILE	11.8
1	A	867	ILE	11.7
1	A	409	LEU	11.4
1	A	407	ALA	11.3
1	A	606	THR	11.3
1	A	488	ALA	11.2
1	A	738	ALA	11.2
1	A	484	LEU	11.1
1	A	588	THR	11.1
1	A	486	PHE	11.0
1	A	650	VAL	11.0
1	A	740	ILE	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	816	VAL	10.8
1	A	747	SER	10.8
1	A	863	ILE	10.8
1	A	515	LEU	10.7
1	A	292	TRP	10.7
1	A	600	GLY	10.6
1	A	857	ALA	10.6
1	A	422	ALA	10.5
1	A	719[A]	LYS	10.4
1	A	604	VAL	10.4
1	A	605	VAL	10.4
1	A	691	ILE	10.4
1	A	803	TRP	10.4
1	A	744	ALA	10.4
1	A	763[A]	SER	10.3
1	A	648	VAL	10.3
1	A	475	TRP	10.3
1	A	840	GLY	10.2
1	A	307	GLY	10.2
1	A	790	THR	10.1
1	A	649	ARG	10.0
1	A	743	GLY	9.9
1	A	425	ALA	9.8
1	A	880	THR	9.8
1	A	511	GLY	9.8
1	A	635	LEU	9.7
1	A	837	PRO	9.6
1	A	601	SER	9.4
1	A	489	LEU	9.4
1	A	828	THR	9.4
1	A	818	ILE	9.3
1	A	637	VAL	9.3
1	A	596	ARG	9.2
1	A	854	THR	9.2
1	A	408	ALA	9.1
1	A	584	THR	9.1
1	A	809	MET	9.1
1	A	297	ASP	9.0
1	A	785[A]	SER	9.0
1	A	646	TRP	9.0
1	A	670	LEU	9.0
1	A	431	PHE	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	806	THR	9.0
1	A	865	THR	8.9
1	A	438	GLU	8.8
1	A	882	TYR	8.8
1	A	641	ILE	8.8
1	A	651	GLY	8.8
1	A	288	HIS	8.8
1	A	513	HIS	8.8
1	A	822	PRO	8.7
1	A	832	SER	8.7
1	A	736	GLY	8.7
1	A	826	ASP	8.7
1	A	361	THR	8.6
1	A	602	GLY	8.5
1	A	358	LYS	8.5
1	A	741[A]	SER	8.5
1	A	636	THR	8.5
1	A	442	HIS	8.5
1	A	476	TYR	8.5
1	A	293	HIS	8.5
1	A	739	ARG	8.4
1	A	885	SER	8.4
1	A	300	TYR	8.4
1	A	888	ARG	8.3
1	A	841	LYS	8.3
1	A	298	HIS	8.2
1	A	647	LEU	8.1
1	A	638	THR	8.1
1	A	805	THR	8.1
1	A	855	SER	8.0
1	A	824	MET	8.0
1	A	290	THR	7.9
1	A	439	ARG	7.9
1	A	482	ARG	7.9
1	A	452	TYR	7.9
1	A	291	SER	7.8
1	A	421	SER	7.8
1	A	697	SER	7.8
1	A	808	ASP	7.8
1	A	306	HIS	7.8
1	A	645	ASN	7.7
1	A	745	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	583	PRO	7.7
1	A	319	SER	7.6
1	A	791	SER	7.6
1	A	318	SER	7.6
1	A	474	ILE	7.6
1	A	829	PRO	7.6
1	A	742	GLN	7.6
1	A	671	ASP	7.5
1	A	598	GLN	7.5
1	A	814	ASN	7.5
1	A	884	PRO	7.4
1	A	856	ARG	7.4
1	A	643	VAL	7.4
1	A	294	TYR	7.4
1	A	436	ASP	7.4
1	A	591	ASP	7.3
1	A	864[A]	GLN	7.3
1	A	403	VAL	7.3
1	A	821	ASN	7.2
1	A	876	ASN	7.2
1	A	317	ALA	7.2
1	A	485	GLU	7.2
1	A	440	ASN	7.2
1	A	835	GLU	7.2
1	A	673	ARG	7.2
1	A	590	MET	7.1
1	A	487	GLU	7.1
1	A	423	ARG	7.1
1	A	283	LYS	7.0
1	A	405	SER	7.0
1	A	453	ASN	6.9
1	A	286	GLN	6.9
1	A	827	LYS	6.9
1	A	881	ASP	6.8
1	A	404	ARG	6.8
1	A	597	ASP	6.8
1	A	800	THR	6.8
1	A	642	ALA	6.7
1	A	510	GLU	6.7
1	A	672	ASP	6.7
1	A	451	VAL	6.7
1	A	360	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	801	HIS	6.7
1	A	426	VAL	6.7
1	A	639	GLU	6.7
1	A	289	GLU	6.6
1	A	402	LYS	6.6
1	A	861	LYS	6.6
1	A	274	LEU	6.6
1	A	406	ASN	6.6
1	A	834	GLU	6.5
1	A	278	GLY	6.5
1	A	603	GLN	6.5
1	A	737	ARG	6.4
1	A	705	GLN	6.4
1	A	435	VAL	6.3
1	A	634	HIS	6.3
1	A	282	GLU	6.3
1	A	890	ARG	6.3
1	A	843	GLU	6.3
1	A	446	LYS	6.3
1	A	296	GLN	6.2
1	A	478	TRP	6.2
1	A	514	LYS	6.2
1	A	887	LYS	6.2
1	A	804	MET	6.2
1	A	815	ARG	6.2
1	A	792	ARG	6.1
1	A	454	MET	6.1
1	A	437	LYS	6.1
1	A	825	GLU	6.0
1	A	494	GLU	6.0
1	A	473	ALA	5.8
1	A	356	LYS	5.7
1	A	807	GLU	5.7
1	A	693	GLN	5.7
1	A	309	TYR	5.7
1	A	428	ASP	5.7
1	A	819	GLN	5.7
1	A	563	LYS	5.6
1	A	445	GLY	5.6
1	A	653	GLU	5.6
1	A	284	ILE	5.6
1	A	544	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	644	LYS	5.6
1	A	424	GLU	5.6
1	A	891	ARG	5.5
1	A	831	GLU	5.5
1	A	652	ARG	5.5
1	A	479	LEU	5.5
1	A	571	LEU	5.5
1	A	698	ARG	5.4
1	A	429	SER	5.4
1	A	640	GLU	5.4
1	A	434	LEU	5.3
1	A	277	ILE	5.2
1	A	433	GLU	5.2
1	A	303	TRP	5.1
1	A	420	LYS	5.0
1	A	556	HIS	5.0
1	A	802	GLU	4.9
1	A	820	GLU	4.9
1	A	399	PHE	4.9
1	A	279	LYS	4.9
1	A	312	LYS	4.9
1	A	383	LYS	4.9
1	A	788	VAL	4.9
1	A	311	THR	4.8
1	A	366	PRO	4.7
1	A	287	GLU	4.7
1	A	443	LEU	4.7
1	A	746	TRP	4.6
1	A	455	MET	4.6
1	A	582	ARG	4.5
1	A	310	GLU	4.5
1	A	447	CYS	4.5
1	A	427	GLU	4.5
1	A	448	GLU	4.4
1	A	509	GLY	4.4
1	A	357	GLU	4.3
1	A	449	THR	4.3
1	A	362	ARG	4.2
1	A	299	PRO	4.2
1	A	542	ILE	4.2
1	A	401	ARG	4.2
1	A	364	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	694	TRP	4.2
1	A	302	THR	4.2
1	A	572	THR	4.2
1	A	337	MET	4.1
1	A	632	ILE	4.1
1	A	365	GLU	4.1
1	A	764	LEU	4.1
1	A	579	ARG	4.1
1	A	593	ILE	4.0
1	A	701	ASN	4.0
1	A	577	VAL	4.0
1	A	301	LYS	3.9
1	A	432	TRP	3.9
1	A	276	ILE	3.9
1	A	376	ILE	3.9
1	A	562	LYS	3.9
1	A	400	THR	3.8
1	A	481	ALA	3.8
1	A	280	ARG	3.8
1	A	370	THR	3.8
1	A	580	VAL	3.8
1	A	575	ASN	3.8
1	A	833	TRP	3.8
1	A	680	ALA	3.8
1	A	558	GLU	3.7
1	A	477	MET	3.7
1	A	396	ARG	3.6
1	A	581	GLN	3.6
1	A	480	GLY	3.5
1	A	633	GLN	3.5
1	A	564	LEU	3.5
1	A	524	LYS	3.5
1	A	371	LYS	3.5
1	A	629	PHE	3.4
1	A	363	THR	3.4
1	A	308	SER	3.3
1	A	717	ILE	3.3
1	A	507	VAL	3.2
1	A	576	LYS	3.2
1	A	689	LYS	3.2
1	A	565	ALA	3.2
1	A	676	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	3.1
1	A	373	LEU	3.1
1	A	275	ASP	3.1
1	A	679	THR	3.1
1	A	553	VAL	3.0
1	A	625	GLY	3.0
1	A	695	GLU	2.9
1	A	547	LEU	2.9
1	A	681	LEU	2.9
1	A	491	PHE	2.9
1	A	537	GLY	2.9
1	A	375	LYS	2.9
1	A	344	THR	2.9
1	A	663	ASP	2.8
1	A	555	ASN	2.8
1	A	368	GLU	2.8
1	A	552	MET	2.8
1	A	699	GLY	2.8
1	A	687	VAL	2.7
1	A	390	THR	2.7
1	A	561	HIS	2.7
1	A	613	THR	2.7
1	A	559	GLY	2.7
1	A	273	ASN	2.7
1	A	566	GLU	2.7
1	A	567	ALA	2.7
1	A	678	LEU	2.7
1	A	810	LEU	2.7
1	A	295	ASP	2.7
1	A	495	ASP	2.6
1	A	551	GLU	2.6
1	A	493	ASN	2.6
1	A	548	LYS	2.6
1	A	630	LYS	2.6
1	A	569	PHE	2.6
1	A	285	LYS	2.6
1	A	545	GLU	2.6
1	A	690	ASP	2.5
1	A	497	TRP	2.5
1	A	397	GLU	2.5
1	A	627	GLY	2.5
1	A	367	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	372	LYS	2.5
1	A	870	VAL	2.5
1	A	496	HIS	2.4
1	A	578	VAL	2.4
1	A	623	MET	2.4
1	A	430	GLY	2.4
1	A	570	LYS	2.3
1	A	398	GLU	2.3
1	A	522	VAL	2.3
1	A	732	ASP	2.3
1	A	343	MET	2.3
1	A	536	ALA	2.3
1	A	716	LEU	2.3
1	A	528	GLY	2.3
1	A	677	ALA	2.2
1	A	540	THR	2.2
1	A	684	MET	2.1
1	A	450	CYS	2.1
1	A	823	TRP	2.1
1	A	377	THR	2.1
1	A	617	ALA	2.1
1	A	886	MET	2.1
1	A	574	GLN	2.1
1	A	757	SER	2.1
1	A	723	VAL	2.0
1	A	715	GLU	2.0
1	A	369	GLY	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 oligosaccharides 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,

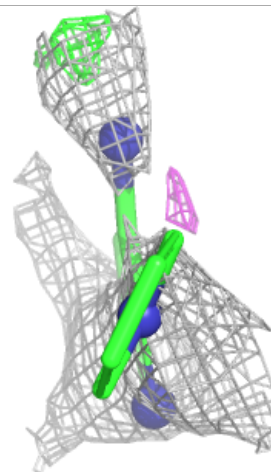
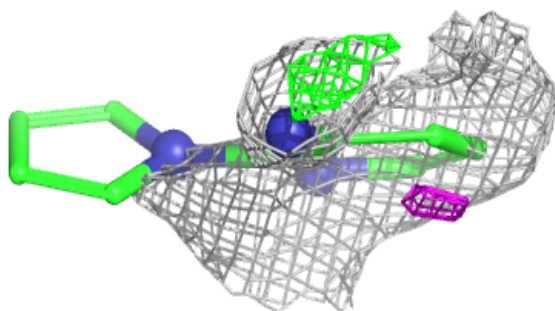
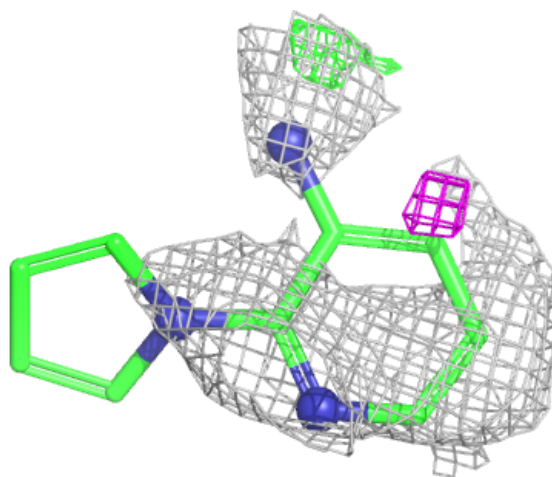
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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
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.

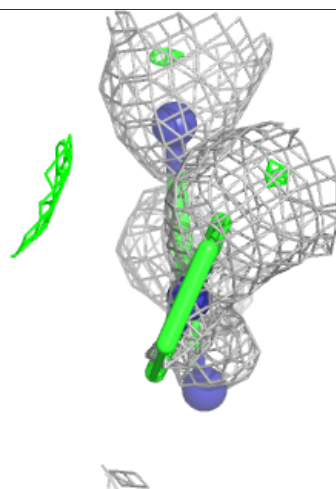
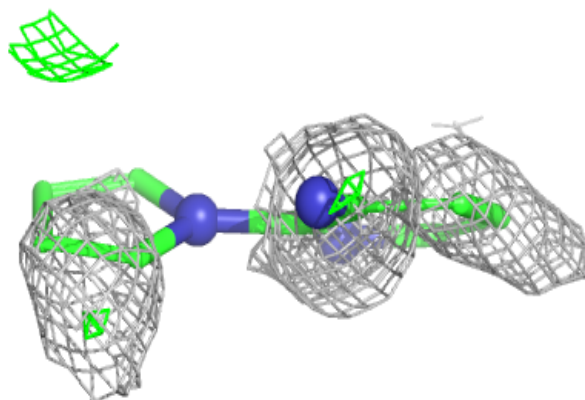
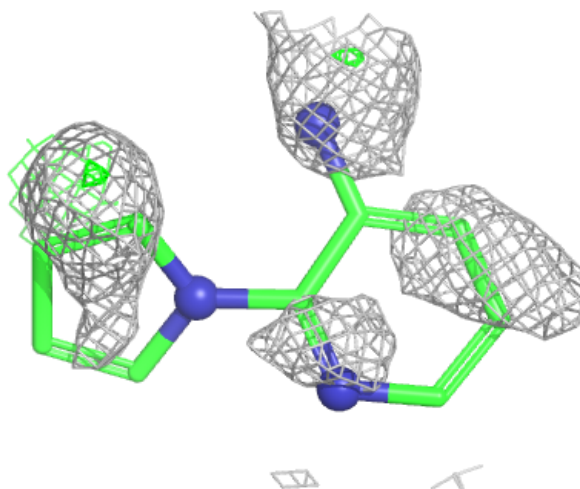
Electron density around A1B0N A 1011:

$2mF_o-DF_c$ (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.