



Full wwPDB X-ray Structure Validation 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 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	:	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)

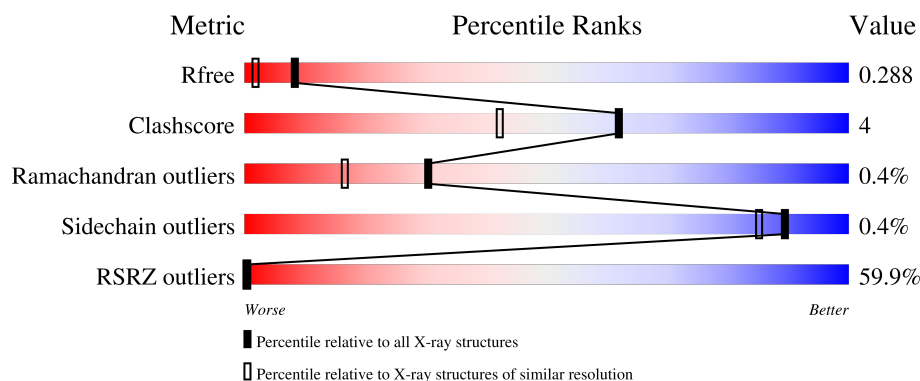
1 Overall quality at a glance

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
			Total	C	N	O	S			
1	A	568	4687	2951	840	862	34	0	5	0

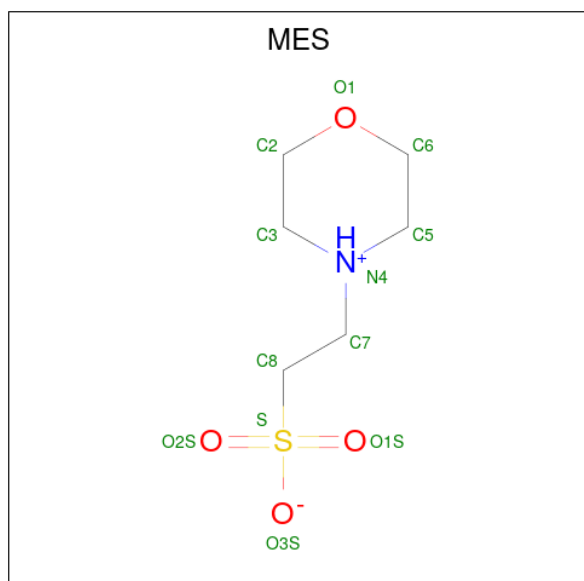
There are 2 discrepancies between the modelled and reference sequences:

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).



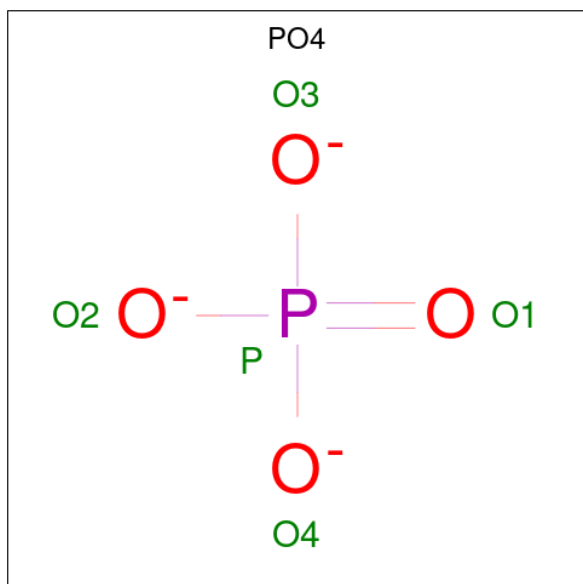
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- 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).

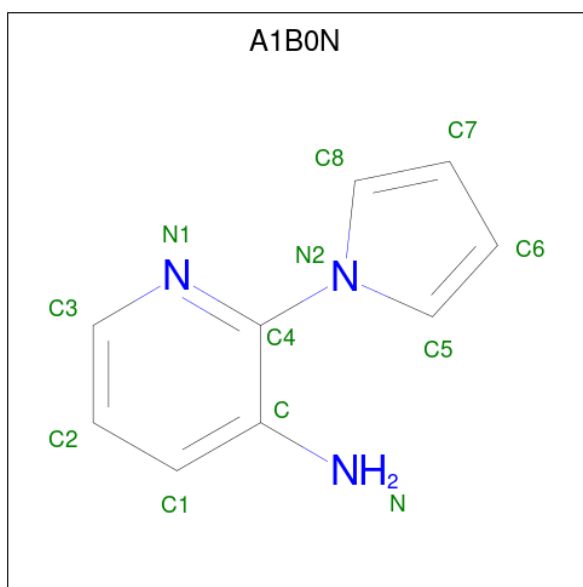


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- 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		

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

Continued on next page...

Continued from previous page...

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.

All (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
1:A:407:ALA:HB1	8:A:1011:A1B0N:C7	2.25	0.67
1:A:664:ASP:OD1	5:A:1006:PO4:O2	2.11	0.67
1:A:318:SER:O	9:A:1101:HOH:O	2.12	0.66
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:406:ASN:HD21	1:A:792:ARG:HA	1.67	0.58
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.91	0.51
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:409:LEU:HB3	9:A:1328:HOH:O	2.14	0.46
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.96	0.46
1:A:510:GLU:O	1:A:514:LYS:HG3	2.18	0.44
1:A:439:ARG:CZ	1:A:487:GLU:OE1	2.66	0.44
1:A:482:ARG:HD3	1:A:482:ARG:HA	1.86	0.44
1:A:644:LYS:O	1:A:648:VAL:HG23	2.18	0.43
1:A:306:HIS:HB2	1:A:592:ILE:O	2.17	0.43
1:A:403:VAL:HA	1:A:409:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:CE1	1:A:591:ASP:OD1	2.63	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
8:A:1011:A1B0N:N	8:A:1011:A1B0N:C8	2.82	0.42
1:A:428:ASP:OD1	1:A:430:GLY:N	2.52	0.42
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.45	0.41
1:A:507:VAL:C	1:A:510:GLU:HG2	2.41	0.41
1:A:507:VAL:O	1:A:510:GLU:HG2	2.20	0.41
1:A:399:PHE:O	1:A:403:VAL:HG13	2.21	0.40
1:A:737:ARG:HD2	1:A:737:ARG:HA	1.77	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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
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

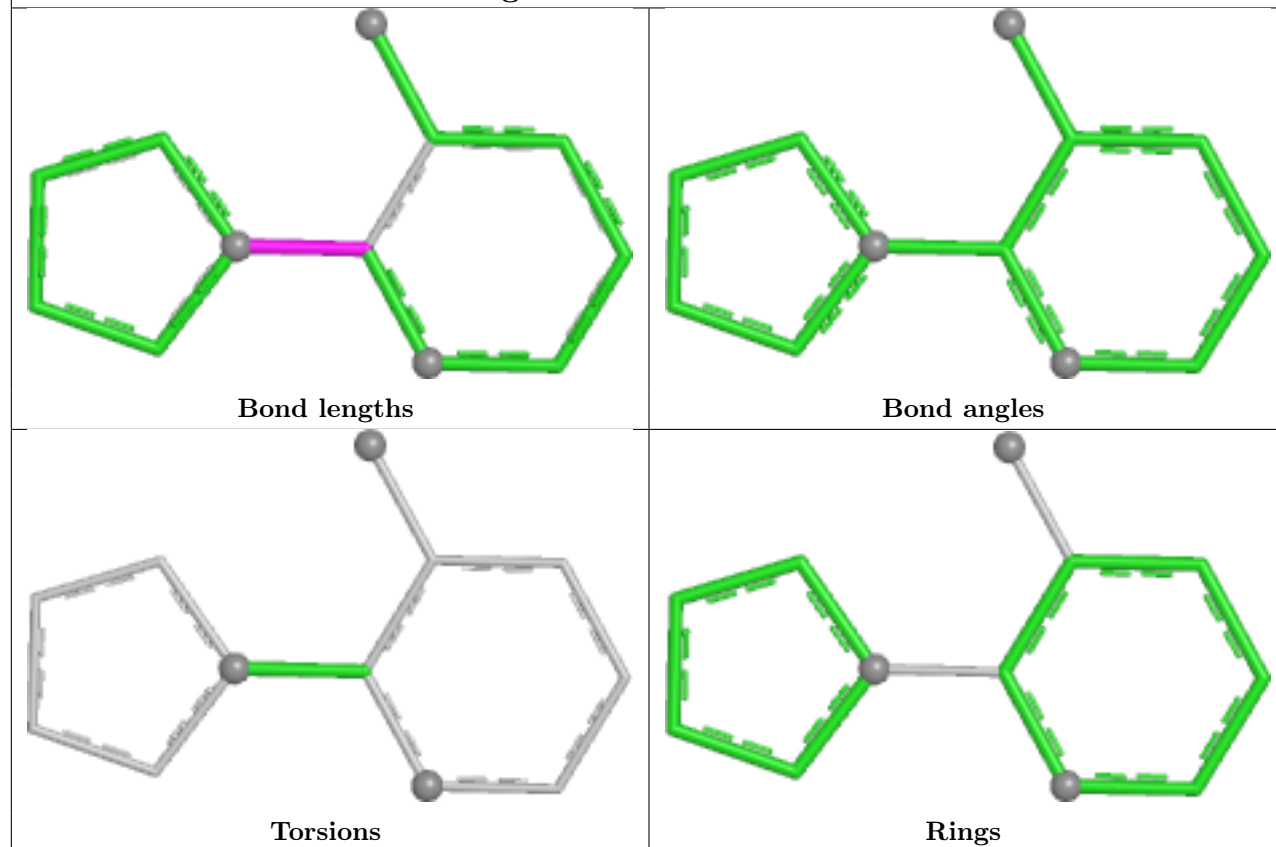
There are no ring outliers.

4 monomers are involved in 9 short contacts:

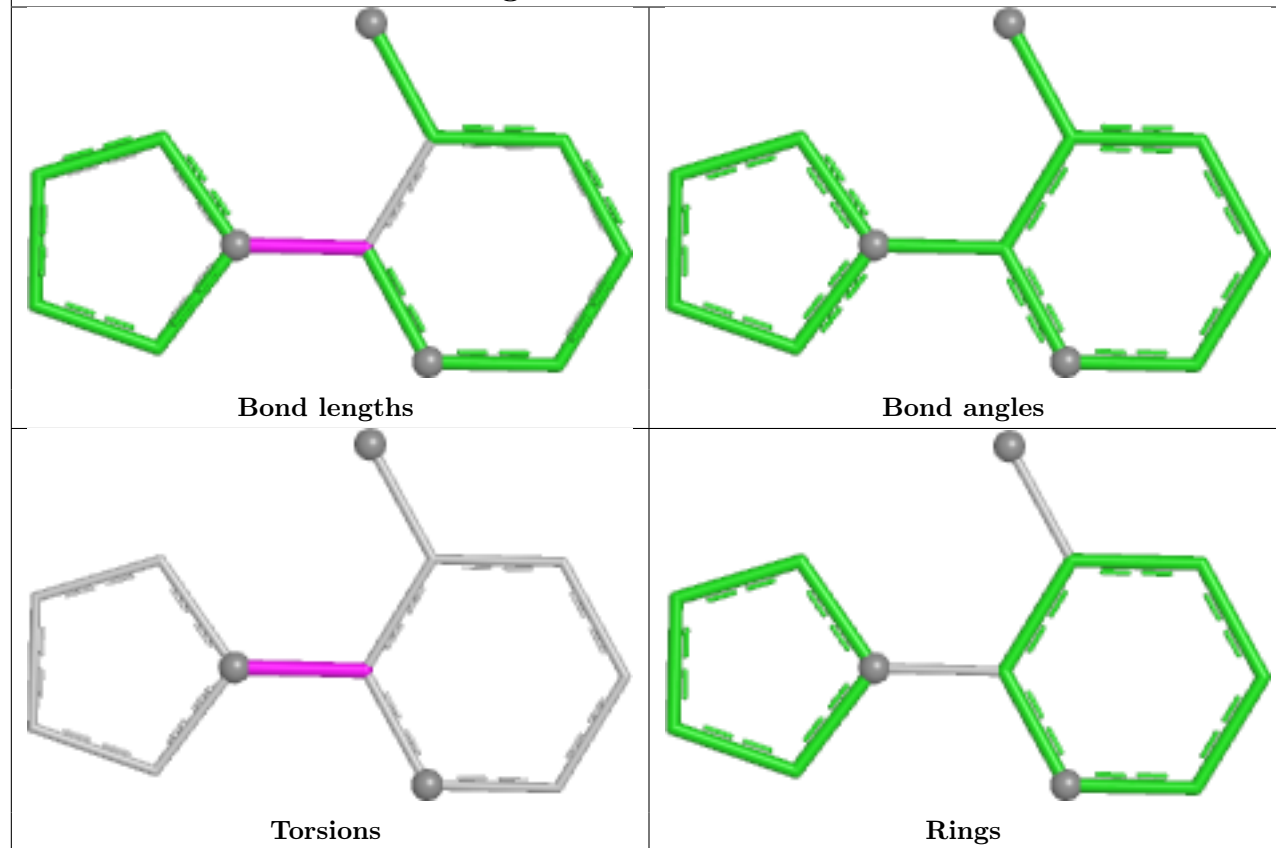
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	3	0
3	A	1003[A]	MES	1	0
5	A	1006	PO4	3	0
8	A	1011	A1B0N	2	0

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

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%)	4.13	340 (59%) 0 0	6, 38, 92, 135	181 (31%)

All (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
1	A	359	VAL	12.7
1	A	305	TYR	12.6
1	A	419	TRP	12.5
1	A	830	VAL	12.5
1	A	512	LEU	12.5
1	A	839	LEU	12.5
1	A	281	ILE	12.3
1	A	889	PHE	12.0
1	A	853	LEU	12.0
1	A	735	ILE	12.0
1	A	592	ILE	11.6
1	A	867	ILE	11.4
1	A	409	LEU	11.1
1	A	606	THR	11.1
1	A	407	ALA	11.0
1	A	488	ALA	10.9
1	A	486	PHE	10.9
1	A	484	LEU	10.8
1	A	738	ALA	10.8
1	A	588	THR	10.8
1	A	740	ILE	10.7
1	A	747	SER	10.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	650	VAL	10.6
1	A	863	ILE	10.5
1	A	816	VAL	10.5
1	A	515	LEU	10.5
1	A	292	TRP	10.4
1	A	719[A]	LYS	10.4
1	A	600	GLY	10.3
1	A	857	ALA	10.3
1	A	763[A]	SER	10.2
1	A	422	ALA	10.2
1	A	803	TRP	10.1
1	A	691	ILE	10.1
1	A	604	VAL	10.1
1	A	605	VAL	10.1
1	A	744	ALA	10.1
1	A	475	TRP	10.0
1	A	649	ARG	10.0
1	A	648	VAL	10.0
1	A	840	GLY	9.9
1	A	790	THR	9.9
1	A	307	GLY	9.9
1	A	743	GLY	9.6
1	A	880	THR	9.6
1	A	425	ALA	9.5
1	A	511	GLY	9.5
1	A	635	LEU	9.4
1	A	837	PRO	9.4
1	A	601	SER	9.3
1	A	596	ARG	9.2
1	A	489	LEU	9.2
1	A	828	THR	9.2
1	A	818	ILE	9.1
1	A	854	THR	9.0
1	A	637	VAL	9.0
1	A	297	ASP	8.9
1	A	809	MET	8.9
1	A	785[A]	SER	8.9
1	A	584	THR	8.9
1	A	408	ALA	8.9
1	A	431	PHE	8.8
1	A	646	TRP	8.8
1	A	670	LEU	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	806	THR	8.8
1	A	438	GLU	8.8
1	A	865	THR	8.7
1	A	882	TYR	8.6
1	A	288	HIS	8.6
1	A	513	HIS	8.6
1	A	832	SER	8.6
1	A	641	ILE	8.6
1	A	826	ASP	8.6
1	A	822	PRO	8.5
1	A	358	LYS	8.5
1	A	651	GLY	8.5
1	A	736	GLY	8.4
1	A	361	THR	8.4
1	A	741[A]	SER	8.4
1	A	739	ARG	8.4
1	A	442	HIS	8.4
1	A	293	HIS	8.3
1	A	636	THR	8.3
1	A	476	TYR	8.3
1	A	885	SER	8.3
1	A	602	GLY	8.3
1	A	841	LYS	8.2
1	A	300	TYR	8.2
1	A	888	ARG	8.2
1	A	298	HIS	8.1
1	A	638	THR	7.9
1	A	647	LEU	7.9
1	A	855	SER	7.9
1	A	805	THR	7.9
1	A	824	MET	7.9
1	A	439	ARG	7.8
1	A	482	ARG	7.8
1	A	290	THR	7.7
1	A	808	ASP	7.7
1	A	291	SER	7.7
1	A	421	SER	7.7
1	A	697	SER	7.7
1	A	452	TYR	7.7
1	A	306	HIS	7.7
1	A	645	ASN	7.6
1	A	319	SER	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	791	SER	7.5
1	A	318	SER	7.5
1	A	745	GLY	7.5
1	A	583	PRO	7.5
1	A	742	GLN	7.4
1	A	671	ASP	7.4
1	A	598	GLN	7.4
1	A	856	ARG	7.4
1	A	474	ILE	7.4
1	A	829	PRO	7.4
1	A	814	ASN	7.3
1	A	436	ASP	7.3
1	A	294	TYR	7.3
1	A	884	PRO	7.2
1	A	591	ASP	7.2
1	A	864[A]	GLN	7.2
1	A	643	VAL	7.2
1	A	485	GLU	7.1
1	A	673	ARG	7.1
1	A	835	GLU	7.1
1	A	821	ASN	7.1
1	A	876	ASN	7.1
1	A	423	ARG	7.0
1	A	487	GLU	7.0
1	A	283	LYS	7.0
1	A	403	VAL	7.0
1	A	440	ASN	7.0
1	A	317	ALA	7.0
1	A	590	MET	7.0
1	A	405	SER	6.9
1	A	827	LYS	6.8
1	A	286	GLN	6.8
1	A	453	ASN	6.8
1	A	404	ARG	6.7
1	A	881	ASP	6.7
1	A	597	ASP	6.7
1	A	510	GLU	6.6
1	A	672	ASP	6.6
1	A	800	THR	6.6
1	A	639	GLU	6.6
1	A	360	ASP	6.6
1	A	402	LYS	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	861	LYS	6.6
1	A	289	GLU	6.6
1	A	801	HIS	6.5
1	A	642	ALA	6.5
1	A	451	VAL	6.5
1	A	834	GLU	6.4
1	A	426	VAL	6.4
1	A	274	LEU	6.4
1	A	406	ASN	6.4
1	A	737	ARG	6.4
1	A	603	GLN	6.4
1	A	705	GLN	6.3
1	A	282	GLU	6.2
1	A	446	LYS	6.2
1	A	278	GLY	6.2
1	A	890	ARG	6.2
1	A	634	HIS	6.2
1	A	843	GLU	6.2
1	A	514	LYS	6.1
1	A	887	LYS	6.1
1	A	435	VAL	6.1
1	A	296	GLN	6.1
1	A	815	ARG	6.1
1	A	792	ARG	6.1
1	A	804	MET	6.0
1	A	437	LYS	6.0
1	A	478	TRP	6.0
1	A	825	GLU	6.0
1	A	454	MET	5.9
1	A	494	GLU	5.9
1	A	356	LYS	5.7
1	A	807	GLU	5.6
1	A	693	GLN	5.6
1	A	563	LYS	5.6
1	A	473	ALA	5.6
1	A	644	LYS	5.6
1	A	428	ASP	5.6
1	A	309	TYR	5.6
1	A	653	GLU	5.6
1	A	819	GLN	5.6
1	A	424	GLU	5.5
1	A	284	ILE	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	544	LEU	5.5
1	A	891	ARG	5.5
1	A	445	GLY	5.4
1	A	831	GLU	5.4
1	A	652	ARG	5.4
1	A	698	ARG	5.4
1	A	640	GLU	5.3
1	A	479	LEU	5.3
1	A	571	LEU	5.3
1	A	429	SER	5.3
1	A	434	LEU	5.2
1	A	433	GLU	5.1
1	A	277	ILE	5.1
1	A	303	TRP	5.0
1	A	420	LYS	4.9
1	A	802	GLU	4.9
1	A	556	HIS	4.9
1	A	820	GLU	4.8
1	A	279	LYS	4.8
1	A	312	LYS	4.8
1	A	383	LYS	4.8
1	A	399	PHE	4.8
1	A	311	THR	4.7
1	A	788	VAL	4.7
1	A	287	GLU	4.6
1	A	366	PRO	4.6
1	A	443	LEU	4.5
1	A	582	ARG	4.5
1	A	455	MET	4.5
1	A	746	TRP	4.5
1	A	310	GLU	4.4
1	A	427	GLU	4.4
1	A	447	CYS	4.4
1	A	448	GLU	4.3
1	A	357	GLU	4.2
1	A	509	GLY	4.2
1	A	449	THR	4.2
1	A	362	ARG	4.2
1	A	401	ARG	4.1
1	A	364	GLN	4.1
1	A	299	PRO	4.0
1	A	542	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	302	THR	4.0
1	A	337	MET	4.0
1	A	572	THR	4.0
1	A	694	TRP	4.0
1	A	365	GLU	4.0
1	A	579	ARG	4.0
1	A	632	ILE	4.0
1	A	764	LEU	3.9
1	A	701	ASN	3.9
1	A	301	LYS	3.9
1	A	593	ILE	3.9
1	A	562	LYS	3.8
1	A	577	VAL	3.8
1	A	432	TRP	3.8
1	A	276	ILE	3.8
1	A	376	ILE	3.8
1	A	280	ARG	3.7
1	A	400	THR	3.7
1	A	370	THR	3.7
1	A	575	ASN	3.7
1	A	481	ALA	3.7
1	A	580	VAL	3.6
1	A	833	TRP	3.6
1	A	558	GLU	3.6
1	A	680	ALA	3.6
1	A	396	ARG	3.6
1	A	477	MET	3.6
1	A	581	GLN	3.5
1	A	524	LYS	3.4
1	A	633	GLN	3.4
1	A	371	LYS	3.4
1	A	480	GLY	3.4
1	A	564	LEU	3.4
1	A	629	PHE	3.3
1	A	363	THR	3.3
1	A	308	SER	3.2
1	A	717	ILE	3.2
1	A	576	LYS	3.1
1	A	689	LYS	3.1
1	A	507	VAL	3.0
1	A	565	ALA	3.0
1	A	676	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	3.0
1	A	373	LEU	3.0
1	A	568	ILE	3.0
1	A	679	THR	2.9
1	A	695	GLU	2.9
1	A	553	VAL	2.8
1	A	375	LYS	2.8
1	A	491	PHE	2.8
1	A	547	LEU	2.8
1	A	681	LEU	2.8
1	A	625	GLY	2.8
1	A	344	THR	2.8
1	A	537	GLY	2.8
1	A	663	ASP	2.7
1	A	368	GLU	2.7
1	A	552	MET	2.7
1	A	555	ASN	2.7
1	A	699	GLY	2.6
1	A	561	HIS	2.6
1	A	566	GLU	2.6
1	A	390	THR	2.6
1	A	613	THR	2.6
1	A	273	ASN	2.6
1	A	687	VAL	2.6
1	A	559	GLY	2.6
1	A	295	ASP	2.6
1	A	551	GLU	2.5
1	A	567	ALA	2.5
1	A	678	LEU	2.5
1	A	810	LEU	2.5
1	A	495	ASP	2.5
1	A	548	LYS	2.5
1	A	630	LYS	2.5
1	A	493	ASN	2.5
1	A	285	LYS	2.5
1	A	569	PHE	2.5
1	A	545	GLU	2.5
1	A	690	ASP	2.5
1	A	397	GLU	2.4
1	A	497	TRP	2.4
1	A	367	LYS	2.4
1	A	372	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	627	GLY	2.4
1	A	496	HIS	2.3
1	A	870	VAL	2.3
1	A	623	MET	2.3
1	A	578	VAL	2.3
1	A	570	LYS	2.3
1	A	430	GLY	2.2
1	A	398	GLU	2.2
1	A	343	MET	2.2
1	A	732	ASP	2.2
1	A	522	VAL	2.2
1	A	716	LEU	2.2
1	A	536	ALA	2.1
1	A	528	GLY	2.1
1	A	677	ALA	2.1
1	A	684	MET	2.1
1	A	450	CYS	2.1
1	A	540	THR	2.0
1	A	823	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

Continued on next page...

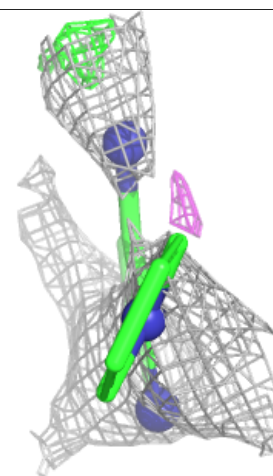
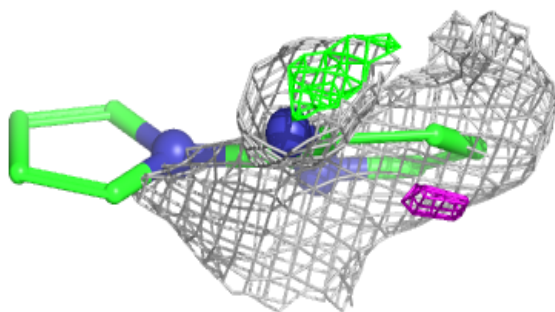
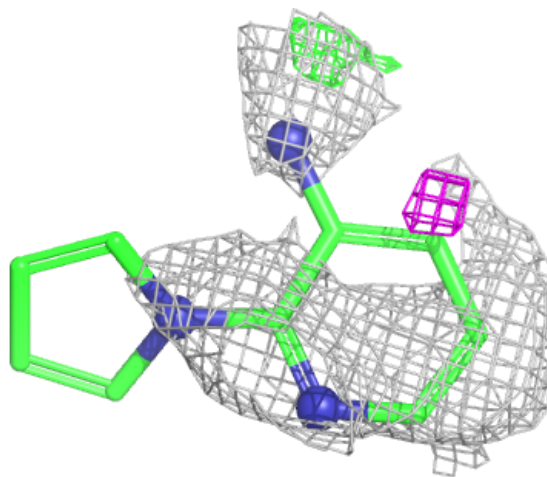
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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.

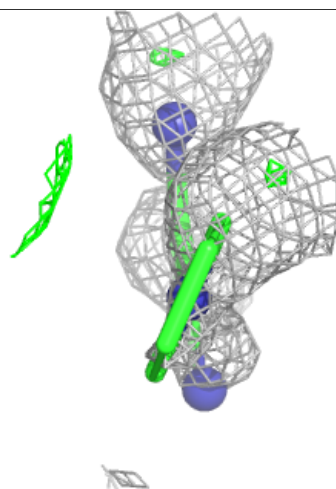
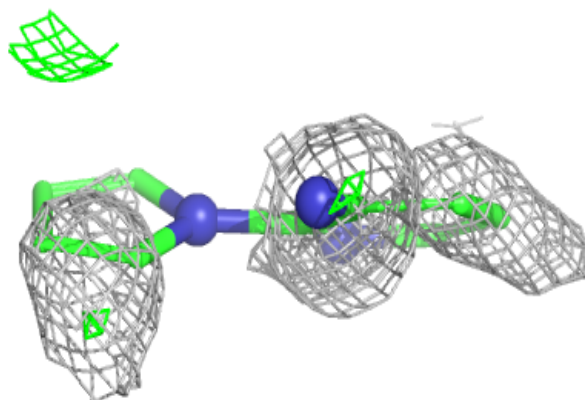
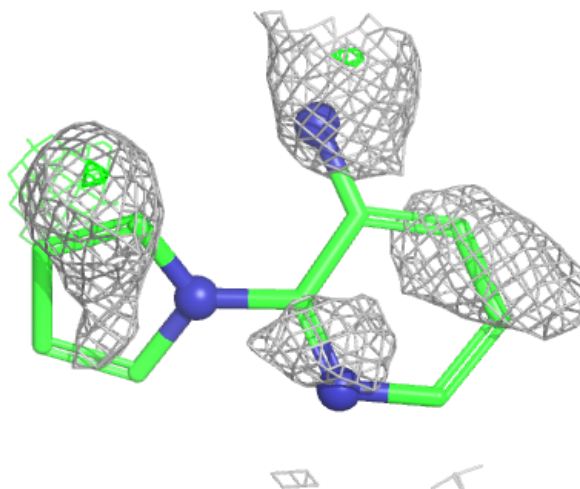
Electron density around A1B0N A 1011:

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.