



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:14 AM EDT

PDB ID : 7I2B
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 Z68404778 (DNV2_NS5A-x0249)
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 : 1.60 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)

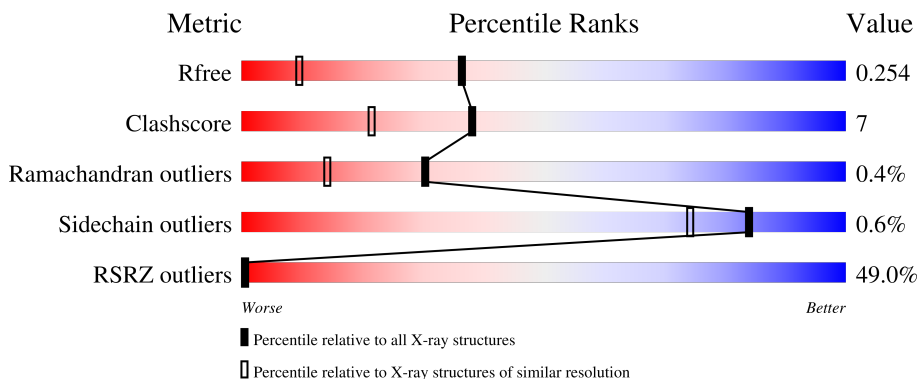
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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
6	PO4	A	1008	-	X	X	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 5223 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	573	4734	2981	849	870	34	0	7	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
			Total	C	N	O	S		
3	A	1	24	12	2	8	2	0	1

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



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



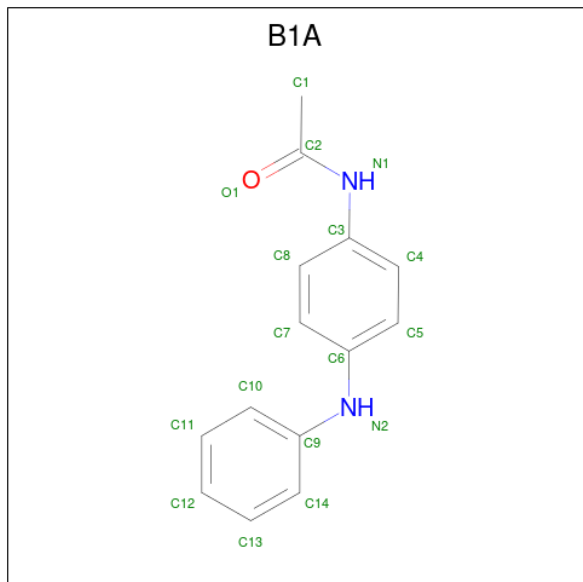
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is {N}-(4-phenylazanylphenyl)ethanamide (three-letter code: B1A) (formula: C₁₄H₁₄N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	34	28	4	2	0	1

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

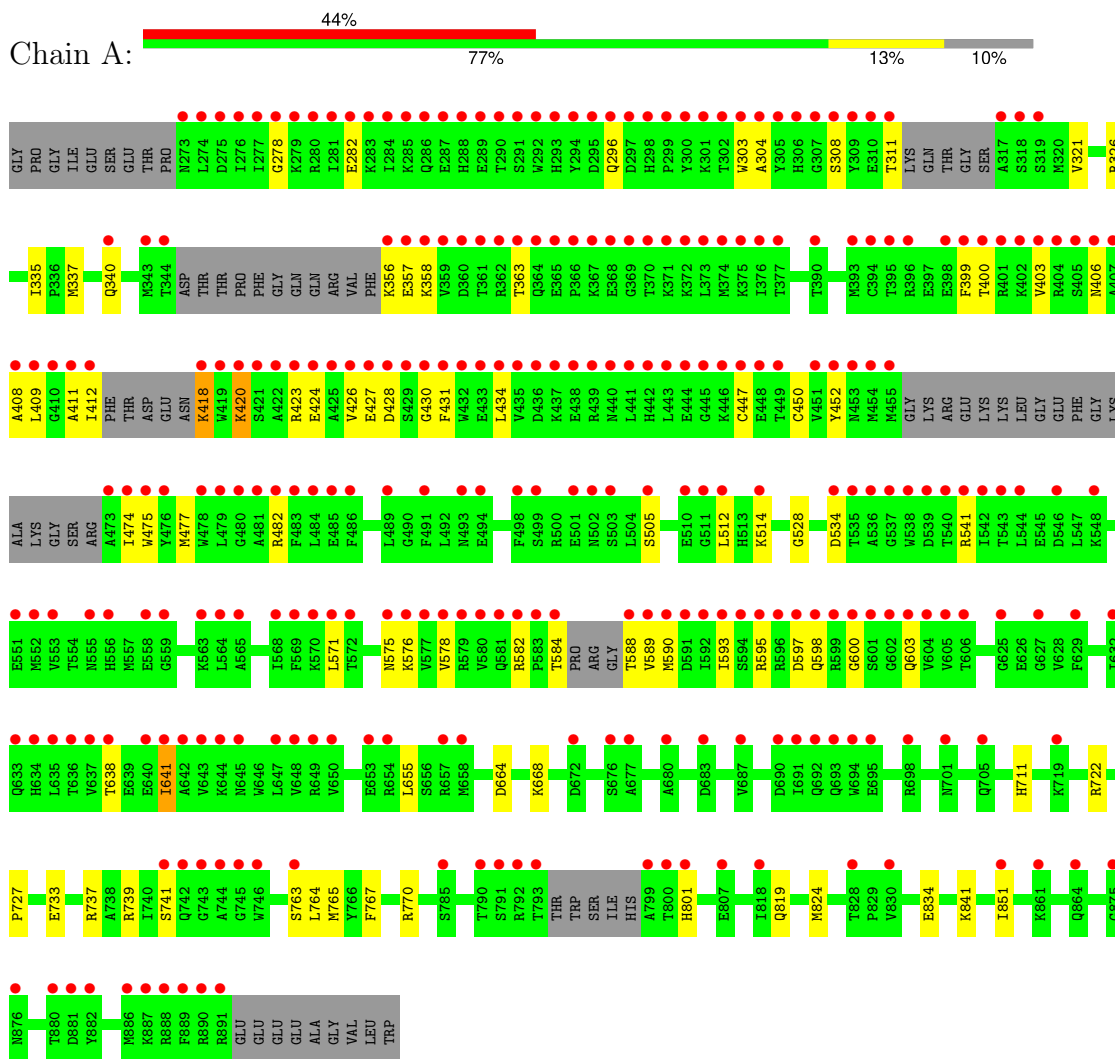
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	392	392	392	0	0

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	82.48Å 116.86Å 148.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 1.60 45.89 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.89-1.60) 99.2 (45.89-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.193 , 0.220 0.232 , 0.254	Depositor DCC
R_{free} test set	4793 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5223	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: PEG, B1A, ZN, PO4, CL, 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	0.75	0/4839	0.81	2/6525 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	739	ARG	NE-CZ-NH2	-5.62	117.49	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	741[B]	SER	Mainchain

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	4734	0	4638	64	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	1	0
5	A	14	0	20	0	0
6	A	10	0	0	3	0
7	A	34	0	0	0	0
8	A	1	0	0	0	0
9	A	392	0	0	10	1
All	All	5223	0	4702	65	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 7.

All (65) 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:664:ASP:OD1	6:A:1008:PO4:O4	1.89	0.91
1:A:340:GLN:OE1	9:A:1101:HOH:O	1.90	0.90
1:A:340:GLN:CD	9:A:1101:HOH:O	2.12	0.87
1:A:412:ILE:O	1:A:412:ILE:HG13	1.82	0.78
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.42	0.77
1:A:474:ILE:HD12	1:A:474:ILE:N	2.05	0.70
1:A:400:THR:O	1:A:403:VAL:HG22	1.92	0.70
1:A:399:PHE:O	1:A:403:VAL:HG13	1.92	0.69
1:A:819:GLN:NE2	9:A:1103:HOH:O	2.29	0.65
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.14	0.64
1:A:308:SER:HA	1:A:590:MET:O	1.97	0.64
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.79	0.64
1:A:474:ILE:HD12	1:A:474:ILE:H	1.62	0.62
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.41	0.60
1:A:475:TRP:CE3	1:A:600:GLY:HA3	2.37	0.60
1:A:356:LYS:O	1:A:357:GLU:HB2	2.03	0.59
1:A:841:LYS:NZ	9:A:1102:HOH:O	2.28	0.59
1:A:428:ASP:OD1	1:A:430:GLY:N	2.34	0.58
1:A:733:GLU:O	1:A:737:ARG:HG3	2.04	0.58
1:A:505:SER:OG	1:A:655:LEU:O	2.19	0.58
1:A:311:THR:HG23	1:A:588:THR:HG22	1.87	0.57
1:A:638:THR:HA	1:A:641:ILE:CG2	2.35	0.56
1:A:834:GLU:HG3	9:A:1153:HOH:O	2.05	0.55
1:A:528:GLY:O	1:A:668:LYS:HE3	2.06	0.54
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASP:OD1	1:A:428:ASP:C	2.47	0.53
1:A:408:ALA:HB3	1:A:603:GLN:HE22	1.74	0.53
1:A:571:LEU:O	1:A:575:ASN:O	2.27	0.53
1:A:764:LEU:HG	1:A:765:MET:CE	2.39	0.52
1:A:418:LYS:O	1:A:418:LYS:HD3	2.09	0.51
1:A:403:VAL:HG12	1:A:409:LEU:CD1	2.41	0.51
1:A:764:LEU:HG	1:A:765:MET:HE3	1.92	0.51
1:A:638:THR:O	1:A:641:ILE:HG23	2.10	0.51
1:A:278:GLY:O	1:A:282:GLU:HG3	2.12	0.49
1:A:475:TRP:CD1	1:A:475:TRP:N	2.80	0.49
1:A:411:ALA:HA	1:A:477:MET:O	2.13	0.48
1:A:403:VAL:HG12	1:A:409:LEU:HD11	1.95	0.47
1:A:356:LYS:O	1:A:357:GLU:OE2	2.32	0.47
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.15	0.47
1:A:308:SER:HB3	1:A:589:VAL:HB	1.96	0.47
1:A:358:LYS:NZ	1:A:541:ARG:HH21	2.13	0.47
1:A:474:ILE:N	1:A:474:ILE:CD1	2.76	0.46
1:A:431:PHE:O	1:A:434:LEU:HB2	2.15	0.46
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.31	0.46
1:A:423:ARG:O	1:A:427:GLU:HG3	2.16	0.45
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.98	0.45
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.34	0.45
1:A:597:ASP:O	1:A:598:GLN:HB2	2.17	0.45
4:A:1004:DMS:H12	9:A:1278:HOH:O	2.16	0.45
1:A:356:LYS:C	1:A:357:GLU:OE2	2.55	0.45
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.52	0.44
1:A:474:ILE:H	1:A:474:ILE:CD1	2.29	0.43
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.84	0.43
1:A:337:MET:HG2	9:A:1359:HOH:O	2.19	0.42
1:A:340:GLN:NE2	9:A:1101:HOH:O	2.46	0.42
1:A:420:LYS:N	1:A:424:GLU:OE1	2.33	0.42
1:A:363:THR:HG23	9:A:1384:HOH:O	2.19	0.42
1:A:763[A]:SER:O	1:A:767:PHE:HB3	2.20	0.41
1:A:477:MET:HB2	1:A:482:ARG:NE	2.36	0.41
1:A:514:LYS:HE2	9:A:1289:HOH:O	2.21	0.41
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.51	0.41
1:A:304:ALA:O	1:A:593:ILE:HA	2.21	0.41
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.51	0.41
1:A:296:GLN:OE1	1:A:296:GLN:HA	2.22	0.40
1:A:722:ARG:HB3	1:A:824:MET:SD	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1139:HOH:O	9:A:1139:HOH:O[2_445]	1.67	0.53

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	566/637 (89%)	547 (97%)	17 (3%)	2 (0%)	30 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LYS
1	A	406	ASN

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	508/554 (92%)	505 (99%)	3 (1%)	84 74

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ILE
1	A	418	LYS
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN

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 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	0.33	0	3,3,3	0.09	0
7	B1A	A	1011[B]	-	18,18,18	0.09	0	23,23,23	0.32	0
5	PEG	A	1007	-	6,6,6	0.24	0	5,5,5	0.18	0
3	MES	A	1003[A]	-	12,12,12	0.85	0	15,16,16	0.77	0
4	DMS	A	1004	-	3,3,3	0.83	0	3,3,3	0.47	0
6	PO4	A	1008	-	4,4,4	6.66	4 (100%)	6,6,6	1.31	1 (16%)
5	PEG	A	1010	-	6,6,6	0.13	0	5,5,5	0.11	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.29	0
6	PO4	A	1009	-	4,4,4	1.15	1 (25%)	6,6,6	0.46	0
7	B1A	A	1011[A]	-	18,18,18	0.07	0	23,23,23	0.28	0
4	DMS	A	1006	-	3,3,3	0.18	0	3,3,3	0.47	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
7	B1A	A	1011[B]	-	-	1/8/8/8	0/2/2/2
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
5	PEG	A	1010	-	-	2/4/4/4	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
7	B1A	A	1011[A]	-	-	0/8/8/8	0/2/2/2
5	PEG	A	1007	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	10.14	1.74	1.50
6	A	1008	PO4	P-O2	6.73	1.74	1.54
6	A	1008	PO4	P-O3	4.94	1.69	1.54
6	A	1008	PO4	P-O4	-2.16	1.48	1.54
6	A	1009	PO4	P-O1	2.10	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1008	PO4	O4-P-O2	2.55	115.83	107.91

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O2S
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1007	PEG	O2-C3-C4-O4
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
5	A	1010	PEG	O1-C1-C2-O2
5	A	1007	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

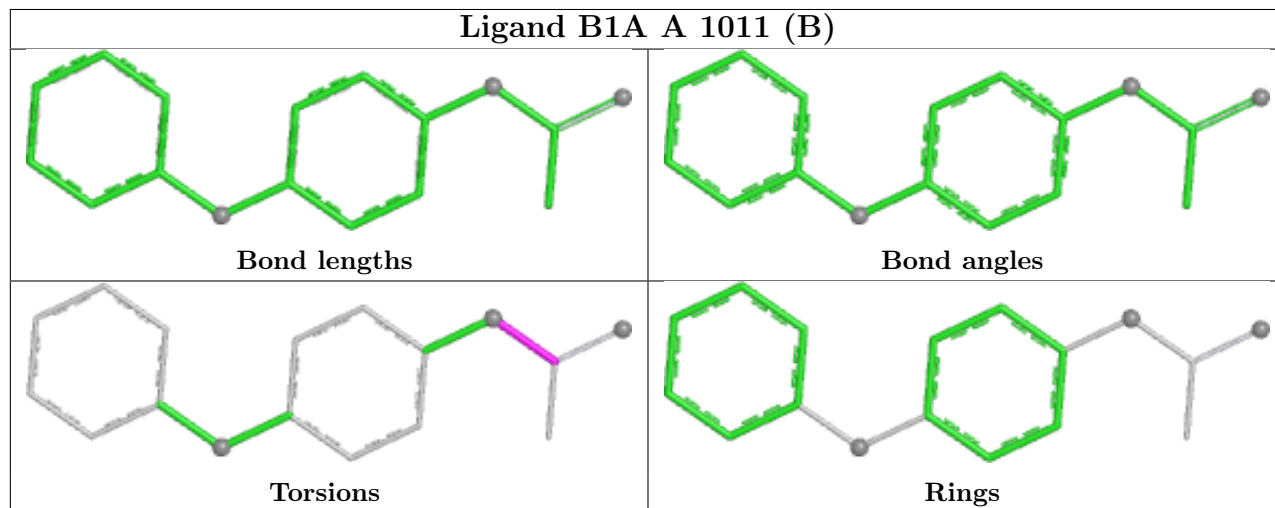
Mol	Chain	Res	Type	Atoms
5	A	1007	PEG	C4-C3-O2-C2
7	A	1011[B]	B1A	O1-C2-N1-C3

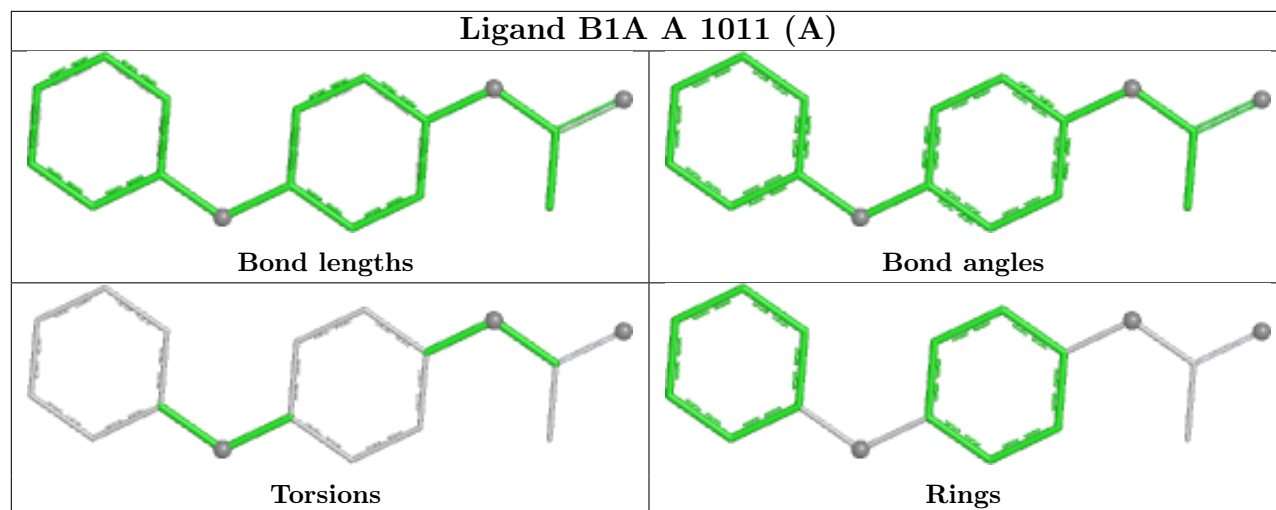
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	1	0
6	A	1008	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	573/637 (89%)	3.02	281 (49%) 0 0	6, 32, 63, 101	185 (32%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512[A]	LEU	12.8
1	A	284	ILE	11.7
1	A	637	VAL	11.2
1	A	281	ILE	11.1
1	A	514	LYS	10.9
1	A	800	THR	10.9
1	A	474	ILE	10.7
1	A	641	ILE	10.7
1	A	801[A]	HIS	10.7
1	A	593	ILE	10.7
1	A	632	ILE	10.5
1	A	319	SER	10.5
1	A	705	GLN	10.2
1	A	441	LEU	10.1
1	A	376	ILE	10.0
1	A	635	LEU	10.0
1	A	799	ALA	9.8
1	A	889	PHE	9.7
1	A	412	ILE	9.7
1	A	407	ALA	9.7
1	A	636	THR	9.5
1	A	409	LEU	9.4
1	A	478	TRP	9.3
1	A	498	PHE	9.3
1	A	373	LEU	9.3
1	A	340	GLN	9.2
1	A	431	PHE	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	9.1
1	A	426	VAL	9.0
1	A	876	ASN	9.0
1	A	594	SER	8.9
1	A	577	VAL	8.9
1	A	719[A]	LYS	8.8
1	A	486	PHE	8.8
1	A	592	ILE	8.7
1	A	292	TRP	8.7
1	A	571	LEU	8.7
1	A	763[A]	SER	8.7
1	A	403	VAL	8.6
1	A	343	MET	8.6
1	A	483	PHE	8.5
1	A	479	LEU	8.3
1	A	480	GLY	8.3
1	A	542	ILE	8.2
1	A	638	THR	8.2
1	A	318	SER	8.1
1	A	543	THR	8.0
1	A	475	TRP	7.9
1	A	377	THR	7.8
1	A	430	GLY	7.8
1	A	283	LYS	7.8
1	A	293	HIS	7.8
1	A	600	GLY	7.8
1	A	276	ILE	7.7
1	A	578	VAL	7.7
1	A	317	ALA	7.7
1	A	301	LYS	7.6
1	A	511	GLY	7.6
1	A	434	LEU	7.6
1	A	538	TRP	7.6
1	A	300	TYR	7.6
1	A	298	HIS	7.6
1	A	400	THR	7.5
1	A	305	TYR	7.5
1	A	606	THR	7.5
1	A	589	VAL	7.4
1	A	399	PHE	7.4
1	A	572	THR	7.4
1	A	499	SER	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	452	TYR	7.3
1	A	505	SER	7.2
1	A	280	ARG	7.1
1	A	601	SER	7.1
1	A	448	GLU	7.1
1	A	411	ALA	7.0
1	A	742	GLN	7.0
1	A	277	ILE	7.0
1	A	580	VAL	7.0
1	A	595	ARG	7.0
1	A	279	LYS	7.0
1	A	274	LEU	6.9
1	A	864[A]	GLN	6.9
1	A	694	TRP	6.9
1	A	374	MET	6.9
1	A	375	LYS	6.8
1	A	484	LEU	6.8
1	A	308	SER	6.8
1	A	442	HIS	6.8
1	A	311	THR	6.7
1	A	303	TRP	6.7
1	A	422	ALA	6.7
1	A	449	THR	6.6
1	A	344	THR	6.6
1	A	405	SER	6.6
1	A	419	TRP	6.5
1	A	745	GLY	6.5
1	A	473	ALA	6.5
1	A	657	ARG	6.4
1	A	741[A]	SER	6.4
1	A	309	TYR	6.3
1	A	588	THR	6.3
1	A	425	ALA	6.3
1	A	476	TYR	6.2
1	A	536	ALA	6.2
1	A	503	SER	6.2
1	A	408	ALA	6.2
1	A	485	GLU	6.1
1	A	363	THR	6.1
1	A	359	VAL	6.1
1	A	481	ALA	6.1
1	A	541	ARG	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	793	THR	6.1
1	A	658	MET	6.0
1	A	791	SER	6.0
1	A	575	ASN	6.0
1	A	358	LYS	6.0
1	A	581	GLN	6.0
1	A	602	GLY	5.9
1	A	282	GLU	5.9
1	A	634	HIS	5.8
1	A	295	ASP	5.8
1	A	785[A]	SER	5.8
1	A	744	ALA	5.7
1	A	576	LYS	5.7
1	A	633	GLN	5.7
1	A	372	LYS	5.6
1	A	306	HIS	5.6
1	A	535	THR	5.6
1	A	360	ASP	5.6
1	A	544	LEU	5.6
1	A	401	ARG	5.6
1	A	603	GLN	5.5
1	A	584	THR	5.5
1	A	278	GLY	5.4
1	A	539	ASP	5.4
1	A	534	ASP	5.4
1	A	361	THR	5.4
1	A	502	ASN	5.4
1	A	275	ASP	5.3
1	A	693	GLN	5.3
1	A	371	LYS	5.3
1	A	546	ASP	5.3
1	A	273	ASN	5.3
1	A	451	VAL	5.3
1	A	302	THR	5.3
1	A	421	SER	5.2
1	A	551	GLU	5.2
1	A	698	ARG	5.2
1	A	423	ARG	5.2
1	A	579	ARG	5.2
1	A	888	ARG	5.1
1	A	365	GLU	5.1
1	A	299	PRO	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	564	LEU	5.1
1	A	427	GLU	5.1
1	A	482	ARG	5.1
1	A	654	ARG	5.1
1	A	583	PRO	5.0
1	A	406	ASN	4.9
1	A	290	THR	4.9
1	A	402	LYS	4.9
1	A	629	PHE	4.9
1	A	597	ASP	4.9
1	A	304	ALA	4.9
1	A	429	SER	4.9
1	A	296	GLN	4.8
1	A	404	ARG	4.8
1	A	596	ARG	4.8
1	A	746	TRP	4.8
1	A	433	GLU	4.8
1	A	648	VAL	4.8
1	A	362	ARG	4.8
1	A	364	GLN	4.8
1	A	890	ARG	4.7
1	A	677	ALA	4.7
1	A	291	SER	4.7
1	A	591	ASP	4.7
1	A	297	ASP	4.7
1	A	599	ARG	4.6
1	A	356	LYS	4.6
1	A	570	LYS	4.6
1	A	598	GLN	4.6
1	A	443	LEU	4.6
1	A	447	CYS	4.6
1	A	653	GLU	4.5
1	A	548	LYS	4.5
1	A	286	GLN	4.5
1	A	285	LYS	4.5
1	A	563	LYS	4.5
1	A	366	PRO	4.5
1	A	455	MET	4.5
1	A	501	GLU	4.5
1	A	428	ASP	4.4
1	A	590	MET	4.4
1	A	556	HIS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	537	GLY	4.4
1	A	582	ARG	4.3
1	A	887	LYS	4.3
1	A	390	THR	4.2
1	A	437	LYS	4.2
1	A	357	GLU	4.2
1	A	440	ASN	4.1
1	A	510	GLU	4.0
1	A	370	THR	3.9
1	A	891	ARG	3.9
1	A	288	HIS	3.9
1	A	410	GLY	3.8
1	A	882	TYR	3.8
1	A	424	GLU	3.8
1	A	446	LYS	3.7
1	A	565	ALA	3.7
1	A	627	GLY	3.7
1	A	687	VAL	3.7
1	A	445	GLY	3.7
1	A	676	SER	3.6
1	A	439	ARG	3.6
1	A	790	THR	3.6
1	A	818	ILE	3.6
1	A	792	ARG	3.5
1	A	647	LEU	3.5
1	A	454	MET	3.5
1	A	552	MET	3.5
1	A	310	GLU	3.5
1	A	287	GLU	3.4
1	A	604	VAL	3.4
1	A	398	GLU	3.4
1	A	453	ASN	3.4
1	A	435	VAL	3.3
1	A	444	GLU	3.3
1	A	368	GLU	3.3
1	A	438	GLU	3.2
1	A	649	ARG	3.2
1	A	830	VAL	3.2
1	A	880	THR	3.2
1	A	650	VAL	3.1
1	A	568	ILE	3.0
1	A	432	TRP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	569	PHE	3.0
1	A	645	ASN	3.0
1	A	851	ILE	3.0
1	A	644	LYS	3.0
1	A	861	LYS	3.0
1	A	396	ARG	2.9
1	A	418	LYS	2.9
1	A	553	VAL	2.9
1	A	540	THR	2.8
1	A	642	ALA	2.8
1	A	558	GLU	2.8
1	A	881	ASP	2.7
1	A	493	ASN	2.7
1	A	555	ASN	2.7
1	A	420	LYS	2.7
1	A	672	ASP	2.7
1	A	605	VAL	2.7
1	A	683	ASP	2.6
1	A	680	ALA	2.6
1	A	436	ASP	2.6
1	A	393	MET	2.5
1	A	625	GLY	2.5
1	A	743	GLY	2.5
1	A	695	GLU	2.5
1	A	692	GLN	2.4
1	A	367	LYS	2.4
1	A	886	MET	2.4
1	A	559	GLY	2.4
1	A	289	GLU	2.4
1	A	701	ASN	2.3
1	A	494	GLU	2.3
1	A	307	GLY	2.3
1	A	489	LEU	2.3
1	A	875	GLY	2.3
1	A	395	THR	2.3
1	A	643	VAL	2.3
1	A	394	CYS	2.2
1	A	690	ASP	2.2
1	A	369	GLY	2.2
1	A	691	ILE	2.1
1	A	828	THR	2.1
1	A	807	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	491	PHE	2.1
1	A	640	GLU	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](#)

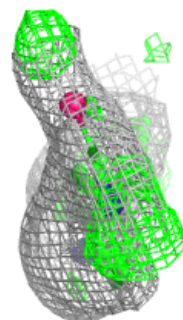
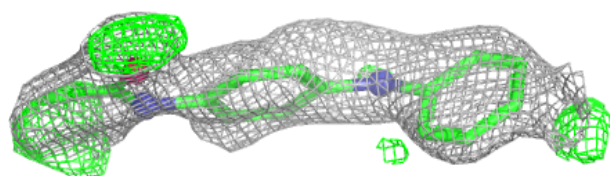
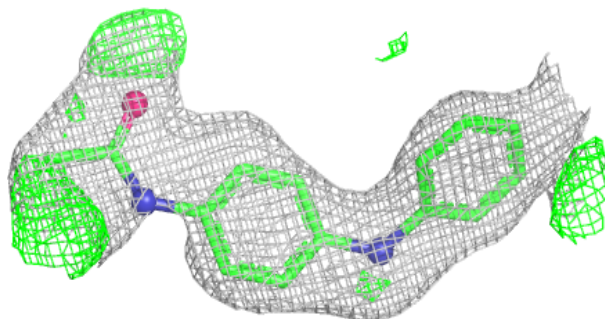
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
7	B1A	A	1011[A]	17/17	0.57	0.28	32,43,47,47	17
7	B1A	A	1011[B]	17/17	0.57	0.28	26,30,32,33	17
6	PO4	A	1009	5/5	0.63	0.17	72,81,90,109	0
4	DMS	A	1005	4/4	0.70	0.29	74,83,95,107	0
5	PEG	A	1007	7/7	0.78	0.17	88,90,91,94	0
6	PO4	A	1008	5/5	0.80	0.16	30,33,44,62	0
5	PEG	A	1010	7/7	0.83	0.15	57,64,72,76	0
4	DMS	A	1004	4/4	0.92	0.16	39,44,45,45	0
4	DMS	A	1006	4/4	0.93	0.13	47,51,57,59	0
3	MES	A	1003[B]	12/12	0.97	0.33	695,733,806,808	12
3	MES	A	1003[A]	12/12	0.97	0.33	20,25,27,29	12
2	ZN	A	1002	1/1	0.98	0.08	51,51,51,51	0
8	CL	A	1012	1/1	0.99	0.05	37,37,37,37	0
2	ZN	A	1001	1/1	1.00	0.02	20,20,20,20	0

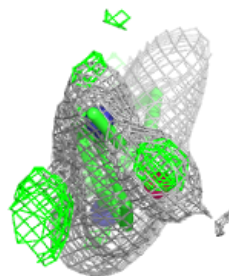
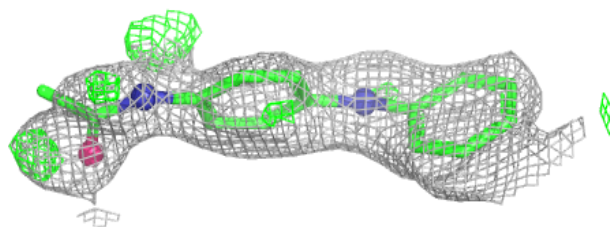
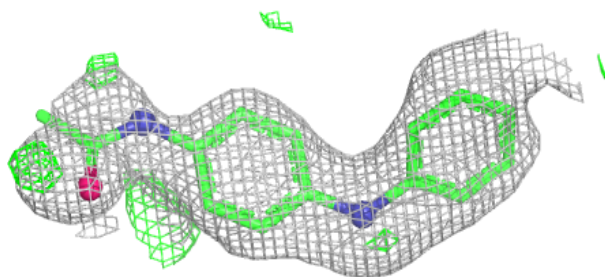
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B1A A 1011 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B1A A 1011 (B):**

$2mF_o-DF_c$ (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.