



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 08:15 PM JST

PDB ID : 9VDS / pdb_00009vds
Title : Crystal structure of voltage-gated sodium channel NavAb N49K/L176W mutant
Authors : Irie, K.
Deposited on : 2025-06-09
Resolution : 3.70 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	:	1.8.5 (274361), CSD as541be (2020)
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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

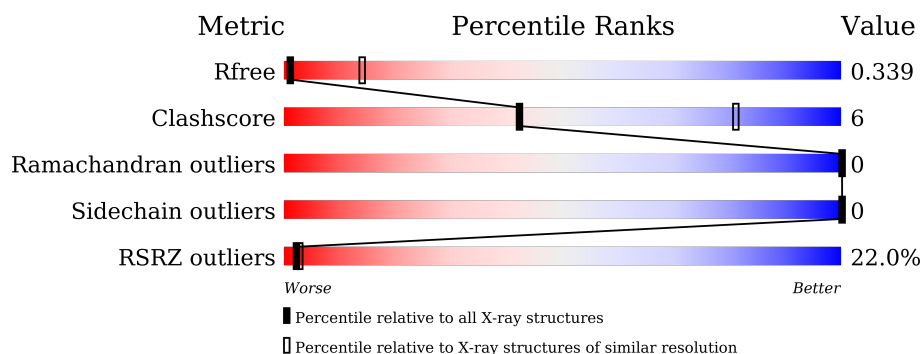
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	269	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1866 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1798	1231	269	286	12	0	0	0

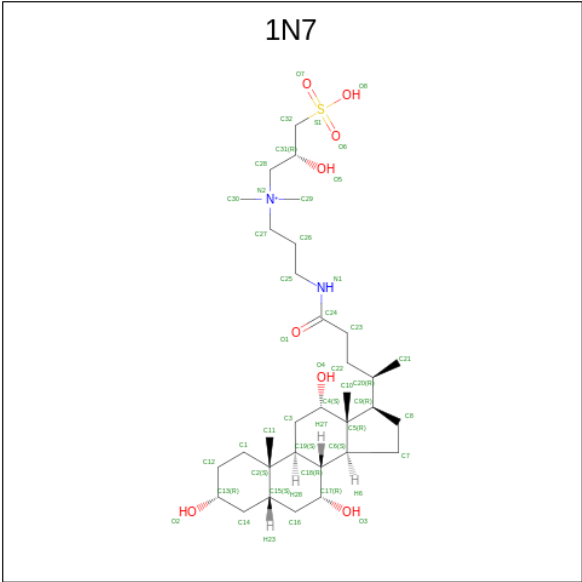
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	999	GLY	-	expression tag	UNP A8EVM5
A	1000	SER	-	expression tag	UNP A8EVM5
A	1049	LYS	ASN	engineered mutation	UNP A8EVM5
A	1176	TRP	LEU	engineered mutation	UNP A8EVM5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

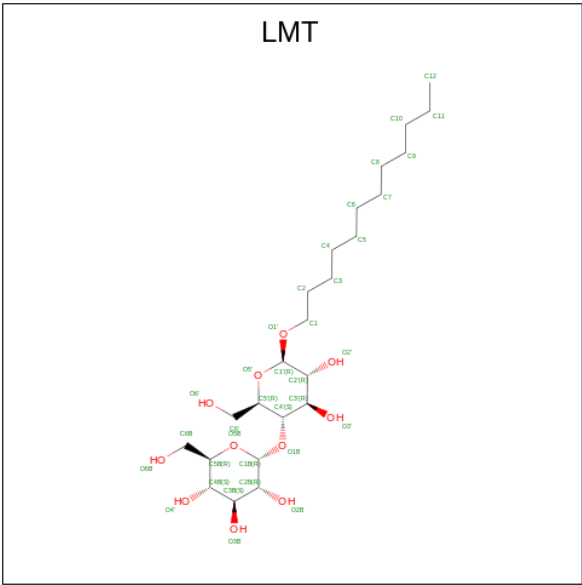
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	27	1	4		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.88Å 126.88Å 204.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.70 29.91 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.91-3.70) 99.3 (29.91-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.313 , 0.339 0.317 , 0.339	Depositor DCC
R_{free} test set	434 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 6.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	1866	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: LMT, 1N7, NA

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	0.14	0/1848	0.29	0/2512

There are no bond length outliers.

There are no bond angle outliers.

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	1798	0	1885	24	0
2	A	1	0	0	0	0
3	A	32	0	44	0	0
4	A	35	0	45	2	0
All	All	1866	0	1974	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (24) 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:1087:SER:HB2	1:A:1105:ARG:HH21	1.60	0.67
1:A:1025:ASN:HD21	1:A:1105:ARG:HH11	1.48	0.61
1:A:1067:HIS:HD1	1:A:1070:SER:HG	1.47	0.60
1:A:1087:SER:O	1:A:1102:ARG:NH1	2.34	0.60
1:A:1130:MET:HB3	1:A:1216:ILE:HD11	1.84	0.58
1:A:1128:PRO:HA	1:A:1131:LEU:HD22	1.85	0.57
1:A:1143:ILE:HG22	1:A:1147:MET:HE2	1.87	0.56
1:A:1060:ILE:HD11	1:A:1108:ARG:HH12	1.71	0.54
1:A:1099:ARG:HB3	1:A:1102:ARG:HE	1.74	0.52
1:A:1122:ALA:O	1:A:1126:VAL:HG23	2.11	0.50
1:A:1032:GLU:O	1:A:1035:LYS:NZ	2.42	0.49
1:A:1188:MET:HA	1:A:1191:TYR:O	2.13	0.48
1:A:1111:THR:O	1:A:1117:ARG:NH2	2.44	0.47
1:A:1087:SER:HB2	1:A:1105:ARG:NH2	2.28	0.46
1:A:1075:PRO:HA	1:A:1078:LEU:HD12	1.99	0.45
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.18	0.44
1:A:1014:PHE:HZ	1:A:1059:GLU:HG2	1.83	0.43
1:A:1194:ALA:HA	4:A:1303:LMT:H11	2.00	0.43
1:A:1045:THR:O	1:A:1049:LYS:HG2	2.19	0.42
1:A:1191:TYR:HB3	4:A:1303:LMT:H2'	2.02	0.42
1:A:1125:SER:O	1:A:1128:PRO:HD2	2.20	0.42
1:A:1074:ASP:OD2	1:A:1076:TRP:HB2	2.19	0.41
1:A:1035:LYS:HD3	1:A:1035:LYS:HA	1.78	0.41
1:A:1067:HIS:HB2	1:A:1071:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/269 (80%)	210 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	200/249 (80%)	200 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1025	ASN
1	A	1225	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1N7	A	1302	-	35,35,46	0.35	0	54,54,72	0.79	1 (1%)
4	LMT	A	1303	-	36,36,36	1.16	4 (11%)	47,47,47	0.95	1 (2%)

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	1N7	A	1302	-	-	3/13/78/92	0/4/4/4
4	LMT	A	1303	-	-	9/21/61/61	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1303	LMT	O3'-C3'	-2.63	1.36	1.43
4	A	1303	LMT	O2'-C2'	-2.44	1.37	1.43
4	A	1303	LMT	O3B-C3B	-2.27	1.37	1.43
4	A	1303	LMT	O2B-C2B	-2.21	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	1N7	C15-C16-C17	-3.51	110.58	114.46
4	A	1303	LMT	C3'-C4'-C5'	-2.81	104.48	110.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1303	LMT	C2'-C1'-O1'-C1
4	A	1303	LMT	O5'-C1'-O1'-C1
4	A	1303	LMT	O5B-C1B-O1B-C4'
4	A	1303	LMT	O5B-C5B-C6B-O6B
3	A	1302	1N7	C22-C23-C24-N1
3	A	1302	1N7	C22-C23-C24-O1
4	A	1303	LMT	C4B-C5B-C6B-O6B
4	A	1303	LMT	C3-C4-C5-C6
4	A	1303	LMT	O5'-C5'-C6'-O6'
4	A	1303	LMT	C2-C1-O1'-C1'

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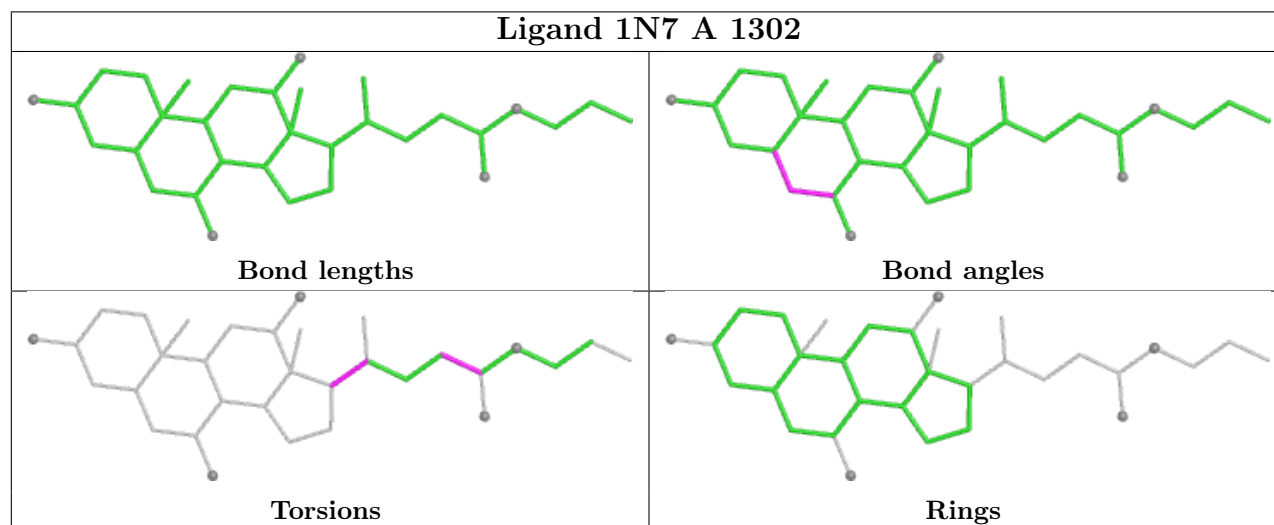
Mol	Chain	Res	Type	Atoms
4	A	1303	LMT	C1-C2-C3-C4
3	A	1302	1N7	C21-C20-C9-C5

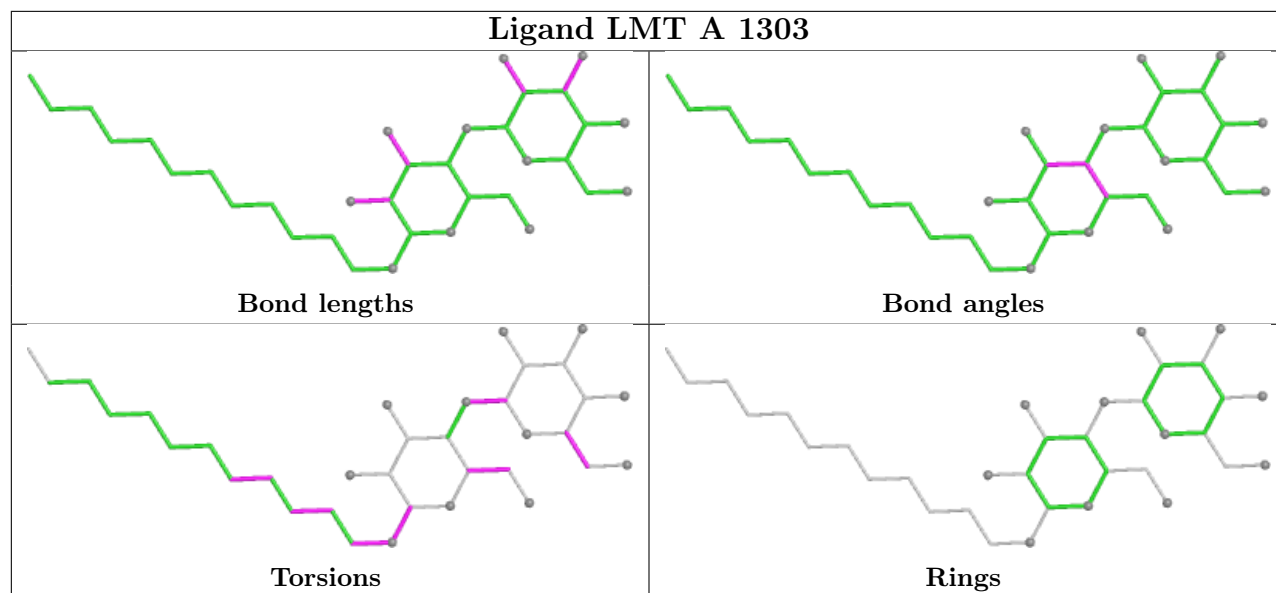
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	LMT	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.





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	218/269 (81%)	1.24	48 (22%) 2 3	102, 159, 222, 254	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1102	ARG	8.0
1	A	1068	ARG	6.2
1	A	1003	LEU	5.1
1	A	1222	ALA	4.7
1	A	1224	LEU	4.3
1	A	1100	VAL	4.2
1	A	1099	ARG	4.1
1	A	1108	ARG	4.1
1	A	1163	LEU	4.0
1	A	1162	THR	3.9
1	A	1158	GLU	3.8
1	A	1101	LEU	3.5
1	A	1150	GLN	3.3
1	A	1211	ASN	3.3
1	A	1063	ARG	3.1
1	A	1221	MET	3.1
1	A	1219	ASP	3.1
1	A	1223	ILE	2.9
1	A	1189	GLU	2.9
1	A	1161	GLY	2.9
1	A	1210	ILE	2.8
1	A	1070	SER	2.8
1	A	1012	SER	2.7
1	A	1062	LEU	2.7
1	A	1121	SER	2.7
1	A	1018	ILE	2.7
1	A	1064	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1056	PHE	2.6
1	A	1067	HIS	2.5
1	A	1178	SER	2.5
1	A	1007	ASN	2.4
1	A	1016	LYS	2.3
1	A	1190	VAL	2.3
1	A	1013	PHE	2.3
1	A	1196	VAL	2.3
1	A	1065	TYR	2.3
1	A	1059	GLU	2.3
1	A	1215	ALA	2.2
1	A	1015	THR	2.2
1	A	1025	ASN	2.2
1	A	1060	ILE	2.1
1	A	1097	ILE	2.1
1	A	1129	GLY	2.1
1	A	1218	VAL	2.1
1	A	1225	ASN	2.0
1	A	1138	THR	2.0
1	A	1069	ILE	2.0
1	A	1117	ARG	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.

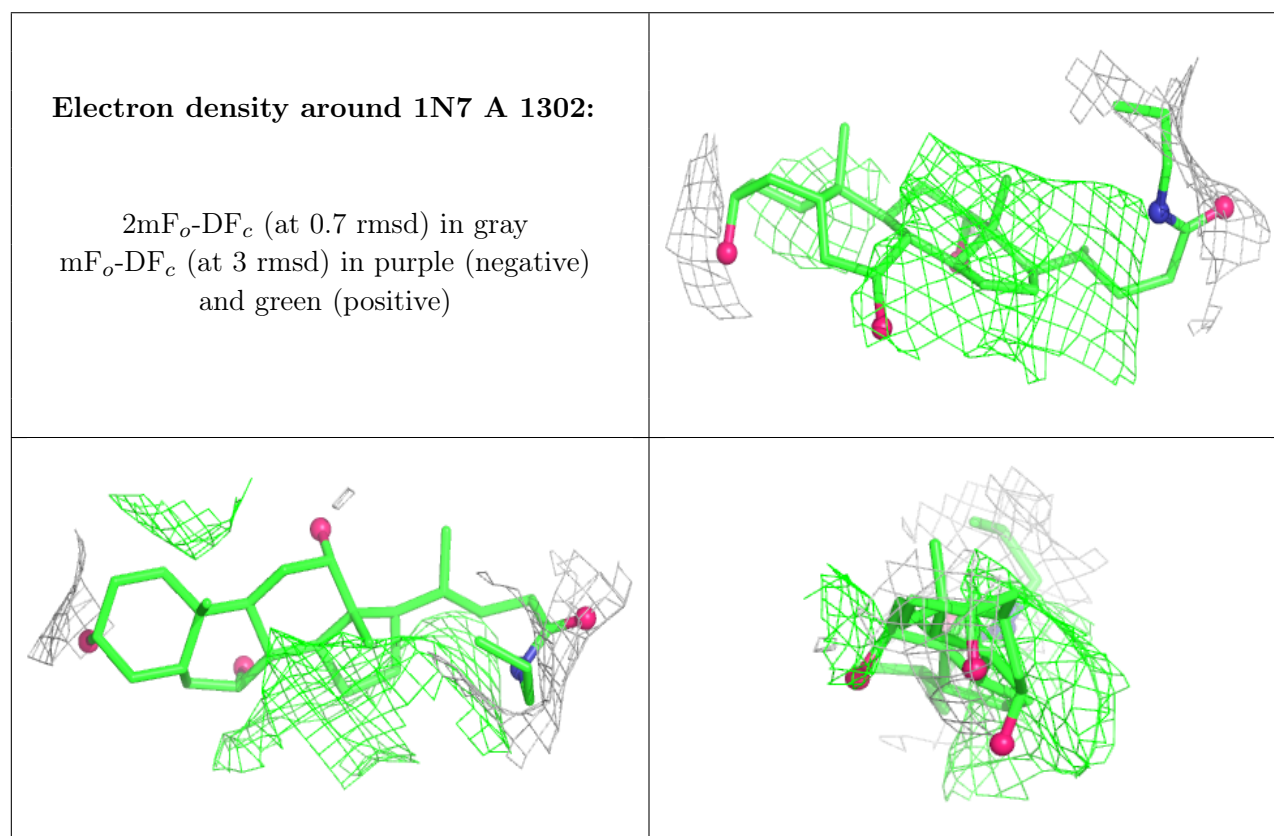
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1N7	A	1302	32/43	0.53	0.22	149,175,180,190	0
4	LMT	A	1303	35/35	0.80	0.19	153,175,199,203	0

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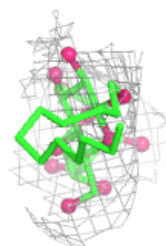
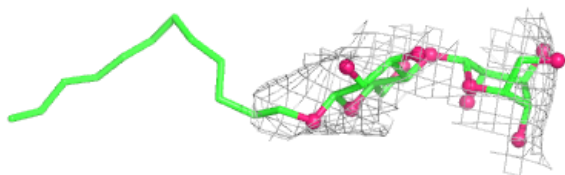
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	A	1301	1/1	0.88	0.79	85,85,85,85	1

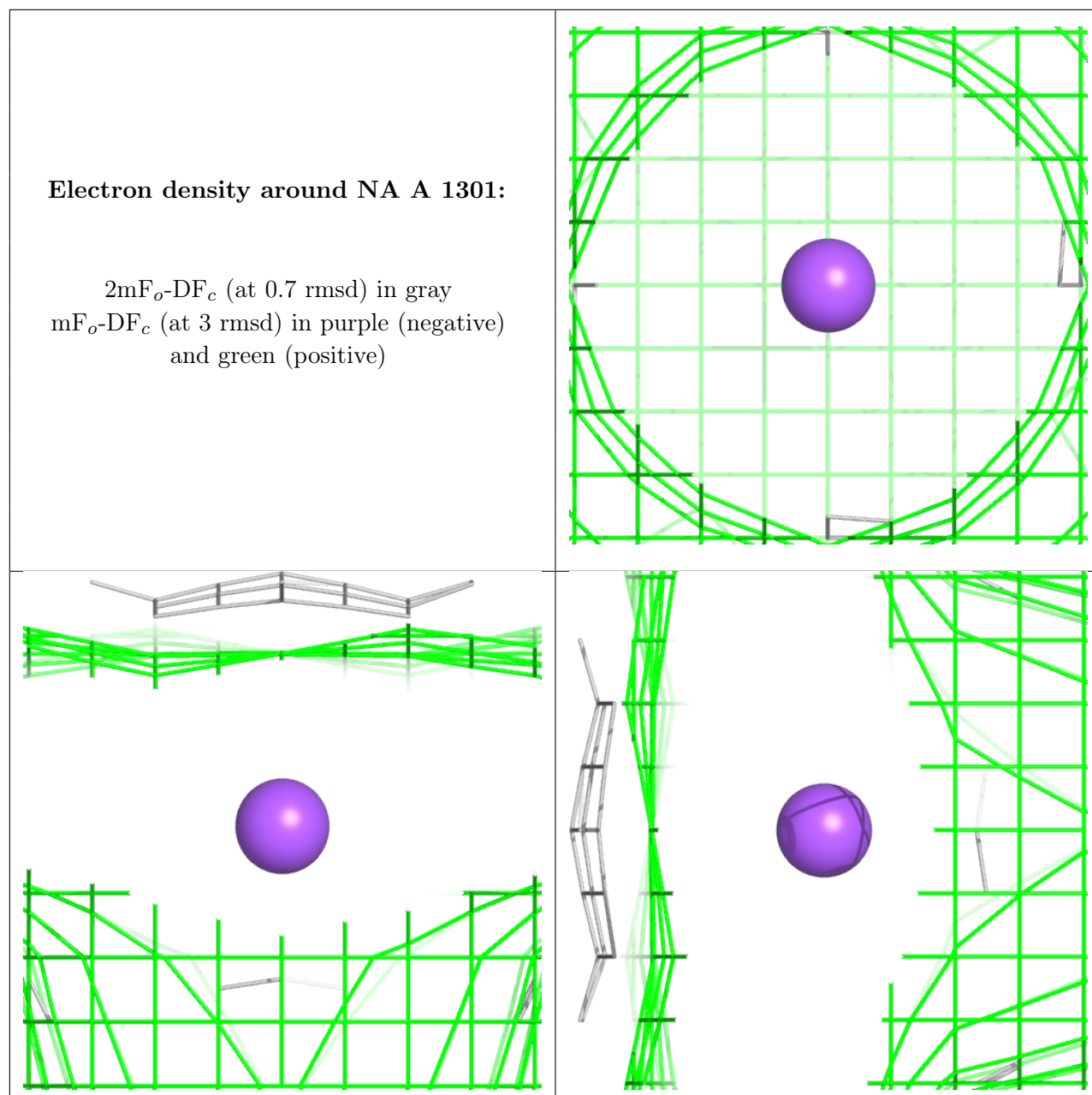
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around LMT A 1303:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.