



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2026 – 04:45 PM JST

PDB ID : 45AM / pdb_000045am
Title : Crystal structure of voltage-gated sodium channel NavAb N49K mutant
Authors : Irie, K.
Deposited on : 2026-08-21
Resolution : 4.20 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 Phenix2.2
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.2
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

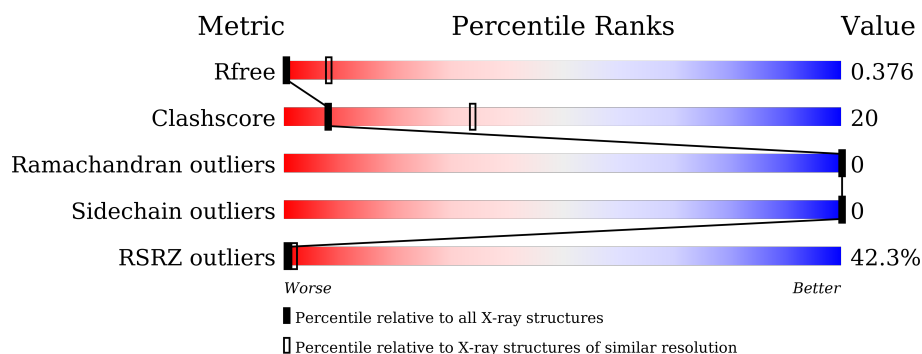
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	229	38% 55% 36% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1779 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.

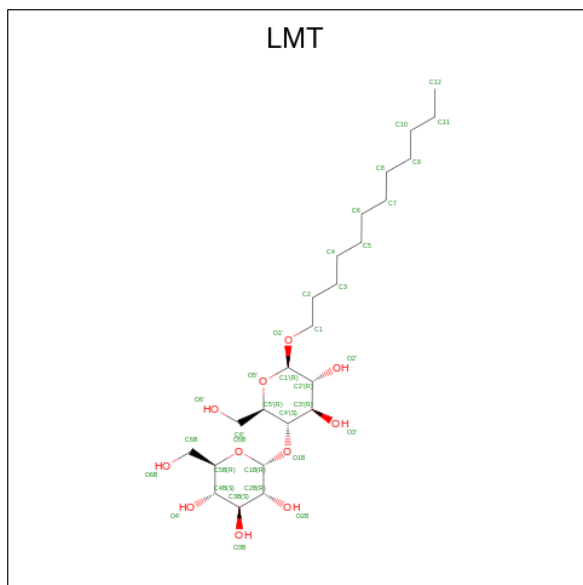
- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1711	1174	254	272	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

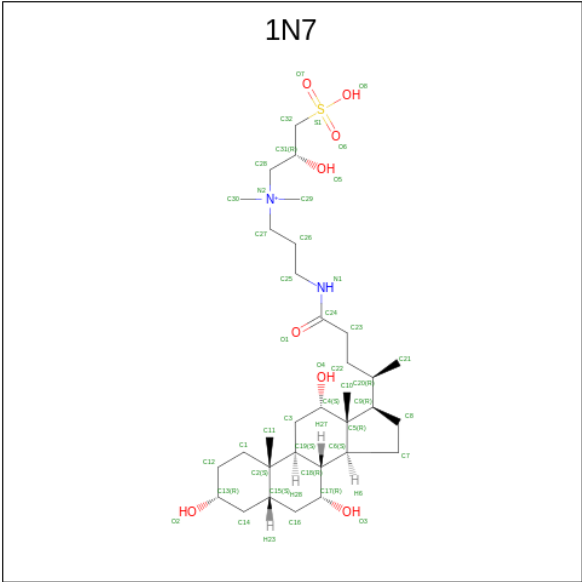
Chain	Residue	Modelled	Actual	Comment	Reference
A	1049	LYS	ASN	engineered mutation	UNP A8EVM5
A	1206	ALA	THR	engineered mutation	UNP A8EVM5

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 3 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



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

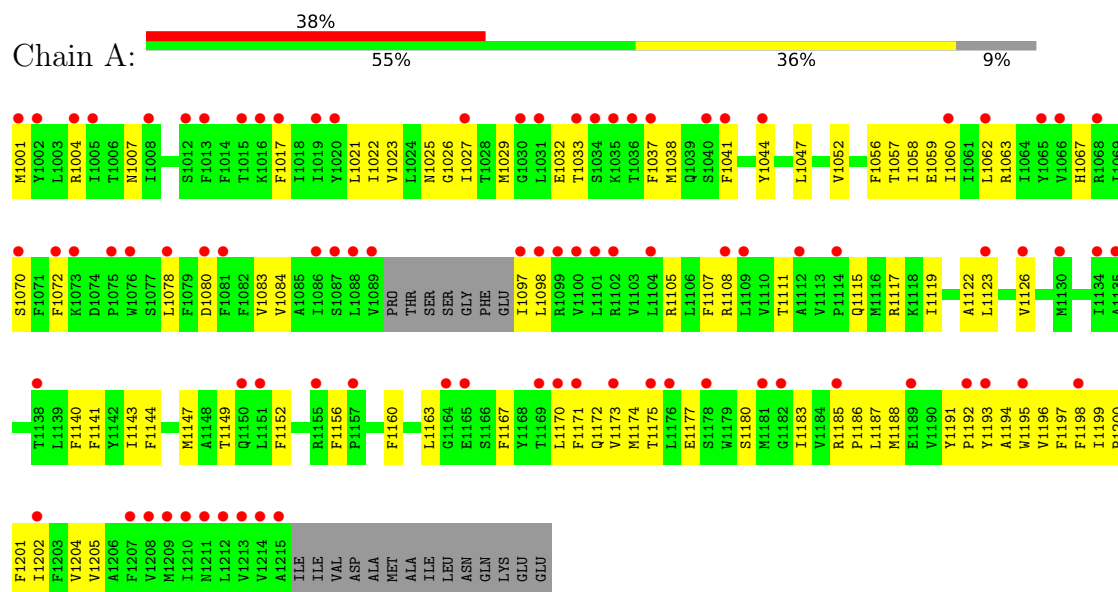
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	1	0
			1	1		

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: 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	128.28Å 128.28Å 202.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.35 – 4.20 45.35 – 4.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (45.35-4.20) 93.2 (45.35-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.353 , 0.372 0.357 , 0.376	Depositor DCC
R_{free} test set	310 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	174.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 40.3	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	0.81	EDS
Total number of atoms	1779	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: 1N7, LMT, CA

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	0.27	0/1759	0.55	1/2390 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1180	SER	N-CA-C	5.41	116.86	111.07

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	1711	0	1791	71	0
2	A	35	0	46	2	0
3	A	32	0	44	1	0
4	A	1	0	0	0	0
All	All	1779	0	1881	72	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 20.

All (72) 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:1060:ILE:HG13	1:A:1084:VAL:HG21	1.56	0.84
1:A:1198:PHE:O	1:A:1202:ILE:N	2.10	0.82
1:A:1025:ASN:HD21	1:A:1105:ARG:HE	1.28	0.82
1:A:1149:THR:HA	1:A:1160:PHE:HB3	1.66	0.77
1:A:1195:TRP:O	1:A:1199:ILE:HG12	1.90	0.72
1:A:1041:PHE:HB3	1:A:1044:TYR:HB3	1.73	0.71
1:A:1149:THR:HG23	1:A:1160:PHE:O	1.90	0.70
1:A:1147:MET:HE3	1:A:1197:PHE:HE1	1.58	0.66
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.22	0.65
1:A:1097:ILE:HG23	1:A:1098:LEU:HD12	1.79	0.65
1:A:1025:ASN:ND2	1:A:1105:ARG:HE	1.96	0.64
1:A:1172:GLN:HG3	1:A:1177:GLU:HB3	1.80	0.64
1:A:1188:MET:HA	1:A:1191:TYR:O	1.99	0.63
1:A:1152:PHE:HB3	1:A:1156:PHE:HD2	1.62	0.62
1:A:1187:LEU:O	1:A:1191:TYR:N	2.33	0.61
1:A:1097:ILE:HG23	1:A:1098:LEU:H	1.64	0.61
1:A:1200:PRO:HB2	2:A:1301:LMT:H123	1.83	0.60
1:A:1072:PHE:CD1	1:A:1078:LEU:HD21	2.37	0.59
1:A:1111:THR:O	1:A:1117:ARG:NH1	2.37	0.57
1:A:1058:ILE:O	1:A:1062:LEU:HG	2.05	0.57
1:A:1194:ALA:HA	2:A:1301:LMT:H42	1.86	0.57
1:A:1141:PHE:HZ	1:A:1174:MET:SD	2.30	0.55
1:A:1025:ASN:HD21	1:A:1105:ARG:NE	1.99	0.55
1:A:1140:PHE:CZ	1:A:1204:VAL:HG11	2.43	0.54
1:A:1060:ILE:HD13	1:A:1063:ARG:HD3	1.90	0.53
1:A:1033:THR:HG22	1:A:1033:THR:O	2.09	0.53
1:A:1183:ILE:O	1:A:1187:LEU:HD23	2.09	0.51
1:A:1152:PHE:HB3	1:A:1156:PHE:CD2	2.44	0.51
1:A:1022:ILE:O	1:A:1025:ASN:HB3	2.11	0.51
1:A:1004:ARG:NH2	1:A:1007:ASN:OD1	2.44	0.51
1:A:1032:GLU:HA	1:A:1038:MET:SD	2.51	0.50
1:A:1195:TRP:CD1	1:A:1195:TRP:H	2.30	0.50
1:A:1119:ILE:O	1:A:1123:LEU:HG	2.12	0.49
1:A:1152:PHE:HB2	1:A:1160:PHE:CD2	2.48	0.49
1:A:1021:LEU:HG	1:A:1052:VAL:HG23	1.95	0.48
1:A:1067:HIS:CD2	1:A:1070:SER:HB3	2.49	0.47
1:A:1025:ASN:HD22	1:A:1056:PHE:HE2	1.63	0.47
1:A:1143:ILE:O	1:A:1147:MET:HG3	2.14	0.47
1:A:1017:PHE:HE2	1:A:1059:GLU:OE2	1.99	0.46
1:A:1171:PHE:O	1:A:1175:THR:HG23	2.16	0.46
1:A:1193:TYR:O	1:A:1196:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:HIS:HB2	1:A:1070:SER:HB3	1.99	0.45
1:A:1029:MET:SD	1:A:1105:ARG:NH2	2.89	0.45
1:A:1037:PHE:CE2	1:A:1041:PHE:HB2	2.52	0.45
1:A:1080:ASP:HA	1:A:1083:VAL:HG22	1.97	0.45
1:A:1122:ALA:O	1:A:1126:VAL:HG23	2.17	0.45
1:A:1152:PHE:O	1:A:1156:PHE:N	2.40	0.45
1:A:1107:PHE:O	1:A:1111:THR:HG23	2.17	0.44
1:A:1183:ILE:O	1:A:1186:PRO:HD2	2.17	0.44
1:A:1199:ILE:HB	1:A:1200:PRO:HD3	1.99	0.44
1:A:1141:PHE:HB3	1:A:1167:PHE:CE1	2.51	0.44
1:A:1056:PHE:O	1:A:1060:ILE:HG12	2.18	0.44
1:A:1200:PRO:O	1:A:1204:VAL:HG23	2.17	0.44
1:A:1188:MET:HA	1:A:1192:PRO:HA	2.00	0.44
1:A:1201:PHE:O	1:A:1205:VAL:HG22	2.18	0.43
1:A:1001:MET:SD	1:A:1001:MET:N	2.92	0.43
1:A:1023:VAL:O	1:A:1027:ILE:HG12	2.19	0.43
1:A:1044:TYR:O	1:A:1047:LEU:HG	2.18	0.42
1:A:1078:LEU:HD23	1:A:1078:LEU:HA	1.74	0.42
1:A:1059:GLU:O	1:A:1063:ARG:HG3	2.19	0.42
1:A:1022:ILE:HD12	1:A:1108:ARG:HB3	2.02	0.42
1:A:1149:THR:OG1	1:A:1163:LEU:HD12	2.19	0.42
1:A:1057:THR:HG22	1:A:1084:VAL:HG13	2.02	0.41
1:A:1029:MET:SD	1:A:1105:ARG:NH1	2.93	0.41
1:A:1144:PHE:HA	1:A:1147:MET:HE2	2.02	0.41
1:A:1185:ARG:HA	1:A:1185:ARG:HD3	1.91	0.41
1:A:1170:LEU:HA	1:A:1173:VAL:HG22	2.03	0.41
1:A:1144:PHE:CE2	1:A:1201:PHE:HB2	2.56	0.41
1:A:1115:GLN:O	1:A:1119:ILE:HG12	2.21	0.41
3:A:1302:1N7:H34	3:A:1302:1N7:H10	1.72	0.41
1:A:1185:ARG:HB2	1:A:1186:PRO:HD3	2.03	0.40
1:A:1026:GLY:HA2	1:A:1029:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

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	204/229 (89%)	202 (99%)	2 (1%)	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	190/209 (91%)	190 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1172	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

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	0.38	0	54,54,72	0.82	1 (1%)
2	LMT	A	1301	-	36,36,36	1.08	4 (11%)	47,47,47	1.05	3 (6%)

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	-	-	4/13/78/92	0/4/4/4
2	LMT	A	1301	-	-	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)
2	A	1301	LMT	O3'-C3'	-2.42	1.37	1.43
2	A	1301	LMT	O2'-C2'	-2.26	1.37	1.43
2	A	1301	LMT	O2B-C2B	-2.25	1.37	1.43
2	A	1301	LMT	O3B-C3B	-2.20	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	1N7	C15-C16-C17	-3.96	110.09	114.46
2	A	1301	LMT	C1'-O5'-C5'	-2.87	108.05	113.69
2	A	1301	LMT	C3'-C4'-C5'	-2.37	105.49	110.93
2	A	1301	LMT	O5B-C5B-C6B	2.14	111.75	106.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

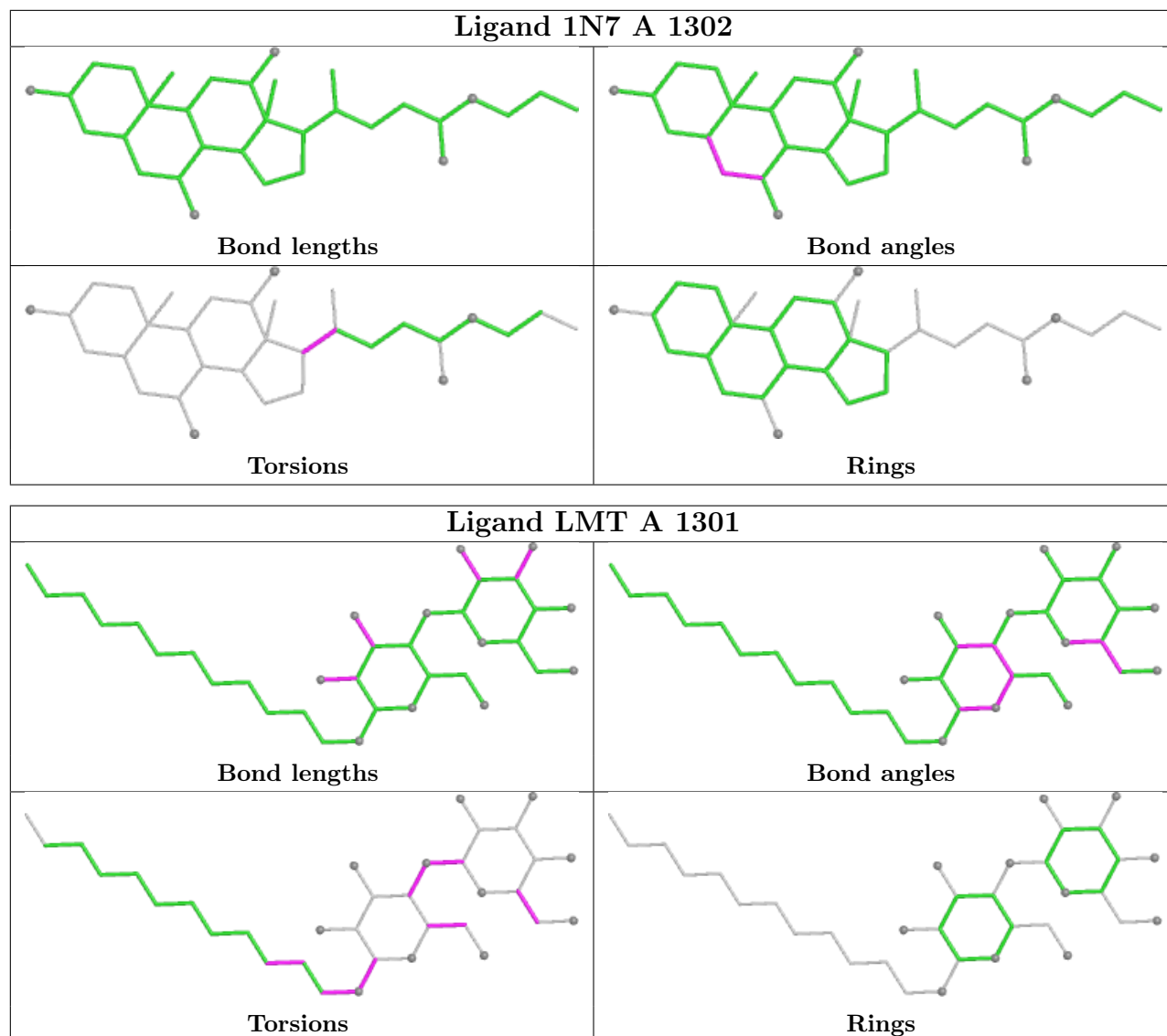
Mol	Chain	Res	Type	Atoms
2	A	1301	LMT	O5B-C1B-O1B-C4'
2	A	1301	LMT	C4B-C5B-C6B-O6B
2	A	1301	LMT	O5B-C5B-C6B-O6B
2	A	1301	LMT	C2'-C1'-O1'-C1
2	A	1301	LMT	O5'-C1'-O1'-C1
2	A	1301	LMT	C2-C1-O1'-C1'
2	A	1301	LMT	C1-C2-C3-C4
2	A	1301	LMT	O5'-C5'-C6'-O6'
3	A	1302	1N7	C22-C20-C9-C5
3	A	1302	1N7	C22-C20-C9-C8
3	A	1302	1N7	C21-C20-C9-C5
3	A	1302	1N7	C21-C20-C9-C8
2	A	1301	LMT	C5'-C4'-O1B-C1B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	1N7	1	0
2	A	1301	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	208/229 (90%)	2.43	88 (42%) 0 2	112, 204, 259, 298	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1099	ARG	25.9
1	A	1211	ASN	14.0
1	A	1098	LEU	13.8
1	A	1089	VAL	13.3
1	A	1214	VAL	13.1
1	A	1097	ILE	12.9
1	A	1065	TYR	11.4
1	A	1100	VAL	11.3
1	A	1213	VAL	9.4
1	A	1101	LEU	7.8
1	A	1016	LYS	7.4
1	A	1102	ARG	7.4
1	A	1215	ALA	7.4
1	A	1210	ILE	7.2
1	A	1068	ARG	5.7
1	A	1086	ILE	5.5
1	A	1012	SER	5.4
1	A	1212	LEU	5.3
1	A	1020	TYR	5.1
1	A	1164	GLY	4.9
1	A	1181	MET	4.9
1	A	1005	ILE	4.8
1	A	1013	PHE	4.6
1	A	1015	THR	4.5
1	A	1017	PHE	4.5
1	A	1135	ALA	4.3
1	A	1019	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1034	SER	4.3
1	A	1173	VAL	4.1
1	A	1207	PHE	4.1
1	A	1126	VAL	4.1
1	A	1073	LYS	4.0
1	A	1176	LEU	3.8
1	A	1155	ARG	3.7
1	A	1189	GLU	3.7
1	A	1008	ILE	3.6
1	A	1075	PRO	3.6
1	A	1088	LEU	3.6
1	A	1178	SER	3.5
1	A	1185	ARG	3.5
1	A	1041	PHE	3.5
1	A	1195	TRP	3.5
1	A	1208	VAL	3.5
1	A	1209	MET	3.5
1	A	1072	PHE	3.3
1	A	1036	THR	3.3
1	A	1044	TYR	3.3
1	A	1112	ALA	3.2
1	A	1066	VAL	3.2
1	A	1062	LEU	3.1
1	A	1033	THR	3.1
1	A	1182	GLY	3.1
1	A	1150	GLN	3.0
1	A	1134	ILE	3.0
1	A	1198	PHE	3.0
1	A	1027	ILE	2.9
1	A	1138	THR	2.9
1	A	1081	PHE	2.8
1	A	1202	ILE	2.8
1	A	1080	ASP	2.8
1	A	1114	PRO	2.8
1	A	1001	MET	2.7
1	A	1004	ARG	2.7
1	A	1076	TRP	2.7
1	A	1030	GLY	2.7
1	A	1130	MET	2.7
1	A	1087	SER	2.7
1	A	1002	TYR	2.7
1	A	1031	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1169	THR	2.7
1	A	1175	THR	2.6
1	A	1040	SER	2.6
1	A	1109	LEU	2.6
1	A	1171	PHE	2.6
1	A	1035	LYS	2.5
1	A	1123	LEU	2.5
1	A	1108	ARG	2.5
1	A	1157	PRO	2.4
1	A	1193	TYR	2.4
1	A	1170	LEU	2.4
1	A	1070	SER	2.3
1	A	1151	LEU	2.3
1	A	1192	PRO	2.2
1	A	1037	PHE	2.2
1	A	1078	LEU	2.2
1	A	1060	ILE	2.1
1	A	1165	GLU	2.1
1	A	1104	LEU	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](#)

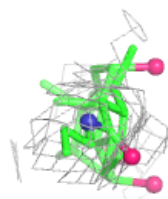
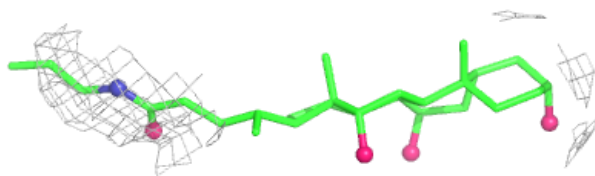
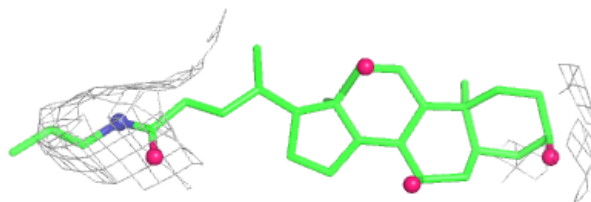
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1N7	A	1302	32/43	0.50	0.22	198,251,265,271	0
2	LMT	A	1301	35/35	0.64	0.29	160,212,229,232	0
4	CA	A	1303	1/1	-	-	136,136,136,136	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.

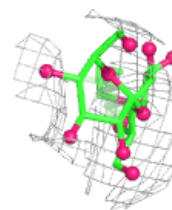
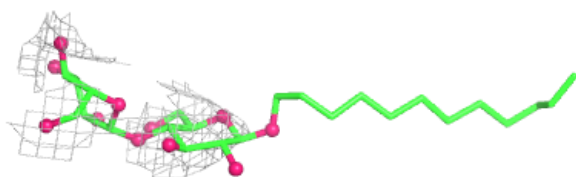
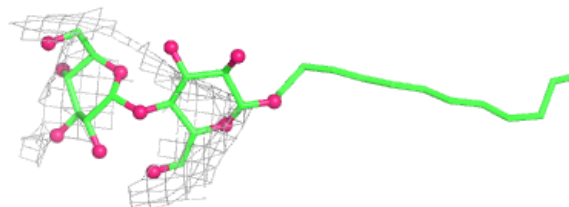
Electron density around 1N7 A 1302:

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



Electron density around LMT A 1301:

$2mF_o-DF_c$ (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.