wwPDB EM Validation Summary Report

Apr 6, 2025 – 01:47 AM JST

PDB ID	:	9IYP / pdb_00009iyp
EMDB ID	:	EMD-61000
Title	:	Structure of the human GluN1-N2B NMDA receptors in the Mg2+ bound state
Authors	:	Huang, X.; Sun, X.; Zhu, S.
Deposited on	:	2024-07-31
Resolution	:	3.27 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
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:

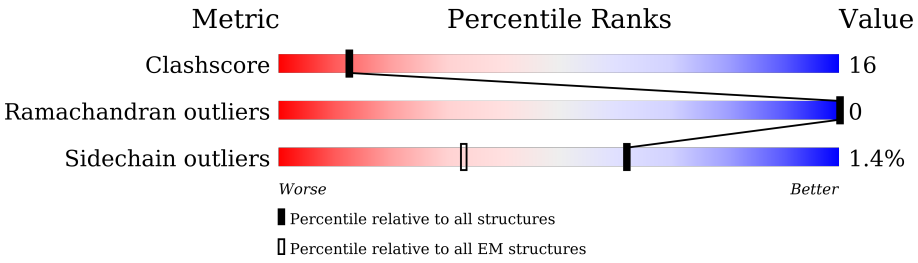
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	814	67% 29%
1	C	814	68% 29%
2	B	808	64% 31%
2	D	808	72% 23% 5%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	7RC	B	901	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23471 atoms, of which 28 are hydrogens and 0 are deuteriums.

In the tables below, 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.

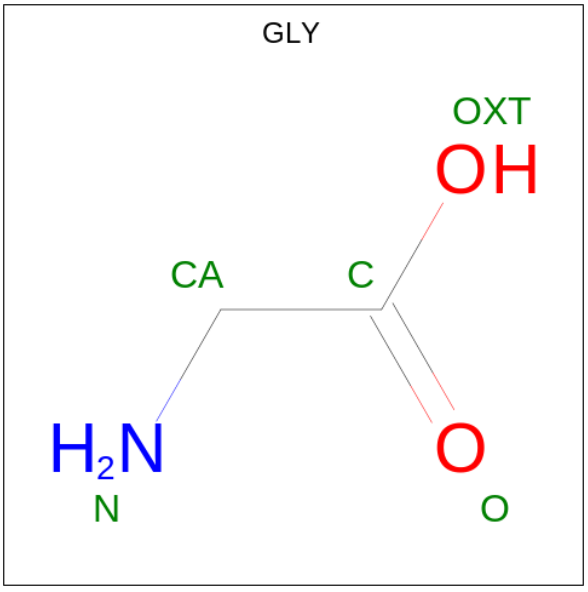
- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	788	Total	C	N	O	S	0	0
			5951	3796	1037	1084	34		
1	C	796	Total	C	N	O	S	0	0
			5954	3805	1035	1083	31		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	772	Total	C	N	O	S	0	0
			5743	3698	935	1072	38		
2	D	770	Total	C	N	O	S	0	0
			5704	3699	932	1038	35		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	

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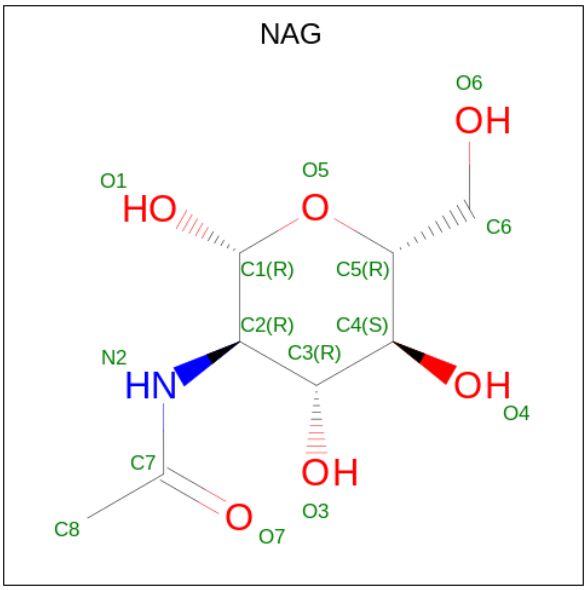
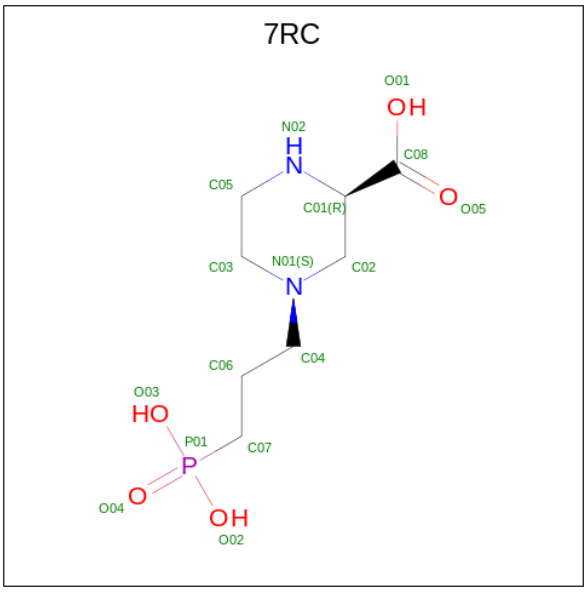
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is (2R)-4-(3-phosphonopropyl)piperazine-2-carboxylic acid (CCD ID: 7RC) (formula: $C_8H_{17}N_2O_5P$).



Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	H	N	O	P	0
			30	8	14	2	5	1	
5	D	1	Total	C	H	N	O	P	0
			30	8	14	2	5	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

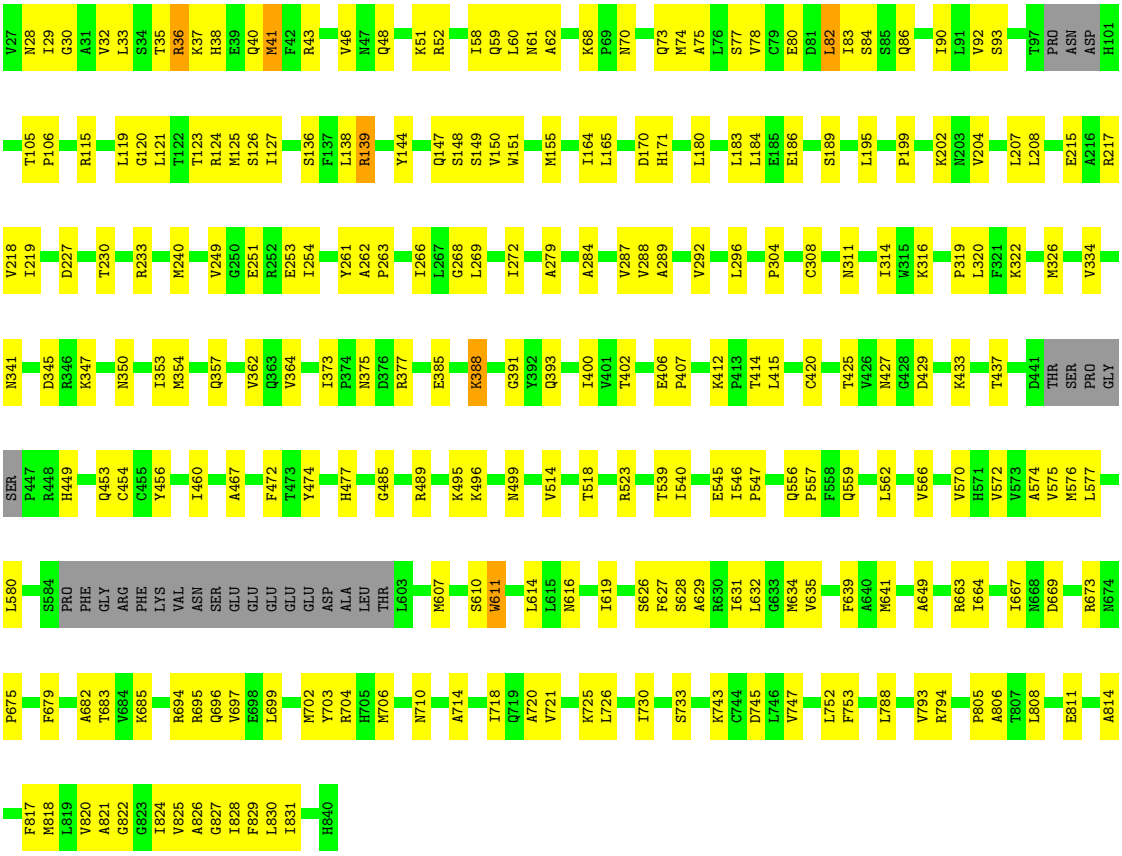
Mol	Chain	Residues	Atoms		AltConf
6	B	4	Total	Mg	0
			4	4	
6	C	1	Total	Mg	0
			1	1	
6	D	2	Total	Mg	0
			2	2	

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. 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. 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.

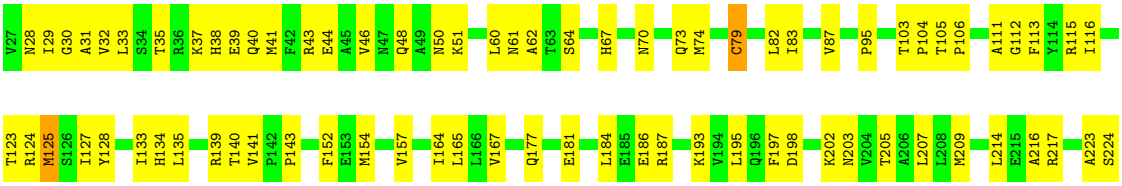
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

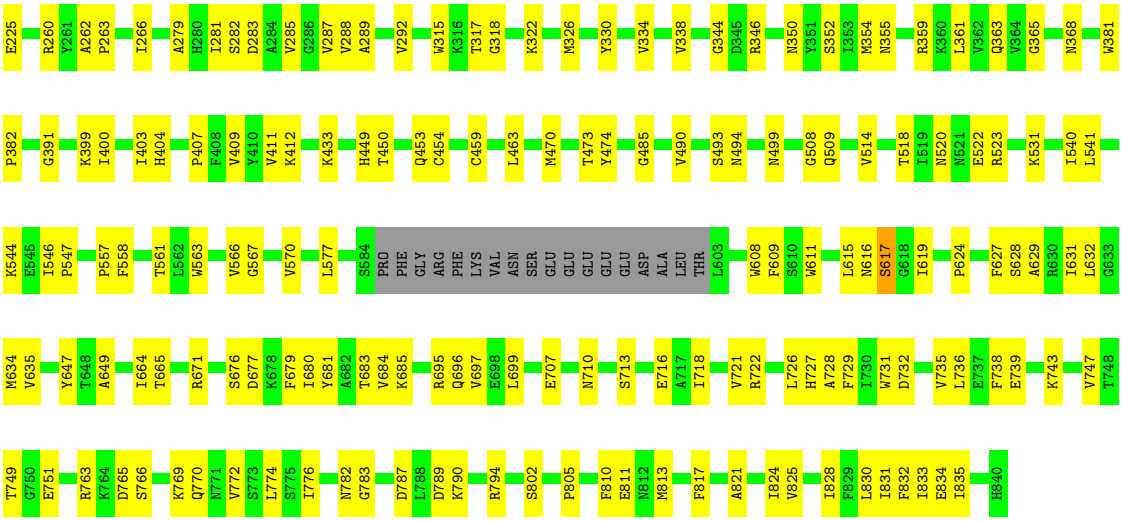
Chain A:



• Molecule 1: Glutamate receptor ionotropic, NMDA 1

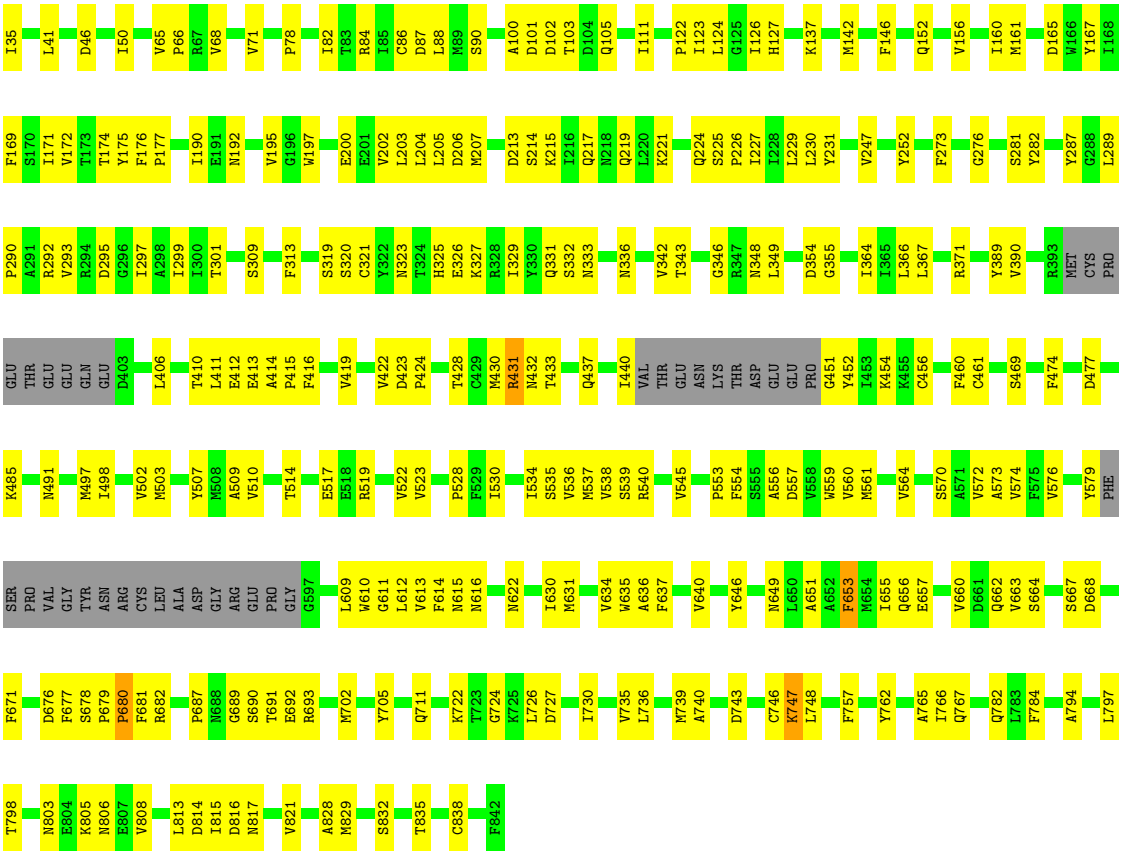
Chain C:





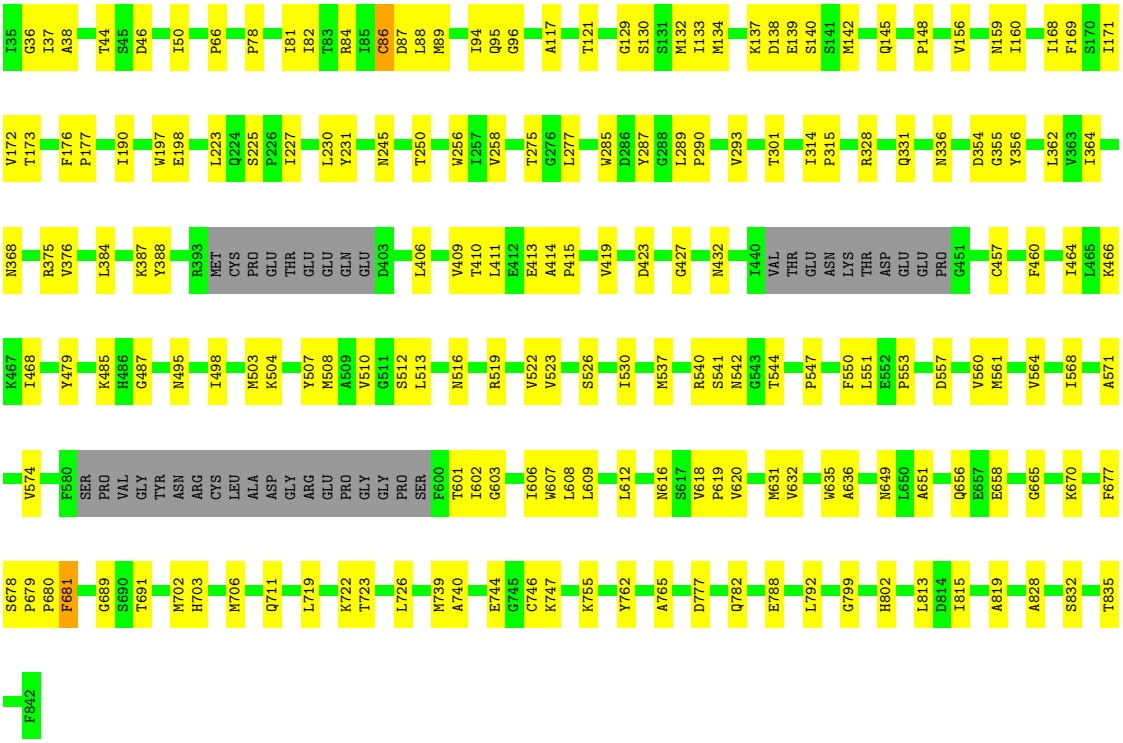
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B:



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:


I35 G36 I37 A38 T44 S45 D46 I50 P66 P78 I81 I82 T83 R84 I85 C86 D87 L88 M89 I94 Q95 G96 A117 T121 G129 S130 S131 M132 I133 M134 K137 D138 E139 S140 S141 M142 Q145 P148 V156 N159 I160 I168 F169 S170 I171
V172 T173 F176 P177 I190 W197 E198 L223 Q224 S225 P226 I227 L230 Y231 N245 T250 W256 I257 V258 T275 G276 L277 W285 D286 Y287 G288 L289 P290 V293 T301 I314 P315 R328 Q331 N336 D354 G355 Y356 L362 V363 I364
N368 R375 V376 L384 K387 Y388 R393 MET CYS PRO GLU THR GLU GLU GLN GLU D403 L406 V409 T410 L411 E412 E413 A414 P415 V419 D423 G427 N432 I440 VAL THR GLU ASN LYS THR ASP GLU GLU PRO G451 C457 F460 I464 L465 K466
K467 I468 Y479 K485 H486 G487 N495 I498 M503 K504 Y507 M508 A509 V510 G511 S512 L513 N516 R519 V522 V523 S526 I530 M537 R540 S541 N542 G543 T544 P547 F550 L551 E552 P553 D557 V560 M561 V564 I568 A571
V574 F580 SER PRO VAL GLY TYR ASN ARG CYS LEU ALA ASP GLY ARG GLU PRO GLY GLY PRO SER F600 T601 I602 G603 I606 W607 L608 L609 L612 N616 S617 V618 P619 V620 M631 V632 W635 A636 N649 L650 A651 Q656 E657 E658 G665 K670 F677
S678 P679 P680 F681 G689 S690 T691 M702 H703 M706 Q711 L719 K722 T723 L726 M739 A740 E744 G745 C746 K747 K755 Y762 A765 D777 Q782 E788 L792 G799 H802 L813 D814 I815 A819 A828 S832 T835
F842

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.00	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, 7RC

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	0.24	0/6074	0.45	0/8252
1	C	0.24	0/6085	0.45	0/8281
2	B	0.24	0/5861	0.42	0/7973
2	D	0.24	0/5831	0.41	0/7944
All	All	0.24	0/23851	0.43	0/32450

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	5951	0	5774	217	0
1	C	5954	0	5693	213	0
2	B	5743	0	5467	214	0
2	D	5704	0	5403	158	0
3	A	5	0	2	3	0
3	C	5	0	2	1	0
4	A	14	0	13	0	0
4	C	28	0	26	1	0
5	B	16	14	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	16	14	0	2	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
All	All	23443	28	22380	755	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 16.

The worst 5 of 755 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:C:518:THR:HG23	3:C:903:GLY:HA3	1.29	1.14
1:C:283:ASP:O	1:C:287:VAL:HG23	1.76	0.85
1:A:518:THR:HG23	3:A:901:GLY:HA3	1.59	0.85
1:C:202:LYS:HE3	1:C:202:LYS:HA	1.59	0.84
1:C:696:GLN:HG3	1:C:699:LEU:HD12	1.59	0.84

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 PDB entries followed by that with respect to all EM entries.

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	780/814 (96%)	745 (96%)	35 (4%)	0	100	100
1	C	792/814 (97%)	754 (95%)	38 (5%)	0	100	100
2	B	764/808 (95%)	709 (93%)	55 (7%)	0	100	100
2	D	762/808 (94%)	732 (96%)	30 (4%)	0	100	100
All	All	3098/3244 (96%)	2940 (95%)	158 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	607/702 (86%)	598 (98%)	9 (2%)	60 77
1	C	592/702 (84%)	584 (99%)	8 (1%)	62 78
2	B	581/704 (82%)	569 (98%)	12 (2%)	48 70
2	D	566/704 (80%)	562 (99%)	4 (1%)	81 88
All	All	2346/2812 (83%)	2313 (99%)	33 (1%)	62 78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	811	GLU
2	D	86	CYS
2	D	739	MET
2	B	430	MET
2	B	313	PHE

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

Mol	Chain	Res	Type
1	A	375	ASN
1	A	559	GLN
2	B	217	GLN
1	C	38	HIS
2	D	432	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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	NAG	C	901	1	14,14,15	0.19	0	17,19,21	0.33	0
4	NAG	C	902	1	14,14,15	0.24	0	17,19,21	0.44	0
3	GLY	C	903	-	4,4,4	1.15	1 (25%)	3,4,4	1.66	1 (33%)
4	NAG	A	902	1	14,14,15	0.18	0	17,19,21	0.42	0
5	7RC	B	901	-	15,16,16	2.13	1 (6%)	17,22,22	1.50	2 (11%)
3	GLY	A	901	-	4,4,4	1.15	1 (25%)	3,4,4	1.65	1 (33%)
5	7RC	D	901	-	15,16,16	2.12	1 (6%)	17,22,22	1.50	1 (5%)

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
4	NAG	C	901	1	-	1/6/23/26	0/1/1/1
4	NAG	C	902	1	-	2/6/23/26	0/1/1/1
3	GLY	C	903	-	-	0/2/2/2	-
4	NAG	A	902	1	-	3/6/23/26	0/1/1/1
5	7RC	B	901	-	-	4/11/21/21	1/1/1/1
3	GLY	A	901	-	-	0/2/2/2	-
5	7RC	D	901	-	-	4/11/21/21	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	7RC	P01-C07	7.51	1.86	1.78
5	D	901	7RC	P01-C07	7.45	1.86	1.78
3	A	901	GLY	OXT-C	-2.17	1.23	1.30
3	C	903	GLY	OXT-C	-2.15	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	901	7RC	P01-C07-C06	-4.40	109.47	114.98
5	B	901	7RC	P01-C07-C06	-4.39	109.49	114.98
3	C	903	GLY	OXT-C-O	-2.12	118.01	123.30
3	A	901	GLY	OXT-C-O	-2.11	118.03	123.30
5	B	901	7RC	O01-C08-C01	2.00	120.06	113.40

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	7RC	N02-C01-C08-O01
5	B	901	7RC	N02-C01-C08-O05
5	D	901	7RC	N02-C01-C08-O05
4	C	902	NAG	O5-C5-C6-O6
4	A	902	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	7RC	C01-C02-C03-C05-N01-N02
5	D	901	7RC	C01-C02-C03-C05-N01-N02

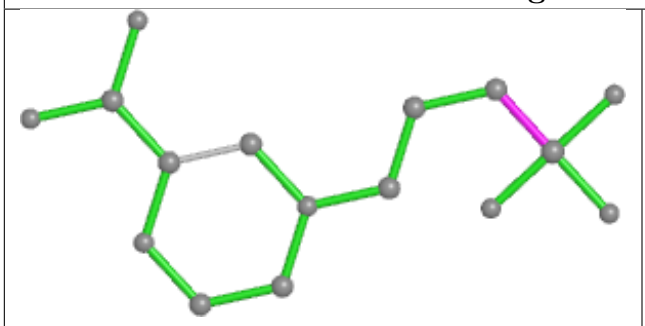
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	901	NAG	1	0
3	C	903	GLY	1	0
5	B	901	7RC	7	0
3	A	901	GLY	3	0
5	D	901	7RC	2	0

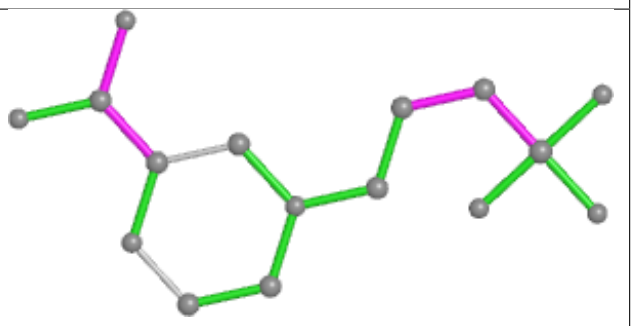
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

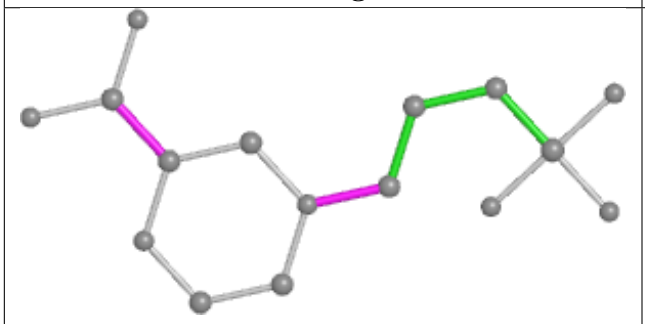
Ligand 7RC B 901



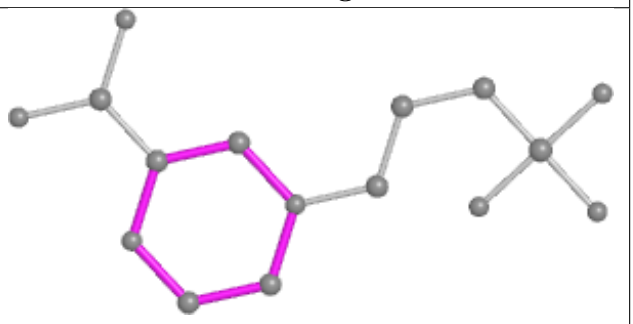
Bond lengths



Bond angles

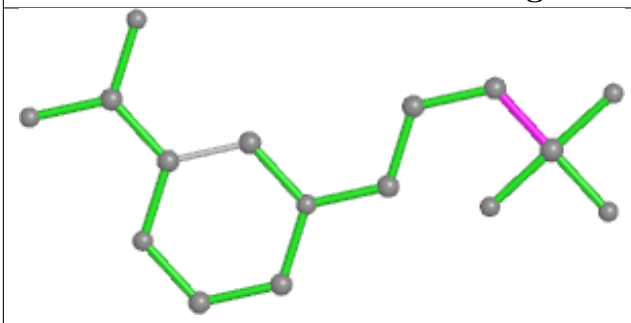


Torsions

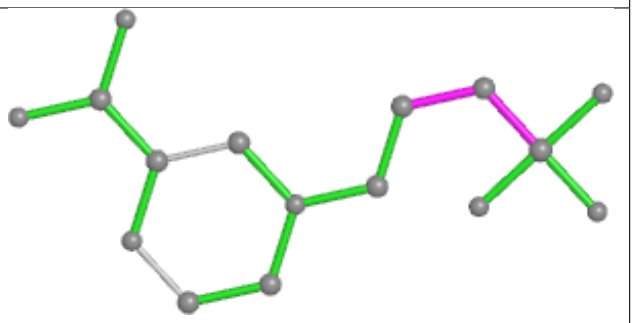


Rings

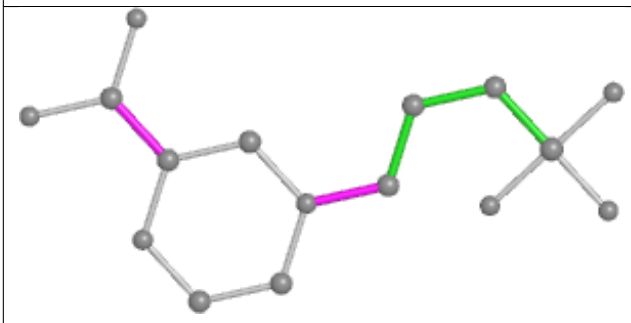
Ligand 7RC D 901



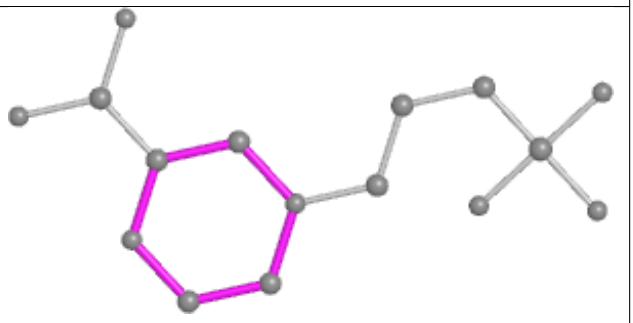
Bond lengths



Bond angles



Torsions



Rings

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.