



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2025 – 01:13 PM EDT

PDB ID : 9D3C / pdb\_00009d3c  
EMDB ID : EMD-46531  
Title : Gly-,Glu-,(S)-(+)-ketamine bound GluN1a-2B-2D NMDAR  
Authors : Hyunook, K.; Hiro, F.  
Deposited on : 2024-08-09  
Resolution : 3.96 Å(reported)  
Based on initial models : 8e96, 7saa

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
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

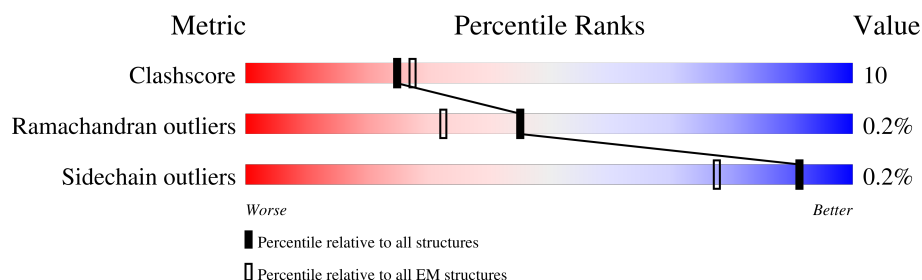
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.96 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	825	71% 23% 6%
1	C	825	72% 25% .
2	B	884	71% 17% 12%
3	D	861	65% 22% 12%
4	E	2	50% 50%

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	GLY	A	901	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24194 atoms, of which 0 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	779	Total	C	N	O	S	0	0
			6033	3841	1046	1114	32		
1	C	803	Total	C	N	O	S	0	0
			6254	3989	1070	1160	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	844	ASN	ARG	engineered mutation	UNP Q05586
A	845	GLY	ARG	engineered mutation	UNP Q05586
A	846	ALA	LYS	engineered mutation	UNP Q05586
C	844	ASN	ARG	engineered mutation	UNP Q05586
C	845	GLY	ARG	engineered mutation	UNP Q05586
C	846	ALA	LYS	engineered mutation	UNP Q05586

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	778	Total	C	N	O	S	0	0
			5969	3837	962	1131	39		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	TRP	-	expression tag	UNP Q13224
B	-7	SER	-	expression tag	UNP Q13224
B	-6	HIS	-	expression tag	UNP Q13224
B	-5	PRO	-	expression tag	UNP Q13224
B	-4	GLN	-	expression tag	UNP Q13224
B	-3	PHE	-	expression tag	UNP Q13224
B	-2	GLU	-	expression tag	UNP Q13224
B	-1	LYS	-	expression tag	UNP Q13224
B	0	GLY	-	expression tag	UNP Q13224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP Q13224
B	2	GLY	-	expression tag	UNP Q13224
B	3	SER	-	expression tag	UNP Q13224
B	4	GLY	-	expression tag	UNP Q13224
B	5	GLY	-	expression tag	UNP Q13224
B	6	GLY	-	expression tag	UNP Q13224
B	7	SER	-	expression tag	UNP Q13224
B	8	GLY	-	expression tag	UNP Q13224
B	9	GLY	-	expression tag	UNP Q13224
B	10	SER	-	expression tag	UNP Q13224
B	11	ALA	-	expression tag	UNP Q13224
B	12	TRP	-	expression tag	UNP Q13224
B	13	SER	-	expression tag	UNP Q13224
B	14	HIS	-	expression tag	UNP Q13224
B	15	PRO	-	expression tag	UNP Q13224
B	16	GLN	-	expression tag	UNP Q13224
B	17	PHE	-	expression tag	UNP Q13224
B	18	GLU	-	expression tag	UNP Q13224
B	19	LYS	-	expression tag	UNP Q13224
B	20	GLY	-	expression tag	UNP Q13224
B	21	ALA	-	expression tag	UNP Q13224
B	22	LEU	-	expression tag	UNP Q13224
B	23	VAL	-	expression tag	UNP Q13224
B	24	PRO	-	expression tag	UNP Q13224
B	25	ARG	-	expression tag	UNP Q13224
B	26	GLY	-	expression tag	UNP Q13224
B	588	SER	CYS	engineered mutation	UNP Q13224
B	838	SER	CYS	engineered mutation	UNP Q13224
B	849	SER	CYS	engineered mutation	UNP Q13224
B	853	GLY	-	expression tag	UNP Q13224
B	854	PRO	-	expression tag	UNP Q13224
B	855	GLY	-	expression tag	UNP Q13224
B	856	SER	-	expression tag	UNP Q13224
B	857	GLY	-	expression tag	UNP Q13224
B	858	ALA	-	expression tag	UNP Q13224
B	859	THR	-	expression tag	UNP Q13224
B	860	ASN	-	expression tag	UNP Q13224
B	861	PHE	-	expression tag	UNP Q13224
B	862	SER	-	expression tag	UNP Q13224
B	863	LEU	-	expression tag	UNP Q13224
B	864	LEU	-	expression tag	UNP Q13224
B	865	LYS	-	expression tag	UNP Q13224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	866	GLN	-	expression tag	UNP Q13224
B	867	ALA	-	expression tag	UNP Q13224
B	868	GLY	-	expression tag	UNP Q13224
B	869	ASP	-	expression tag	UNP Q13224
B	870	VAL	-	expression tag	UNP Q13224
B	871	GLU	-	expression tag	UNP Q13224
B	872	GLU	-	expression tag	UNP Q13224
B	873	ASN	-	expression tag	UNP Q13224
B	874	PRO	-	expression tag	UNP Q13224
B	875	GLY	-	expression tag	UNP Q13224

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	755	Total	C	N	O	S	0	0
			5752	3690	980	1054	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	881	GLU	-	expression tag	UNP O15399
D	882	THR	-	expression tag	UNP O15399
D	883	SER	-	expression tag	UNP O15399
D	884	GLN	-	expression tag	UNP O15399
D	885	VAL	-	expression tag	UNP O15399
D	886	ALA	-	expression tag	UNP O15399
D	887	PRO	-	expression tag	UNP O15399
D	888	ALA	-	expression tag	UNP O15399

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



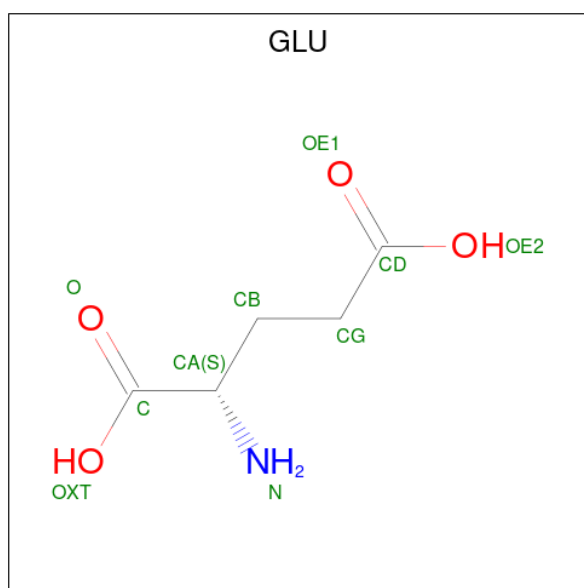
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

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

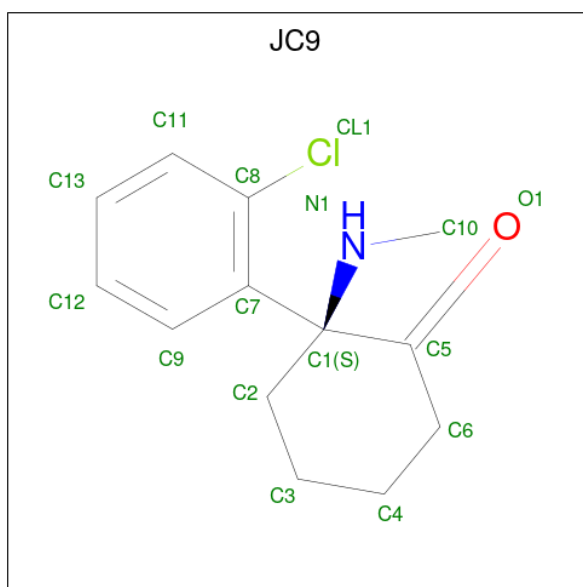
- Molecule 7 is GLUTAMIC ACID (CCD ID: GLU) (formula:  $C_5H_9NO_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			10	5	1	4	
7	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 8 is (2 {S})-2-(2-chlorophenyl)-2-(methylamino)cyclohexan-1-one (CCD ID: JC9) (formula:  $C_{13}H_{16}ClNO$ ) (labeled as "Ligand of Interest" by depositor).



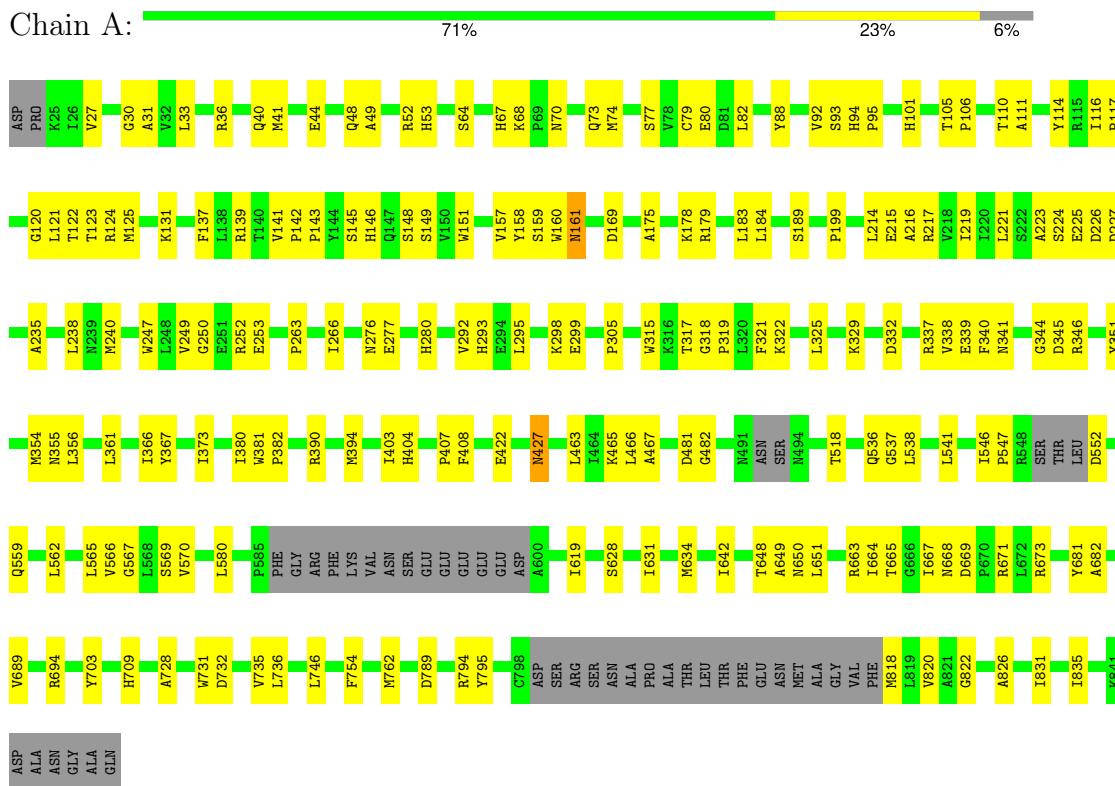


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
8	B	1	16	13	1	1	1	0

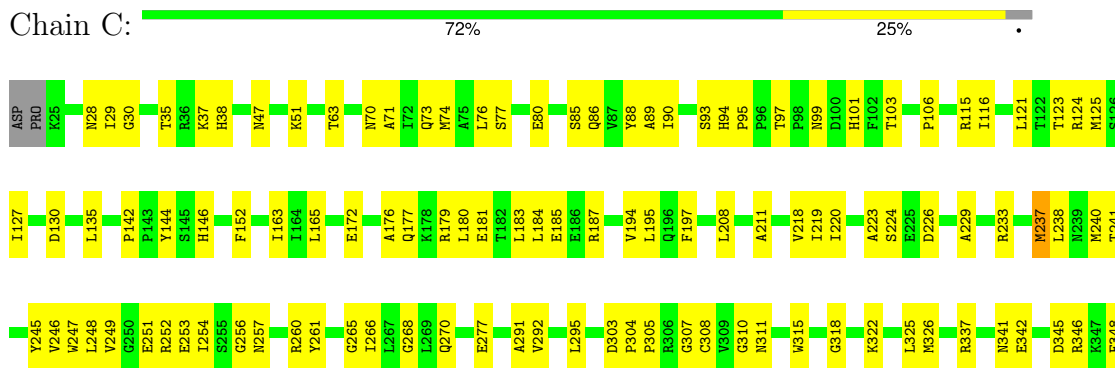
### 3 Residue-property plots

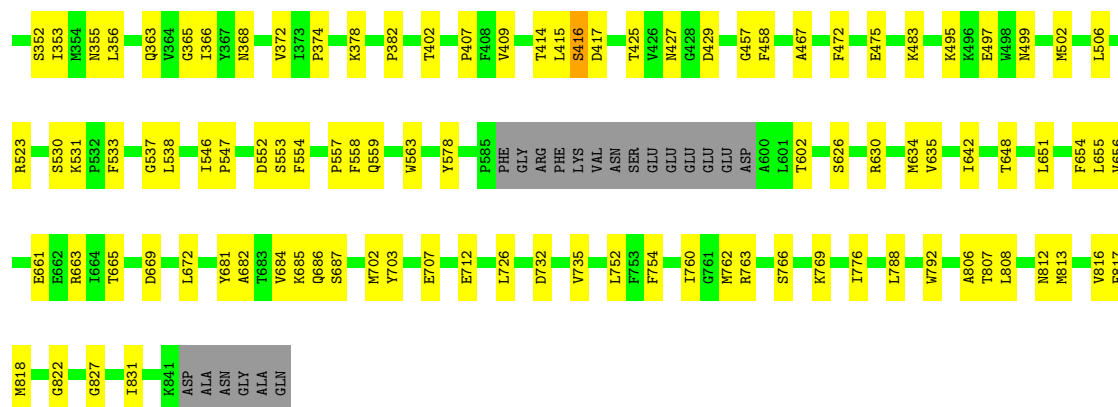
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



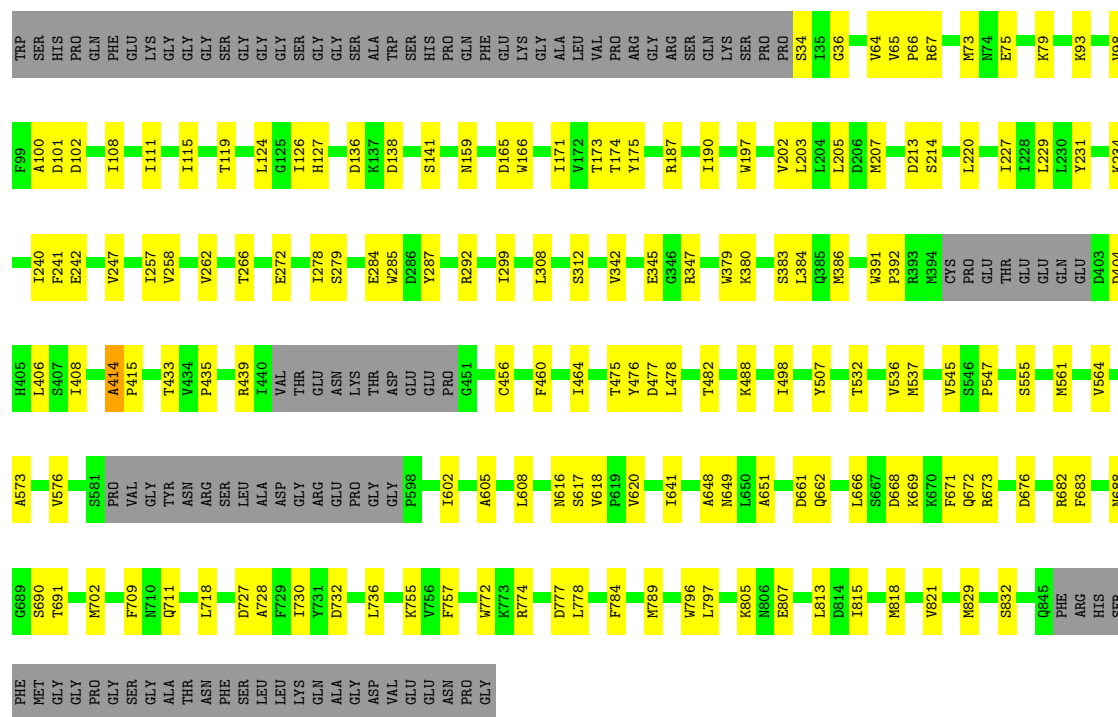
- Molecule 1: Glutamate receptor ionotropic, NMDA 1





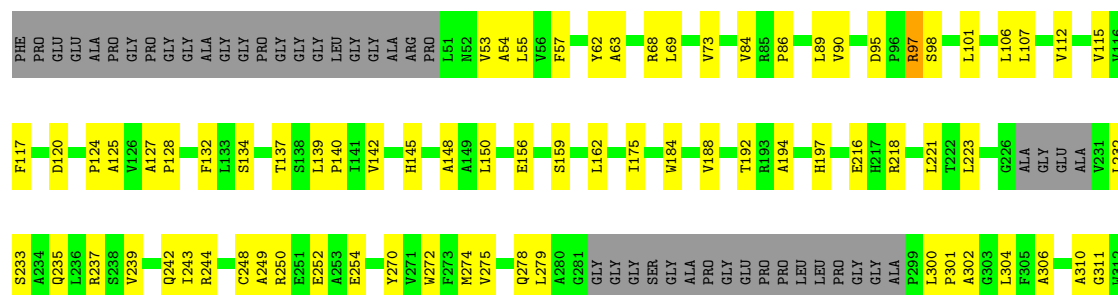
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

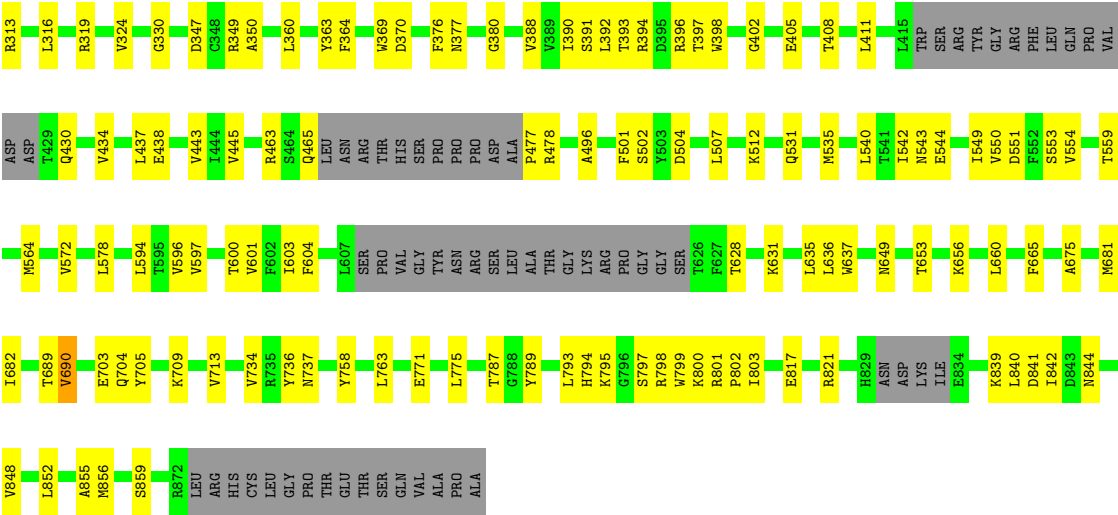
Chain B: 71% 17% 12%



• Molecule 3: Glutamate receptor ionotropic, NMDA 2D

Chain D: 65% 22% 12%





● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	77.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 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: JC9, NAG

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	0.32	0/6165	0.52	0/8365
1	C	0.31	0/6397	0.52	0/8685
2	B	0.30	0/6096	0.48	0/8279
3	D	0.30	0/5879	0.52	1/8003 (0.0%)
All	All	0.31	0/24537	0.51	1/33332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	477	PRO	N-CA-CB	5.98	110.48	103.30

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	6033	0	5917	134	0
1	C	6254	0	6156	143	0
2	B	5969	0	5790	105	0
3	D	5752	0	5647	134	0
4	E	28	0	25	1	0
5	A	5	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	2	2	0
6	A	56	0	52	0	0
6	B	14	0	13	2	0
6	C	42	0	39	0	0
7	B	10	0	5	2	0
7	D	10	0	5	0	0
8	B	16	0	0	1	0
All	All	24194	0	23653	494	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 10.

The worst 5 of 494 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:337:ARG:HE	1:C:348:PHE:HB3	1.36	0.85
1:C:341:ASN:OD1	1:C:342:GLU:N	2.16	0.77
1:C:28:ASN:ND2	1:C:85:SER:OG	2.19	0.75
1:A:650:ASN:HD21	2:B:813:LEU:HD21	1.51	0.75
3:D:89:LEU:HD21	3:D:106:LEU:HG	1.70	0.73

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	769/825 (93%)	694 (90%)	74 (10%)	1 (0%)	48 81
1	C	799/825 (97%)	724 (91%)	74 (9%)	1 (0%)	48 81
2	B	770/884 (87%)	709 (92%)	60 (8%)	1 (0%)	48 81
3	D	741/861 (86%)	667 (90%)	72 (10%)	2 (0%)	37 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3079/3395 (91%)	2794 (91%)	280 (9%)	5 (0%)	45	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	SER
1	A	663	ARG
3	D	690	VAL
2	B	414	ALA
3	D	705	TYR

### 5.3.2 Protein sidechains ⓘ

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	641/710 (90%)	639 (100%)	2 (0%)	91	92
1	C	674/710 (95%)	672 (100%)	2 (0%)	91	92
2	B	638/760 (84%)	637 (100%)	1 (0%)	92	94
3	D	599/701 (85%)	598 (100%)	1 (0%)	92	94
All	All	2552/2881 (89%)	2546 (100%)	6 (0%)	91	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	237	MET
1	C	702	MET
3	D	97	ARG
1	A	427	ASN
1	A	161	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:



Mol	Chain	Res	Type
1	C	363	GLN
1	C	28	ASN
2	B	616	ASN
2	B	359	HIS
2	B	649	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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	E	1	3,4	14,14,15	0.50	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.80	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
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	-2.26	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

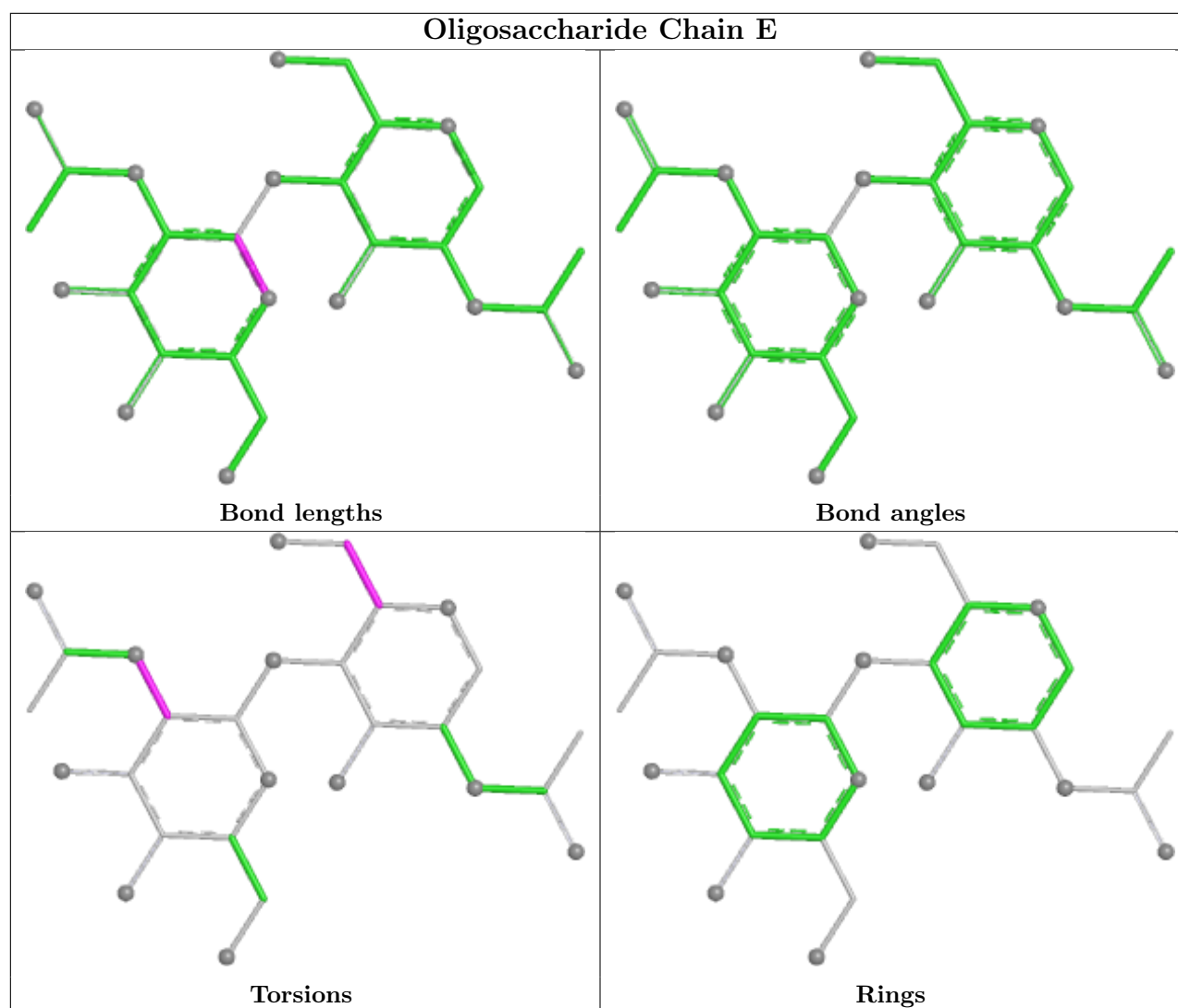
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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	NAG	A	903	1	14,14,15	0.28	0	17,19,21	0.53	0
6	NAG	B	902	2	14,14,15	0.58	1 (7%)	17,19,21	0.64	0
6	NAG	C	904	1	14,14,15	0.23	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GLU	B	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.29	1 (12%)
6	NAG	A	904	1	14,14,15	0.24	0	17,19,21	0.44	0
5	GLY	C	901	-	4,4,4	1.17	1 (25%)	3,4,4	1.65	1 (33%)
6	NAG	C	903	1	14,14,15	0.45	0	17,19,21	0.50	0
6	NAG	A	905	1	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
6	NAG	C	902	1	14,14,15	0.29	0	17,19,21	0.32	0
6	NAG	A	902	1	14,14,15	0.22	0	17,19,21	0.44	0
8	JC9	B	903	-	15,17,17	1.44	2 (13%)	15,24,24	1.50	2 (13%)
5	GLY	A	901	-	4,4,4	1.20	1 (25%)	3,4,4	1.75	2 (66%)
7	GLU	D	901	-	8,9,9	1.13	1 (12%)	8,11,11	1.19	1 (12%)

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	NAG	A	903	1	-	4/6/23/26	0/1/1/1
6	NAG	B	902	2	-	4/6/23/26	0/1/1/1
6	NAG	C	904	1	-	3/6/23/26	0/1/1/1
7	GLU	B	901	-	-	0/9/9/9	-
6	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	GLY	C	901	-	-	0/2/2/2	-
6	NAG	C	903	1	-	0/6/23/26	0/1/1/1
6	NAG	A	905	1	-	1/6/23/26	0/1/1/1
6	NAG	C	902	1	-	2/6/23/26	0/1/1/1
6	NAG	A	902	1	-	1/6/23/26	0/1/1/1
8	JC9	B	903	-	-	3/6/23/23	0/2/2/2
5	GLY	A	901	-	-	2/2/2/2	-
7	GLU	D	901	-	-	0/9/9/9	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	903	JC9	C6-C5	4.01	1.56	1.50
7	B	901	GLU	OXT-C	-2.37	1.23	1.30
5	A	901	GLY	OXT-C	-2.28	1.23	1.30
7	D	901	GLU	OXT-C	-2.26	1.23	1.30
5	C	901	GLY	OXT-C	-2.23	1.23	1.30

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	903	JC9	C9-C7-C8	3.48	120.21	116.51
8	B	903	JC9	C1-C7-C8	-3.31	120.40	123.43
7	B	901	GLU	OXT-C-O	-2.75	117.84	124.08
7	D	901	GLU	OXT-C-O	-2.61	118.15	124.08
6	A	905	NAG	C2-N2-C7	2.60	126.39	122.90

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

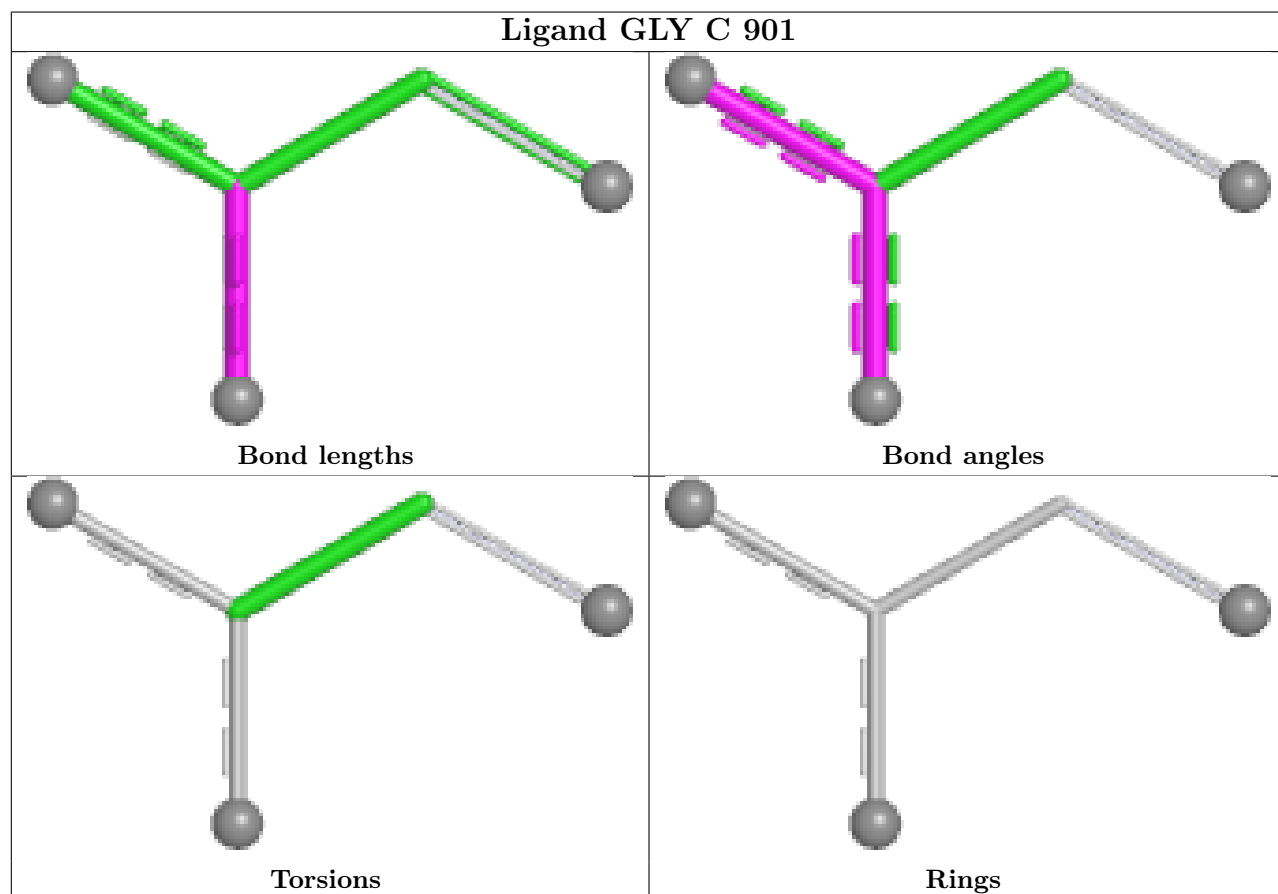
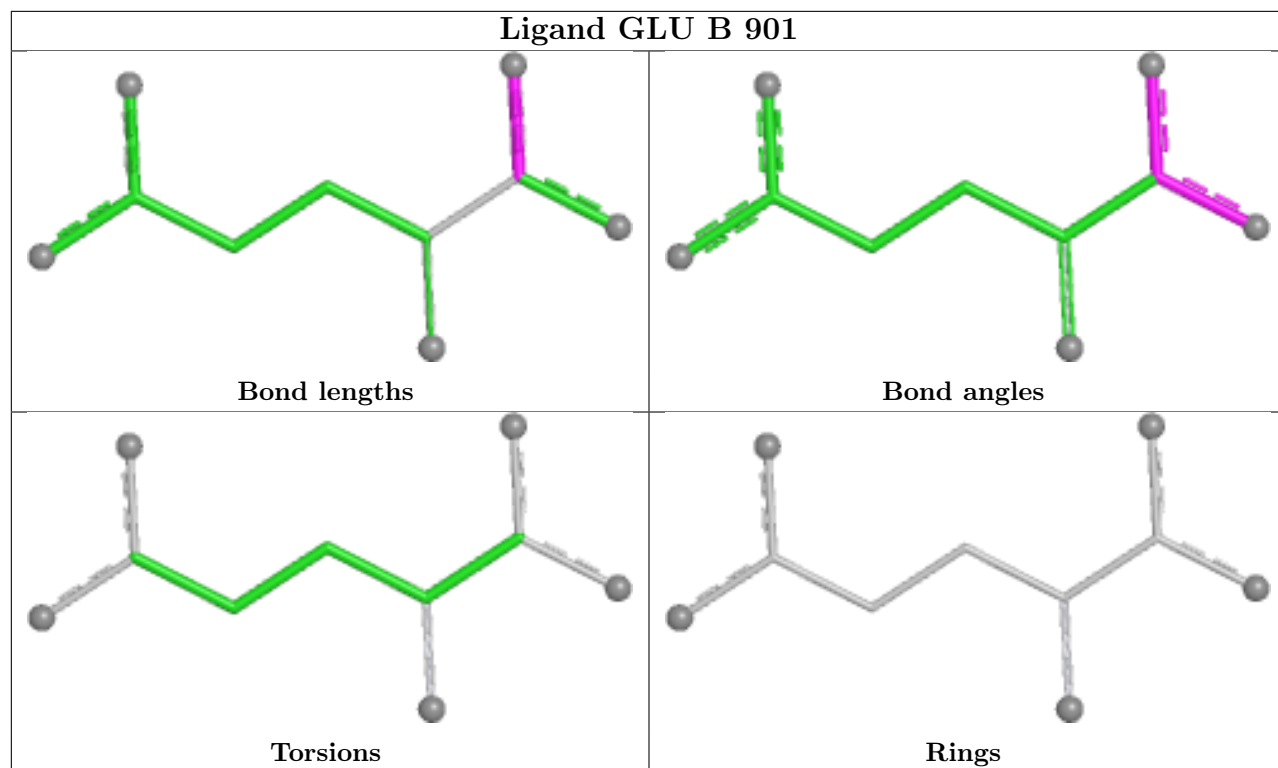
Mol	Chain	Res	Type	Atoms
5	A	901	GLY	O-C-CA-N
5	A	901	GLY	OXT-C-CA-N
6	A	905	NAG	C1-C2-N2-C7
8	B	903	JC9	N1-C1-C7-C8
8	B	903	JC9	C5-C1-C7-C8

There are no ring outliers.

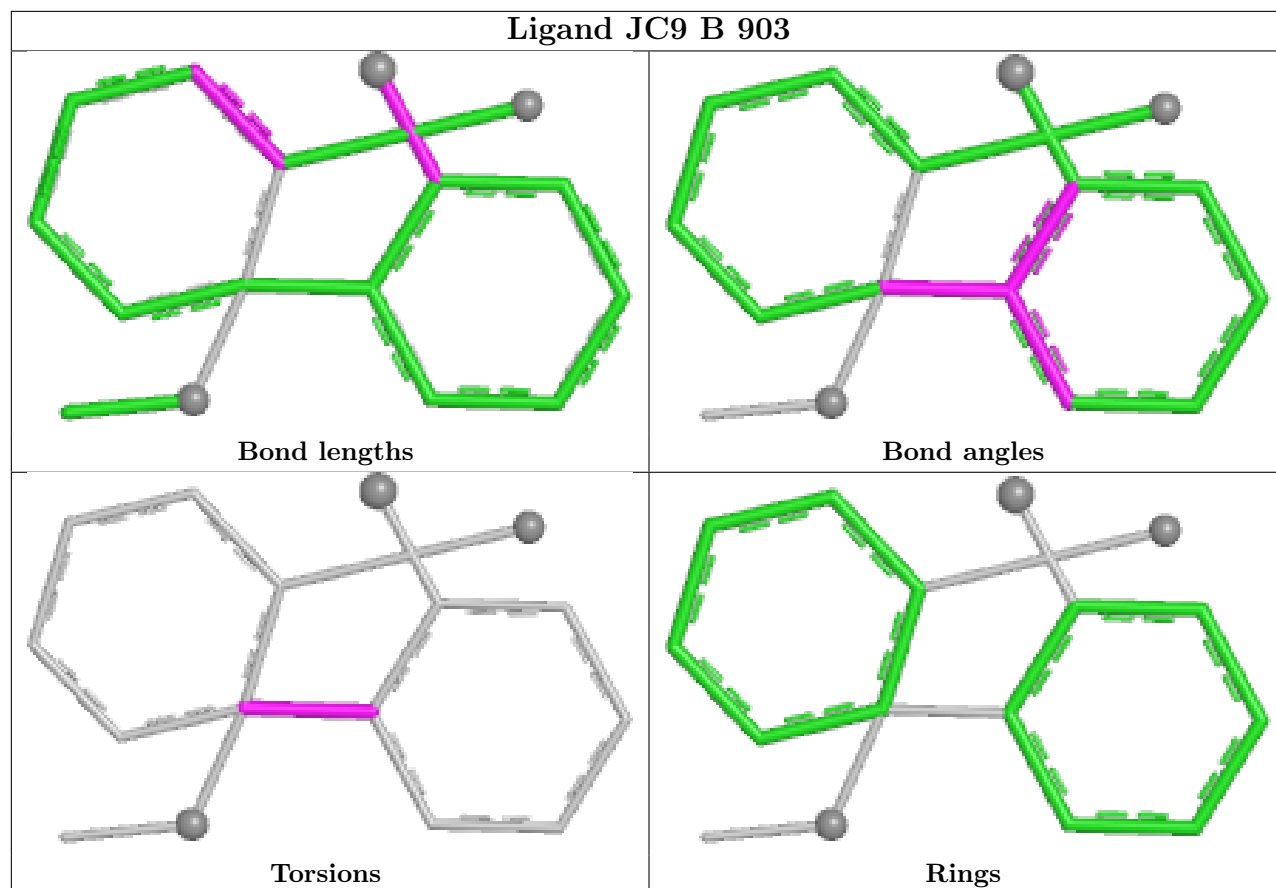
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	902	NAG	2	0
7	B	901	GLU	2	0
5	C	901	GLY	2	0
8	B	903	JC9	1	0
5	A	901	GLY	1	0

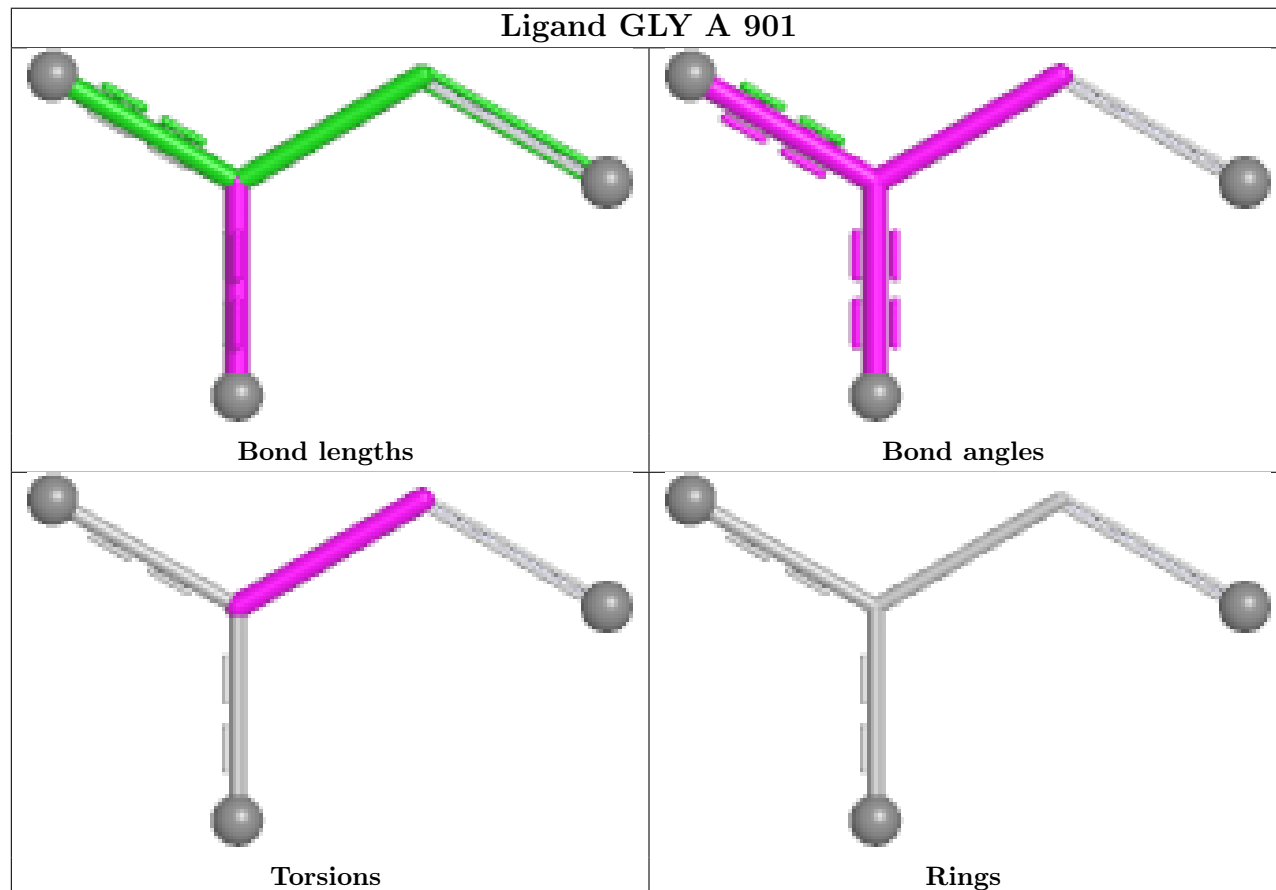
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

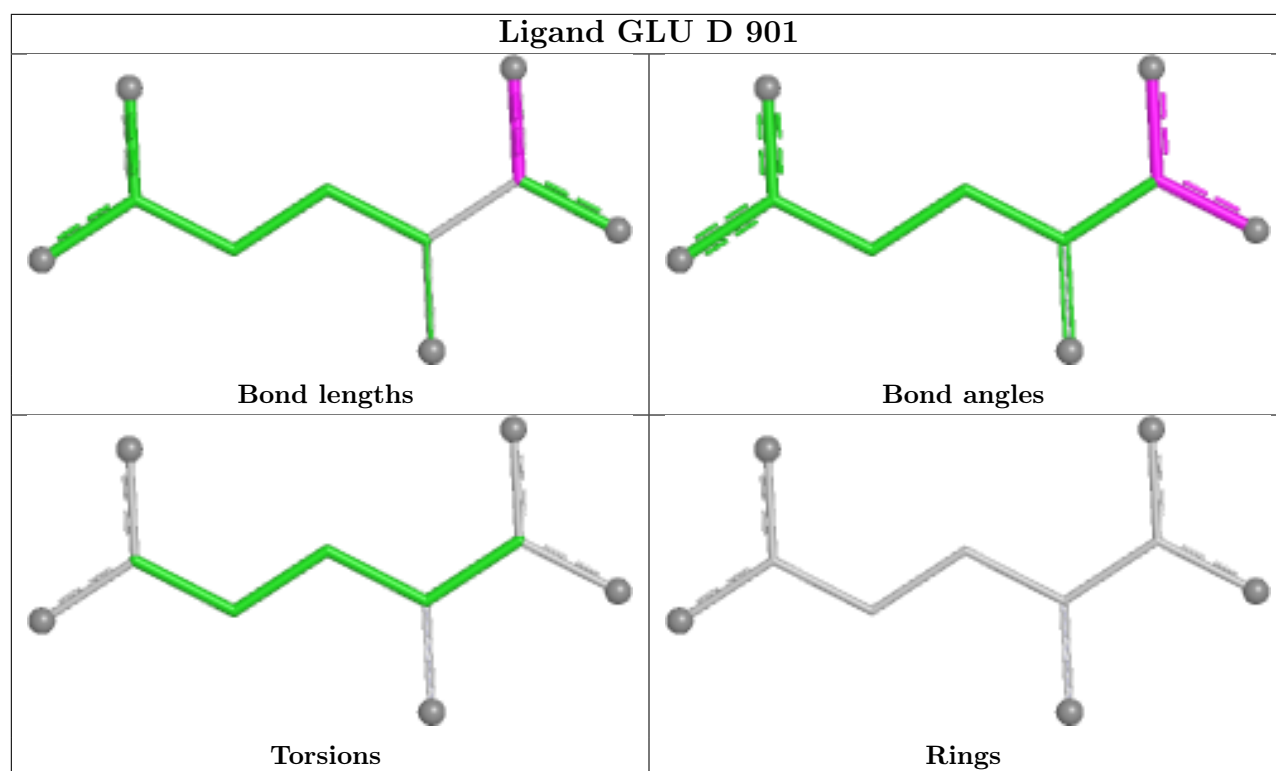


## Ligand JC9 B 903



## Ligand GLY A 901





## 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-46531. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.