



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2019 – 05:06 PM EST

PDB ID : 6MMX  
EMDB ID: : EMD-9165  
Title : Triheteromeric NMDA receptor GluN1/GluN2A/GluN2A\* in the 'Extended' conformation, in complex with glycine and glutamate, in the presence of 1 micromolar zinc chloride, and at pH 7.4  
Authors : Jalali-Yazdi, F.; Chowdhury, S.; Yoshioka, C.; Gouaux, E.  
Deposited on : 2018-10-01  
Resolution : 6.99 Å (reported)  
Based on PDB ID : 5UOW, 4PE5, 5TQ0, 5I57

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4



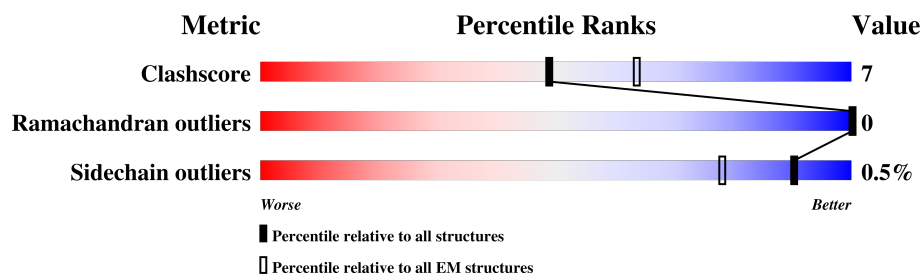
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.99 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	838	71% 21% 7%
1	C	838	79% 14% 7%
2	B	837	75% 17% 8%
2	D	837	73% 17% 9%



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25011 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	777	Total	C	N	O	S	0	0
			6158	3931	1060	1132	35		
1	C	783	Total	C	N	O	S	0	0
			6206	3960	1072	1139	35		

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

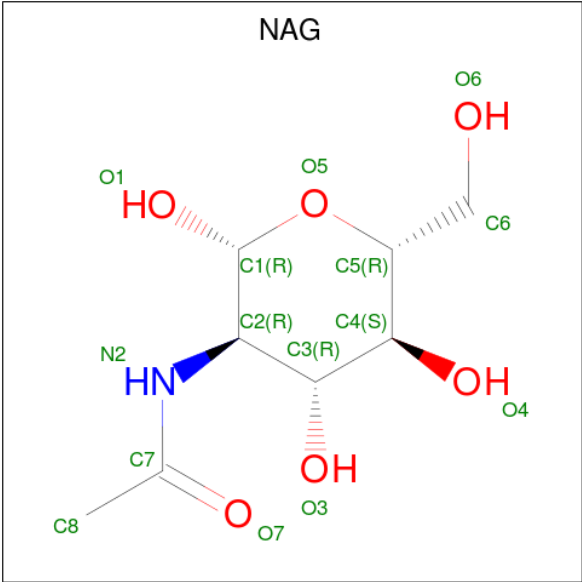
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	771	Total	C	N	O	S	0	0
			6090	3931	993	1130	36		
2	D	761	Total	C	N	O	S	0	0
			6011	3884	983	1109	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	ALA	HIS	engineered mutation	UNP Q00959
B	687	ALA	ASN	engineered mutation	UNP Q00959
B	758	THR	SER	conflict	UNP Q00959
D	128	ALA	HIS	engineered mutation	UNP Q00959
D	687	ALA	ASN	engineered mutation	UNP Q00959
D	758	THR	SER	conflict	UNP Q00959

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	A	1	Total	C	N	O	0
			210	120	15	75	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			210	120	15	75	
3	B	1	Total	C	N	O	0
			84	48	6	30	
3	B	1	Total	C	N	O	0
			84	48	6	30	
3	B	1	Total	C	N	O	0
			84	48	6	30	
3	B	1	Total	C	N	O	0
			84	48	6	30	
3	B	1	Total	C	N	O	0
			84	48	6	30	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	C	1	Total	C	N	O	0
			182	104	13	65	
3	D	1	Total	C	N	O	0
			70	40	5	25	

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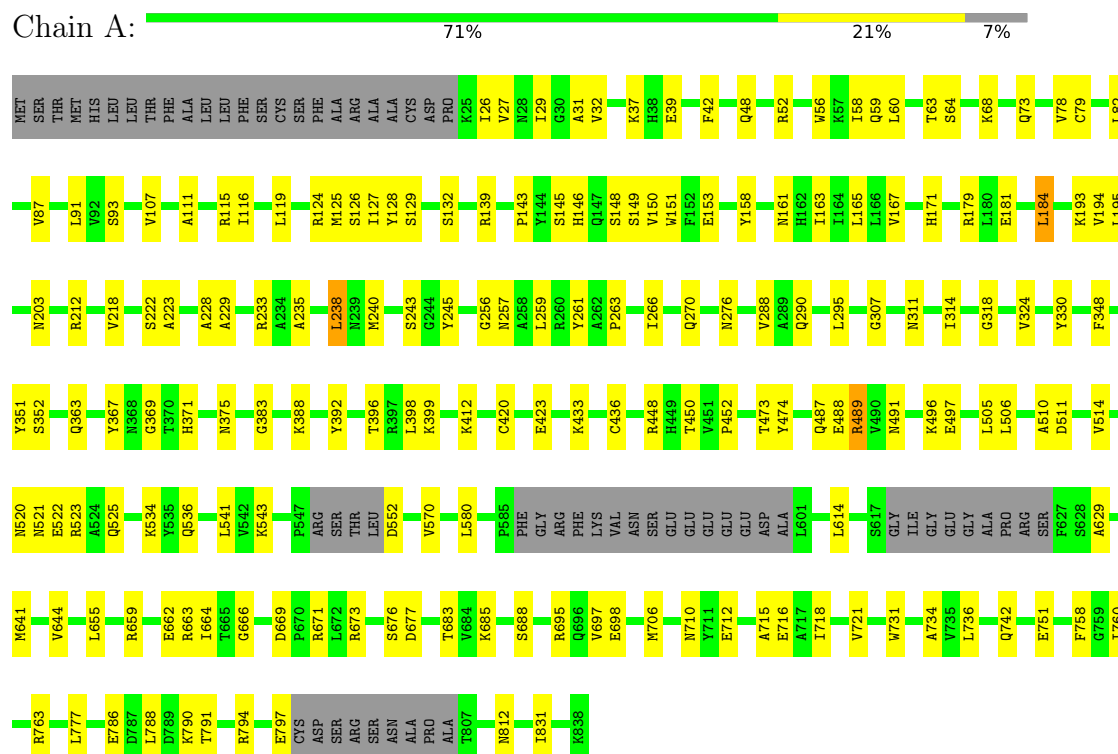
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			70	40	5	25	
3	D	1	Total	C	N	O	0
			70	40	5	25	
3	D	1	Total	C	N	O	0
			70	40	5	25	
3	D	1	Total	C	N	O	0
			70	40	5	25	



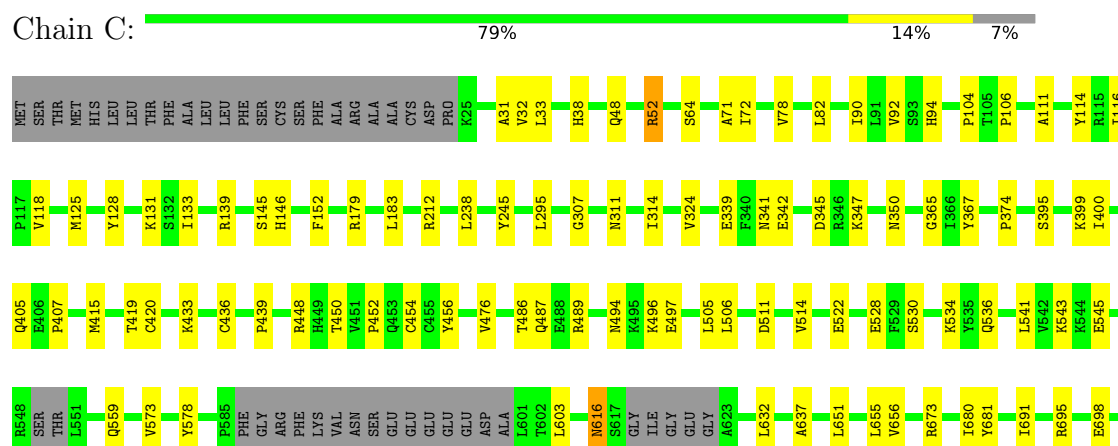
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

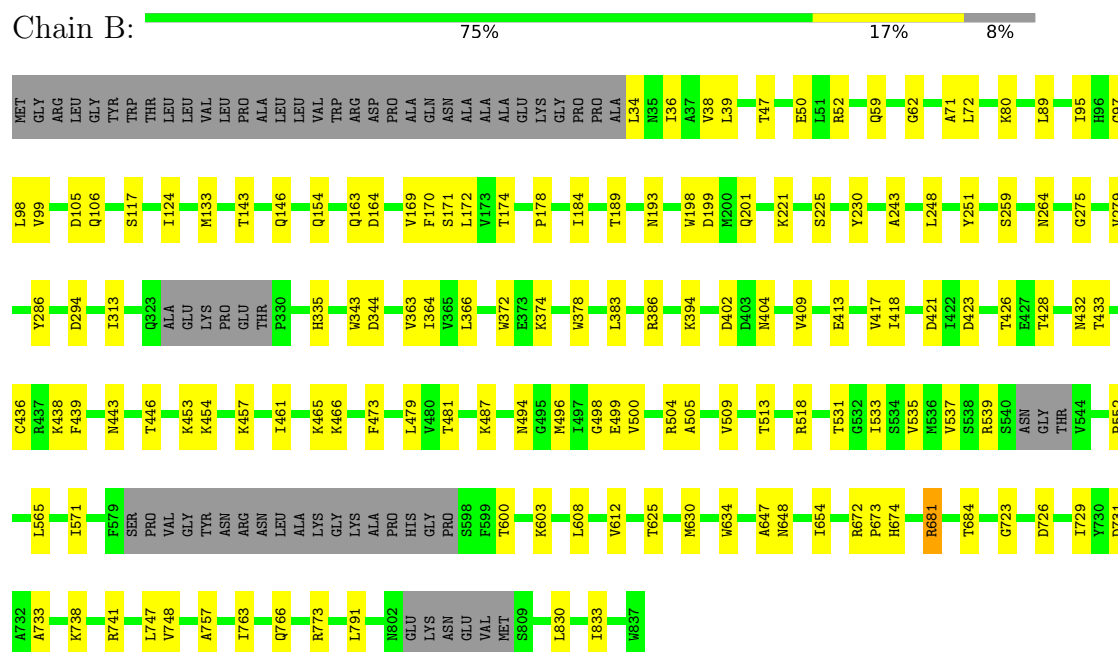


- Molecule 1: Glutamate receptor ionotropic, NMDA 1

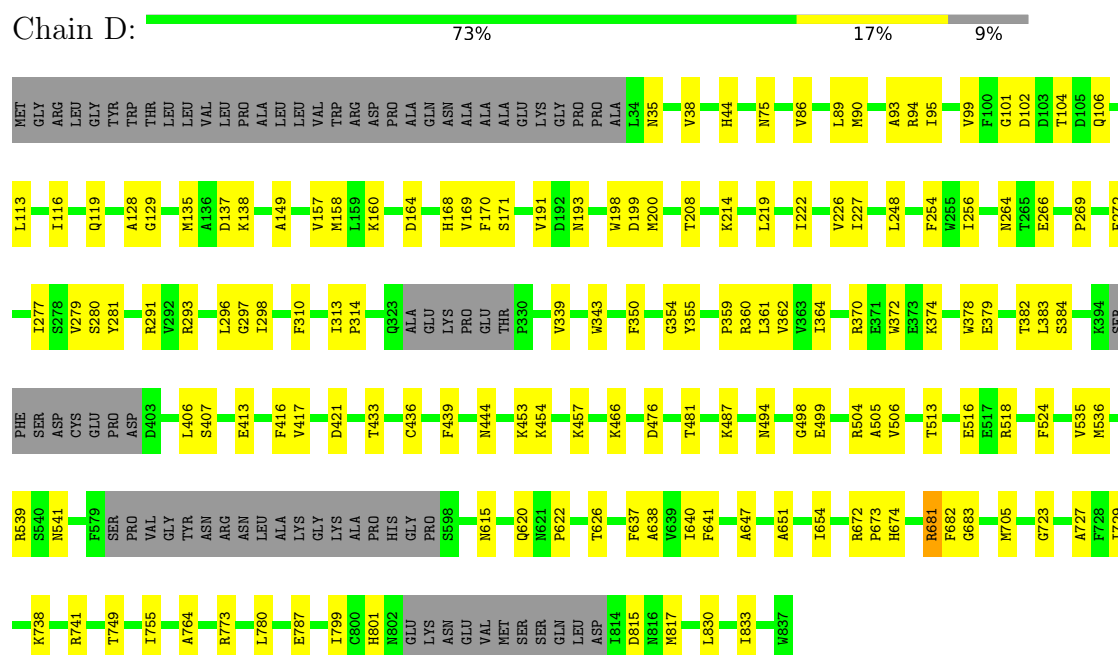




- Molecule 2: Glutamate receptor ionotropic, NMDA 2A



- Molecule 2: Glutamate receptor ionotropic, NMDA 2A





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 BASE (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

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.28	0/6295	0.51	2/8526 (0.0%)
1	C	0.28	0/6344	0.50	1/8592 (0.0%)
2	B	0.27	0/6233	0.48	0/8462
2	D	0.27	0/6152	0.49	0/8352
All	All	0.27	0/25024	0.50	3/33932 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	CA-CB-CG	5.96	129.02	115.30
1	C	651	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	184	LEU	CA-CB-CG	5.38	127.66	115.30

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	6158	0	6131	108	0
1	C	6206	0	6185	74	0
2	B	6090	0	6024	82	0
2	D	6011	0	5962	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	210	0	190	3	0
3	B	84	0	77	0	0
3	C	182	0	167	0	0
3	D	70	0	65	0	0
All	All	25011	0	24801	332	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 7.

The worst 5 of 332 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)
2:B:773:ARG:NH1	1:C:528:GLU:OE2	2.10	0.85
1:A:487:GLN:HA	1:A:497:GLU:O	1.82	0.80
1:C:559:GLN:NE2	2:D:815:ASP:OD2	2.21	0.73
2:D:272:PHE:HB2	2:D:370:ARG:HH12	1.57	0.70
1:A:399:LYS:N	1:A:511:ASP:OD2	2.23	0.69

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 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	767/838 (92%)	702 (92%)	65 (8%)	0	100	100
1	C	773/838 (92%)	725 (94%)	48 (6%)	0	100	100
2	B	761/837 (91%)	708 (93%)	53 (7%)	0	100	100
2	D	751/837 (90%)	694 (92%)	57 (8%)	0	100	100
All	All	3052/3350 (91%)	2829 (93%)	223 (7%)	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	673/722 (93%)	667 (99%)	6 (1%)	81	90
1	C	678/722 (94%)	674 (99%)	4 (1%)	87	93
2	B	674/724 (93%)	672 (100%)	2 (0%)	93	96
2	D	663/724 (92%)	661 (100%)	2 (0%)	93	96
All	All	2688/2892 (93%)	2674 (100%)	14 (0%)	90	95

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	625	THR
2	B	681	ARG
1	C	813	MET
1	A	491	ASN
1	C	616	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	387	HIS
2	B	736	ASN
2	D	697	ASN
2	B	709	ASN
1	C	73	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

39 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	$\# Z  > 2$
3	NAG	A	901	1,3	14,14,15	0.45	0	17,19,21	0.75	0
3	NAG	A	902	3	14,14,15	0.64	1 (7%)	17,19,21	0.75	0
3	NAG	A	903	1	14,14,15	0.37	0	17,19,21	1.14	1 (5%)
3	NAG	A	904	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
3	NAG	A	905	1	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
3	NAG	A	906	1	14,14,15	0.35	0	17,19,21	0.75	1 (5%)
3	NAG	A	907	1,3	14,14,15	0.36	0	17,19,21	1.33	3 (17%)
3	NAG	A	908	3	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
3	NAG	A	909	1,3	14,14,15	0.48	0	17,19,21	1.30	2 (11%)
3	NAG	A	910	3	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
3	NAG	A	911	1,3	14,14,15	0.46	0	17,19,21	0.97	2 (11%)
3	NAG	A	912	3	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
3	NAG	A	913	1	14,14,15	0.40	0	17,19,21	1.10	1 (5%)
3	NAG	A	914	1	14,14,15	0.42	0	17,19,21	1.31	1 (5%)
3	NAG	A	915	1	14,14,15	0.39	0	17,19,21	2.25	2 (11%)
3	NAG	B	901	2	14,14,15	0.56	0	17,19,21	1.10	2 (11%)
3	NAG	B	902	2	14,14,15	0.49	0	17,19,21	0.74	0
3	NAG	B	903	3,2	14,14,15	0.55	0	17,19,21	1.64	4 (23%)
3	NAG	B	904	3	14,14,15	0.43	0	17,19,21	0.82	0
3	NAG	B	905	2	14,14,15	0.37	0	17,19,21	0.78	0
3	NAG	B	906	2	14,14,15	0.38	0	17,19,21	0.75	0
3	NAG	C	901	1	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
3	NAG	C	902	1,3	14,14,15	0.36	0	17,19,21	0.80	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	903	3	14,14,15	0.47	0	17,19,21	1.10	1 (5%)
3	NAG	C	904	1	14,14,15	0.47	0	17,19,21	0.78	0
3	NAG	C	905	1	14,14,15	0.48	0	17,19,21	1.28	2 (11%)
3	NAG	C	906	1	14,14,15	0.45	0	17,19,21	1.32	2 (11%)
3	NAG	C	907	1	14,14,15	0.40	0	17,19,21	0.69	0
3	NAG	C	908	1,3	14,14,15	0.42	0	17,19,21	1.90	2 (11%)
3	NAG	C	909	3	14,14,15	0.45	0	17,19,21	0.82	0
3	NAG	C	910	1	14,14,15	0.37	0	17,19,21	1.32	1 (5%)
3	NAG	C	911	1	14,14,15	0.31	0	17,19,21	0.83	1 (5%)
3	NAG	C	912	1	14,14,15	0.68	1 (7%)	17,19,21	1.66	3 (17%)
3	NAG	C	913	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
3	NAG	D	901	2	14,14,15	0.54	0	17,19,21	1.33	3 (17%)
3	NAG	D	902	2	14,14,15	0.33	0	17,19,21	0.71	1 (5%)
3	NAG	D	903	2	14,14,15	0.44	0	17,19,21	1.56	2 (11%)
3	NAG	D	904	2	14,14,15	0.34	0	17,19,21	0.81	1 (5%)
3	NAG	D	905	2	14,14,15	0.40	0	17,19,21	0.95	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
3	NAG	A	901	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	902	3	-	4/6/23/26	0/1/1/1
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
3	NAG	A	904	1	-	2/6/23/26	0/1/1/1
3	NAG	A	905	1	-	2/6/23/26	0/1/1/1
3	NAG	A	906	1	-	2/6/23/26	0/1/1/1
3	NAG	A	907	1,3	-	5/6/23/26	0/1/1/1
3	NAG	A	908	3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	1,3	-	5/6/23/26	0/1/1/1
3	NAG	A	910	3	-	2/6/23/26	0/1/1/1
3	NAG	A	911	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	912	3	-	0/6/23/26	0/1/1/1
3	NAG	A	913	1	-	3/6/23/26	0/1/1/1
3	NAG	A	914	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	915	1	-	4/6/23/26	0/1/1/1
3	NAG	B	901	2	-	4/6/23/26	0/1/1/1
3	NAG	B	902	2	-	4/6/23/26	0/1/1/1
3	NAG	B	903	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	904	3	-	3/6/23/26	0/1/1/1
3	NAG	B	905	2	-	2/6/23/26	0/1/1/1
3	NAG	B	906	2	-	2/6/23/26	0/1/1/1
3	NAG	C	901	1	-	3/6/23/26	0/1/1/1
3	NAG	C	902	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	903	3	-	4/6/23/26	0/1/1/1
3	NAG	C	904	1	-	3/6/23/26	0/1/1/1
3	NAG	C	905	1	-	4/6/23/26	0/1/1/1
3	NAG	C	906	1	-	3/6/23/26	0/1/1/1
3	NAG	C	907	1	-	2/6/23/26	0/1/1/1
3	NAG	C	908	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	909	3	-	3/6/23/26	0/1/1/1
3	NAG	C	910	1	-	2/6/23/26	0/1/1/1
3	NAG	C	911	1	-	3/6/23/26	0/1/1/1
3	NAG	C	912	1	-	3/6/23/26	0/1/1/1
3	NAG	C	913	1	-	2/6/23/26	0/1/1/1
3	NAG	D	901	2	-	3/6/23/26	0/1/1/1
3	NAG	D	902	2	-	2/6/23/26	0/1/1/1
3	NAG	D	903	2	-	5/6/23/26	0/1/1/1
3	NAG	D	904	2	-	2/6/23/26	0/1/1/1
3	NAG	D	905	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	912	NAG	C1-C2	2.03	1.55	1.52
3	A	902	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	915	NAG	C1-O5-C5	8.17	123.30	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	908	NAG	C1-O5-C5	6.99	121.70	112.20
3	C	910	NAG	C1-O5-C5	5.03	119.05	112.20
3	D	903	NAG	C1-O5-C5	4.35	118.11	112.20
3	A	903	NAG	C1-O5-C5	4.03	117.68	112.20

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	910	NAG	C8-C7-N2-C2
3	C	910	NAG	O7-C7-N2-C2
3	C	911	NAG	C8-C7-N2-C2
3	C	911	NAG	O7-C7-N2-C2
3	C	903	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAG	1	0
3	A	902	NAG	1	0
3	A	907	NAG	1	0
3	A	908	NAG	1	0
3	A	909	NAG	1	0

## 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.