wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 08:31 AM UTC

PDB ID	:	4TLM / pdb_00004tlm
Title	:	Crystal structure of GluN1/GluN2B NMDA receptor, structure 2
Authors	:	Gouaux, E.; Lee, C.-H.; Lu, W.
Deposited on	:	2014-05-30
Resolution	:	3.77 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

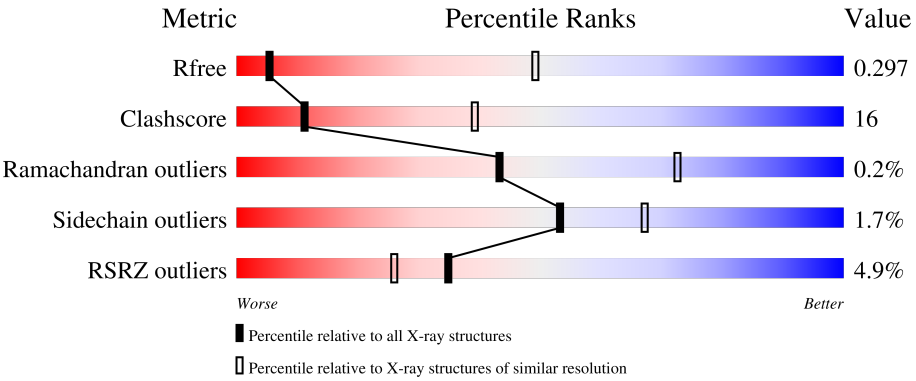
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.77 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

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 <=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	823	2% 68% 28%
1	C	823	6% 69% 21% 9%
2	B	824	5% 67% 22% 9%
2	D	824	5% 67% 23% 9%

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	QEM	C	903	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19547 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 receptor subunit GluN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			5383	3411	945	1004	23			
1	C	750	Total	C	N	O	S	0	0	0
			4582	2855	818	893	16			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	engineered mutation	UNP C0KD18
A	51	PHE	LYS	engineered mutation	UNP C0KD18
A	52	PHE	ARG	engineered mutation	UNP C0KD18
A	300	GLN	ASN	engineered mutation	UNP C0KD18
A	350	GLN	ASN	engineered mutation	UNP C0KD18
A	368	ASP	ASN	engineered mutation	UNP C0KD18
A	440	ASP	ASN	engineered mutation	UNP C0KD18
A	469	ASP	ASN	engineered mutation	UNP C0KD18
A	493	ALA	LYS	engineered mutation	UNP C0KD18
A	494	ALA	LYS	engineered mutation	UNP C0KD18
A	495	ALA	GLU	engineered mutation	UNP C0KD18
A	602	ARG	GLY	engineered mutation	UNP C0KD18
A	609	LEU	ILE	engineered mutation	UNP C0KD18
A	648	ARG	ASP	engineered mutation	UNP C0KD18
A	761	GLU	ASN	engineered mutation	UNP C0KD18
A	829	SER	-	insertion	UNP C0KD18
A	830	ARG	-	insertion	UNP C0KD18
A	831	ALA	-	insertion	UNP C0KD18
A	832	GLU	-	insertion	UNP C0KD18
A	833	ALA	-	insertion	UNP C0KD18
A	834	LYS	-	insertion	UNP C0KD18
A	835	ARG	-	insertion	UNP C0KD18
A	836	MET	-	insertion	UNP C0KD18
A	837	LYS	-	insertion	UNP C0KD18
A	838	GLY	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	839	LEU	-	expression tag	UNP C0KD18
A	840	GLU	-	expression tag	UNP C0KD18
A	841	VAL	-	expression tag	UNP C0KD18
A	842	LEU	-	expression tag	UNP C0KD18
A	843	PHE	-	expression tag	UNP C0KD18
A	844	GLN	-	expression tag	UNP C0KD18
C	22	ALA	CYS	engineered mutation	UNP C0KD18
C	51	PHE	LYS	engineered mutation	UNP C0KD18
C	52	PHE	ARG	engineered mutation	UNP C0KD18
C	300	GLN	ASN	engineered mutation	UNP C0KD18
C	350	GLN	ASN	engineered mutation	UNP C0KD18
C	368	ASP	ASN	engineered mutation	UNP C0KD18
C	440	ASP	ASN	engineered mutation	UNP C0KD18
C	469	ASP	ASN	engineered mutation	UNP C0KD18
C	493	ALA	LYS	engineered mutation	UNP C0KD18
C	494	ALA	LYS	engineered mutation	UNP C0KD18
C	495	ALA	GLU	engineered mutation	UNP C0KD18
C	602	ARG	GLY	engineered mutation	UNP C0KD18
C	609	LEU	ILE	engineered mutation	UNP C0KD18
C	648	ARG	ASP	engineered mutation	UNP C0KD18
C	761	GLU	ASN	engineered mutation	UNP C0KD18
C	829	SER	-	insertion	UNP C0KD18
C	830	ARG	-	insertion	UNP C0KD18
C	831	ALA	-	insertion	UNP C0KD18
C	832	GLU	-	insertion	UNP C0KD18
C	833	ALA	-	insertion	UNP C0KD18
C	834	LYS	-	insertion	UNP C0KD18
C	835	ARG	-	insertion	UNP C0KD18
C	836	MET	-	insertion	UNP C0KD18
C	837	LYS	-	insertion	UNP C0KD18
C	838	GLY	-	expression tag	UNP C0KD18
C	839	LEU	-	expression tag	UNP C0KD18
C	840	GLU	-	expression tag	UNP C0KD18
C	841	VAL	-	expression tag	UNP C0KD18
C	842	LEU	-	expression tag	UNP C0KD18
C	843	PHE	-	expression tag	UNP C0KD18
C	844	GLN	-	expression tag	UNP C0KD18

- Molecule 2 is a protein called receptor subunit GluN2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	749	Total	C	N	O	S	0	0	0
			4752	2998	811	923	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	753	Total	C	N	O	S	0	0	0
			4664	2932	803	914	15			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	216	CYS	LYS	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	UNP A7XY94
B	486	VAL	THR	engineered mutation	UNP A7XY94
B	601	LEU	VAL	engineered mutation	UNP A7XY94
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
B	826	TYR	-	insertion	UNP A7XY94
B	827	LYS	-	insertion	UNP A7XY94
B	828	SER	-	insertion	UNP A7XY94
B	829	ARG	-	insertion	UNP A7XY94
B	830	ALA	-	insertion	UNP A7XY94
B	831	GLU	-	insertion	UNP A7XY94
B	832	ALA	-	insertion	UNP A7XY94
B	833	LYS	-	insertion	UNP A7XY94
B	834	ARG	-	insertion	UNP A7XY94
B	835	MET	-	insertion	UNP A7XY94
B	836	LYS	-	insertion	UNP A7XY94
B	837	GLY	-	expression tag	UNP A7XY94
B	838	LEU	-	expression tag	UNP A7XY94
B	839	GLU	-	expression tag	UNP A7XY94
B	840	VAL	-	expression tag	UNP A7XY94
B	841	LEU	-	expression tag	UNP A7XY94
B	842	PHE	-	expression tag	UNP A7XY94
B	843	GLN	-	expression tag	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	UNP A7XY94
D	69	GLN	ASN	engineered mutation	UNP A7XY94
D	216	CYS	LYS	engineered mutation	UNP A7XY94
D	343	ASP	ASN	engineered mutation	UNP A7XY94

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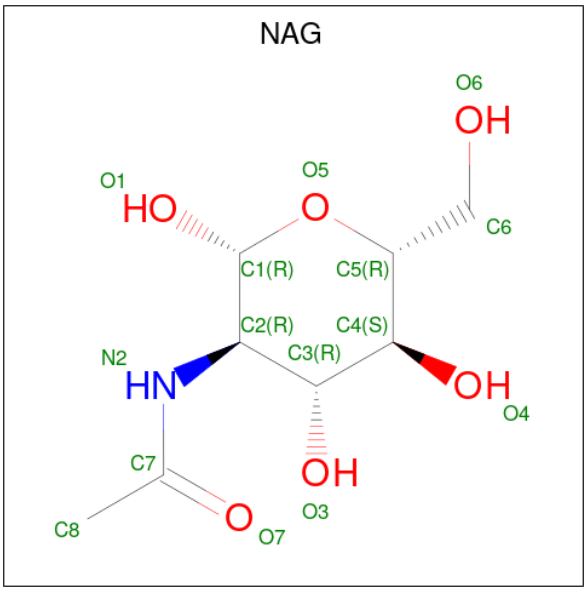
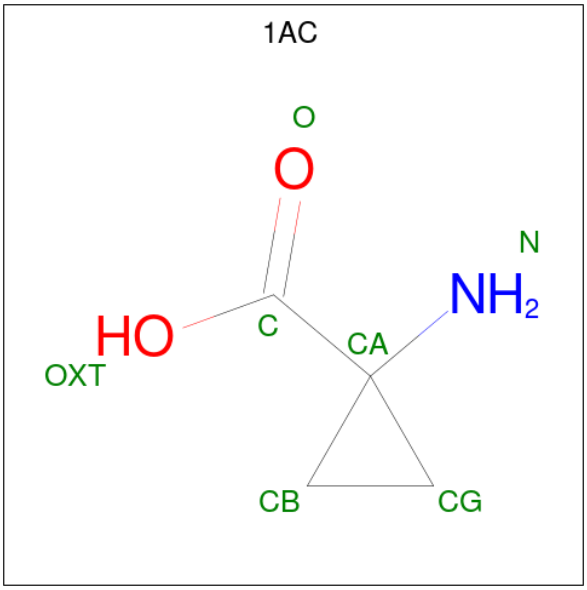
Chain	Residue	Modelled	Actual	Comment	Reference
D	486	VAL	THR	engineered mutation	UNP A7XY94
D	601	LEU	VAL	engineered mutation	UNP A7XY94
D	640	ARG	GLU	engineered mutation	UNP A7XY94
D	641	ARG	GLU	engineered mutation	UNP A7XY94
D	826	TYR	-	insertion	UNP A7XY94
D	827	LYS	-	insertion	UNP A7XY94
D	828	SER	-	insertion	UNP A7XY94
D	829	ARG	-	insertion	UNP A7XY94
D	830	ALA	-	insertion	UNP A7XY94
D	831	GLU	-	insertion	UNP A7XY94
D	832	ALA	-	insertion	UNP A7XY94
D	833	LYS	-	insertion	UNP A7XY94
D	834	ARG	-	insertion	UNP A7XY94
D	835	MET	-	insertion	UNP A7XY94
D	836	LYS	-	insertion	UNP A7XY94
D	837	GLY	-	expression tag	UNP A7XY94
D	838	LEU	-	expression tag	UNP A7XY94
D	839	GLU	-	expression tag	UNP A7XY94
D	840	VAL	-	expression tag	UNP A7XY94
D	841	LEU	-	expression tag	UNP A7XY94
D	842	PHE	-	expression tag	UNP A7XY94
D	843	GLN	-	expression tag	UNP A7XY94

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



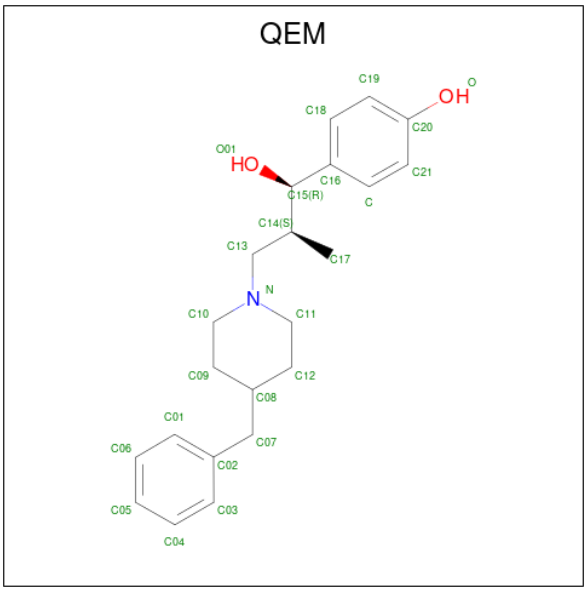
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 1-AMINOCYCLOPROPANECARBOXYLIC ACID (CCD ID: 1AC) (formula: $C_4H_7NO_2$).



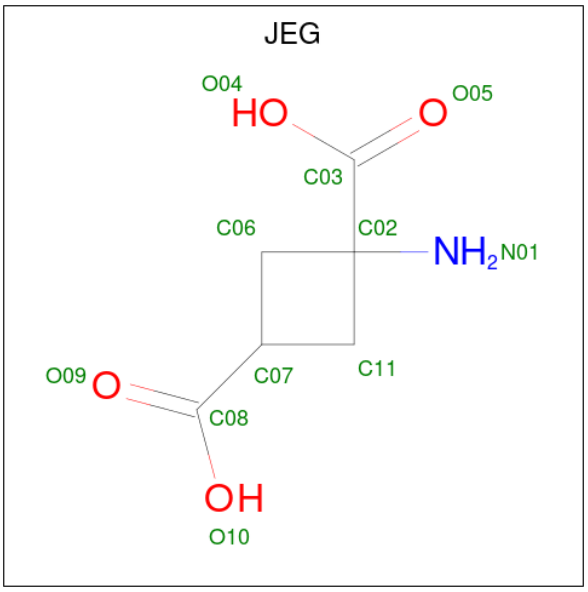
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 4 1 2	0	0

- Molecule 5 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (CCD ID: QEM) (formula: $C_{22}H_{29}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 25 22 1 2	0	0
5	C	1	Total C N O 25 22 1 2	0	0

- Molecule 6 is trans-1-aminocyclobutane-1,3-dicarboxylic acid (CCD ID: JEG) (formula: $C_6H_9NO_4$).



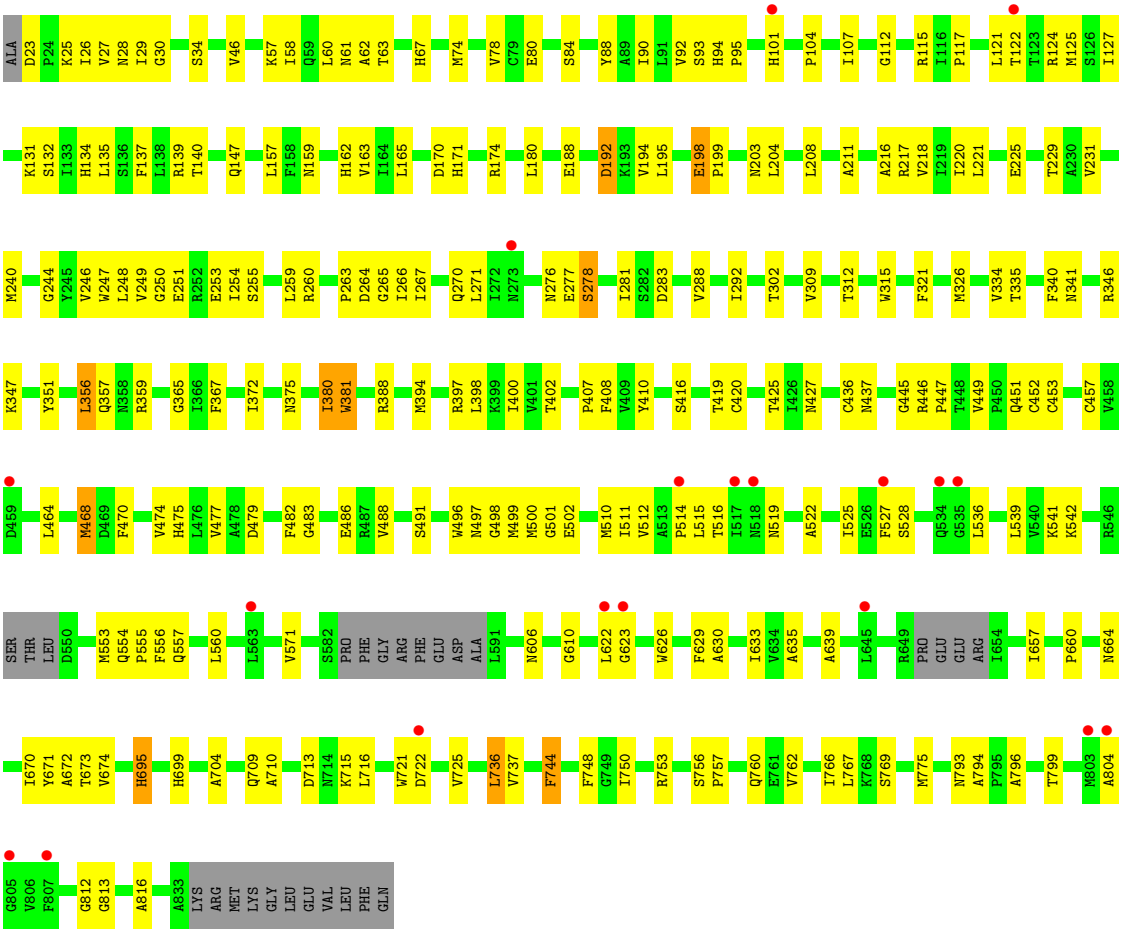
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O 11 6 1 4	0	0

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.

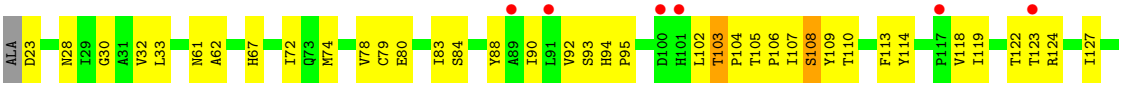
• Molecule 1: receptor subunit GluN1

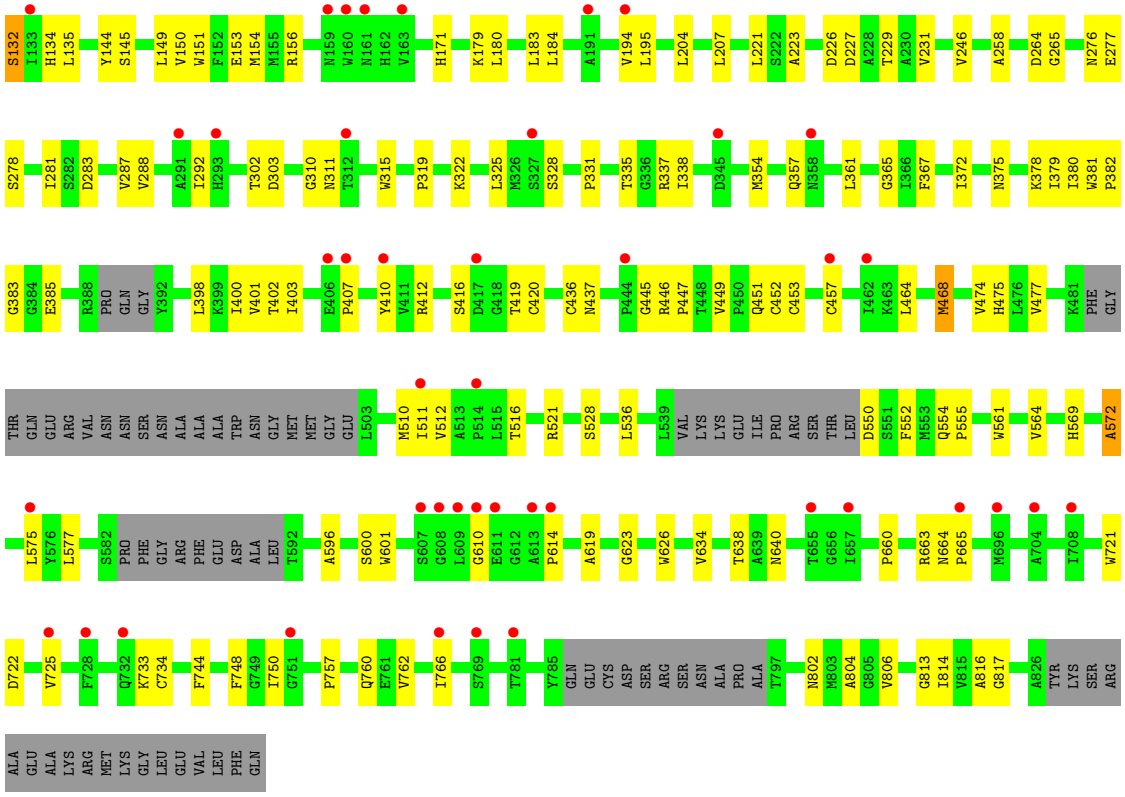
Chain A:



• Molecule 1: receptor subunit GluN1

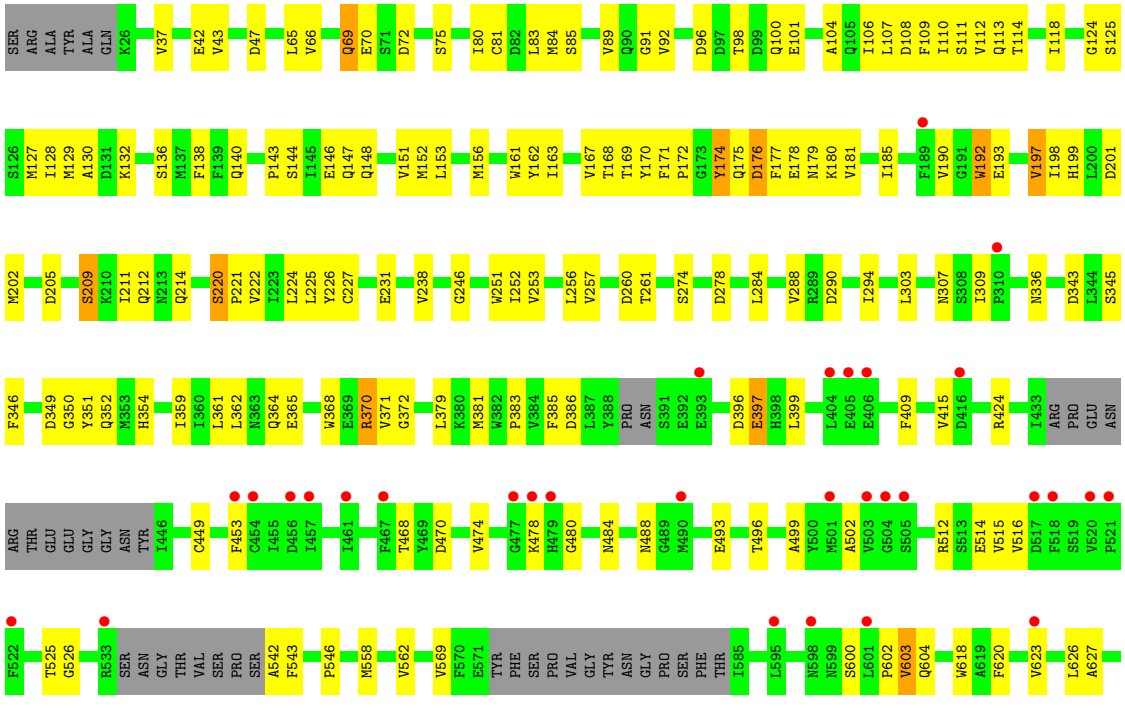
Chain C:

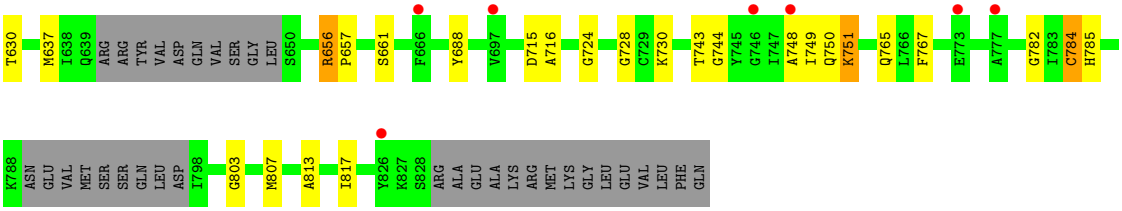




• Molecule 2: receptor subunit GluN2B

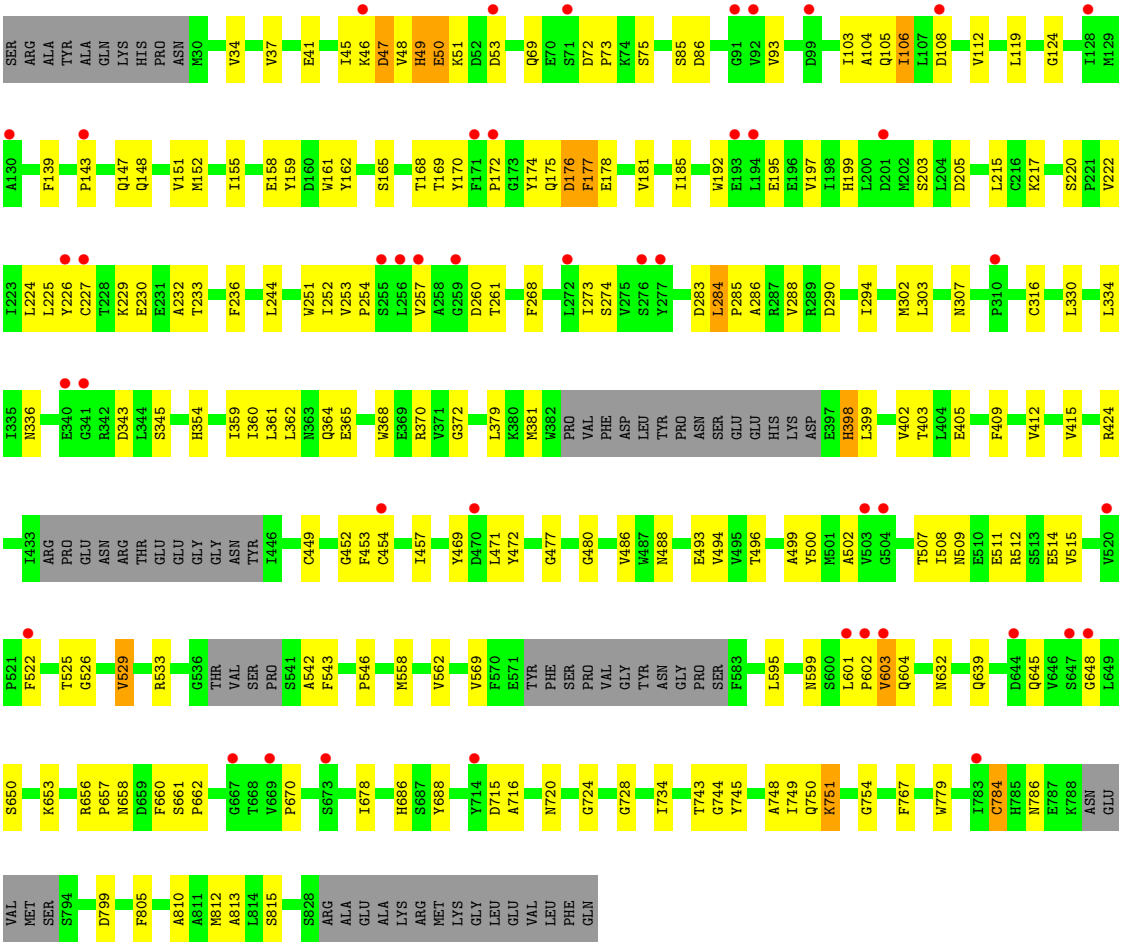
Chain B:





• Molecule 2: receptor subunit GluN2B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.49Å 118.43Å 226.59Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	29.96 – 3.77 29.96 – 3.77	Depositor EDS
% Data completeness (in resolution range)	83.2 (29.96-3.77) 83.0 (29.96-3.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1723)	Depositor
R, R_{free}	0.253 , 0.292 0.261 , 0.297	Depositor DCC
R_{free} test set	2393 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å^2)	102.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 154.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19547	wwPDB-VP
Average B, all atoms (Å^2)	218.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: QEM, 1AC, JEG, 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	0.45	0/5494	1.06	30/7543 (0.4%)
1	C	0.52	2/4653 (0.0%)	1.17	24/6433 (0.4%)
2	B	0.46	0/4832	1.13	32/6668 (0.5%)
2	D	0.49	1/4735 (0.0%)	1.16	32/6550 (0.5%)
All	All	0.48	3/19714 (0.0%)	1.13	118/27194 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
2	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	596	ALA	CA-CB	-7.36	1.41	1.53
1	C	572	ALA	CA-CB	-5.62	1.44	1.53
2	D	49	HIS	CA-C	-5.47	1.46	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	103	THR	CA-C-N	-12.67	104.81	121.91
1	C	103	THR	C-N-CA	-12.67	104.81	121.91
2	B	603	VAL	N-CA-C	11.48	124.78	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	69	GLN	N-CA-C	10.58	122.89	111.36
2	D	69	GLN	N-CA-C	-8.90	101.66	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	542	LYS	Peptide
2	B	246	GLY	Peptide
2	B	603	VAL	Peptide
2	D	603	VAL	Peptide

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	5383	0	4571	169	0
1	C	4582	0	3453	137	0
2	B	4752	0	3629	156	0
2	D	4664	0	3494	127	0
3	A	42	0	39	6	0
3	B	14	0	13	1	0
3	C	28	0	26	3	0
3	D	14	0	13	1	0
4	A	7	0	6	2	0
5	A	25	0	29	4	0
5	C	25	0	29	15	0
6	D	11	0	6	0	0
All	All	19547	0	15308	568	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 568 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:110:THR:HA	5:C:903:QEM:H03	1.31	1.10
1:C:32:VAL:HG21	1:C:74:MET:HE1	1.42	0.99
1:C:74:MET:HE3	1:C:107:ILE:HG13	1.45	0.95
5:C:903:QEM:H10	2:D:105:GLN:OE1	1.67	0.95
1:C:74:MET:HG3	1:C:107:ILE:HD11	1.50	0.94

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	788/823 (96%)	763 (97%)	24 (3%)	1 (0%)	48 79
1	C	738/823 (90%)	718 (97%)	20 (3%)	0	100 100
2	B	735/824 (89%)	705 (96%)	28 (4%)	2 (0%)	36 67
2	D	741/824 (90%)	712 (96%)	27 (4%)	2 (0%)	36 67
All	All	3002/3294 (91%)	2898 (96%)	99 (3%)	5 (0%)	43 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	399	LEU
1	A	799	THR
2	B	397	GLU
2	D	533	ARG
2	B	43	VAL

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	434/705 (62%)	427 (98%)	7 (2%)	55	68
1	C	294/705 (42%)	290 (99%)	4 (1%)	59	70
2	B	328/724 (45%)	322 (98%)	6 (2%)	51	66
2	D	307/724 (42%)	301 (98%)	6 (2%)	48	64
All	All	1363/2858 (48%)	1340 (98%)	23 (2%)	53	67

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	452	CYS
2	D	197	VAL
1	C	561	TRP
2	D	370	ARG
1	A	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	336	ASN
2	D	681	ASN
1	C	273	ASN
2	D	306	HIS
1	C	67	HIS

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)

11 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	903	-	14,14,15	3.34	2 (14%)	17,19,21	2.22	4 (23%)
6	JEG	D	902	-	9,11,11	2.70	5 (55%)	9,17,17	2.40	3 (33%)
3	NAG	A	901	1	14,14,15	0.21	0	17,19,21	0.69	0
3	NAG	D	901	2	14,14,15	0.44	0	17,19,21	0.67	0
5	QEM	A	905	-	27,27,27	0.84	1 (3%)	35,36,36	1.25	5 (14%)
3	NAG	B	901	-	14,14,15	1.55	1 (7%)	17,19,21	1.13	1 (5%)
3	NAG	C	902	-	14,14,15	1.76	2 (14%)	17,19,21	0.64	0
4	1AC	A	904	-	5,7,7	2.39	2 (40%)	6,11,11	3.33	3 (50%)
3	NAG	A	902	-	14,14,15	0.94	1 (7%)	17,19,21	0.71	1 (5%)
3	NAG	C	901	1	14,14,15	0.47	0	17,19,21	0.37	0
5	QEM	C	903	-	27,27,27	0.85	1 (3%)	35,36,36	1.18	4 (11%)

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	903	-	-	3/6/23/26	0/1/1/1
6	JEG	D	902	-	-	0/9/20/20	0/1/1/1
3	NAG	A	901	1	-	1/6/23/26	0/1/1/1
3	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	QEM	A	905	-	-	4/16/26/26	0/3/3/3
3	NAG	B	901	-	-	0/6/23/26	0/1/1/1
3	NAG	C	902	-	-	2/6/23/26	0/1/1/1
4	1AC	A	904	-	-	2/4/10/10	0/1/1/1
3	NAG	A	902	-	-	2/6/23/26	0/1/1/1
3	NAG	C	901	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	QEM	C	903	-	-	5/16/26/26	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	NAG	O5-C1	-11.84	1.23	1.43
3	B	901	NAG	O5-C1	-5.75	1.34	1.43
3	C	902	NAG	O5-C1	-5.72	1.34	1.43
6	D	902	JEG	C07-C08	-4.06	1.44	1.51
3	A	903	NAG	C1-C2	-3.71	1.47	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	903	NAG	C1-O5-C5	-6.97	102.85	112.19
4	A	904	1AC	CG-CA-CB	6.33	62.34	59.24
6	D	902	JEG	C06-C07-C08	5.63	128.79	116.96
3	B	901	NAG	C1-O5-C5	4.08	117.66	112.19
5	A	905	QEM	C11-N-C10	3.69	116.80	108.84

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	NAG	C3-C2-N2-C7
4	A	904	1AC	OXT-C-CA-CG
4	A	904	1AC	O-C-CA-CG
5	C	903	QEM	C13-C14-C15-O01
3	A	902	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	NAG	1	0
3	A	901	NAG	3	0
3	D	901	NAG	1	0
5	A	905	QEM	4	0
3	B	901	NAG	1	0
3	C	902	NAG	2	0
4	A	904	1AC	2	0

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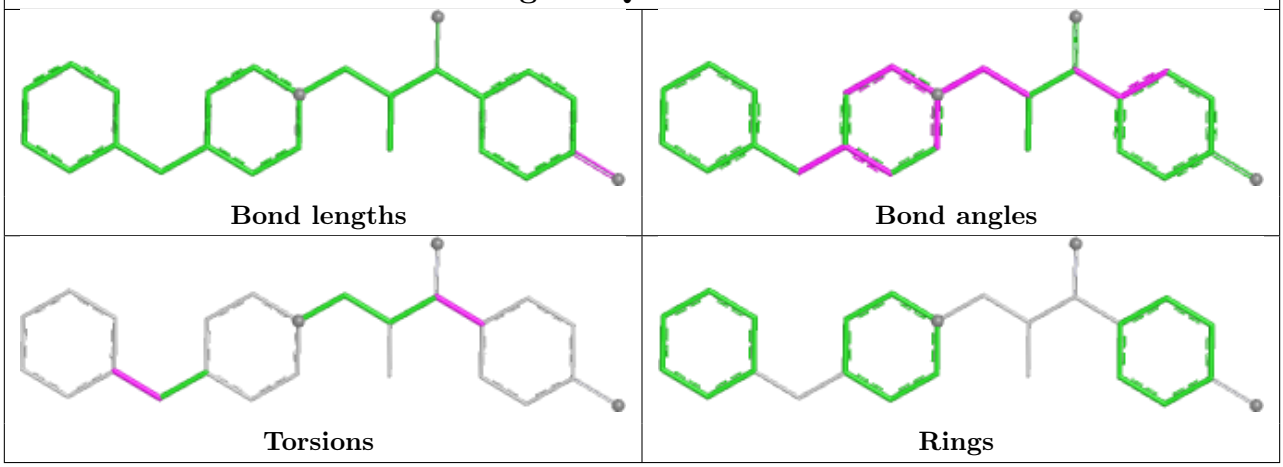
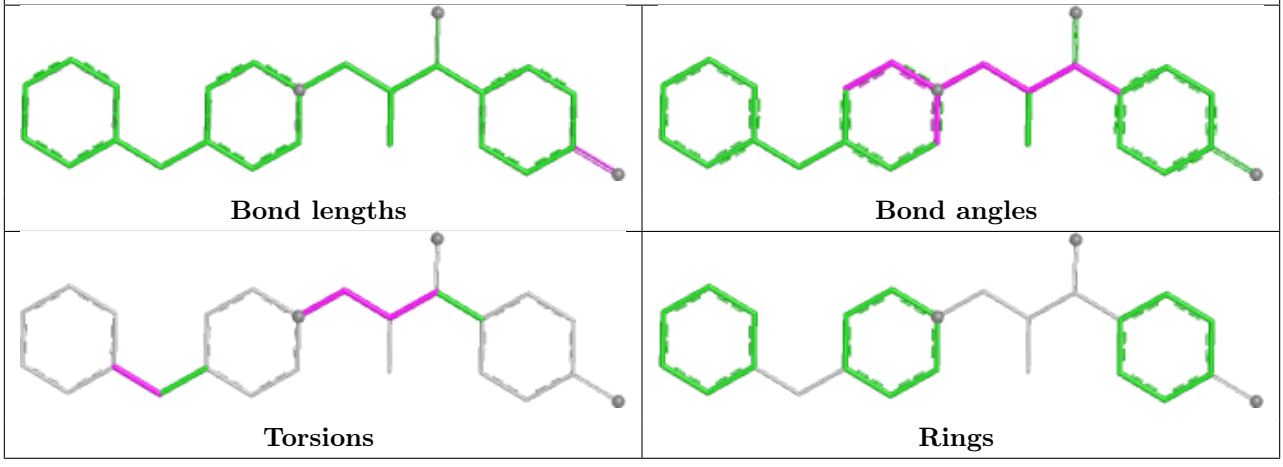
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	NAG	2	0
3	C	901	NAG	1	0
5	C	903	QEM	15	0

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 QEM A 905



Ligand QEM C 903



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, 95^{th} 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	796/823 (96%)	0.02	19 (2%)	59	40	41, 153, 321, 553	0
1	C	750/823 (91%)	0.39	49 (6%)	25	21	150, 269, 396, 519	0
2	B	749/824 (90%)	0.26	38 (5%)	33	25	63, 240, 383, 454	0
2	D	753/824 (91%)	0.24	44 (5%)	29	23	109, 220, 338, 497	0
All	All	3048/3294 (92%)	0.23	150 (4%)	35	26	41, 226, 370, 553	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	504	GLY	11.4
1	C	407	PRO	9.2
1	A	803	MET	8.2
2	B	405	GLU	8.1
1	C	607	SER	7.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

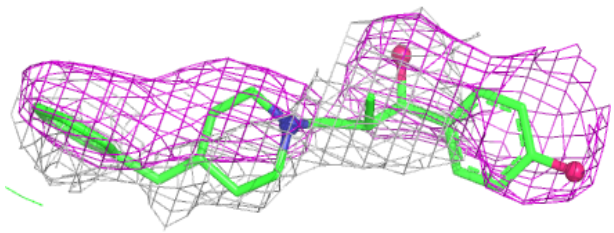
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

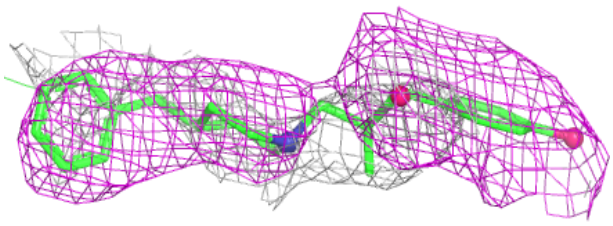
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	902	14/15	0.51	0.10	189,204,228,252	0
5	QEM	C	903	25/25	0.59	0.18	74,100,146,157	0
3	NAG	A	902	14/15	0.63	0.17	126,164,180,199	0
3	NAG	D	901	14/15	0.68	0.16	324,362,384,386	0
3	NAG	B	901	14/15	0.69	0.08	173,193,216,246	0
3	NAG	C	901	14/15	0.70	0.10	160,237,260,283	0
3	NAG	A	901	14/15	0.74	0.14	130,153,198,212	0
3	NAG	A	903	14/15	0.86	0.08	99,135,215,230	0
5	QEM	A	905	25/25	0.87	0.18	0,28,59,62	0
6	JEG	D	902	11/11	0.92	0.13	167,188,232,237	0
4	1AC	A	904	7/7	0.95	0.12	158,161,184,208	0

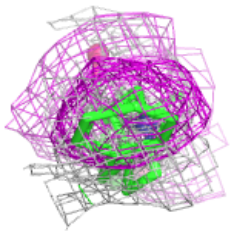
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QEM C 903:

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

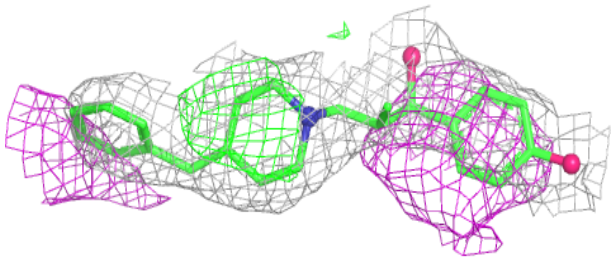


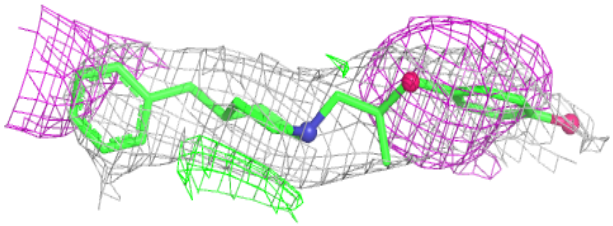


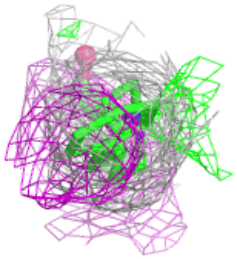


Electron density around QEM A 905:

$2mF_o$-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.