



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:36 PM GMT

PDB ID : 4PE5
Title : Crystal Structure of GluN1a/GluN2B NMDA Receptor Ion Channel
Authors : Karakas, E.; Furukawa, H.
Deposited on : 2014-04-22
Resolution : 3.96 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

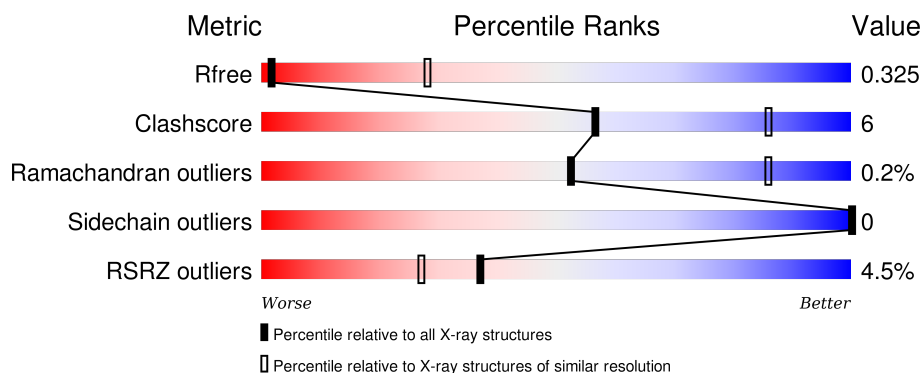
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	825	 4% 79% 11% 10%
1	C	825	 6% 82% 10% 9%
2	B	820	 2% 78% 10% 12%
2	D	820	 4% 79% 10% 11%

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
7	MAN	B	918	-	-	X	-
7	MAN	B	919	-	-	X	-
8	QEL	C	939	-	-	-	X
9	GLU	B	921	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20246 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5049	3173	884	967	25			
1	C	754	Total	C	N	O	S	0	0	0
			5026	3175	874	954	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP P35439
A	239	ASP	ASN	engineered mutation	UNP P35439
A	350	GLN	ASN	engineered mutation	UNP P35439
A	471	GLN	ASN	engineered mutation	UNP P35439
A	491	GLN	ASN	engineered mutation	UNP P35439
A	561	CYS	THR	engineered mutation	UNP P35439
A	594	GLN	GLU	engineered mutation	UNP P35439
A	595	SER	GLU	engineered mutation	UNP P35439
A	597	SER	GLU	engineered mutation	UNP P35439
A	598	THR	GLU	engineered mutation	UNP P35439
A	771	GLN	ASN	engineered mutation	UNP P35439
A	810	CYS	PHE	engineered mutation	UNP P35439
A	844	ASN	ARG	engineered mutation	UNP P35439
A	845	GLY	ARG	engineered mutation	UNP P35439
A	846	ALA	LYS	engineered mutation	UNP P35439
C	61	GLN	ASN	engineered mutation	UNP P35439
C	239	ASP	ASN	engineered mutation	UNP P35439
C	350	GLN	ASN	engineered mutation	UNP P35439
C	471	GLN	ASN	engineered mutation	UNP P35439
C	491	GLN	ASN	engineered mutation	UNP P35439
C	561	CYS	THR	engineered mutation	UNP P35439
C	594	GLN	GLU	engineered mutation	UNP P35439
C	595	SER	GLU	engineered mutation	UNP P35439
C	597	SER	GLU	engineered mutation	UNP P35439
C	598	THR	GLU	engineered mutation	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	GLN	ASN	engineered mutation	UNP P35439
C	810	CYS	PHE	engineered mutation	UNP P35439
C	844	ASN	ARG	engineered mutation	UNP P35439
C	845	GLY	ARG	engineered mutation	UNP P35439
C	846	ALA	LYS	engineered mutation	UNP P35439

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	720	Total	C	N	O	S	0	0	0
			4798	3048	788	933	29			
2	D	727	Total	C	N	O	S	0	0	0
			4777	3027	809	912	29			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	214	CYS	SER	engineered mutation	UNP Q00960
B	348	ASP	ASN	engineered mutation	UNP Q00960
B	?	-	CYS	deletion	UNP Q00960
B	?	-	PRO	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	557	CYS	ASP	engineered mutation	UNP Q00960
B	588	SER	CYS	engineered mutation	UNP Q00960
B	815	CYS	ILE	engineered mutation	UNP Q00960
B	838	SER	CYS	engineered mutation	UNP Q00960
B	849	SER	CYS	engineered mutation	UNP Q00960
D	214	CYS	SER	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960
D	?	-	CYS	deletion	UNP Q00960
D	?	-	PRO	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	557	CYS	ASP	engineered mutation	UNP Q00960
D	588	SER	CYS	engineered mutation	UNP Q00960
D	815	CYS	ILE	engineered mutation	UNP Q00960
D	838	SER	CYS	engineered mutation	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	849	SER	CYS	engineered mutation	UNP Q00960

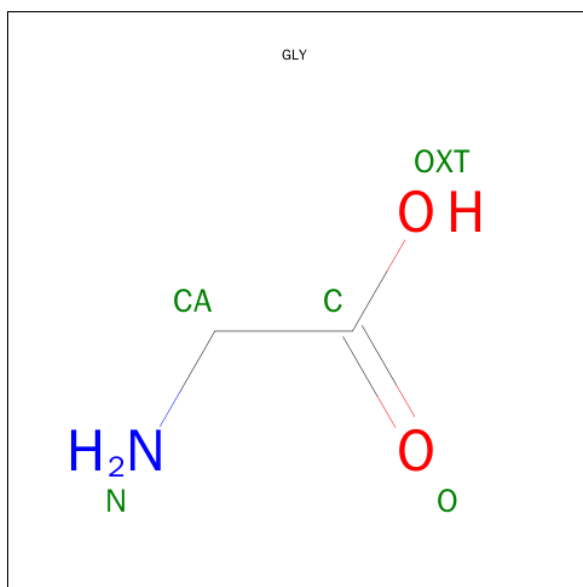
- Molecule 3 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	11	Total W 11 11	0	0
3	A	37	Total W 37 37	0	0
3	C	36	Total W 36 36	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

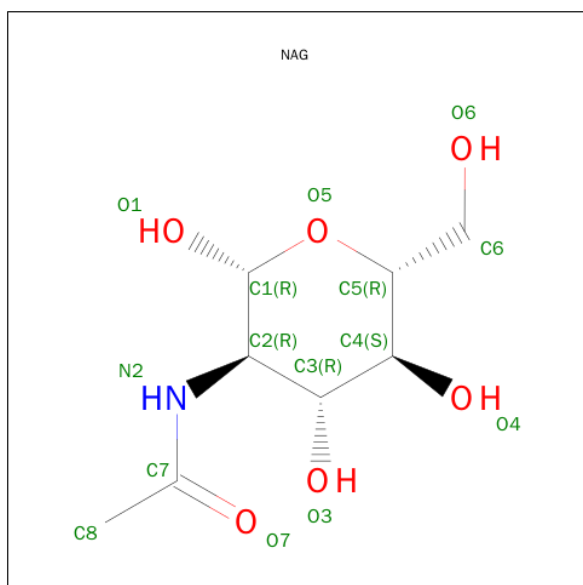
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total C N O 50 28 2 20	0	0
4	C	4	Total C N O 50 28 2 20	0	0
4	D	4	Total C N O 50 28 2 20	0	0

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

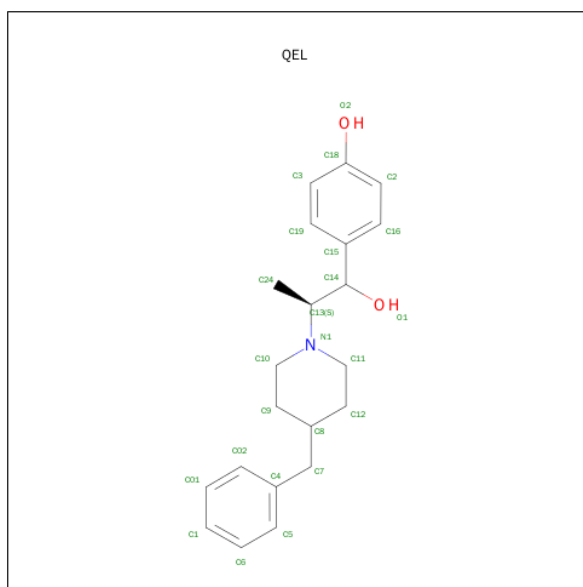


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1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

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

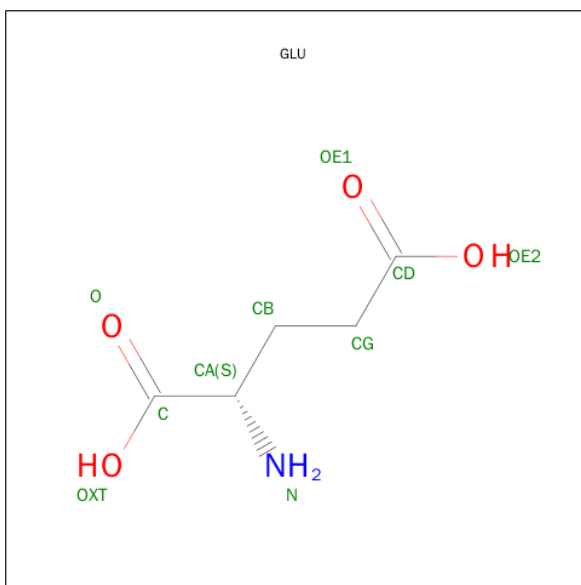
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	6	Total	C	N	O	0	0
			72	40	2	30		
7	B	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (three-letter code: QEL) (formula: C₂₁H₂₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			24	21	1	2		
8	C	1	Total	C	N	O	0	0
			24	21	1	2		

- Molecule 9 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



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

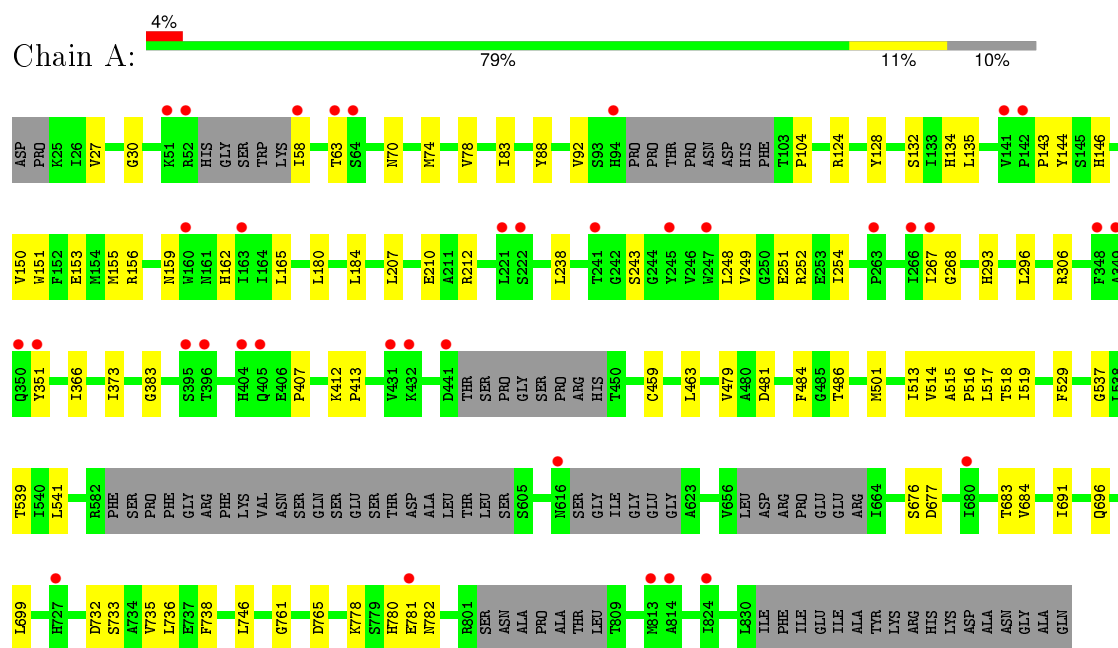
- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	2	Total	C	N	O	0	0
			28	16	2	10		

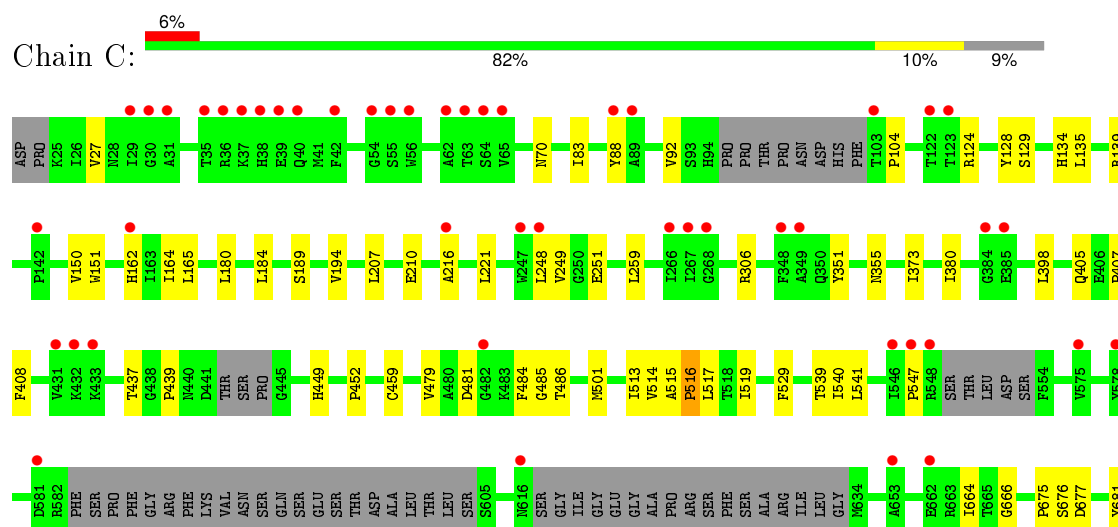
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Glutamate receptor ionotropic, NMDA 1

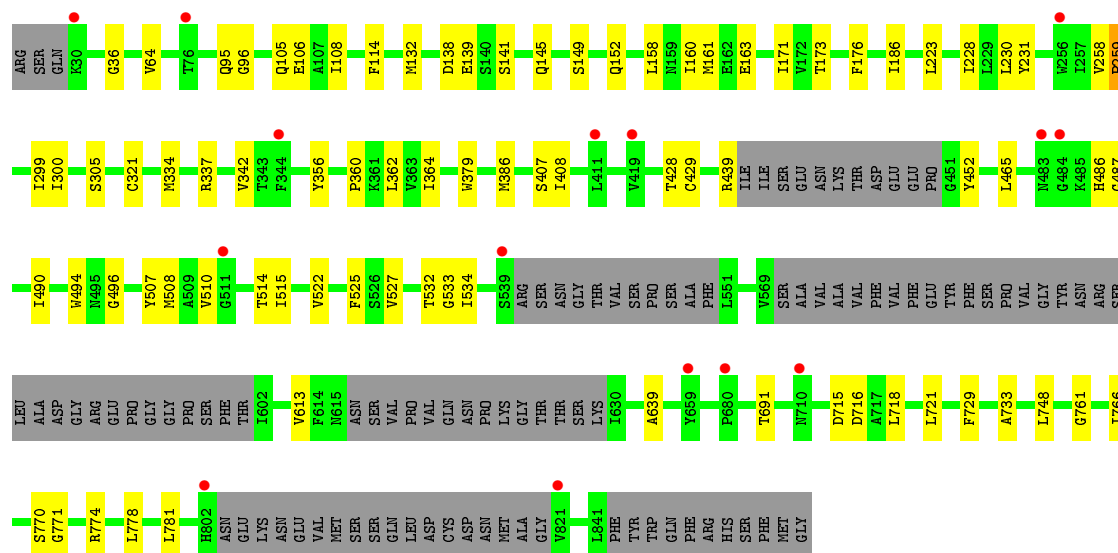
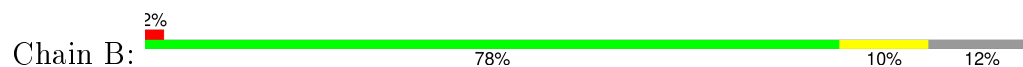


- Molecule 1: Glutamate receptor ionotropic, NMDA 1

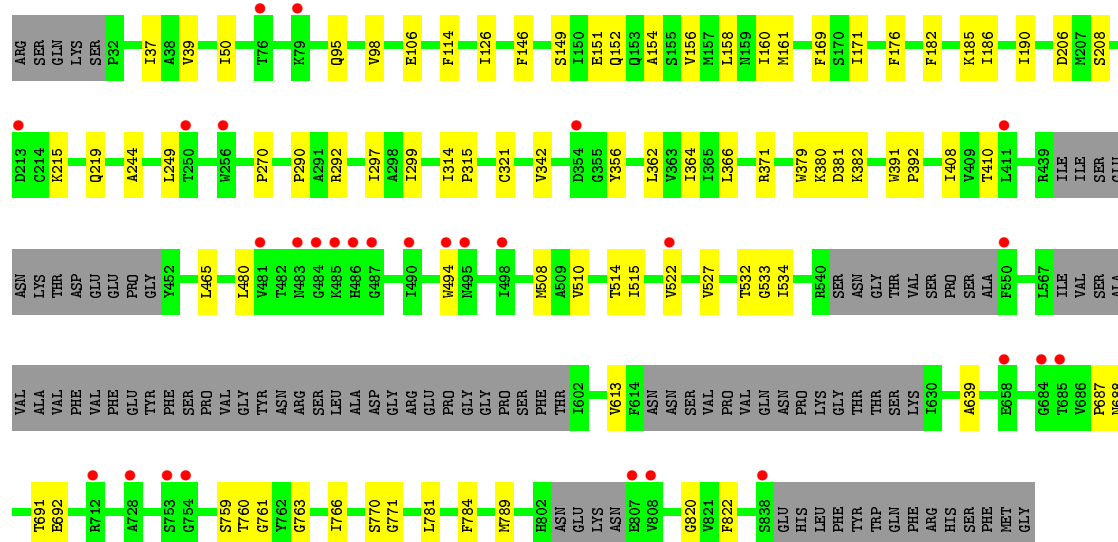
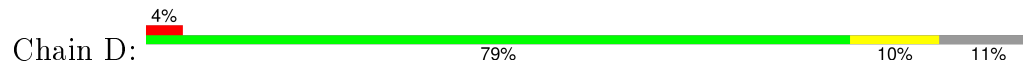




• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.83Å 163.19Å 163.14Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	29.72 – 3.96 47.55 – 3.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.72-3.96) 98.2 (47.55-3.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.256 , 0.295 0.292 , 0.325	Depositor DCC
R_{free} test set	2625 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	196.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 128.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 52201 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20246	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QEL, BMA, NAG, W, MAN

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	0.22	0/5138	0.42	0/7050
1	C	0.21	0/5118	0.41	0/7035
2	B	0.20	0/4884	0.35	0/6718
2	D	0.21	0/4862	0.40	0/6682
All	All	0.21	0/20002	0.40	0/27485

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 [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	5049	0	4271	55	0
1	C	5026	0	4204	49	0
2	B	4798	0	3981	51	0
2	D	4777	0	3881	56	0
3	A	37	0	0	0	0
3	B	11	0	0	0	0
3	C	36	0	0	0	0
4	A	50	0	43	1	0
4	C	50	0	43	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	50	0	43	1	0
5	A	5	0	2	2	0
5	C	5	0	2	0	0
6	A	42	0	39	0	0
6	B	28	0	26	0	0
6	C	14	0	13	0	0
6	D	28	0	26	0	0
7	A	72	0	61	0	0
7	B	72	0	61	12	0
8	B	24	0	26	6	0
8	C	24	0	26	6	0
9	B	10	0	5	2	0
9	D	10	0	5	1	0
10	C	28	0	25	2	0
All	All	20246	0	16783	224	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 6.

The worst 5 of 224 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)
7:B:918:MAN:H61	7:B:919:MAN:H3	1.37	1.00
2:D:514:THR:HG1	9:D:907:GLU:N	1.69	0.90
7:B:918:MAN:H61	7:B:919:MAN:C3	2.00	0.86
2:B:114:PHE:CB	8:B:920:QEL:H6	2.10	0.80
4:C:943:NAG:C3	4:C:944:BMA:H2	2.16	0.75

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	727/825 (88%)	667 (92%)	59 (8%)	1 (0%)	56	89
1	C	742/825 (90%)	681 (92%)	58 (8%)	3 (0%)	39	79
2	B	708/820 (86%)	656 (93%)	50 (7%)	2 (0%)	46	82
2	D	715/820 (87%)	656 (92%)	58 (8%)	1 (0%)	56	89
All	All	2892/3290 (88%)	2660 (92%)	225 (8%)	7 (0%)	52	86

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	547	PRO
2	B	490	ILE
2	D	381	ASP
2	B	259	PRO
1	C	516	PRO

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 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	422/710 (59%)	422 (100%)	0	100	100
1	C	402/710 (57%)	402 (100%)	0	100	100
2	B	394/716 (55%)	394 (100%)	0	100	100
2	D	368/716 (51%)	368 (100%)	0	100	100
All	All	1586/2852 (56%)	1586 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	355	ASN
2	D	486	HIS
2	D	180	GLN

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Mol	Chain	Res	Type
1	A	355	ASN
2	D	311	HIS

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 ⓘ

26 carbohydrates 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	A	938	1,4	14,14,15	0.30	0	15,19,21	0.39	0
4	NAG	A	939	4	14,14,15	0.27	0	15,19,21	0.52	0
4	BMA	A	940	4	11,11,12	0.26	0	14,15,17	0.60	0
4	MAN	A	941	4	11,11,12	0.25	0	14,15,17	0.60	0
7	NAG	A	946	1,7	14,14,15	0.66	1 (7%)	15,19,21	0.97	1 (6%)
7	NAG	A	947	7	14,14,15	0.30	0	15,19,21	0.21	0
7	BMA	A	948	7	11,11,12	1.03	1 (9%)	14,15,17	1.95	4 (28%)
7	MAN	A	949	7	11,11,12	0.68	0	14,15,17	1.10	2 (14%)
7	MAN	A	950	7	11,11,12	0.67	0	14,15,17	1.09	2 (14%)
7	MAN	A	951	7	11,11,12	0.67	0	14,15,17	1.11	2 (14%)
7	NAG	B	914	2,7	14,14,15	0.28	0	15,19,21	0.29	0
7	NAG	B	915	7	14,14,15	0.25	0	15,19,21	0.26	0
7	BMA	B	916	7	11,11,12	0.26	0	14,15,17	0.60	0
7	MAN	B	917	7	11,11,12	0.25	0	14,15,17	0.60	0
7	MAN	B	918	7	11,11,12	0.27	0	14,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	B	919	7	11,11,12	0.25	0	14,15,17	0.74	0
10	NAG	C	937	1,10	14,14,15	0.30	0	15,19,21	0.95	1 (6%)
10	NAG	C	938	10	14,14,15	0.37	0	15,19,21	0.29	0
4	NAG	C	942	1,4	14,14,15	0.19	0	15,19,21	0.29	0
4	NAG	C	943	4	14,14,15	0.40	0	15,19,21	0.87	0
4	BMA	C	944	4	11,11,12	0.26	0	14,15,17	0.81	0
4	MAN	C	945	4	11,11,12	0.67	0	14,15,17	1.09	2 (14%)
4	NAG	D	903	2,4	14,14,15	0.20	0	15,19,21	0.44	0
4	NAG	D	904	4	14,14,15	0.27	0	15,19,21	0.53	0
4	BMA	D	905	4	11,11,12	0.26	0	14,15,17	0.60	0
4	MAN	D	906	4	11,11,12	0.26	0	14,15,17	0.61	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	A	938	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	939	4	-	0/6/23/26	0/1/1/1
4	BMA	A	940	4	-	0/2/19/22	0/1/1/1
4	MAN	A	941	4	-	0/2/19/22	0/1/1/1
7	NAG	A	946	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	947	7	-	0/6/23/26	0/1/1/1
7	BMA	A	948	7	-	0/2/19/22	0/1/1/1
7	MAN	A	949	7	-	0/2/19/22	0/1/1/1
7	MAN	A	950	7	-	0/2/19/22	0/1/1/1
7	MAN	A	951	7	-	0/2/19/22	0/1/1/1
7	NAG	B	914	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	915	7	-	0/6/23/26	0/1/1/1
7	BMA	B	916	7	-	0/2/19/22	0/1/1/1
7	MAN	B	917	7	-	0/2/19/22	0/1/1/1
7	MAN	B	918	7	-	0/2/19/22	0/1/1/1
7	MAN	B	919	7	-	0/2/19/22	0/1/1/1
10	NAG	C	937	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	938	10	-	0/6/23/26	0/1/1/1
4	NAG	C	942	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	943	4	-	0/6/23/26	0/1/1/1
4	BMA	C	944	4	-	0/2/19/22	0/1/1/1
4	MAN	C	945	4	-	0/2/19/22	0/1/1/1
4	NAG	D	903	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	904	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	D	905	4	-	0/2/19/22	0/1/1/1
4	MAN	D	906	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	946	NAG	C1-C2	2.17	1.55	1.52
7	A	948	BMA	C4-C5	2.33	1.58	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	945	MAN	O2-C2-C3	-2.24	105.62	110.12
7	A	950	MAN	O2-C2-C3	-2.23	105.62	110.12
7	A	951	MAN	O2-C2-C3	-2.19	105.71	110.12
7	A	949	MAN	O2-C2-C3	-2.19	105.72	110.12
4	C	945	MAN	C1-O5-C5	2.38	115.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	938	NAG	1	0
7	B	916	BMA	2	0
7	B	917	MAN	2	0
7	B	918	MAN	10	0
7	B	919	MAN	10	0
10	C	937	NAG	2	0
4	C	943	NAG	4	0
4	C	944	BMA	4	0
4	D	903	NAG	1	0

5.6 Ligand geometry

Of 98 ligands modelled in this entry, 84 are monoatomic - leaving 14 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
5	GLY	A	942	-	1,4,4	0.53	0	0,4,4	0.00	-
6	NAG	A	943	1	14,14,15	0.27	0	15,19,21	0.40	0
6	NAG	A	944	1	14,14,15	0.21	0	15,19,21	0.26	0
6	NAG	A	945	1	14,14,15	0.23	0	15,19,21	0.60	1 (6%)
6	NAG	B	912	2	14,14,15	0.20	0	15,19,21	0.22	0
6	NAG	B	913	2	14,14,15	0.21	0	15,19,21	0.33	0
8	QEL	B	920	-	26,26,26	2.61	8 (30%)	34,35,35	1.82	8 (23%)
9	GLU	B	921	-	3,9,9	0.36	0	2,11,11	0.06	0
8	QEL	C	939	-	26,26,26	2.46	8 (30%)	34,35,35	1.91	8 (23%)
5	GLY	C	940	-	1,4,4	0.53	0	0,4,4	0.00	-
6	NAG	C	941	1	14,14,15	0.22	0	15,19,21	0.35	0
6	NAG	D	901	2	14,14,15	0.27	0	15,19,21	0.19	0
6	NAG	D	902	2	14,14,15	0.54	0	15,19,21	0.89	1 (6%)
9	GLU	D	907	-	3,9,9	0.37	0	2,11,11	0.03	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
5	GLY	A	942	-	-	0/0/2/2	0/0/0/0
6	NAG	A	943	1	-	0/6/23/26	0/1/1/1
6	NAG	A	944	1	-	0/6/23/26	0/1/1/1
6	NAG	A	945	1	-	0/6/23/26	0/1/1/1
6	NAG	B	912	2	-	0/6/23/26	0/1/1/1
6	NAG	B	913	2	-	0/6/23/26	0/1/1/1
8	QEL	B	920	-	-	0/16/26/26	0/3/3/3
9	GLU	B	921	-	-	0/3/9/9	0/0/0/0
8	QEL	C	939	-	-	0/16/26/26	0/3/3/3
5	GLY	C	940	-	-	0/0/2/2	0/0/0/0
6	NAG	C	941	1	-	0/6/23/26	0/1/1/1
6	NAG	D	901	2	-	0/6/23/26	0/1/1/1
6	NAG	D	902	2	-	0/6/23/26	0/1/1/1
9	GLU	D	907	-	-	0/3/9/9	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	920	QEL	O1-C14	-9.92	1.22	1.42
8	C	939	QEL	O1-C14	-8.92	1.24	1.42
8	B	920	QEL	C14-C13	-3.47	1.49	1.54
8	C	939	QEL	C14-C13	-3.46	1.49	1.54
8	B	920	QEL	C3-C18	-3.07	1.32	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	939	QEL	C24-C13-C14	-4.44	104.64	111.80
8	B	920	QEL	C24-C13-C14	-4.40	104.70	111.80
8	B	920	QEL	C12-C8-C7	-4.32	102.14	111.84
8	C	939	QEL	C12-C8-C7	-4.31	102.16	111.84
8	C	939	QEL	C19-C15-C14	-2.44	117.15	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	942	GLY	2	0
8	B	920	QEL	6	0
9	B	921	GLU	2	0
8	C	939	QEL	6	0
9	D	907	GLU	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	743/825 (90%)	-0.00	36 (4%) 34 25	125, 207, 315, 377	0
1	C	754/825 (91%)	0.13	52 (6%) 20 13	122, 208, 319, 371	0
2	B	720/820 (87%)	-0.16	15 (2%) 67 55	107, 181, 281, 330	0
2	D	727/820 (88%)	-0.08	29 (3%) 42 31	109, 188, 296, 327	0
All	All	2944/3290 (89%)	-0.03	132 (4%) 37 27	107, 198, 305, 377	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	SER	10.1
1	C	63	THR	7.3
1	C	40	GLN	6.7
1	C	216	ALA	6.2
1	C	62	ALA	5.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MAN	A	941	11/12	0.72	0.41	-	350,359,369,372	0
4	BMA	C	944	11/12	0.81	0.36	-	329,341,349,357	0
4	NAG	D	904	14/15	0.65	0.20	-	326,333,354,356	0
4	NAG	D	903	14/15	0.88	0.41	-	315,318,332,336	0
10	NAG	C	938	14/15	0.86	0.15	-	261,293,304,310	0
7	MAN	B	917	11/12	0.54	0.20	-	341,359,367,368	0
7	NAG	B	915	14/15	0.80	0.47	-	338,346,358,359	0
4	BMA	A	940	11/12	0.44	0.24	-	344,347,352,356	0
4	MAN	D	906	11/12	0.88	0.57	-	337,350,357,358	0
7	NAG	A	947	14/15	0.72	0.37	-	333,348,360,363	0
4	NAG	A	939	14/15	0.78	0.26	-	332,342,355,358	0
7	NAG	A	946	14/15	0.87	0.77	-	326,338,347,348	0
7	MAN	B	919	11/12	0.73	0.23	-	334,337,358,366	0
4	NAG	C	942	14/15	0.81	0.26	-	328,347,354,358	0
4	MAN	C	945	11/12	0.56	0.33	-	351,356,359,359	0
7	BMA	B	916	11/12	0.61	0.32	-	352,360,364,366	0
7	MAN	A	950	11/12	0.58	0.34	-	348,357,368,370	0
7	BMA	A	948	11/12	0.67	0.34	-	359,362,364,364	0
7	MAN	B	918	11/12	0.60	0.41	-	352,356,361,365	0
7	MAN	A	949	11/12	0.64	0.28	-	332,362,370,371	0
7	NAG	B	914	14/15	0.86	0.32	-	315,322,327,332	0
10	NAG	C	937	14/15	0.93	0.15	-	250,262,281,288	0
4	NAG	A	938	14/15	0.81	0.21	-	315,315,334,335	0
4	NAG	C	943	14/15	0.70	0.22	-	340,349,351,352	0
7	MAN	A	951	11/12	0.84	0.12	-	328,350,358,360	0
4	BMA	D	905	11/12	0.80	0.49	-	339,348,354,356	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	GLU	B	921	10/10	0.89	0.46	1.43	183,200,227,229	0
8	QEL	C	939	24/24	0.85	0.41	1.40	107,135,151,160	0
8	QEL	B	920	24/24	0.86	0.31	0.87	100,133,155,170	0
5	GLY	A	942	5/5	0.93	0.23	-0.67	166,169,185,190	0
9	GLU	D	907	10/10	0.85	0.21	-0.95	196,208,232,234	0
5	GLY	C	940	5/5	0.93	0.22	-1.14	180,183,189,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	W	A	903	1/1	0.98	0.15	-	336,336,336,336	1
3	W	A	904	1/1	0.99	0.10	-	214,214,214,214	1
3	W	C	912	1/1	0.93	0.06	-	549,549,549,549	1
3	W	C	905	1/1	0.96	0.13	-	550,550,550,550	1
3	W	B	905	1/1	0.95	0.08	-	398,398,398,398	1
3	W	A	926	1/1	0.99	0.05	-	443,443,443,443	1
3	W	C	907	1/1	0.94	0.06	-	537,537,537,537	1
3	W	A	922	1/1	0.95	0.10	-	542,542,542,542	1
3	W	B	906	1/1	0.96	0.07	-	550,550,550,550	1
3	W	A	912	1/1	0.99	0.10	-	196,196,196,196	1
3	W	C	926	1/1	0.99	0.13	-	449,449,449,449	1
3	W	A	920	1/1	0.95	0.07	-	549,549,549,549	1
3	W	A	929	1/1	0.97	0.07	-	492,492,492,492	1
3	W	C	906	1/1	0.94	0.06	-	550,550,550,550	1
3	W	A	925	1/1	0.95	0.11	-	463,463,463,463	1
3	W	B	910	1/1	1.00	0.06	-	520,520,520,520	1
3	W	A	930	1/1	0.95	0.09	-	450,450,450,450	1
6	NAG	D	901	14/15	0.82	0.49	-	220,253,260,261	0
3	W	C	921	1/1	0.98	0.04	-	386,386,386,386	1
3	W	A	933	1/1	0.90	0.07	-	486,486,486,486	1
3	W	C	911	1/1	0.98	0.07	-	550,550,550,550	1
3	W	A	915	1/1	0.99	0.06	-	550,550,550,550	1
3	W	A	910	1/1	0.96	0.11	-	171,171,171,171	1
6	NAG	B	913	14/15	0.82	0.30	-	197,221,231,235	0
3	W	C	910	1/1	0.77	0.08	-	447,447,447,447	1
3	W	C	909	1/1	0.97	0.04	-	550,550,550,550	1
3	W	A	923	1/1	0.93	0.16	-	515,515,515,515	1
3	W	C	920	1/1	0.98	0.04	-	473,473,473,473	1
3	W	C	933	1/1	0.99	0.03	-	529,529,529,529	1
3	W	A	932	1/1	0.99	0.04	-	473,473,473,473	1
6	NAG	A	944	14/15	0.64	0.41	-	270,308,315,318	0
3	W	A	936	1/1	0.99	0.07	-	473,473,473,473	1
6	NAG	D	902	14/15	0.83	0.26	-	210,244,253,265	0
3	W	C	919	1/1	0.99	0.05	-	467,467,467,467	1
3	W	B	909	1/1	0.98	0.05	-	550,550,550,550	1
3	W	A	916	1/1	0.97	0.06	-	542,542,542,542	1
3	W	A	937	1/1	0.93	0.13	-	408,408,408,408	1
3	W	A	935	1/1	0.97	0.05	-	495,495,495,495	1
3	W	A	907	1/1	0.95	0.15	-	212,212,212,212	1
6	NAG	A	943	14/15	0.82	0.26	-	229,244,260,264	0
3	W	A	931	1/1	0.99	0.09	-	456,456,456,456	1
3	W	A	927	1/1	0.99	0.05	-	491,491,491,491	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	W	C	935	1/1	0.98	0.07	-	479,479,479,479	1
3	W	A	905	1/1	0.97	0.13	-	209,209,209,209	1
3	W	A	919	1/1	0.95	0.08	-	522,522,522,522	1
3	W	A	921	1/1	0.99	0.04	-	550,550,550,550	1
3	W	C	931	1/1	0.98	0.08	-	475,475,475,475	1
3	W	C	930	1/1	0.99	0.02	-	465,465,465,465	1
3	W	A	902	1/1	0.99	0.11	-	205,205,205,205	1
6	NAG	C	941	14/15	0.82	0.25	-	281,293,309,312	0
3	W	A	924	1/1	0.98	0.06	-	526,526,526,526	1
3	W	C	932	1/1	0.98	0.05	-	540,540,540,540	1
3	W	B	907	1/1	0.98	0.04	-	550,550,550,550	1
3	W	B	903	1/1	0.99	0.10	-	438,438,438,438	1
3	W	C	924	1/1	0.99	0.04	-	465,465,465,465	1
3	W	B	901	1/1	0.98	0.07	-	312,312,312,312	1
3	W	B	911	1/1	0.98	0.05	-	489,489,489,489	1
3	W	C	915	1/1	0.99	0.03	-	496,496,496,496	1
3	W	B	908	1/1	0.96	0.05	-	511,511,511,511	1
3	W	C	904	1/1	0.97	0.07	-	533,533,533,533	1
3	W	A	901	1/1	0.99	0.17	-	337,337,337,337	1
3	W	B	904	1/1	0.93	0.13	-	417,417,417,417	1
3	W	C	925	1/1	0.99	0.03	-	475,475,475,475	1
3	W	A	914	1/1	0.96	0.11	-	514,514,514,514	1
3	W	C	922	1/1	0.99	0.04	-	378,378,378,378	1
3	W	C	923	1/1	0.97	0.05	-	320,320,320,320	1
3	W	C	936	1/1	0.97	0.05	-	478,478,478,478	1
3	W	C	902	1/1	0.90	0.09	-	525,525,525,525	1
3	W	A	911	1/1	0.98	0.10	-	251,251,251,251	1
3	W	A	913	1/1	0.97	0.18	-	509,509,509,509	1
3	W	A	917	1/1	0.95	0.10	-	523,523,523,523	1
6	NAG	B	912	14/15	0.84	0.24	-	224,261,273,280	0
3	W	C	913	1/1	0.98	0.10	-	366,366,366,366	1
3	W	A	908	1/1	1.00	0.08	-	260,260,260,260	1
3	W	C	917	1/1	0.95	0.09	-	433,433,433,433	1
3	W	A	906	1/1	0.98	0.14	-	213,213,213,213	1
3	W	C	934	1/1	0.96	0.05	-	466,466,466,466	1
3	W	C	916	1/1	0.99	0.05	-	456,456,456,456	1
3	W	B	902	1/1	0.96	0.11	-	404,404,404,404	1
6	NAG	A	945	14/15	0.36	0.27	-	293,330,339,339	0
3	W	C	914	1/1	0.99	0.03	-	484,484,484,484	1
3	W	C	903	1/1	0.92	0.09	-	516,516,516,516	1
3	W	A	934	1/1	0.98	0.07	-	394,394,394,394	1
3	W	C	928	1/1	0.98	0.07	-	441,441,441,441	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	W	C	908	1/1	0.94	0.06	-	550,550,550,550	1
3	W	C	918	1/1	0.99	0.07	-	398,398,398,398	1
3	W	C	901	1/1	0.94	0.12	-	489,489,489,489	1
3	W	C	929	1/1	0.99	0.03	-	426,426,426,426	1
3	W	C	927	1/1	0.98	0.06	-	494,494,494,494	1
3	W	A	928	1/1	0.98	0.03	-	426,426,426,426	1
3	W	A	918	1/1	0.96	0.08	-	549,549,549,549	1
3	W	A	909	1/1	0.98	0.11	-	312,312,312,312	1

6.5 Other polymers

There are no such residues in this entry.