



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

Nov 1, 2017 – 11:44 PM EDT

PDB ID : 5VHZ  
EMDB ID: : EMD-8688  
Title : GluA2-2xGSG1L bound to L-Quisqualate  
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.  
Deposited on : unknown  
Resolution : 8.40 Å(reported)

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

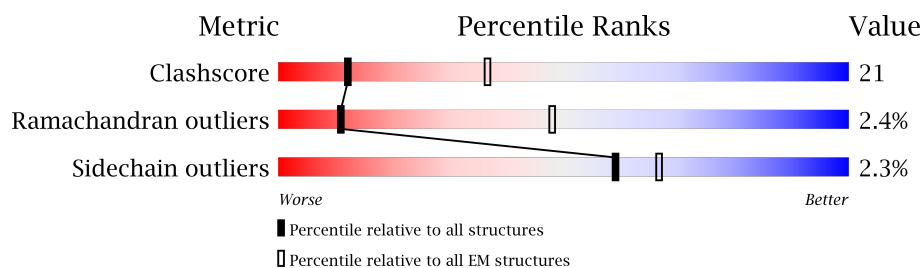
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1057	
1	B	1057	
1	C	1057	
1	D	1057	
1	E	1057	
1	F	1057	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27460 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 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	E	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		
1	F	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

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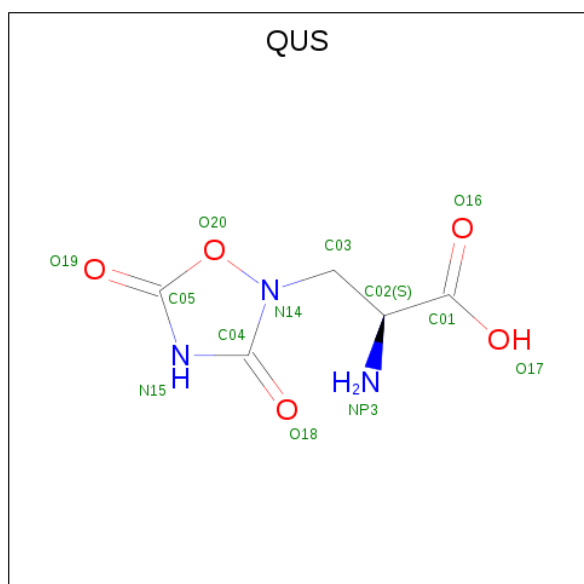
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491
F	-588	GLU	ASN	conflict	UNP P19491
F	-447	LEU	VAL	conflict	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	THR	deletion	UNP P19491
F	?	-	GLU	deletion	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	PRO	deletion	UNP P19491
F	?	-	SER	deletion	UNP P19491
F	-445	GLU	GLY	conflict	UNP P19491
F	-444	ASP	ASN	conflict	UNP P19491
F	-437	GLN	ASN	conflict	UNP P19491
F	-2	GLY	-	linker	UNP P19491
F	-1	THR	-	linker	UNP P19491
F	0	GLY	-	linker	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>5</sub>).

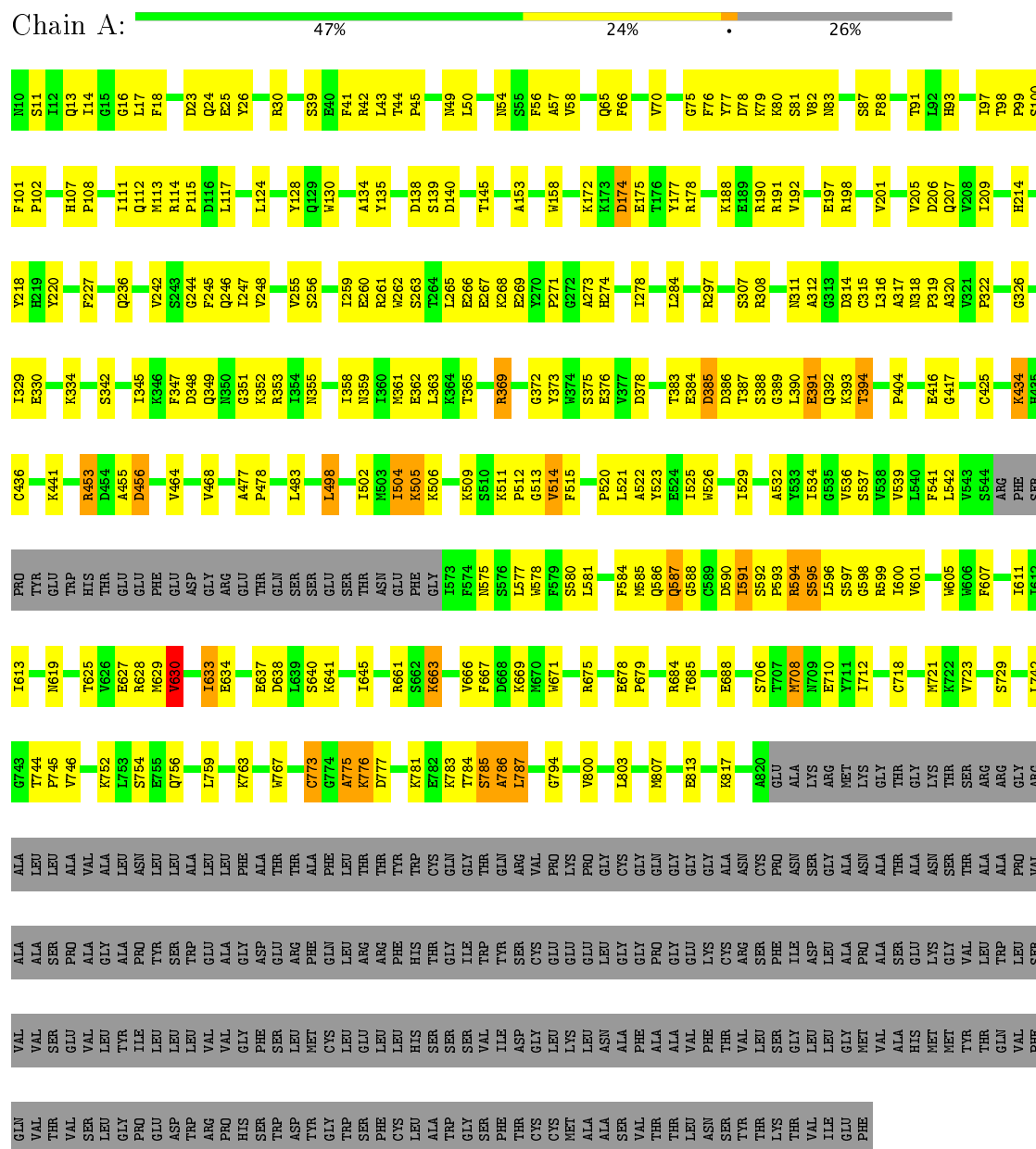


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 13	C 5	N 3	O 5	0
2	B	1	Total 13	C 5	N 3	O 5	0
2	C	1	Total 13	C 5	N 3	O 5	0
2	D	1	Total 13	C 5	N 3	O 5	0

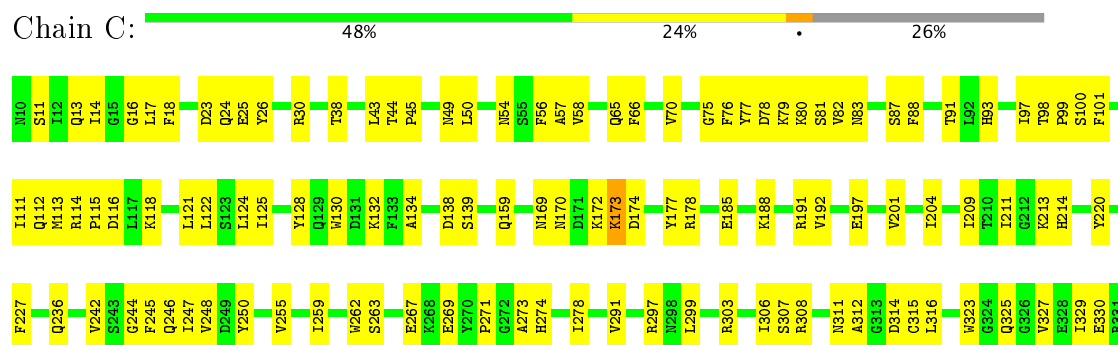
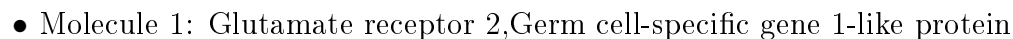
### 3 Residue-property plots

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 2, Germ cell-specific gene 1-like protein

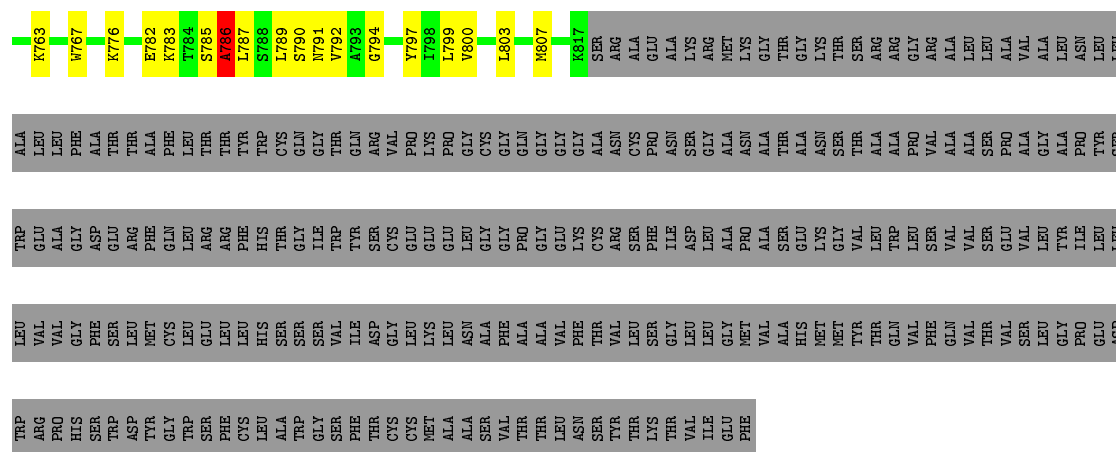


- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

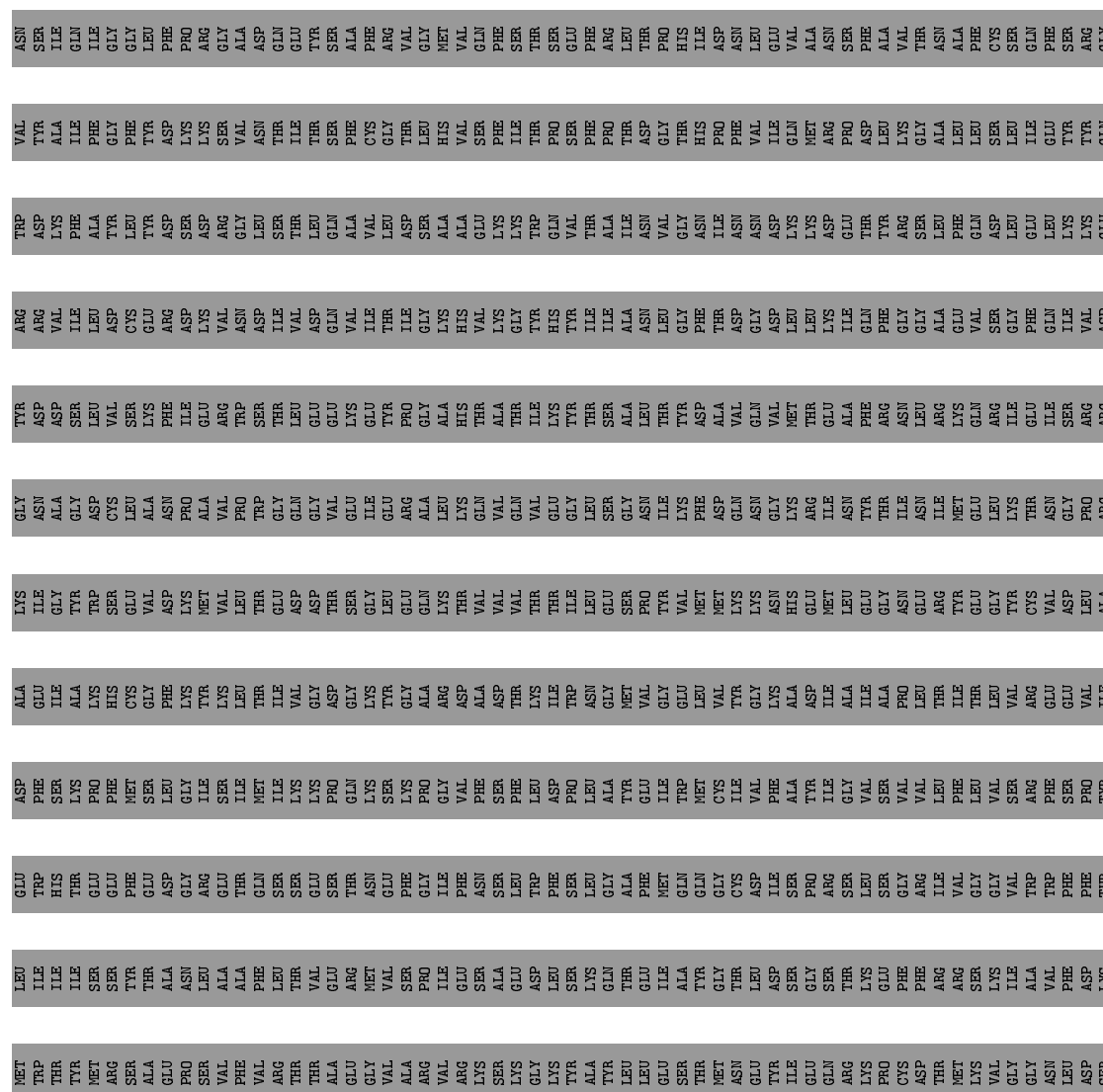


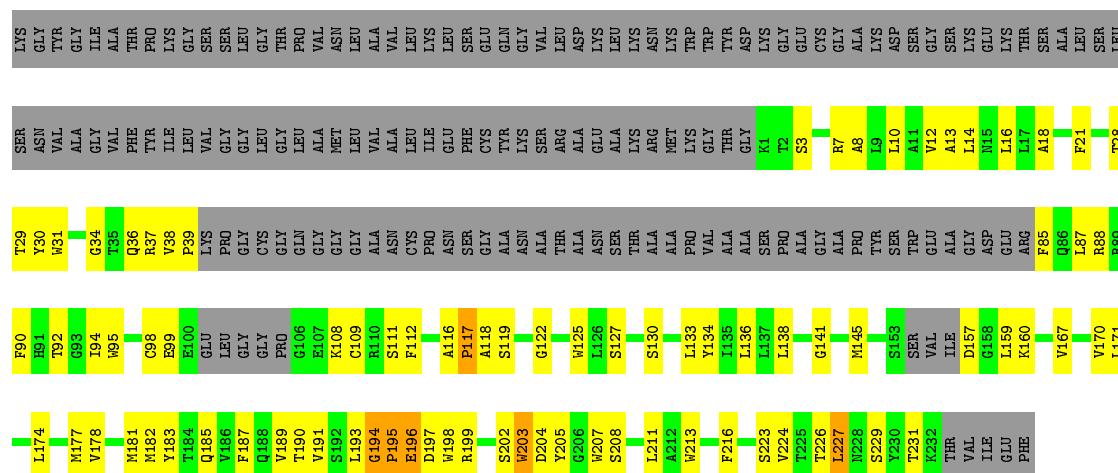






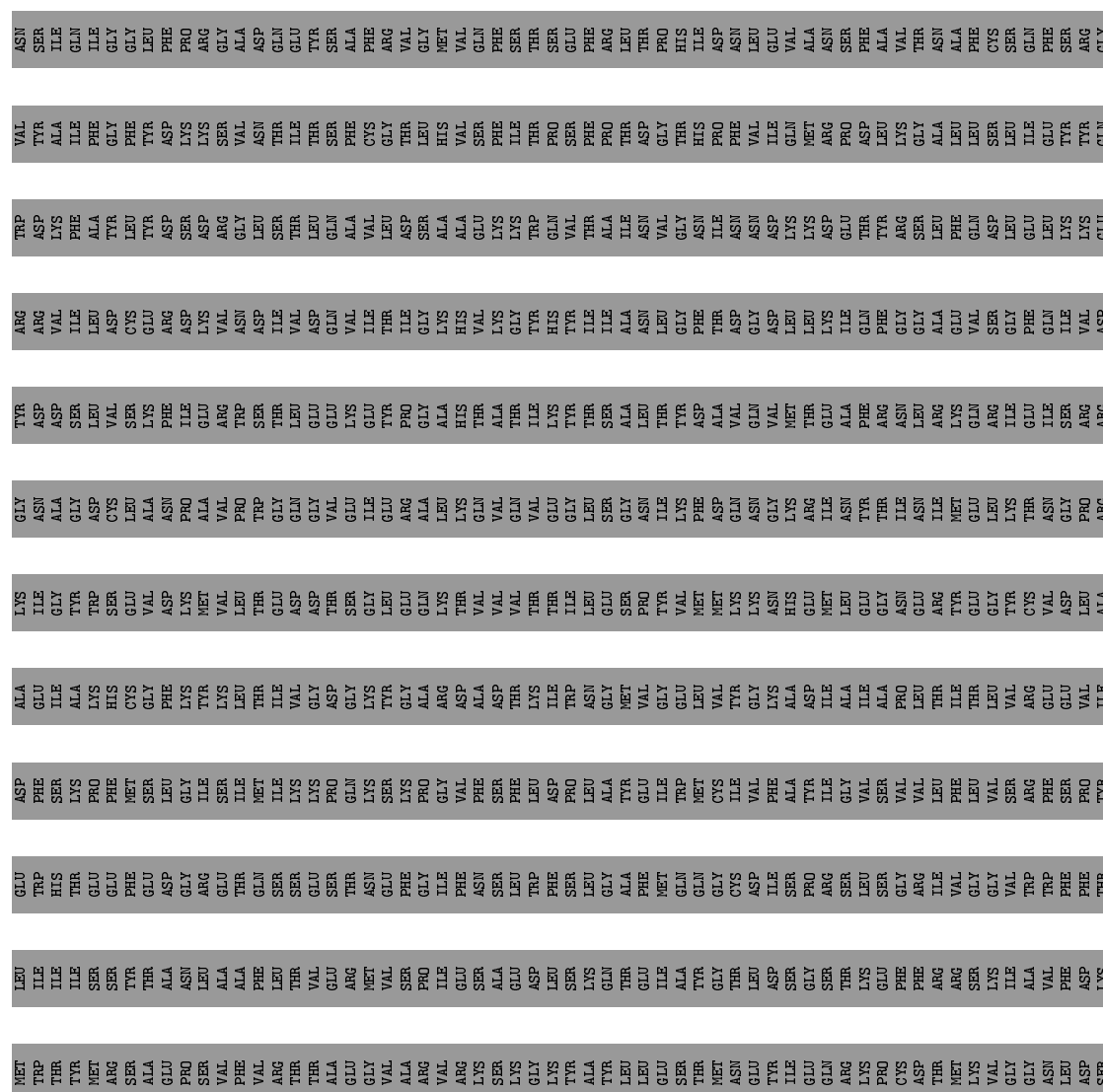
- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein





- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

Chain F:  9% 8% 83%



L174	H91	Y30	LYS	SER	LYS
M177	T92	W31	ASN	ASN	GLY
V178	G93		VAL	VAL	TVR
	I94	G34	ALA	ALA	GLY
M181	W95	T35	GLY	GLY	ILE
M182	C98	Q36	VAL	VAL	ALA
Y183	E99	R37	PHE	PHE	THR
T184	Y183	V38	TVR	TVR	PRO
Q185	E100	P39	ILE	ILE	LYS
V186	GLU	LYS	LEU	LEU	GLY
F187	LEU	PRO	VAL	VAL	SER
Q188	GLY	GLY	GLY	GLY	SER
V189	PRO	GLY	LEU	LEU	LEU
T190	G106	GLN	GLY	GLY	THR
	E107	GLY	LEU	LEU	PRO
L193	K108	GLY	ALA	ALA	VAL
G194	C109	GLY	MET	MET	ASN
P195	R110	ALA	LEU	LEU	LEU
E196	S111	ASN	VAL	VAL	ALA
D197	F112	CYS	ALA	ALA	VAL
W198		PRO	LEU	LEU	LEU
R199	A116	ASN	ILE	ILE	LYS
	P117	SER	GLU	GLU	LEU
S202	A118	GLY	PHE	PHE	SER
W203	S119	ALA	CYS	CYS	GLU
D204		ASN	TVR	TVR	GLN
Y205	G122	ALA	LYS	LYS	GLY
G206		THR	SER	SER	VAL
W207	W125	ALA	ARG	ARG	LEU
S208	L126	ASN	ALA	ALA	ASP
	S127	SER	GLU	GLU	LYS
L211		THR	ALA	ALA	LEU
A212	S130	ALA	LYS	LYS	LYS
W213		ALA	ARG	ARG	ASN
	L133	PRO	MET	MET	LYS
F216	Y134	VAL	LYS	LYS	TRP
S223	L135	ALA	GLY	GLY	TRP
W224	L137	SER	THR	THR	TVR
T225	L138	PRO	GLY	GLY	ASP
T226		ALA	K1	K1	LYS
L227	G141	ALA	T2	T2	GLY
M228		GLY	S3	S3	GLU
S229		ALA			CYS
Y230	M145	PRO	R7	R7	GLY
T231	S153	TVR	A8	A8	ALA
K232	SER	SER	V12	V12	LYS
THR	VAL	TRP	A13	A13	ASP
VAL	ILE	GLU			SER
ILE	D157	GLY	L16	L16	GLY
GLU	G158	ASP	L17	L17	LYS
PHE	L159	GLU	A18	A18	GLU
	K160	ARG			LYS
		F85	F21	F21	THR
	V167	G86			SER
	V170	L87	A25	A25	ALA
	L171	R88			LEU
		R89	T28	T28	SER
		F92	T30	T30	LEU

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: QUS

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	0.32	0/6287	0.50	0/8493
1	B	0.33	0/6265	0.56	4/8464 (0.0%)
1	C	0.32	0/6287	0.50	1/8493 (0.0%)
1	D	0.35	1/6265 (0.0%)	0.57	5/8464 (0.1%)
1	E	0.29	0/1443	0.49	0/1959
1	F	0.29	0/1443	0.48	0/1959
All	All	0.33	1/27990 (0.0%)	0.53	10/37832 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	786	ALA	C-N	-11.69	1.07	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	LYS	C-N-CD	-17.67	81.72	120.60
1	D	506	LYS	C-N-CD	-17.65	81.76	120.60
1	B	631	SER	C-N-CD	-16.78	83.69	120.60
1	D	631	SER	C-N-CD	-16.76	83.72	120.60
1	D	786	ALA	O-C-N	-8.83	108.58	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	786	ALA	Mainchain

## 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	6159	0	6157	283	0
1	B	6137	0	6132	321	0
1	C	6159	0	6157	309	0
1	D	6137	0	6131	291	0
1	E	1408	0	1406	61	0
1	F	1408	0	1406	54	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
2	D	13	0	6	0	0
All	All	27460	0	27413	1177	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 21.

The worst 5 of 1177 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:506:LYS:CE	1:C:721:MET:HB2	1.20	1.65
1:A:506:LYS:CE	1:A:721:MET:HB2	1.16	1.58
1:A:506:LYS:HE3	1:A:721:MET:CB	1.33	1.57
1:C:506:LYS:HE3	1:C:721:MET:CB	1.35	1.56
1:A:506:LYS:CE	1:A:721:MET:CB	1.86	1.53

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	779/1057 (74%)	716 (92%)	47 (6%)	16 (2%)	8	45
1	B	776/1057 (73%)	723 (93%)	39 (5%)	14 (2%)	10	49
1	C	779/1057 (74%)	716 (92%)	45 (6%)	18 (2%)	7	43
1	D	776/1057 (73%)	723 (93%)	35 (4%)	18 (2%)	7	43
1	E	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	3	28
1	F	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	3	28
All	All	3452/6342 (54%)	3190 (92%)	180 (5%)	82 (2%)	11	42

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	456	ASP
1	A	514	VAL
1	A	630	VAL
1	A	776	LYS

### 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	666/888 (75%)	648 (97%)	18 (3%)	50	74
1	B	664/888 (75%)	645 (97%)	19 (3%)	48	73
1	C	666/888 (75%)	648 (97%)	18 (3%)	50	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	664/888 (75%)	652 (98%)	12 (2%)	64	84
1	E	152/888 (17%)	151 (99%)	1 (1%)	87	93
1	F	152/888 (17%)	152 (100%)	0	100	100
All	All	2964/5328 (56%)	2896 (98%)	68 (2%)	59	79

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	633	ILE
1	C	390	LEU
1	D	508	GLN
1	B	634	GLU
1	B	684	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	HIS
1	C	311	ASN
1	E	15	ASN
1	C	83	ASN
1	C	325	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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
2	QUS	A	1101	-	3,13,13	1.39	0	0,18,18	0.00	-
2	QUS	B	1101	-	3,13,13	1.40	0	0,18,18	0.00	-
2	QUS	C	1101	-	3,13,13	1.38	0	0,18,18	0.00	-
2	QUS	D	1101	-	3,13,13	1.40	0	0,18,18	0.00	-

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
2	QUS	A	1101	-	-	0/2/8/8	0/0/1/1
2	QUS	B	1101	-	-	0/2/8/8	0/0/1/1
2	QUS	C	1101	-	-	0/2/8/8	0/0/1/1
2	QUS	D	1101	-	-	0/2/8/8	0/0/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	786:ALA	C	787:LEU	N	1.07