



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 07:55 PM BST

PDB ID : 5FTI
Title : Crystal structure of the GluA2 K738M-T744K LBD in complex with glutamate (lithium form)
Authors : Nayeem, N.; Green, T.
Deposited on : 2016-01-13
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

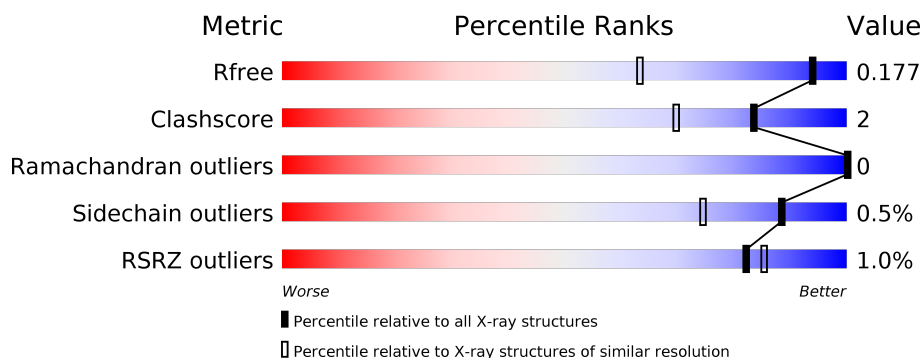
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	291	
1	B	291	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4885 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	13	1
			2099	1351	339	391	18			
1	B	258	Total	C	N	O	S	0	7	1
			2044	1310	335	382	17			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	MET	-	expression tag	UNP P19491
A	363	HIS	-	expression tag	UNP P19491
A	364	HIS	-	expression tag	UNP P19491
A	365	HIS	-	expression tag	UNP P19491
A	366	HIS	-	expression tag	UNP P19491
A	367	HIS	-	expression tag	UNP P19491
A	368	HIS	-	expression tag	UNP P19491
A	369	HIS	-	expression tag	UNP P19491
A	370	HIS	-	expression tag	UNP P19491
A	371	SER	-	expression tag	UNP P19491
A	372	SER	-	expression tag	UNP P19491
A	373	GLY	-	expression tag	UNP P19491
A	374	LEU	-	expression tag	UNP P19491
A	375	VAL	-	expression tag	UNP P19491
A	376	PRO	-	expression tag	UNP P19491
A	377	ARG	-	expression tag	UNP P19491
A	378	GLY	-	expression tag	UNP P19491
A	379	SER	-	expression tag	UNP P19491
A	380	ALA	-	expression tag	UNP P19491
A	381	MET	-	expression tag	UNP P19491
A	382	GLY	-	expression tag	UNP P19491
A	389	ARG	GLY	engineered mutation	UNP P19491
A	390	GLY	LEU	engineered mutation	UNP P19491
A	391	ALA	GLU	engineered mutation	UNP P19491
A	555	GLY	-	linker	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	566	THR	-	linker	UNP P19491
A	738	MET	LYS	engineered mutation	UNP P19491
A	744	LYS	THR	engineered mutation	UNP P19491
B	362	MET	-	expression tag	UNP P19491
B	363	HIS	-	expression tag	UNP P19491
B	364	HIS	-	expression tag	UNP P19491
B	365	HIS	-	expression tag	UNP P19491
B	366	HIS	-	expression tag	UNP P19491
B	367	HIS	-	expression tag	UNP P19491
B	368	HIS	-	expression tag	UNP P19491
B	369	HIS	-	expression tag	UNP P19491
B	370	HIS	-	expression tag	UNP P19491
B	371	SER	-	expression tag	UNP P19491
B	372	SER	-	expression tag	UNP P19491
B	373	GLY	-	expression tag	UNP P19491
B	374	LEU	-	expression tag	UNP P19491
B	375	VAL	-	expression tag	UNP P19491
B	376	PRO	-	expression tag	UNP P19491
B	377	ARG	-	expression tag	UNP P19491
B	378	GLY	-	expression tag	UNP P19491
B	379	SER	-	expression tag	UNP P19491
B	380	ALA	-	expression tag	UNP P19491
B	381	MET	-	expression tag	UNP P19491
B	382	GLY	-	expression tag	UNP P19491
B	389	ARG	GLY	engineered mutation	UNP P19491
B	390	GLY	LEU	engineered mutation	UNP P19491
B	391	ALA	GLU	engineered mutation	UNP P19491
B	555	GLY	-	linker	UNP P19491
B	566	THR	-	linker	UNP P19491
B	738	MET	LYS	engineered mutation	UNP P19491
B	744	LYS	THR	engineered mutation	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



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

- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Li	0	0
			1	1		
3	A	1	Total	Li	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

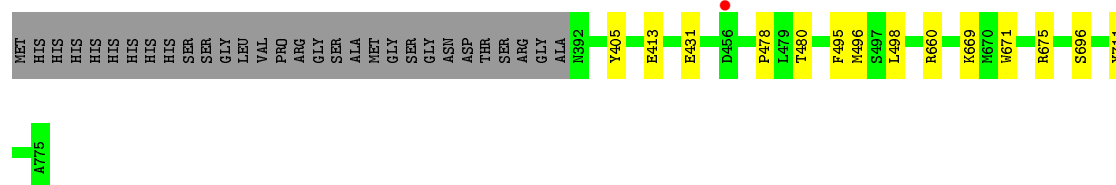
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	386	Total	O	0	0
			386	386		
6	B	302	Total	O	0	0
			302	302		

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.

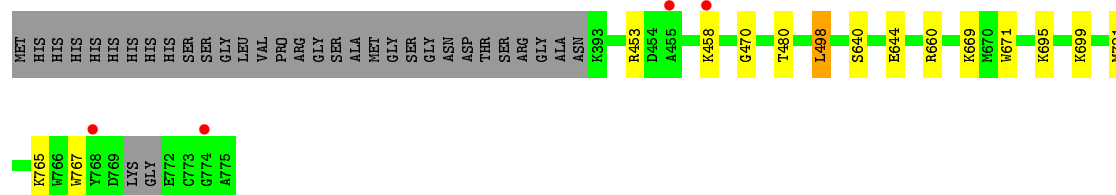
- Molecule 1: GLUTAMATE RECEPTOR 2

Chain A: 



- Molecule 1: GLUTAMATE RECEPTOR 2

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.32Å 47.56Å 96.75Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	66.99 – 1.35 66.99 – 1.35	Depositor EDS
% Data completeness (in resolution range)	94.7 (66.99-1.35) 94.7 (66.99-1.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.35Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.161 , 0.177 0.162 , 0.177	Depositor DCC
R_{free} test set	2538 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4885	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, SO4, LI

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	0.58	0/2177	0.72	2/2927 (0.1%)
1	B	0.49	0/2101	0.64	1/2824 (0.0%)
All	All	0.54	0/4278	0.68	3/5751 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	660	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	498	LEU	CA-CB-CG	-5.14	103.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2099	0	2173	10	0
1	B	2044	0	2104	11	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	6	0	8	2	0
5	B	6	0	8	2	0
6	A	386	0	0	4	0
6	B	302	0	0	4	0
All	All	4885	0	4303	20	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 2.

All (20) 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:A:696[B]:SER:OG	6:A:2263:HOH:O	1.99	0.77
1:A:711[B]:TYR:OH	6:A:2013:HOH:O	1.94	0.74
1:B:721[A]:MET:SD	6:B:2122:HOH:O	2.48	0.70
1:B:671:TRP:HZ2	5:B:904:GOL:H2	1.59	0.67
1:A:413:GLU:OE2	1:B:765:LYS:HE3	1.97	0.65
1:B:644:GLU:OE2	1:B:699:LYS:NZ	2.30	0.61
1:A:495:PHE:CD1	1:A:496[B]:MET:HG3	2.37	0.60
1:A:671:TRP:HZ2	5:A:904:GOL:H2	1.65	0.60
1:B:640:SER:O	1:B:669:LYS:HE3	2.10	0.52
1:A:669:LYS:NZ	6:A:2209:HOH:O	2.44	0.50
1:A:675:ARG:NH2	5:A:904:GOL:O1	2.47	0.48
1:A:480:THR:HG1	2:A:900:GLU:N	2.13	0.46
1:B:470:GLY:HA2	6:B:2084:HOH:O	2.15	0.46
1:B:453:ARG:HH21	1:B:458:LYS:HG2	1.81	0.46
1:B:767:TRP:O	6:B:2293:HOH:O	2.20	0.44
1:B:660:ARG:HE	5:B:904:GOL:H32	1.84	0.43
1:A:431:GLU:OE2	6:A:2046:HOH:O	2.22	0.43
1:B:695:LYS:NZ	6:B:2221:HOH:O	2.50	0.42
1:B:480:THR:HG1	2:B:900:GLU:N	2.18	0.41
1:A:405[B]:TYR:CE1	1:A:478:PRO:HB3	2.57	0.40

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 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	272/291 (94%)	270 (99%)	2 (1%)	0	100	100
1	B	261/291 (90%)	258 (99%)	3 (1%)	0	100	100
All	All	533/582 (92%)	528 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	232/242 (96%)	231 (100%)	1 (0%)	91	81
1	B	224/242 (93%)	223 (100%)	1 (0%)	91	81
All	All	456/484 (94%)	454 (100%)	2 (0%)	88	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	B	498	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	GOL	B	904	-	5,5,5	0.35	0	5,5,5	0.36	0
4	SO4	B	902	-	4,4,4	0.13	0	6,6,6	0.37	0
4	SO4	A	902	-	4,4,4	0.23	0	6,6,6	0.50	0
5	GOL	A	904	-	5,5,5	0.36	0	5,5,5	0.30	0
4	SO4	B	903	-	4,4,4	0.17	0	6,6,6	0.19	0
2	GLU	B	900	-	2,9,9	0.19	0	2,11,11	0.77	0
4	SO4	A	903	-	4,4,4	0.15	0	6,6,6	0.12	0
2	GLU	A	900	-	2,9,9	0.33	0	2,11,11	1.00	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	GOL	B	904	-	-	0/4/4/4	-
2	GLU	A	900	-	-	0/3/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	B	900	-	-	0/3/9/9	-
5	GOL	A	904	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	904	GOL	C1-C2-C3-O3
5	A	904	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	904	GOL	2	0
5	A	904	GOL	2	0
2	B	900	GLU	1	0
2	A	900	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	261/291 (89%)	-0.33	1 (0%) 92 93	11, 17, 39, 75	0
1	B	258/291 (88%)	-0.38	4 (1%) 72 76	14, 22, 46, 73	0
All	All	519/582 (89%)	-0.36	5 (0%) 82 85	11, 20, 44, 75	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	768	TYR	4.8
1	A	456	ASP	4.5
1	B	774	GLY	4.2
1	B	455	ALA	2.9
1	B	458	LYS	2.8

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](#)

There are no monosaccharides in this entry.

6.4 Ligands [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. 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	B-factors(\AA^2)	Q<0.9
4	SO4	A	903	5/5	0.75	0.13	71,74,77,78	5
5	GOL	A	904	6/6	0.79	0.11	42,51,52,58	0
5	GOL	B	904	6/6	0.79	0.13	49,53,56,65	0
3	LI	B	901	1/1	0.94	0.28	11,11,11,11	1
4	SO4	B	903	5/5	0.96	0.08	29,33,39,43	5
3	LI	A	901	1/1	0.96	0.43	10,10,10,10	1
2	GLU	B	900	10/10	0.97	0.05	16,17,19,19	0
4	SO4	B	902	5/5	0.97	0.08	24,26,30,33	5
2	GLU	A	900	10/10	0.98	0.06	11,12,15,15	0
4	SO4	A	902	5/5	0.99	0.07	17,18,21,23	5

6.5 Other polymers [i](#)

There are no such residues in this entry.