



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 06:57 PM BST

PDB ID : 5CMK  
Title : Crystal structure of the GluK2EM LBD dimer assembly complex with glutamate and LY466195  
Authors : Chittori, S.; Mayer, M.L.  
Deposited on : 2015-07-16  
Resolution : 1.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

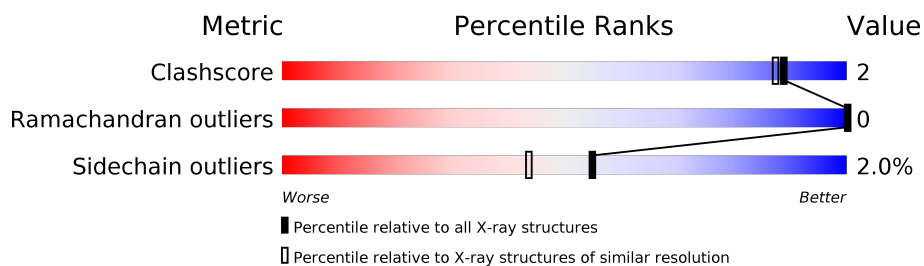
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8890 atoms, of which 4184 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, kainate 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	H	N	O	S	0	8	0
			4101	1299	2060	340	391	11			
1	B	253	Total	C	H	N	O	S	0	14	0
			4178	1323	2094	347	403	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P42260
A	91	THR	ALA	engineered mutation	UNP P42260
A	118	GLY	-	linker	UNP P42260
A	119	THR	-	linker	UNP P42260
A	142	SER	ALA	engineered mutation	UNP P42260
A	174	SER	ASN	engineered mutation	UNP P42260
A	188	LEU	PHE	engineered mutation	UNP P42260
B	1	GLY	-	expression tag	UNP P42260
B	91	THR	ALA	engineered mutation	UNP P42260
B	118	GLY	-	linker	UNP P42260
B	119	THR	-	linker	UNP P42260
B	142	SER	ALA	engineered mutation	UNP P42260
B	174	SER	ASN	engineered mutation	UNP P42260
B	188	LEU	PHE	engineered mutation	UNP P42260

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			18	5	8	1	4		

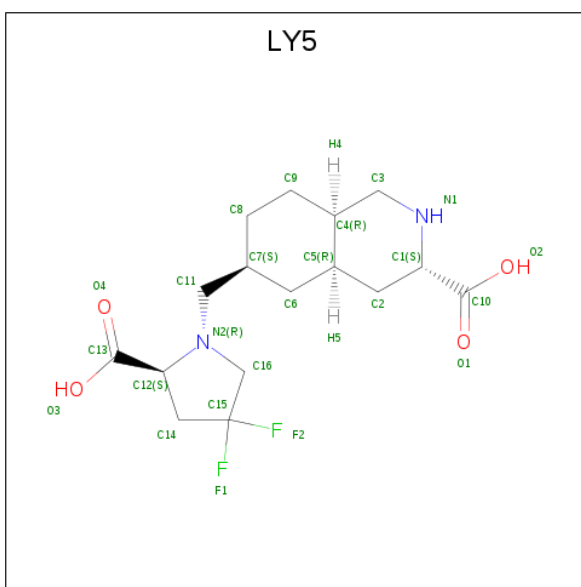
- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is (3S,4aR,6S,8aR)-6-{[(2S)-2-carboxy-4,4-difluoropyrrolidin-1-yl]methyl}decahydroisoquinoline-3-carboxylic acid (three-letter code: LY5) (formula: C<sub>16</sub>H<sub>24</sub>F<sub>2</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	F	H	N	O	0	0
			46	16	2	22	2	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total 232	O 232	0	2
7	B	301	Total 301	O 301	0	4

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.76Å 102.76Å 281.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 1.80	Depositor
% Data completeness (in resolution range)	99.9 (29.86-1.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.164 , 0.187	Depositor
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.077	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LY5, CL, 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	0.61	0/2113	0.69	1/2847 (0.0%)
1	B	0.65	0/2173	0.70	0/2926
All	All	0.63	0/4286	0.70	1/5773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	2041	2060	2026	7	0
1	B	2084	2094	2031	10	0
2	A	10	8	5	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	24	22	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	0	0
7	A	232	0	0	2	1
7	B	301	0	0	3	1
All	All	4706	4184	4084	16	1

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.

The worst 5 of 16 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:B:41:ARG:NH2	7:B:402:HOH:O	2.16	0.78
1:B:148:LYS:NZ	7:B:403:HOH:O	2.22	0.71
1:A:65:ASP:OD2	1:A:68:ASN:ND2	2.24	0.71
1:B:168:SER:O	1:B:180:ARG:NH1	2.30	0.63
1:B:176[A]:GLU:OE2	7:B:401:HOH:O	2.16	0.60

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:617:HOH:O	7:B:677:HOH:O[6_555]	2.16	0.04

## 4.3 Torsion angles [i](#)

### 4.3.1 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	257/259 (99%)	252 (98%)	5 (2%)	0	100	100
1	B	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
All	All	522/518 (101%)	511 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 4.3.2 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	230/227 (101%)	224 (97%)	6 (3%)	46	32
1	B	236/227 (104%)	233 (99%)	3 (1%)	69	62
All	All	466/454 (103%)	457 (98%)	9 (2%)	55	46

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	SER
1	B	190	MET
1	B	18	LEU
1	A	122	ASP
1	A	166	ARG

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

#### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 4.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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.

## 4.7 Other polymers

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.