

wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 07:06 AM EDT

:	3PD8
:	X-ray structure of the ligand-binding core of GluA2 in complex with (S)-7-
	HPCA at 2.5 A resolution
:	Frydenvang, K.; Kastrup, J.S.
:	2010-10-22
:	2.48 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 (1)) were used in the production of this report:

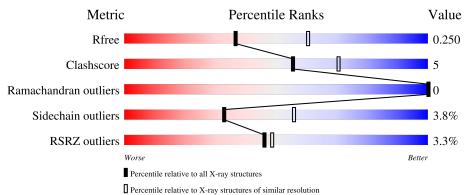
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.48 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469(2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	А	261	85%	13%	••
1	В	261	86%	13%	•
1	С	261	^{2%} 87%	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
5	ACY	А	263	-	-	Х	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6551 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	259	Total	С	Ν	0	\mathbf{S}	0	0	0
	А	239	2022	1288	337	383	14	0	0	0
1	Р	261	Total	С	Ν	0	S	0	0	0
	D	201	2035	1295	340	386	14	0		
1	1 C	C 960	Total	С	Ν	0	S	0	1	0
	260	2039	1299	340	386	14	0	1	0	

• Molecule 1 is a protein called Glutamate receptor 2.

There are 0	discremancies	hetween	the modelled	and	reference sequences:
There are 9	discrepancies	Detween	the modelled	and	reference sequences.

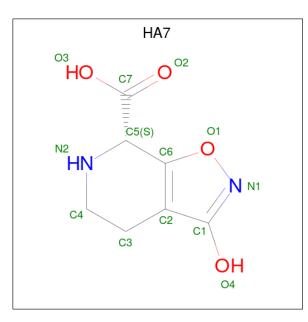
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P19491
А	115	GLY	-	linker	UNP P19491
А	116	THR	-	linker	UNP P19491
В	-1	ALA	-	expression tag	UNP P19491
В	115	GLY	-	linker	UNP P19491
В	116	THR	-	linker	UNP P19491
С	-1	ALA	-	expression tag	UNP P19491
С	115	GLY	-	linker	UNP P19491
С	116	THR	-	linker	UNP P19491

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

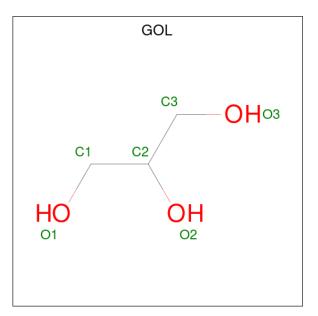
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	2	Total Zn 2 2	0	0
2	С	2	Total Zn 2 2	0	0

• Molecule 3 is (7S)-3-hydroxy-4,5,6,7-tetrahydroisoxazolo[5,4-c]pyridine-7-carboxylic acid (three-letter code: HA7) (formula: $C_7H_8N_2O_4$).





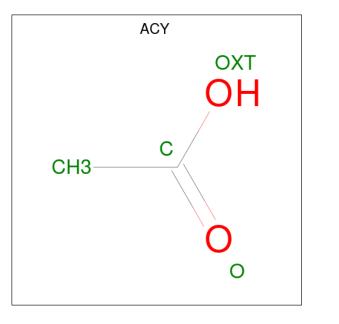
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O 13 7 2 4	0	0
3	В	1	Total C N O 13 7 2 4	0	0
3	С	1	Total C N O 13 7 2 4	0	0



Mo	bl	Chain	Residues	Atoms			ZeroOcc	AltConf
4		А	1	Total 6	C 3	0 3	0	0

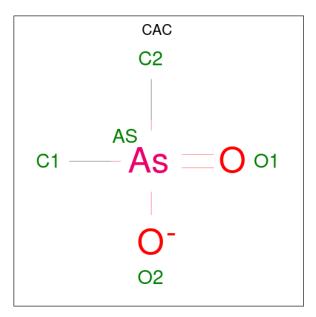


• Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	С	1	Total 5	As 1	С 2	O 2	0	0

• Molecule 7 is water.

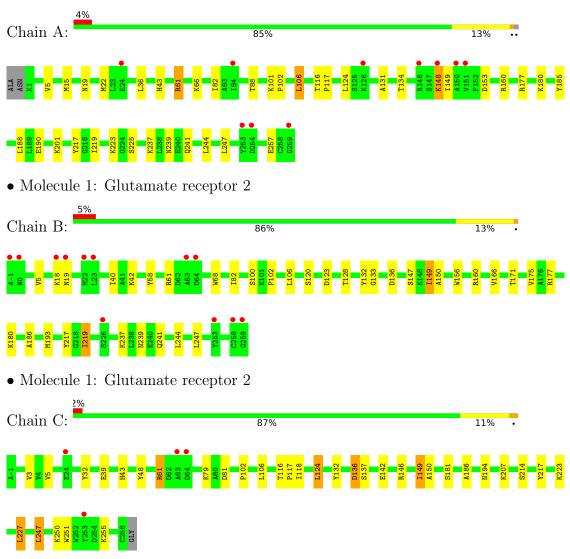


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	102	Total O 102 102	0	0
7	В	120	Total O 120 120	0	0
7	С	174	Total O 174 174	0	0



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: Glutamate receptor 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	114.62Å 164.00 Å 47.62 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 - 2.48	Depositor
Resolution (A)	29.32 - 2.48	EDS
% Data completeness	97.9 (29.32-2.48)	Depositor
(in resolution range)	97.9 (29.32-2.48)	EDS
R _{merge}	0.11	Depositor
R _{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	$3.13 (at 2.48 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
D D.	0.175 , 0.261	Depositor
R, R_{free}	0.162 , 0.250	DCC
R_{free} test set	1641 reflections (5.10%)	wwPDB-VP
Wilson B-factor $(Å^2)$	28.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 60.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.55% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: HA7, ACY, GOL, CAC, ZN $\,$

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/2058	0.49	0/2767	
1	В	0.32	0/2071	0.49	0/2785	
1	С	0.32	0/2075	0.50	0/2791	
All	All	0.31	0/6204	0.49	0/8343	

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	А	2022	0	2056	23	0
1	В	2035	0	2067	22	0
1	С	2039	0	2074	19	0
2	А	1	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	А	13	0	6	1	0
3	В	13	0	6	1	0
3	С	13	0	6	0	0
4	А	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	4	0	3	2	0
6	С	5	0	0	0	0
7	А	102	0	0	1	0
7	В	120	0	0	1	0
7	С	174	0	0	1	0
All	All	6551	0	6226	63	0

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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 5.

The worst 5 of 63 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:19:ASN:HB2	1:A:22:MET:HE2	1.61	0.81	
1:A:61:ARG:HD3	1:A:66:LYS:HA	1.63	0.81	
1:B:133:GLY:HA3	1:B:166:VAL:O	1.99	0.63	
1:B:40:ILE:HD12	1:B:219:ILE:HD12	1.80	0.63	
1:C:251:TRP:CZ3	1:C:255:LYS:HE3	2.34	0.62	

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	Perce	ntiles
1	А	257/261~(98%)	249~(97%)	8(3%)	0	100	100
1	В	259/261~(99%)	253~(98%)	6~(2%)	0	100	100
1	С	259/261~(99%)	252 (97%)	7 (3%)	0	100	100
All	All	775/783~(99%)	754 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.



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	А	217/218~(100%)	208~(96%)	9~(4%)	30 53
1	В	218/218~(100%)	211 (97%)	7(3%)	39 63
1	С	$219/218\ (100\%)$	210 (96%)	9 (4%)	30 53
All	All	654/654~(100%)	629~(96%)	25~(4%)	33 56

5 of 25 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	219	ILE
1	С	79	LYS
1	С	247	LEU
1	С	61	ARG
1	С	106	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	А	241	GLN
1	С	19	ASN

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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).

Mal	Mol Type Chain		Res	Link	Bo	ond leng	ths	Bond angles		
	Type	e Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	CAC	С	263	2	0,4,4	-	-	0,6,6	-	-
3	HA7	В	262	-	11,14,14	1.94	4 (36%)	12,20,20	2.82	3 (25%)
4	GOL	А	262	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.19	0
5	ACY	А	263	-	3,3,3	0.78	0	3,3,3	0.77	0
3	HA7	С	262	-	11,14,14	2.27	4 (36%)	12,20,20	2.96	4 (33%)
3	HA7	А	261	-	11,14,14	2.09	4 (36%)	12,20,20	2.93	4 (33%)

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	HA7	С	262	-	-	1/3/14/14	0/2/2/2
3	HA7	В	262	-	-	1/3/14/14	0/2/2/2
4	GOL	А	262	-	-	0/4/4/4	-
3	HA7	А	261	-	-	1/3/14/14	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	261	HA7	C2-C1	-3.93	1.38	1.43
3	С	262	HA7	O1-C6	3.83	1.38	1.34
3	С	262	HA7	C2-C1	-3.70	1.38	1.43
3	С	262	HA7	O4-C1	-3.46	1.23	1.33
3	А	261	HA7	O4-C1	-3.44	1.23	1.33

The worst 5 of 11 bond angle outliers are listed below:



3PD8

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	261	HA7	O1-C6-C5	8.44	132.96	120.29
3	В	262	HA7	O1-C6-C5	8.36	132.84	120.29
3	С	262	HA7	O1-C6-C5	8.35	132.82	120.29
3	С	262	HA7	C3-C2-C6	3.66	124.73	121.85
3	А	261	HA7	C3-C2-C6	3.54	124.63	121.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	262	HA7	N2-C5-C7-O2
3	А	261	HA7	N2-C5-C7-O2
3	В	262	HA7	N2-C5-C7-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	262	HA7	1	0
5	А	263	ACY	2	0
3	А	261	HA7	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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	259/261~(99%)	-0.05	10 (3%) 39 41	14, 33, 71, 100	0
1	В	$261/261 \ (100\%)$	-0.12	12 (4%) 32 34	13, 29, 63, 98	0
1	С	260/261~(99%)	-0.19	4 (1%) 73 75	12, 24, 56, 127	0
All	All	780/783~(99%)	-0.12	26 (3%) 46 49	12, 28, 65, 127	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	64	ASP	5.2
1	А	253	TYR	4.9
1	В	64	ASP	4.5
1	В	0	ASN	4.3
1	А	259	GLY	3.7

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, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
4	GOL	А	262	6/6	0.88	0.21	42,60,69,82	0
3	HA7	С	262	13/13	0.94	0.20	$15,\!22,\!40,\!48$	0
2	ZN	А	260	1/1	0.95	0.04	71, 71, 71, 71	0
3	HA7	А	261	13/13	0.96	0.20	$15,\!25,\!39,\!45$	0
3	HA7	В	262	13/13	0.97	0.23	10,22,38,41	0
2	ZN	С	261	1/1	0.98	0.05	27,27,27,27	0
5	ACY	А	263	4/4	0.98	0.09	32,44,48,49	0
6	CAC	С	263	5/5	0.98	0.14	$6,\!45,\!55,\!55$	0
2	ZN	В	261	1/1	0.99	0.04	45,45,45,45	0
2	ZN	В	260	1/1	0.99	0.07	27,27,27,27	0
2	ZN	С	260	1/1	1.00	0.07	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

