



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:36 am GMT

PDB ID : 5KCA
Title : Crystal structure of the Cbln1 C1q domain trimer in complex with the amino-terminal domain (ATD) of iGluR Delta-2 (GluD2)
Authors : Elegheert, J.; Aricescu, A.R.
Deposited on : 2016-06-05
Resolution : 3.10 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

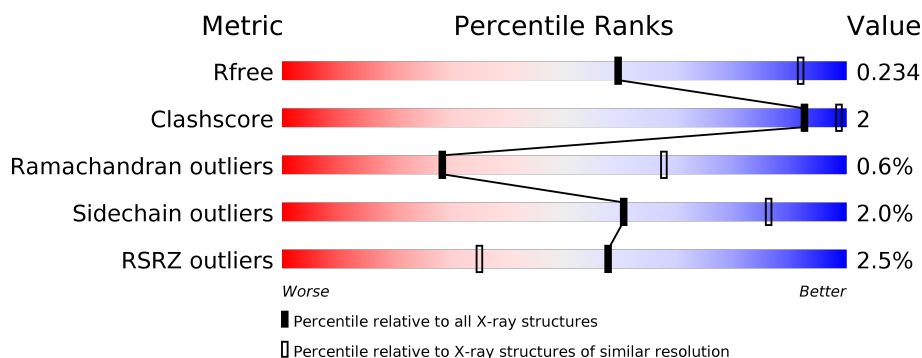
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	878	<div> <div>2%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6332 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 Cerebellin-1,Cerebellin-1,Cerebellin-1,Glutamate receptor ionotropic, delta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	807	Total	C	N	O	S	0	1	0
			6331	4016	1097	1186	32			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLU	-	expression tag	UNP P23435
A	57	THR	-	expression tag	UNP P23435
A	194	GLY	-	linker	UNP P23435
A	195	SER	-	linker	UNP P23435
A	196	GLU	-	linker	UNP P23435
A	197	LEU	-	linker	UNP P23435
A	198	GLY	-	linker	UNP P23435
A	336	GLY	-	linker	UNP P23435
A	337	SER	-	linker	UNP P23435
A	338	ALA	-	linker	UNP P23435
A	339	SER	-	linker	UNP P23435
A	340	GLY	-	linker	UNP P23435
A	478	GLY	-	linker	UNP P23435
A	479	THR	-	linker	UNP P23435
A	480	GLY	-	linker	UNP P23435
A	481	GLY	-	linker	UNP P23435
A	482	SER	-	linker	UNP P23435
A	483	GLY	-	linker	UNP P23435
A	484	GLY	-	linker	UNP P23435
A	485	SER	-	linker	UNP P23435
A	486	GLY	-	linker	UNP P23435
A	487	GLY	-	linker	UNP P23435
A	488	SER	-	linker	UNP P23435
A	489	GLY	-	linker	UNP P23435
A	490	GLY	-	linker	UNP P23435
A	491	SER	-	linker	UNP P23435

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Chain	Residue	Modelled	Actual	Comment	Reference
A	492	GLY	-	linker	UNP P23435
A	493	GLY	-	linker	UNP P23435
A	494	SER	-	linker	UNP P23435
A	495	GLY	-	linker	UNP P23435
A	496	GLY	-	linker	UNP P23435
A	497	SER	-	linker	UNP P23435
A	498	GLY	-	linker	UNP P23435
A	499	GLY	-	linker	UNP P23435
A	500	SER	-	linker	UNP P23435
A	501	GLY	-	linker	UNP P23435
A	502	GLY	-	linker	UNP P23435
A	503	SER	-	linker	UNP P23435
A	504	GLY	-	linker	UNP P23435
A	505	GLY	-	linker	UNP P23435
A	506	SER	-	linker	UNP P23435
A	507	GLY	-	linker	UNP P23435
A	508	GLY	-	linker	UNP P23435
A	509	SER	-	linker	UNP P23435
A	927	LYS	-	expression tag	UNP O43424
A	928	HIS	-	expression tag	UNP O43424
A	929	HIS	-	expression tag	UNP O43424
A	930	HIS	-	expression tag	UNP O43424
A	931	HIS	-	expression tag	UNP O43424
A	932	HIS	-	expression tag	UNP O43424
A	933	HIS	-	expression tag	UNP O43424

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.68Å 142.68Å 276.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.02 – 3.10 46.05 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.02-3.10) 99.4 (46.05-3.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1772)	Depositor
R, R_{free}	0.204 , 0.231 0.207 , 0.234	Depositor DCC
R_{free} test set	1545 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.28	0/6460	0.50	0/8742

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

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	6331	0	6178	22	0
2	A	1	0	0	0	0
All	All	6332	0	6178	22	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 (22) 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:150:ARG:O	1:A:150:ARG:NE	2.26	0.69
1:A:150:ARG:NH1	1:A:426:PHE:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:NH2	1:A:435:GLU:OE2	2.31	0.63
1:A:215:GLU:OE1	1:A:834:HIS:NE2	2.33	0.61
1:A:542:GLU:OE1	1:A:788:ASN:ND2	2.36	0.58
1:A:526:ASP:OD1	1:A:810:ASN:ND2	2.39	0.54
1:A:274:MET:HE3	1:A:312:LYS:HE2	1.95	0.48
1:A:352:ARG:HG3	1:A:464:TRP:NE1	2.28	0.48
1:A:98:ASP:O	1:A:102:SER:N	2.48	0.46
1:A:429:ASP:O	1:A:430:GLN:HB2	2.17	0.45
1:A:660:SER:OG	1:A:688:ASN:OD1	2.33	0.45
1:A:793:SER:HA	1:A:796:CYS:SG	2.57	0.45
1:A:843:ARG:O	1:A:846:SER:N	2.45	0.44
1:A:382:ASP:O	1:A:386:SER:N	2.51	0.44
1:A:240:ASP:O	1:A:244:SER:N	2.51	0.43
1:A:68:ARG:HG3	1:A:180:TRP:CD1	2.54	0.43
1:A:758:GLU:HG3	1:A:762:ARG:HE	1.85	0.42
1:A:259:HIS:CE1	1:A:294:ALA:CB	3.03	0.41
1:A:429:ASP:OD1	1:A:430:GLN:N	2.53	0.41
1:A:778:GLN:HG2	1:A:779:ASN:N	2.36	0.41
1:A:890:ASN:O	1:A:891:TYR:HB3	2.19	0.41
1:A:908:VAL:HG23	1:A:909:THR:N	2.35	0.41

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	796/878 (91%)	755 (95%)	36 (4%)	5 (1%)	28 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	TYR

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Mol	Chain	Res	Type
1	A	406	TYR
1	A	291	THR
1	A	125	GLN
1	A	779	ASN

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	686/742 (92%)	672 (98%)	14 (2%)	60 86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	68	ARG
1	A	70	THR
1	A	79	ASN
1	A	124	ARG
1	A	150	ARG
1	A	207	SER
1	A	314	GLU
1	A	352	ARG
1	A	409	GLN
1	A	687	GLU
1	A	715	ARG
1	A	836	MET
1	A	912	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	160	GLN
1	A	302	GLN

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Mol	Chain	Res	Type
1	A	890	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	807/878 (91%)	-0.03	20 (2%) 58 35	24, 57, 113, 175	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	891	TYR	4.3
1	A	890	ASN	3.7
1	A	431	ASP	3.6
1	A	622	SER	3.6
1	A	407	ASN	3.4
1	A	740	PHE	2.9
1	A	78	SER	2.9
1	A	892	GLY	2.9
1	A	624	ARG	2.8
1	A	845	ASN	2.8
1	A	625	ASN	2.8
1	A	623	ASN	2.5
1	A	337	SER	2.5
1	A	81	THR	2.3
1	A	247	ILE	2.3
1	A	406	TYR	2.2
1	A	305	LYS	2.2
1	A	79	ASN	2.2
1	A	76	GLU	2.1
1	A	365	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
2	CA	A	1001	1/1	0.87	0.35	0.32	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.