



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 10:41 PM GMT

PDB ID : 2E4Y
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 2R,4R-APDC
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

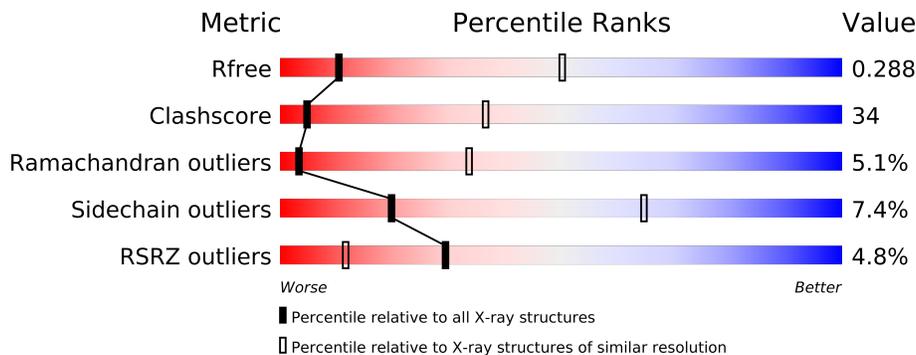
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	801	-	X
3	52A	B	2001	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7823 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

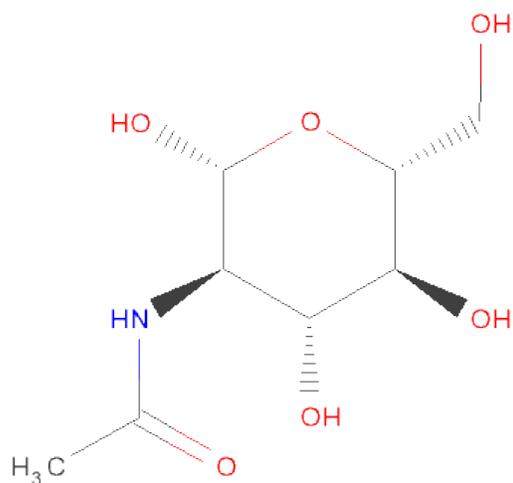
- Molecule 1 is a protein called Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	518	4118	2606	709	776	27	23	0	0
1	B	459	3667	2325	642	685	15	23	0	0

There are 12 discrepancies between the modelled and reference sequences:

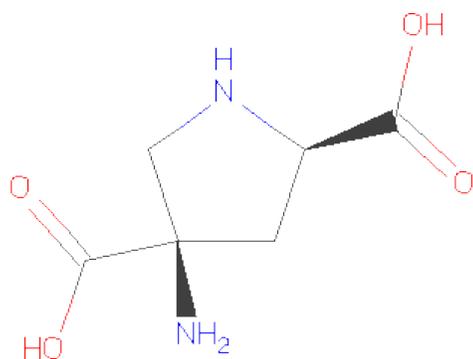
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	UNP P31422
B	439	GLN	ASN	ENGINEERED	UNP P31422
B	576	LEU	-	CLONING ARTIFACT	UNP P31422
B	577	VAL	-	CLONING ARTIFACT	UNP P31422
B	578	PRO	-	CLONING ARTIFACT	UNP P31422
B	579	ARG	-	CLONING ARTIFACT	UNP P31422

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is (2R,4R)-4-AMINOPYRROLIDINE-2,4-DICARBOXYLICACID (three-letter code: 52A) (formula: C₆H₁₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	6	2	4	0	0
3	B	1	12	6	2	4	0	0

CYS	W483	L418	F333	I260	S179
MET	G484	C419	D334	R261	D180
ASP	H486	M422	R336	L264	K181
CYS	W486	K423	Y336	L267	Y184
GLY	A487	I424	F337	P267	D185
PRO	E488	L425	L340	V271	Y186
GLY	T489	D426	N341	V272	F187
GLN	T490	G427	P342	V273	A188
TRP	S491	K428	Y343	L274	R189
THR	L492	K429	N344	F275	T190
PRO	D493	L430	N345	M276	V191
ALA	V494	Y431	P349	D279	P192
ASP	D495	K432	W350	D280	P193
LEU	S496	Y434	W355	F195	D194
SER	T497	L436	E356	Y196	F196
GLY	H498	K437	F359	A200	A200
CYS	W499	I438	Q360	H201	H201
TVR	W499	Q439	C361	I204	I204
ASN	M502	F440	S362	L205	L205
LEU	P505	T441	R289	F208	F208
PRO	P505	A442	L363	M209	M209
GLU	Q508	P443	Q364	W210	W210
ASP	Q508	F444	N365	V213	V213
ILE	Q508	M445	K366	S214	S214
LYS	Q508	N446	R367	T215	T215
TRP	Q508	M447	K368	V216	V216
GLU	Q508	A450	H369	A217	A217
ASP	Q508	D451	R370	S218	S218
ALA	Q508	S452	Q371	E219	E219
LEU	Q508	I453	V372	G220	G220
VAL	Q508	V454	D374	D221	D221
PRO	Q508	K455	L377	Y222	Y222
ARG	Q508	F456	K378	I227	I227
		D457	L379	F230	F230
		T458	E387	E231	E231
		F459	S388	A242	A242
		D461	K389	T243	T243
		G464	I390	A244	A244
		R465	M391	E245	E245
		Y466	F392	K246	K246
		N467	A399	V247	V247
		V468	M400	G248	G248
		F469	A403	R249	R249
		M470	L404	S250	S250
		L471	H405	N251	N251
		Q472	A408	I252	I252
		Q473	L411	R253	R253
		G476	C412	K254	K254
		K477	P413	S255	S255
		Y478	Q332	V259	V259
		S479	H338		
		Y480	F329		
			V330		
			R331		
			Q332		

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.39Å 91.80Å 112.97Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	12.00 – 3.40 84.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.40) 99.5 (84.33-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.284 0.236 , 0.288	Depositor DCC
R_{free} test set	1632 reflections (7.35%)	DCC
Wilson B-factor (Å ²)	122.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 114.3	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23829 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAG, 52A

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	0.52	0/4212	0.71	2/5704 (0.0%)
1	B	0.37	0/3745	0.65	2/5062 (0.0%)
All	All	0.46	0/7957	0.68	4/10766 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	CYS	CA-CB-SG	-7.22	101.01	114.00
1	A	419	CYS	CA-CB-SG	-7.08	101.25	114.00
1	A	546	CYS	CA-CB-SG	-7.05	101.30	114.00
1	B	412	CYS	CA-CB-SG	-5.14	104.75	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4118	0	3994	302	0
1	B	3667	0	3605	227	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	8	2	0
3	B	12	0	8	1	0
All	All	7823	0	7628	526	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 526 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:437:LYS:HA	1:B:437:LYS:HE3	1.40	1.02
1:B:181:LYS:HE2	1:B:459:PHE:O	1.64	0.98
1:A:437:LYS:HA	1:A:437:LYS:HE3	1.44	0.97
1:A:519:LYS:HD2	1:A:546:CYS:HB2	1.45	0.96
1:A:181:LYS:HE2	1:A:459:PHE:O	1.67	0.95

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	514/555 (93%)	415 (81%)	71 (14%)	28 (5%)	3	31
1	B	455/555 (82%)	368 (81%)	66 (14%)	21 (5%)	4	37
All	All	969/1110 (87%)	783 (81%)	137 (14%)	49 (5%)	3	33

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	A	292	ASN
1	A	361	CYS
1	A	443	PRO
1	A	494	VAL

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	A	447/481 (93%)	411 (92%)	36 (8%)	17	60
1	B	394/481 (82%)	368 (93%)	26 (7%)	24	70
All	All	841/962 (87%)	779 (93%)	62 (7%)	20	65

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	502	ASN
1	A	546	CYS
1	B	454	VAL
1	A	522	GLN
1	B	67	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	GLN
1	B	251	ASN
1	B	344	ASN
1	A	473	GLN
1	B	365	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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)

3 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
3	52A	A	1001	-	12,12,12	0.85	0	18,18,18	1.38	2 (11%)
2	NAG	A	801	1	12,14,15	0.52	0	15,19,21	0.58	0
3	52A	B	2001	-	12,12,12	0.84	0	18,18,18	1.37	2 (11%)

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	52A	A	1001	-	-	0/10/21/21	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	52A	B	2001	-	-	0/10/21/21	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	52A	CA-CB1-CG1	-3.63	101.73	104.89
3	A	1001	52A	CA-CB1-CG1	-3.62	101.73	104.89
3	A	1001	52A	OXT-C-CA	2.59	119.79	113.70
3	B	2001	52A	OXT-C-CA	2.45	119.45	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	518/555 (93%)	0.24	6 (1%) 75 39	38, 98, 201, 397	5 (0%)
1	B	459/555 (82%)	0.62	41 (8%) 10 5	52, 151, 269, 371	5 (1%)
All	All	977/1110 (88%)	0.42	47 (4%) 29 12	38, 117, 249, 397	10 (1%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	ARG	10.9
1	B	365	ASN	5.8
1	B	369	HIS	5.0
1	B	310	VAL	4.7
1	B	370	ARG	4.6

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

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	801	14/15	0.41	3.72	210,210,210,210	0
3	52A	B	2001	12/12	0.54	0.76	94,94,94,94	0
3	52A	A	1001	12/12	0.30	0.47	64,64,64,64	0

6.5 Other polymers

There are no such residues in this entry.