Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2024 – 08:57 AM EDT

PDB ID	:	5KZN
Title	:	Metabotropic Glutamate Receptor
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Deposited on	:	2016-07-25
Resolution	:	2.80 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 (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:

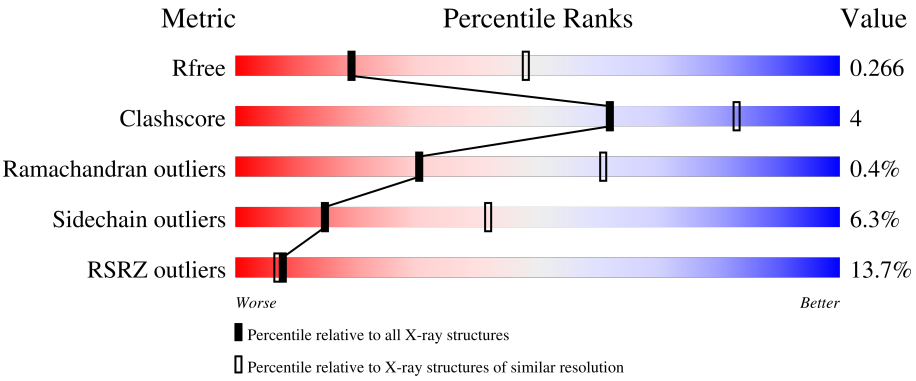
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	A	570	12% 75% 12% • 12%

Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3908 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.

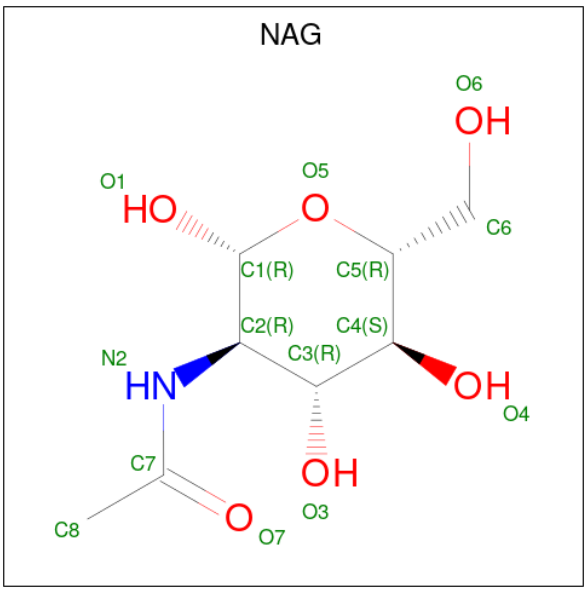
- Molecule 1 is a protein called Metabotropic glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	503	3843	2446	670	705	22	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	563	GLU	TRP	conflict	UNP Q14416
A	565	HIS	-	expression tag	UNP Q14416
A	566	HIS	-	expression tag	UNP Q14416
A	567	HIS	-	expression tag	UNP Q14416
A	568	HIS	-	expression tag	UNP Q14416
A	569	HIS	-	expression tag	UNP Q14416
A	570	HIS	-	expression tag	UNP Q14416

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

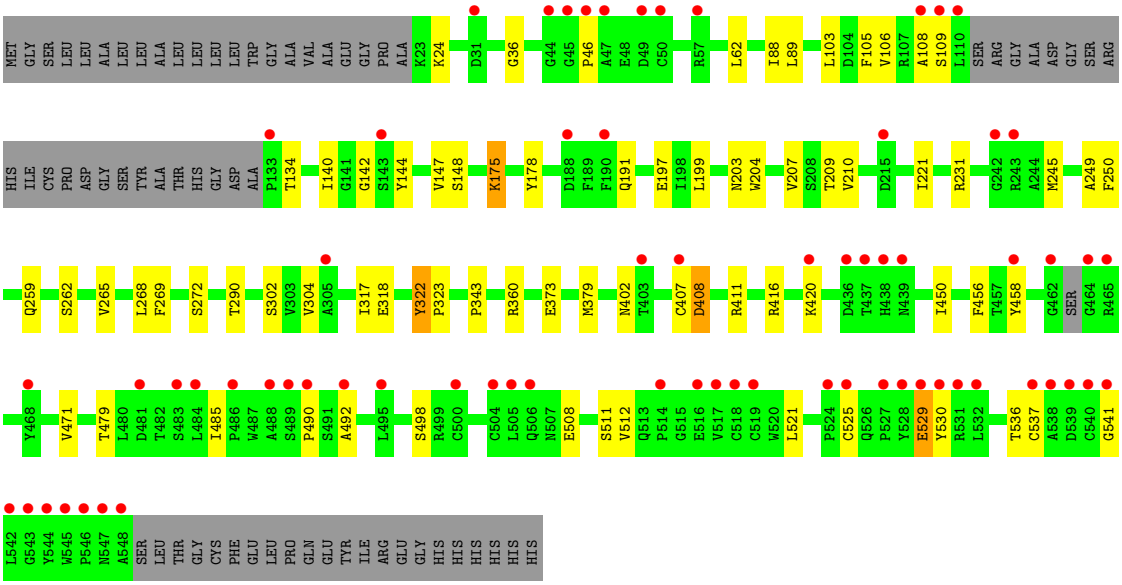
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	36	Total O 36 36	0	0

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: Metabotropic glutamate receptor 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	129.85Å 129.85Å 252.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.17 – 2.80 25.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.17-2.80) 99.8 (25.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.220 , 0.249 0.227 , 0.266	Depositor DCC
R_{free} test set	1598 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	85.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 79.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3908	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, NAG

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	0.54	0/3941	0.73	0/5361

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ASN	Sidechain

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	3843	0	3618	30	0
2	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	36	0	0	0	0
All	All	3908	0	3644	30	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 4.

All (30) 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:191:GLN:HB2	1:A:317:ILE:HD11	1.69	0.73
1:A:199:LEU:HD13	1:A:207:VAL:HG11	1.86	0.57
1:A:245:MET:HG2	1:A:249:ALA:HB3	1.89	0.55
1:A:210:VAL:HB	1:A:268:LEU:HD22	1.89	0.54
1:A:144:TYR:HB2	1:A:147:VAL:HG13	1.90	0.54
1:A:142:GLY:HA3	1:A:148:SER:OG	2.09	0.53
1:A:408:ASP:HA	1:A:411:ARG:HB2	1.91	0.53
1:A:108:ALA:HB1	1:A:134:THR:O	2.09	0.53
1:A:525:CYS:HB3	1:A:529:GLU:HB3	1.91	0.52
1:A:490:PRO:C	1:A:492:ALA:H	2.15	0.49
1:A:197:GLU:HG2	1:A:231:ARG:HH21	1.76	0.49
1:A:103:LEU:HA	1:A:106:VAL:HG22	1.93	0.49
1:A:209:THR:HB	1:A:221:ILE:HD11	1.94	0.49
1:A:24:LYS:HD3	1:A:343:PRO:HB2	1.94	0.48
1:A:62:LEU:CD1	1:A:88:ILE:HG21	2.43	0.48
1:A:265:VAL:HG22	1:A:290:THR:HB	1.94	0.48
1:A:175:LYS:HE3	1:A:178:TYR:O	2.14	0.46
1:A:207:VAL:HG12	1:A:265:VAL:HB	1.97	0.45
1:A:416:ARG:O	1:A:420:LYS:HG2	2.17	0.45
1:A:318:GLU:HB2	1:A:456:PHE:HE2	1.83	0.44
1:A:511:SER:HB3	1:A:521:LEU:HB2	2.01	0.43
1:A:304:VAL:O	1:A:304:VAL:HG12	2.18	0.43
1:A:322:TYR:CE1	1:A:379:MET:HG3	2.53	0.43
1:A:529:GLU:HG2	1:A:537:CYS:HB3	2.01	0.43
1:A:245:MET:HB3	1:A:250:PHE:CE1	2.55	0.42
1:A:36:GLY:HA2	1:A:140:ILE:O	2.20	0.42
1:A:304:VAL:HG11	1:A:458:TYR:CZ	2.55	0.41
1:A:322:TYR:CD1	1:A:322:TYR:C	2.95	0.41
1:A:89:LEU:HD12	1:A:105:PHE:CZ	2.57	0.40
1:A:204:TRP:CD2	1:A:265:VAL:HG21	2.57	0.40

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	497/570 (87%)	467 (94%)	28 (6%)	2 (0%)	30 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	541	GLY

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	381/463 (82%)	357 (94%)	24 (6%)	15 42

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	175	LYS
1	A	259	GLN
1	A	262	SER
1	A	269	PHE
1	A	272	SER

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Mol	Chain	Res	Type
1	A	302	SER
1	A	322	TYR
1	A	323	PRO
1	A	360	ARG
1	A	373	GLU
1	A	402	ASN
1	A	407	CYS
1	A	408	ASP
1	A	450	ILE
1	A	471	VAL
1	A	479	THR
1	A	485	ILE
1	A	498	SER
1	A	508	GLU
1	A	512	VAL
1	A	529	GLU
1	A	530	TYR
1	A	536	THR

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	NAG	A	602	1	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
2	NAG	A	601	1	14,14,15	0.41	0	17,19,21	1.29	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
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAG	C1-O5-C5	3.95	117.49	112.19
2	A	601	NAG	O5-C1-C2	2.92	115.80	111.29
2	A	602	NAG	C1-C2-N2	-2.65	106.25	110.43

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	503/570 (88%)	0.59	69 (13%) 8 7	57, 91, 148, 203	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	TYR	7.6
1	A	547	ASN	6.9
1	A	545	TRP	6.8
1	A	548	ALA	6.7
1	A	110	LEU	6.2
1	A	546	PRO	5.9
1	A	462	GLY	5.7
1	A	532	LEU	5.2
1	A	506	GLN	4.6
1	A	133	PRO	4.5
1	A	538	ALA	4.5
1	A	530	TYR	4.5
1	A	492	ALA	4.4
1	A	49	ASP	4.4
1	A	542	LEU	4.3
1	A	50	CYS	4.0
1	A	31	ASP	4.0
1	A	481	ASP	4.0
1	A	539	ASP	3.9
1	A	527	PRO	3.9
1	A	528	TYR	3.8
1	A	519	CYS	3.8
1	A	407	CYS	3.5
1	A	464	GLY	3.4
1	A	46	PRO	3.4
1	A	143	SER	3.4
1	A	108	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	525	CYS	3.2
1	A	483	SER	3.1
1	A	465	ARG	3.1
1	A	484	LEU	3.0
1	A	518	CYS	2.9
1	A	541	GLY	2.9
1	A	537	CYS	2.9
1	A	242	GLY	2.8
1	A	109	SER	2.8
1	A	489	SER	2.7
1	A	543	GLY	2.7
1	A	540	CYS	2.7
1	A	517	VAL	2.7
1	A	458	TYR	2.6
1	A	514	PRO	2.6
1	A	437	THR	2.6
1	A	438	HIS	2.6
1	A	468	TYR	2.5
1	A	436	ASP	2.5
1	A	45	GLY	2.5
1	A	490	PRO	2.4
1	A	504	CYS	2.4
1	A	529	GLU	2.4
1	A	505	LEU	2.3
1	A	44	GLY	2.3
1	A	190	PHE	2.3
1	A	439	ASN	2.3
1	A	215	ASP	2.3
1	A	531	ARG	2.3
1	A	305	ALA	2.2
1	A	516	GLU	2.2
1	A	188	ASP	2.2
1	A	420	LYS	2.1
1	A	524	PRO	2.1
1	A	403	THR	2.1
1	A	243	ARG	2.1
1	A	500	CYS	2.1
1	A	495	LEU	2.0
1	A	488	ALA	2.0
1	A	486	PRO	2.0
1	A	47	ALA	2.0
1	A	57	ARG	2.0

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	B-factors(Å^2)	Q<0.9
2	NAG	A	602	14/15	0.50	0.19	129,136,136,137	0
2	NAG	A	601	14/15	0.72	0.14	111,123,129,129	0
3	MG	A	603	1/1	0.98	0.06	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.