



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3JAE
EMDB ID: : EMD-6345
Title : Structure of alpha-1 glycine receptor by single particle electron cryo-microscopy, glycine-bound state
Authors : Du, J.; Lu, W.; Wu, S.P.; Cheng, Y.F.; Gouaux, E.
Deposited on : 2015-06-08
Resolution : 3.90 Å(reported)
Based on PDB ID : 3RHW

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

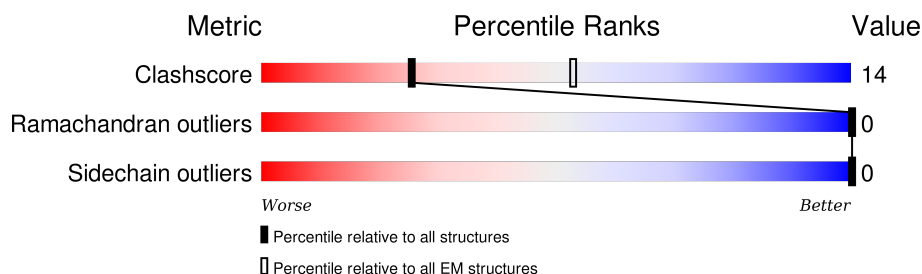
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	342	75% 24% .
1	B	342	73% 26% .
1	C	342	75% 24% .
1	D	342	73% 25% .
1	E	342	75% 24% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	B	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	C	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	D	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		
1	E	338	Total	C	N	O	S	0	0
			2537	1656	424	444	13		

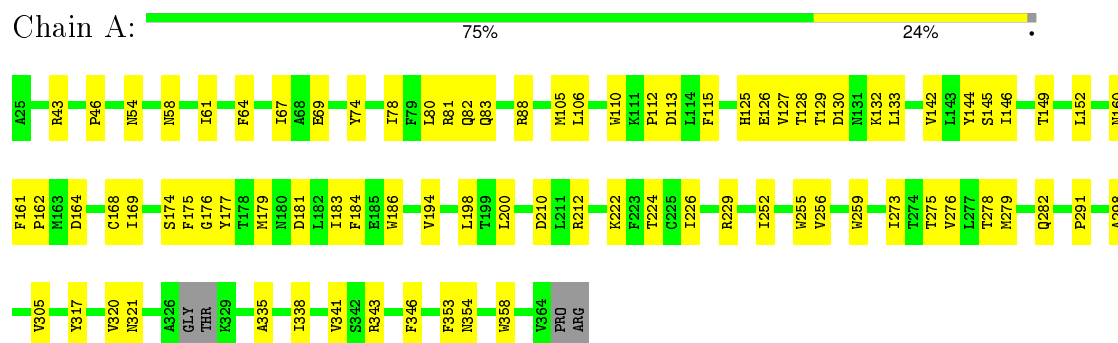
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			28	16	2	10	
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	C	2	Total	C	N	O	0
			28	16	2	10	
2	D	2	Total	C	N	O	0
			28	16	2	10	
2	E	2	Total	C	N	O	0
			28	16	2	10	

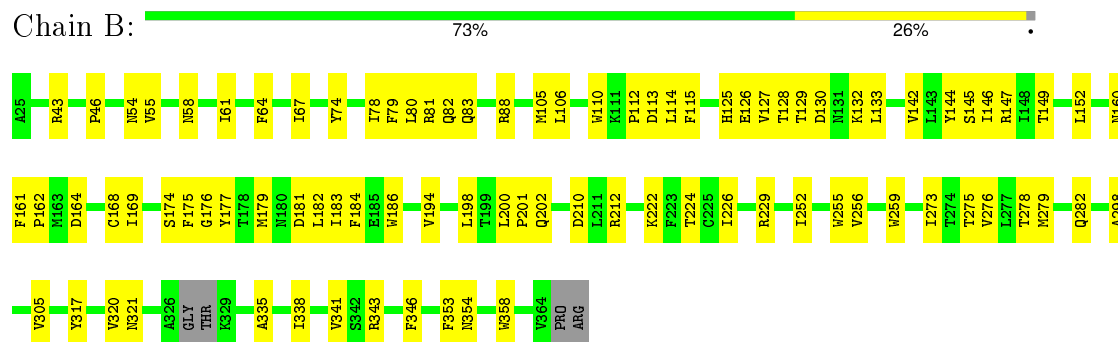
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

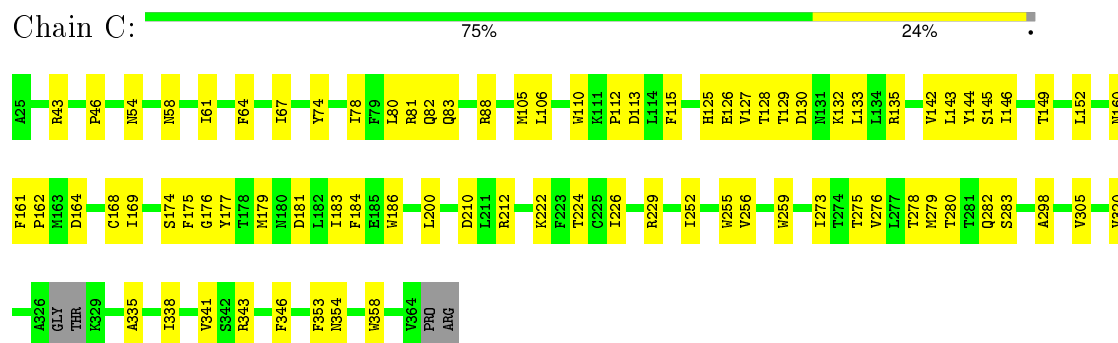
• Molecule 1: Glycine receptor subunit alphaZ1




• Molecule 1: Glycine receptor subunit alphaZ1



• Molecule 1: Glycine receptor subunit alphaZ1



• Molecule 1: Glycine receptor subunit alphaZ1

Chain E: 

V305	P162	A25
Y317	M163	R43
V320	D164	P46
N321	C168	M54
A326	L169	V55
GLY	S174	N58
THR	F175	I61
K329	G176	F64
A335	Y177	I67
I338	T178	Y74
V341	M180	I78
S342	D181	F79
R343	L182	L80
F346	I183	R81
F353	F184	Q82
V364	E185	Q83
PRO	G186	R88
ARG	V194	M105
	L198	L106
	T199	W110
	L200	K111
	P201	P112
	Q202	D213
	D210	L114
	L211	F115
	R212	L125
	K222	E126
	F223	V127
	T224	T128
	C225	T129
	I226	D130
	R229	K131
	I282	K132
	W255	L133
	V256	V142
	K259	L143
	T273	Y144
	T274	S145
	T275	I146
	V276	T149
	I277	L152
	T278	M160
	T279	F161
	Q282	
	A288	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	58188	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.31	0/2601	0.54	0/3557
1	B	0.32	0/2601	0.54	0/3557
1	C	0.31	0/2601	0.54	0/3557
1	D	0.31	0/2601	0.54	0/3557
1	E	0.32	0/2601	0.54	0/3557
All	All	0.31	0/13005	0.54	0/17785

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	A	2537	0	2391	67	0
1	B	2537	0	2391	70	0
1	C	2537	0	2391	69	0
1	D	2537	0	2391	71	0
1	E	2537	0	2391	68	0
2	A	28	0	25	2	0
2	B	28	0	25	2	0
2	C	28	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	2	0
2	E	28	0	25	2	0
All	All	12825	0	12080	338	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 14.

The worst 5 of 338 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:169:ILE:HG21	1:A:229:ARG:HH11	1.36	0.91
1:E:169:ILE:HG21	1:E:229:ARG:HH11	1.36	0.90
1:D:169:ILE:HG21	1:D:229:ARG:HH11	1.36	0.90
1:B:169:ILE:HG21	1:B:229:ARG:HH11	1.36	0.90
1:C:169:ILE:HG21	1:C:229:ARG:HH11	1.36	0.90

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 PDB entries followed by that with respect to all EM entries.

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	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	B	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	C	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	D	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
1	E	334/342 (98%)	331 (99%)	3 (1%)	0	100	100
All	All	1670/1710 (98%)	1655 (99%)	15 (1%)	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 PDB entries followed by that with respect to all EM entries.

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	246/304 (81%)	246 (100%)	0	100	100
1	B	246/304 (81%)	246 (100%)	0	100	100
1	C	246/304 (81%)	246 (100%)	0	100	100
1	D	246/304 (81%)	246 (100%)	0	100	100
1	E	246/304 (81%)	246 (100%)	0	100	100
All	All	1230/1520 (81%)	1230 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	ASN
1	C	160	ASN
1	D	160	ASN
1	B	160	ASN
1	D	54	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](#)

10 carbohydrates 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
2	NAG	A	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	A	502	2	14,14,15	0.61	0	15,19,21	0.58	0
2	NAG	B	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	B	502	2	14,14,15	0.61	0	15,19,21	0.58	0
2	NAG	C	501	2	14,14,15	0.37	0	15,19,21	1.33	1 (6%)
2	NAG	C	502	2	14,14,15	0.60	0	15,19,21	0.58	0
2	NAG	D	501	2	14,14,15	0.39	0	15,19,21	1.32	1 (6%)
2	NAG	D	502	2	14,14,15	0.60	0	15,19,21	0.58	0
2	NAG	E	501	2	14,14,15	0.38	0	15,19,21	1.32	1 (6%)
2	NAG	E	502	2	14,14,15	0.62	0	15,19,21	0.58	0

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	501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	501	2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	NAG	C	501	2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	2	-	0/6/23/26	0/1/1/1
2	NAG	D	501	2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	2	-	0/6/23/26	0/1/1/1
2	NAG	E	501	2	-	0/6/23/26	0/1/1/1
2	NAG	E	502	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C2-N2-C7	4.51	128.97	123.11
2	A	501	NAG	C2-N2-C7	4.51	128.97	123.11
2	E	501	NAG	C2-N2-C7	4.51	128.97	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAG	C2-N2-C7	4.52	128.98	123.11
2	C	501	NAG	C2-N2-C7	4.55	129.02	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	2	0
2	B	501	NAG	2	0
2	C	501	NAG	2	0
2	D	501	NAG	2	0
2	E	501	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.