# wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Feb 10, 2019 – 02:00 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6N51 |
| EMDB ID: | : | EMD-0345 |
| Title | : | Metabotropic Glutamate Receptor 5 bound to L-quisqualate and Nb43 |
| Authors | : | Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Weis, W.I.; Skiniotis, G.S.; Mathiesen, J.M.; Kobilka, B.K. |
| Deposited on | : | 2018-11-20 |
| Resolution | : | 4.00 Å(reported) |

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

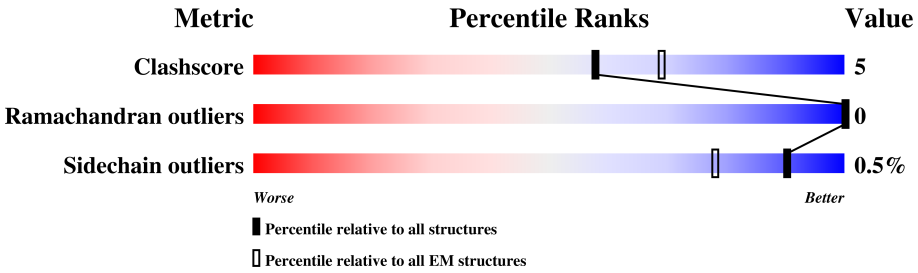
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.3 (157068), CSD as539be (2018) |
| Percentile statistics | : | 20171227.v01 (using entries in the PDB archive December 27th 2017) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20031633 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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 | 136327 | 1886 |
| Ramachandran outliers | 132723 | 1663 |
| Sidechain outliers | 132532 | 1531 |

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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 804 | 85% 13% . |
| 1 | B | 804 | 84% 14% . |
| 2 | C | 123 | 81% 19% |
| 2 | D | 123 | 85% 15% |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14087 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.

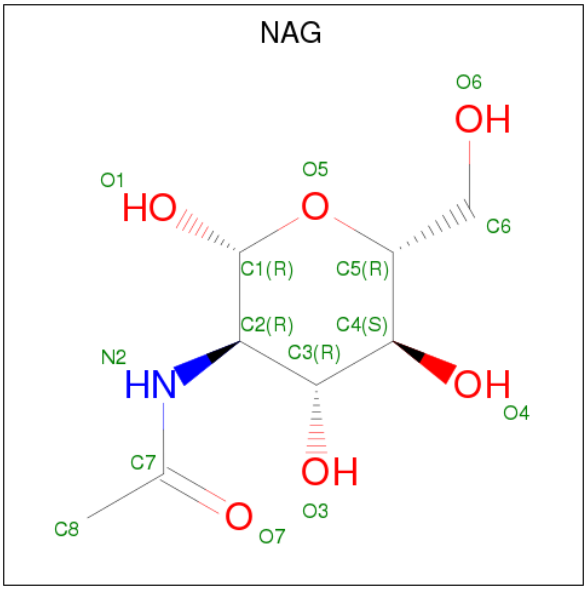
- Molecule 1 is a protein called Metabotropic glutamate receptor 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | B | 793 | Total | C | N | O | S | 0 | 0 |
| | | | 6075 | 3878 | 1030 | 1108 | 59 | | |
| 1 | A | 791 | Total | C | N | O | S | 0 | 0 |
| | | | 6060 | 3870 | 1028 | 1103 | 59 | | |

- Molecule 2 is a protein called Nanobody 43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 939 | 583 | 164 | 187 | 5 | | |
| 2 | D | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 931 | 578 | 162 | 186 | 5 | | |

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |

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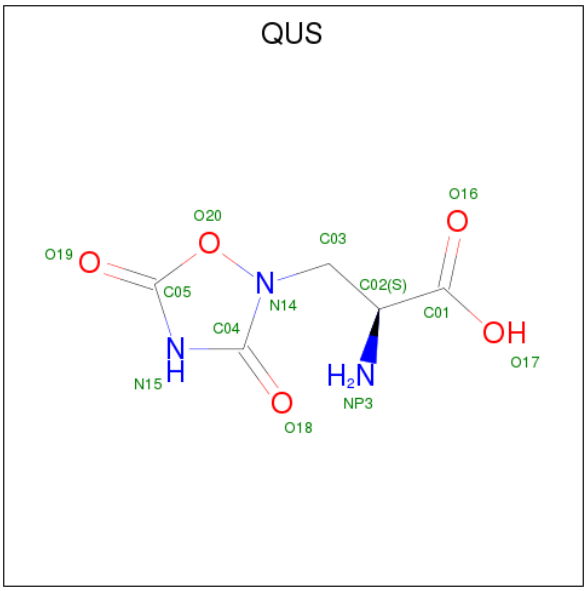
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 3 | A | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 3 | A | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |

- Molecule 4 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: $C_5H_7N_3O_5$).



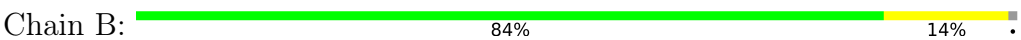

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 4 | B | 1 | Total | C | N | O | 0 |
| | | | 13 | 5 | 3 | 5 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 13 | 5 | 3 | 5 | |

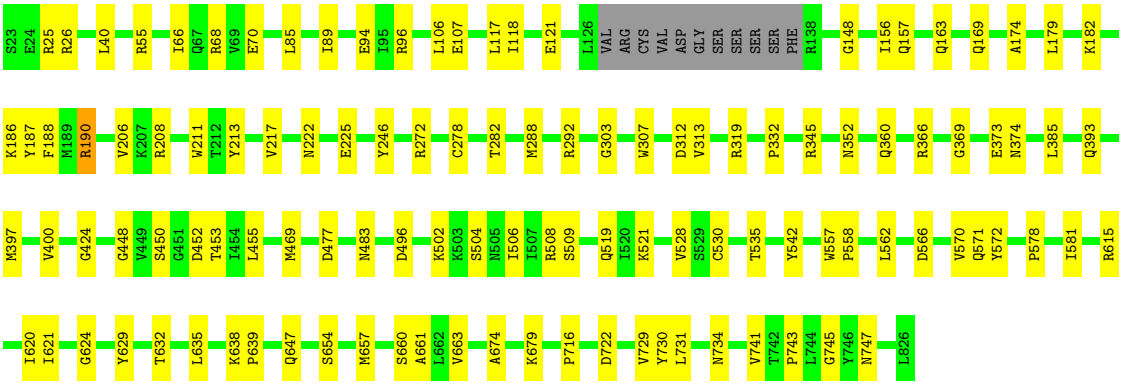
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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: Metabotropic glutamate receptor 5

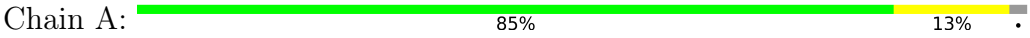
Chain B:

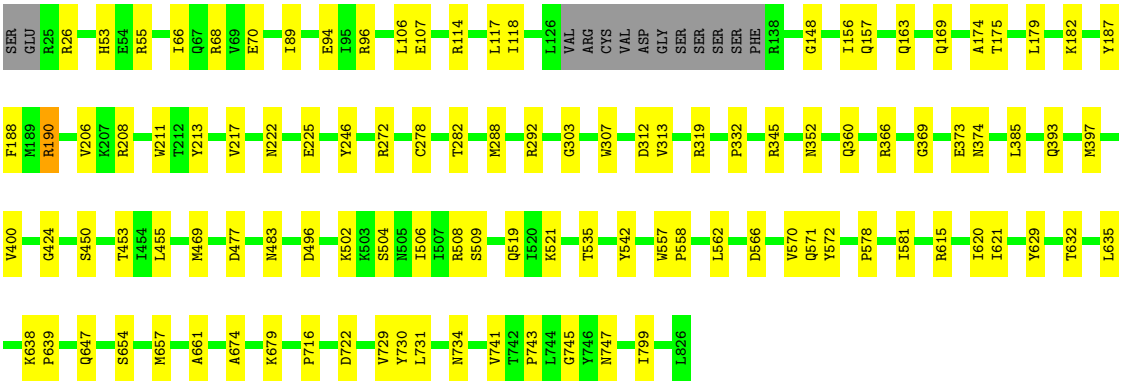



• Molecule 1: Metabotropic glutamate receptor 5

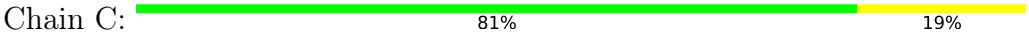
Chain A:




• Molecule 2: Nanobody 43

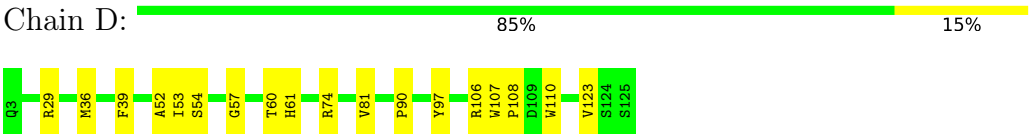
Chain C:





• Molecule 2: Nanobody 43

Chain D:


85%
15%
Q3
R29
M36
F39
A52
I53
S54
G57
T60
H61
R74
V81
P90
Y97
R106
W107
P108
D109
W110
V123
S124
S125

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 73472 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | 47169 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUS, 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 | 0.34 | 0/6194 | 0.52 | 0/8397 |
| 1 | B | 0.34 | 0/6209 | 0.52 | 0/8417 |
| 2 | C | 0.31 | 0/961 | 0.51 | 0/1300 |
| 2 | D | 0.31 | 0/953 | 0.52 | 0/1291 |
| All | All | 0.34 | 0/14317 | 0.52 | 0/19405 |

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 | 6060 | 0 | 5921 | 62 | 0 |
| 1 | B | 6075 | 0 | 5932 | 70 | 0 |
| 2 | C | 939 | 0 | 880 | 12 | 0 |
| 2 | D | 931 | 0 | 863 | 13 | 0 |
| 3 | A | 28 | 0 | 26 | 0 | 0 |
| 3 | B | 28 | 0 | 26 | 0 | 0 |
| 4 | A | 13 | 0 | 6 | 1 | 0 |
| 4 | B | 13 | 0 | 6 | 0 | 0 |
| All | All | 14087 | 0 | 13660 | 150 | 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 5.

The worst 5 of 150 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:B:360:GLN:HE22 | 1:B:366:ARG:HA | 1.55 | 0.72 |
| 1:A:360:GLN:HE22 | 1:A:366:ARG:HA | 1.55 | 0.69 |
| 1:B:288:MET:HG2 | 1:B:292:ARG:HE | 1.57 | 0.68 |
| 1:B:360:GLN:HE21 | 1:B:374:ASN:HB3 | 1.59 | 0.68 |
| 1:A:360:GLN:HE21 | 1:A:374:ASN:HB3 | 1.59 | 0.67 |

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 | 787/804 (98%) | 731 (93%) | 56 (7%) | 0 | 100 | 100 |
| 1 | B | 789/804 (98%) | 733 (93%) | 56 (7%) | 0 | 100 | 100 |
| 2 | C | 121/123 (98%) | 114 (94%) | 7 (6%) | 0 | 100 | 100 |
| 2 | D | 121/123 (98%) | 117 (97%) | 4 (3%) | 0 | 100 | 100 |
| All | All | 1818/1854 (98%) | 1695 (93%) | 123 (7%) | 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 | 643/701 (92%) | 640 (100%) | 3 (0%) | 90 95 |
| 1 | B | 645/701 (92%) | 642 (100%) | 3 (0%) | 90 95 |
| 2 | C | 97/97 (100%) | 96 (99%) | 1 (1%) | 78 89 |
| 2 | D | 95/97 (98%) | 95 (100%) | 0 | 100 100 |
| All | All | 1480/1596 (93%) | 1473 (100%) | 7 (0%) | 90 95 |

5 of 7 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 106 | ARG |
| 1 | A | 615 | ARG |
| 1 | A | 190 | ARG |
| 1 | B | 508 | ARG |
| 1 | A | 508 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 53 | HIS |
| 1 | A | 360 | GLN |
| 1 | A | 159 | GLN |
| 1 | B | 360 | GLN |
| 1 | A | 157 | GLN |

### 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)

6 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 | NAG | A | 901 | 1 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.37 | 0 |
| 3 | NAG | A | 902 | 1 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.56 | 0 |
| 4 | QUS | A | 903 | - | 4,13,13 | 0.85 | 0 | 0,18,18 | 0.00 | - |
| 3 | NAG | B | 901 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.37 | 0 |
| 3 | NAG | B | 902 | 1 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.54 | 0 |
| 4 | QUS | B | 903 | - | 4,13,13 | 0.81 | 0 | 0,18,18 | 0.00 | - |

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 | NAG | A | 901 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | A | 902 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | QUS | A | 903 | - | - | 0/1/8/8 | 0/1/1/1 |
| 3 | NAG | B | 901 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | B | 902 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | QUS | B | 903 | - | - | 0/1/8/8 | 0/1/1/1 |

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.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | A | 903 | QUS | 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.