



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jun 26, 2018 – 12:41 PM EDT

PDB ID : 6DDE
EMDB ID: : EMD-7868
Title : Mu Opioid Receptor-Gi Protein Complex
Authors : Koehl, A.; Hu, H.; Maeda, S.; Manglik, A.; Zhang, Y.; Kobilka, B.K.; Skiniotis, G.; Weis, W.I.
Deposited on : 2018-05-10
Resolution : 3.50 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 ⓘ 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-20031172

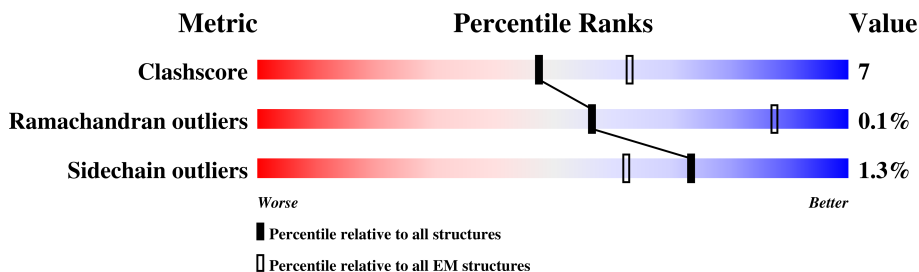
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	354	51% 10% 39%
2	B	344	74% 23% .
3	C	71	65% 10% 25%
4	E	259	80% 9% 10%
5	R	356	70% 9% 21%
6	D	5	80% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8489 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1679	1075	288	304	12		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	336	Total	C	N	O	S	0	0
			2547	1577	458	493	19		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	53	Total	C	N	O	S	0	0
			381	243	67	68	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	232	Total	C	N	O	S	0	0
			1748	1116	295	328	9		

- Molecule 5 is a protein called Mu-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	281	Total	C	N	O	S	0	0
			2097	1379	344	357	17		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	46	GLU	-	insertion	UNP P42866
R	47	ASN	-	insertion	UNP P42866
R	48	LEU	-	insertion	UNP P42866
R	49	TYR	-	insertion	UNP P42866
R	50	PHE	-	insertion	UNP P42866
R	51	GLN	-	insertion	UNP P42866

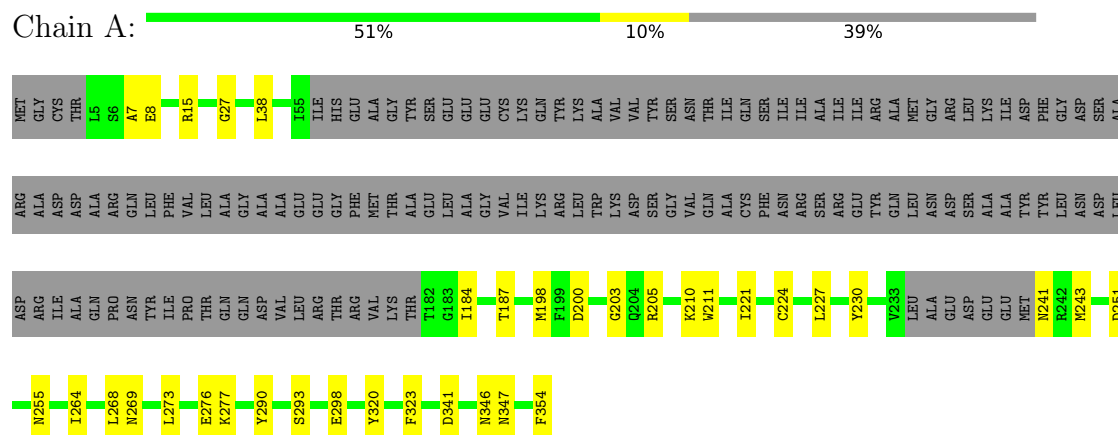
- Molecule 6 is a protein called DAMGO.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	5	Total	C	N	O	0	0
			37	26	5	6		

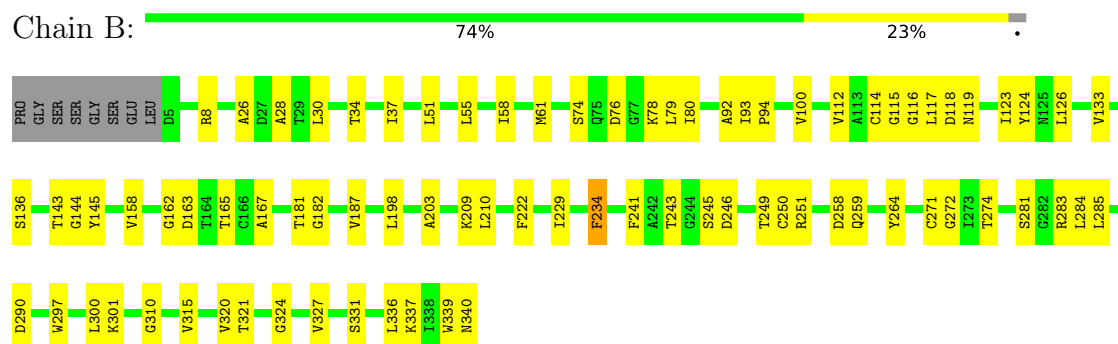
3 Residue-property plots [i](#)

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.

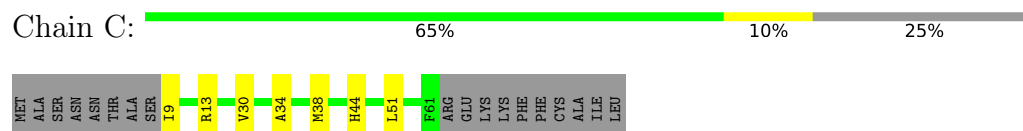
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



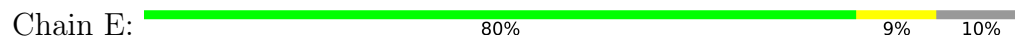
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

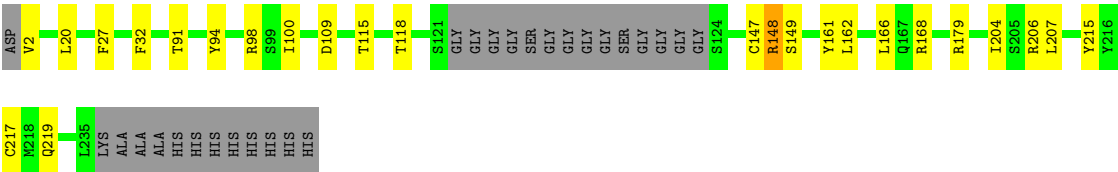


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

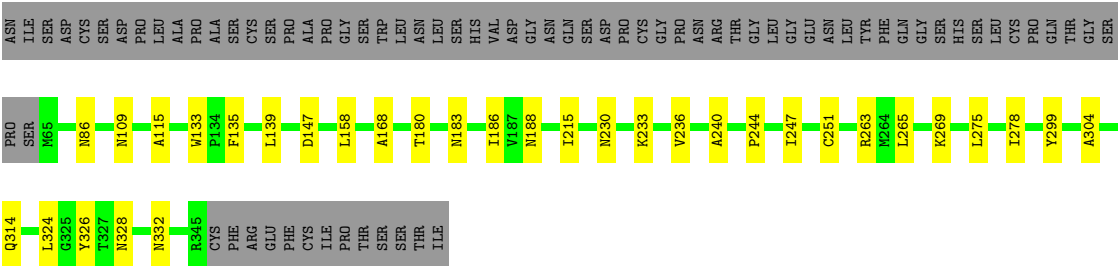


- Molecule 4: scFv16

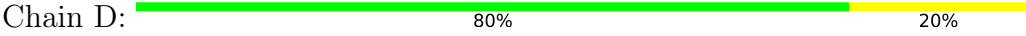




● Molecule 5: Mu-type opioid receptor



● Molecule 6: DAMGO



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	359406	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	48076	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: DAL, ETA, MEA

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	0.32	0/1708	0.54	0/2296
2	B	0.37	0/2594	0.63	0/3520
3	C	0.37	0/387	0.51	0/527
4	E	0.42	0/1792	0.69	0/2434
5	R	0.30	0/2147	0.54	0/2942
6	D	0.34	0/15	0.54	0/17
All	All	0.36	0/8643	0.60	0/11736

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	1679	0	1634	24	0
2	B	2547	0	2437	55	0
3	C	381	0	378	6	0
4	E	1748	0	1671	21	0
5	R	2097	0	2002	20	0
6	D	37	0	34	1	0
All	All	8489	0	8156	113	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 7.

The worst 5 of 113 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)
4:E:147:CYS:HG	4:E:217:CYS:HG	1.06	0.88
4:E:147:CYS:HG	4:E:217:CYS:CB	1.91	0.83
2:B:79:LEU:HD12	2:B:79:LEU:O	1.78	0.83
4:E:162:LEU:HD11	4:E:217:CYS:SG	2.20	0.82
4:E:20:LEU:CD1	4:E:94:TYR:HD2	2.07	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	211/354 (60%)	197 (93%)	14 (7%)	0	100	100
2	B	334/344 (97%)	301 (90%)	33 (10%)	0	100	100
3	C	51/71 (72%)	46 (90%)	5 (10%)	0	100	100
4	E	228/259 (88%)	221 (97%)	7 (3%)	0	100	100
5	R	279/356 (78%)	261 (94%)	17 (6%)	1 (0%)	36	75
6	D	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1104/1389 (80%)	1027 (93%)	76 (7%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	R	269	LYS

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 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	172/305 (56%)	170 (99%)	2 (1%)	74	88
2	B	268/285 (94%)	264 (98%)	4 (2%)	67	86
3	C	36/58 (62%)	36 (100%)	0	100	100
4	E	184/209 (88%)	181 (98%)	3 (2%)	65	85
5	R	205/320 (64%)	203 (99%)	2 (1%)	78	90
6	D	1/1 (100%)	1 (100%)	0	100	100
All	All	866/1178 (74%)	855 (99%)	11 (1%)	73	88

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	PHE
2	B	340	ASN
4	E	219	GLN
2	B	30	LEU
4	E	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	340	ASN
3	C	18	GLN
5	R	150	ASN
2	B	266	HIS
2	B	295	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
6	DAL	D	2	6	4,4,5	0.91	0	1,4,6	0.22	0
6	MEA	D	4	6	12,12,13	0.86	1 (8%)	13,14,16	0.75	0
6	ETA	D	5	6	3,3,3	0.88	0	2,2,2	0.77	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
6	DAL	D	2	6	-	0/0/2/4	0/0/0/0
6	MEA	D	4	6	-	0/4/8/10	0/1/1/1
6	ETA	D	5	6	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	4	MEA	CA-C	2.06	1.53	1.50

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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.