wwPDB EM Validation Summary Report

Oct 7, 2024 – 02:09 PM JST

PDB ID	:	8JMT
EMDB ID	:	EMD-36426
Title	:	Structure of the adhesion GPCR ADGRL3 in the apo state
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Deposited on	:	2023-06-05
Resolution	:	3.36 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

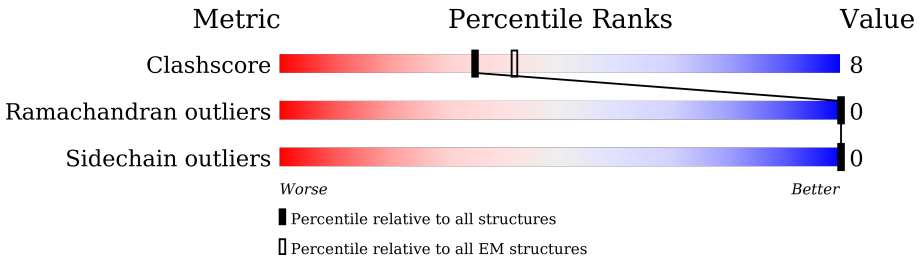
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.36 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	758	24% 7% 69%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1894 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 Adhesion G protein-coupled receptor L3,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	234	1894	1284	296	297	17	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ASP	-	expression tag	UNP E7ES20
A	480	TYR	-	expression tag	UNP E7ES20
A	481	LYS	-	expression tag	UNP E7ES20
A	482	ASP	-	expression tag	UNP E7ES20
A	483	ASP	-	expression tag	UNP E7ES20
A	484	ASP	-	expression tag	UNP E7ES20
A	485	ASP	-	expression tag	UNP E7ES20
A	486	LYS	-	expression tag	UNP E7ES20
A	842	ALA	THR	engineered mutation	UNP E7ES20
A	1051	TRP	MET	engineered mutation	UNP P0ABE7
A	1088	SER	-	linker	UNP P0ABE7
A	1089	GLY	-	linker	UNP P0ABE7
A	1090	SER	-	linker	UNP P0ABE7
A	1091	GLY	-	linker	UNP P0ABE7
A	1139	ILE	HIS	engineered mutation	UNP P0ABE7
A	1143	LEU	-	insertion	UNP P0ABE7
A	1144	GLU	-	insertion	UNP P0ABE7
A	1146	ALA	-	linker	UNP P0ABE7
A	1219	ALA	-	expression tag	UNP E7ES20
A	1220	ALA	-	expression tag	UNP E7ES20
A	1221	SER	-	expression tag	UNP E7ES20
A	1222	ARG	-	expression tag	UNP E7ES20
A	1223	LEU	-	expression tag	UNP E7ES20
A	1224	GLU	-	expression tag	UNP E7ES20
A	1225	GLU	-	expression tag	UNP E7ES20
A	1226	GLU	-	expression tag	UNP E7ES20
A	1227	LEU	-	expression tag	UNP E7ES20

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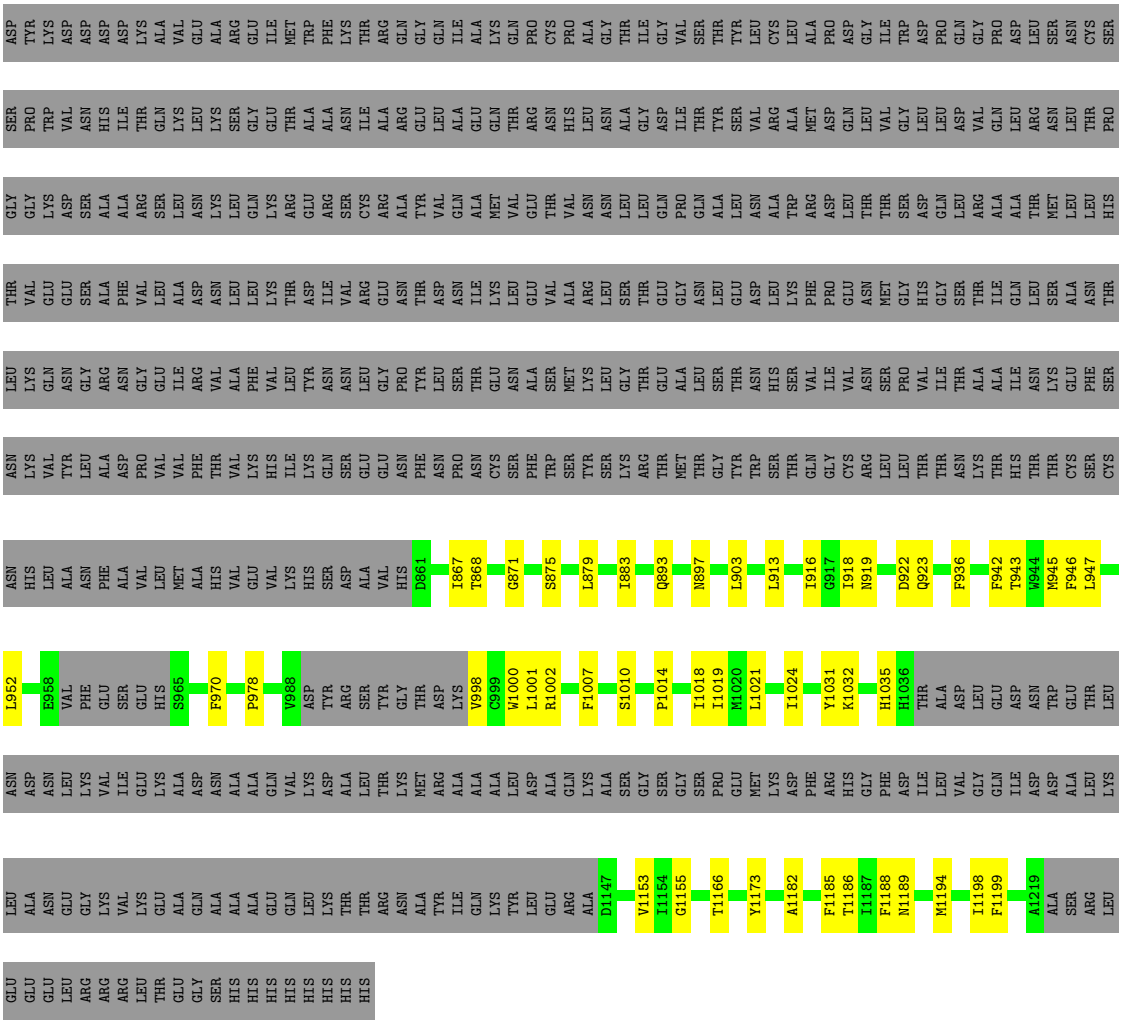
Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	ARG	-	expression tag	UNP E7ES20
A	1229	ARG	-	expression tag	UNP E7ES20
A	1230	ARG	-	expression tag	UNP E7ES20
A	1231	LEU	-	expression tag	UNP E7ES20
A	1232	THR	-	expression tag	UNP E7ES20
A	1233	GLU	-	expression tag	UNP E7ES20
A	1234	GLY	-	expression tag	UNP E7ES20
A	1235	SER	-	expression tag	UNP E7ES20
A	1236	HIS	-	expression tag	UNP E7ES20
A	1237	HIS	-	expression tag	UNP E7ES20
A	1238	HIS	-	expression tag	UNP E7ES20
A	1239	HIS	-	expression tag	UNP E7ES20
A	1240	HIS	-	expression tag	UNP E7ES20
A	1241	HIS	-	expression tag	UNP E7ES20
A	1242	HIS	-	expression tag	UNP E7ES20
A	1243	HIS	-	expression tag	UNP E7ES20

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. 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: Adhesion G protein-coupled receptor L3,Soluble cytochrome b562

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	706010	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)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/1943	0.46	0/2633

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	1894	0	1961	30	0
All	All	1894	0	1961	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 8.

The worst 5 of 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:1185:PHE:O	1:A:1189:ASN:ND2	2.20	0.74
1:A:1001:LEU:HD12	1:A:1002:ARG:H	1.55	0.69
1:A:1194:MET:HG3	1:A:1198:ILE:HD12	1.76	0.66
1:A:1031:TYR:O	1:A:1035:HIS:ND1	2.30	0.59
1:A:998:VAL:HG22	1:A:1000:TRP:H	1.69	0.57

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	226/758 (30%)	218 (96%)	8 (4%)	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	203/649 (31%)	203 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1189	ASN
1	A	1204	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 oligosaccharides 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.