



wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 12:16 AM JST

PDB ID : 8IBV
EMDB ID : EMD-35346
Title : Cryo-EM structure of the motilin-bound motilin receptor-Gq protein complex
Authors : Jiang, Y.; Xu, H.E.; You, C.; Xu, Y.
Deposited on : 2023-02-10
Resolution : 3.19 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

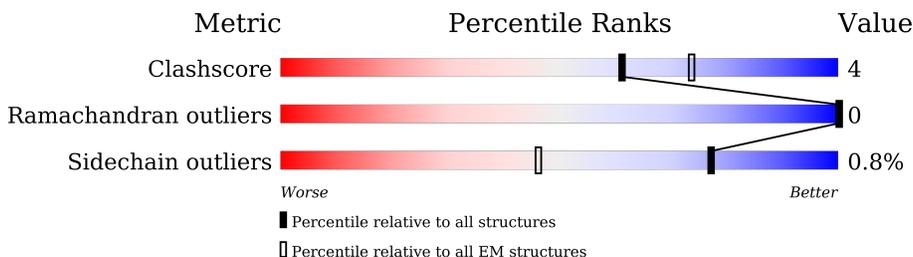
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	R	741	
2	C	22	
3	A	361	
4	B	371	
5	E	247	
6	G	70	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18081 atoms, of which 9023 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 Soluble cytochrome b562, Motilin receptor, Soluble cytochrome b562, motilin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	R	279	4539	1472	2322	371	358	16	0	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-155	MET	-	initiating methionine	UNP P0ABE7
R	-154	LYS	-	expression tag	UNP P0ABE7
R	-153	THR	-	expression tag	UNP P0ABE7
R	-152	ILE	-	expression tag	UNP P0ABE7
R	-151	ILE	-	expression tag	UNP P0ABE7
R	-150	ALA	-	expression tag	UNP P0ABE7
R	-149	LEU	-	expression tag	UNP P0ABE7
R	-148	SER	-	expression tag	UNP P0ABE7
R	-147	TYR	-	expression tag	UNP P0ABE7
R	-146	ILE	-	expression tag	UNP P0ABE7
R	-145	PHE	-	expression tag	UNP P0ABE7
R	-144	CYS	-	expression tag	UNP P0ABE7
R	-143	LEU	-	expression tag	UNP P0ABE7
R	-142	VAL	-	expression tag	UNP P0ABE7
R	-141	PHE	-	expression tag	UNP P0ABE7
R	-140	ALA	-	expression tag	UNP P0ABE7
R	-139	ASP	-	expression tag	UNP P0ABE7
R	-138	TYR	-	expression tag	UNP P0ABE7
R	-137	LYS	-	expression tag	UNP P0ABE7
R	-136	ASP	-	expression tag	UNP P0ABE7
R	-135	ASP	-	expression tag	UNP P0ABE7
R	-134	ASP	-	expression tag	UNP P0ABE7
R	-133	ASP	-	expression tag	UNP P0ABE7
R	-132	ALA	-	expression tag	UNP P0ABE7
R	-131	LYS	-	expression tag	UNP P0ABE7
R	-130	LEU	-	expression tag	UNP P0ABE7
R	-129	GLN	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-128	THR	-	expression tag	UNP P0ABE7
R	-127	MET	-	expression tag	UNP P0ABE7
R	-126	HIS	-	expression tag	UNP P0ABE7
R	-125	HIS	-	expression tag	UNP P0ABE7
R	-124	HIS	-	expression tag	UNP P0ABE7
R	-123	HIS	-	expression tag	UNP P0ABE7
R	-122	HIS	-	expression tag	UNP P0ABE7
R	-121	HIS	-	expression tag	UNP P0ABE7
R	-120	HIS	-	expression tag	UNP P0ABE7
R	-119	HIS	-	expression tag	UNP P0ABE7
R	-118	HIS	-	expression tag	UNP P0ABE7
R	-117	HIS	-	expression tag	UNP P0ABE7
R	-110	TRP	MET	conflict	UNP P0ABE7
R	-15	ILE	HIS	conflict	UNP P0ABE7
R	-11	LEU	-	linker	UNP P0ABE7
R	-10	ALA	-	linker	UNP P0ABE7
R	-9	SER	-	linker	UNP P0ABE7
R	-8	GLU	-	linker	UNP P0ABE7
R	-7	ASN	-	linker	UNP P0ABE7
R	-6	LEU	-	linker	UNP P0ABE7
R	-5	TYR	-	linker	UNP P0ABE7
R	-4	PHE	-	linker	UNP P0ABE7
R	-3	GLN	-	linker	UNP P0ABE7
R	-2	GLY	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	THR	-	linker	UNP P0ABE7

- Molecule 2 is a protein called Motilin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	19	332	107	165	29	30	1	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(q) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	A	232	3815	1207	1907	338	355	8	0	0

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	B	338	5089	1597	2498	467	506	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	GLY	-	expression tag	UNP P62873
B	3	SER	-	expression tag	UNP P62873
B	4	LEU	-	expression tag	UNP P62873
B	5	LEU	-	expression tag	UNP P62873
B	6	GLN	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	SER	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873
B	359	SER	-	expression tag	UNP P62873
B	360	GLY	-	expression tag	UNP P62873
B	361	VAL	-	expression tag	UNP P62873
B	362	SER	-	expression tag	UNP P62873
B	363	GLY	-	expression tag	UNP P62873
B	364	TRP	-	expression tag	UNP P62873
B	365	ARG	-	expression tag	UNP P62873
B	366	LEU	-	expression tag	UNP P62873
B	367	PHE	-	expression tag	UNP P62873
B	368	LYS	-	expression tag	UNP P62873
B	369	LYS	-	expression tag	UNP P62873
B	370	ILE	-	expression tag	UNP P62873
B	371	SER	-	expression tag	UNP P62873

- Molecule 5 is a protein called Scfv16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	230	3479	1123	1711	293	343	9	0	0

- Molecule 6 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	54	827	253	420	71	80	3	0	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1174882	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 ($e^-/\text{\AA}^2$)	1.39	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	R	0.43	2/2271 (0.1%)	0.53	1/3092 (0.0%)
2	C	0.40	0/170	0.72	1/226 (0.4%)
3	A	0.23	0/1942	0.37	0/2614
4	B	0.23	0/2637	0.42	0/3576
5	E	0.25	0/1811	0.41	0/2455
6	G	0.25	0/411	0.35	0/555
All	All	0.30	2/9242 (0.0%)	0.44	2/12518 (0.0%)

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	R	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	96	TYR	CB-CG	-5.75	1.43	1.51
1	R	226	GLU	CA-C	5.49	1.67	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	12	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	R	236	ARG	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	233	ARG	Sidechain

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	R	2217	2322	2318	30	0
2	C	167	165	165	0	0
3	A	1908	1907	1905	10	0
4	B	2591	2498	2496	26	0
5	E	1768	1711	1709	10	0
6	G	407	420	419	3	0
All	All	9058	9023	9012	76	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.

The worst 5 of 76 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)
3:A:216:ASN:OD1	4:B:62:LYS:NZ	2.21	0.73
1:R:124:ALA:O	1:R:128:HIS:ND1	2.24	0.71
3:A:259:ASN:OD1	3:A:260:LYS:N	2.28	0.65
5:E:5:GLU:N	5:E:5:GLU:OE1	2.30	0.63
5:E:88:GLU:OE1	5:E:88:GLU:N	2.33	0.61

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	R	271/741 (37%)	264 (97%)	7 (3%)	0	100	100
2	C	17/22 (77%)	17 (100%)	0	0	100	100
3	A	228/361 (63%)	225 (99%)	3 (1%)	0	100	100
4	B	336/371 (91%)	336 (100%)	0	0	100	100
5	E	224/247 (91%)	222 (99%)	2 (1%)	0	100	100
6	G	52/70 (74%)	52 (100%)	0	0	100	100
All	All	1128/1812 (62%)	1116 (99%)	12 (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	R	239/615 (39%)	235 (98%)	4 (2%)	56	78
2	C	18/20 (90%)	18 (100%)	0	100	100
3	A	210/316 (66%)	207 (99%)	3 (1%)	62	82
4	B	279/302 (92%)	278 (100%)	1 (0%)	89	94
5	E	194/198 (98%)	194 (100%)	0	100	100
6	G	43/57 (75%)	43 (100%)	0	100	100
All	All	983/1508 (65%)	975 (99%)	8 (1%)	77	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	110	TYR
3	A	356	ARG
3	A	324	HIS
1	R	234	GLU
3	A	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	324	HIS
4	B	96	HIS
4	B	161	GLN
5	E	76	ASN
5	E	142	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.