



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 10:59 AM JST

PDB ID : 8XVH
EMDB ID : EMD-38704
Title : Cryo-EM structure of ETBR bound with Endothelin1
Authors : Hou, J.Y.; Liu, S.H.; Wu, L.J.; Liu, Z.J.; Hua, T.
Deposited on : 2024-01-15
Resolution : 3.26 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:

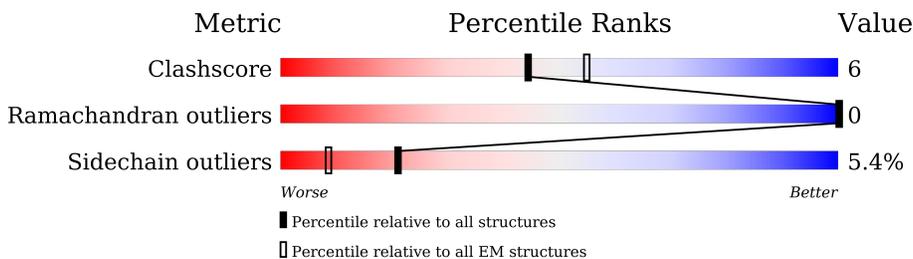
EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 3.26 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	A	261	
2	B	346	
3	G	71	
4	N	157	
5	T	21	
6	R	837	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8544 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 Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	233	1935	1221	348	359	7	0	0

- 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
			Total	C	N	O	S		
2	B	338	2600	1604	467	508	21	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ILE	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	ARG	-	expression tag	UNP P62873
B	-2	ALA	-	expression tag	UNP P62873
B	-1	ARG	-	expression tag	UNP P62873
B	0	GLY	-	expression tag	UNP P62873
B	1	PHE	-	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
			Total	C	N	O	S		
3	G	57	436	273	77	83	3	0	0

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	126	961	599	168	188	6	0	0

- Molecule 5 is a protein called Endothelin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	T	21	171	109	25	32	5	0	0

- Molecule 6 is a protein called Exo-alpha-sialidase,Endothelin receptor type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	305	2441	1621	395	405	20	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-412	MET	-	initiating methionine	UNP Q59310
R	-411	LYS	-	expression tag	UNP Q59310
R	-410	THR	-	expression tag	UNP Q59310
R	-409	ILE	-	expression tag	UNP Q59310
R	-408	ILE	-	expression tag	UNP Q59310
R	-407	ALA	-	expression tag	UNP Q59310
R	-406	LEU	-	expression tag	UNP Q59310
R	-405	SER	-	expression tag	UNP Q59310
R	-404	TYR	-	expression tag	UNP Q59310
R	-403	ILE	-	expression tag	UNP Q59310
R	-402	PHE	-	expression tag	UNP Q59310
R	-401	CYS	-	expression tag	UNP Q59310
R	-400	LEU	-	expression tag	UNP Q59310
R	-399	VAL	-	expression tag	UNP Q59310
R	-398	PHE	-	expression tag	UNP Q59310
R	-397	ALA	-	expression tag	UNP Q59310
R	-396	ASP	-	expression tag	UNP Q59310
R	-395	TYR	-	expression tag	UNP Q59310
R	-394	LYS	-	expression tag	UNP Q59310
R	-393	ASP	-	expression tag	UNP Q59310
R	-392	ASP	-	expression tag	UNP Q59310
R	-391	ASP	-	expression tag	UNP Q59310
R	-390	ASP	-	expression tag	UNP Q59310
R	-389	ALA	-	expression tag	UNP Q59310
R	-388	GLY	-	expression tag	UNP Q59310

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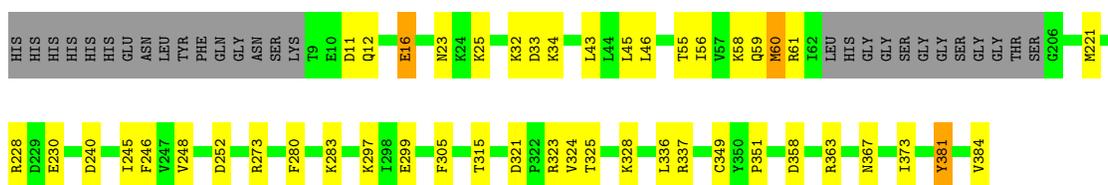
Chain	Residue	Modelled	Actual	Comment	Reference
R	-387	ARG	-	expression tag	UNP Q59310
R	-386	ALA	-	expression tag	UNP Q59310
R	-235	SER	GLY	conflict	UNP Q59310
R	407	LEU	-	expression tag	UNP P24530
R	408	GLU	-	expression tag	UNP P24530
R	409	VAL	-	expression tag	UNP P24530
R	410	LEU	-	expression tag	UNP P24530
R	411	PHE	-	expression tag	UNP P24530
R	412	GLN	-	expression tag	UNP P24530
R	413	GLY	-	expression tag	UNP P24530
R	414	PRO	-	expression tag	UNP P24530
R	415	HIS	-	expression tag	UNP P24530
R	416	HIS	-	expression tag	UNP P24530
R	417	HIS	-	expression tag	UNP P24530
R	418	HIS	-	expression tag	UNP P24530
R	419	HIS	-	expression tag	UNP P24530
R	420	HIS	-	expression tag	UNP P24530
R	421	HIS	-	expression tag	UNP P24530
R	422	HIS	-	expression tag	UNP P24530
R	423	HIS	-	expression tag	UNP P24530
R	424	HIS	-	expression tag	UNP P24530

3 Residue-property plots

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.

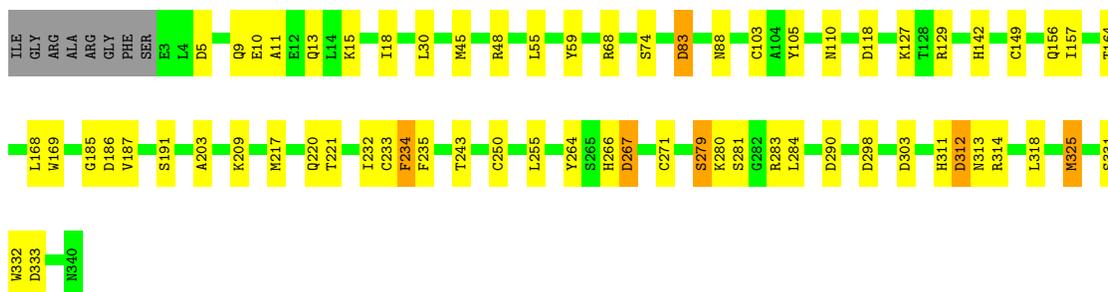
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A: 



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

Chain B: 



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

Chain G: 



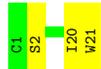
- Molecule 4: Nanobody 35

Chain N: 

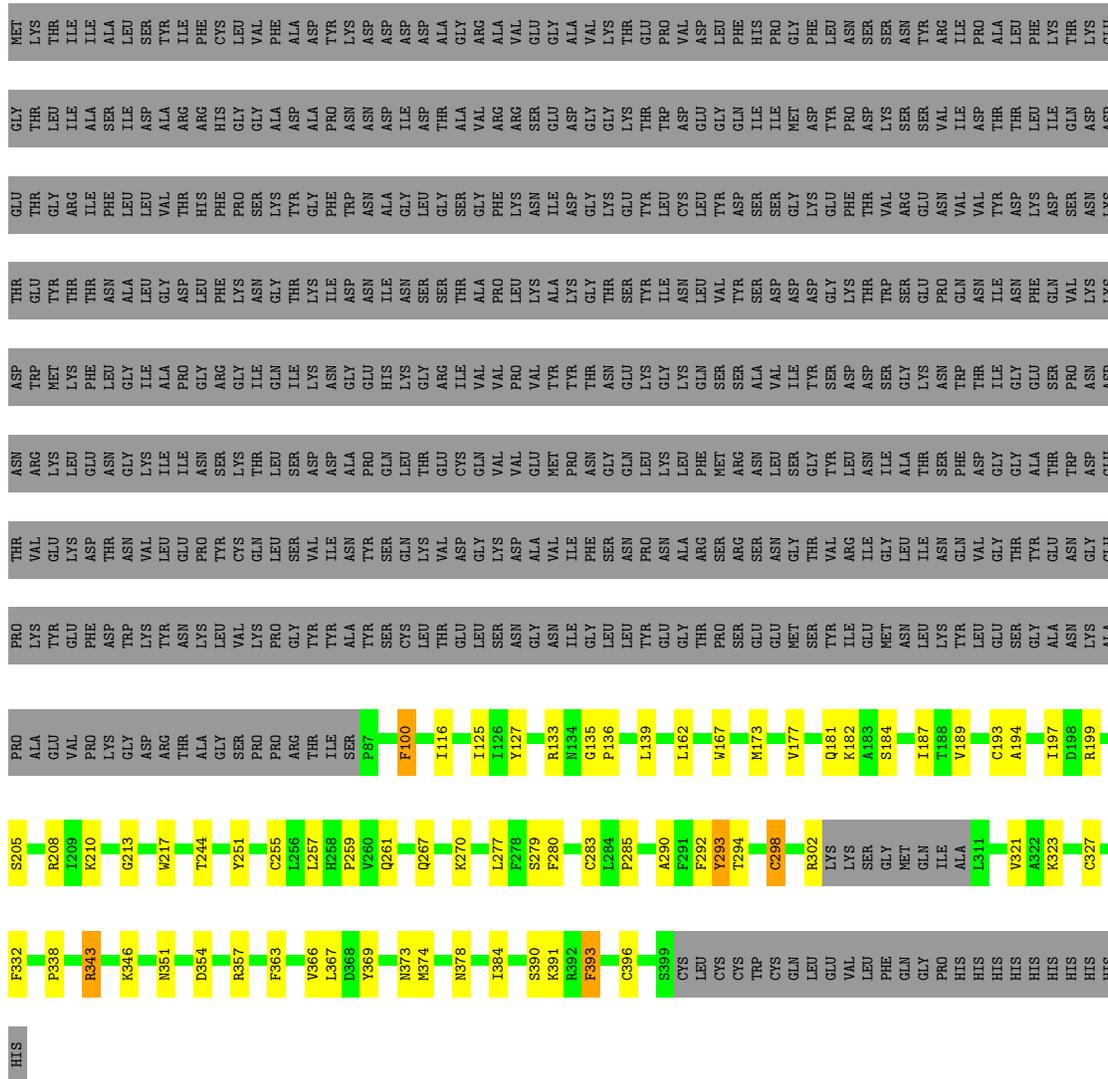




• Molecule 5: Endothelin-1



• Molecule 6: Exo-alpha-sialidase, Endothelin receptor type B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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	A	0.26	0/1971	0.54	1/2652 (0.0%)
2	B	0.24	0/2647	0.53	0/3589
3	G	0.25	0/442	0.46	0/597
4	N	0.25	0/981	0.52	0/1329
5	T	0.25	0/175	0.40	0/234
6	R	0.25	0/2501	0.45	0/3400
All	All	0.25	0/8717	0.51	1/11801 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASP	CB-CG-OD1	5.89	123.60	118.30

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	1935	0	1915	27	0
2	B	2600	0	2505	37	0
3	G	436	0	448	7	0
4	N	961	0	928	11	0
5	T	171	0	157	4	0
6	R	2441	0	2562	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8544	0	8515	106	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 6.

The worst 5 of 106 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:363:ARG:O	1:A:367:ASN:ND2	2.14	0.80
1:A:23:ASN:HD22	2:B:88:ASN:HB2	1.51	0.74
5:T:2:SER:HB3	6:R:257:LEU:HB3	1.72	0.71
6:R:384:ILE:HD12	6:R:384:ILE:H	1.60	0.65
6:R:354:ASP:HB3	6:R:357:ARG:HB3	1.79	0.64

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	229/261 (88%)	226 (99%)	3 (1%)	0	100	100
2	B	336/346 (97%)	322 (96%)	14 (4%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	124/157 (79%)	120 (97%)	4 (3%)	0	100	100
5	T	19/21 (90%)	19 (100%)	0	0	100	100
6	R	301/837 (36%)	297 (99%)	4 (1%)	0	100	100
All	All	1064/1693 (63%)	1039 (98%)	25 (2%)	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	210/231 (91%)	200 (95%)	10 (5%)	21	48
2	B	281/286 (98%)	263 (94%)	18 (6%)	14	39
3	G	46/58 (79%)	45 (98%)	1 (2%)	47	68
4	N	104/127 (82%)	101 (97%)	3 (3%)	37	61
5	T	21/21 (100%)	21 (100%)	0	100	100
6	R	274/731 (38%)	255 (93%)	19 (7%)	13	37
All	All	936/1454 (64%)	885 (95%)	51 (5%)	21	45

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	22	GLU
6	R	173	MET
6	R	391	LYS
4	N	35	ASN
6	R	100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	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](#)

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.