Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:06 PM JST

PDB ID	:	8HN1
EMDB ID	:	EMD-34906
Title	:	Cryo-EM structure of AdTx1-alpha1AAR-Nb6
Authors	:	Liu, X.; Shi, M.
Deposited on	:	2022-12-06
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation 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:

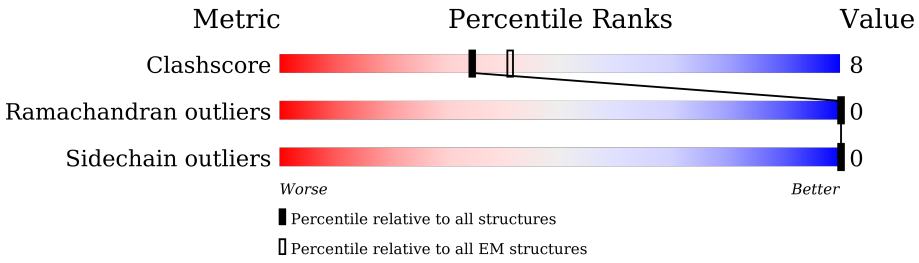
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.90 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	C	71	76% 15% 8%
2	A	346	66% 15% 19%
3	D	133	69% 14% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3560 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 Toxin AdTx1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	65	Total	C	N	O	S	1	0
			510	313	87	102	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP P85092
C	-4	PRO	-	expression tag	UNP P85092
C	-3	GLY	-	expression tag	UNP P85092
C	-2	SER	-	expression tag	UNP P85092
C	-1	GLY	-	expression tag	UNP P85092
C	0	SER	-	expression tag	UNP P85092

- Molecule 2 is a protein called Alpha-1A adrenergic receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	280	Total	C	N	O	S	0	0
			2217	1480	362	360	15		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P35348
A	-6	TYR	-	expression tag	UNP P35348
A	-5	LYS	-	expression tag	UNP P35348
A	-4	ASP	-	expression tag	UNP P35348
A	-3	ASP	-	expression tag	UNP P35348
A	-2	ASP	-	expression tag	UNP P35348
A	-1	ASP	-	expression tag	UNP P35348
A	0	ALA	-	expression tag	UNP P35348
A	7	GLN	ASN	conflict	UNP P35348
A	13	GLN	ASN	conflict	UNP P35348
A	22	GLN	ASN	conflict	UNP P35348

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Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ARG	SER	conflict	UNP P35348
A	115	TRP	MET	conflict	UNP P35348
A	?	-	GLU	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	ARG	deletion	UNP P35348
A	?	-	GLY	deletion	UNP P35348
A	?	-	LEU	deletion	UNP P35348
A	?	-	LYS	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	GLY	deletion	UNP P35348
A	?	-	LEU	deletion	UNP P35348
A	?	-	LYS	deletion	UNP P35348
A	?	-	THR	deletion	UNP P35348
A	?	-	ASP	deletion	UNP P35348
A	?	-	LYS	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	ASP	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	GLU	deletion	UNP P35348
A	?	-	GLN	deletion	UNP P35348
A	?	-	VAL	deletion	UNP P35348
A	?	-	THR	deletion	UNP P35348
A	?	-	LEU	deletion	UNP P35348
A	?	-	ARG	deletion	UNP P35348
A	?	-	ILE	deletion	UNP P35348
A	?	-	HIS	deletion	UNP P35348
A	?	-	ARG	deletion	UNP P35348
A	?	-	LYS	deletion	UNP P35348
A	?	-	ASN	deletion	UNP P35348
A	?	-	ALA	deletion	UNP P35348
A	?	-	PRO	deletion	UNP P35348
A	?	-	ALA	deletion	UNP P35348
A	?	-	GLY	deletion	UNP P35348
A	?	-	GLY	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	GLY	deletion	UNP P35348
A	?	-	MET	deletion	UNP P35348
A	?	-	ALA	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	?	-	ALA	deletion	UNP P35348
A	?	-	LYS	deletion	UNP P35348
A	?	-	THR	deletion	UNP P35348

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P35348
A	?	-	THR	deletion	UNP P35348
A	?	-	HIS	deletion	UNP P35348
A	?	-	PHE	deletion	UNP P35348
A	?	-	SER	deletion	UNP P35348
A	218	SER	LYS	conflict	UNP P35348
A	219	GLY	PHE	conflict	UNP P35348
A	224	ASP	-	insertion	UNP P35348
A	225	ARG	-	insertion	UNP P35348
A	226	ASN	-	insertion	UNP P35348
A	227	LEU	-	insertion	UNP P35348
A	228	ARG	-	insertion	UNP P35348
A	372	HIS	-	expression tag	UNP P35348
A	373	HIS	-	expression tag	UNP P35348
A	374	HIS	-	expression tag	UNP P35348
A	375	HIS	-	expression tag	UNP P35348
A	376	HIS	-	expression tag	UNP P35348
A	377	HIS	-	expression tag	UNP P35348
A	378	HIS	-	expression tag	UNP P35348

- Molecule 3 is a protein called Nb6.

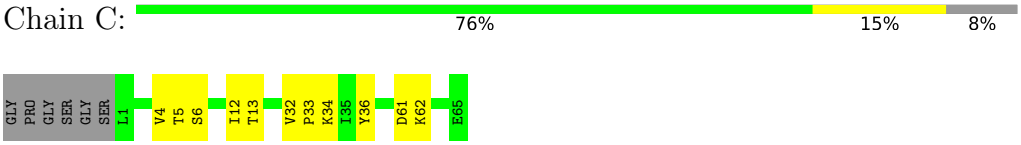
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	111	Total	C	N	O	S	0	0
			833	521	144	164	4		

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.

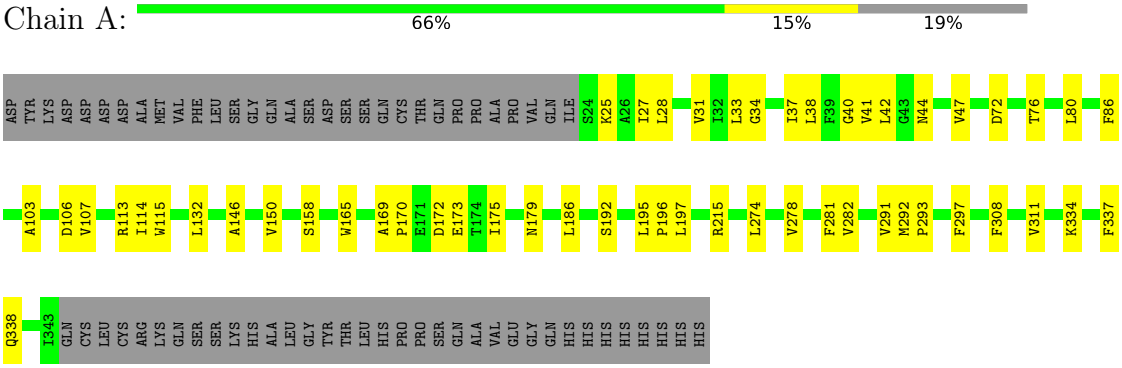
- Molecule 1: Toxin AdTx1

Chain C:



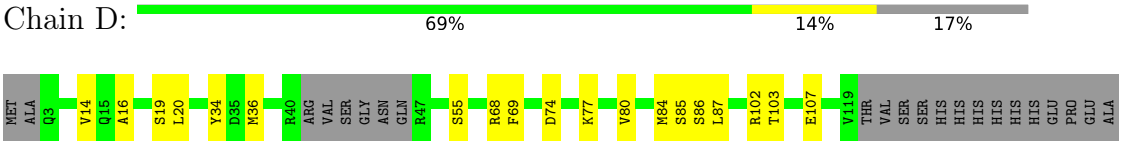
- Molecule 2: Alpha-1A adrenergic receptor

Chain A:



- Molecule 3: Nb6

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	616710	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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	C	0.28	0/523	0.53	0/707
2	A	0.27	0/2278	0.48	0/3106
3	D	0.25	0/847	0.53	0/1146
All	All	0.26	0/3648	0.49	0/4959

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	C	510	0	485	9	0
2	A	2217	0	2309	35	0
3	D	833	0	774	17	0
All	All	3560	0	3568	56	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.

All (56) 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:D:103:THR:OG1	3:D:107:GLU:OE1	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:ARG:O	3:D:85:SER:OG	2.03	0.76
3:D:68:ARG:NH2	3:D:86:SER:O	2.23	0.70
3:D:84:MET:CE	3:D:87:LEU:HD23	2.24	0.68
2:A:197:LEU:HD11	2:A:282:VAL:HG22	1.77	0.67
1:C:4:VAL:HG13	1:C:12:ILE:HG23	1.79	0.63
2:A:40:GLY:O	2:A:44:ASN:ND2	2.30	0.63
2:A:291:VAL:HG11	2:A:311:VAL:HG21	1.81	0.63
2:A:215:ARG:O	3:D:102:ARG:NH2	2.32	0.62
3:D:74:ASP:OD2	3:D:77:LYS:NZ	2.29	0.61
2:A:33:LEU:O	2:A:37:ILE:HG13	2.01	0.60
2:A:37:ILE:O	2:A:41:VAL:HG23	2.04	0.58
3:D:84:MET:HE3	3:D:87:LEU:HD23	1.85	0.58
2:A:72:ASP:OD1	2:A:113:ARG:NE	2.40	0.55
3:D:84:MET:HE2	3:D:87:LEU:HD23	1.89	0.54
1:C:34:LYS:NZ	2:A:106:ASP:OD2	2.31	0.54
3:D:16:ALA:HA	3:D:87:LEU:HB2	1.90	0.53
3:D:14:VAL:HG11	3:D:20:LEU:HD21	1.90	0.53
2:A:132:LEU:H	2:A:132:LEU:HD23	1.74	0.52
2:A:107:VAL:HG12	2:A:158:SER:HB2	1.92	0.52
2:A:165:TRP:O	2:A:179:ASN:ND2	2.43	0.51
3:D:19:SER:O	3:D:20:LEU:HD22	2.11	0.51
2:A:34:GLY:O	2:A:38:LEU:HD23	2.11	0.51
1:C:4:VAL:HG13	1:C:12:ILE:CG2	2.42	0.50
2:A:115:TRP:HB3	2:A:150:VAL:HG13	1.93	0.50
2:A:146:ALA:O	2:A:150:VAL:HG23	2.12	0.49
1:C:5:THR:OG1	1:C:13:THR:O	2.31	0.49
2:A:274:LEU:O	2:A:278:VAL:HG23	2.14	0.48
2:A:186:LEU:HD13	2:A:297:PHE:HZ	1.77	0.47
2:A:76:THR:HG22	2:A:80:LEU:HD12	1.96	0.47
2:A:186:LEU:HD13	2:A:297:PHE:CZ	2.49	0.47
3:D:19:SER:C	3:D:20:LEU:HD22	2.35	0.47
3:D:84:MET:CE	3:D:87:LEU:HA	2.45	0.47
2:A:25:LYS:HA	2:A:28:LEU:HD21	1.97	0.46
2:A:103:ALA:O	2:A:107:VAL:HG23	2.15	0.46
1:C:33:PRO:HA	2:A:86:PHE:CE2	2.50	0.46
2:A:292:MET:HB3	2:A:293:PRO:HD3	1.97	0.45
2:A:169:ALA:N	2:A:170:PRO:HD2	2.31	0.45
3:D:69:PHE:CE1	3:D:84:MET:SD	3.10	0.45
3:D:36:MET:CE	3:D:80:VAL:HB	2.47	0.44
2:A:47:VAL:HG22	2:A:337:PHE:HZ	1.82	0.44
2:A:38:LEU:O	2:A:42:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:LEU:HB3	2:A:196:PRO:HD3	2.00	0.43
3:D:34:TYR:O	3:D:55:SER:N	2.51	0.43
2:A:114:ILE:HD12	2:A:281:PHE:CZ	2.55	0.42
1:C:36:TYR:CZ	2:A:175:ILE:HG23	2.55	0.41
2:A:27:ILE:O	2:A:31:VAL:HG23	2.20	0.41
2:A:334:LYS:O	2:A:338:GLN:HG2	2.21	0.41
2:A:114:ILE:HG21	2:A:192:SER:O	2.20	0.41
2:A:169:ALA:N	2:A:170:PRO:CD	2.84	0.41
1:C:61:ASP:OD1	1:C:62:LYS:HG3	2.21	0.40
1:C:32:VAL:HG22	2:A:308:PHE:HE2	1.86	0.40
1:C:5:THR:O	1:C:6:SER:OG	2.30	0.40
2:A:172:ASP:O	2:A:173:GLU:HB3	2.21	0.40
2:A:173:GLU:O	2:A:173:GLU:HG3	2.21	0.40
3:D:84:MET:SD	3:D:85:SER:N	2.93	0.40

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	C	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
2	A	278/346 (80%)	266 (96%)	12 (4%)	0	100	100
3	D	107/133 (80%)	104 (97%)	3 (3%)	0	100	100
All	All	449/550 (82%)	431 (96%)	18 (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	C	61/63 (97%)	61 (100%)	0	100	100
2	A	243/301 (81%)	243 (100%)	0	100	100
3	D	82/109 (75%)	82 (100%)	0	100	100
All	All	386/473 (82%)	386 (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
2	A	54	HIS
2	A	179	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.