



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 01:39 PM JST

PDB ID : 8ZSS
EMDB ID : EMD-60426
Title : Cryo-EM structure of the RO5263397-bound hTAAR1-Gs complex
Authors : Jiang, K.X.; Zheng, Y.; Xu, F.
Deposited on : 2024-06-05
Resolution : 3.07 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**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

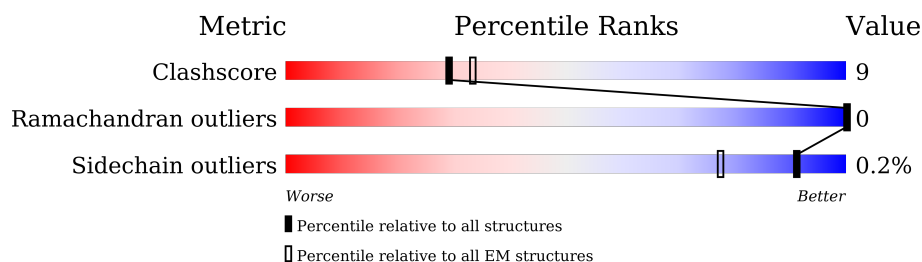
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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	247	77% 15% 7%
2	B	345	73% 24% .
3	G	71	65% 15% 20%
4	N	139	64% 25% . 9%
5	R	495	46% 11% 43%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8057 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1868	1176	334	351	7		

- 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
			2568	1584	459	504	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	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	G	57	Total	C	N	O	S	0	0
			432	270	76	83	3		

- Molecule 4 is a protein called Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	127	Total	C	N	O	S	0	0
			955	594	166	190	5		

- Molecule 5 is a protein called Soluble cytochrome b562,Trace amine-associated receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	282	Total	C	N	O	S	0	0
			2220	1487	345	363	25		

There are 54 discrepancies between the modelled and reference sequences:

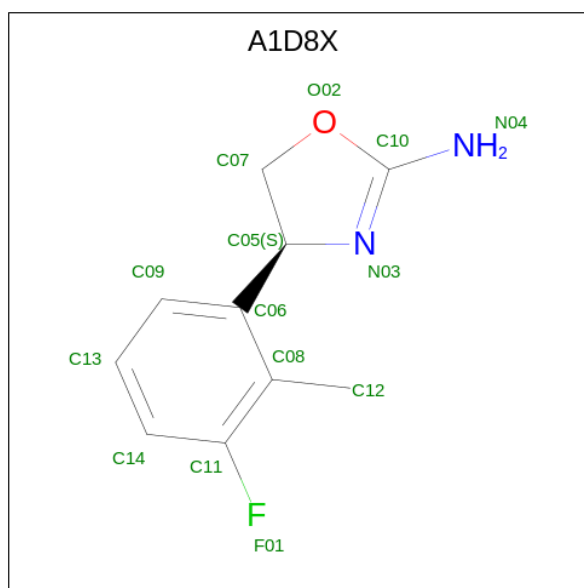
Chain	Residue	Modelled	Actual	Comment	Reference
R	-155	MET	-	initiating methionine	UNP P0ABE7
R	-154	LYS	-	expression tag	UNP P0ABE7
R	-153	THR	-	expression tag	UNP P0ABE7
R	-152	ILE	-	expression tag	UNP P0ABE7
R	-151	ILE	-	expression tag	UNP P0ABE7
R	-150	ALA	-	expression tag	UNP P0ABE7
R	-149	LEU	-	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	LYS	-	expression tag	UNP P0ABE7
R	-131	HIS	-	expression tag	UNP P0ABE7
R	-130	HIS	-	expression tag	UNP P0ABE7
R	-129	HIS	-	expression tag	UNP P0ABE7
R	-128	HIS	-	expression tag	UNP P0ABE7
R	-127	HIS	-	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	LEU	-	expression tag	UNP P0ABE7
R	-120	GLU	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-119	VAL	-	expression tag	UNP P0ABE7
R	-118	LEU	-	expression tag	UNP P0ABE7
R	-117	PHE	-	expression tag	UNP P0ABE7
R	-116	GLN	-	expression tag	UNP P0ABE7
R	-115	GLY	-	expression tag	UNP P0ABE7
R	-114	PRO	-	expression tag	UNP P0ABE7
R	-107	TRP	MET	conflict	UNP P0ABE7
R	-12	ILE	HIS	conflict	UNP P0ABE7
R	-8	LEU	-	linker	UNP P0ABE7
R	-7	MET	-	linker	UNP P0ABE7
R	-6	GLY	-	linker	UNP P0ABE7
R	-5	GLN	-	linker	UNP P0ABE7
R	-4	PRO	-	linker	UNP P0ABE7
R	-3	GLY	-	linker	UNP P0ABE7
R	-2	ASN	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	SER	-	linker	UNP P0ABE7
R	1	ALA	-	linker	UNP P0ABE7

- Molecule 6 is (4 {S})-4-(3-fluoranyl-2-methyl-phenyl)-1,3-oxazolidin-2-amine (three-letter code: A1D8X) (formula: C₁₀H₁₁FN₂O).

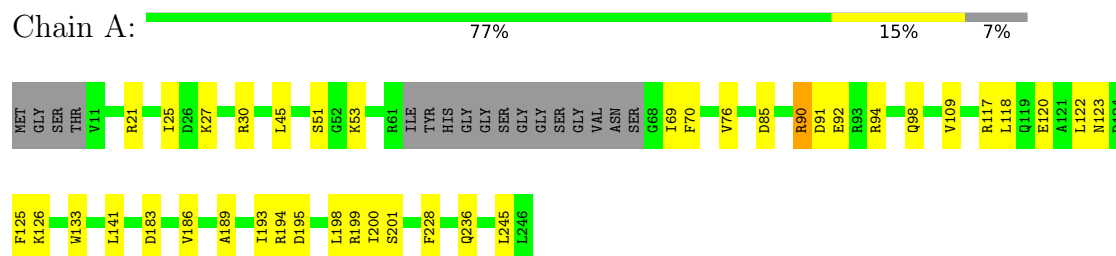


Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	F	N	O	0
			14	10	1	2	1	

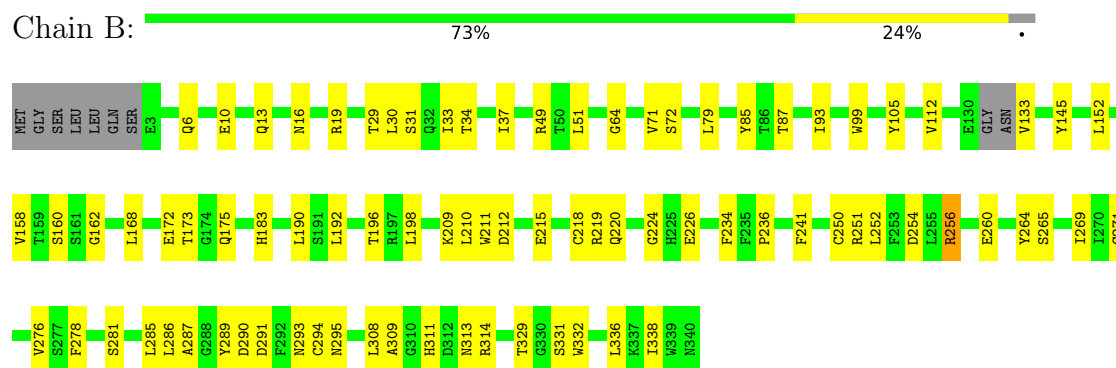
3 Residue-property plots

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.

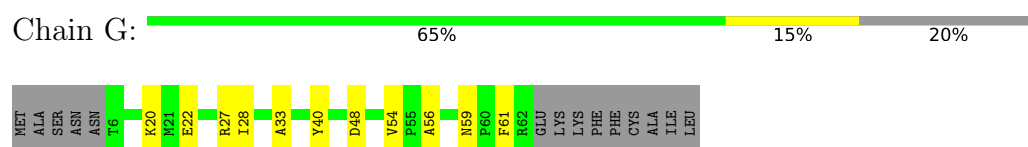
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



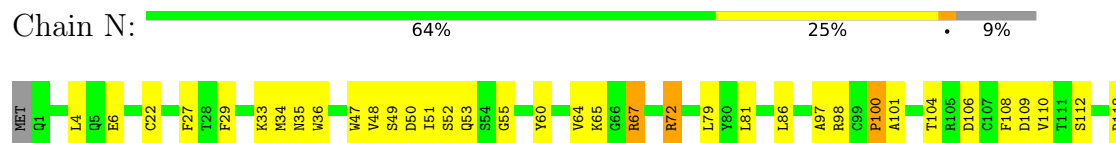
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



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



- Molecule 4: Nb35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193651	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: A1D8X

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	0.31	0/1904	0.54	0/2565
2	B	0.28	0/2614	0.54	0/3546
3	G	0.28	0/438	0.49	0/593
4	N	0.30	0/975	0.53	1/1323 (0.1%)
5	R	0.33	0/2285	0.47	0/3108
All	All	0.30	0/8216	0.52	1/11135 (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	A	0	1
2	B	0	1
4	N	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	N	100	PRO	C-N-CA	-6.03	106.63	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	256	ARG	Sidechain
4	N	67	ARG	Sidechain
4	N	72	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	A	1868	0	1819	27	0
2	B	2568	0	2449	54	0
3	G	432	0	437	8	0
4	N	955	0	906	27	0
5	R	2220	0	2226	39	0
6	R	14	0	0	0	0
All	All	8057	0	7837	144	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 9.

The worst 5 of 144 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)
5:R:57:PRO:HB3	5:R:140:ILE:HG13	1.67	0.77
4:N:29:PHE:HE1	4:N:72:ARG:HG3	1.57	0.70
5:R:158:MET:HG3	5:R:163:LEU:HB3	1.76	0.67
5:R:210:TYR:CD1	5:R:253:LEU:HD22	2.31	0.65
2:B:34:THR:OG1	2:B:37:ILE:CG1	2.46	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	226/247 (92%)	216 (96%)	10 (4%)	0	100	100
2	B	332/345 (96%)	321 (97%)	11 (3%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	125/139 (90%)	119 (95%)	6 (5%)	0	100	100
5	R	278/495 (56%)	269 (97%)	9 (3%)	0	100	100
All	All	1016/1297 (78%)	980 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	198/213 (93%)	198 (100%)	0	100	100
2	B	275/287 (96%)	275 (100%)	0	100	100
3	G	45/58 (78%)	44 (98%)	1 (2%)	47	68
4	N	102/116 (88%)	101 (99%)	1 (1%)	73	85
5	R	241/438 (55%)	241 (100%)	0	100	100
All	All	861/1112 (77%)	859 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	20	LYS
4	N	108	PHE

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	89	GLN
2	B	119	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](#)

1 ligand is 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	A1D8X	R	401	-	14,15,15	7.92	10 (71%)	17,21,21	5.34	3 (17%)

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	A1D8X	R	401	-	-	1/4/13/13	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	A1D8X	C10-N03	22.20	1.46	1.29
6	R	401	A1D8X	C09-C06	9.98	1.52	1.39
6	R	401	A1D8X	C14-C11	7.15	1.52	1.37
6	R	401	A1D8X	C10-N04	6.94	1.45	1.33
6	R	401	A1D8X	C13-C14	6.91	1.53	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	A1D8X	O02-C10-N03	-18.72	108.32	117.80
6	R	401	A1D8X	O02-C10-N04	10.59	125.56	114.75
6	R	401	A1D8X	C09-C06-C05	-2.18	117.87	120.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	A1D8X	N03-C05-C06-C09

There are no ring outliers.

No monomer is involved in short contacts.

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.