



Full wwPDB EM Validation Report ⓘ

Dec 24, 2023 – 12:08 AM JST

PDB ID : 8W87
EMDB ID : EMD-37347
Title : Cryo-EM structure of the METH-TAAR1 complex
Authors : Liu, H.; Zheng, Y.; Wang, Y.; Wang, Y.; He, X.; Xu, P.; Huang, S.; Yuan, Q.;
Zhang, X.; Wang, S.; Xu, H.E.; Xu, F.
Deposited on : 2023-09-01
Resolution : 2.80 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**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

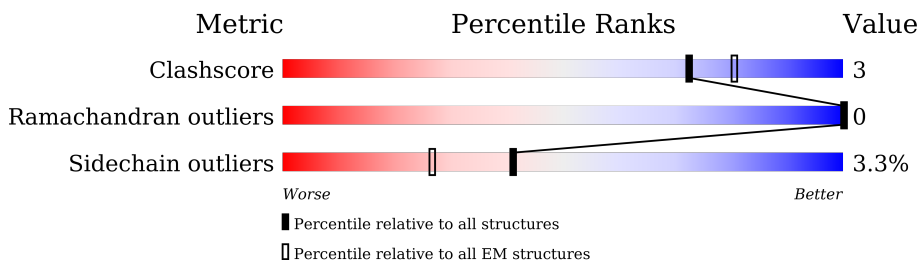
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	361	61% 35%
2	B	345	88% 10%
3	G	71	77% 20%
4	N	139	81% 10% 9%
5	R	339	74% 10% 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8228 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
			Total	C	N	O	S		
1	A	234	1906	1197	344	358	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	2593	1601	467	504	21	0	0

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
			Total	C	N	O	S		
3	G	57	436	273	77	83	3	0	0

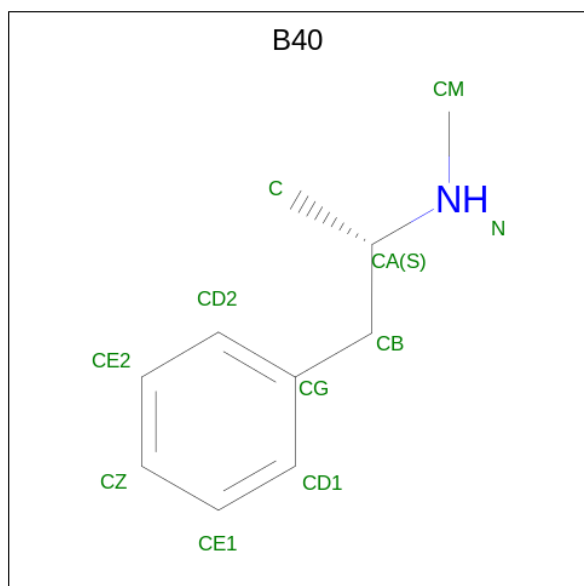
- Molecule 4 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	127	967	602	169	190	6	0	0

- Molecule 5 is a protein called Trace amine-associated receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	289	2315	1552	357	380	26	0	0

- Molecule 6 is (2S)-N-methyl-1-phenylpropan-2-amine (three-letter code: B40) (formula: C₁₀H₁₅N).

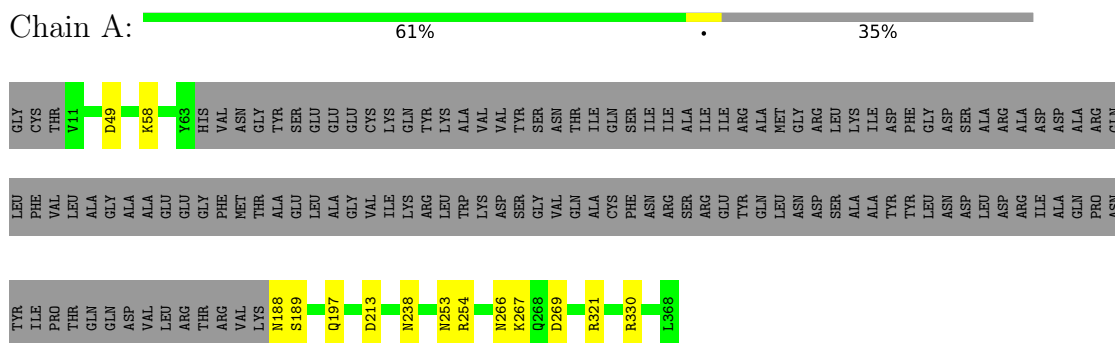


Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
6	R	1	11	10	1	0

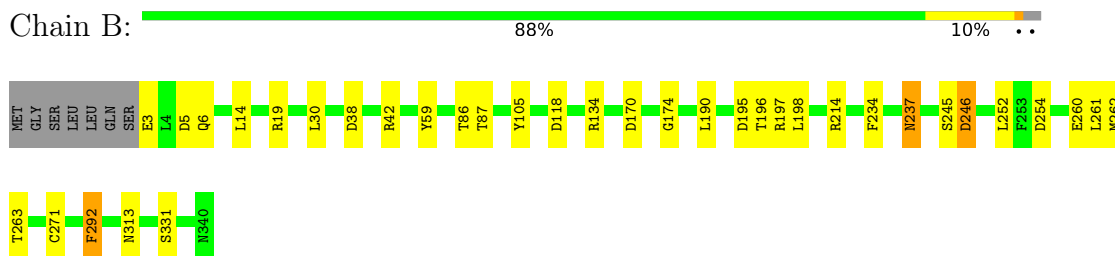
3 Residue-property plots [i](#)

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.

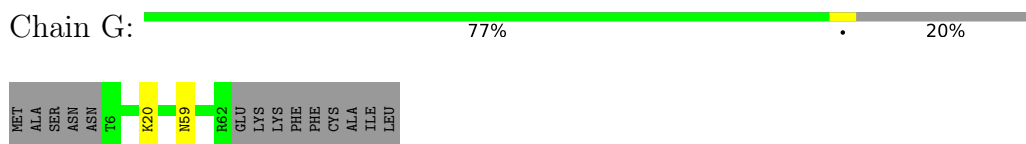
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



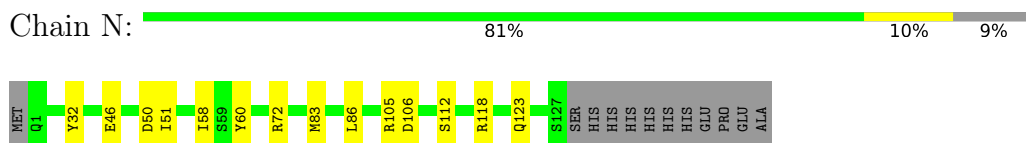
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



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

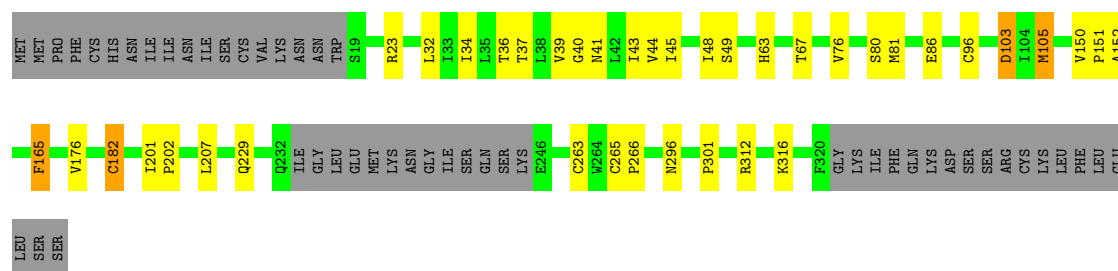


- Molecule 4: Nanobody35



- Molecule 5: Trace amine-associated receptor 1

Chain R:  74% 10% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	306504	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 ($e^-/\text{\AA}^2$)	50	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B40

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	0/1942	0.50	0/2615
2	B	0.26	0/2640	0.53	0/3580
3	G	0.26	0/442	0.45	0/597
4	N	0.28	0/987	0.51	0/1337
5	R	0.29	0/2384	0.45	0/3240
All	All	0.27	0/8395	0.49	0/11369

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 [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	1906	0	1861	5	0
2	B	2593	0	2499	19	0
3	G	436	0	448	2	0
4	N	967	0	937	7	0
5	R	2315	0	2332	22	0
6	R	11	0	15	2	0
All	All	8228	0	8092	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 3.

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)
5:R:76:VAL:HG11	5:R:103:ASP:OD1	2.02	0.60
2:B:252:LEU:CD2	2:B:261:LEU:HD12	2.33	0.58
4:N:50:ASP:OD1	4:N:51:ILE:N	2.38	0.57
2:B:5:ASP:OD1	2:B:6:GLN:N	2.38	0.56
2:B:195:ASP:O	2:B:196:THR:OG1	2.19	0.56
5:R:23:ARG:NH1	5:R:86:GLU:OE2	2.40	0.55
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.89	0.54
4:N:83:MET:HB3	4:N:86:LEU:HD11	1.90	0.54
5:R:45:ILE:HD11	5:R:67:THR:HA	1.90	0.53
4:N:105:ARG:HB2	4:N:105:ARG:NH1	2.24	0.53
1:A:188:ASN:O	1:A:189:SER:OG	2.23	0.52
5:R:39:VAL:O	5:R:43:ILE:CD1	2.58	0.52
2:B:14:LEU:HD11	3:G:20:LYS:HG3	1.92	0.51
5:R:39:VAL:O	5:R:43:ILE:HD12	2.13	0.49
3:G:59:ASN:C	3:G:59:ASN:OD1	2.52	0.48
5:R:39:VAL:HG13	5:R:40:GLY:N	2.29	0.48
5:R:312:ARG:O	5:R:316:LYS:HD2	2.13	0.48
5:R:37:THR:O	5:R:41:ASN:ND2	2.48	0.47
5:R:34:ILE:HD12	5:R:81:MET:HE2	1.96	0.47
1:A:330:ARG:HB2	1:A:330:ARG:NH1	2.29	0.47
2:B:237:ASN:O	2:B:237:ASN:ND2	2.47	0.47
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.32	0.47
6:R:501:B40:HD2	6:R:501:B40:HA	1.66	0.47
2:B:252:LEU:HD23	2:B:261:LEU:HD12	1.96	0.46
2:B:245:SER:OG	2:B:246:ASP:N	2.51	0.45
2:B:197:ARG:O	2:B:198:LEU:HD12	2.16	0.44
1:A:269:ASP:N	1:A:269:ASP:OD1	2.49	0.44
2:B:87:THR:O	2:B:87:THR:CG2	2.65	0.44
5:R:32:LEU:O	5:R:36:THR:HG22	2.17	0.44
4:N:106:ASP:OD1	4:N:106:ASP:N	2.39	0.44
5:R:150:VAL:HB	5:R:151:PRO:HD3	1.99	0.44
2:B:30:LEU:HD23	2:B:262:MET:HE3	2.00	0.44
4:N:32:TYR:O	4:N:72:ARG:NH2	2.49	0.43
1:A:253:ASN:OD1	1:A:254:ARG:N	2.52	0.43
5:R:176:VAL:HG13	5:R:182:CYS:HA	2.00	0.43
5:R:229:GLN:C	5:R:229:GLN:OE1	2.57	0.43
1:A:266:ASN:OD1	1:A:267:LYS:N	2.46	0.42
5:R:201:ILE:HB	5:R:202:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:HB2	2:B:19:ARG:NH1	2.34	0.42
6:R:501:B40:HMB	6:R:501:B40:HB	1.68	0.42
4:N:58:ILE:HD12	4:N:60:TYR:OH	2.19	0.42
5:R:265:CYS:N	5:R:266:PRO:HD2	2.35	0.42
2:B:87:THR:O	2:B:87:THR:HG22	2.20	0.42
2:B:3:GLU:N	2:B:3:GLU:OE1	2.53	0.42
5:R:43:ILE:HD12	5:R:43:ILE:N	2.35	0.41
5:R:43:ILE:HD12	5:R:43:ILE:H	1.84	0.41
5:R:263:CYS:HB3	5:R:296:ASN:HB2	2.02	0.41
2:B:38:ASP:OD1	2:B:38:ASP:N	2.49	0.41
2:B:86:THR:O	2:B:87:THR:HB	2.19	0.41
5:R:48:ILE:HG21	5:R:63:HIS:HB2	2.03	0.41
2:B:292:PHE:HB3	2:B:313:ASN:O	2.21	0.41
2:B:170:ASP:O	2:B:174:GLY:N	2.44	0.40
5:R:44:VAL:HG21	5:R:301:PRO:HB3	2.03	0.40
5:R:105:MET:HG3	5:R:152:ALA:HA	2.03	0.40
5:R:165:PHE:C	5:R:165:PHE:CD1	2.94	0.40
4:N:112:SER:O	4:N:118:ARG:NH2	2.50	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	A	230/361 (64%)	228 (99%)	2 (1%)	0	100	100
2	B	336/345 (97%)	326 (97%)	10 (3%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	125/139 (90%)	122 (98%)	3 (2%)	0	100	100
5	R	285/339 (84%)	280 (98%)	5 (2%)	0	100	100
All	All	1031/1255 (82%)	1011 (98%)	20 (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	203/310 (66%)	197 (97%)	6 (3%)	41	75
2	B	279/287 (97%)	266 (95%)	13 (5%)	26	59
3	G	46/58 (79%)	46 (100%)	0	100	100
4	N	105/116 (90%)	103 (98%)	2 (2%)	57	85
5	R	255/309 (82%)	247 (97%)	8 (3%)	40	74
All	All	888/1080 (82%)	859 (97%)	29 (3%)	41	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	58	LYS
1	A	197	GLN
1	A	213	ASP
1	A	238	ASN
1	A	321	ARG
2	B	42	ARG
2	B	59	TYR
2	B	105	TYR
2	B	118	ASP
2	B	134	ARG
2	B	190	LEU
2	B	214	ARG
2	B	234	PHE
2	B	237	ASN
2	B	246	ASP
2	B	271	CYS
2	B	292	PHE
2	B	331	SER
4	N	46	GLU
4	N	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	49	SER
5	R	80	SER
5	R	96	CYS
5	R	103	ASP
5	R	105	MET
5	R	165	PHE
5	R	182	CYS
5	R	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	B40	R	501	-	11,11,11	0.97	1 (9%)	12,13,13	1.13	1 (8%)

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	B40	R	501	-	-	6/6/6/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	B40	CA-N	-3.02	1.44	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	B40	C-CA-N	-2.97	104.29	112.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	501	B40	CB-CA-N-CM
6	R	501	B40	N-CA-CB-CG
6	R	501	B40	C-CA-CB-CG
6	R	501	B40	C-CA-N-CM
6	R	501	B40	CA-CB-CG-CD1
6	R	501	B40	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	B40	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.