



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:15 AM UTC

PDB ID : 4DBB / pdb_00004dbb
Title : The PTB domain of Mint1 is autoinhibited by a helix in the C-terminal linker region
Authors : Tomchick, D.R.; Rizo, J.; Ho, A.; Xu, Y.
Deposited on : 2012-01-13
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

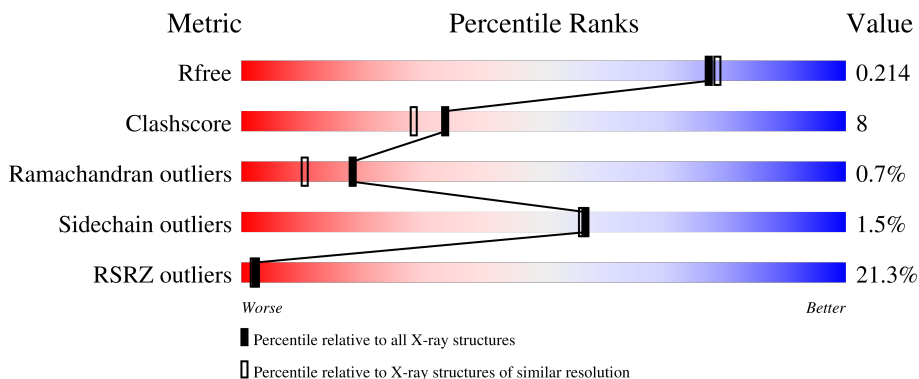
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2558 atoms, of which 1248 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Amyloid beta A4 precursor protein-binding family A member 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	150	2413	754	1210	207	232	10	0	1	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP O35430
A	?	-	SER	deletion	UNP O35430
A	?	-	GLN	deletion	UNP O35430
A	?	-	GLU	deletion	UNP O35430
A	?	-	ASN	deletion	UNP O35430
A	?	-	VAL	deletion	UNP O35430
A	?	-	GLU	deletion	UNP O35430
A	?	-	ALA	deletion	UNP O35430
A	?	-	SER	deletion	UNP O35430
A	?	-	HIS	deletion	UNP O35430
A	?	-	PRO	deletion	UNP O35430
A	?	-	SER	deletion	UNP O35430
A	?	-	GLN	deletion	UNP O35430
A	?	-	ASP	deletion	UNP O35430
A	?	-	ALA	deletion	UNP O35430
A	?	-	LYS	deletion	UNP O35430
A	?	-	ARG	deletion	UNP O35430

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

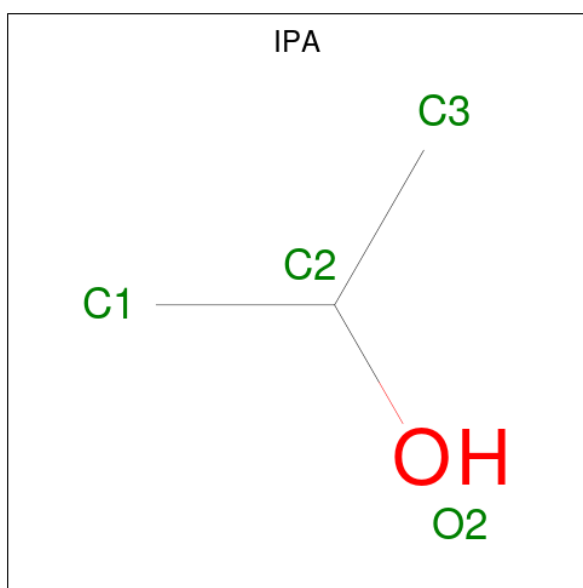
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			12	3	8	1		
4	A	1	Total	C	H	O	0	0
			12	3	8	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		


- Molecule 6 is water.

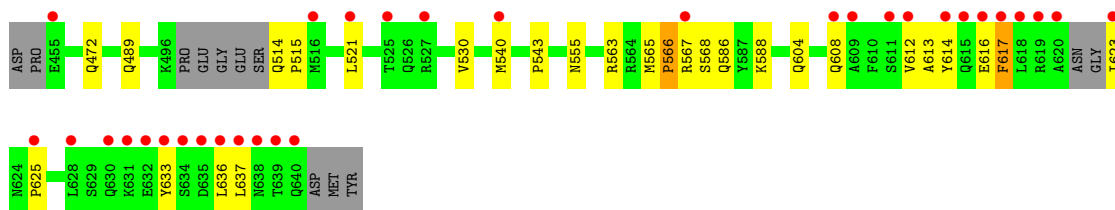
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Amyloid beta A4 precursor protein-binding family A member 1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.73Å 64.73Å 115.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.02 – 1.90 33.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (33.02-1.90) 91.7 (33.02-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.197 , 0.225 0.184 , 0.214	Depositor DCC
R_{free} test set	934 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2558	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: IPA, CL, GOL, ACY

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	0.94	0/1218	0.91	0/1640

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	1203	1210	1207	19	1
2	A	1	0	0	0	0
3	A	8	6	6	1	0
4	A	8	16	16	1	0
5	A	12	16	16	2	0
6	A	78	0	0	0	0
All	All	1310	1248	1245	19	1

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 (19) 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:613:ALA:O	1:A:616:GLU:HB2	1.96	0.65
1:A:608:GLN:HE22	4:A:704:IPA:H33	1.62	0.64
1:A:614:TYR:OH	1:A:636:LEU:HB3	2.00	0.61
1:A:566:PRO:HB2	1:A:586:GLN:OE1	2.04	0.57
1:A:633:TYR:CE2	1:A:637:LEU:HD11	2.42	0.55
1:A:530:VAL:HG21	1:A:540:MET:HE2	1.89	0.54
1:A:617:PHE:HE2	1:A:625:PRO:HG3	1.76	0.51
1:A:543:PRO:HG3	5:A:707:GOL:H2	1.93	0.50
1:A:521:LEU:CD1	1:A:530:VAL:HG22	2.44	0.47
1:A:563:ARG:HE	3:A:703:ACY:C	2.27	0.47
1:A:472:GLN:OE1	1:A:588:LYS:HD3	2.16	0.45
1:A:567:ARG:O	1:A:568:SER:HB2	2.17	0.45
1:A:604:GLN:O	1:A:608:GLN:HG3	2.17	0.44
1:A:543:PRO:CG	5:A:707:GOL:H2	2.48	0.44
1:A:623:ILE:O	1:A:625:PRO:HD3	2.19	0.43
1:A:565:MET:C	1:A:566:PRO:O	2.60	0.42
1:A:614:TYR:HH	1:A:636:LEU:HB3	1.85	0.42
1:A:565:MET:HB2	1:A:586:GLN:O	2.20	0.42
1:A:514:GLN:HA	1:A:515:PRO:HD2	1.95	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:HE21	1:A:555:ASN:H[7_555]	1.27	0.33

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 X-ray entries followed by that with respect to entries of similar resolution.

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	145/162 (90%)	138 (95%)	6 (4%)	1 (1%)	18 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	135/144 (94%)	133 (98%)	2 (2%)	57 56

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

Mol	Chain	Res	Type
1	A	612	VAL
1	A	617	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	487	GLN
1	A	608	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

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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
5	GOL	A	707	-	5,5,5	0.42	0	5,5,5	0.46	0
4	IPA	A	705	-	3,3,3	0.53	0	3,3,3	0.33	0
4	IPA	A	704	-	3,3,3	0.56	0	3,3,3	0.30	0
3	ACY	A	703	-	3,3,3	0.80	0	3,3,3	0.56	0
3	ACY	A	702	-	3,3,3	0.83	0	3,3,3	1.05	0
5	GOL	A	706	-	5,5,5	0.49	0	5,5,5	0.75	0

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
5	GOL	A	706	-	-	2/4/4/4	-
5	GOL	A	707	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	706	GOL	O1-C1-C2-O2
5	A	706	GOL	O1-C1-C2-C3
5	A	707	GOL	O1-C1-C2-O2
5	A	707	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	GOL	2	0
4	A	704	IPA	1	0
3	A	703	ACY	1	0

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/162 (92%)	0.85	32 (21%) 2 2	24, 43, 135, 181	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	639	THR	6.1
1	A	623	ILE	6.0
1	A	617	PHE	5.7
1	A	618	LEU	5.5
1	A	640	GLN	5.3
1	A	615	GLN	4.9
1	A	631	LYS	4.8
1	A	620	ALA	4.7
1	A	634	SER	4.5
1	A	612	VAL	4.2
1	A	630	GLN	3.9
1	A	625	PRO	3.8
1	A	635	ASP	3.6
1	A	455	GLU	3.5
1	A	608	GLN	3.5
1	A	633	TYR	3.5
1	A	637	LEU	3.3
1	A	516[A]	MET	3.2
1	A	614	TYR	3.1
1	A	525	THR	3.1
1	A	628	LEU	3.1
1	A	611	SER	3.1
1	A	638	ASN	3.0
1	A	636	LEU	2.9
1	A	521	LEU	2.8
1	A	616	GLU	2.4
1	A	567	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	540	MET	2.3
1	A	619	ARG	2.2
1	A	609	ALA	2.2
1	A	527	ARG	2.1
1	A	632	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	707	6/6	0.57	0.16	51,69,82,83	0
3	ACY	A	703	4/4	0.79	0.15	47,57,68,73	0
4	IPA	A	704	4/4	0.87	0.21	52,66,66,77	0
4	IPA	A	705	4/4	0.88	0.16	45,57,69,77	0
5	GOL	A	706	6/6	0.90	0.12	48,59,68,82	0
3	ACY	A	702	4/4	0.95	0.10	33,39,43,47	0
2	CL	A	701	1/1	0.95	0.08	34,34,34,34	1

6.5 Other polymers [i](#)

There are no such residues in this entry.