



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 PM UTC

PDB ID : 7U8T / pdb_00007u8t
Title : Vps13 adaptor binding domain in complex with Mcp1 PxP motif peptide
Authors : Adlakha, J.; Reinisch, K.M.
Deposited on : 2022-03-09
Resolution : 3.00 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
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

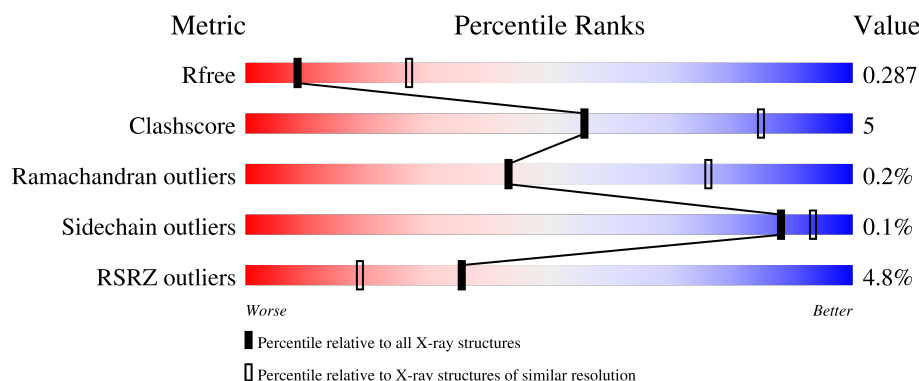
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	717	3% 68% 7% 25%
1	B	717	4% 75% 9% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8697 atoms, of which 0 are hydrogens and 0 are deuteriums.

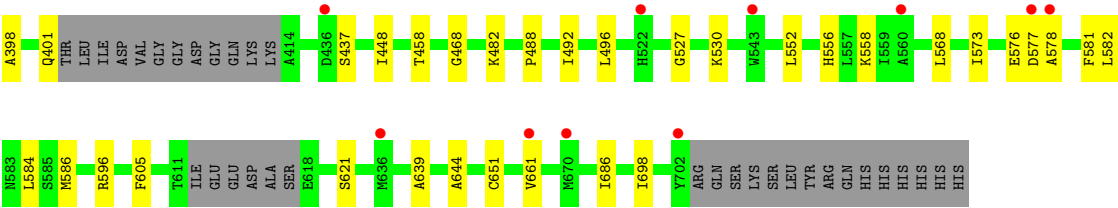
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mcp1 PxP motif, Putative vacuolar protein sorting-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4162	2675	710	767	10			
1	B	605	Total	C	N	O	S	0	0	0
			4535	2911	763	846	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP G0S0T5
A	712	HIS	-	expression tag	UNP G0S3B8
A	713	HIS	-	expression tag	UNP G0S3B8
A	714	HIS	-	expression tag	UNP G0S3B8
A	715	HIS	-	expression tag	UNP G0S3B8
A	716	HIS	-	expression tag	UNP G0S3B8
A	717	HIS	-	expression tag	UNP G0S3B8
B	1	MET	-	initiating methionine	UNP G0S0T5
B	712	HIS	-	expression tag	UNP G0S3B8
B	713	HIS	-	expression tag	UNP G0S3B8
B	714	HIS	-	expression tag	UNP G0S3B8
B	715	HIS	-	expression tag	UNP G0S3B8
B	716	HIS	-	expression tag	UNP G0S3B8
B	717	HIS	-	expression tag	UNP G0S3B8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.73Å 91.22Å 132.77Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	48.36 – 3.00 48.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.36-3.00) 98.6 (48.36-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4411	Depositor
R, R_{free}	0.250 , 0.285 0.259 , 0.287	Depositor DCC
R_{free} test set	1904 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8697	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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](#)

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	0.30	0/4266	0.55	1/5819 (0.0%)
1	B	0.28	0/4647	0.50	2/6357 (0.0%)
All	All	0.29	0/8913	0.53	3/12176 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLN	N-CA-C	-5.94	106.67	114.04
1	B	138	LYS	N-CA-CB	-5.38	102.82	110.46
1	B	135	ASP	N-CA-C	-5.00	107.67	112.97

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	4162	0	3987	36	0
1	B	4535	0	4186	43	0
All	All	8697	0	8173	79	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 5.

All (79) 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:B:577:ASP:O	1:B:577:ASP:OD1	1.90	0.90
1:A:169:LEU:HD11	1:A:190:LYS:HE2	1.64	0.77
1:B:558:LYS:HD3	1:B:639:ALA:HB3	1.65	0.76
1:B:135:ASP:OD1	1:B:137:ILE:HG22	1.88	0.73
1:B:22:TYR:HB2	1:B:66:TRP:O	1.92	0.70
1:A:123:LEU:HG	1:A:125:LYS:HE2	1.75	0.68
1:B:146:LEU:HG	1:B:253:PRO:HB2	1.74	0.67
1:A:229:TYR:HB2	1:A:232:GLU:CG	2.28	0.64
1:A:380:THR:HA	1:A:488:PRO:HD3	1.80	0.63
1:A:229:TYR:HB2	1:A:232:GLU:HG2	1.82	0.61
1:B:133:GLY:HA3	1:B:139:TYR:HE2	1.65	0.61
1:B:468:GLY:HA3	1:B:578:ALA:HB1	1.84	0.58
1:A:222:LEU:HB2	1:A:236:PHE:HB2	1.85	0.58
1:A:169:LEU:HD11	1:A:190:LYS:CE	2.33	0.57
1:A:461:ARG:HH21	1:A:523:TRP:HE1	1.54	0.56
1:B:496:LEU:HB3	1:B:586:MET:HE2	1.87	0.55
1:B:398:ALA:HB3	1:B:401:GLN:NE2	2.21	0.55
1:A:87:SER:HB3	1:A:104:ARG:HE	1.71	0.55
1:A:168:LEU:HD21	1:A:204:TRP:CZ2	2.41	0.54
1:A:451:THR:HB	1:A:578:ALA:HB2	1.90	0.53
1:B:146:LEU:HD12	1:B:187:ALA:HB1	1.90	0.53
1:B:386:VAL:H	1:B:401:GLN:NE2	2.06	0.53
1:B:448:ILE:HD11	1:B:482:LYS:HG2	1.90	0.53
1:A:318:PHE:HA	1:A:344:ASP:HA	1.90	0.52
1:B:130:ILE:HA	1:B:139:TYR:O	2.10	0.52
1:B:527:GLY:O	1:B:530:LYS:NZ	2.43	0.52
1:A:229:TYR:CD2	1:A:232:GLU:HG3	2.44	0.52
1:B:162:ASP:HB3	1:B:167:HIS:HB3	1.92	0.52
1:A:315:ASP:O	1:A:316:THR:HG23	2.10	0.52
1:B:386:VAL:H	1:B:401:GLN:HE22	1.58	0.52
1:B:158:LEU:HD11	1:B:192:LEU:HD23	1.92	0.51
1:A:556:HIS:HB3	1:A:568:LEU:HD11	1.92	0.51
1:B:318:PHE:HA	1:B:344:ASP:HA	1.91	0.51
1:B:34:ILE:HD12	1:B:58:LEU:HD13	1.92	0.51
1:A:221:THR:OG1	1:A:237:ARG:NH1	2.44	0.50
1:A:459:ALA:O	1:A:461:ARG:NH1	2.44	0.50
1:A:34:ILE:HG12	1:A:90:VAL:HG22	1.93	0.49
1:B:151:ASP:OD2	1:B:258:LYS:NZ	2.40	0.49
1:A:229:TYR:CB	1:A:232:GLU:HG2	2.42	0.49
1:B:221:THR:OG1	1:B:237:ARG:NH1	2.42	0.48
1:B:552:LEU:HD23	1:B:573:ILE:HG22	1.96	0.48
1:A:167:HIS:CD2	1:A:168:LEU:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:SER:HA	1:B:458:THR:HA	1.96	0.47
1:A:437:SER:HA	1:A:458:THR:HA	1.96	0.46
1:B:344:ASP:OD1	1:B:348:MET:N	2.47	0.46
1:B:380:THR:HA	1:B:488:PRO:HD3	1.96	0.46
1:B:576:GLU:HB3	1:B:581:PHE:HE1	1.80	0.46
1:B:282:ASN:O	1:B:283:LYS:C	2.58	0.46
1:A:226:SER:HB3	1:A:229:TYR:O	2.15	0.46
1:A:169:LEU:CD1	1:A:190:LYS:HE2	2.41	0.45
1:B:110:GLU:HB3	1:B:127:LEU:HD11	1.98	0.45
1:A:209:LEU:HD23	1:A:257:LEU:HD23	1.99	0.45
1:B:306:THR:HA	1:B:327:ASN:O	2.16	0.45
1:B:621:SER:HA	1:B:644:ALA:HB3	1.98	0.45
1:A:229:TYR:HB2	1:A:232:GLU:HB2	1.99	0.44
1:A:119:THR:OG1	1:A:120:GLN:N	2.51	0.44
1:A:315:ASP:O	1:A:316:THR:CG2	2.65	0.44
1:B:492:ILE:HD11	1:B:584:LEU:HD11	1.99	0.44
1:B:468:GLY:CA	1:B:578:ALA:HB1	2.48	0.44
1:B:398:ALA:HB3	1:B:401:GLN:HE21	1.82	0.43
1:B:596:ARG:HD3	1:B:698:ILE:HG12	2.00	0.43
1:A:342:VAL:HG23	1:A:350:LEU:HB3	2.01	0.43
1:A:552:LEU:HD23	1:A:573:ILE:HG22	2.00	0.43
1:B:90:VAL:HG21	1:B:142:LEU:HD21	2.01	0.43
1:A:35:SER:HB3	1:A:55:THR:HG22	2.00	0.43
1:B:605:PHE:HA	1:B:651:CYS:O	2.19	0.42
1:A:22:TYR:HB2	1:A:66:TRP:O	2.20	0.42
1:A:489:ARG:O	1:A:580:ILE:N	2.53	0.42
1:B:573:ILE:HG12	1:B:582:LEU:HD23	2.02	0.41
1:A:229:TYR:HB2	1:A:232:GLU:CB	2.50	0.41
1:B:110:GLU:OE1	1:B:254:TYR:OH	2.33	0.41
1:B:133:GLY:HA3	1:B:139:TYR:CE2	2.52	0.41
1:A:149:GLU:HB2	1:A:258:LYS:HA	2.01	0.41
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.88	0.41
1:B:661:VAL:HG11	1:B:686:ILE:HG21	2.03	0.41
1:A:98:GLN:HG3	1:A:117:PRO:HD3	2.02	0.41
1:B:279:ASP:N	1:B:279:ASP:OD1	2.53	0.41
1:A:344:ASP:OD1	1:A:347:GLY:N	2.54	0.41
1:B:556:HIS:HB3	1:B:568:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	528/717 (74%)	503 (95%)	24 (4%)	1 (0%)	43	76
1	B	587/717 (82%)	561 (96%)	25 (4%)	1 (0%)	43	76
All	All	1115/1434 (78%)	1064 (95%)	49 (4%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LEU
1	B	283	LYS

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 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	433/630 (69%)	432 (100%)	1 (0%)	87	92
1	B	453/630 (72%)	453 (100%)	0	100	100
All	All	886/1260 (70%)	885 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	167	HIS
1	A	339	HIS
1	A	345	ASN
1	A	378	ASN
1	A	525	GLN
1	B	244	GLN
1	B	330	ASN
1	B	339	HIS
1	B	401	GLN
1	B	423	ASN
1	B	588	GLN
1	B	695	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 [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.

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	540/717 (75%)	0.27	25 (4%)	37 20	30, 94, 154, 210	0
1	B	605/717 (84%)	0.37	30 (4%)	34 18	71, 106, 158, 211	0
All	All	1145/1434 (79%)	0.32	55 (4%)	35 19	30, 100, 157, 211	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	GLY	5.2
1	A	460	ASN	4.7
1	A	232	GLU	4.5
1	A	231	GLY	4.5
1	A	230	GLY	4.4
1	B	661	VAL	4.0
1	B	702	TYR	3.8
1	B	250	ARG	3.6
1	A	490	TYR	3.4
1	B	102	SER	3.4
1	A	54	MET	3.4
1	B	86	ASN	3.3
1	A	383	ASP	3.3
1	A	521	LEU	3.2
1	A	364	GLY	3.1
1	B	228	GLN	2.8
1	B	113	PHE	2.8
1	A	136	ASN	2.8
1	A	86	ASN	2.7
1	B	146	LEU	2.7
1	B	136	ASN	2.7
1	A	554	ILE	2.6
1	B	189	PHE	2.6
1	A	133	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	2.6
1	B	284	GLN	2.5
1	B	56	LEU	2.5
1	A	539	VAL	2.5
1	B	87	SER	2.4
1	A	315	ASP	2.4
1	B	285	GLU	2.4
1	B	577	ASP	2.3
1	B	199	GLY	2.3
1	A	394	SER	2.3
1	A	303	LEU	2.3
1	A	113	PHE	2.3
1	A	500	ILE	2.2
1	A	53	THR	2.2
1	A	69	GLU	2.2
1	A	513	LEU	2.2
1	B	578	ALA	2.2
1	B	543	TRP	2.2
1	B	670	MET	2.2
1	B	436	ASP	2.2
1	B	277	ILE	2.1
1	A	132	LEU	2.1
1	B	132	LEU	2.1
1	B	232	GLU	2.1
1	A	522	HIS	2.1
1	B	636	MET	2.1
1	B	560	ALA	2.1
1	B	253	PRO	2.1
1	B	184	VAL	2.1
1	B	288	ASN	2.0
1	B	522	HIS	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.