



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 05:33 AM UTC

PDB ID : 8ESE / pdb_00008ese
Title : Crystal structure of human Vps29 bound to a peptide from Vps35L
Authors : Healy, M.D.; Collins, B.M.
Deposited on : 2022-10-13
Resolution : 1.35 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

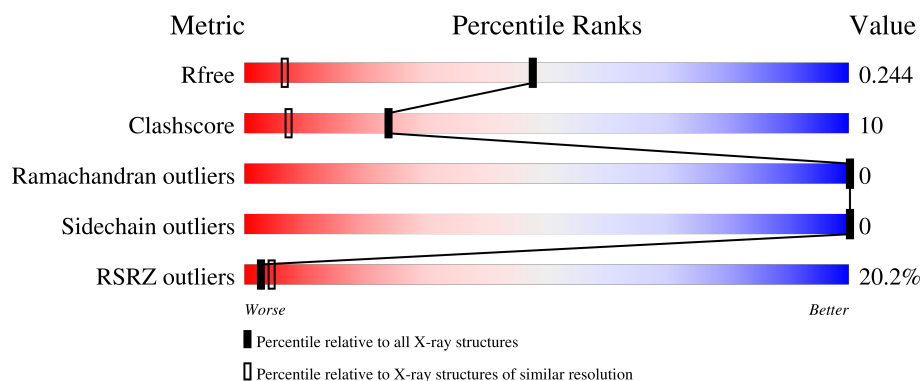
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	X	23	30% 61% 35%
2	Z	184	18% 88% 11% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3589 atoms, of which 1822 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 VPS35 endosomal protein-sorting factor-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	15	Total	C	H	N	O	0	0	0
			239	82	119	18	20			

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Z	183	Total	C	H	N	O	S	0	0	0
			2921	942	1465	245	263	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-1	GLY	-	expression tag	UNP Q9UBQ0
Z	0	HIS	-	expression tag	UNP Q9UBQ0

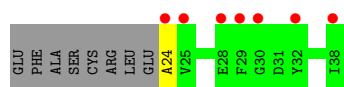
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	11	Total	H	O	0	0
			23	12	11		
3	Z	180	Total	H	O	0	0
			406	226	180		

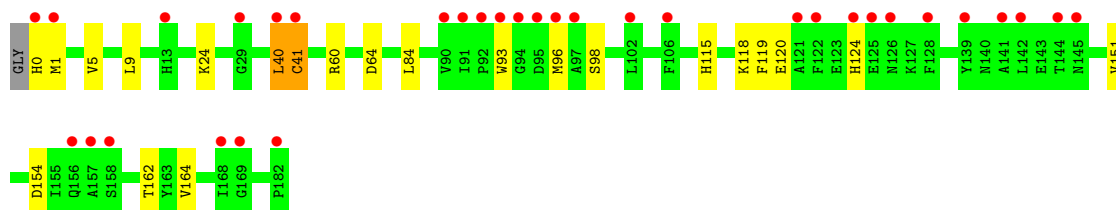
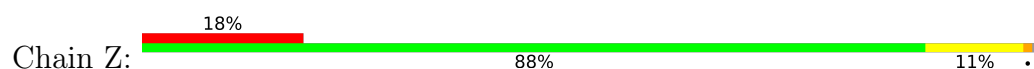
3 Residue-property plots [i](#)

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: VPS35 endosomal protein-sorting factor-like



- Molecule 2: Vacuolar protein sorting-associated protein 29



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.72Å 55.28Å 82.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 1.35 45.95 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.95-1.35) 97.8 (45.95-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.215 , 0.241 0.216 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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	X	0.90	0/125	1.04	0/171
2	Z	1.30	2/1491 (0.1%)	1.20	4/2023 (0.2%)
All	All	1.27	2/1616 (0.1%)	1.19	4/2194 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	84	LEU	C-O	5.36	1.29	1.24
2	Z	5	VAL	C-O	5.08	1.29	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	40	LEU	N-CA-C	-11.24	99.11	111.36
2	Z	41	CYS	CA-C-O	-7.41	109.92	120.51
2	Z	40	LEU	CB-CA-C	-5.72	101.13	110.85
2	Z	41	CYS	CB-CA-C	5.17	120.71	110.42

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	X	120	119	118	1	0
2	Z	1456	1465	1466	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	11	12	0	1	0
3	Z	180	226	0	17	4
All	All	1767	1822	1584	32	4

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 10.

All (32) 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)
2:Z:1:MET:SD	3:Z:247:HOH:O	1.91	1.20
2:Z:24:LYS:NZ	3:Z:201:HOH:O	1.84	1.06
1:X:24:ALA:N	3:X:101:HOH:O	1.93	1.01
2:Z:60:ARG:HG2	3:Z:273:HOH:O	1.69	0.90
2:Z:40:LEU:O	3:Z:202:HOH:O	1.89	0.89
2:Z:60:ARG:CG	3:Z:273:HOH:O	2.23	0.85
2:Z:60:ARG:CD	3:Z:273:HOH:O	2.27	0.81
2:Z:60:ARG:HD2	3:Z:273:HOH:O	1.85	0.75
2:Z:98:SER:OG	3:Z:203:HOH:O	2.08	0.72
2:Z:40:LEU:CA	3:Z:202:HOH:O	2.44	0.65
2:Z:118:LYS:HD3	2:Z:118:LYS:C	2.23	0.63
2:Z:24:LYS:NZ	3:Z:206:HOH:O	2.28	0.63
2:Z:40:LEU:HA	3:Z:202:HOH:O	1.99	0.61
2:Z:40:LEU:O	2:Z:41:CYS:HB2	2.00	0.60
2:Z:118:LYS:HD3	2:Z:119:PHE:O	2.03	0.58
2:Z:98:SER:CB	3:Z:203:HOH:O	2.53	0.56
2:Z:40:LEU:C	3:Z:202:HOH:O	2.37	0.56
2:Z:119:PHE:CZ	2:Z:164:VAL:HG21	2.41	0.55
2:Z:118:LYS:HD3	2:Z:119:PHE:N	2.21	0.55
2:Z:0:HIS:CA	3:Z:204:HOH:O	2.55	0.55
2:Z:0:HIS:N	3:Z:204:HOH:O	2.14	0.53
2:Z:40:LEU:O	2:Z:41:CYS:CB	2.54	0.53
2:Z:96:MET:HE2	2:Z:124:HIS:ND1	2.25	0.52
2:Z:98:SER:HA	3:Z:203:HOH:O	2.10	0.52
2:Z:118:LYS:CD	2:Z:119:PHE:O	2.59	0.50
2:Z:151:VAL:HG13	2:Z:162:THR:HG23	1.95	0.48
2:Z:9:LEU:N	2:Z:9:LEU:HD12	2.29	0.47
2:Z:0:HIS:HB3	2:Z:154:ASP:OD2	2.15	0.45
2:Z:93:TRP:CG	2:Z:115:HIS:HE2	2.35	0.45
2:Z:41:CYS:HA	2:Z:64:ASP:HA	1.98	0.44
2:Z:119:PHE:O	2:Z:120:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:0:HIS:HA	3:Z:204:HOH:O	2.19	0.41

All (4) 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)
3:Z:272:HOH:O	3:Z:316:HOH:O[4_555]	2.00	0.20
3:Z:275:HOH:O	3:Z:331:HOH:H2[3_545]	1.45	0.15
3:Z:275:HOH:O	3:Z:331:HOH:O[3_545]	2.05	0.15
3:Z:305:HOH:O	3:Z:365:HOH:O[3_555]	2.07	0.13

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	X	13/23 (56%)	13 (100%)	0	0	100	100
2	Z	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
All	All	194/207 (94%)	190 (98%)	4 (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 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	X	13/20 (65%)	13 (100%)	0	100	100
2	Z	161/161 (100%)	161 (100%)	0	100	100
All	All	174/181 (96%)	174 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	72	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	X	15/23 (65%)	2.08	7 (46%) 0 0	21, 31, 48, 50	0
2	Z	183/184 (99%)	1.15	33 (18%) 3 6	12, 23, 57, 87	0
All	All	198/207 (95%)	1.22	40 (20%) 3 4	12, 24, 57, 87	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	93	TRP	10.0
2	Z	141	ALA	7.0
2	Z	182	PRO	6.8
2	Z	157	ALA	6.3
1	X	38	ILE	5.6
2	Z	94	GLY	5.4
2	Z	91	ILE	5.3
1	X	29	PHE	5.2
2	Z	142	LEU	5.2
2	Z	90	VAL	4.3
2	Z	41	CYS	4.0
2	Z	145	ASN	3.8
2	Z	124	HIS	3.4
2	Z	92	PRO	3.4
2	Z	97	ALA	3.4
2	Z	158	SER	3.2
1	X	24	ALA	3.1
2	Z	144	THR	3.1
1	X	30	GLY	2.9
2	Z	122	PHE	2.8
2	Z	96	MET	2.8
2	Z	126	ASN	2.8
2	Z	125	GLU	2.7
2	Z	95	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	Z	156	GLN	2.5
2	Z	106	PHE	2.4
2	Z	0	HIS	2.4
1	X	25	VAL	2.4
2	Z	169	GLY	2.4
2	Z	128	PHE	2.3
2	Z	168	ILE	2.3
2	Z	40	LEU	2.3
2	Z	139	TYR	2.3
2	Z	13	HIS	2.1
2	Z	102	LEU	2.1
1	X	32	TYR	2.1
2	Z	1	MET	2.1
1	X	28	GLU	2.1
2	Z	121	ALA	2.0
2	Z	29	GLY	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.