

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	5OSH
Title	:	Structure of retromer VPS29-VPS35C subunits complexed with RidL N-
		terminal domain (1-236)
Authors	:	Romano-Moreno, M.; Rojas, A.L.; Lucas, M.; Isupov, M.N.; Hierro, A.
Deposited on	:	2017-08-17
Resolution	:	4.30 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 on 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 <=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	А	182	83%	16% •
1	D	182	81%	19%
1	G	182	5% 85%	15% •
1	J	182	92%	8%
2	В	299	85%	13% •
2	Е	299	86%	11% ••



Mol	Chain	Length	Quality of chain		
2	Н	299	5% 88%	8%	••
2	K	299	85%	12%	•••
3	С	223	83%	13%	••
3	F	223	^{2%} 7 6% 1 7%	ά •	•
3	Ι	223	2% 85%	13%	•
3	L	223	79% 13	% •	6%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22276 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	100	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	102	1447	936	242	263	6	0	0	0
1	л	189	Total	С	Ν	Ο	S	0	0	0
		102	1447	936	242	263	6	0	0	0
1	C	199	Total	С	Ν	Ο	S	0	0	0
	G	102	1447	936	242	263	6	0	0	0
1	т	199	Total	С	Ν	Ο	S	0	0	0
	I J	182	1447	936	242	263	6	0		U

• Molecule 1 is a protein called Vacuolar protein sorting-associated protein 29.

• Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	р	200	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	299	2424	1539	423	452	10	0	0	0
0	Б	20.4	Total	С	Ν	0	S	0	0	0
	Ľ	294	2383	1514	418	441	10	0	0	U
0	и	200	Total	С	Ν	Ο	S	0	0	0
	11	290	2344	1491	408	435	10	0	0	0
0	2 K	20.2	Total	С	Ν	Ο	S	0	0	0
		293	2374	1509	417	438	10	U	0	0

• Molecule 3 is a protein called Interaptin.

Mol	Chain	Residues		Atoms					AltConf	Trace
9	C	917	Total	С	Ν	Ο	\mathbf{S}	0	0	0
3		211	1750	1103	299	344	4	0	0	0
2	Б	214	Total	С	Ν	Ο	S	0	0	0
J	Г	214	1723	1085	294	340	4	0		0
2	т	222	Total	С	Ν	Ο	S	0	0	0
3	1	223	1802	1135	306	356	5	0	0	0
2	3 L	L 209	Total	С	Ν	Ο	S	0	0	0
J			1688	1062	288	334	4	0	0	0





Chain	Residue	Modelled	Actual	Comment	Reference
С	1	MET	-	initiating methionine	UNP G8UZ99
С	2	ALA	-	expression tag	UNP G8UZ99
F	1	MET	-	initiating methionine	UNP G8UZ99
F	2	ALA	-	expression tag	UNP G8UZ99
Ι	1	MET	-	initiating methionine	UNP G8UZ99
Ι	2	ALA	-	expression tag	UNP G8UZ99
L	1	MET	-	initiating methionine	UNP G8UZ99
L	2	ALA	-	expression tag	UNP G8UZ99

There are 8 discrepancies between the modelled and reference sequences:



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Vacuolar protein sorting-associated protein 29



Line E482 Line E482 M7 F484 M7 F485 M7 F486 M7 F486 M7 F486 M7 F486 M7 F486 M7 F486 M7 F496 F73 F496 F73 F496 M66 F496 M7 F496 M66 F496 M76 F507 M76 F507 M76 F507 M76 F507 M653 F563 F77 F563 F77 F563 F563 F563 F563 F563 F611 S612 F613 F630 F630 F630 F631 F630 F633 F633 F647 F630 F633 F647

• Molecule 2: Vacuolar protein sorting-associated protein 35



E758 8759 8759 8759 8759 1774 1774 1778 1778 1778 1779 1779

• Molecule 2: Vacuolar protein sorting-associated protein 35



 \bullet Molecule 2: Vacuolar protein sorting-associated protein 35







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	90.20Å 173.24Å 445.77Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
\mathbf{B} as a solution (\mathbf{A})	222.89 - 4.30	Depositor
	112.79 - 4.30	EDS
$\% { m Data \ completeness}$	$100.0\ (222.89-4.30)$	Depositor
(in resolution range)	$100.0\ (112.79-4.30)$	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.24 (at 4.30 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R R.	0.254 , 0.311	Depositor
Π, Π_{free}	0.249 , 0.294	DCC
R_{free} test set	2460 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	216.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 238.4	EDS
L-test for $twinning^2$	$ < L >=0.44, < L^2>=0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22276	wwPDB-VP
Average B, all atoms $(Å^2)$	266.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Mol Chain		lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.54	0/1481	0.78	0/2008	
1	D	0.56	0/1481	0.77	0/2008	
1	G	0.53	0/1481	0.71	0/2008	
1	J	0.45	0/1481	0.63	0/2008	
2	В	0.56	0/2471	0.69	0/3327	
2	Ε	0.54	0/2429	0.69	0/3270	
2	Н	0.50	0/2390	0.64	0/3219	
2	Κ	0.54	0/2420	0.64	0/3258	
3	С	0.55	0/1783	0.71	0/2401	
3	F	0.56	0/1755	0.71	0/2362	
3	Ι	0.57	0/1835	0.70	0/2469	
3	L	0.51	0/1717	0.65	0/2311	
All	All	0.54	0/22724	0.69	0/30649	

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	А	1447	0	1459	13	0
1	D	1447	0	1459	15	0
1	G	1447	0	1459	10	0
1	J	1447	0	1459	7	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	2424	0	2407	16	0
2	Е	2383	0	2379	10	0
2	Н	2344	0	2336	9	0
2	Κ	2374	0	2373	18	0
3	С	1750	0	1726	8	0
3	F	1723	0	1704	16	0
3	Ι	1802	0	1783	14	0
3	L	1688	0	1673	7	0
All	All	22276	0	22217	131	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.

The worst 5 of 131 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)
3:I:11:LYS:NZ	3:I:88:TYR:OH	2.19	0.75
3:L:176:ASN:ND2	3:L:178:SER:OG	2.26	0.69
1:A:134:SER:OG	1:A:137:GLY:N	2.30	0.64
1:G:27:VAL:HG22	1:G:28:PRO:HD2	1.84	0.60
3:L:58:VAL:HG21	3:L:95:LEU:HD11	1.83	0.59

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 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	Perc	entiles
1	А	180/182~(99%)	160 (89%)	17 (9%)	3 (2%)	9	43
1	D	180/182~(99%)	157 (87%)	21 (12%)	2 (1%)	14	52
1	G	180/182~(99%)	160 (89%)	18 (10%)	2 (1%)	14	52



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
1	J	180/182~(99%)	157 (87%)	20 (11%)	3 (2%)	9	43
2	В	297/299~(99%)	259 (87%)	34 (11%)	4 (1%)	12	48
2	E	292/299~(98%)	265~(91%)	25~(9%)	2(1%)	22	62
2	Н	288/299~(96%)	265~(92%)	20 (7%)	3 (1%)	15	54
2	K	291/299~(97%)	264 (91%)	25~(9%)	2(1%)	22	62
3	С	215/223~(96%)	190 (88%)	24 (11%)	1 (0%)	29	68
3	F	212/223~(95%)	182~(86%)	26~(12%)	4 (2%)	8	41
3	Ι	221/223~(99%)	198~(90%)	19 (9%)	4 (2%)	8	42
3	L	205/223~(92%)	184 (90%)	19 (9%)	2 (1%)	15	54
All	All	2741/2816 (97%)	2441 (89%)	268 (10%)	32 (1%)	13	50

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	157	ALA
2	В	496	HIS
1	D	157	ALA
3	F	50	ASP
3	F	71	SER

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	А	160/160~(100%)	151 (94%)	9 (6%)	21 48
1	D	160/160~(100%)	157~(98%)	3 (2%)	57 75
1	G	160/160~(100%)	151 (94%)	9 (6%)	21 48
1	J	160/160~(100%)	158~(99%)	2(1%)	69 82
2	В	260/260~(100%)	240~(92%)	20 (8%)	13 39
2	Е	256/260~(98%)	237 (93%)	19 (7%)	13 40
2	Н	252/260~(97%)	241 (96%)	11 (4%)	28 54



Mol	Chain	Analysed	Rotameric	Outliers	Percentil	es
2	K	255/260~(98%)	237~(93%)	18 (7%)	14 41	
3	С	192/198~(97%)	172~(90%)	20 (10%)	7 27	
3	F	190/198~(96%)	169~(89%)	21 (11%)	6 25	
3	Ι	198/198~(100%)	184~(93%)	14 (7%)	14 41	
3	L	187/198~(94%)	166~(89%)	21 (11%)	6 25	
All	All	2430/2472~(98%)	2263~(93%)	167 (7%)	15 42	

5 of 167 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
3	F	58	VAL
1	G	16	ASN
3	L	155	GLU
3	F	75	PHE
3	F	126	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
2	Е	598	ASN
3	F	176	ASN
3	L	134	ASN
3	F	68	HIS
3	F	208	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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	182/182~(100%)	0.21	0 100 100	124, 191, 258, 292	0
1	D	182/182~(100%)	0.07	0 100 100	126, 182, 255, 298	0
1	G	182/182~(100%)	0.29	10 (5%) 25 22	185, 263, 320, 362	0
1	J	182/182~(100%)	0.33	18 (9%) 7 7	219, 314, 372, 462	0
2	В	299/299~(100%)	0.21	5 (1%) 70 61	140, 230, 338, 449	0
2	Е	294/299~(98%)	0.13	1 (0%) 94 90	121, 229, 313, 387	0
2	Н	290/299~(96%)	0.29	14 (4%) 30 26	165, 275, 377, 435	0
2	K	293/299~(97%)	0.62	37 (12%) 3 5	235, 343, 441, 539	0
3	С	217/223~(97%)	0.04	3 (1%) 75 66	132, 216, 314, 371	0
3	F	214/223~(95%)	0.17	4 (1%) 66 58	148, 226, 334, 438	0
3	Ι	223/223~(100%)	-0.00	4 (1%) 68 60	210, 307, 384, 453	0
3	L	209/223~(93%)	0.20	10 (4%) 30 26	209, 315, 401, 451	0
All	All	$276\overline{7/2816}~(98\%)$	0.22	106 (3%) 40 32	121, 261, 385, 539	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	679	SER	9.8
2	Н	681	ARG	7.1
2	Κ	687	GLY	6.1
2	К	694	LYS	5.9
2	Κ	686	ASN	5.2

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 carbohydrates 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.

