wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 05:29 PM UTC

PDB ID	:	6LPC / pdb_00006lpc
Title	:	Crystal Structure of rat Munc18-1 with K332E/K333E mutation
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Deposited on	:	2020-01-09
Resolution	:	3.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

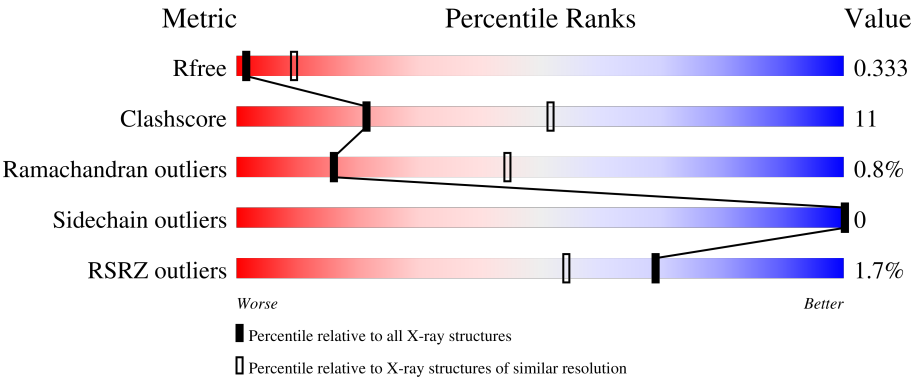
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 <=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	594	2% 68% 22% 10%
1	B	594	% 62% 16% 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7114 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 Syntaxin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			3814	2423	621	748	22			
1	B	467	Total	C	N	O	S	0	0	0
			3300	2081	548	654	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	GLU	LYS	engineered mutation	UNP P61765
A	333	GLU	LYS	engineered mutation	UNP P61765
B	332	GLU	LYS	engineered mutation	UNP P61765
B	333	GLU	LYS	engineered mutation	UNP P61765

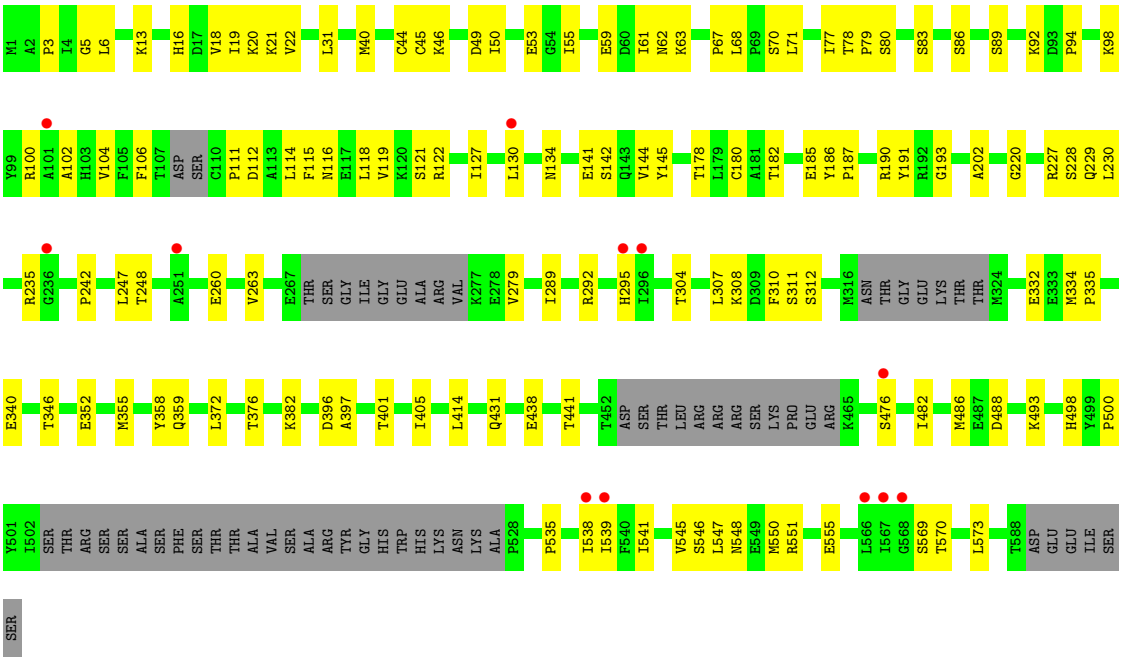
3 Residue-property plots (i)

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: Syntaxin-binding protein 1

Chain A:

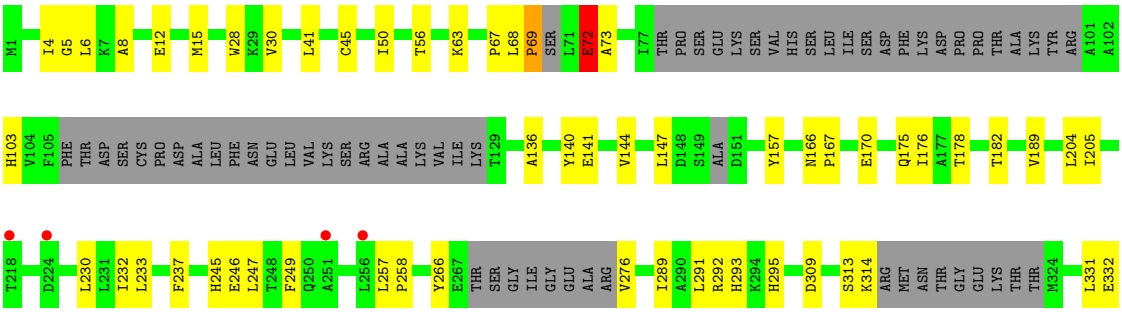


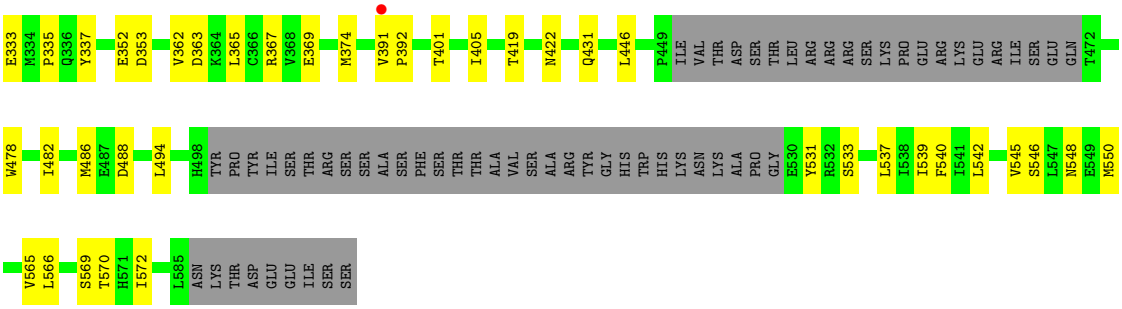


• Molecule 1: Syntaxin-binding protein 1

Chain B:






E333 M334 P335 Q336 Y337 E352 D353 V362 D363 K364 L365 C366 R367 V368 E369 M374 V391 P392 T401 I405 T419 N422 Q431 L446 P449 ILE VAL THR ASP SER THR LEU ARG ARG ARG SER LYS PRO GLU ARG LYS GLU ARG ILE SER GLU GLN T472
W478 I482 M486 E487 D488 L494 H498 TYR PRO TYR ILE SER THR ARG SER SER ALA SER PHE SER THR THR ALA VAL SER ALA ARG TYR GLY HIS TRP HIS LYS ASN LYS ALA PRO GLY E530 Y531 R532 S533 L537 I538 I539 F540 I541 L542 V545 S546 L547 N548 E549 M550
V565 L566 S569 T570 H571 I572 L585 ASN LYS THR ASP GLU GLU ILE SER SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	80.47Å 80.47Å 247.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.40 49.07 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.07-3.40) 99.9 (49.07-3.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.281 , 0.331 0.283 , 0.333	Depositor DCC
R_{free} test set	1104 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	126.2	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 151.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.22	0/3887	0.46	0/5324
1	B	0.28	0/3354	0.51	3/4590 (0.1%)
All	All	0.25	0/7241	0.48	3/9914 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	GLU	N-CA-C	6.61	119.61	110.35
1	B	431	GLN	N-CA-C	6.33	118.94	111.02
1	B	69	PRO	N-CA-C	5.38	125.55	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3814	0	3389	90	0
1	B	3300	0	2856	61	0
All	All	7114	0	6245	146	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 11.

The worst 5 of 146 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:289:ILE:HA	1:B:292:ARG:HD2	1.61	0.82
1:B:6:LEU:HD21	1:B:566:LEU:HD21	1.61	0.81
1:A:68:LEU:HD13	1:A:70:SER:H	1.49	0.75
1:B:136:ALA:HB1	1:B:175:GLN:HG2	1.68	0.73
1:A:62:ASN:CB	1:A:86:SER:HB2	2.20	0.72

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	Percentiles	
1	A	521/594 (88%)	461 (88%)	56 (11%)	4 (1%)	16	44
1	B	449/594 (76%)	401 (89%)	44 (10%)	4 (1%)	14	42
All	All	970/1188 (82%)	862 (89%)	100 (10%)	8 (1%)	16	44

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	B	63	LYS
1	A	431	GLN
1	A	79	PRO
1	A	100	ARG

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	358/533 (67%)	358 (100%)	0	100	100
1	B	298/533 (56%)	298 (100%)	0	100	100
All	All	656/1066 (62%)	656 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	206	GLN
1	A	442	ASN
1	A	445	HIS
1	A	558	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	533/594 (89%)	0.08	12 (2%) 61 46	30, 130, 157, 179	0
1	B	467/594 (78%)	0.16	5 (1%) 78 65	89, 138, 193, 244	0
All	All	1000/1188 (84%)	0.12	17 (1%) 69 54	30, 134, 182, 244	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	SER	3.1
1	A	251	ALA	2.7
1	A	568	GLY	2.6
1	A	567	ILE	2.5
1	B	251	ALA	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.