



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:24 PM GMT

PDB ID : 3SWH
Title : Munc13-1, MUN domain, C-terminal module
Authors : Tomchick, D.R.; Rizo, J.; Li, W.
Deposited on : 2011-07-13
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

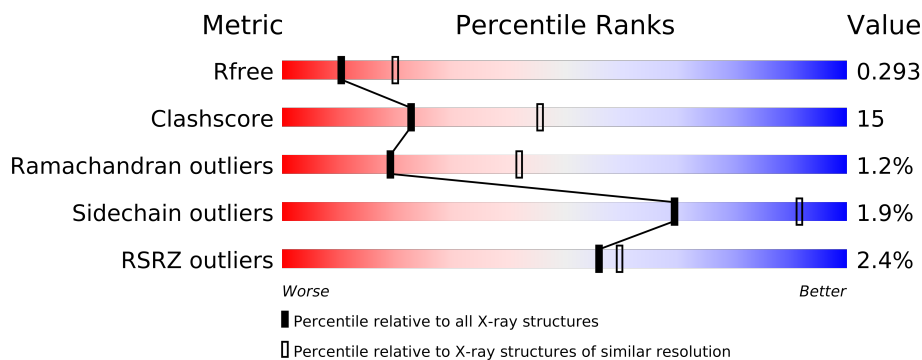
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4852 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein unc-13 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2370	1516	394	445	15			
1	B	297	Total	C	N	O	S	0	0	0
			2383	1523	395	450	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1408	GLU	-	LINKER	UNP Q62768
A	1409	PHE	-	LINKER	UNP Q62768
B	1408	GLU	-	LINKER	UNP Q62768
B	1409	PHE	-	LINKER	UNP Q62768

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	43	Total	O	0	0
			43	43		

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	160.79Å 160.79Å 42.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 2.65 40.85 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.12-2.65) 89.7 (40.85-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.244 , 0.302 0.237 , 0.293	Depositor DCC
R_{free} test set	1442 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.6	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 28876 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4852	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0681e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.44	0/2412	0.58	0/3249
1	B	0.46	0/2424	0.63	0/3267
All	All	0.45	0/4836	0.61	0/6516

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2370	0	0	40	0
1	B	2383	0	0	31	0
2	A	56	0	0	4	0
2	B	43	0	0	12	0
All	All	4852	0	0	70	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1483:LYS:NZ	1:B:1499:GLU:OE1	1.82	1.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1266:CYS:SG	2:A:60:HOH:O	2.16	1.04
1:B:1217:LYS:NZ	2:B:81:HOH:O	2.08	0.87
1:A:1397:ASN:OD1	2:A:21:HOH:O	1.91	0.86
1:A:1494:LYS:NZ	1:B:1485:TYR:OH	2.12	0.82
1:B:1468:THR:N	2:B:93:HOH:O	2.23	0.72
1:A:1183:ARG:NH1	1:A:1204:ASP:OD2	2.23	0.71
1:B:1352:SER:N	2:B:66:HOH:O	2.26	0.69
1:B:1492:GLY:O	2:B:70:HOH:O	2.13	0.66
1:B:1380:GLU:OE1	2:B:68:HOH:O	2.13	0.65
1:B:1294:GLU:OE1	2:B:15:HOH:O	2.15	0.64
1:B:1257:CYS:O	1:B:1259:LYS:N	2.34	0.60
1:A:1184:ASP:OD2	1:A:1201:SER:OG	2.20	0.59
1:A:1334:ASP:O	1:A:1337:SER:OG	2.19	0.59
1:B:1494:LYS:NZ	2:B:73:HOH:O	2.36	0.58
1:B:1257:CYS:C	1:B:1259:LYS:N	2.56	0.57
1:B:1405:LEU:O	1:B:1456:LYS:NZ	2.37	0.57
1:B:1199:SER:OG	1:B:1271:ASN:ND2	2.38	0.57
1:A:1483:LYS:NZ	1:A:1499:GLU:OE2	2.39	0.56
1:B:1252:ASP:O	1:B:1255:SER:OG	2.24	0.55
1:B:1484:GLN:OE1	1:B:1495:LYS:NZ	2.42	0.53
1:B:1193:SER:OG	1:B:1196:ALA:N	2.42	0.53
1:A:1234:PHE:O	1:A:1237:THR:N	2.42	0.52
1:B:1173:SER:O	1:B:1177:LEU:N	2.42	0.52
1:A:1340:LYS:NZ	2:A:53:HOH:O	2.43	0.52
1:B:1376:ALA:O	2:B:82:HOH:O	2.19	0.51
1:A:1163:ILE:CD1	1:A:1229:HIS:CD2	2.94	0.50
1:B:1352:SER:N	1:B:1355:GLN:OE1	2.45	0.50
1:B:1278:GLN:NE2	2:B:27:HOH:O	2.45	0.50
1:A:1317:PHE:O	1:A:1320:SER:OG	2.30	0.49
1:B:1494:LYS:NZ	2:B:70:HOH:O	2.46	0.49
1:A:1258:SER:C	1:A:1260:GLU:N	2.66	0.49
1:A:1406:PRO:O	1:A:1409:PHE:N	2.46	0.48
1:A:1279:LEU:O	1:A:1282:MET:N	2.47	0.48
1:B:1178:HIS:NE2	1:B:1244:GLN:OE1	2.46	0.48
1:A:1362:GLN:N	1:A:1363:PRO:CD	2.77	0.47
1:A:1385:LYS:O	1:A:1389:LYS:CG	2.62	0.47
1:A:1168:GLU:O	1:A:1172:VAL:N	2.47	0.47
1:A:1352:SER:O	1:A:1355:GLN:N	2.48	0.47
1:A:1509:TYR:O	1:A:1512:SER:OG	2.32	0.47
1:B:1358:ASP:O	2:B:94:HOH:O	2.20	0.47
1:A:1268:LEU:O	1:A:1271:ASN:N	2.49	0.46
1:A:1313:LEU:O	1:A:1317:PHE:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1502:PRO:O	1:A:1506:SER:N	2.50	0.45
1:B:1296:SER:O	1:B:1300:LYS:N	2.50	0.45
1:A:1258:SER:O	1:A:1260:GLU:N	2.50	0.45
1:B:1183:ARG:NH1	1:B:1204:ASP:OD2	2.49	0.45
1:A:1273:GLN:OE1	1:A:1276:ARG:NH1	2.50	0.45
1:A:1202:VAL:CG1	1:A:1202:VAL:O	2.66	0.45
1:A:1369:ASP:O	1:A:1373:THR:OG1	2.36	0.44
1:B:1472:CYS:O	1:B:1476:GLU:N	2.50	0.44
1:A:1169:ASN:O	1:A:1173:SER:N	2.51	0.44
1:B:1508:ARG:NE	2:B:76:HOH:O	2.51	0.43
1:A:1371:ASN:O	1:A:1374:LEU:N	2.51	0.43
1:A:1268:LEU:O	1:A:1269:MET:C	2.57	0.43
1:A:1382:THR:CG2	1:A:1386:ARG:NE	2.82	0.43
1:A:1170:GLU:OE1	1:A:1233:ARG:NH1	2.52	0.43
1:A:1307:ASN:ND2	2:A:18:HOH:O	2.51	0.42
1:A:1193:SER:OG	1:A:1196:ALA:N	2.53	0.42
1:B:1193:SER:OG	1:B:1195:HIS:N	2.53	0.42
1:A:1497:PHE:CD2	1:A:1497:PHE:C	2.93	0.42
1:A:1380:GLU:O	1:A:1381:LYS:C	2.58	0.42
1:A:1475:VAL:O	1:A:1475:VAL:CG1	2.69	0.41
1:B:1280:GLU:CG	1:B:1303:GLN:NE2	2.84	0.41
1:A:1296:SER:O	1:A:1299:LEU:N	2.54	0.41
1:A:1211:GLN:O	1:A:1212:SER:C	2.59	0.40
1:B:1159:GLU:O	1:B:1160:PRO:C	2.59	0.40
1:A:1217:LYS:C	1:A:1219:LEU:N	2.74	0.40
1:A:1352:SER:O	1:A:1354:ALA:N	2.55	0.40
1:B:1476:GLU:OE2	1:B:1508:ARG:NH1	2.54	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	289/341 (85%)	252 (87%)	34 (12%)	3 (1%)	22	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/341 (85%)	255 (88%)	32 (11%)	4 (1%)	16	37
All	All	580/682 (85%)	507 (87%)	66 (11%)	7 (1%)	19	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1258	SER
1	B	1469	PRO
1	A	1288	GLY
1	A	1353	VAL
1	B	1222	PRO
1	A	1259	LYS
1	B	1293	ALA

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	268/307 (87%)	263 (98%)	5 (2%)	69	91
1	B	270/307 (88%)	265 (98%)	5 (2%)	69	91
All	All	538/614 (88%)	528 (98%)	10 (2%)	69	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1200	CYS
1	A	1201	SER
1	A	1245	TYR
1	A	1372	LEU
1	A	1514	TYR
1	B	1167	ASP
1	B	1221	CYS
1	B	1472	CYS
1	B	1483	LYS
1	B	1501	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	295/341 (86%)	0.20	7 (2%) 56 60	45, 76, 121, 163	0
1	B	297/341 (87%)	0.27	7 (2%) 56 60	45, 76, 123, 157	0
All	All	592/682 (86%)	0.23	14 (2%) 56 60	45, 76, 122, 163	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1457	ASP	3.9
1	B	1339	VAL	3.5
1	B	1516	GLN	3.2
1	A	1458	HIS	3.0
1	A	1157	TRP	2.9
1	B	1215	ILE	2.6
1	B	1226	ILE	2.5
1	A	1353	VAL	2.4
1	B	1157	TRP	2.4
1	B	1340	LYS	2.2
1	A	1230	TYR	2.1
1	A	1295	ALA	2.1
1	B	1230	TYR	2.1
1	A	1219	LEU	2.0

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 carbohydrates 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.