



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:29 AM GMT

PDB ID : 3B5N
Title : Structure of the yeast plasma membrane SNARE complex
Authors : Strop, P.; Brunger, A.T.
Deposited on : 2007-10-26
Resolution : 1.60 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>

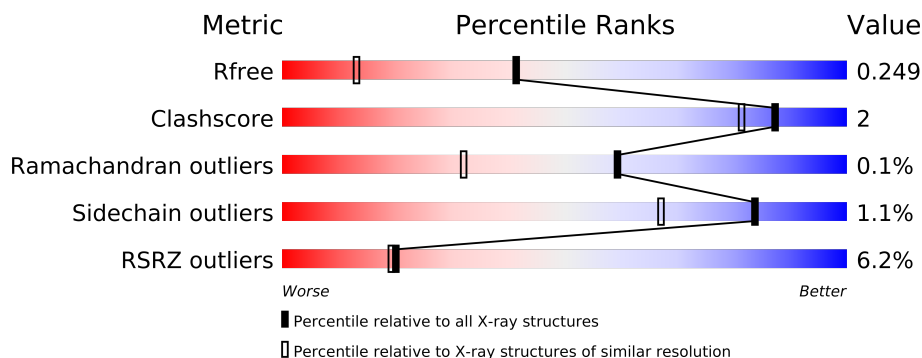
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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	61	
1	E	61	
1	I	61	
2	B	69	
2	F	69	
2	J	69	
3	C	70	
3	G	70	
3	K	70	
4	D	64	
4	H	64	
4	L	64	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6656 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 Synaptobrevin homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	S	0	0	0
			473	284	93	94	2			
1	E	58	Total	C	N	O	S	0	0	0
			452	273	87	90	2			
1	I	58	Total	C	N	O	S	0	0	0
			452	273	87	90	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP P31109
E	26	GLY	-	EXPRESSION TAG	UNP P31109
I	26	GLY	-	EXPRESSION TAG	UNP P31109

- Molecule 2 is a protein called Protein SSO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			545	333	94	116	2			
2	F	68	Total	C	N	O	S	0	0	0
			533	327	90	114	2			
2	J	64	Total	C	N	O	S	0	0	0
			509	312	86	109	2			

- Molecule 3 is a protein called Protein transport protein SEC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	70	Total	C	N	O	S	0	1	0
			542	329	101	108	4			
3	G	69	Total	C	N	O	S	0	2	0
			532	324	97	107	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	65	Total	C	N	O	S	0	1	0
			503	305	93	101	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	GLY	-	EXPRESSION TAG	UNP P40357
C	432	SER	-	EXPRESSION TAG	UNP P40357
C	500	GLN	-	EXPRESSION TAG	UNP P40357
G	431	GLY	-	EXPRESSION TAG	UNP P40357
G	432	SER	-	EXPRESSION TAG	UNP P40357
G	500	GLN	-	EXPRESSION TAG	UNP P40357
K	431	GLY	-	EXPRESSION TAG	UNP P40357
K	432	SER	-	EXPRESSION TAG	UNP P40357
K	500	GLN	-	EXPRESSION TAG	UNP P40357

- Molecule 4 is a protein called Protein transport protein SEC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	64	Total	C	N	O	S	0	0	0
			511	305	94	109	3			
4	H	63	Total	C	N	O	S	0	1	0
			514	308	96	107	3			
4	L	62	Total	C	N	O	S	0	0	0
			498	297	92	106	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	587	GLY	-	EXPRESSION TAG	UNP P40357
D	588	SER	-	EXPRESSION TAG	UNP P40357
H	587	GLY	-	EXPRESSION TAG	UNP P40357
H	588	SER	-	EXPRESSION TAG	UNP P40357
L	587	GLY	-	EXPRESSION TAG	UNP P40357
L	588	SER	-	EXPRESSION TAG	UNP P40357

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	59	Total 59	O 59	0	0
5	C	53	Total 53	O 53	0	0
5	D	57	Total 57	O 57	0	0
5	E	54	Total 54	O 54	0	0
5	F	78	Total 78	O 78	0	0
5	G	58	Total 58	O 58	0	0
5	H	72	Total 72	O 72	0	0
5	I	25	Total 25	O 25	0	0
5	J	19	Total 19	O 19	0	0
5	K	28	Total 28	O 28	0	0
5	L	43	Total 43	O 43	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

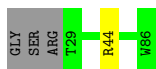
- Molecule 1: Synaptobrevin homolog 1

Chain A: 



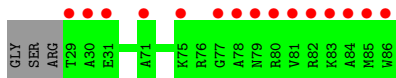
- Molecule 1: Synaptobrevin homolog 1

Chain E: 



- Molecule 1: Synaptobrevin homolog 1

Chain I: 



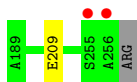
- Molecule 2: Protein SSO1

Chain B: 



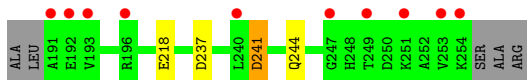
- Molecule 2: Protein SSO1

Chain F: 



- Molecule 2: Protein SSO1

Chain J: 



- Molecule 3: Protein transport protein SEC9

Chain C: 



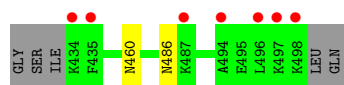
- Molecule 3: Protein transport protein SEC9

Chain G: 



- Molecule 3: Protein transport protein SEC9

Chain K: 



- Molecule 4: Protein transport protein SEC9

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 4: Protein transport protein SEC9

Chain H: 



- Molecule 4: Protein transport protein SEC9

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.96Å 48.11Å 110.27Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	34.57 – 1.60 34.57 – 1.60	Depositor EDS
% Data completeness (in resolution range)	85.0 (34.57-1.60) 85.0 (34.57-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.60Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.248 0.210 , 0.249	Depositor DCC
R_{free} test set	4519 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 90056 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6656	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.27	0/475	0.39	0/633
1	E	0.31	0/454	0.45	0/606
1	I	0.24	0/454	0.39	0/606
2	B	0.28	0/547	0.38	0/734
2	F	0.33	0/535	0.41	0/720
2	J	0.23	0/511	0.35	0/687
3	C	0.29	0/546	0.39	0/725
3	G	0.31	0/539	0.38	0/718
3	K	0.25	0/507	0.37	0/675
4	D	0.34	0/511	0.41	0/682
4	H	0.31	0/517	0.45	0/691
4	L	0.26	0/498	0.35	0/666
All	All	0.29	0/6094	0.39	0/8143

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	473	0	0	0	0
1	E	452	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	452	0	0	0	0
2	B	545	0	0	0	0
2	F	533	0	0	1	0
2	J	509	0	0	3	0
3	C	542	0	0	2	0
3	G	532	0	7	6	0
3	K	503	0	0	1	0
4	D	511	0	9	0	0
4	H	514	0	0	7	0
4	L	498	0	0	0	0
5	A	46	0	0	0	0
5	B	59	0	0	0	0
5	C	53	0	0	1	0
5	D	57	0	0	0	0
5	E	54	0	0	0	0
5	F	78	0	0	0	0
5	G	58	0	0	1	0
5	H	72	0	0	2	0
5	I	25	0	0	0	0
5	J	19	0	0	1	0
5	K	28	0	0	0	0
5	L	43	0	0	0	0
All	All	6656	0	16	15	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 2.

All (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:625[A]:ARG:CG	4:H:625[A]:ARG:NH1	2.61	0.62
3:G:495:GLU:O	3:G:499:LEU:HG	2.04	0.58
3:G:476:GLU:OE1	4:H:625[A]:ARG:NH1	2.37	0.57
4:H:625[A]:ARG:NH1	5:H:687:HOH:O	2.42	0.52
2:J:237:ASP:O	2:J:241:ASP:OD1	2.29	0.50
3:G:459:MET:SD	4:H:611:MET:SD	3.15	0.45
4:H:588:SER:N	5:H:699:HOH:O	2.49	0.45
1:E:44:ARG:NH2	2:F:209:GLU:OE2	2.50	0.45
2:J:244:GLN:CB	5:J:260:HOH:O	2.64	0.44
3:G:467:HIS:CD2	5:G:536:HOH:O	2.70	0.44
3:C:434:LYS:NZ	3:C:438:GLN:NE2	2.68	0.42
3:G:469[B]:SER:OG	4:H:618:GLU:OE2	2.38	0.41
2:J:218:GLU:OE2	3:K:460[A]:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:431:GLY:N	5:C:533:HOH:O	2.54	0.41
3:G:469[B]:SER:OG	4:H:622:GLN:NE2	2.54	0.41

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	59/61 (97%)	59 (100%)	0	0	100	100
1	E	56/61 (92%)	56 (100%)	0	0	100	100
1	I	56/61 (92%)	56 (100%)	0	0	100	100
2	B	67/69 (97%)	67 (100%)	0	0	100	100
2	F	66/69 (96%)	66 (100%)	0	0	100	100
2	J	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
3	C	69/70 (99%)	69 (100%)	0	0	100	100
3	G	69/70 (99%)	69 (100%)	0	0	100	100
3	K	64/70 (91%)	64 (100%)	0	0	100	100
4	D	62/64 (97%)	62 (100%)	0	0	100	100
4	H	62/64 (97%)	62 (100%)	0	0	100	100
4	L	60/64 (94%)	58 (97%)	1 (2%)	1 (2%)	14	2
All	All	752/792 (95%)	749 (100%)	2 (0%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	648	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	48/48 (100%)	48 (100%)	0	100	100
1	E	46/48 (96%)	46 (100%)	0	100	100
1	I	46/48 (96%)	46 (100%)	0	100	100
2	B	60/60 (100%)	60 (100%)	0	100	100
2	F	59/60 (98%)	59 (100%)	0	100	100
2	J	57/60 (95%)	56 (98%)	1 (2%)	71	44
3	C	60/59 (102%)	57 (95%)	3 (5%)	34	9
3	G	60/59 (102%)	60 (100%)	0	100	100
3	K	56/59 (95%)	55 (98%)	1 (2%)	71	44
4	D	59/59 (100%)	59 (100%)	0	100	100
4	H	60/59 (102%)	58 (97%)	2 (3%)	50	20
4	L	58/59 (98%)	56 (97%)	2 (3%)	49	19
All	All	669/678 (99%)	660 (99%)	9 (1%)	84	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	456[A]	ARG
3	C	456[B]	ARG
3	C	473	ASN
4	H	625[A]	ARG
4	H	625[B]	ARG
2	J	241	ASP
3	K	486	ASN
4	L	589	GLU
4	L	623	GLN

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	61/61 (100%)	0.18	1 (1%) 68 68	27, 36, 54, 58	0
1	E	58/61 (95%)	-0.20	0 100 100	25, 33, 52, 69	0
1	I	58/61 (95%)	0.98	15 (25%) 1 1	28, 55, 109, 138	0
2	B	69/69 (100%)	-0.12	2 (2%) 49 48	26, 36, 55, 70	0
2	F	68/69 (98%)	-0.09	2 (2%) 49 48	24, 32, 55, 77	0
2	J	64/69 (92%)	0.75	10 (15%) 3 2	34, 59, 101, 122	0
3	C	70/70 (100%)	-0.08	0 100 100	24, 33, 51, 67	0
3	G	69/70 (98%)	0.12	4 (5%) 22 21	23, 32, 60, 92	0
3	K	65/70 (92%)	0.55	7 (10%) 6 5	31, 48, 85, 110	0
4	D	64/64 (100%)	0.02	0 100 100	20, 34, 47, 51	0
4	H	63/64 (98%)	-0.16	0 100 100	25, 34, 47, 65	0
4	L	62/64 (96%)	0.49	7 (11%) 6 5	27, 43, 90, 100	0
All	All	771/792 (97%)	0.19	48 (6%) 20 19	20, 38, 79, 138	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	499	LEU	7.8
2	J	254	LYS	6.4
3	K	496	LEU	6.1
1	I	86	TRP	5.6
3	K	497	LYS	5.3
2	J	253	VAL	4.9
1	I	30	ALA	4.9
3	K	494	ALA	4.5
4	L	588	SER	4.5
3	K	435	PHE	4.0
1	I	77	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	J	251	LYS	3.8
1	I	84	ALA	3.7
1	I	80	ARG	3.7
4	L	592	LEU	3.7
3	K	498	LYS	3.6
2	F	256	ALA	3.5
4	L	647	LEU	3.4
1	I	78	ALA	3.3
2	J	249	THR	3.2
4	L	648	ALA	3.1
2	J	193	VAL	3.1
2	J	192	GLU	3.1
4	L	644	THR	2.9
2	J	196	ARG	2.9
1	I	75	LYS	2.9
1	I	29	THR	2.9
1	I	79	ASN	2.8
2	B	189	ALA	2.8
1	I	31	GLU	2.7
1	I	82	ARG	2.7
2	J	240	LEU	2.7
1	I	71	ALA	2.6
4	L	646	ARG	2.6
2	J	191	ALA	2.5
4	L	591	GLU	2.5
3	G	498	LYS	2.4
1	A	86	TRP	2.4
2	J	247	GLY	2.3
1	I	83	LYS	2.3
1	I	81	VAL	2.3
3	G	435	PHE	2.2
2	F	255	SER	2.2
3	K	487	LYS	2.1
1	I	85	MET	2.1
3	K	434	LYS	2.0
2	B	191	ALA	2.0
3	G	432	SER	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.