



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1FVF / pdb_00001fvf
Title : CRYSTAL STRUCTURE ANALYSIS OF NEURONAL SEC1 FROM THE SQUID L. PEALEI
Authors : Bracher, A.; Weissenhorn, W.
Deposited on : 2000-09-19
Resolution : 3.20 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 ⓘ 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

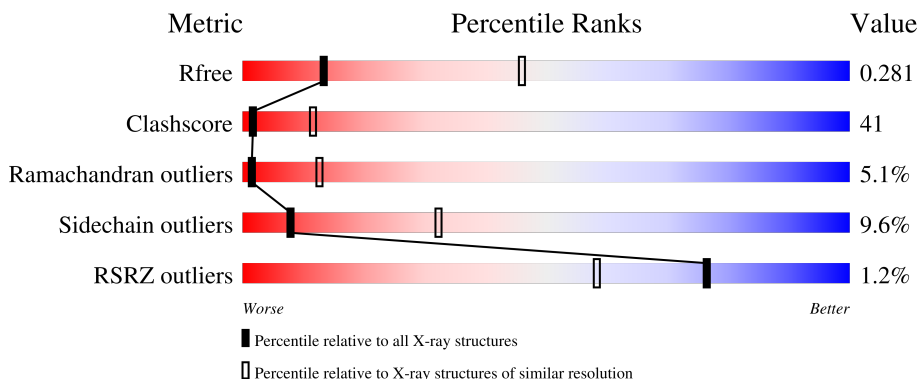
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	A	591	% 38% 42% 10% • 8%
1	B	591	% 39% 40% 12% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8786 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 SEC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4393	2783	759	823	28			
1	B	543	Total	C	N	O	S	0	0	0
			4393	2783	759	823	28			

K587	SER	I448	T374	R312	H242	G162	I75	MET
I588	VAL	I449	D375	MEI	E243	I163	P76	A2
S589	ARG	Q450	A376	GLY	I244	P164		L3
N590	TYR	D451	D377	THR	T245	N165	S80	K4
P591	GLY	G452	G378	ALA	F246	V81	K82	T5
	HIS	G453	E379	ALA	Q247	R168	C93	A6
	TRP		K380	ASP	K248	C169	L84	V7
	HIS	K456	I381	LYS	K249	A170	R85	
	LYS	I457	R382	ALA	E171	A176	A86	I11
	LYS	Q458	D383	GLY	E257	L176	D87	M12
	LYS	Q459	H384	I1E	E258	C177	F88	V15
	GLN	H462	M385	LYS	D259	A178	O89	Y16
	ALA	I463	R386	ASP	V260	T179	N90	L17
	SER	H464	N387	L325	Y261	L180	P91	
	TYR	N465	I388	S326	Y263	R187	N93	K21
	LYS	R466	V389	Q327	V264		O95	N22
	SER	R467	I391	M328	ASN		Y96	A23
	LYS	R468	L392	K330	THR	D183		E24
	G536	R469	L393	K331	GLY	E194		W25
P537			D394	M332	GLY	N195		K26
	I540		K395	P333	ASN	F198	I101	V27
			Q396	Q334	GLU	F102	F103	V30
	V544		I397	Y335	VAL	T104	E105	D31
G545				Q336	PRO	L201	A106	Q32
G546	G545	K402	K403	K337	E273	V202		S34
I547		R479	R404	E338	K274	Q203		M35
		W480	I405	E339	E275	Q204		R36
E551		Y483	I406	S340	V276	K205		M37
M552		M484	L407	K341	D279	L206		V38
R553		K485	L408	S342	E280	D207		S39
		D486	L409	S343	K281	K208		A40
		I487	I410	T344	W285	Y209		C41
		M488	I411	H345	E286	R210		C42
V558		V492	H412	H347	E287	D212		M44
T559			K413	L348	W288	D213		H45
T561		I416			R289			E46
K563		N420	L421		H290	G217		E50
N564		L425	V425		Q291	E218		L54
N565					H292	E219		V55
W566					I293	P220		E56
E567					K294	K222		D57
V568					V295	D223		F58
I569					W296	R224		N59
L570					S297	S225		R60
G571					Q298	Q226		R61
S572					N299	L227		R62
T573					V300	L228		E63
H574					T301	I229		P64
I575					L304			L65
L576					K365	R232		P66
T577					V366			E69
P578					E367			I74
E579					K305			
G580					Q368			
I581					D369			
L582					L370			
					F307			
					L444			
					G445			
					V446			
					A371			
					E310			
					G373			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.52Å 118.52Å 192.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.20 12.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (12.00-3.20) 93.7 (12.00-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 3.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.288 0.240 , 0.281	Depositor DCC
R_{free} test set	1202 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8786	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	A	0.53	0/4481	1.05	31/6050 (0.5%)
1	B	0.50	1/4481 (0.0%)	1.05	30/6050 (0.5%)
All	All	0.51	1/8962 (0.0%)	1.05	61/12100 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	544	VAL	CA-CB	5.39	1.59	1.53

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	N-CA-C	10.02	122.28	111.36
1	B	193	ASP	N-CA-C	9.85	121.78	111.14
1	A	207	ASP	N-CA-C	-8.84	101.62	111.07
1	A	346	LEU	N-CA-C	-8.52	101.96	111.07
1	B	207	ASP	N-CA-C	-8.36	102.12	111.07

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	A	4393	0	4393	371	0
1	B	4393	0	4393	374	0
All	All	8786	0	8786	721	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 41.

The worst 5 of 721 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:A:209:TYR:HB3	1:A:216:MET:HE1	1.42	1.02
1:A:89:GLN:HE21	1:A:89:GLN:HA	1.25	1.00
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.27	0.98
1:B:209:TYR:HB3	1:B:216:MET:HE1	1.43	0.98
1:A:577:THR:HG22	1:A:580:GLY:H	1.32	0.94

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	535/591 (90%)	424 (79%)	85 (16%)	26 (5%)	1	13
1	B	535/591 (90%)	423 (79%)	83 (16%)	29 (5%)	1	12
All	All	1070/1182 (90%)	847 (79%)	168 (16%)	55 (5%)	1	13

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ALA
1	A	93	ASN
1	A	220	PRO
1	A	223	ASP
1	A	376	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	485/523 (93%)	440 (91%)	45 (9%)	8	33
1	B	485/523 (93%)	437 (90%)	48 (10%)	7	31
All	All	970/1046 (93%)	877 (90%)	93 (10%)	8	32

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	LEU
1	B	330	LYS
1	B	193	ASP
1	B	243	GLU
1	B	375	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	299	ASN
1	B	439	ASN
1	B	336	GLN
1	B	359	HIS
1	B	462	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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 [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>2	OWAB(Å ²)	Q<0.9
1	A	543/591 (91%)	-0.15	7 (1%) 75 55	30, 63, 104, 131	1 (0%)
1	B	543/591 (91%)	-0.22	6 (1%) 78 61	28, 65, 105, 131	1 (0%)
All	All	1086/1182 (91%)	-0.18	13 (1%) 76 58	28, 64, 105, 131	2 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	GLY	4.9
1	A	506	GLY	4.5
1	A	377	ASP	3.8
1	B	506	GLY	3.6
1	B	89	GLN	3.6

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.