



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:26 am BST

PDB ID : 2SCP
Title : STRUCTURE OF A SARCOPLASMIC CALCIUM-BINDING PROTEIN FROM NEREIS DIVERSICOLOR REFINED AT 2.0 ANGSTROMS RESOLUTION
Authors : Cook, W.J.; Vijay-Kumar, S.
Deposited on : 1991-08-22
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) 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

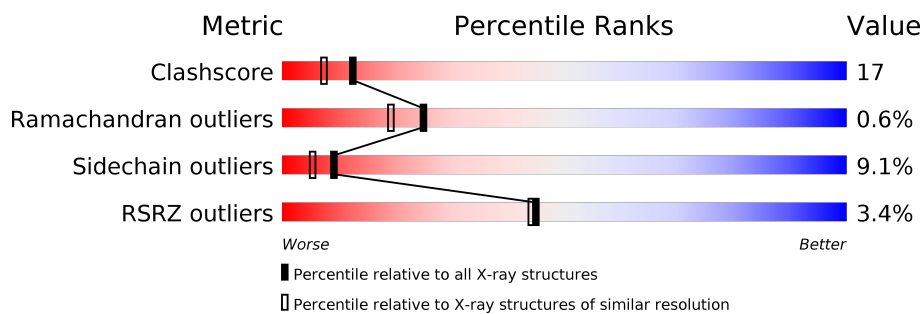
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	174	
1	B	174	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2955 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 SARCOPLASMIC CALCIUM-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1368	868	218	272	10			
1	B	174	Total	C	N	O	S	0	0	0
			1368	868	218	272	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	89	Total	O	0	0
			89	89		

- Molecule 1: SARCOPLASMIC CALCIUM-BINDING PROTEIN

A102	M106	E107	D108	M109	M110	I111	S112	R113	D114	E115	I118	L125	D126	K127	T128	M129	I137	D138	L144	L145	D161	V174	S1	D2	L3	T10	M13	R14	I15	R25	E26	D27	E33	R34	F35	S39	E40	N41	K42	K47	V48	L49	P50	D51	D58	P59	F60	K68	D71	E72	T73	I76	M77	S78	M79	K80	E81	K84	N85	P86	E87	A88	V91	G94	P95	L96	P97	E101
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Molecule 1: SARCOPLASMIC CALCIUM-BINDING PROTEIN

L96	P97	F99	F100	K101	A102	V103	D104	T105	M106	D107	D108	R113	D114	G121	M122	L125	D126	K127	T128	M129	A130	P131	A136	M141	L147	E148	E149	F150	V151	D156	F157	D163	S164	T165	M166	K167	P172	L173	V174	L96	P97	F99	F100	K101	A102	V103	D104	T105	M106	D107	D108	R113	D114	G121	M122	L125	D126	K127	T128	M129	A130	P131	A136	M141	L147	E148	E149	F150	V151	D156	F157	D163	S164	T165	M166	K167	P172	L173	V174
S1	K7	T10	Y11	F12	R14	F17	D18	K19	M26	E29	S30	P31	A32	E33	R34	F35	E38	S39	E40	M41	K42	A43	E44	H45	A46	L49	S53	F60	L61	T62	A63	V64	A65	G66	G67	X68	M77	X80	K84	X85	P86	X89	G94	D95																																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.60 Å 56.00 Å 65.80 Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 5.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 88.5 (5.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.68 , 114.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2955	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

¹Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.00	1/1396 (0.1%)	1.44	14/1880 (0.7%)
1	B	0.94	0/1396	1.47	13/1880 (0.7%)
All	All	0.97	1/2792 (0.0%)	1.46	27/3760 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	VAL	C-O	6.04	1.34	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	B	114	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	18	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	129	MET	CA-CB-CG	7.78	126.53	113.30
1	B	113	ARG	NE-CZ-NH2	-7.77	116.41	120.30

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	1368	0	1310	35	0
1	B	1368	0	1310	56	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	124	0	0	7	0
3	B	89	0	0	2	0
All	All	2955	0	2620	90	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 17.

The worst 5 of 90 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:129:MET:HB3	3:A:316:HOH:O	1.59	1.01
1:B:121:GLY:HA3	1:B:127:LYS:NZ	1.76	0.99
1:B:136:ALA:HB1	1:B:165:THR:HG22	1.46	0.97
1:B:86:PRO:O	1:B:89:LYS:HG3	1.64	0.95
1:B:45:HIS:CD2	1:B:105:THR:HG23	2.06	0.90

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	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	25	19
1	B	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	25	19
All	All	344/348 (99%)	331 (96%)	11 (3%)	2 (1%)	25	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	GLU
1	A	2	ASP

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	148/148 (100%)	135 (91%)	13 (9%)	10	6
1	B	148/148 (100%)	134 (90%)	14 (10%)	8	5
All	All	296/296 (100%)	269 (91%)	27 (9%)	9	5

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	B	40	GLU
1	B	105	THR
1	B	19	LYS
1	A	33	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	85	ASN
1	B	45	HIS
1	A	109	ASN
1	B	77	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	174/174 (100%)	-0.36	0 100 100	8, 16, 30, 34	0
1	B	174/174 (100%)	0.22	12 (6%) 16 16	11, 26, 31, 32	0
All	All	348/348 (100%)	-0.07	12 (3%) 45 44	8, 20, 31, 34	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	GLU	3.8
1	B	43	ALA	2.7
1	B	66	GLY	2.6
1	B	128	THR	2.6
1	B	141	ASN	2.5

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	B	194	1/1	0.96	0.23	9,9,9,9	0
2	CA	A	192	1/1	0.98	0.16	2,2,2,2	0
2	CA	B	195	1/1	0.99	0.28	2,2,2,2	0
2	CA	A	191	1/1	0.99	0.15	2,2,2,2	0
2	CA	B	193	1/1	0.99	0.22	2,2,2,2	0
2	CA	A	190	1/1	1.00	0.20	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.