WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 08:15 pm BST

PDB ID	:	2X3X
Title	:	structure of mouse syndapin I (crystal form 1)
Authors	:	Ma, Q.; Rao, Y.; Vahedi-Faridi, A.; Saenger, W.; Haucke, V.
Deposited on	:	2010-01-28
Resolution	:	3.35 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:

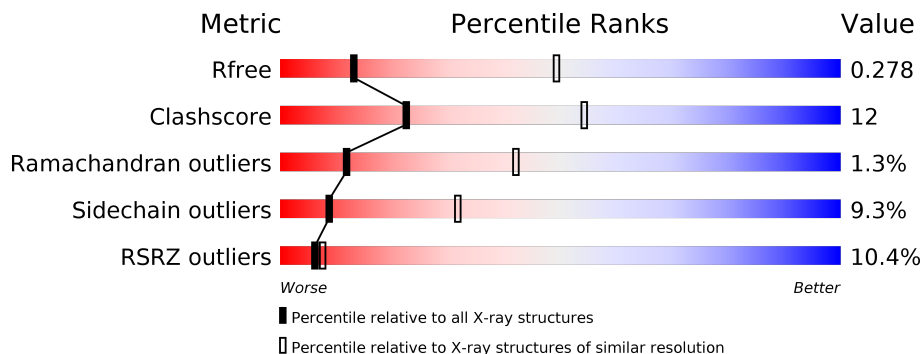|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.35 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		12
Ramachandran outliers		1.3%
Sidechain outliers		9.3%
RSRZ outliers		10.4%

Worse   *Better*

∎ Percentile relative to all X-ray structures

❏ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 <=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	337	2% — 58% / 26% / • / 14%
1	B	337	4% — 60% / 18% / • / 19%
1	C	337	11% — 61% / 23% / • / 14%
2	D	60	10% — 67% / 22% / 5% / 7%
2	E	60	62% — 68% / 17% / 8% / 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8006 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.
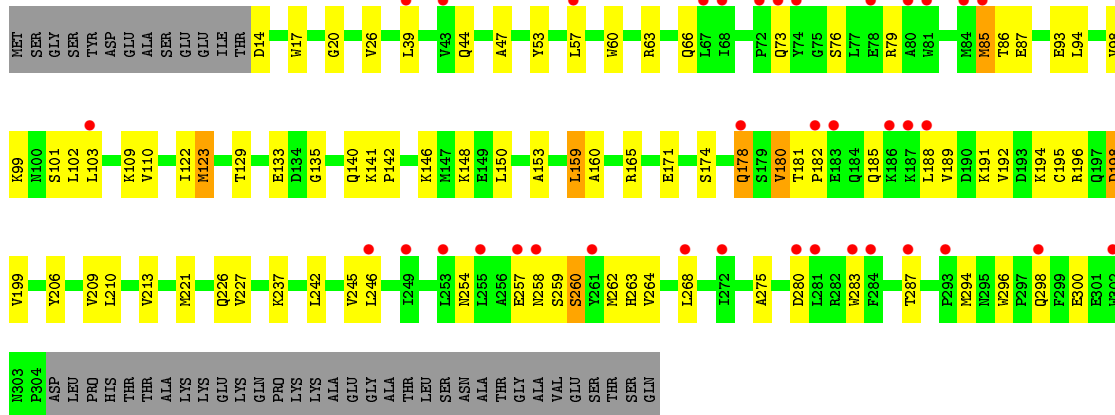
- Molecule 1 is a protein called PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2418	1514	430	457	17			
1	B	274	Total	C	N	O	S	0	0	0
			2277	1431	403	427	16			
1	C	291	Total	C	N	O	S	0	0	0
			2417	1513	430	457	17			

- Molecule 2 is a protein called PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	56	Total	C	N	O	S	0	0	0
			447	276	76	94	1			
2	E	56	Total	C	N	O	S	0	0	0
			447	276	76	94	1			

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 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: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1

- Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1

- Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1

Chain C:

● Molecule 2: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1

Chain D:

● Molecule 2: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	83.08Å 154.54Å 255.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.13 – 3.35 73.17 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.13-3.35) 98.5 (73.17-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.221 , 0.277 0.225 , 0.278	Depositor DCC
R_{free} test set	1192 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	1.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 104.0	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8006	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.42	0/2466	0.54	0/3305
1	B	0.40	0/2323	0.52	0/3114
1	C	0.36	0/2465	0.49	0/3304
2	D	0.34	0/454	0.57	0/611
2	E	0.39	0/454	0.53	0/611
All	All	0.39	0/8162	0.52	0/10945

There are no bond length outliers.

There are no bond angle outliers.

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	2418	0	2377	76	0
1	B	2277	0	2234	51	0
1	C	2417	0	2372	50	0
2	D	447	0	410	13	0
2	E	447	0	410	13	0
All	All	8006	0	7803	184	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 12.

The worst 5 of 184 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:35:LEU:HD11	1:B:72:PRO:HD2	1.34	1.05
1:A:150:LEU:HD11	1:A:210:LEU:HD22	1.46	0.97
2:D:387:VAL:HG13	2:D:438:VAL:HG13	1.54	0.89
2:D:387:VAL:HG13	2:D:438:VAL:CG1	2.04	0.88
1:A:143:TRP:CZ3	1:A:217:THR:HG23	2.08	0.86

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	289/337 (86%)	262 (91%)	22 (8%)	5 (2%)	9	36
1	B	270/337 (80%)	249 (92%)	18 (7%)	3 (1%)	14	46
1	C	289/337 (86%)	260 (90%)	26 (9%)	3 (1%)	15	49
2	D	54/60 (90%)	52 (96%)	2 (4%)	0	100	100
2	E	54/60 (90%)	48 (89%)	5 (9%)	1 (2%)	8	34
All	All	956/1131 (84%)	871 (91%)	73 (8%)	12 (1%)	12	42

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	ASN
1	A	183	GLU
1	B	122	ILE
1	B	76	SER
1	C	178	GLN

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	258/295 (88%)	238 (92%)	20 (8%)	12	40
1	B	241/295 (82%)	220 (91%)	21 (9%)	10	35
1	C	257/295 (87%)	232 (90%)	25 (10%)	8	30
2	D	45/47 (96%)	39 (87%)	6 (13%)	4	16
2	E	45/47 (96%)	38 (84%)	7 (16%)	2	11
All	All	846/979 (86%)	767 (91%)	79 (9%)	9	32

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	GLU
1	C	66	GLN
2	E	396	GLN
1	B	166	LEU
1	B	268	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	C	73	GLN
2	D	436	ASN
1	B	233	GLN
1	B	278	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 carbohydrates 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	291/337 (86%)	0.56	8 (2%)	54	57	87, 102, 115, 127	0
1	B	274/337 (81%)	0.58	13 (4%)	31	34	87, 102, 120, 136	0
1	C	291/337 (86%)	0.76	37 (12%)	3	4	86, 103, 121, 124	0
2	D	56/60 (93%)	0.95	6 (10%)	6	7	96, 102, 111, 116	0
2	E	56/60 (93%)	2.77	37 (66%)	0	0	92, 102, 108, 113	0
All	All	968/1131 (85%)	0.78	101 (10%)	6	7	86, 102, 119, 136	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ASP	6.4
2	E	437	TYR	6.4
1	B	189	VAL	6.0
1	A	298	GLN	5.8
2	E	391	TYR	5.8

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.