Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 03:23 am GMT

PDB ID	:	2YOA
Title	:	Synaptotagmin-1 C2B domain with phosphoserine
Authors	:	Honigmann, A.; van den Bogaart, G.; Iraheta, E.; Risselada, H.J.; Milovanovic, D.; Mueller, V.; Muellar, S.; Diederichsen, U.; Fasshauer, D.; Grubmuller, H.; Hell, S.W.; Eggeling, C.; Kuhnel, K.; Jahn, R.
Deposited on	:	2012-10-22
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (i)) were used in the production of this report:

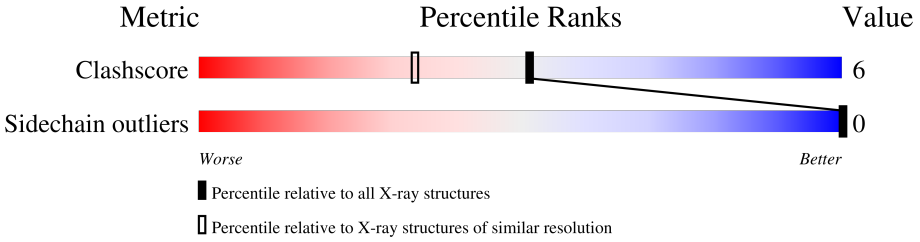
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	3144 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2713 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 SYNAPTOTAGMIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1208	777	205	219	7	0	2	0
1	B	149	1205	775	205	220	5	0	2	0

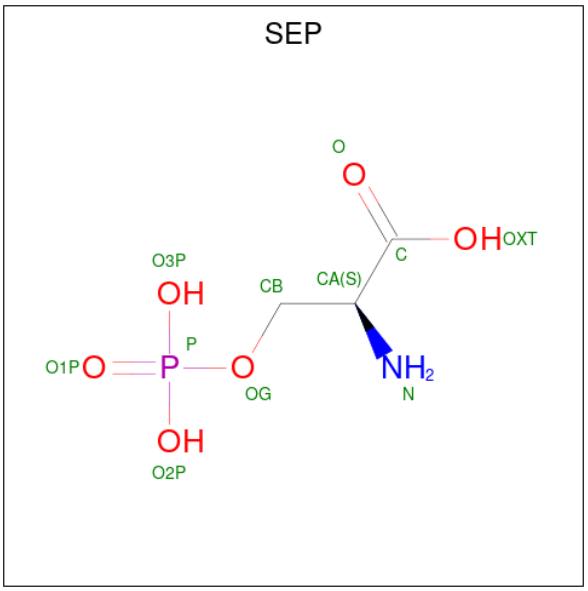
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	MET	-	expression tag	UNP P21707
B	270	MET	-	expression tag	UNP P21707

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

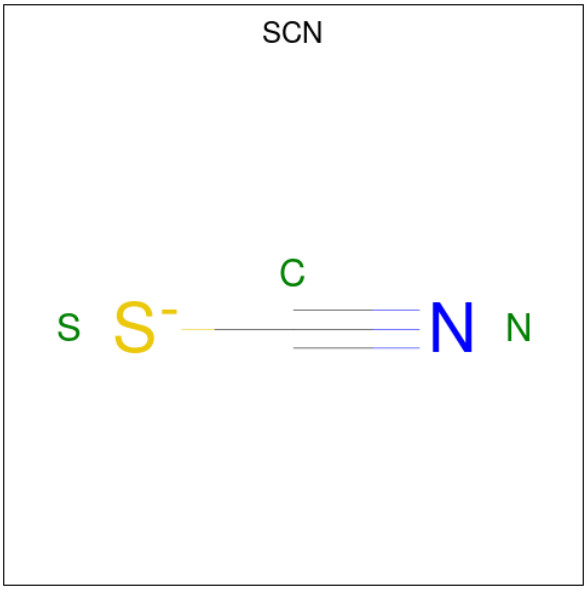
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	4	4	4	0	0
2	B	3	3	3	0	0

- Molecule 3 is PHOSPHOSERINE (three-letter code: SEP) (formula: $C_3H_8NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	11	3	1	6	1	0	0
			Total	C	N	O	P		
3	B	1	11	3	1	6	1	0	0

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
4	A	1	3	1	1	1	0	0
			Total	C	N	S		
4	A	1	3	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
4	B	1	3	1	1	1	0	0
			Total	C	N	S		
4	B	1	3	1	1	1	0	0
			Total	C	N	S		
4	B	1	3	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	131	131	131	0	0
			Total	O		
5	B	125	125	125	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.00Å 97.00Å 89.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.50 – 1.50	Depositor
% Data completeness (in resolution range)	100.0 (44.50-1.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.87 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.204	Depositor
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.305	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2713	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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 77.53 % 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 8.3477e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

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

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	0.43	0/1231	0.62	0/1660
1	B	0.42	0/1228	0.61	0/1658
All	All	0.42	0/2459	0.62	0/3318

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1208	0	1245	13	0
1	B	1205	0	1241	15	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	11	0	5	0	0
3	B	11	0	5	0	0
4	A	6	0	0	0	0
4	B	9	0	0	0	0
5	A	131	0	0	0	0
5	B	125	0	0	2	0
All	All	2713	0	2496	28	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 6.

All (28) 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:B:315:HIS:HB3	1:B:317:MET:HE3	1.33	1.06
1:B:315:HIS:HB3	1:B:317:MET:CE	1.84	1.05
1:B:317:MET:SD	1:B:322:ARG:HG2	2.19	0.82
1:B:416:MET:HA	1:B:416:MET:HE2	1.70	0.73
1:A:317[B]:MET:SD	1:A:322:ARG:HG2	2.32	0.69
1:B:315:HIS:HB3	1:B:317:MET:HE2	1.71	0.67
1:A:318:GLN:CG	1:A:355[A]:VAL:HG12	2.27	0.65
1:B:409:VAL:CG2	1:B:412:GLU:HG3	2.29	0.62
1:B:416:MET:HA	1:B:416:MET:CE	2.30	0.62
1:B:409:VAL:HG23	1:B:412:GLU:HG3	1.82	0.60
1:B:315:HIS:HD2	5:B:2035:HOH:O	1.91	0.53
1:B:418:ALA:O	1:B:419:VAL:HG22	2.10	0.50
1:A:318:GLN:NE2	1:A:351:GLN:OE1	2.34	0.50
1:A:318:GLN:HG2	1:A:355[A]:VAL:HG12	1.95	0.48
1:A:318:GLN:HG3	1:A:355[A]:VAL:HG12	1.97	0.47
1:A:316:LEU:CD1	1:A:355[B]:VAL:HG13	2.44	0.47
1:B:315:HIS:CD2	5:B:2035:HOH:O	2.66	0.46
1:A:316:LEU:HD23	1:A:324:LYS:HD2	1.98	0.46
1:A:316:LEU:HD12	1:A:355[B]:VAL:HG13	1.97	0.46
1:B:310:PRO:HD2	1:B:331:LYS:O	2.19	0.43
1:A:379:GLY:HA2	1:A:390:TRP:CD2	2.54	0.43
1:B:310:PRO:HA	1:B:362:LEU:O	2.18	0.43
1:A:310:PRO:HA	1:A:362:LEU:O	2.19	0.42
1:A:318:GLN:HB2	1:A:323:LEU:HD11	2.00	0.42
1:B:302:MET:HG3	1:B:373:ILE:HG12	2.02	0.42
1:A:316:LEU:CD2	1:A:324:LYS:HD2	2.50	0.41
1:A:302:MET:HG3	1:A:373:ILE:HG12	2.02	0.40
1:B:315:HIS:CB	1:B:317:MET:HE2	2.48	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 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	127/135 (94%)	127 (100%)	0	100	100
1	B	134/135 (99%)	134 (100%)	0	100	100
All	All	261/270 (97%)	261 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	315	HIS

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.