wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 07:01 AM EDT

PDB ID	:	3HN8
Title	:	Crystal structure of synaptotagmin
Authors	:	Strop, P.; Vrljic, M.; Ernst, J.; Brunger, A.T.
Deposited on	:	2009-05-30
Resolution	:	3.50 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 (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 (1)) were used in the production of this report:

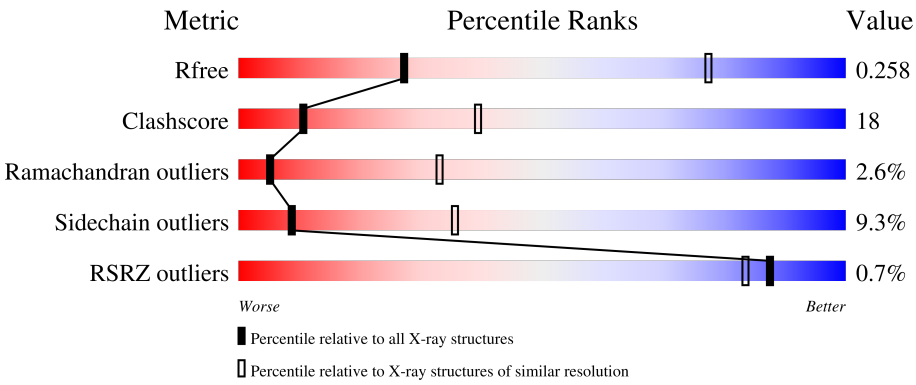
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 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))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	296	54% 35% • 6%
1	B	296	% 55% 34% 5% 6%
1	C	296	% 56% 34% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6672 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	279	2217	1417	385	409	6	0	0	0
1	B	279	2217	1417	385	409	6	0	0	0
1	C	279	2217	1417	385	409	6	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	6	6	6	0	0
2	B	6	6	6	0	0
2	C	6	6	6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

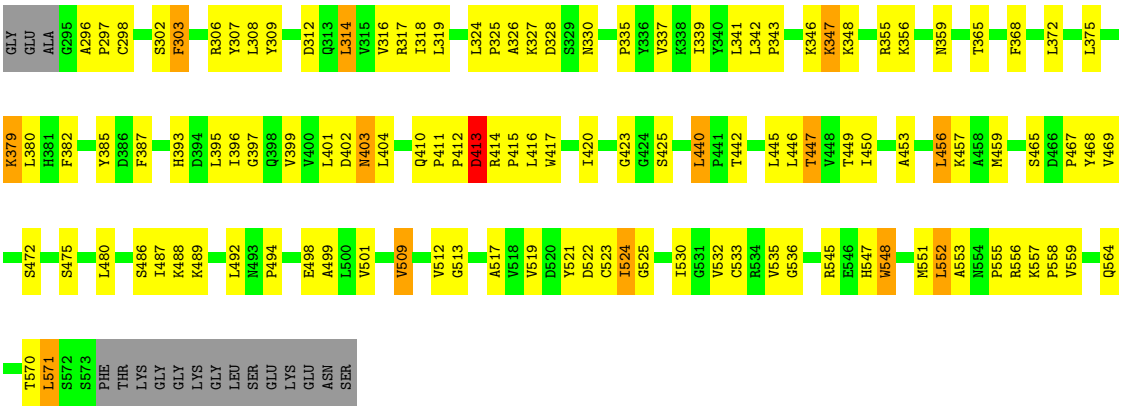
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

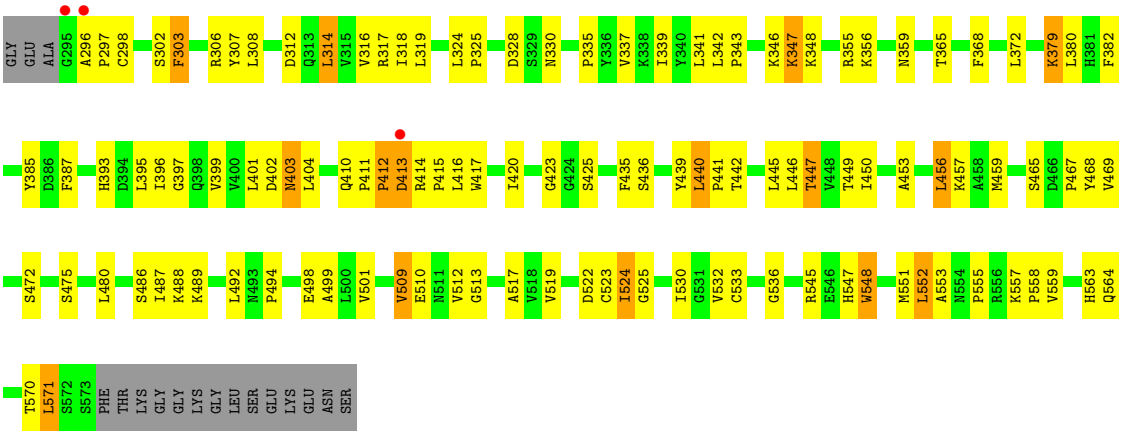
• Molecule 1: Synaptotagmin-3

Chain A:



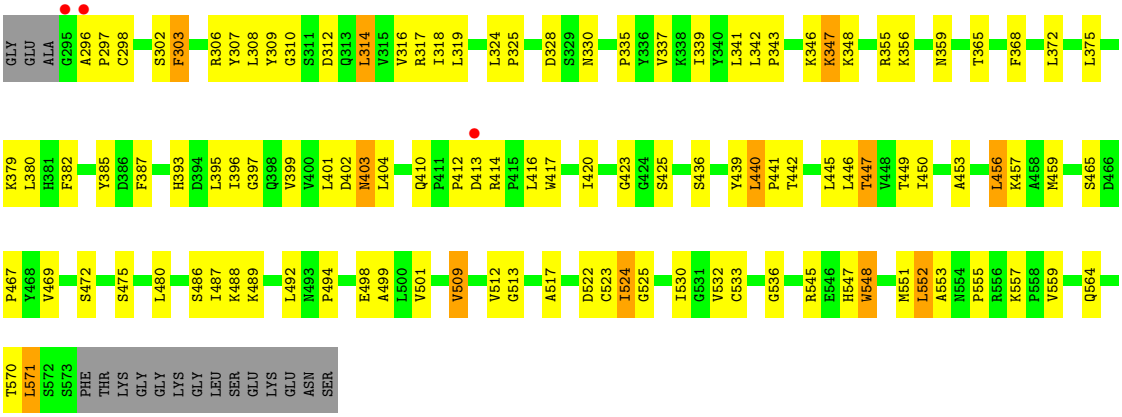
• Molecule 1: Synaptotagmin-3

Chain B:



• Molecule 1: Synaptotagmin-3

Chain C:


GLY
GLU
ALA
G295
A296
P297
C298
S302
F303
R306
Y307
L308
Y309
G310
S311
D312
Q313
L314
V315
V316
R317
I318
L319
L324
P325
D328
S329
N330
P335
Y336
V337
K338
I339
Y340
L341
L342
P343
K346
K347
K348
R355
K356
N359
T365
F368
L372
L375
K379
L380
H381
F382
Y385
D386
F387
H393
D394
L395
I396
G397
Q398
V399
V400
L401
D402
M403
L404
Q410
P411
P412
D413
R414
P415
L416
W417
I420
G423
G424
S425
S436
Y439
L440
P441
T442
L445
L446
T447
V448
T449
I450
A453
L456
K457
A458
M459
S465
D466
P467
Y468
V469
S472
S475
L480
S486
I487
K488
K489
L492
N493
P494
E498
A499
L500
V501
V509
V512
G513
A517
D522
C523
I524
G525
I530
G531
V532
C533
G536
R545
E546
H547
W548
M551
L552
A553
N554
P555
R556
K557
P558
V559
Q564
T570
L571
S572
S573
PHE
THR
LYS
GLY
GLY
LYS
GLY
LEU
SER
GLU
LYS
GLU
ASN
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	205.68Å 205.68Å 143.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.50 29.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-3.50) 99.8 (29.82-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 3.47Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.259 0.233 , 0.258	Depositor DCC
R_{free} test set	3930 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	79.4	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.8	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	0.90	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

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

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	0/2268	0.50	0/3076
1	B	0.26	0/2268	0.49	0/3076
1	C	0.27	0/2268	0.50	0/3076
All	All	0.26	0/6804	0.50	0/9228

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	ASP	Peptide

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	2217	0	2228	89	0
1	B	2217	0	2228	82	0
1	C	2217	0	2228	84	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	6672	0	6684	246	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 18.

The worst 5 of 246 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:556:ARG:HG3	1:C:310:GLY:HA2	1.38	1.01
1:A:556:ARG:HB2	1:C:310:GLY:H	1.46	0.80
1:A:556:ARG:CG	1:C:310:GLY:HA2	2.10	0.80
1:B:303:PHE:HA	1:B:319:LEU:HG	1.65	0.79
1:A:303:PHE:HA	1:A:319:LEU:HG	1.65	0.78

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	277/296 (94%)	234 (84%)	36 (13%)	7 (2%)	5 34
1	B	277/296 (94%)	231 (83%)	38 (14%)	8 (3%)	4 31
1	C	277/296 (94%)	234 (84%)	36 (13%)	7 (2%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	831/888 (94%)	699 (84%)	110 (13%)	22 (3%)	5 33

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	LYS
1	A	524	ILE
1	B	347	LYS
1	B	524	ILE
1	C	347	LYS

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	244/256 (95%)	220 (90%)	24 (10%)	8 33
1	B	244/256 (95%)	222 (91%)	22 (9%)	9 37
1	C	244/256 (95%)	222 (91%)	22 (9%)	9 37
All	All	732/768 (95%)	664 (91%)	68 (9%)	9 35

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	440	LEU
1	C	446	LEU
1	C	548	TRP
1	B	303	PHE
1	A	571	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 21 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	279/296 (94%)	-0.51	0	100	100	54, 79, 141, 221	0
1	B	279/296 (94%)	-0.40	3 (1%)	80	75	54, 89, 160, 218	0
1	C	279/296 (94%)	-0.46	3 (1%)	80	75	53, 78, 147, 230	0
All	All	837/888 (94%)	-0.46	6 (0%)	87	83	53, 82, 148, 230	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	GLY	5.0
1	C	295	GLY	4.6
1	C	413	ASP	2.5
1	B	296	ALA	2.2
1	C	296	ALA	2.1

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 monosaccharides 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(Å^2)	Q<0.9
2	CA	A	603	1/1	0.87	0.08	79,79,79,79	0
2	CA	C	602	1/1	0.87	0.10	64,64,64,64	0
2	CA	B	606	1/1	0.88	0.08	57,57,57,57	0
2	CA	C	606	1/1	0.88	0.10	35,35,35,35	0
2	CA	B	603	1/1	0.91	0.08	76,76,76,76	0
2	CA	B	601	1/1	0.91	0.07	50,50,50,50	0
2	CA	B	605	1/1	0.92	0.06	51,51,51,51	0
2	CA	C	601	1/1	0.92	0.17	50,50,50,50	0
2	CA	C	603	1/1	0.93	0.15	98,98,98,98	0
2	CA	A	601	1/1	0.94	0.10	50,50,50,50	0
2	CA	A	602	1/1	0.95	0.07	51,51,51,51	0
2	CA	A	606	1/1	0.95	0.15	57,57,57,57	0
2	CA	A	600	1/1	0.96	0.15	58,58,58,58	0
2	CA	C	605	1/1	0.97	0.13	65,65,65,65	0
2	CA	A	605	1/1	0.97	0.12	55,55,55,55	0
3	ZN	B	700	1/1	0.97	0.10	74,74,74,74	0
2	CA	B	602	1/1	0.98	0.06	52,52,52,52	0
2	CA	B	600	1/1	0.98	0.12	53,53,53,53	0
2	CA	C	600	1/1	0.98	0.12	51,51,51,51	0
3	ZN	C	700	1/1	0.98	0.09	58,58,58,58	0
3	ZN	A	700	1/1	0.99	0.10	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.