



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 02:06 PM EST

PDB ID : 6X03
Title : Nup84-Nup133 (aa521-1157) from *S. cerevisiae* bound by VHH-SAN8 and VHH-SAN9
Authors : Nordeen, S.A.; Schwartz, T.U.
Deposited on : 2020-05-15
Resolution : 7.30 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 ⓘ 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	:	2.14.6
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)	:	2.14.6

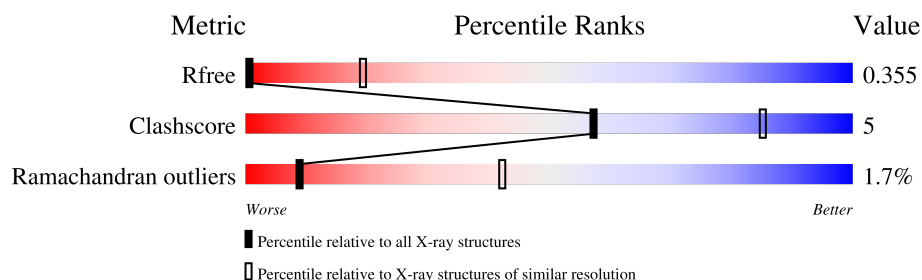
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.30 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	726	
2	B	643	
3	C	131	
4	D	128	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7091 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 Nucleoporin NUP84.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	0	0	0
			3234	1934	650	650			

- Molecule 2 is a protein called Nucleoporin NUP133.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	602	Total	C	N	O	0	0	0
			2993	1789	602	602			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	515	MET	-	expression tag	UNP P36161
B	516	ALA	-	expression tag	UNP P36161
B	517	ASP	-	expression tag	UNP P36161
B	518	PRO	-	expression tag	UNP P36161
B	519	GLY	-	expression tag	UNP P36161
B	520	PHE	-	expression tag	UNP P36161

- Molecule 3 is a protein called VHH-SAN8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	90	Total	C	N	O	0	0	0
			440	260	90	90			

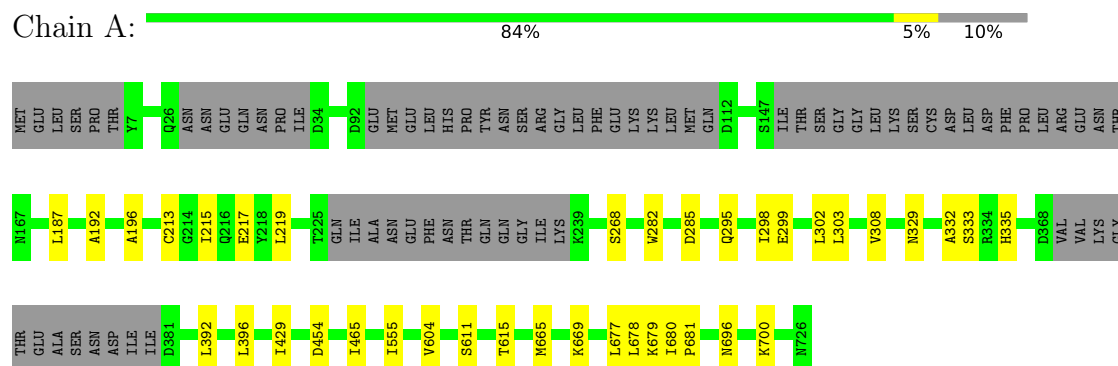
- Molecule 4 is a protein called VHH-SAN9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	87	Total	C	N	O	0	0	0
			424	250	87	87			

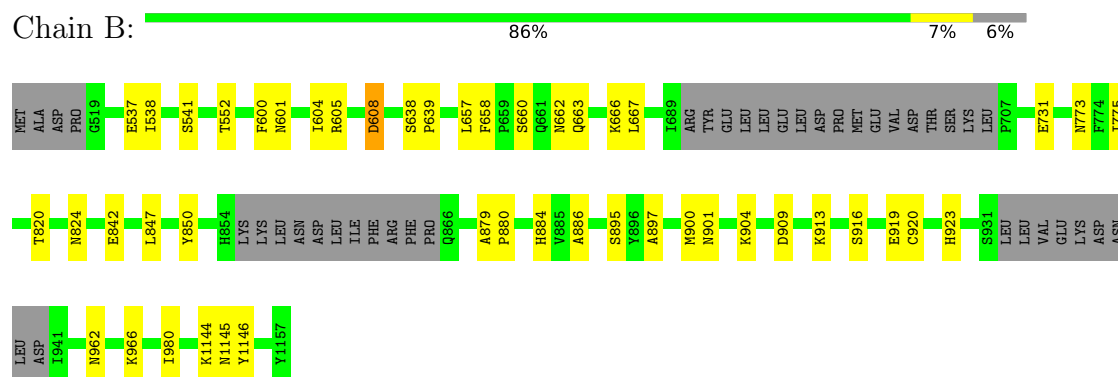
3 Residue-property plots [i](#)

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. 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. 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.

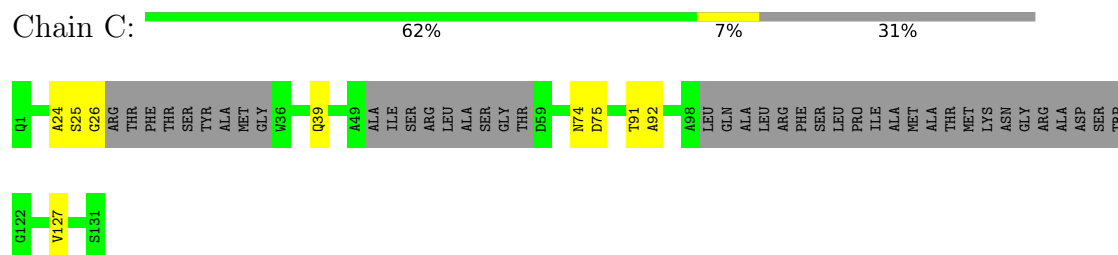
• Molecule 1: Nucleoporin NUP84



• Molecule 2: Nucleoporin NUP133



• Molecule 3: VHH-SAN8



• Molecule 4: VHH-SAN9



Q1	V2	Q3	G26	GLY	THR	LEU	SER	THR	THR	LEU	ALA	MET	GLY	W36	A49	ARG	ILE	GLY	TRP	THR	ASN	GLY	ASP	THR	G59	D73	ASN	VAL	LYS	N77	T98	ARG	ARG	PRO	TYR	GLY	SER	THR	LEU	TYR	PRO	PRO	ASN	THR	GLU	SER	ALA	HIS	ASP	ASN	TRP	G119	S128
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.25Å 295.20Å 295.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.80 – 7.30 147.80 – 7.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (147.80-7.30) 99.7 (147.80-7.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 7.44Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.335 , 0.353 0.335 , 0.355	Depositor DCC
R_{free} test set	936 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	763.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.62 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7091	wwPDB-VP
Average B, all atoms (Å ²)	668.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	0.24	0/3228	0.43	0/4500
2	B	0.26	0/2989	0.49	1/4168 (0.0%)
3	C	0.25	0/436	0.47	0/598
4	D	0.34	0/419	0.55	0/572
All	All	0.25	0/7072	0.46	1/9838 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	658	PHE	C-N-CA	7.67	154.20	122.00

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	3234	0	1392	18	0
2	B	2993	0	1244	27	0
3	C	440	0	211	4	0
4	D	424	0	202	4	0
All	All	7091	0	3049	50	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 5.

All (50) 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)
2:B:662:ASN:O	2:B:666:LYS:CB	1.83	1.25
1:A:298:ILE:O	1:A:302:LEU:CB	1.99	1.10
2:B:662:ASN:O	2:B:666:LYS:N	1.97	0.96
1:A:329:ASN:CB	4:D:77:ASN:N	2.35	0.89
2:B:537:GLU:O	2:B:541:SER:O	1.94	0.86
2:B:663:GLN:O	2:B:667:LEU:N	2.08	0.85
1:A:282:TRP:CB	1:A:335:HIS:CB	2.57	0.82
1:A:696:ASN:HA	1:A:700:LYS:HA	1.61	0.80
2:B:662:ASN:O	2:B:666:LYS:CA	2.30	0.78
1:A:332:ALA:O	4:D:73:ASP:C	2.23	0.76
2:B:601:ASN:O	2:B:605:ARG:N	2.18	0.75
1:A:333:SER:CB	4:D:73:ASP:CB	2.64	0.75
1:A:268:SER:O	1:A:295:GLN:CB	2.34	0.75
1:A:192:ALA:O	1:A:196:ALA:N	2.20	0.73
1:A:299:GLU:O	1:A:303:LEU:CB	2.42	0.67
2:B:962:ASN:O	2:B:966:LYS:CB	2.45	0.65
2:B:847:LEU:O	2:B:850:TYR:N	2.31	0.64
2:B:657:LEU:O	2:B:660:SER:O	2.18	0.61
2:B:662:ASN:CB	2:B:731:GLU:CB	2.79	0.61
2:B:919:GLU:O	2:B:923:HIS:N	2.32	0.61
1:A:298:ILE:O	1:A:302:LEU:N	2.36	0.59
1:A:213:CYS:O	1:A:217:GLU:N	2.34	0.59
2:B:604:ILE:O	2:B:608:ASP:N	2.27	0.58
2:B:847:LEU:O	2:B:850:TYR:CB	2.52	0.57
2:B:900:MET:O	2:B:904:LYS:N	2.30	0.56
3:C:24:ALA:O	3:C:26:GLY:N	2.39	0.56
1:A:392:LEU:O	1:A:396:LEU:N	2.36	0.55
2:B:897:ALA:O	2:B:901:ASN:N	2.39	0.55
2:B:886:ALA:HB1	2:B:901:ASN:CB	2.37	0.55
3:C:74:ASN:O	3:C:75:ASP:CB	2.55	0.54
2:B:916:SER:O	2:B:920:CYS:N	2.28	0.53
1:A:215:ILE:O	1:A:219:LEU:N	2.44	0.51
2:B:1144:LYS:O	2:B:1146:TYR:N	2.43	0.51
2:B:820:THR:O	2:B:824:ASN:N	2.44	0.51
2:B:657:LEU:C	2:B:660:SER:H	2.13	0.51
2:B:600:PHE:O	2:B:604:ILE:N	2.37	0.49
2:B:663:GLN:O	2:B:667:LEU:CB	2.61	0.49
1:A:665:MET:O	1:A:669:LYS:N	2.46	0.48
2:B:538:ILE:HA	2:B:541:SER:O	2.14	0.48
2:B:909:ASP:HA	2:B:913:LYS:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:O	1:A:679:LYS:N	2.45	0.45
3:C:91:THR:HA	3:C:127:VAL:O	2.16	0.45
1:A:611:SER:O	1:A:615:THR:N	2.44	0.44
2:B:884:HIS:C	2:B:886:ALA:H	2.21	0.44
2:B:657:LEU:O	2:B:660:SER:N	2.43	0.43
2:B:847:LEU:C	2:B:850:TYR:H	2.21	0.43
4:D:36:TRP:N	4:D:49:ALA:O	2.51	0.43
1:A:187:LEU:O	1:A:192:ALA:HB3	2.19	0.42
3:C:39:GLN:O	3:C:92:ALA:HB1	2.21	0.41
1:A:298:ILE:O	1:A:302:LEU:CA	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	638/726 (88%)	576 (90%)	52 (8%)	10 (2%)	9	44
2	B	594/643 (92%)	520 (88%)	62 (10%)	12 (2%)	7	38
3	C	82/131 (63%)	76 (93%)	5 (6%)	1 (1%)	13	50
4	D	77/128 (60%)	74 (96%)	2 (3%)	1 (1%)	12	48
All	All	1391/1628 (85%)	1246 (90%)	121 (9%)	24 (2%)	9	42

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	638	SER
2	B	639	PRO
2	B	773	ASN
2	B	879	ALA
2	B	880	PRO

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	308	VAL
1	A	604	VAL
2	B	552	THR
2	B	980	ILE
2	B	1145	ASN
3	C	25	SER
4	D	3	GLN
2	B	775	ILE
2	B	895	SER
1	A	429	ILE
1	A	678	LEU
2	B	608	ASP
2	B	842	GLU
1	A	465	ILE
1	A	555	ILE
1	A	454	ASP
1	A	681	PRO
1	A	680	ILE

5.3.2 Protein sidechains [i](#)

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

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](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.