



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:16 PM EDT

PDB ID : 6X06
Title : Nup120 (aa1-757) from *S. cerevisiae* bound by VHH-SAN11
Authors : Knockenhauer, K.E.; Nordeen, S.A.; Schwartz, T.U.
Deposited on : 2020-05-15
Resolution : 4.27 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

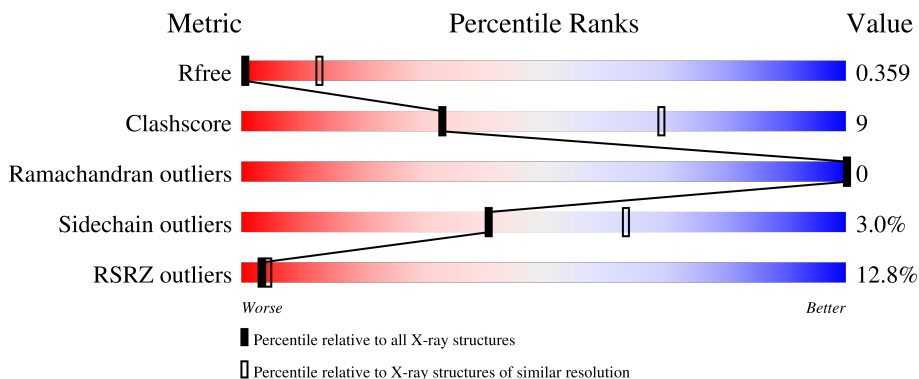
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.27 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	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)
RSRZ outliers	127900	1072 (4.80-3.70)

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 $\leq 5\%$. 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	758	<p>9% (red), 65% (green), 16% (yellow), 19% (grey)</p>
2	K	124	<p>22% (red), 72% (green), 25% (yellow), .. (grey)</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5650 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 NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	615	4803	3109	756	924	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P35729

- Molecule 2 is a protein called VHH-SAN11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	121	847	528	150	166	3	0	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	193.17Å 193.17Å 78.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.65 – 4.27 83.65 – 4.27	Depositor EDS
% Data completeness (in resolution range)	98.4 (83.65-4.27) 98.4 (83.65-4.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.30Å)	Xtrriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.334 , 0.359 0.334 , 0.359	Depositor DCC
R_{free} test set	1154 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	196.9	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 227.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5650	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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	0.25	0/4900	0.44	0/6677
2	K	0.27	0/863	0.51	0/1173
All	All	0.25	0/5763	0.45	0/7850

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	4803	0	4557	70	0
2	K	847	0	734	27	0
All	All	5650	0	5291	94	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 9.

All (94) 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:439:ASP:OD2	1:A:442:TYR:HB3	1.20	1.28
1:A:439:ASP:OD2	1:A:442:TYR:CB	2.02	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:CB	2:K:29:PHE:CD1	2.52	0.92
1:A:438:GLU:CB	2:K:29:PHE:CE1	2.65	0.80
2:K:123:VAL:HG12	2:K:124:SER:N	1.97	0.78
1:A:433:ILE:HG13	2:K:105:VAL:HG13	1.66	0.77
2:K:98:ALA:O	2:K:112:TYR:N	2.21	0.72
1:A:351:LEU:HB3	1:A:366:LEU:HB2	1.73	0.70
1:A:439:ASP:O	1:A:443:LEU:HD23	1.90	0.70
1:A:169:VAL:HG12	1:A:171:PRO:HD2	1.72	0.70
2:K:35:GLY:H	2:K:97:ALA:HB3	1.60	0.66
2:K:121:VAL:HG12	2:K:122:THR:N	2.09	0.66
2:K:23:VAL:HG13	2:K:78:THR:HG22	1.76	0.66
1:A:466:TYR:HB3	1:A:470:ILE:HB	1.79	0.65
1:A:62:LEU:HD13	1:A:135:LEU:HD22	1.79	0.65
2:K:123:VAL:CG1	2:K:124:SER:N	2.60	0.64
1:A:108:LEU:HD13	1:A:121:VAL:HG23	1.79	0.64
1:A:391:SER:O	1:A:451:ARG:NH2	2.31	0.64
2:K:123:VAL:HG12	2:K:124:SER:H	1.61	0.64
1:A:616:LEU:HD11	1:A:676:ALA:HB2	1.79	0.64
2:K:104:VAL:HG22	2:K:106:TYR:H	1.63	0.63
1:A:439:ASP:CG	1:A:442:TYR:HB3	2.15	0.63
1:A:169:VAL:HB	1:A:173:PHE:HB3	1.79	0.63
2:K:123:VAL:CG1	2:K:124:SER:H	2.12	0.63
1:A:240:ASN:N	1:A:241:CYS:HA	2.14	0.63
2:K:91:THR:HG23	2:K:121:VAL:HA	1.81	0.63
1:A:19:GLU:HB2	1:A:20:PRO:HD2	1.82	0.62
1:A:54:SER:HA	1:A:73:SER:HB2	1.81	0.61
1:A:427:LEU:HD21	1:A:449:ILE:HG13	1.82	0.60
1:A:623:LEU:HD12	1:A:664:LEU:HD22	1.83	0.60
1:A:100:ALA:O	1:A:124:LYS:N	2.35	0.59
2:K:54:SER:H	2:K:72:ARG:HH21	1.51	0.59
1:A:347:SER:HA	1:A:369:ASN:HA	1.84	0.58
1:A:593:PRO:HG2	1:A:707:SER:HB2	1.85	0.58
1:A:541:PRO:HB2	1:A:544:MET:HG2	1.86	0.57
1:A:291:LEU:HD12	1:A:297:LEU:HD12	1.86	0.57
1:A:435:ALA:HB3	1:A:439:ASP:HB2	1.87	0.56
2:K:121:VAL:CG1	2:K:122:THR:N	2.68	0.56
1:A:608:ASP:HB3	1:A:611:THR:HB	1.87	0.55
1:A:555:LYS:HA	1:A:559:GLU:HB3	1.88	0.55
1:A:16:GLU:HA	1:A:417:THR:HG21	1.88	0.54
1:A:55:GLU:HG2	1:A:104:GLN:HG3	1.89	0.54
2:K:32:TYR:HB2	2:K:99:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TYR:HB3	1:A:673:CYS:HB2	1.91	0.53
1:A:113:VAL:HG12	1:A:114:GLU:HG3	1.89	0.53
1:A:288:VAL:HG11	1:A:351:LEU:HD21	1.91	0.52
1:A:413:SER:OG	1:A:672:LYS:NZ	2.43	0.52
2:K:88:PRO:HA	2:K:122:THR:OG1	2.10	0.51
2:K:109:HIS:O	2:K:109:HIS:ND1	2.44	0.50
2:K:7:THR:HG22	2:K:8:GLY:H	1.76	0.49
1:A:298:PHE:CD1	1:A:323:LEU:HD21	2.47	0.49
1:A:71:HIS:CE1	1:A:478:PRO:HA	2.48	0.49
1:A:632:GLN:O	1:A:636:THR:HG23	2.13	0.48
1:A:554:PHE:O	1:A:559:GLU:N	2.46	0.48
1:A:244:LYS:HB3	1:A:253:LEU:HD23	1.96	0.47
1:A:364:GLN:NE2	1:A:380:GLU:OE2	2.41	0.47
1:A:11:LEU:HA	1:A:613:ILE:HD13	1.96	0.47
2:K:121:VAL:CG1	2:K:122:THR:H	2.28	0.46
1:A:335:VAL:HG12	1:A:337:THR:HG23	1.97	0.46
1:A:59:CYS:SG	1:A:67:TYR:HB3	2.55	0.46
2:K:14:ALA:N	2:K:123:VAL:O	2.46	0.45
1:A:243:LEU:HG	1:A:257:TYR:HB2	1.99	0.45
1:A:333:ASP:OD1	1:A:334:LEU:N	2.48	0.45
1:A:336:LEU:HD13	1:A:351:LEU:HD13	1.98	0.44
1:A:474:ASN:HA	1:A:481:HIS:HD1	1.83	0.44
1:A:66:GLU:HG2	1:A:139:PHE:CE1	2.52	0.44
1:A:79:LEU:HB2	1:A:95:ILE:O	2.18	0.44
1:A:291:LEU:HB3	1:A:297:LEU:HB2	2.00	0.44
1:A:108:LEU:HD12	1:A:109:THR:N	2.32	0.44
1:A:386:LEU:HD22	1:A:621:GLN:HA	2.00	0.44
1:A:583:LEU:O	1:A:587:ILE:HG12	2.18	0.44
1:A:626:HIS:ND1	1:A:710:TYR:OH	2.33	0.43
1:A:348:TYR:HB2	1:A:370:ASP:HA	1.99	0.43
1:A:28:VAL:HG23	1:A:98:PRO:HD3	2.01	0.43
1:A:336:LEU:HD11	1:A:349:LEU:HD13	2.00	0.43
1:A:248:LEU:HA	1:A:250:SER:N	2.34	0.42
1:A:642:LEU:HD13	1:A:647:PHE:CE2	2.54	0.42
2:K:60:TYR:OH	2:K:70:ILE:HG22	2.19	0.42
1:A:187:LYS:HD2	1:A:187:LYS:HA	1.80	0.42
1:A:555:LYS:O	1:A:559:GLU:HG2	2.19	0.42
2:K:35:GLY:N	2:K:97:ALA:HB3	2.31	0.42
2:K:83:MET:HB3	2:K:86:LEU:HD21	2.02	0.42
1:A:288:VAL:HG23	1:A:336:LEU:HD22	2.02	0.42
1:A:298:PHE:HZ	1:A:353:VAL:HG11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD11	1:A:469:GLU:HA	2.01	0.42
2:K:15:GLY:N	2:K:86:LEU:O	2.42	0.42
1:A:248:LEU:HA	1:A:249:THR:C	2.40	0.41
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.82	0.41
2:K:121:VAL:HG12	2:K:122:THR:H	1.84	0.41
1:A:420:PHE:HA	1:A:450:LEU:HD21	2.03	0.41
2:K:32:TYR:HB2	2:K:99:PRO:CD	2.50	0.41
1:A:328:ILE:HD13	1:A:328:ILE:HA	1.97	0.40
1:A:176:VAL:HG13	1:A:184:LEU:HB3	2.03	0.40
1:A:398:VAL:HG13	1:A:666:ASN:ND2	2.37	0.40

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	595/758 (78%)	546 (92%)	49 (8%)	0	100	100
2	K	117/124 (94%)	103 (88%)	14 (12%)	0	100	100
All	All	712/882 (81%)	649 (91%)	63 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	525/711 (74%)	511 (97%)	14 (3%)	44	66
2	K	73/97 (75%)	69 (94%)	4 (6%)	21	50
All	All	598/808 (74%)	580 (97%)	18 (3%)	41	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	111	GLN
1	A	120	ASN
1	A	236	VAL
1	A	249	THR
1	A	278	GLU
1	A	440	GLU
1	A	472	LEU
1	A	476	PHE
1	A	483	LEU
1	A	519	THR
1	A	567	LEU
1	A	664	LEU
1	A	695	TYR
2	K	47	PHE
2	K	96	CYS
2	K	112	TYR
2	K	114	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	369	ASN
1	A	375	ASN
2	K	120	GLN

5.3.3 RNA ⓘ

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

6.1 Protein, DNA and RNA chains

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	615/758 (81%)	0.56	67 (10%) 5 6	144, 238, 310, 359	0
2	K	121/124 (97%)	1.03	27 (22%) 0 1	182, 248, 301, 339	0
All	All	736/882 (83%)	0.64	94 (12%) 3 4	144, 241, 310, 359	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	10	GLY	10.4
2	K	119	THR	8.7
2	K	120	GLN	6.6
1	A	341	GLU	6.3
1	A	254	ILE	5.6
1	A	340	LEU	5.6
1	A	65	SER	5.6
1	A	438	GLU	5.3
2	K	30	ARG	5.1
2	K	118	GLY	4.8
1	A	400	LYS	4.8
1	A	225	SER	4.5
2	K	34	MET	4.4
2	K	11	LEU	4.3
2	K	51	ILE	4.1
2	K	29	PHE	4.0
1	A	361	SER	3.9
2	K	60	TYR	3.9
1	A	280	LEU	3.8
1	A	99	ASN	3.7
1	A	372	SER	3.6
1	A	139	PHE	3.6
1	A	164	HIS	3.6
2	K	70	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	3.6
1	A	255	GLN	3.5
1	A	320	PRO	3.5
2	K	32	TYR	3.5
2	K	121	VAL	3.5
1	A	692	PHE	3.4
1	A	251	PHE	3.3
1	A	243	LEU	3.3
1	A	318	ASN	3.2
1	A	245	ILE	3.2
1	A	100	ALA	3.2
1	A	324	SER	3.1
2	K	94	TYR	3.1
1	A	66	GLU	3.1
1	A	278	GLU	3.0
1	A	187	LYS	3.0
1	A	226	CYS	3.0
2	K	117	GLN	3.0
1	A	373	PHE	3.0
2	K	97	ALA	2.9
1	A	296	GLY	2.9
1	A	334	LEU	2.9
1	A	299	GLN	2.8
1	A	377	GLU	2.8
1	A	244	LYS	2.8
1	A	316	GLN	2.8
1	A	237	LEU	2.8
1	A	154	ASN	2.8
2	K	45	ARG	2.8
1	A	321	THR	2.7
1	A	298	PHE	2.7
2	K	19	ARG	2.7
1	A	253	LEU	2.7
1	A	290	LEU	2.7
1	A	437	ASN	2.7
2	K	102	GLY	2.6
1	A	371	GLU	2.6
1	A	227	LYS	2.6
1	A	252	THR	2.6
1	A	28	VAL	2.6
1	A	102	MET	2.6
2	K	77	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	2.5
2	K	124	SER	2.5
2	K	12	VAL	2.5
1	A	300	MET	2.5
1	A	432	ILE	2.4
1	A	261	SER	2.4
2	K	58	THR	2.4
1	A	460	ALA	2.3
1	A	323	LEU	2.3
1	A	353	VAL	2.3
1	A	364	GLN	2.3
1	A	346	ALA	2.3
2	K	101	GLY	2.3
1	A	171	PRO	2.2
1	A	436	HIS	2.2
2	K	9	GLY	2.2
1	A	473	VAL	2.2
1	A	672	LYS	2.2
1	A	593	PRO	2.2
1	A	454	LYS	2.2
1	A	345	GLU	2.2
2	K	33	THR	2.2
1	A	276	VAL	2.2
1	A	236	VAL	2.1
1	A	463	ILE	2.1
1	A	63	SER	2.1
1	A	228	LEU	2.1
2	K	61	GLY	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.