



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:43 am GMT

PDB ID : 5C3L
Title : Structure of the metazoan Nup62.Nup58.Nup54 nucleoporin complex.
Authors : Chug, H.; Trakhanov, S.; Hulsmann, B.B.; Pleiner, T.; Gorlich, D.
Deposited on : 2015-06-17
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

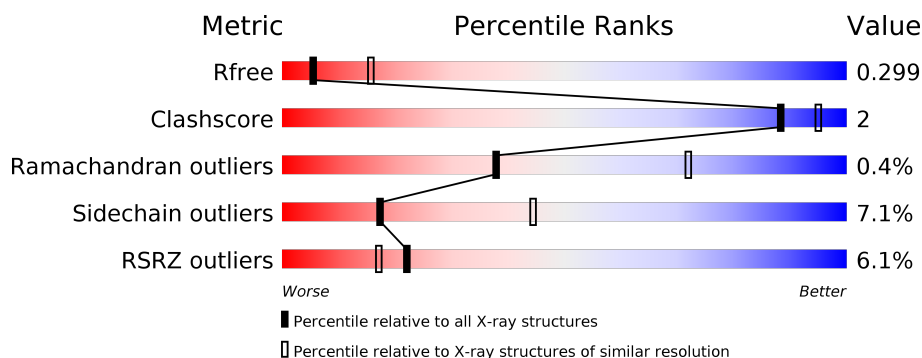
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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. 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	333	
2	B	142	
3	C	150	
4	D	119	
5	H	14	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8051 atoms, of which 4031 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 Nup54.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	134	2214	682	1128	195	205	4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLY	-	expression tag	UNP K9ZTJ6
A	142	SER	-	expression tag	UNP K9ZTJ6
A	143	MET	-	expression tag	UNP K9ZTJ6
A	144	GLY	-	expression tag	UNP K9ZTJ6
A	145	THR	-	expression tag	UNP K9ZTJ6

- Molecule 2 is a protein called Nucleoporin Nup58.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	124	2018	628	1015	176	196	3	0	0	0

- Molecule 3 is a protein called Nucleoporin Nup62.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	122	2038	636	1011	180	208	3	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	339	ALA	-	expression tag	UNP Q91349
C	340	GLY	-	expression tag	UNP Q91349
C	341	THR	-	expression tag	UNP Q91349

- Molecule 4 is a protein called Nanobody Nb15.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	112	Total	C	H	N	O	S	0	0	0
			1642	515	808	148	167	4			

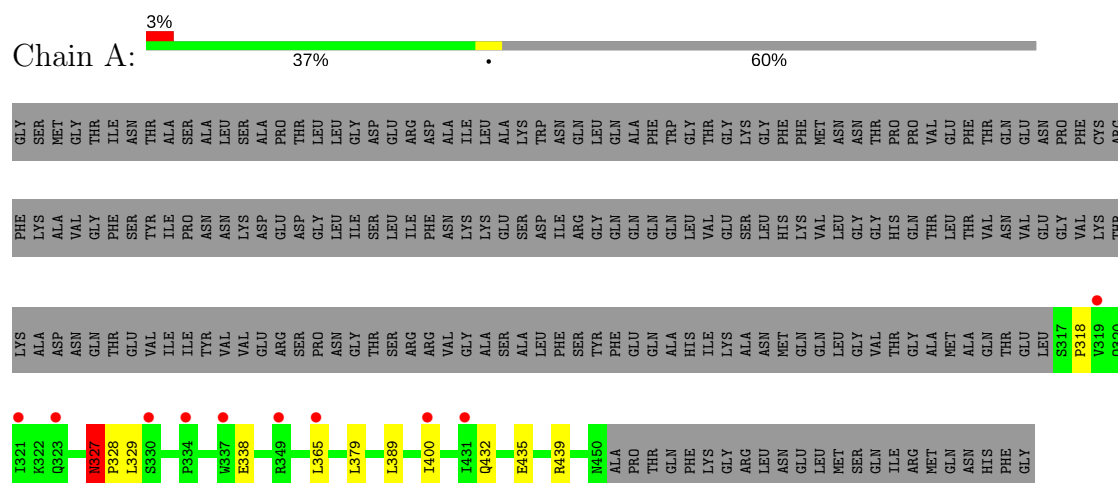
- Molecule 5 is a protein called Part of Nup54 N-terminus with weak electron density, built as poly-alanine..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	14	Total	C	H	N	O	0	0	0
			139	42	69	14	14			

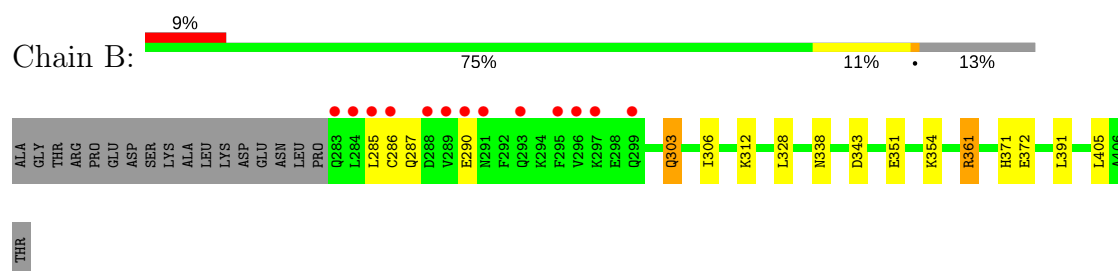
3 Residue-property plots [i](#)

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.

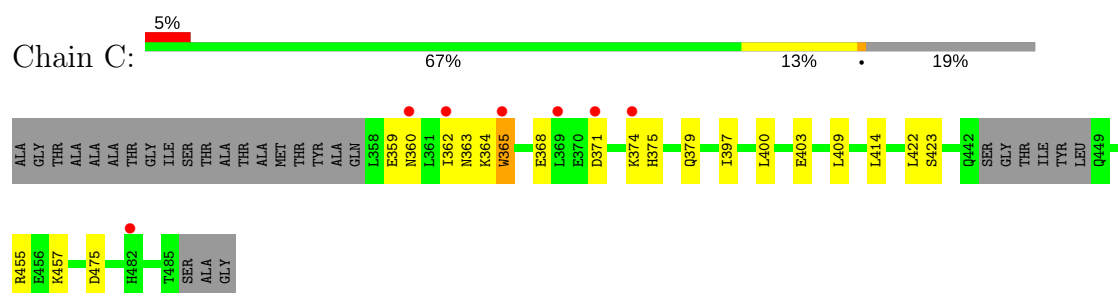
• Molecule 1: Nup54



• Molecule 2: Nucleoporin Nup58



• Molecule 3: Nucleoporin Nup62



• Molecule 4: Nanobody Nb15

Chain D:

87%

7%

6%



- Molecule 5: Part of Nup54 N-terminus with weak electron density, built as poly-alanine.

Chain H:

86%

14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.57Å 167.57Å 142.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.88 – 2.90 50.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.88-2.90) 99.7 (50.88-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.265 , 0.301 0.290 , 0.299	Depositor DCC
R_{free} test set	1334 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8051	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	0.33	0/1099	0.49	0/1480
2	B	0.33	0/1014	0.47	0/1363
3	C	0.34	0/1037	0.47	0/1391
4	D	0.41	0/848	0.55	0/1146
All	All	0.35	0/3998	0.49	0/5380

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	1086	1128	1129	7	0
2	B	1003	1015	1018	7	0
3	C	1027	1011	1015	8	0
4	D	834	808	810	3	0
5	H	70	69	17	1	0
All	All	4020	4031	3989	18	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 2.

All (18) 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)
3:C:364:LYS:NZ	3:C:368:GLU:OE2	2.25	0.68
1:A:435:GLU:OE1	3:C:455:ARG:NH1	2.38	0.57
2:B:303:GLN:OE1	3:C:375:HIS:ND1	2.44	0.49
4:D:51:ILE:HD11	4:D:55:GLY:HA2	1.95	0.48
2:B:306:ILE:HG21	3:C:379:GLN:CD	2.33	0.48
2:B:351:GLU:OE2	2:B:354:LYS:NZ	2.32	0.48
1:A:327:ASN:N	1:A:327:ASN:OD1	2.48	0.46
1:A:439:ARG:HH12	3:C:457:LYS:HB3	1.81	0.45
2:B:328:LEU:HD21	3:C:403:GLU:HG3	1.99	0.45
1:A:379:LEU:HD21	3:C:397:ILE:HD13	1.98	0.45
1:A:327:ASN:CB	1:A:328:PRO:CD	2.96	0.44
3:C:362:ILE:HA	3:C:365:TRP:HD1	1.83	0.43
4:D:67:ARG:NH1	4:D:90:ASP:OD2	2.37	0.43
5:H:118:UNK:C	5:H:120:UNK:H	2.31	0.43
1:A:400:ILE:CD1	2:B:338:ASN:HB2	2.49	0.42
1:A:327:ASN:HB3	1:A:328:PRO:CD	2.50	0.41
2:B:361:ARG:NH1	4:D:50:ASP:OD2	2.54	0.41
2:B:371:HIS:CE1	2:B:372:GLU:HG3	2.56	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	132/333 (40%)	122 (92%)	8 (6%)	2 (2%)	12	39
2	B	122/142 (86%)	120 (98%)	2 (2%)	0	100	100
3	C	118/150 (79%)	114 (97%)	4 (3%)	0	100	100
4	D	110/119 (92%)	109 (99%)	1 (1%)	0	100	100
All	All	482/744 (65%)	465 (96%)	15 (3%)	2 (0%)	38	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	PRO
1	A	327	ASN

5.3.2 Protein sidechains ⓘ

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	124/291 (43%)	118 (95%)	6 (5%)	30	64
2	B	111/126 (88%)	101 (91%)	10 (9%)	11	33
3	C	115/131 (88%)	103 (90%)	12 (10%)	8	25
4	D	89/92 (97%)	86 (97%)	3 (3%)	42	76
All	All	439/640 (69%)	408 (93%)	31 (7%)	17	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	329	LEU
1	A	338	GLU
1	A	365	LEU
1	A	389	LEU
1	A	432	GLN
2	B	285	LEU
2	B	286	CYS
2	B	287	GLN
2	B	290	GLU
2	B	303	GLN
2	B	312	LYS
2	B	343	ASP
2	B	361	ARG
2	B	391	LEU
2	B	405	LEU
3	C	359	GLU
3	C	360	ASN
3	C	363	ASN
3	C	365	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	371	ASP
3	C	374	LYS
3	C	400	LEU
3	C	409	LEU
3	C	414	LEU
3	C	422	LEU
3	C	423	SER
3	C	475	ASP
4	D	53	SER
4	D	89	GLU
4	D	96	CYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	134/333 (40%)	0.64	10 (7%) 15 11	55, 93, 140, 150	0
2	B	124/142 (87%)	0.87	13 (10%) 7 5	55, 79, 159, 175	0
3	C	122/150 (81%)	0.51	7 (5%) 24 19	57, 85, 138, 160	0
4	D	112/119 (94%)	0.27	0 100 100	56, 69, 87, 103	0
5	H	0/14	-	-	-	-
All	All	492/758 (64%)	0.58	30 (6%) 22 17	55, 80, 144, 175	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	PHE	6.8
2	B	291	ASN	6.6
3	C	371	ASP	6.6
1	A	323	GLN	6.3
2	B	284	LEU	5.7
2	B	289	VAL	5.5
1	A	349	ARG	5.2
2	B	286	CYS	5.1
3	C	369	LEU	5.0
2	B	293	GLN	4.4
2	B	296	VAL	4.3
2	B	285	LEU	4.1
3	C	362	ILE	3.8
3	C	374	LYS	3.2
2	B	288	ASP	3.0
1	A	431	ILE	3.0
2	B	290	GLU	3.0
1	A	337	TRP	2.9
3	C	482	HIS	2.9
1	A	319	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	297	LYS	2.4
1	A	365	LEU	2.3
1	A	400	ILE	2.3
3	C	365	TRP	2.2
2	B	299	GLN	2.2
1	A	330	SER	2.2
1	A	334	PRO	2.2
2	B	283	GLN	2.2
1	A	321	ILE	2.0
3	C	360	ASN	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 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.