



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:03 PM 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

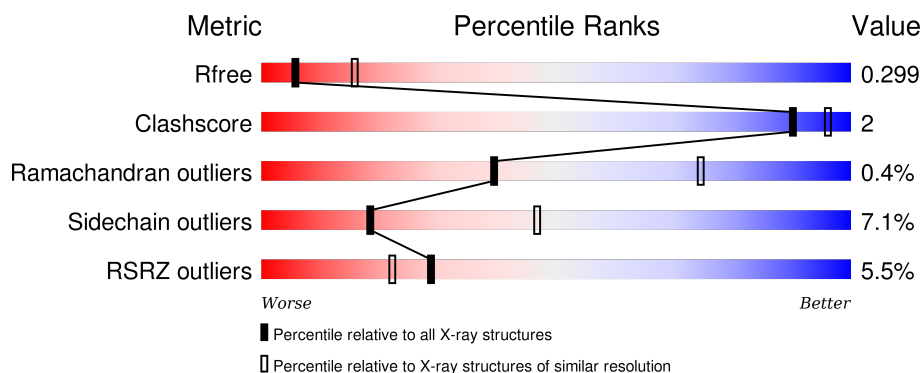
1 Overall quality at a glance ⓘ

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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	<div> <div>2%</div> <div>37%</div> <div>60%</div> </div>
2	B	142	<div> <div>9%</div> <div>75%</div> <div>11%</div> <div>13%</div> </div>
3	C	150	<div> <div>4%</div> <div>67%</div> <div>13%</div> <div>19%</div> </div>
4	D	119	<div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
5	H	14	<div> <div>86%</div> <div>14%</div> </div>

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
1	A	134	Total	C	H	N	O	S	0	0	0
			2214	682	1128	195	205	4			

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
2	B	124	Total	C	H	N	O	S	0	0	0
			2018	628	1015	176	196	3			

- Molecule 3 is a protein called Nucleoporin Nup62.

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

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			

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 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 29540 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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%)	13	42
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%)	39	74

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%)	31	67
2	B	111/126 (88%)	101 (91%)	10 (9%)	12	34
3	C	115/131 (88%)	103 (90%)	12 (10%)	9	26
4	D	89/92 (97%)	86 (97%)	3 (3%)	44	79
All	All	439/640 (69%)	408 (93%)	31 (7%)	18	47

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

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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 [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 carbohydrates 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	134/333 (40%)	0.63	8 (5%) 25 18	55, 93, 140, 150	0
2	B	124/142 (87%)	0.82	13 (10%) 8 5	55, 79, 159, 175	0
3	C	122/150 (81%)	0.49	6 (4%) 33 27	57, 85, 138, 160	0
4	D	112/119 (94%)	0.29	0 100 100	56, 69, 87, 103	0
5	H	0/14	-	-	-	-
All	All	492/758 (64%)	0.57	27 (5%) 29 22	55, 80, 144, 175	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	GLN	6.9
2	B	291	ASN	6.7
2	B	284	LEU	6.2
2	B	295	PHE	6.1
3	C	371	ASP	5.9
1	A	349	ARG	5.3
2	B	286	CYS	5.3
2	B	289	VAL	5.2
3	C	362	ILE	4.2
2	B	285	LEU	4.1
3	C	369	LEU	4.0
2	B	290	GLU	3.4
1	A	319	VAL	3.2
3	C	482	HIS	3.2
2	B	288	ASP	3.2
2	B	296	VAL	3.0
2	B	293	GLN	2.9
3	C	374	LYS	2.9
3	C	360	ASN	2.8
1	A	431	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	337	TRP	2.6
2	B	283	GLN	2.4
1	A	320	GLN	2.3
2	B	299	GLN	2.2
1	A	365	LEU	2.2
1	A	334	PRO	2.1
2	B	297	LYS	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.