Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 08:05 am BST

PDB ID	:	4JNV
Title	:	Crystal structure of the human Nup57CCS3* coiled-coil segment, space group C2
Authors	:	Stuwe, T.; Bley, C.J.; Mayo, D.J.; Hoelz, A.
Deposited on	:	2013-03-15
Resolution	:	1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

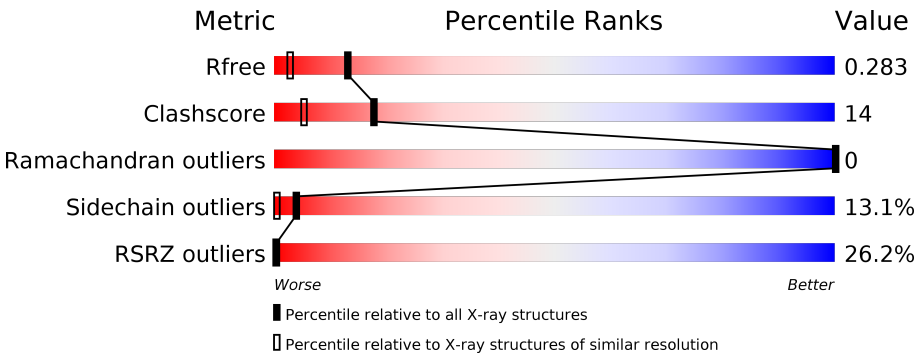
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	40	23%; 45%, 23%, 10%, 23%
1	B	40	15%; 60%, 25%, 15%
1	C	40	20%; 48%, 33%, 20%
1	D	40	25%; 45%, 30%, •, 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2234 atoms, of which 1130 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 p54.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	31	Total C H N O 529 166 270 45 48	0	0	0
1	B	34	Total C H N O Se 595 182 305 50 57 1	0	1	0
1	C	32	Total C H N O 558 175 282 48 53	0	1	0
1	D	31	Total C H N O Se 530 161 273 46 49 1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	SER	-	EXPRESSION TAG	UNP Q7Z3B4
A	484	MSE	LEU	CONFLICT	UNP Q7Z3B4
B	451	SER	-	EXPRESSION TAG	UNP Q7Z3B4
B	484	MSE	LEU	CONFLICT	UNP Q7Z3B4
C	451	SER	-	EXPRESSION TAG	UNP Q7Z3B4
C	484	MSE	LEU	CONFLICT	UNP Q7Z3B4
D	451	SER	-	EXPRESSION TAG	UNP Q7Z3B4
D	484	MSE	LEU	CONFLICT	UNP Q7Z3B4

- Molecule 2 is water.

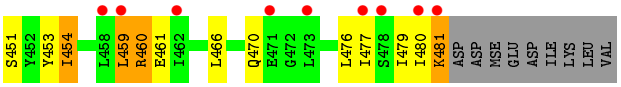
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	14	Total O 14 14	0	0
2	D	5	Total O 5 5	0	0

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.

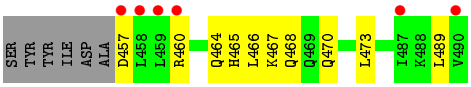
- Molecule 1: Nucleoporin p54

Chain A:



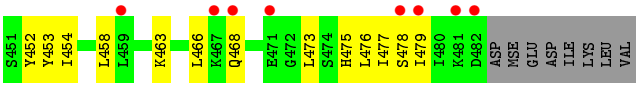
- Molecule 1: Nucleoporin p54

Chain B:



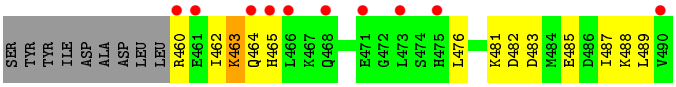
- Molecule 1: Nucleoporin p54

Chain C:



- Molecule 1: Nucleoporin p54

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.51Å 36.62Å 63.18Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	19.81 – 1.85 19.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.81-1.85) 92.8 (19.81-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.237 , 0.277 0.247 , 0.283	Depositor DCC
R_{free} test set	1305 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.49 , 68.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2234	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.05% 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)

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	0.44	0/262	0.49	0/350
1	B	0.40	0/290	0.56	0/384
1	C	0.35	0/279	0.46	0/373
1	D	0.32	0/257	0.50	0/339
All	All	0.38	0/1088	0.50	0/1446

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	259	270	268	17	0
1	B	290	305	301	6	0
1	C	276	282	279	14	0
1	D	257	273	270	11	0
2	A	3	0	0	0	0
2	B	14	0	0	0	0
2	D	5	0	0	1	0
All	All	1104	1130	1118	30	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 14.

All (30) 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:476:LEU:HD11	1:B:465:HIS:HB3	1.68	0.74
1:D:482:ASP:OD1	1:D:483:ASP:N	2.22	0.72
1:A:476:LEU:HD11	1:B:465:HIS:CB	2.30	0.61
1:A:477:ILE:O	1:D:463:LYS:NZ	2.33	0.61
1:C:454:ILE:HD12	2:D:502:HOH:O	2.02	0.59
1:A:480:ILE:HG21	1:D:460:ARG:HG2	1.86	0.57
1:A:460:ARG:HD2	1:A:461:GLU:N	2.20	0.56
1:C:476:LEU:HD11	1:D:462:ILE:HG23	1.90	0.53
1:A:459:LEU:HD21	1:C:458:LEU:HD23	1.91	0.52
1:A:466:LEU:HD22	1:D:476:LEU:HD23	1.92	0.52
1:B:467:LYS:HG2	1:B:468:GLN:N	2.25	0.51
1:A:480:ILE:O	1:A:481:LYS:C	2.48	0.51
1:C:476:LEU:CD1	1:D:462:ILE:HG12	2.42	0.49
1:C:454:ILE:HD13	1:D:487:ILE:HD13	1.95	0.49
1:A:454:ILE:CD1	1:C:454:ILE:HG23	2.43	0.48
1:A:476:LEU:HD21	1:B:466:LEU:HG	1.95	0.48
1:A:479:ILE:CG2	1:A:479:ILE:O	2.62	0.48
1:C:475:HIS:NE2	1:C:479:ILE:HD11	2.28	0.47
1:C:473:LEU:O	1:C:477:ILE:HG23	2.17	0.45
1:D:481:LYS:O	1:D:485:GLU:HG3	2.18	0.44
1:A:480:ILE:CG2	1:D:460:ARG:HD2	2.48	0.43
1:B:473:LEU:HD11	1:C:466:LEU:HD22	2.01	0.43
1:D:482:ASP:C	1:D:482:ASP:OD1	2.56	0.43
1:A:454:ILE:HD12	1:C:454:ILE:HG23	2.01	0.43
1:A:451:SER:O	1:A:451:SER:OG	2.36	0.42
1:C:477:ILE:HG13	1:C:478:SER:N	2.35	0.41
1:A:453:TYR:HB3	1:C:453:TYR:HB3	2.02	0.41
1:A:476:LEU:CD1	1:B:465:HIS:HB3	2.46	0.41
1:C:452:TYR:CE1	1:D:489:LEU:HD13	2.56	0.41
1:A:459:LEU:HD22	1:C:454:ILE:HG21	2.03	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	29/40 (72%)	29 (100%)	0	0	100	100
1	B	33/40 (82%)	33 (100%)	0	0	100	100
1	C	31/40 (78%)	31 (100%)	0	0	100	100
1	D	29/40 (72%)	28 (97%)	1 (3%)	0	100	100
All	All	122/160 (76%)	121 (99%)	1 (1%)	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	29/37 (78%)	24 (83%)	5 (17%)	2	0
1	B	34/37 (92%)	29 (85%)	5 (15%)	3	0
1	C	31/37 (84%)	29 (94%)	2 (6%)	17	4
1	D	30/37 (81%)	26 (87%)	4 (13%)	4	0
All	All	124/148 (84%)	108 (87%)	16 (13%)	4	0

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	ILE
1	A	459	LEU
1	A	460	ARG
1	A	470	GLN
1	A	481	LYS
1	B	457	ASP
1	B	460	ARG
1	B	464	GLN
1	B	470	GLN
1	B	489	LEU

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Mol	Chain	Res	Type
1	C	463	LYS
1	C	468	GLN
1	D	463	LYS
1	D	464	GLN
1	D	465	HIS
1	D	488	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	HIS
1	B	464	GLN
1	B	465	HIS
1	B	468	GLN
1	D	475	HIS

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 (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	31/40 (77%)	1.51	9 (29%)	0	0	18, 40, 66, 77	0
1	B	33/40 (82%)	1.08	6 (18%)	1	1	10, 27, 60, 70	0
1	C	32/40 (80%)	1.34	8 (25%)	0	0	15, 49, 69, 79	0
1	D	30/40 (75%)	1.51	10 (33%)	0	0	18, 53, 81, 92	0
All	All	126/160 (78%)	1.36	33 (26%)	0	0	10, 43, 76, 92	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	LYS	5.6
1	D	475	HIS	4.9
1	B	458	LEU	4.8
1	A	477	ILE	4.7
1	D	471	GLU	4.3
1	D	466	LEU	3.7
1	B	490	VAL	3.4
1	C	481	LYS	3.3
1	B	457	ASP	3.2
1	D	461	GLU	3.2
1	C	482	ASP	2.9
1	D	468	GLN	2.9
1	A	459	LEU	2.9
1	A	480	ILE	2.9
1	D	460	ARG	2.8
1	C	471	GLU	2.7
1	D	465	HIS	2.7
1	C	479	ILE	2.5
1	C	467	LYS	2.5
1	D	490	VAL	2.5
1	B	459	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	460	ARG	2.4
1	A	473	LEU	2.4
1	A	478	SER	2.3
1	D	464	GLN	2.3
1	A	471	GLU	2.3
1	C	468	GLN	2.3
1	C	478	SER	2.2
1	B	487	ILE	2.1
1	D	473	LEU	2.1
1	A	458	LEU	2.1
1	C	459	LEU	2.1
1	A	462	ILE	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.