



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:57 am BST

PDB ID : 3JRO
Title : NUP84-NUP145C-SEC13 edge element of the NPC lattice
Authors : Brohawn, S.G.; Schwartz, T.U.
Deposited on : 2009-09-08
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

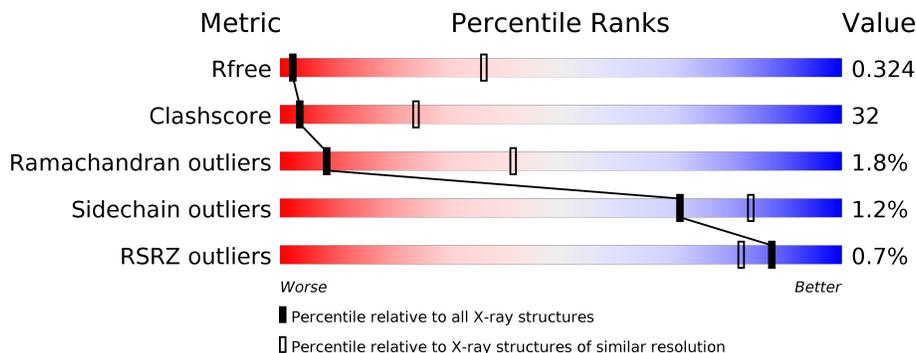
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 $\leq 5\%$. 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	753	 54% 38% • 7%
2	C	426	 35% 50% • 11%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8671 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 Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	701	5623	3598	943	1068	9	5	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1100	GLY	-	LINKER	UNP P49687
A	1101	GLY	-	LINKER	UNP P49687
A	1102	GLY	-	LINKER	UNP P49687
A	1103	GLY	-	LINKER	UNP P49687
A	1104	SER	-	LINKER	UNP P49687
A	1105	GLY	-	LINKER	UNP P49687
A	1106	GLY	-	LINKER	UNP P49687
A	1107	GLY	-	LINKER	UNP P49687
A	1108	GLY	-	LINKER	UNP P49687

- Molecule 2 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	C	379	3048	1949	504	584	4	7	0	0	0

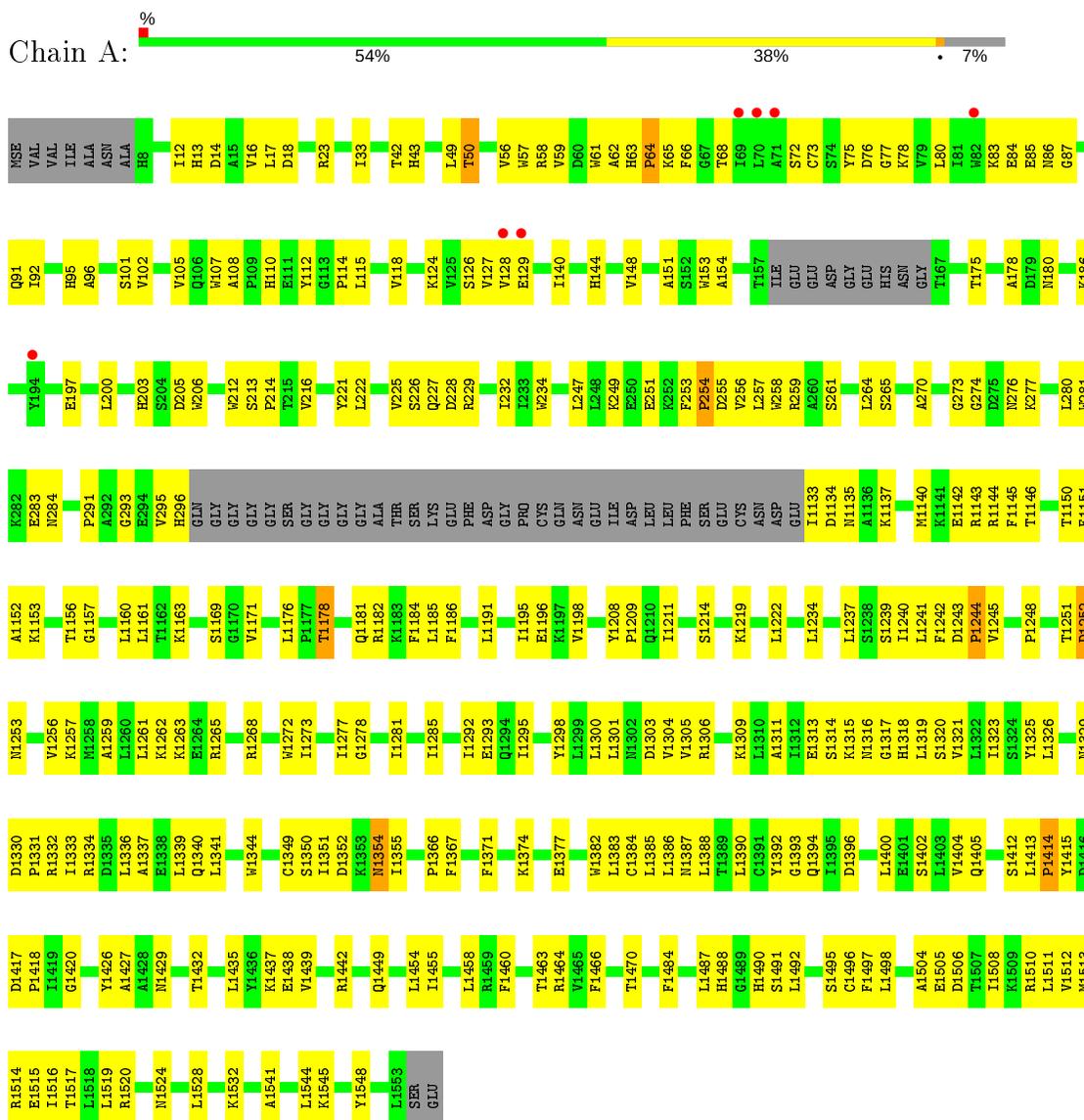
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P52891
C	0	SER	-	EXPRESSION TAG	UNP P52891

3 Residue-property plots

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: Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145



- Molecule 2: Nucleoporin NUP84



K421	R344	E261	V132	GLY
G424	V345	L202	M133	SER
	L346	N205	E134	MSE
	M347	I206	R135	GLU
	I351	S207	P136	LEU
	L355	I208	LYS	SER
	P356	C209	ASN	PRO
	I359	M210	VAL	THR
	H360	I211	P140	TYR
	V363	G214	T141	GLN
	V370	I215	S142	THR
	LYS	Q216	K143	GLU
	GLY	E217	W144	ARG
	THR	Y218	L145	PHE
	GLU	L219	M146	THR
	ALA	N220	S147	LYS
	SER	P221	G151	PHE
	ASN	V222	G152	SER
	ASN	I223	L153	ASP
	ASP	I227	K154	THR
	ILE	F231	S155	LEU
	ILE	M232	C156	LYS
	D331	T233	D157	GLU
	R337	Q234	L158	PHE
	I338	Q235	D159	LYS
	V339	G236	F160	ILE
	T390	I237	P161	GLU
	F391	K238	L162	GLN
	L392	R239	H163	ASN
	A393	H240	Y164	ASN
	I394	S241	V171	GLU
	G395	L242	K172	GLN
	L396	V243	F105	PRO
	D397	R244	L104	D34
	I398	R246	F106	P35
	I399	T246	E106	F36
	N400	S249	K107	R37
	P401	L250	K108	I38
	V404	S251	L109	I39
	E405	Q252	M110	R40
	V407	Q253	K114	E41
	D408	A254	Q115	F42
		G255	L116	R43
		L256	Y117	A46
		A332	Q118	L49
		S333	Y119	A50
		R334	M120	L53
		H335	I121	A54
		P336	I122	N55
		S337	M123	S56
		F338	A192	G57
		S339	I193	D68
		E340	A196	E59
		H341	L197	S60
		P342	E198	N61
		I343	E199	
			A200	
			E260	
			R261	
			A262	
			I263	
			Y264	
			S265	
			Y266	
			L267	
			S268	
			G269	

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 170.47Å 270.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.89 – 4.00 49.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-4.00) 99.9 (49.89-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 4.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.329 0.274 , 0.324	Depositor DCC
R_{free} test set	1586 reflections (7.83%)	wwPDB-VP
Wilson B-factor (Å ²)	133.7	Xtrriage
Anisotropy	0.702	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 123.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0/5744	0.41	0/7776
2	C	0.28	0/3101	0.49	0/4202
All	All	0.25	0/8845	0.44	0/11978

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	5623	0	5577	286	0
2	C	3048	0	3033	306	0
All	All	8671	0	8610	555	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 32.

The worst 5 of 555 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:C:104:LEU:HA	2:C:219:LEU:HD12	1.19	1.09
2:C:215:ILE:HG21	2:C:267:LEU:HD13	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:HB2	2:C:160:PHE:HB2	1.44	0.99
2:C:412:LEU:HB3	2:C:416:TYR:HE2	1.32	0.94
1:A:1251:THR:H	1:A:1257:LYS:HE2	1.35	0.91

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	695/753 (92%)	608 (88%)	78 (11%)	9 (1%)	12	48
2	C	373/426 (88%)	297 (80%)	66 (18%)	10 (3%)	5	34
All	All	1068/1179 (91%)	905 (85%)	144 (14%)	19 (2%)	8	41

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	218	TYR
2	C	281	ASP
2	C	55	ASN
2	C	171	VAL
2	C	222	VAL

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	621/655 (95%)	618 (100%)	3 (0%)	88	93
2	C	345/384 (90%)	336 (97%)	9 (3%)	46	67
All	All	966/1039 (93%)	954 (99%)	12 (1%)	71	84

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	163	ARG
2	C	170	ASP
2	C	301	TYR
2	C	99	TYR
2	C	280	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	234	GLN
2	C	360	HIS
2	C	273	ASN
2	C	118	GLN
2	C	240	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	696/753 (92%)	-0.23	7 (1%) 82 74	159, 188, 244, 325	0
2	C	372/426 (87%)	-0.37	1 (0%) 94 90	134, 171, 248, 370	0
All	All	1068/1179 (90%)	-0.28	8 (0%) 87 82	134, 183, 246, 370	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	3.0
1	A	71	ALA	2.7
1	A	194	TYR	2.6
1	A	82	TRP	2.6
1	A	69	ILE	2.3

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.