

wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 03:04 AM EST

PDB ID	:	3F3F
Title	:	Crystal structure of the nucleoporin pair Nup85-Seh1, space group P21
Authors	:	Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.
Deposited on	:	2008-10-30
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	Qual	ity of chain		
			2%			
1	А	351	48%	37%	• 1	2%
			6%			
1	В	351	44%	42%	•	13%
			.%			
1	Ε	351	46%	38%	• 1	L3%
			3%			
1	F	351	41%	43%	•]	L3%
			5%			
2	С	570	54%	28%	• 1	7%



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Mol	Chain	Length	Quality of	' chain	
9	П	570	7%	210/	120/
	D	570	54%	31%	• 13%
	~		5%		
2	G	570	55%	26%	• 16%
			9%		
2	Н	570	54%	28%	• 15%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25239 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	200	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	300	2448	1549	425	463	11	0	0	0
1	Р	207	Total	С	Ν	0	S	0	0	0
1	D	307	2438	1543	423	461	11	0	0	0
1	F	206	Total	С	Ν	0	S	0	0	0
	E	300	2432	1540	422	459	11	0	0	0
1	F	306	Total	С	Ν	0	S	0	0	0
	T,	500	2430	1538	422	459	11	U	0	0

• Molecule 1 is a protein called Nucleoporin SEH1.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	PRO	-	expression tag	UNP P53011
А	1A	HIS	-	expression tag	UNP P53011
В	1A	PRO	-	expression tag	UNP P53011
В	1B	HIS	-	expression tag	UNP P53011
Е	1A	PRO	-	expression tag	UNP P53011
E	1B	HIS	-	expression tag	UNP P53011
F	0	PRO	-	expression tag	UNP P53011
F	1A	HIS	-	expression tag	UNP P53011

• Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	С	475	Total	С	Ν	0	\mathbf{S}	0	0	0
	U	475	3812	2451	608	732	21	0	0	0
2	Л	405	Total	С	Ν	0	S	0	0	0
	D	495	3959	2533	633	770	23	0	0	0
9	С	476	Total	С	Ν	0	S	0	0	0
	G	470	3820	2447	613	738	22	0	0	0
2	Ц	487	Total	С	Ν	0	S	0	0	0
	Н	H 487	3900	2501	624	753	22	0	U	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 SEH1







• Molecule 2: Nucleoporin NUP85



Chain G:

<mark>465</mark> 165 266

(35.1 125.1

Chain H:





MET LEU SER ALA HIS ASN ILE ILE

GLU SER ALA ASN ASN ARG ALA ALA ALA CLY CLY CLY SER SER



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	79.84Å 166.19Å 188.90Å	Depositor
a, b, c, α , β , γ	90.00° 93.02° 90.00°	Depositor
Bosolution (Å)	50.00 - 2.90	Depositor
Resolution (A)	48.31 - 2.89	EDS
% Data completeness	(Not available) $(50.00-2.90)$	Depositor
(in resolution range)	89.0 (48.31-2.89)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$2.69 (at 2.91 \text{\AA})$	Xtriage
Refinement program	CNS 1.2	Depositor
R R.	0.246 , 0.265	Depositor
n, n_{free}	0.248 , 0.267	DCC
R_{free} test set	10747 reflections $(9.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	80.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 59.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25239	wwPDB-VP
Average B, all atoms $(Å^2)$	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/2510	0.71	0/3403	
1	В	0.42	0/2501	0.71	0/3391	
1	Е	0.45	0/2495	0.72	0/3383	
1	F	0.45	0/2492	0.71	0/3379	
2	С	0.44	0/3889	0.64	1/5265~(0.0%)	
2	D	0.43	0/4037	0.65	0/5463	
2	G	0.43	0/3896	0.63	0/5268	
2	Н	0.44	0/3978	0.63	0/5384	
All	All	0.44	0/25798	0.67	1/34936~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	С	454	LEU	N-CA-C	5.65	126.26	111.00

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	А	2448	0	2385	110	0
1	В	2438	0	2373	138	0
1	Е	2432	0	2368	120	0
1	F	2430	0	2366	147	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
2	С	3812	0	3761	151	0	
2	D	3959	0	3892	167	0	
2	G	3820	0	3750	148	0	
2	Н	3900	0	3846	167	0	
All	All	25239	0	24741	1082	0	

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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 22.

The worst 5 of 1082 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:D:450:MET:HG3	2:D:451:LEU:H	1.26	0.99
2:D:59:GLU:HG3	2:D:60:LYS:H	1.28	0.98
2:G:169:VAL:HG12	2:G:170:ASN:H	1.25	0.97
2:C:240:PHE:O	2:C:241:GLU:HG3	1.66	0.95
2:D:515:THR:HG22	2:D:516:ASN:H	1.32	0.92

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	Per	$\operatorname{centiles}$
1	А	304/351~(87%)	266 (88%)	31 (10%)	7 (2%)	6	23
1	В	303/351~(86%)	265 (88%)	33 (11%)	5 (2%)	9	31
1	Е	302/351~(86%)	263 (87%)	30 (10%)	9(3%)	4	17
1	F	302/351~(86%)	267 (88%)	26 (9%)	9(3%)	4	17
2	С	467/570~(82%)	406 (87%)	53 (11%)	8 (2%)	9	31
2	D	489/570~(86%)	419 (86%)	58 (12%)	12 (2%)	5	21



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	P	erc	entil	\mathbf{es}
2	G	468/570~(82%)	406 (87%)	52 (11%)	10 (2%)		7	26	
2	Н	481/570~(84%)	406 (84%)	60 (12%)	15 (3%)		4	16	
All	All	3116/3684 (85%)	2698 (87%)	343 (11%)	75 (2%)		6	22	

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5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	43	SER
1	В	43	SER
2	С	272	PRO
2	С	455	PHE
2	D	272	PRO

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	270/307~(88%)	261~(97%)	9~(3%)	38 72
1	В	269/307~(88%)	260~(97%)	9~(3%)	38 72
1	Ε	268/307~(87%)	257~(96%)	11 (4%)	30 64
1	F	267/307~(87%)	255~(96%)	12 (4%)	27 61
2	С	424/510~(83%)	415 (98%)	9(2%)	53 81
2	D	441/510~(86%)	431 (98%)	10 (2%)	50 80
2	G	424/510~(83%)	414 (98%)	10 (2%)	49 79
2	Η	434/510~(85%)	425 (98%)	9 (2%)	53 81
All	All	2797/3268~(86%)	2718 (97%)	79 (3%)	43 76

 $5~{\rm of}~79$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	F	313	ASN
2	Н	55	ASP



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Mol	Chain	Res	Type
1	F	334	THR
2	G	488	LEU
2	Н	269	ASP

Sometimes 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 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 (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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
1	А	308/351~(87%)	0.32	6 (1%) 66 65	77, 104, 136, 169	0
1	В	307/351~(87%)	0.39	20 (6%) 18 14	79, 107, 137, 180	0
1	Е	306/351~(87%)	0.29	4 (1%) 77 77	75, 105, 134, 172	0
1	F	306/351~(87%)	0.26	9 (2%) 51 47	82, 107, 137, 180	0
2	С	475/570~(83%)	0.34	31 (6%) 18 14	74, 102, 159, 171	0
2	D	495/570~(86%)	0.40	40 (8%) 12 9	75, 106, 168, 191	0
2	G	476/570~(83%)	0.41	29 (6%) 21 17	70, 102, 159, 190	0
2	Н	487/570~(85%)	0.50	53 (10%) 5 4	77, 106, 174, 192	0
All	All	3160/3684~(85%)	0.37	192 (6%) 21 17	70, 105, 160, 192	0

The worst 5 of 192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	166	GLN	9.3
2	G	546	MET	8.4
2	G	545	GLN	7.2
2	D	133	ASN	6.9
2	Н	45	GLY	6.6

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.

