



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 10:31 PM UTC

PDB ID : 3F3F / pdb_00003f3f
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

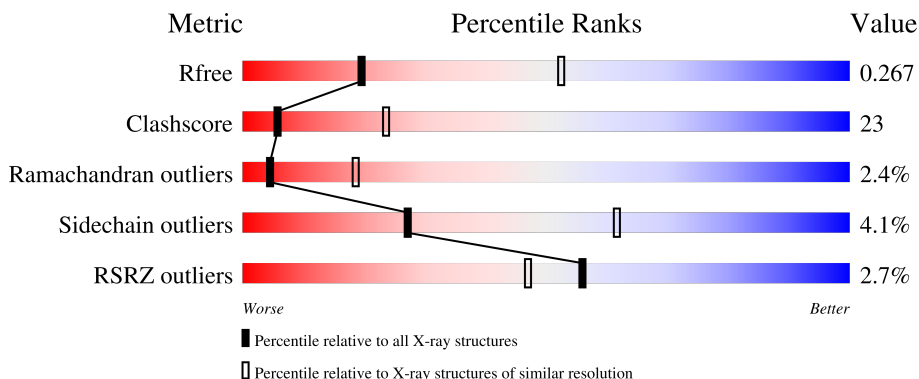
1 Overall quality at a glance

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.





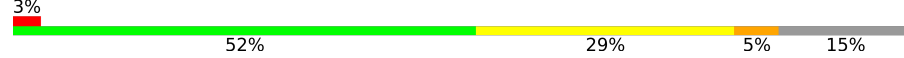
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	351	 2% 44% 39% 12%
1	B	351	 % 42% 41% 13%
1	E	351	 2% 44% 38% 13%
1	F	351	 2% 38% 43% 5% 13%
2	C	570	 3% 51% 28% 17%

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Mol	Chain	Length	Quality of chain
2	D	570	
2	G	570	
2	H	570	

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.

- Molecule 1 is a protein called Nucleoporin SEH1.

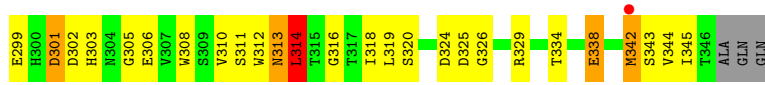
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2448	1549	425	463	11	0	0	0
1	B	307	2438	1543	423	461	11	0	0	0
1	E	306	2432	1540	422	459	11	0	0	0
1	F	306	2430	1538	422	459	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

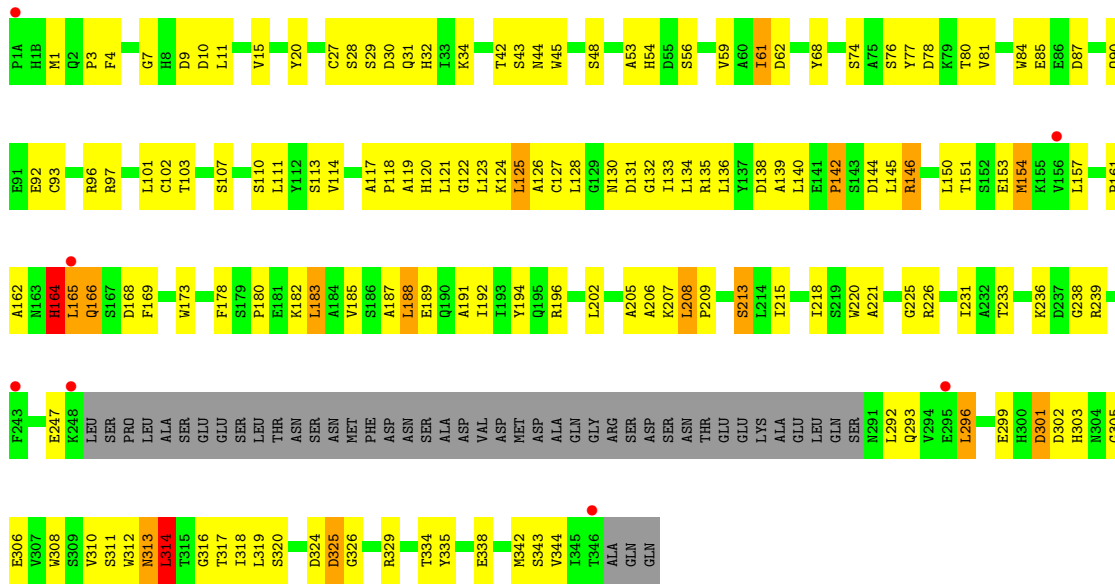
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P53011
A	1A	HIS	-	expression tag	UNP P53011
B	1A	PRO	-	expression tag	UNP P53011
B	1B	HIS	-	expression tag	UNP P53011
E	1A	PRO	-	expression tag	UNP P53011
E	1B	HIS	-	expression tag	UNP P53011
F	0	PRO	-	expression tag	UNP P53011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

- Molecule 2 is a protein called Nucleoporin NUP85.

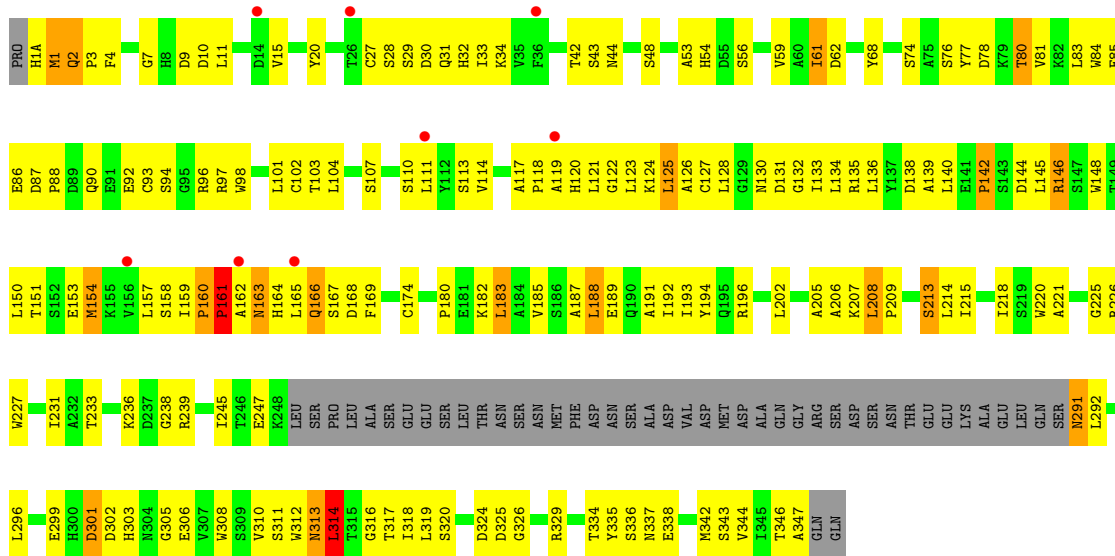
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	475	3812	2451	608	732	21	0	0	0
2	D	495	3959	2533	633	770	23	0	0	0
2	G	476	3820	2447	613	738	22	0	0	0
2	H	487	3900	2501	624	753	22	0	0	0



• Molecule 1: Nucleoporin SEH1

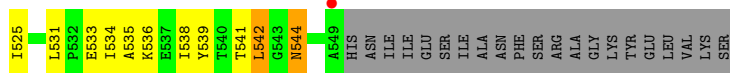


• Molecule 1: Nucleoporin SEH1

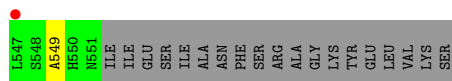
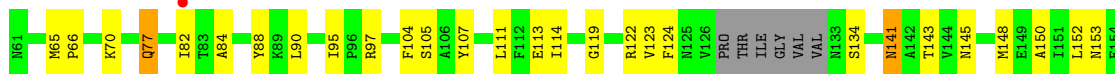


• Molecule 2: Nucleoporin NUP85

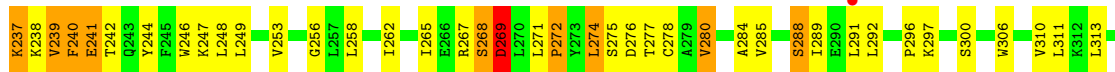
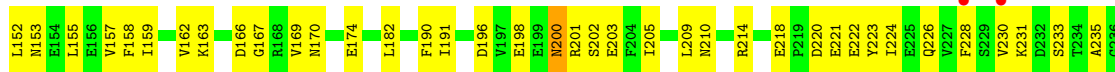


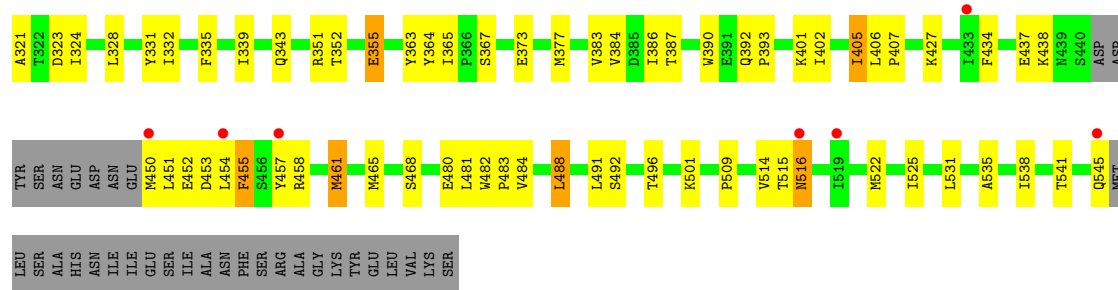


● Molecule 2: Nucleoporin NUP85



● Molecule 2: Nucleoporin NUP85





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.84Å 166.19Å 188.90Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 89.6 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.91Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.265 0.248 , 0.267	Depositor DCC
R_{free} test set	10747 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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	0.54	0/2510	1.03	13/3403 (0.4%)
1	B	0.48	1/2501 (0.0%)	1.01	10/3391 (0.3%)
1	E	0.54	0/2495	1.02	9/3383 (0.3%)
1	F	0.50	0/2492	1.00	10/3379 (0.3%)
2	C	0.53	1/3889 (0.0%)	1.04	18/5265 (0.3%)
2	D	0.50	0/4037	1.06	20/5463 (0.4%)
2	G	0.56	0/3896	1.02	19/5268 (0.4%)
2	H	0.51	0/3978	1.00	15/5384 (0.3%)
All	All	0.52	2/25798 (0.0%)	1.02	114/34936 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	MET	SD-CE	5.14	1.92	1.79
2	C	377	MET	SD-CE	5.04	1.92	1.79

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	454	LEU	N-CA-C	11.64	126.26	111.24
2	D	228	PHE	N-CA-C	9.16	122.57	111.40
2	C	453	ASP	N-CA-C	8.85	122.33	108.79
2	H	288	SER	N-CA-C	-8.65	100.85	111.40
2	G	461	MET	N-CA-C	-8.57	102.60	113.23

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	2448	0	2385	118	0
1	B	2438	0	2373	145	0
1	E	2432	0	2368	126	0
1	F	2430	0	2366	157	0
2	C	3812	0	3761	162	0
2	D	3959	0	3892	182	0
2	G	3820	0	3750	162	0
2	H	3900	0	3846	177	0
All	All	25239	0	24741	1157	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 23.

The worst 5 of 1157 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
1:B:159:ILE:C	1:B:161:PRO:HD3	1.93	0.94

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	304/351 (87%)	266 (88%)	31 (10%)	7 (2%)	5 19
1	B	303/351 (86%)	265 (88%)	33 (11%)	5 (2%)	7 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	302/351 (86%)	263 (87%)	30 (10%)	9 (3%)	3	14
1	F	302/351 (86%)	267 (88%)	26 (9%)	9 (3%)	3	14
2	C	467/570 (82%)	406 (87%)	53 (11%)	8 (2%)	7	26
2	D	489/570 (86%)	419 (86%)	58 (12%)	12 (2%)	4	17
2	G	468/570 (82%)	406 (87%)	52 (11%)	10 (2%)	5	21
2	H	481/570 (84%)	406 (84%)	60 (12%)	15 (3%)	3	14
All	All	3116/3684 (85%)	2698 (87%)	343 (11%)	75 (2%)	4	18

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	B	43	SER
2	C	272	PRO
2	C	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/307 (88%)	256 (95%)	14 (5%)	21	52
1	B	269/307 (88%)	257 (96%)	12 (4%)	24	58
1	E	268/307 (87%)	255 (95%)	13 (5%)	22	54
1	F	267/307 (87%)	251 (94%)	16 (6%)	17	47
2	C	424/510 (83%)	409 (96%)	15 (4%)	32	66
2	D	441/510 (86%)	426 (97%)	15 (3%)	32	66
2	G	424/510 (83%)	410 (97%)	14 (3%)	33	67
2	H	434/510 (85%)	419 (96%)	15 (4%)	32	66
All	All	2797/3268 (86%)	2683 (96%)	114 (4%)	27	61

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	80	THR
2	H	488	LEU
1	F	61	ILE
2	H	387	THR
2	H	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	342	ASN
2	H	260	GLN
1	E	163	ASN
2	H	545	GLN
2	G	308	ASN

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 oligosaccharides 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

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	308/351 (87%)	0.48	8 (2%) 57 48	77, 104, 136, 169	0
1	B	307/351 (87%)	0.21	3 (0%) 79 73	79, 107, 137, 180	0
1	E	306/351 (87%)	0.35	7 (2%) 61 52	75, 105, 134, 172	0
1	F	306/351 (87%)	0.40	8 (2%) 57 48	82, 107, 137, 180	0
2	C	475/570 (83%)	0.18	17 (3%) 46 38	74, 102, 159, 171	0
2	D	495/570 (86%)	0.19	13 (2%) 57 48	75, 106, 168, 191	0
2	G	476/570 (83%)	0.27	12 (2%) 58 48	70, 102, 159, 190	0
2	H	487/570 (85%)	0.23	16 (3%) 49 40	77, 106, 174, 192	0
All	All	3160/3684 (85%)	0.27	84 (2%) 56 47	70, 105, 160, 192	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	549	ALA	6.0
2	G	539	TYR	5.4
1	F	165	LEU	4.2
2	H	48	LEU	4.1
1	F	162	ALA	4.0

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.