



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:59 AM UTC

PDB ID : 7F60 / pdb_00007f60
Title : Crystal structure of auxiliary protein in complex with human nuclear protein
Authors : Gao, X.; Cui, S.
Deposited on : 2021-06-23
Resolution : 2.85 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 ⓘ 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
Xtriage (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

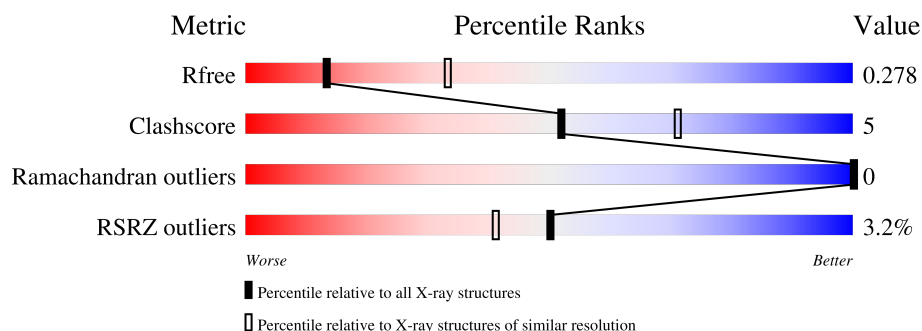
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	368	2% 79% 11% 10%
1	B	368	2% 77% 12% 10%
2	C	1817	• 97%
2	D	1817	• 97%
3	E	61	3% 10% 5% 85%
3	F	61	2% 8% • 89%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6151 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 mRNA export factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2616	1655	456	488	17			
1	B	330	Total	C	N	O	S	0	0	0
			2608	1651	454	486	17			

- Molecule 2 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	48	Total	C	N	O	S	0	0	0
			383	235	66	80	2			
2	D	52	Total	C	N	O	S	0	0	0
			411	252	70	86	3			

- Molecule 3 is a protein called ORF6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	S	0	0	0
			75	44	10	20	1			
3	F	7	Total	C	N	O	S	0	0	0
			58	35	8	14	1			



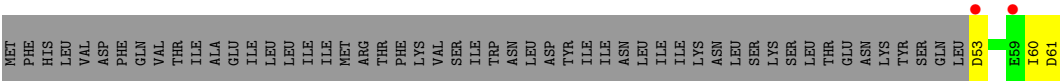
THR	GLN	LYS	ARG	LEU	TRP
THR	VAL	LEU	HIS	TRP	GLN
ASP	ASP	ILE	CYS	GLU	SER
SER	CYS	ILE	GLN	VAL	TYR
THR	SER	ARG	LEU	LEU	LEU
PRO	GLY	HIS	LEU	ARG	GLY
ASP	ASN	LEU	GLU	ALA	LYS
PRO	ASP	ALA	THR	LEU	SER
GLN	LEU	SER	PRO	LEU	GLN
ARG	GLU	ASP	GLU	ASN	ILE
VAL	GLN	ALA	SER	THR	VAL
PRO	LEU	ILE	TRP	HIS	CYS
LEU	HIS	ILE	ALA	LEU	CYS
ARG	ILE	ASN	LYS	GLU	SER
LEU	LYS	GLU	GLU	ALA	GLN
LEU	THR	ASN	THR	GLN	ASN
ALA	VAL	TYR	PHE	CYS	ASP
PRO	SER	ASP	LEU	GLU	SER
HIS	LEU	TYR	THR	GLY	GLN
ILE	CYS	LEU	GLN	VAL	THR
GLY	SER	LEU	LYS	VAL	ARG
ARG	LEU	GLY	LEU	GLN	SER
LEU	ILE	PHE	ARG	ALA	ILE
PRO	GLU	LEU	VAL	SER	HIS
MET	GLN	LEU	PRO	TYR	LEU
PRO	ILE	ASP	ALA	ALA	CYS
GLU	ILE	GLN	LYS	GLY	PHE
ASP	CYS	ALA	TRP	GLN	LEU
TYR	TYR	PRO	ILE	LEU	LEU
ALA	SER	PRO	HIS	GLU	LYS
MET	ALA	GLU	GLU	SER	LEU
ASP	LYS	ARG	ALA	GLU	TYR
GLU	ASP	SER	LYS	GLY	PRO
LEU	ARG	SER	ALA	LEU	ASP
ARG	LEU	LEU	VAL	TRP	ILE
SER	ALA	ILE	ARG	GLU	SER
LEU	GLN	GLN	ALA	TRP	ARG
THR	SER	ASP	HIS	TYR	SER
GLN	SER	TRP	MET	ILE	ALA
ALA	THR	TRP	LEU	ASP	ALA
LEU	VAL	GLU	LEU	ASN	LEU
VAL	LEU	THR	ALA	PHE	ARG
GLY	LEU	ASP	LEU	ASN	SER
SER	ARG	TYR	LEU	SER	GLN
LEU	VAL	THR	CYS	ILE	ASN
			GLY	THR	THR
			ILE	ALA	ASP
			LEU	GLU	SER
			LYS	LEU	ASP
			GLU	ALA	ARG
			HIS	VAL	TYR
			ARG	THR	TYR
			ASN	GLN	ASN
			GLY	ASN	GLN
			TRP	GLN	GLN
			ILE	LEU	LEU
			ASP	LEU	LEU
			GLN	GLN	PRO
			VAL	GLU	TYR
			ALA	GLY	LEU
			THR	GLY	LEU
			PRO	THR	CYS
			GLY	VAL	LEU
			ASP	GLY	SER
			TRP	ALA	TRP
			ARG	GLU	GLN
			ILE	LEU	LEU
			GLY	GLY	GLY
			THR	THR	THR
			ASN	ASN	ASN
			GLN	GLN	GLN
			VAL	VAL	VAL
			ASP	ASP	ASP
			LEU	LEU	LEU
			GLY	GLY	GLY
			TRP	TRP	TRP
			ILE	ILE	ILE
			ASP	ASP	ASP
			GLN	GLN	GLN
			VAL	VAL	VAL
			THR	THR	THR
			ASN	ASN	ASN
			GLY	GLY	GLY
			TRP	TRP	TRP
			ILE	ILE	ILE
			ASP	ASP	ASP
			GLN	GLN	GLN
			VAL	VAL	VAL
			THR	THR	THR
			ASN	ASN	ASN
			GLY	GLY	GLY
			TRP	TRP	TRP
			ILE	ILE	ILE
			ASP	ASP	ASP
			GLN	GLN	GLN
			VAL	VAL	VAL
			THR	THR	THR
			ASN	ASN	ASN
			GLY	GLY	GLY
			TRP	TRP	TRP
			ILE	ILE	ILE
			ASP	ASP	ASP
			GLN	GLN	GLN
			VAL	VAL	VAL
			THR	THR	THR
			ASN	ASN	ASN
			GLY	GLY	

- Molecule 2: Nuclear pore complex protein Nup98-Nup96

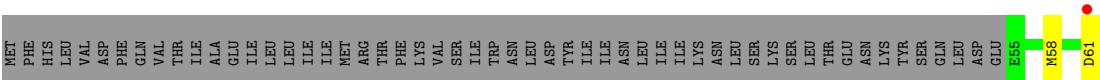
Chain D: 97%

[illegible]





● Molecule 3: ORF6 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.34Å 87.53Å 48.23Å 90.00° 93.68° 90.00°	Depositor
Resolution (Å)	48.24 – 2.85 48.24 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.24-2.85) 99.2 (48.24-2.85)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.236 , 0.276 0.235 , 0.278	Depositor DCC
R_{free} test set	906 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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	0.11	0/2691	0.33	0/3658
1	B	0.10	0/2683	0.30	0/3647
2	C	0.07	0/387	0.26	0/519
2	D	0.08	0/415	0.24	0/557
3	E	0.21	0/75	0.42	0/100
3	F	0.11	0/58	0.21	0/77
All	All	0.10	0/6309	0.31	0/8558

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	2616	0	2514	22	0
1	B	2608	0	2508	32	0
2	C	383	0	376	6	0
2	D	411	0	406	3	0
3	E	75	0	60	2	0
3	F	58	0	50	4	0
All	All	6151	0	5914	62	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 5.

All (62) 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:B:239:ARG:NH1	3:F:61:ASP:OD2	2.10	0.84
1:A:110:ALA:HB3	1:A:124:ALA:HB3	1.67	0.75
1:B:171:GLU:HG3	1:B:172:ARG:HD2	1.77	0.66
3:E:53:ASP:OD1	3:E:53:ASP:N	2.28	0.65
1:B:110:ALA:HB3	1:B:124:ALA:HB3	1.80	0.63
1:B:50:PRO:HG3	1:B:325:HIS:HB2	1.80	0.63
2:D:194:GLU:N	2:D:194:GLU:OE1	2.35	0.60
1:A:263:ASN:HB2	1:A:271:GLN:HG3	1.84	0.60
1:A:107:ASP:OD1	1:A:109:THR:OG1	2.20	0.59
1:A:101:VAL:HG23	1:A:115:LEU:HD11	1.85	0.58
1:B:88:PRO:HD2	1:B:106:CYS:HB2	1.85	0.58
1:A:165:MET:HE1	1:A:200:GLN:HB2	1.85	0.57
2:C:198:LYS:NZ	2:C:206:GLU:OE2	2.34	0.57
1:A:262:SER:O	1:A:263:ASN:ND2	2.38	0.56
1:B:172:ARG:HD2	1:B:172:ARG:H	1.71	0.56
3:F:61:ASP:OD1	3:F:61:ASP:N	2.38	0.56
1:B:282:HIS:HE1	1:B:359:ALA:HA	1.70	0.56
1:A:50:PRO:HG3	1:A:325:HIS:HB2	1.87	0.56
1:B:149:TRP:HA	1:B:172:ARG:HB2	1.89	0.55
1:A:88:PRO:HD2	1:A:106:CYS:HB2	1.90	0.53
2:D:171:ASP:OD1	2:D:172:THR:N	2.43	0.52
1:B:83:GLN:NE2	1:B:118:ASN:OD1	2.41	0.52
1:A:54:GLY:C	1:A:55:ASN:HD22	2.18	0.52
1:B:165:MET:HE1	1:B:201:PRO:HG2	1.91	0.52
1:B:255:PHE:HE2	3:F:58:MET:HE1	1.74	0.52
1:B:61:SER:OG	1:B:65:ASP:OD1	2.27	0.51
2:D:167:PRO:HG2	2:D:186:HIS:HB3	1.92	0.51
1:A:136:ILE:HG12	1:A:178:VAL:HG11	1.91	0.51
1:B:274:TYR:HB3	1:B:293:SER:HB2	1.93	0.51
1:A:86:THR:HA	1:B:84:MET:HE3	1.93	0.51
1:B:239:ARG:HD3	3:F:61:ASP:OD2	2.11	0.51
3:E:60:ILE:HG12	3:E:61:ASP:N	2.26	0.51
1:A:184:VAL:HG22	1:A:194:VAL:HG22	1.93	0.51
1:A:301:ASP:HB3	1:A:306:THR:HG22	1.93	0.50
1:B:174:TYR:CZ	1:B:188:ALA:HB2	2.46	0.50
1:B:282:HIS:CD2	1:B:284:VAL:HG12	2.47	0.49
1:B:211:LEU:HD13	1:B:235:SER:HB3	1.95	0.49
1:A:324:ASN:OD1	1:A:329:ILE:N	2.44	0.49
1:A:106:CYS:HA	1:A:129:PRO:HB3	1.95	0.49
1:B:62:TRP:HA	1:B:88:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HB2	1:A:123:ILE:HD13	1.96	0.47
2:C:200:LEU:HD12	2:C:200:LEU:H	1.80	0.47
1:B:174:TYR:CZ	2:C:199:SER:HB3	2.51	0.45
1:B:324:ASN:ND2	1:B:326:ASN:OD1	2.39	0.44
1:B:92:VAL:HG12	1:B:103:THR:HA	1.98	0.44
1:B:40:ASP:OD1	1:B:345:TYR:OH	2.34	0.44
2:C:168:THR:HG22	2:C:185:LYS:HD3	2.00	0.44
1:B:165:MET:HE3	1:B:167:LEU:HG	1.99	0.44
1:A:315:ASP:OD1	1:A:315:ASP:N	2.51	0.44
1:B:338:TRP:HZ3	2:C:207:ASP:OD2	2.02	0.43
1:A:281:PHE:CE1	1:A:288:LEU:HB3	2.54	0.43
1:B:198:GLU:O	1:B:200:GLN:N	2.51	0.43
1:B:342:HIS:ND1	2:C:160:THR:OG1	2.44	0.43
1:B:157:ASP:HB3	1:B:164:MET:SD	2.60	0.42
1:A:290:THR:OG1	1:A:300:TRP:NE1	2.51	0.42
1:B:165:MET:HE2	1:B:165:MET:HB3	1.96	0.41
1:B:34:VAL:HG22	1:B:77:THR:HG21	2.02	0.41
1:B:34:VAL:HB	1:B:353:ILE:HB	2.02	0.41
1:B:106:CYS:HA	1:B:129:PRO:HB3	2.01	0.41
1:A:114:ASP:OD2	1:A:117:SER:OG	2.31	0.41
1:A:307:LYS:HE3	1:A:307:LYS:HB3	1.88	0.41
1:A:215:HIS:NE2	1:A:233:LEU:HD21	2.36	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	327/368 (89%)	319 (98%)	8 (2%)	0	100	100
1	B	326/368 (89%)	319 (98%)	7 (2%)	0	100	100
2	C	44/1817 (2%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	48/1817 (3%)	45 (94%)	3 (6%)	0	100	100
3	E	7/61 (12%)	7 (100%)	0	0	100	100
3	F	5/61 (8%)	5 (100%)	0	0	100	100
All	All	757/4492 (17%)	737 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [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	331/368 (89%)	0.38	9 (2%)	56	47	24, 35, 61, 89	0
1	B	330/368 (89%)	0.40	6 (1%)	67	61	24, 36, 56, 92	0
2	C	48/1817 (2%)	0.61	4 (8%)	17	13	32, 47, 69, 86	0
2	D	52/1817 (2%)	0.69	3 (5%)	29	21	29, 53, 88, 113	0
3	E	9/61 (14%)	1.30	2 (22%)	2	2	51, 57, 78, 80	0
3	F	7/61 (11%)	0.87	1 (14%)	6	4	46, 57, 61, 79	0
All	All	777/4492 (17%)	0.44	25 (3%)	50	41	24, 38, 67, 113	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	3.7
1	A	262	SER	3.4
1	B	60	GLY	3.3
2	C	172	THR	3.3
1	B	357	ASN	3.1
3	E	59	GLU	3.0
1	A	357	ASN	3.0
3	E	53	ASP	3.0
1	A	315	ASP	2.9
3	F	61	ASP	2.9
2	D	174	VAL	2.7
2	C	163	LYS	2.7
2	D	173	MET	2.6
2	C	181	ASN	2.6
1	A	263	ASN	2.6
1	B	345	TYR	2.5
1	B	365	ARG	2.5
1	B	251	ALA	2.4
1	A	359	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	365	ARG	2.4
2	D	172	THR	2.3
1	A	75	GLY	2.2
2	C	207	ASP	2.2
1	A	292	GLY	2.2
1	B	262	SER	2.2

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.