



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

PDB ID : 3IKO
Title : Crystal structure of the heterotrimeric Sec13-Nup145C-Nup84 nucleoporin complex
Authors : Nagy, V.; Hsia, K.-C.; Debler, E.W.; Davenport, A.; Blobel, G.; Hoelz, A.
Deposited on : 2009-08-06
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

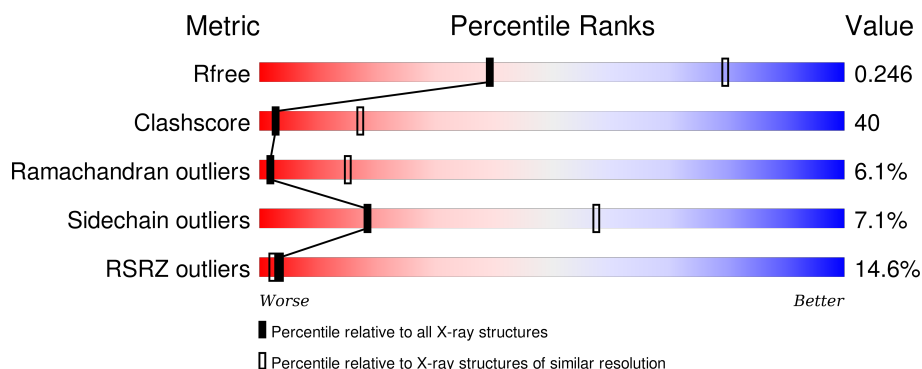
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	297	<div> <div>31%</div> <div> <div>32%</div> <div>54%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	297	<div> <div>34%</div> <div> <div>34%</div> <div>52%</div> <div>7%</div> <div>8%</div> </div> </div>
1	G	297	<div> <div>39%</div> <div> <div>31%</div> <div>54%</div> <div>7%</div> <div>8%</div> </div> </div>
2	B	442	<div> <div>3%</div> <div> <div>43%</div> <div>46%</div> <div>8%</div> <div>••</div> </div> </div>
2	E	442	<div> <div>8%</div> <div> <div>43%</div> <div>44%</div> <div>8%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	442	<div><div></div><div>18%</div><div>42%</div><div>43%</div><div>9%</div><div>5%</div></div>
3	C	460	<div><div></div><div>3%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div>
3	F	460	<div><div></div><div>5%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div>
3	I	460	<div><div></div><div>4%</div><div>44%</div><div>38%</div><div>7%</div><div>10%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27032 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	D	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	G	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	9	0	0
			3528	2254	587	675	12			
2	E	423	Total	C	N	O	S	9	0	0
			3438	2201	570	656	11			
2	H	420	Total	C	N	O	S	9	0	0
			3409	2182	566	650	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	EXPRESSION TAG	UNP P49687
B	112	GLY	-	EXPRESSION TAG	UNP P49687
B	113	SER	-	EXPRESSION TAG	UNP P49687
B	114	SER	-	EXPRESSION TAG	UNP P49687
B	115	HIS	-	EXPRESSION TAG	UNP P49687
B	116	HIS	-	EXPRESSION TAG	UNP P49687
B	117	HIS	-	EXPRESSION TAG	UNP P49687
B	118	HIS	-	EXPRESSION TAG	UNP P49687
B	119	HIS	-	EXPRESSION TAG	UNP P49687
B	120	HIS	-	EXPRESSION TAG	UNP P49687
B	121	SER	-	EXPRESSION TAG	UNP P49687
B	122	GLN	-	EXPRESSION TAG	UNP P49687

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	ASP	-	EXPRESSION TAG	UNP P49687
B	124	PRO	-	EXPRESSION TAG	UNP P49687
E	111	MET	-	EXPRESSION TAG	UNP P49687
E	112	GLY	-	EXPRESSION TAG	UNP P49687
E	113	SER	-	EXPRESSION TAG	UNP P49687
E	114	SER	-	EXPRESSION TAG	UNP P49687
E	115	HIS	-	EXPRESSION TAG	UNP P49687
E	116	HIS	-	EXPRESSION TAG	UNP P49687
E	117	HIS	-	EXPRESSION TAG	UNP P49687
E	118	HIS	-	EXPRESSION TAG	UNP P49687
E	119	HIS	-	EXPRESSION TAG	UNP P49687
E	120	HIS	-	EXPRESSION TAG	UNP P49687
E	121	SER	-	EXPRESSION TAG	UNP P49687
E	122	GLN	-	EXPRESSION TAG	UNP P49687
E	123	ASP	-	EXPRESSION TAG	UNP P49687
E	124	PRO	-	EXPRESSION TAG	UNP P49687
H	111	MET	-	EXPRESSION TAG	UNP P49687
H	112	GLY	-	EXPRESSION TAG	UNP P49687
H	113	SER	-	EXPRESSION TAG	UNP P49687
H	114	SER	-	EXPRESSION TAG	UNP P49687
H	115	HIS	-	EXPRESSION TAG	UNP P49687
H	116	HIS	-	EXPRESSION TAG	UNP P49687
H	117	HIS	-	EXPRESSION TAG	UNP P49687
H	118	HIS	-	EXPRESSION TAG	UNP P49687
H	119	HIS	-	EXPRESSION TAG	UNP P49687
H	120	HIS	-	EXPRESSION TAG	UNP P49687
H	121	SER	-	EXPRESSION TAG	UNP P49687
H	122	GLN	-	EXPRESSION TAG	UNP P49687
H	123	ASP	-	EXPRESSION TAG	UNP P49687
H	124	PRO	-	EXPRESSION TAG	UNP P49687

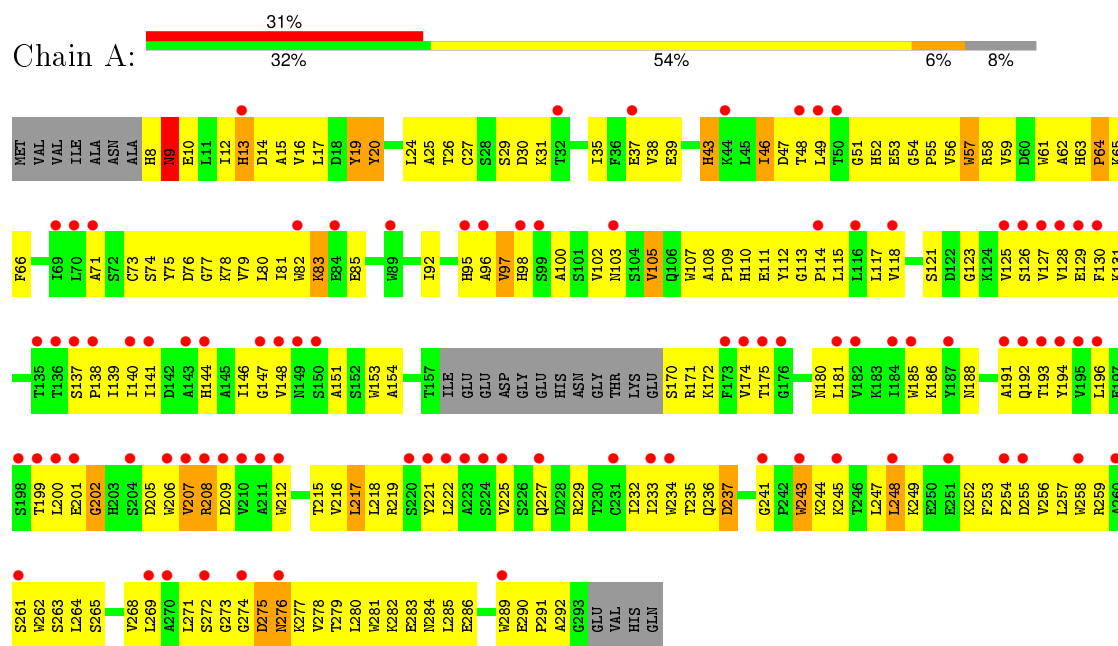
- Molecule 3 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			
3	F	419	Total	C	N	O	S	0	0	0
			3404	2178	558	656	12			
3	I	414	Total	C	N	O	S	0	0	0
			3369	2155	554	649	11			

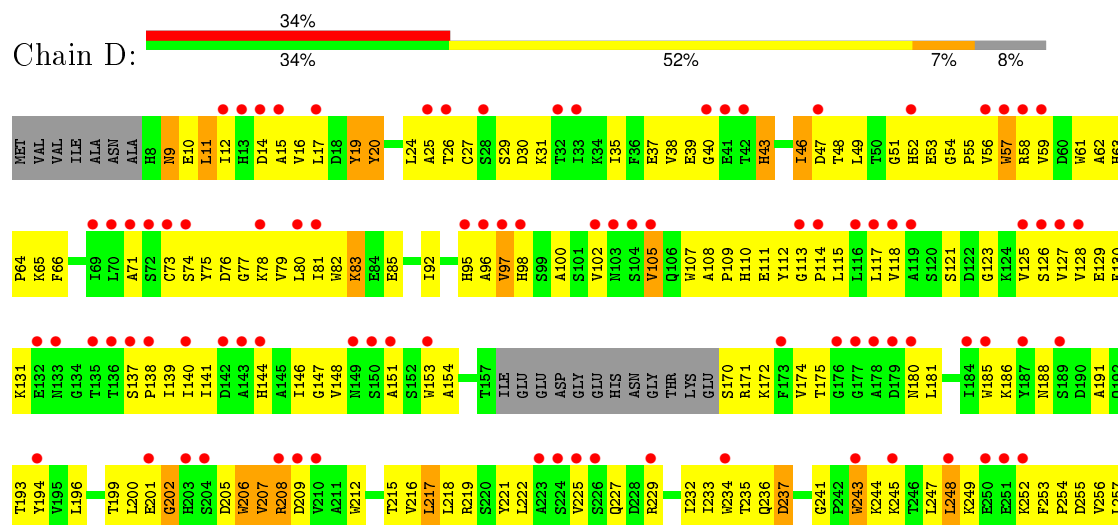
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Protein transport protein SEC13

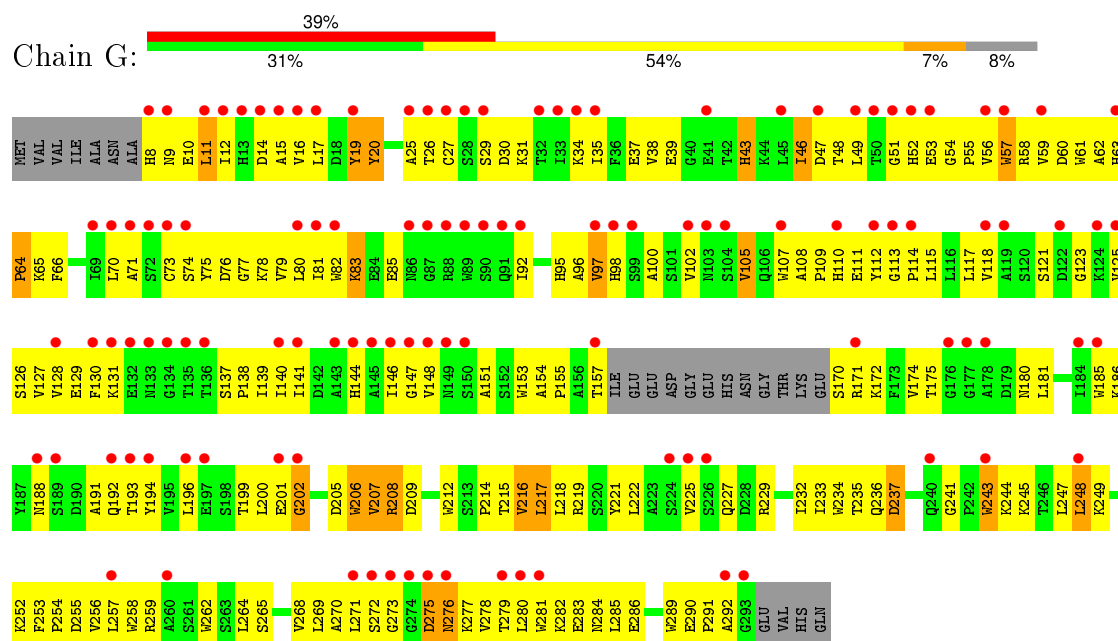


• Molecule 1: Protein transport protein SEC13

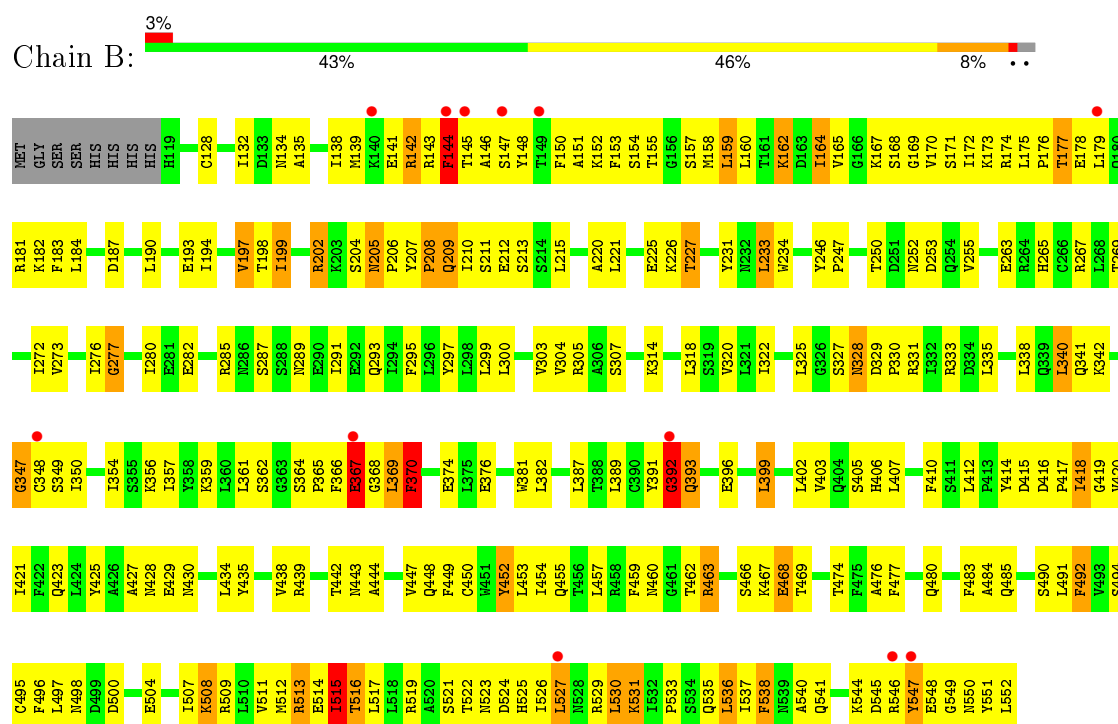




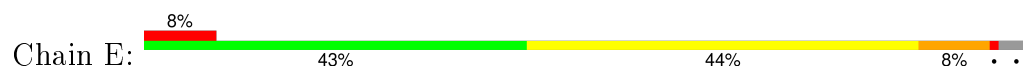
• Molecule 1: Protein transport protein SEC13

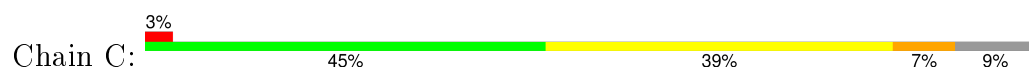
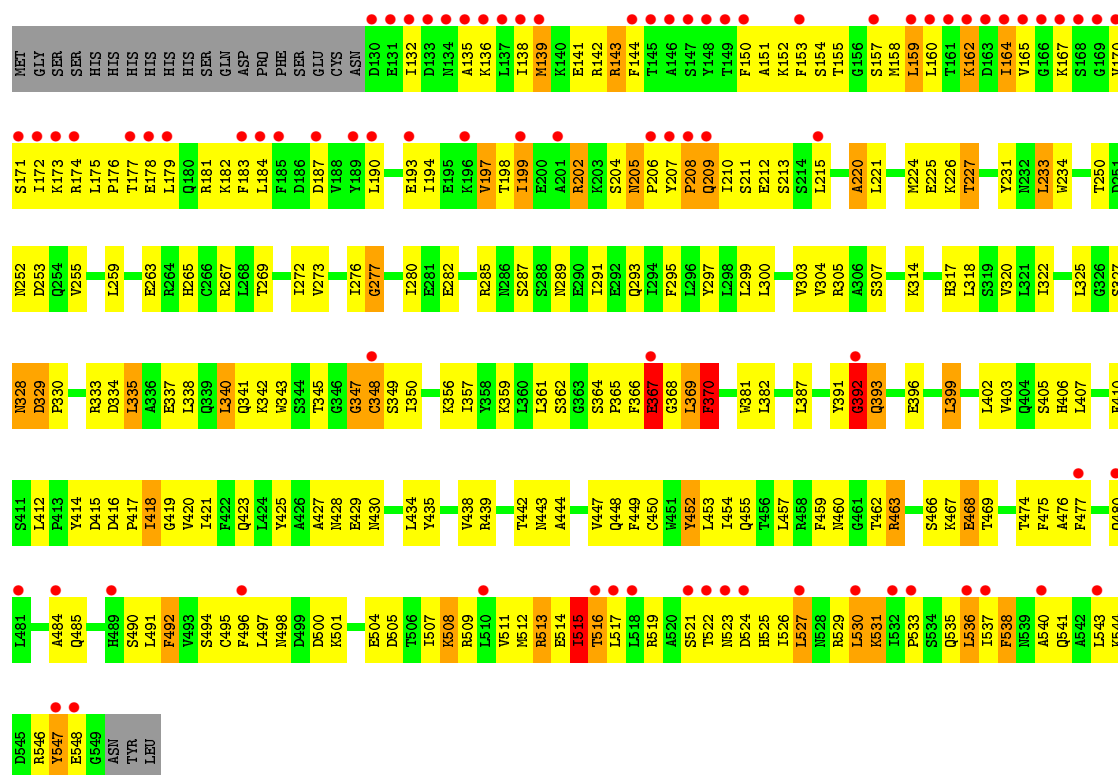


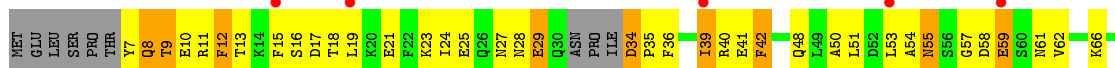
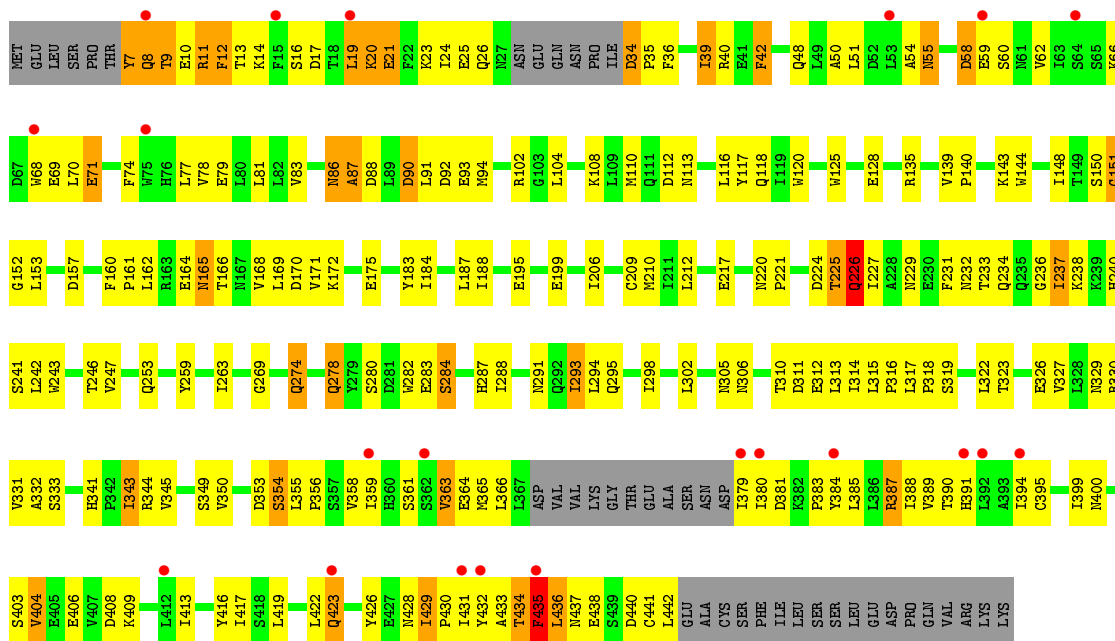
• Molecule 2: Nucleoporin NUP145C



• Molecule 2: Nucleoporin NUP145C







D408	K409	H341	H243	G151	L70
L412	L413	I343	T246	G152	E71
I413	I413	R344	V247	L153	F74
Y416	Y416	V345	S251	D159	L77
I417	I417	S349	Y259	F160	V78
S418	S418	V350	E260	P161	E79
L419	L419	D353	R261	L162	L80
L420	L420	A262	L263	E164	L81
K421	K421	S354	L355	N165	L82
L422	L422	L355	I263	T166	V83
Q423	Q423	P356	G269	M167	N86
G424	G424	S357	Q274	V168	L89
L425	L425	V358	Q274	L169	L89
Y426	Y426	I359	Q274	V171	D90
E427	E427	H360	Q278	K172	L91
N428	N428	S361	Y279	D92	D92
I429	I429	S362	S280	E175	E93
P430	P430	V363	D281	Y183	N94
I431	I431	E364	W282	I184	L96
Y432	Y432	N365	E283	I188	Y99
A433	A433	L366	S284	L189	
T434	T434	L367	H287	E199	R102
F435	F435	ASP	I289	G103	G103
L436	L436	VAL	N291	L104	L104
ASN	ASN	LYS	Q292	I206	K108
GLU	GLU	GLY	I293	C209	L109
SER	SER	THR	L294	P210	M110
ASP	ASP	GLU	Q295	I211	Q111
CYS	CYS	ALA	L298	D112	D112
LEU	LEU	SER		N113	N113
GLU	GLU	ASN		E217	K114
ALA	ALA	ASP			Q115
CYS	CYS	ILE		P221	L116
SER	SER	ILE		V222	Y117
PHE	PHE	ILE		I223	Q118
ILE	ILE	D381	N305	D224	I119
LEU	LEU	R382	N306	T225	W120
SER	SER	P383	T310	I227	W125
SER	SER	Y384	D311	A228	E128
LEU	LEU	L385	E312	E230	R135
GLU	GLU	L386	L313	F231	N135
ASP	ASP	R387	L314	N232	V139
PRO	PRO	I388	L315	Q234	P140
GLN	GLN	V389	L317	G236	K143
VAL	VAL	T390	P316	I237	W144
ARG	ARG	H391	L317	K238	L145
LYS	LYS	C395	T323	H239	I148
LYS	LYS	I399	E326	H240	S150
		N400	V327	L242	
		S403	N329		
		V404	L328		
		E405	R330		
		A406	V331		
		V407	A332		
			S333		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.40Å 194.05Å 327.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 48.79 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.20) 96.2 (48.79-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.273 0.243 , 0.246	Depositor DCC
R_{free} test set	5204 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 110.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 104908 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27032	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.48	0/2220	0.68	1/3028 (0.0%)
1	D	0.47	0/2220	0.67	0/3028
1	G	0.47	0/2220	0.67	0/3028
2	B	0.55	0/3598	0.74	1/4856 (0.0%)
2	E	0.57	0/3504	0.75	1/4728 (0.0%)
2	H	0.56	0/3474	0.74	1/4688 (0.0%)
3	C	0.63	0/3472	0.76	0/4714
3	F	0.63	0/3472	0.77	3/4714 (0.1%)
3	I	0.62	0/3437	0.76	0/4666
All	All	0.57	0/27617	0.74	7/37450 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	392	GLY	N-CA-C	5.99	128.08	113.10
2	H	392	GLY	N-CA-C	5.98	128.05	113.10
2	B	392	GLY	N-CA-C	5.96	128.01	113.10
3	F	435	PHE	N-CA-C	5.71	126.41	111.00
3	F	436	LEU	N-CA-C	5.29	125.28	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	435	PHE	Mainchain
3	F	435	PHE	Mainchain

5.2 Too-close contacts

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	2160	0	2096	239	0
1	D	2160	0	2096	228	0
1	G	2160	0	2096	226	0
2	B	3528	0	3521	301	0
2	E	3438	0	3452	293	0
2	H	3409	0	3426	313	0
3	C	3404	0	3378	249	0
3	F	3404	0	3380	246	0
3	I	3369	0	3341	243	0
All	All	27032	0	26786	2165	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 40.

The worst 5 of 2165 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:E:369:LEU:O	2:E:369:LEU:HG	1.36	1.13
2:E:208:PRO:HB3	2:E:531:LYS:HB2	1.32	1.10
1:A:131:LYS:HE3	1:A:137:SER:HB2	1.38	1.06
2:H:208:PRO:HB3	2:H:531:LYS:HB2	1.32	1.06
2:H:139:MET:HG2	2:H:144:PHE:O	1.56	1.05

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	270/297 (91%)	199 (74%)	51 (19%)	20 (7%)	1	9
1	D	270/297 (91%)	200 (74%)	51 (19%)	19 (7%)	1	10
1	G	270/297 (91%)	200 (74%)	50 (18%)	20 (7%)	1	9
2	B	432/442 (98%)	346 (80%)	55 (13%)	31 (7%)	1	10
2	E	421/442 (95%)	343 (82%)	48 (11%)	30 (7%)	1	10
2	H	418/442 (95%)	339 (81%)	49 (12%)	30 (7%)	1	10
3	C	413/460 (90%)	341 (83%)	55 (13%)	17 (4%)	3	27
3	F	413/460 (90%)	343 (83%)	53 (13%)	17 (4%)	3	27
3	I	408/460 (89%)	334 (82%)	56 (14%)	18 (4%)	3	24
All	All	3315/3597 (92%)	2645 (80%)	468 (14%)	202 (6%)	2	15

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	254	PRO
2	B	209	GLN
2	B	348	CYS
2	B	367	GLU

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	233/252 (92%)	221 (95%)	12 (5%)	29	69
1	D	233/252 (92%)	222 (95%)	11 (5%)	32	73
1	G	233/252 (92%)	223 (96%)	10 (4%)	35	75
2	B	397/404 (98%)	362 (91%)	35 (9%)	12	45
2	E	386/404 (96%)	352 (91%)	34 (9%)	12	45
2	H	383/404 (95%)	350 (91%)	33 (9%)	13	46
3	C	387/425 (91%)	361 (93%)	26 (7%)	20	60
3	F	387/425 (91%)	359 (93%)	28 (7%)	18	57
3	I	382/425 (90%)	358 (94%)	24 (6%)	22	63
All	All	3021/3243 (93%)	2808 (93%)	213 (7%)	18	57

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	335	LEU
3	F	12	PHE
3	I	90	ASP
2	E	367	GLU
2	E	447	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	9	ASN
1	D	149	ASN
3	F	300	ASN
3	C	235	GLN
2	E	328	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	274/297 (92%)	1.71	92 (33%) 0 0	103, 167, 201, 202	0
1	D	274/297 (92%)	1.85	102 (37%) 0 0	101, 185, 202, 202	0
1	G	274/297 (92%)	1.97	116 (42%) 0 0	127, 193, 202, 202	0
2	B	434/442 (98%)	0.21	12 (2%) 56 42	44, 102, 181, 202	2 (0%)
2	E	423/442 (95%)	0.43	35 (8%) 14 7	49, 94, 192, 202	2 (0%)
2	H	420/442 (95%)	0.87	80 (19%) 2 1	46, 122, 200, 202	2 (0%)
3	C	419/460 (91%)	0.15	13 (3%) 52 38	9, 95, 175, 202	19 (4%)
3	F	419/460 (91%)	0.22	21 (5%) 32 19	11, 96, 178, 201	19 (4%)
3	I	414/460 (90%)	0.14	17 (4%) 41 27	48, 95, 181, 202	0
All	All	3351/3597 (93%)	0.71	488 (14%) 3 2	9, 124, 201, 202	44 (1%)

The worst 5 of 488 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	148	VAL	11.0
1	D	73	CYS	10.7
1	D	41	GLU	10.3
1	D	136	THR	10.0
2	E	138	ILE	9.5

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.