



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 14, 2016 – 08:44 PM EDT

PDB ID : 4XMM
Title : Structure of the yeast coat nucleoporin complex, space group C2
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;
Hoelz, A.
Deposited on : 2015-01-14
Resolution : 7.38 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
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)	:	rb-20027790

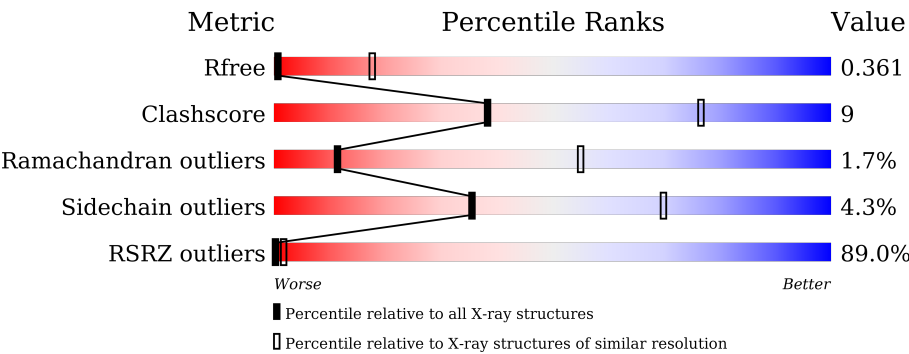
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.38 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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>92%</div><div><div>64%</div><div>25%</div><div>•</div><div>8%</div></div></div>
2	B	652	<div><div>70%</div><div><div>56%</div><div>19%</div><div>•</div><div>22%</div></div></div>
3	C	349	<div><div>83%</div><div><div>61%</div><div>26%</div><div>•</div><div>12%</div></div></div>
4	D	715	<div><div>81%</div><div><div>66%</div><div>19%</div><div>•</div><div>13%</div></div></div>
5	E	1045	<div><div>69%</div><div><div>71%</div><div>14%</div><div>•</div><div>14%</div></div></div>
6	F	454	<div><div>82%</div><div><div>68%</div><div>21%</div><div>•</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
7	H	271	<div> <div>70%</div> <div>71%8%20%</div> </div>
8	L	217	<div> <div>85%</div> <div>86%10%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26139 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			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	511	Total	C	N	O	S	0	0	0
			3805	2417	648	730	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	307	Total	C	N	O	S	0	0	0
			2438	1543	422	462	11			

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	620	Total	C	N	O	S	0	0	0
			4535	2884	753	877	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	MET	-	initiating methionine	UNP P46673
D	31	GLY	-	expression tag	UNP P46673
D	32	SER	-	expression tag	UNP P46673
D	33	SER	-	expression tag	UNP P46673
D	34	HIS	-	expression tag	UNP P46673
D	35	HIS	-	expression tag	UNP P46673
D	36	HIS	-	expression tag	UNP P46673
D	37	HIS	-	expression tag	UNP P46673
D	38	HIS	-	expression tag	UNP P46673
D	39	HIS	-	expression tag	UNP P46673
D	40	SER	-	expression tag	UNP P46673
D	41	ASP	-	expression tag	UNP P46673
D	42	GLN	-	expression tag	UNP P46673
D	43	PRO	-	expression tag	UNP P46673

- Molecule 5 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729
E	1	THR	-	expression tag	UNP P35729

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891

- Molecule 7 is a protein called Antibody 57 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	217	Total	C	N	O	S	0	0	0
			1576	988	267	315	6			

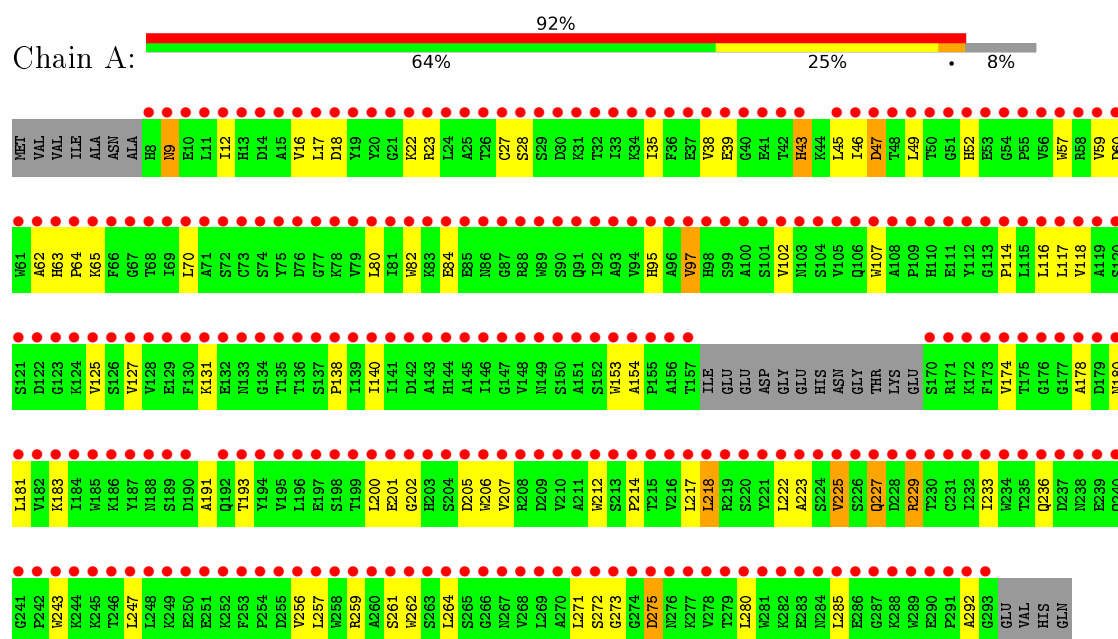
- Molecule 8 is a protein called Antibody 57 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	210	Total	C	N	O	S	0	0	0
			1599	996	270	327	6			

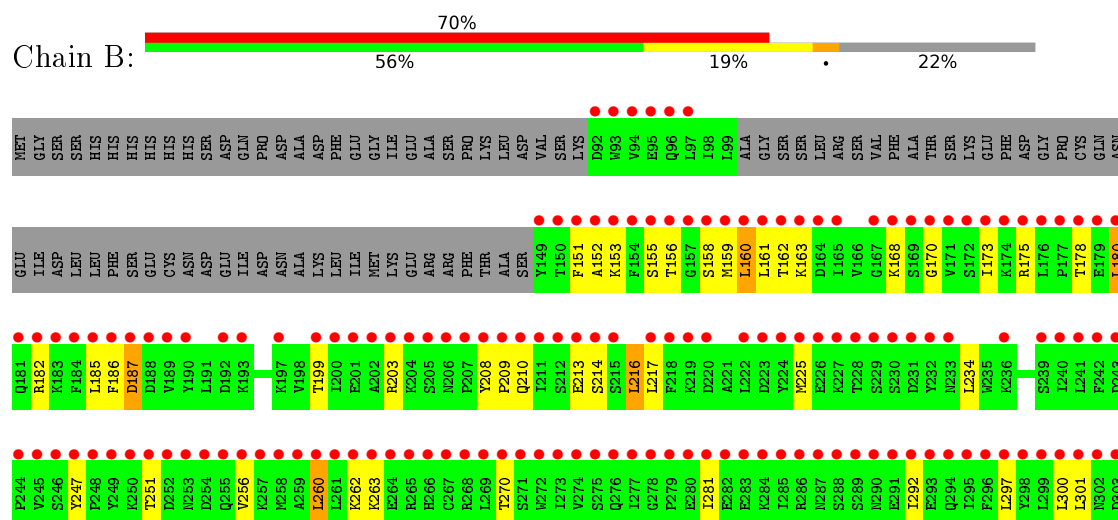
3 Residue-property plots

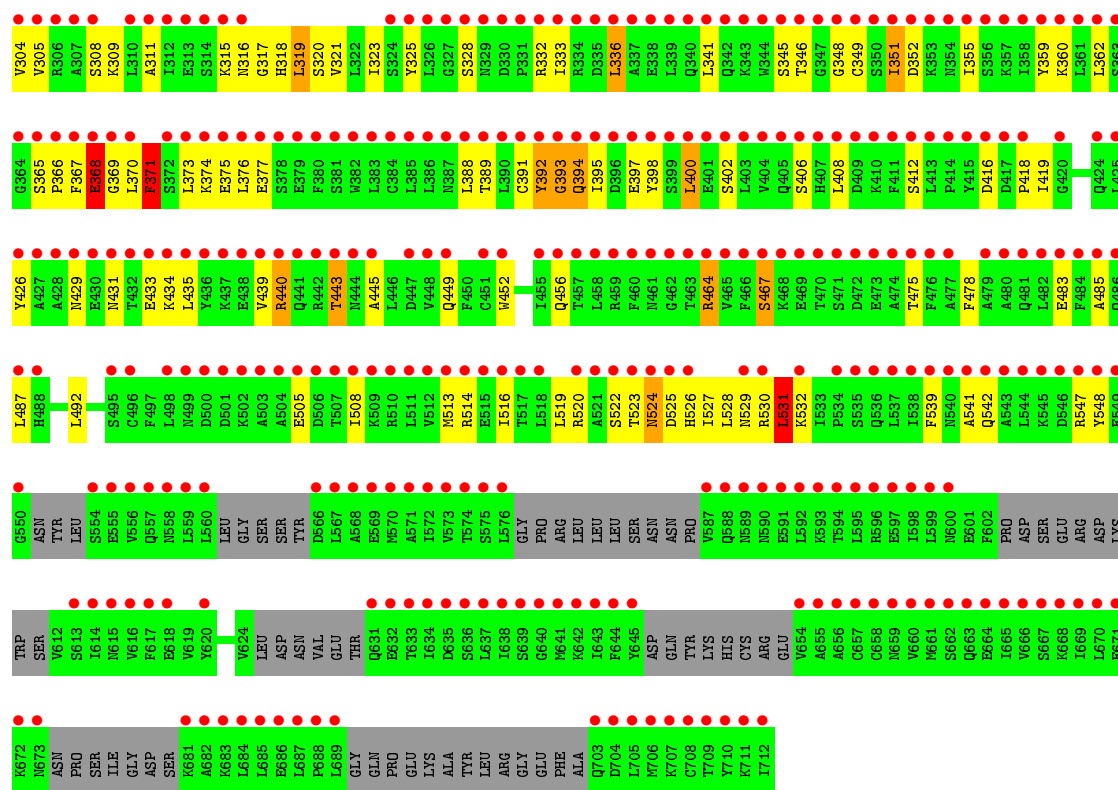
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

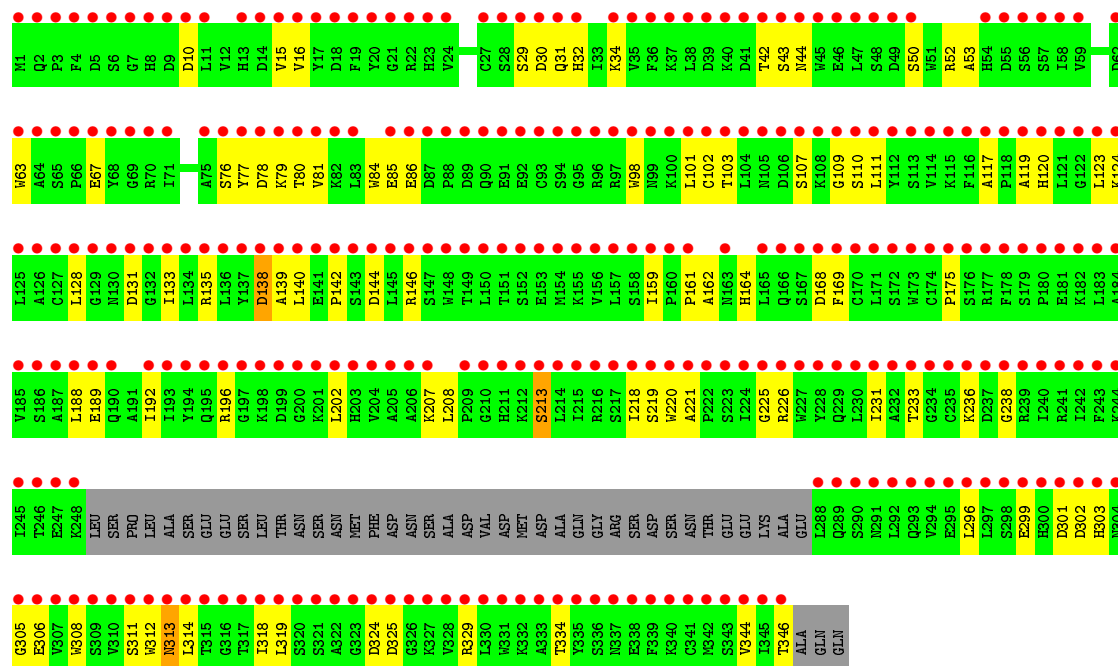
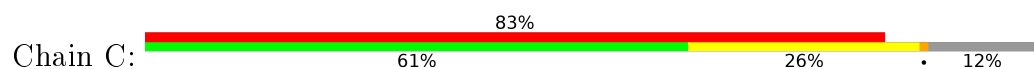


• Molecule 2: Nucleoporin NUP145

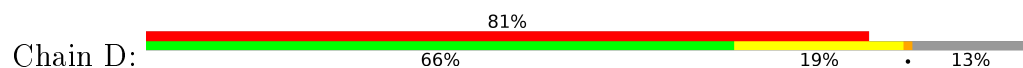


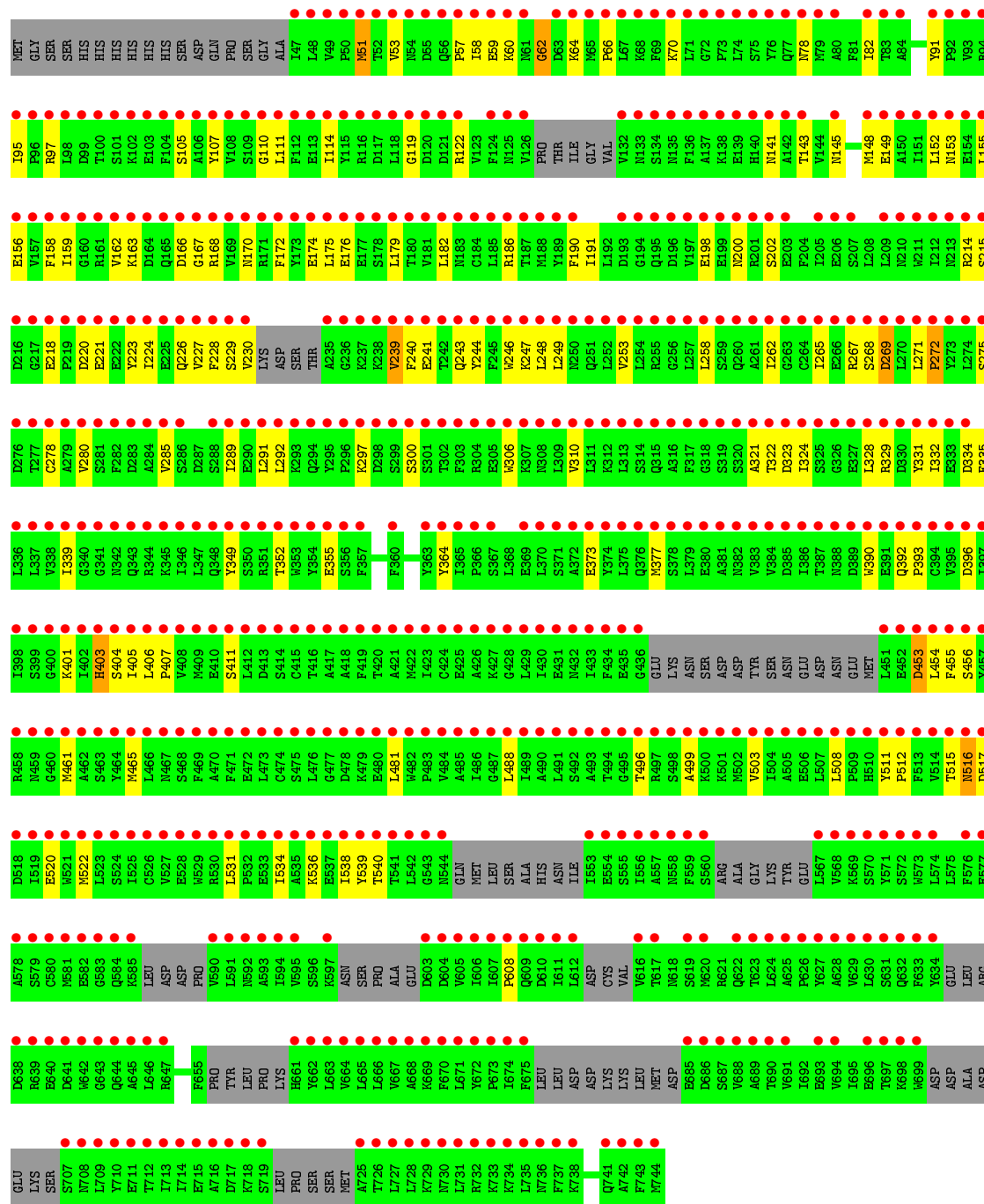


• Molecule 3: Nucleoporin SEH1



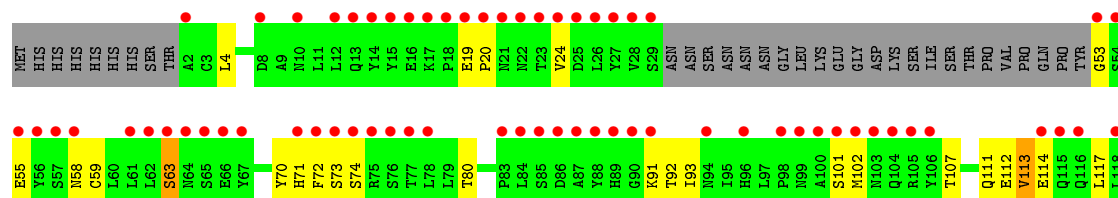
• Molecule 4: Nucleoporin NUP85





• Molecule 5: Nucleoporin NUP120

Chain E:

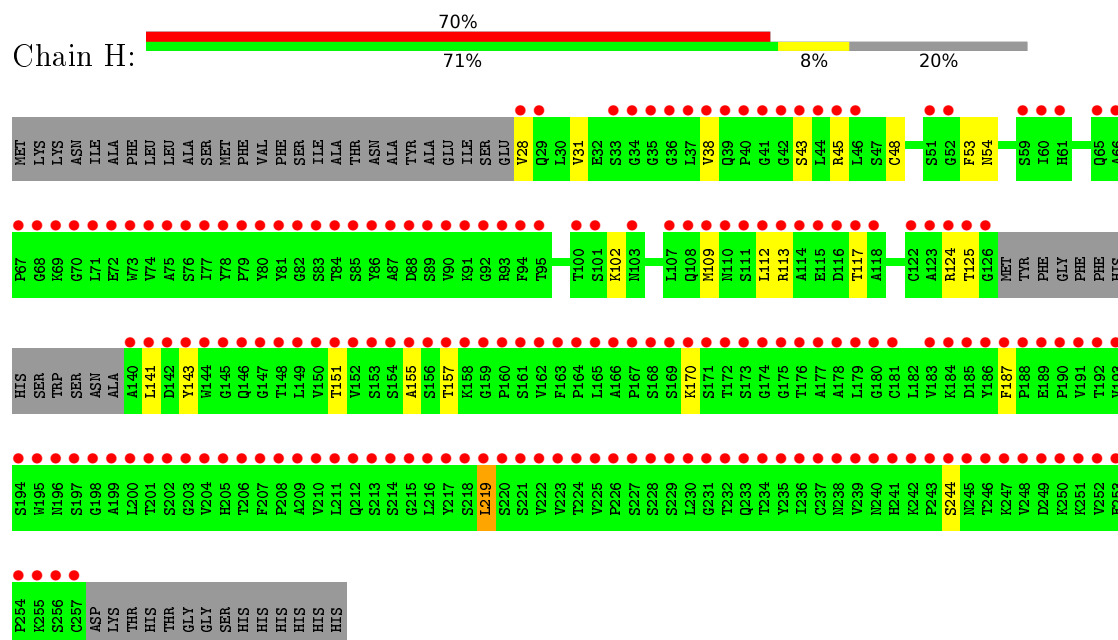


ILE	TRP	ASP	D833	F770	F710	E645	D685	L525	K454	D393	P320	T249	L183	V119
LEU	GLU	THR	ARG	D771	N711	I646	L586	R526	T455	D394	T321	S260	L184	
ASN		VAL	ASN	Q772	ALA	F647	I587	S527	A456	D395	N322	F251	G185	L123
SER			SER	S773	SER	G648	N588	I528	F457	D396	L323	T252	L186	
LYS			SER	Y774	ILE	Q649	N589	S529	N458	D397	S324	L253	K187	D126
VAL				Y775	T715	H650	O590	K531	N459	D398	A325	L254	K188	G125
V1025				E776	E716	I651	N591	F532	A460	D399	S326	Q255	Y189	S127
T1026				F777	N717	S652	K592	F533	S461	D400	A327	D256	F128	
T1027				F778	N718	T653	K593	D534	S462	D401	L328	Y257	D189	
T1028				H779	F719	L654	O594	D535	L463	D402	S329	D258	Y192	L129
D1029				H780	D720	L655	I595	I536	T464	D403	K330	M259	H193	T130
I1030				D781	M721	D656	F596	I537	L465	V404	S330	V260	Y194	L131
I1031				T782	T722	L657	N597	T537	Y466	E405	V335	G260	F195	Q132
R1032				P783	F723	H658	K598	G538	Y467	R406	L336	Q262	F196	L133
D1033				G784	F724	F659	K599	E539	D468	R407	S263	G263	L197	P134
L1034				A785	R725	K660	D600	L540	D469	F408	R337	S264	L198	L135
R1035				T786	T726	Q661	F601	P541	E470	D409	P339	S265	F199	S136
G1036				Y787	S727	F662	I602	D542	I471	N410	P340	D266	F199	L137
LEU				Y788	ILE	L663	S603	S543		L411	E341	P267	D201	L138
				Y789	ILE	L664	A604	N544	N474	K412	L342	P268	D202	L139
				Y790	ILE	L665	L605	T545	C475	S413	N343	S269	S203	S140
				Y791	ASN	L666	K606	T546	F476	R414	V344	F270	Y204	S141
				Y792	THR	L667	F607	V547	Q477	V415	E345	R271	L205	N143
				Y793	THR	Y668	D608	K548	P478	D416	A346	K272	K206	L144
				Y794	THR	R669	O609	E549	Y479	T417	S347	V273	S207	L145
				Y795	THR	Q670	F610	F550	M480	Q418	Y348	E274	G147	N146
				Y796	THR	D671	T611	T551	V490	E421	I352	A275	R210	G148
				Y797	THR	K672	S612	D552		R422		V276	F211	G149
				Y798	THR	C673	L613	I553	W493	A423	W355	L280	F212	F150
				Y799	THR	L674	S615	K555		Q424	K356	Y283	S213	H151
				Y800	THR	L675	L616	N556	N486	Q425	S357	N284	R214	L152
				Y801	THR	A676	L617	C557	N487	L426	G358	N285	S215	Q153
				Y802	THR	E677	S618	L558	H498	L427	T359	T286	S216	N154
				Y803	THR	L678	L619	E559	S499	S428	A360	L287	K217	P155
				Y804	THR	L680	H620	N560	E500	E429	K361	V288	S218	P156
				Y805	THR	K681	Q621	Q561	T501	N430	K362		D219	Y157
				Y806	THR	D682	L622	F562	D502	K431			Y220	F158
				Y807	THR	S683	L623	E563	G503	L432	N369	L291	D221	T159
				Y808	THR	S684	L624	L564	S504	L433	D370	P292	S222	V160
				Y809	THR	E685	L625	T565	E505	N434	E371	L293	V223	R161
				Y810	THR	F686	H626	N566	L506	A435	S372	E294	V224	V162
				Y811	THR	S687	L627	L567	F507	H436		N295	L228	P163
				Y812	THR	F688	L628	K568	K508	N437	N375	G296	L229	H164
				Y813	THR	G689	L629	I569	Y509	E438	Y376	L297	F229	
				Y814	THR	V690	L630	L570	L510	D439	E377		H230	F167
				Y815	THR	K691	L631	D571	R511	E440	W378	M300	E231	Y168
				Y816	THR	F692	Q632	D572	T512	E441	I379		R232	V169
				Y817	THR	F693	L633	E573	L513	Y442	E380	L304	Y233	S170
				Y818	THR	M694	L634	L574	M514	L443	S381	V305	P171	P172
				Y819	THR	Y701	L635	N575	G515	A444		ASP	T238	Q173
				Y820	THR	T702	L636	N576	F516	N445	K384	SER	Q239	F173
				Y821	THR	D703	L637	F577	A517	L446	S385	SER	N240	S174
				Y822	THR	F692	L638	D578	S518	E447	L386	GLY	C241	
				Y823	THR	S704	L639	I579	T519	T448	V387	ILE	H242	F177
				Y824	THR	L705	L640	P580	L520	L449	D388		L178	L177
				Y825	THR	I706	L641	P581	S521	L450	L389	T312	E279	E279
				Y826	THR	N707	L642	V581	M522	R451	Q390	T313	D180	D180
				Y827	THR	S707	L643	V582	M523	D452	S391	T314	G181	G181
				Y828	THR	D708	L644	N584	V524	V453	E392		L248	L248
				Y829	THR	V709	L645							
				Y830	THR									
				Y831	THR									
				Y832	THR									
				Y833	THR									
				Y834	THR									
				Y835	THR									
				Y836	THR									
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				Y907	THR									

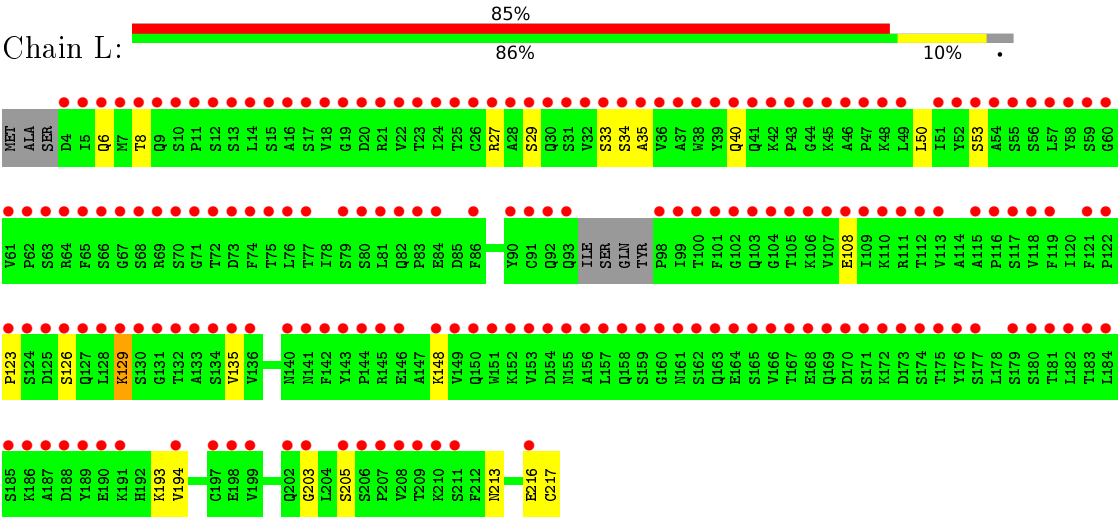
Chain F:



Chain H:



● Molecule 8: Antibody 57 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.65Å 186.30Å 199.57Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	67.52 – 7.38 68.01 – 7.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.52-7.38) 99.7 (68.01-7.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 7.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, R_{free}	0.330 , 0.353 0.328 , 0.361	Depositor DCC
R_{free} test set	1021 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	734.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	26139	wwPDB-VP
Average B, all atoms (Å ²)	716.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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

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	0.32	0/2220	0.62	0/3028
2	B	0.37	0/3860	0.66	2/5224 (0.0%)
3	C	0.28	0/2499	0.64	0/3388
4	D	0.30	0/4602	0.58	2/6246 (0.0%)
5	E	0.33	0/6730	0.55	1/9158 (0.0%)
6	F	0.35	0/3472	0.64	2/4714 (0.0%)
7	H	0.31	0/1610	0.62	1/2194 (0.0%)
8	L	0.29	0/1631	0.60	0/2210
All	All	0.32	0/26624	0.60	8/36162 (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
2	B	0	2
5	E	0	2
6	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	167	GLY	N-CA-C	-6.40	97.09	113.10
4	D	608	PRO	N-CA-CB	6.10	110.62	103.30
2	B	187	ASP	CB-CG-OD2	6.04	123.73	118.30
7	H	219	LEU	CA-CB-CG	6.04	129.19	115.30
5	E	818	PRO	N-CA-CB	5.78	110.23	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide
5	E	190	ASP	Mainchain
5	E	264	ASP	Sidechain
6	F	151	GLY	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	60	0
2	B	3805	0	3499	106	0
3	C	2438	0	2378	56	0
4	D	4535	0	4073	104	0
5	E	6622	0	5907	80	0
6	F	3404	0	3378	77	2
7	H	1576	0	1532	13	0
8	L	1599	0	1554	9	2
All	All	26139	0	24417	462	2

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 9.

The worst 5 of 462 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)
5:E:537:THR:HG22	5:E:743:ASN:HA	1.54	0.86
5:E:293:LEU:HD13	5:E:297:LEU:HD12	1.59	0.85
4:D:517:ASP:OD1	7:H:54:ASN:N	2.10	0.85
4:D:159:ILE:HG12	4:D:175:LEU:HB3	1.59	0.84
4:D:156:GLU:OE2	4:D:214:ARG:NH1	2.13	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:233:THR:OG1	8:L:203:GLY:O[4_455]	2.05	0.15
6:F:232:ASN:O	8:L:205:SER:N[4_455]	2.08	0.12

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%)	228 (84%)	36 (13%)	6 (2%)	8	49
2	B	491/652 (75%)	451 (92%)	30 (6%)	10 (2%)	9	51
3	C	303/349 (87%)	266 (88%)	31 (10%)	6 (2%)	9	51
4	D	592/715 (83%)	532 (90%)	50 (8%)	10 (2%)	11	55
5	E	858/1045 (82%)	798 (93%)	49 (6%)	11 (1%)	15	60
6	F	413/454 (91%)	368 (89%)	34 (8%)	11 (3%)	6	45
7	H	213/271 (79%)	206 (97%)	7 (3%)	0	100	100
8	L	206/217 (95%)	198 (96%)	6 (3%)	2 (1%)	19	65
All	All	3346/4000 (84%)	3047 (91%)	243 (7%)	56 (2%)	11	55

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	C	43	SER

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%)	224 (96%)	9 (4%)	39	72
2	B	367/594 (62%)	332 (90%)	35 (10%)	11	41
3	C	269/305 (88%)	261 (97%)	8 (3%)	48	77
4	D	424/642 (66%)	414 (98%)	10 (2%)	57	82
5	E	639/980 (65%)	616 (96%)	23 (4%)	42	74
6	F	387/418 (93%)	367 (95%)	20 (5%)	29	65
7	H	175/224 (78%)	170 (97%)	5 (3%)	50	78
8	L	184/191 (96%)	179 (97%)	5 (3%)	52	79
All	All	2678/3606 (74%)	2563 (96%)	115 (4%)	35	70

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	51	MET
5	E	127	SER
7	H	113	ARG
4	D	143	THR
4	D	488	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	313	ASN
4	D	467	ASN
5	E	575	ASN
2	B	542	GLN
5	E	588	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 ⓘ

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	274/297 (92%)	15.07	272 (99%) 0 0	629, 712, 763, 800	0
2	B	511/652 (78%)	9.33	459 (89%) 0 1	374, 655, 746, 784	0
3	C	307/349 (87%)	10.24	290 (94%) 0 1	631, 756, 814, 905	0
4	D	620/715 (86%)	9.98	581 (93%) 0 1	388, 746, 989, 1000	0
5	E	896/1045 (85%)	8.87	726 (81%) 0 2	422, 725, 816, 883	0
6	F	419/454 (92%)	12.15	373 (89%) 0 2	545, 699, 803, 877	0
7	H	217/271 (80%)	8.87	189 (87%) 0 2	528, 677, 821, 884	0
8	L	210/217 (96%)	8.38	185 (88%) 0 2	526, 676, 756, 791	0
All	All	3454/4000 (86%)	10.12	3075 (89%) 0 2	374, 711, 890, 1000	0

The worst 5 of 3075 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	75.7
5	E	519	THR	62.9
1	A	27	CYS	59.4
1	A	100	ALA	58.7
2	B	153	LYS	56.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.