



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2024 – 11:32 PM JST

PDB ID : 7FIK
EMDB ID : EMD-31600
Title : The cryo-EM structure of the CR subunit from *X. laevis* NPC
Authors : Shi, Y.; Huang, G.; Zhan, X.
Deposited on : 2021-07-31
Resolution : 3.70 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

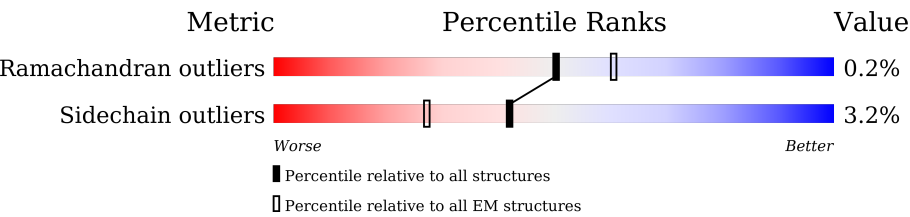
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.




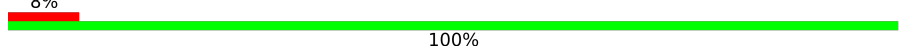
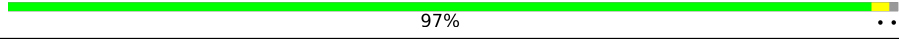











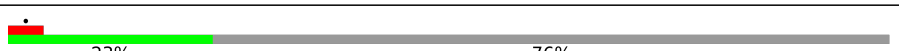


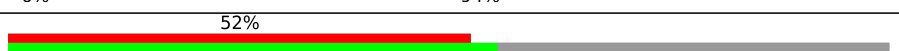

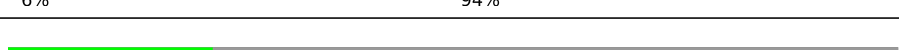

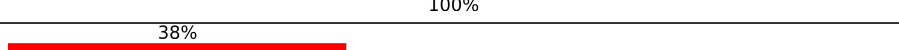
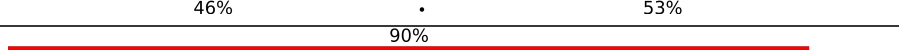
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2011	
1	a	2011	
2	B	653	
2	b	653	
3	C	375	
3	c	375	
4	D	360	
4	d	360	
5	E	1435	

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Mol	Chain	Length	Quality of chain
5	e	1435	
6	F	326	
6	f	326	
7	G	1742	
7	g	1742	
8	H	320	
8	h	320	
9	I	916	
9	i	916	
10	J	1140	
11	K	2905	
11	L	2905	
11	M	2905	
11	N	2905	
11	O	2905	
12	P	820	
12	S	820	
12	p	820	
12	s	820	
13	W	1388	
14	X	161	
15	Y	728	
16	j	1140	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 116163 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 MGC83295 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1795	Total	C	N	O	S	0	0
			9238	5541	1851	1841	5		
1	a	1725	Total	C	N	O	S	0	0
			8811	5278	1770	1757	6		

- Molecule 2 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	598	Total	C	N	O	S	0	0
			4799	3051	833	878	37		
2	b	595	Total	C	N	O	S	0	0
			4549	2894	793	829	33		

- Molecule 3 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2557	1590	461	488	18		
3	c	309	Total	C	N	O	S	0	0
			2445	1518	443	468	16		

- Molecule 4 is a protein called Nucleoporin SEH1-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	316	Total	C	N	O	S	0	0
			2473	1550	443	463	17		
4	d	312	Total	C	N	O	S	0	0
			2435	1531	435	451	18		

- Molecule 5 is a protein called outer Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1310	Total	C	N	O	S	0	0
			7891	4857	1495	1522	17		
5	e	1247	Total	C	N	O	S	0	0
			8134	5074	1497	1533	30		

- Molecule 6 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	326	Total	C	N	O		0	0
			1607	954	326	327			
6	f	322	Total	C	N	O	S	0	0
			2524	1612	436	461	15		

- Molecule 7 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	567	Total	C	N	O	S	0	0
			4209	2659	769	764	17		
7	g	603	Total	C	N	O	S	0	0
			4770	3022	868	856	24		

- Molecule 8 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	288	Total	C	N	O	S	0	0
			2235	1417	383	423	12		
8	h	288	Total	C	N	O	S	0	0
			2259	1429	385	433	12		

- Molecule 9 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	729	Total	C	N	O	0	0
			3626	2168	729	729		
9	i	673	Total	C	N	O	0	0
			3347	2001	673	673		

- Molecule 10 is a protein called nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	1015	Total	C	N	O	0	0
			5029	2999	1015	1015		

- Molecule 11 is a protein called Nup358 complex, clamps.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	697	Total	C	N	O	0	0
			3460	2066	697	697		
11	L	679	Total	C	N	O	0	0
			3372	2014	679	679		
11	M	654	Total	C	N	O	0	0
			3246	1938	654	654		
11	N	701	Total	C	N	O	0	0
			3480	2078	701	701		
11	O	683	Total	C	N	O	0	0
			3391	2025	683	683		

- Molecule 12 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	593	Total	C	N	O		0	0
			2945	1759	593	593			
12	S	52	Total	C	N	O	S	0	0
			432	272	77	81	2		
12	s	52	Total	C	N	O	S	0	0
			432	272	77	81	2		
12	p	456	Total	C	N	O		0	0
			2267	1355	456	456			

- Molecule 13 is a protein called Nup155-prov protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	324	Total	C	N	O	S	0	0
			2636	1688	447	485	16		

- Molecule 14 is a protein called Nup98.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	161	Total	C	N	O	0	0
			794	472	161	161		

- Molecule 15 is a protein called Nucleoporin Nup88A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	339	Total	C	N	O	0	0
			1676	998	339	339		

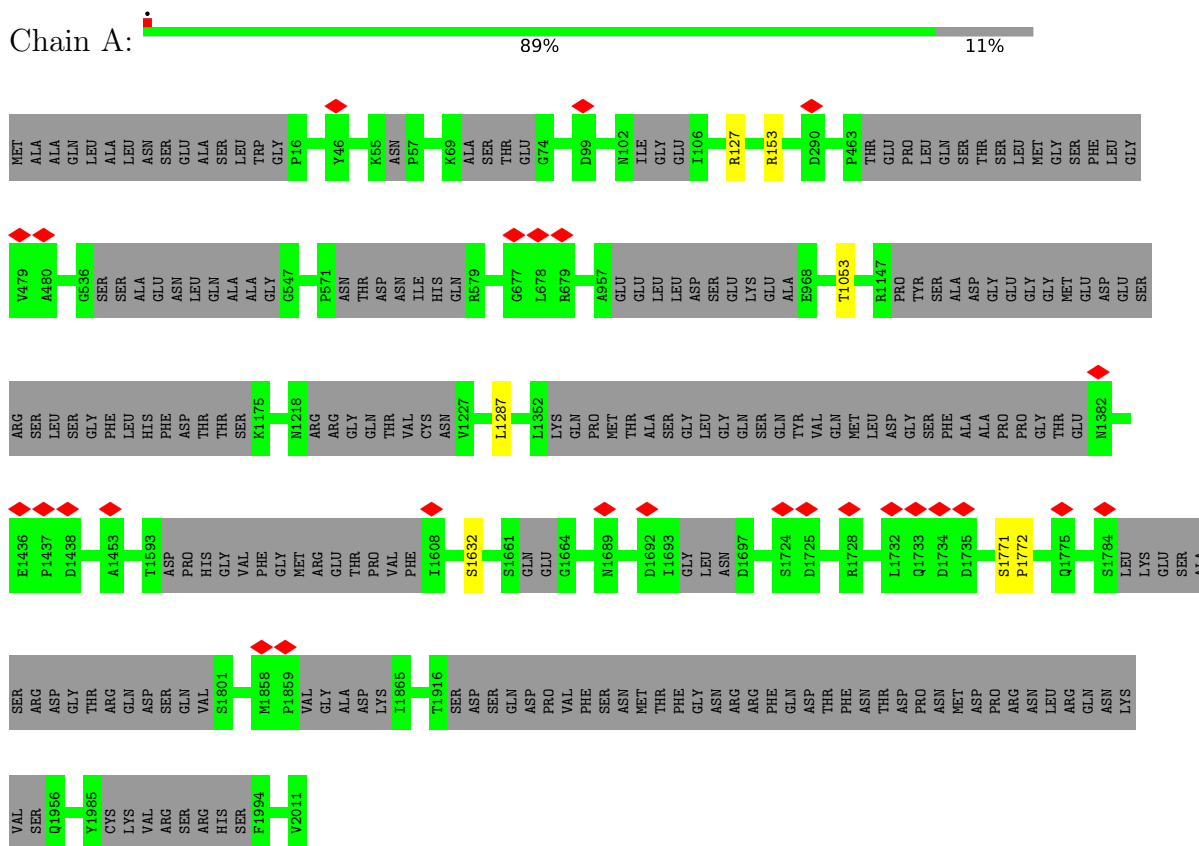
- Molecule 16 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	j	1028	5094	3038	1028	1028	0	0

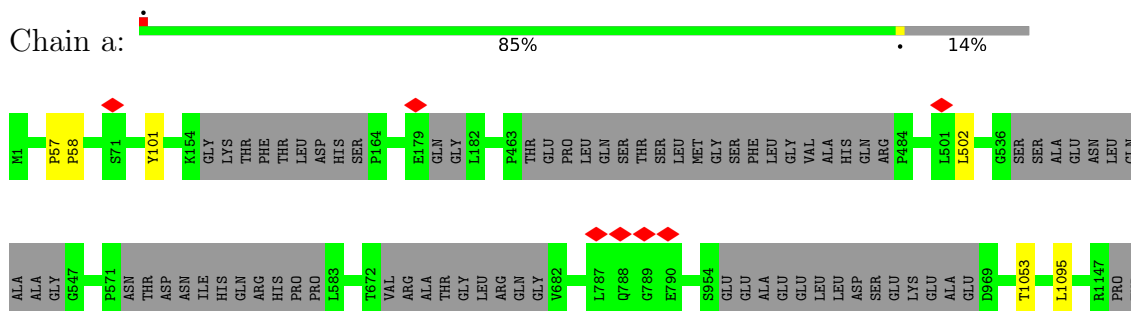
3 Residue-property plots

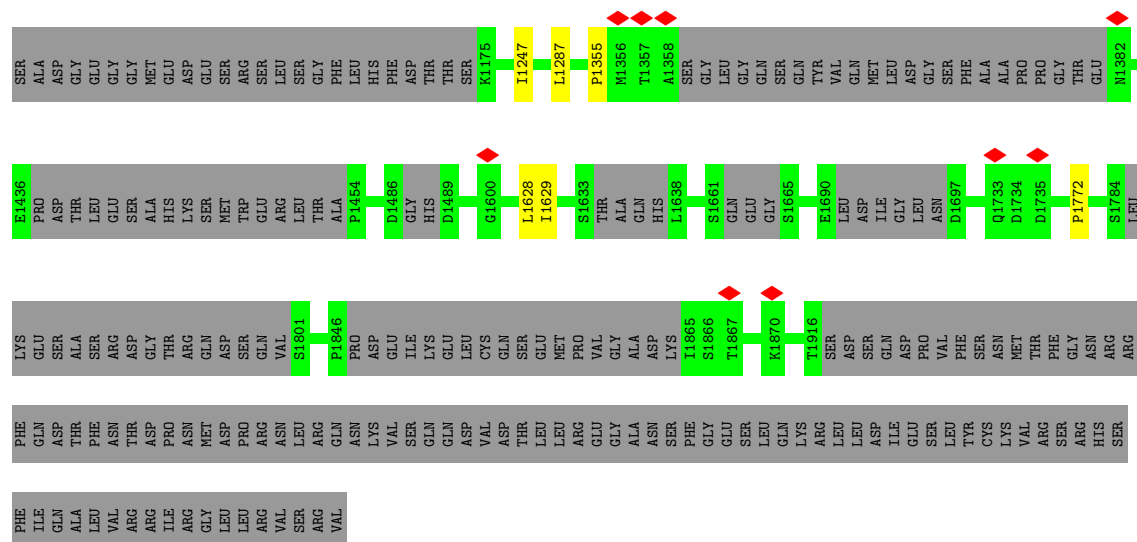
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: MGC83295 protein

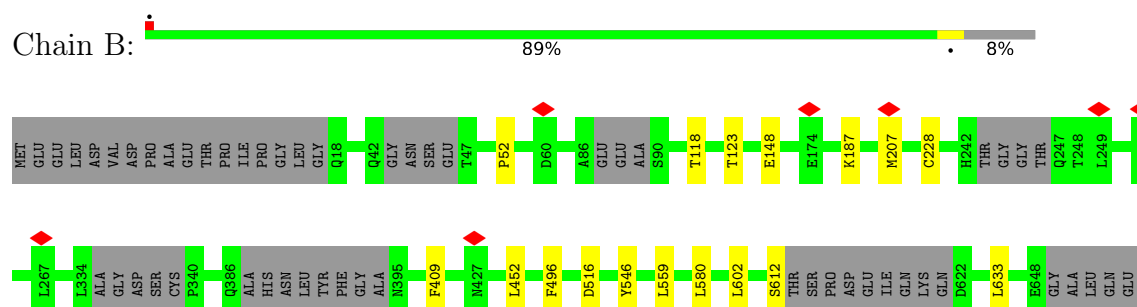


- Molecule 1: MGC83295 protein

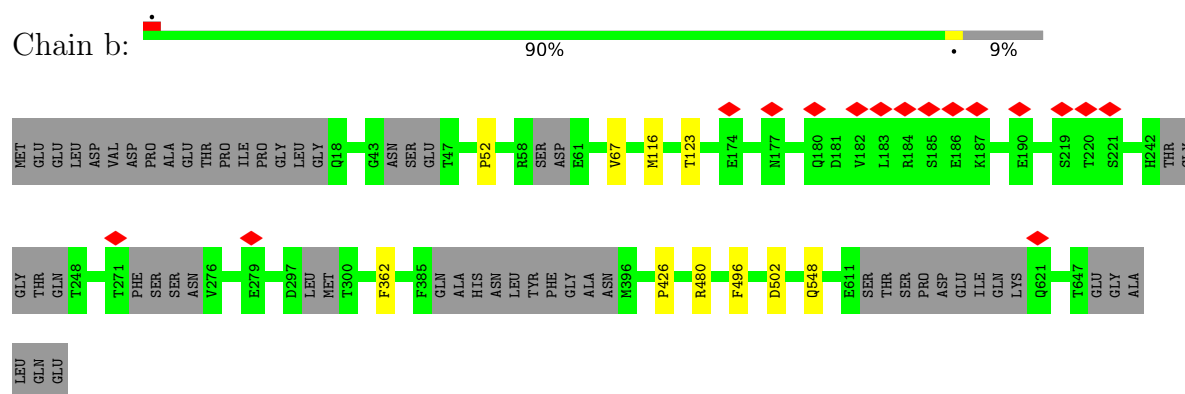




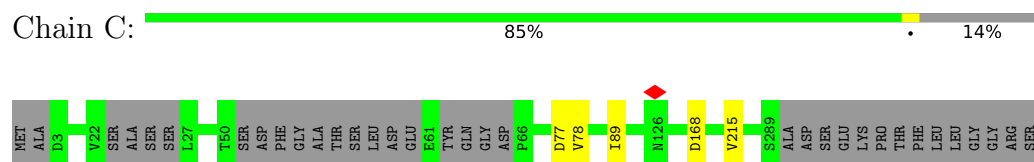
- Molecule 2: Nuclear pore complex protein Nup85

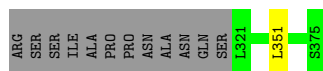


- Molecule 2: Nuclear pore complex protein Nup85



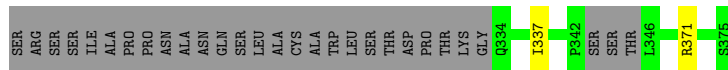
- Molecule 3: MGC154553 protein





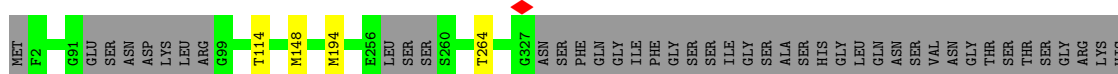
• Molecule 3: MGC154553 protein

Chain c: 80% 18%



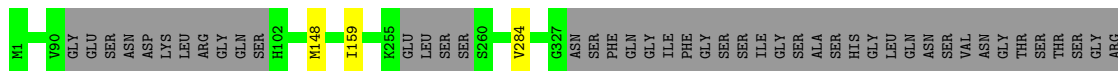
• Molecule 4: Nucleoporin SEH1-B

Chain D: 87% 12%



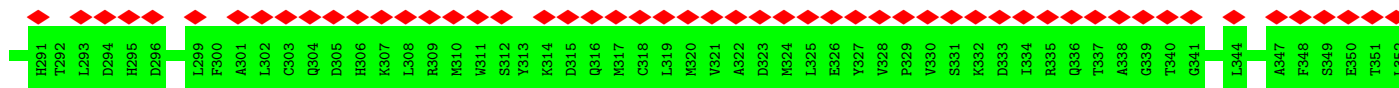
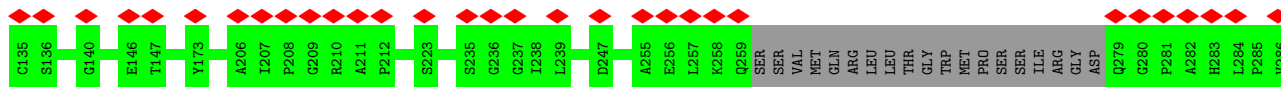
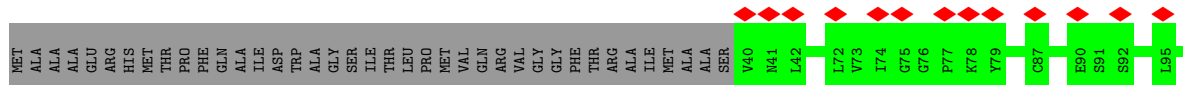
• Molecule 4: Nucleoporin SEH1-B

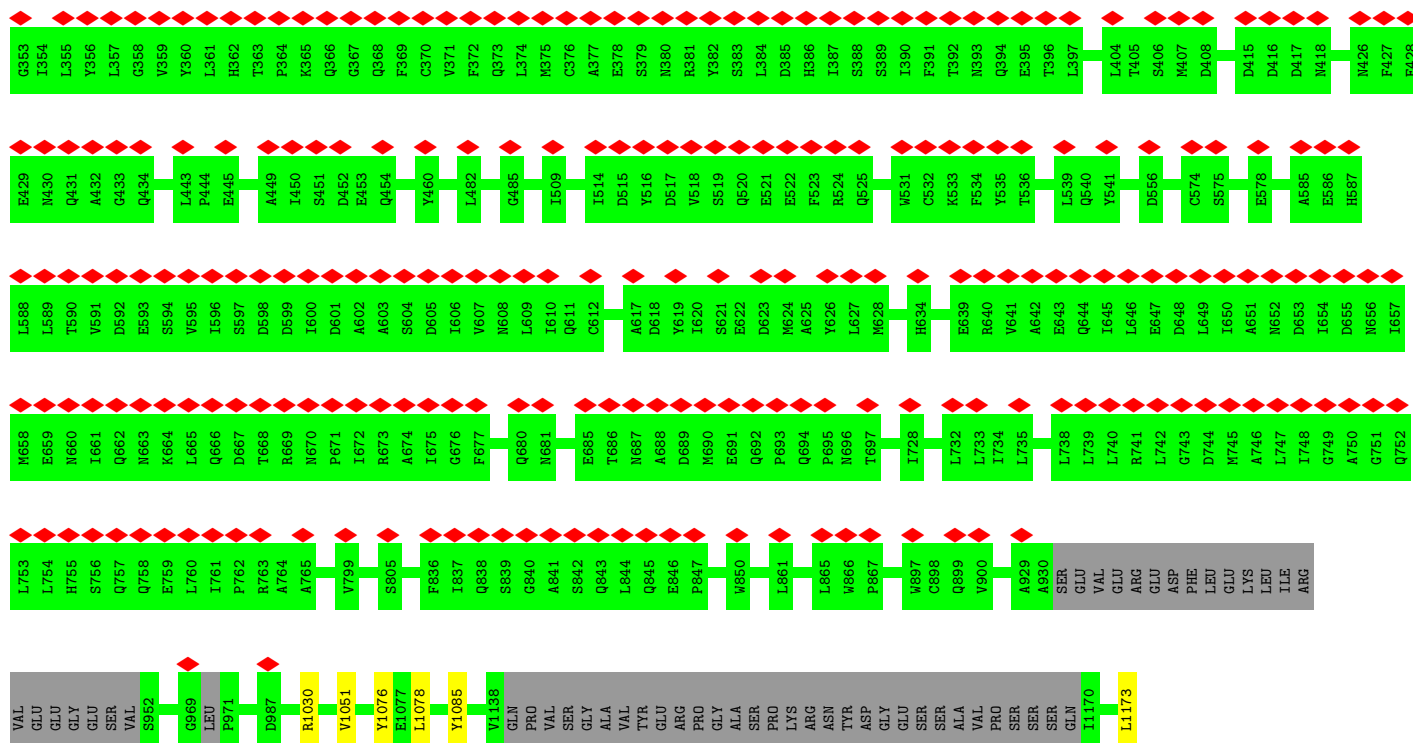
Chain d: 86% 13%



• Molecule 5: outer Nup160

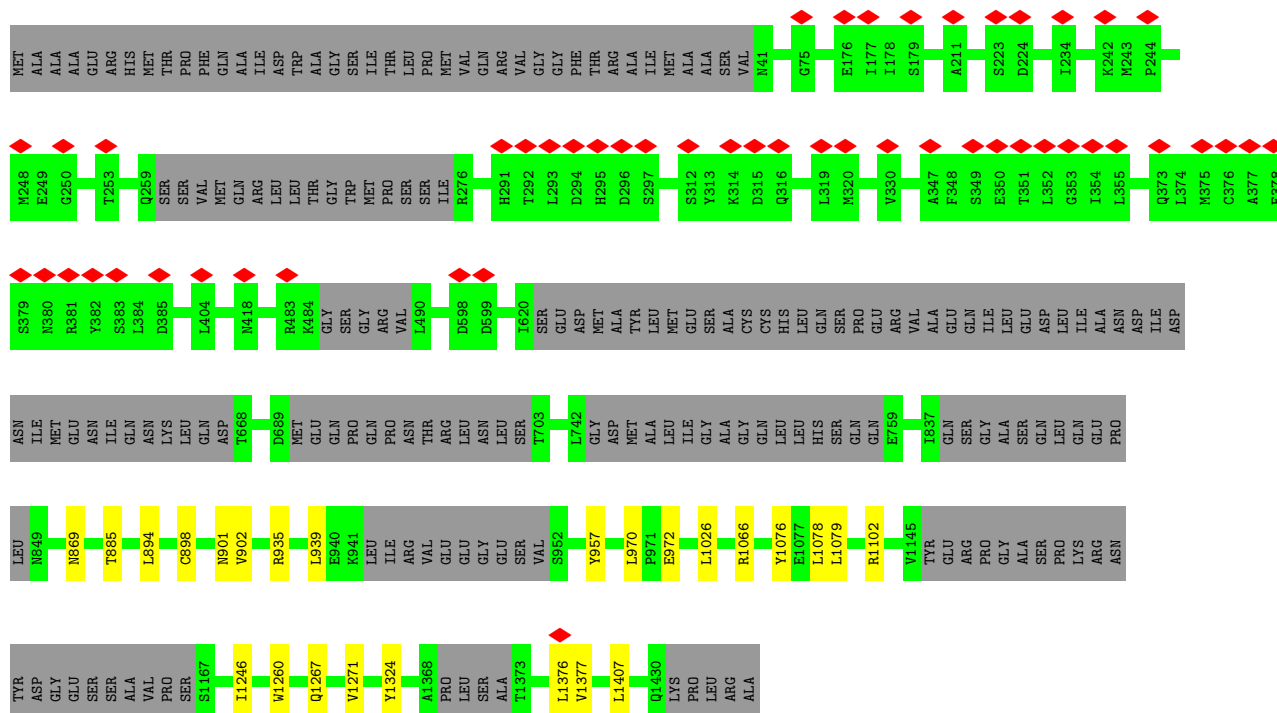
Chain E: 24% 90% 9%



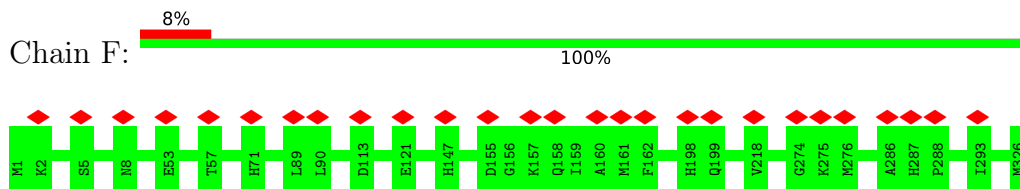


• Molecule 5: outer Nup160

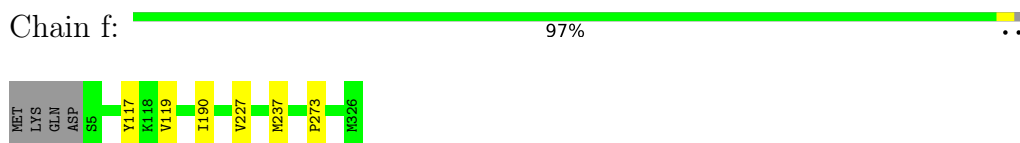
Chain e: 85% 13%



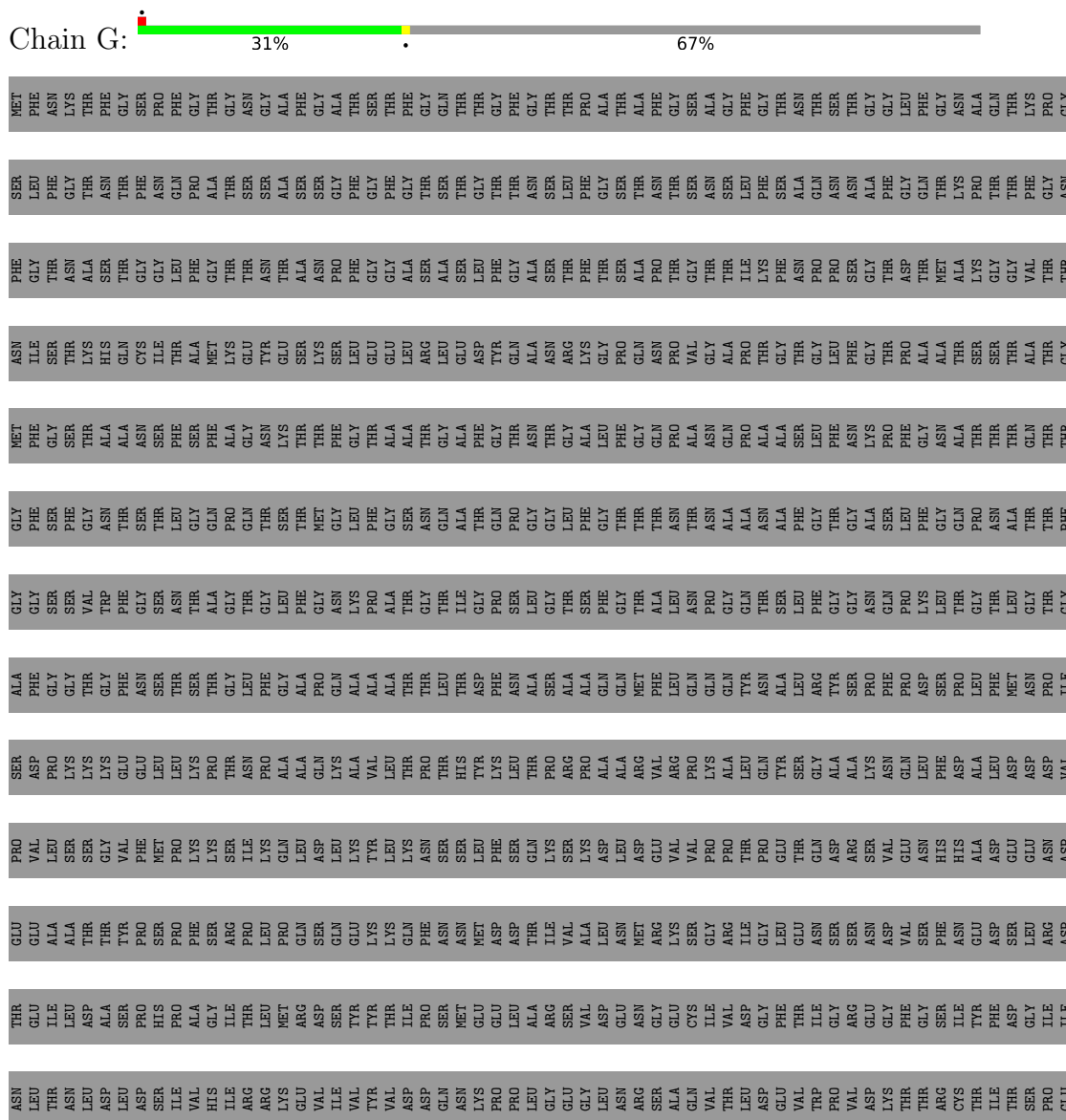
- Molecule 6: MGC83926 protein

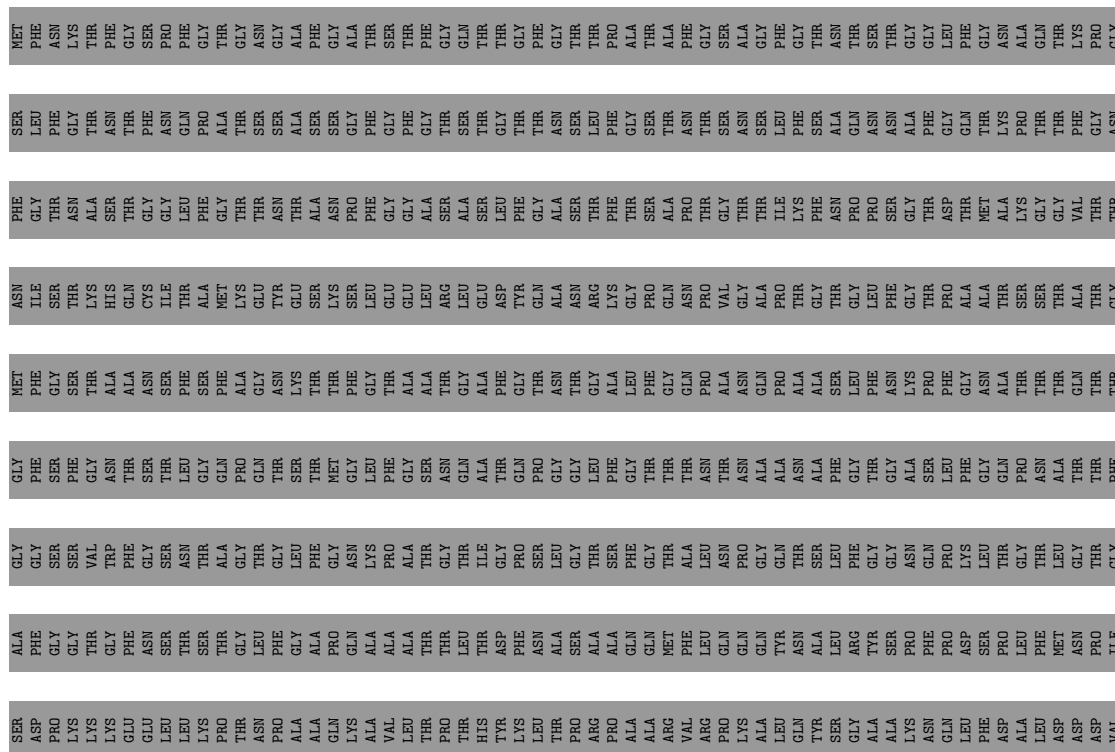
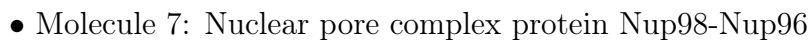


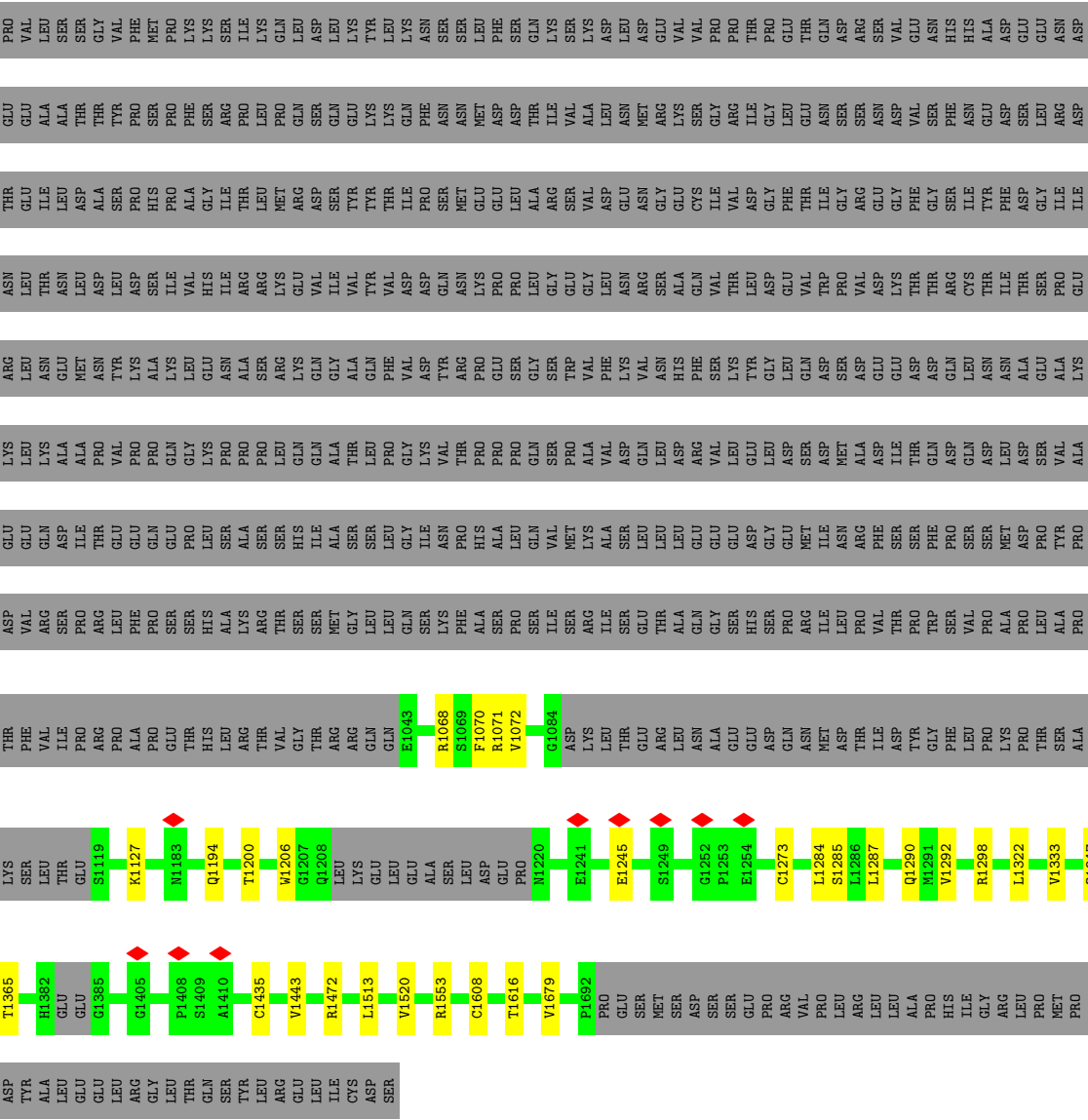
- Molecule 6: MGC83926 protein



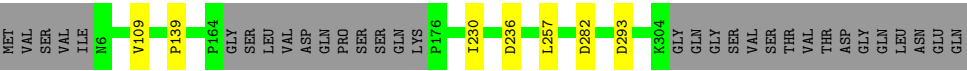
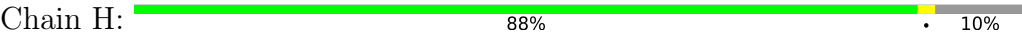
- Molecule 7: Nuclear pore complex protein Nup98-Nup96



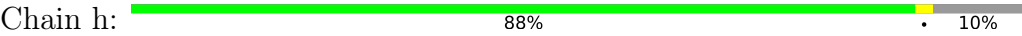




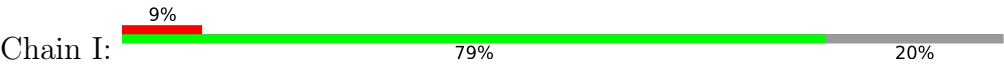
• Molecule 8: Protein SEC13 homolog

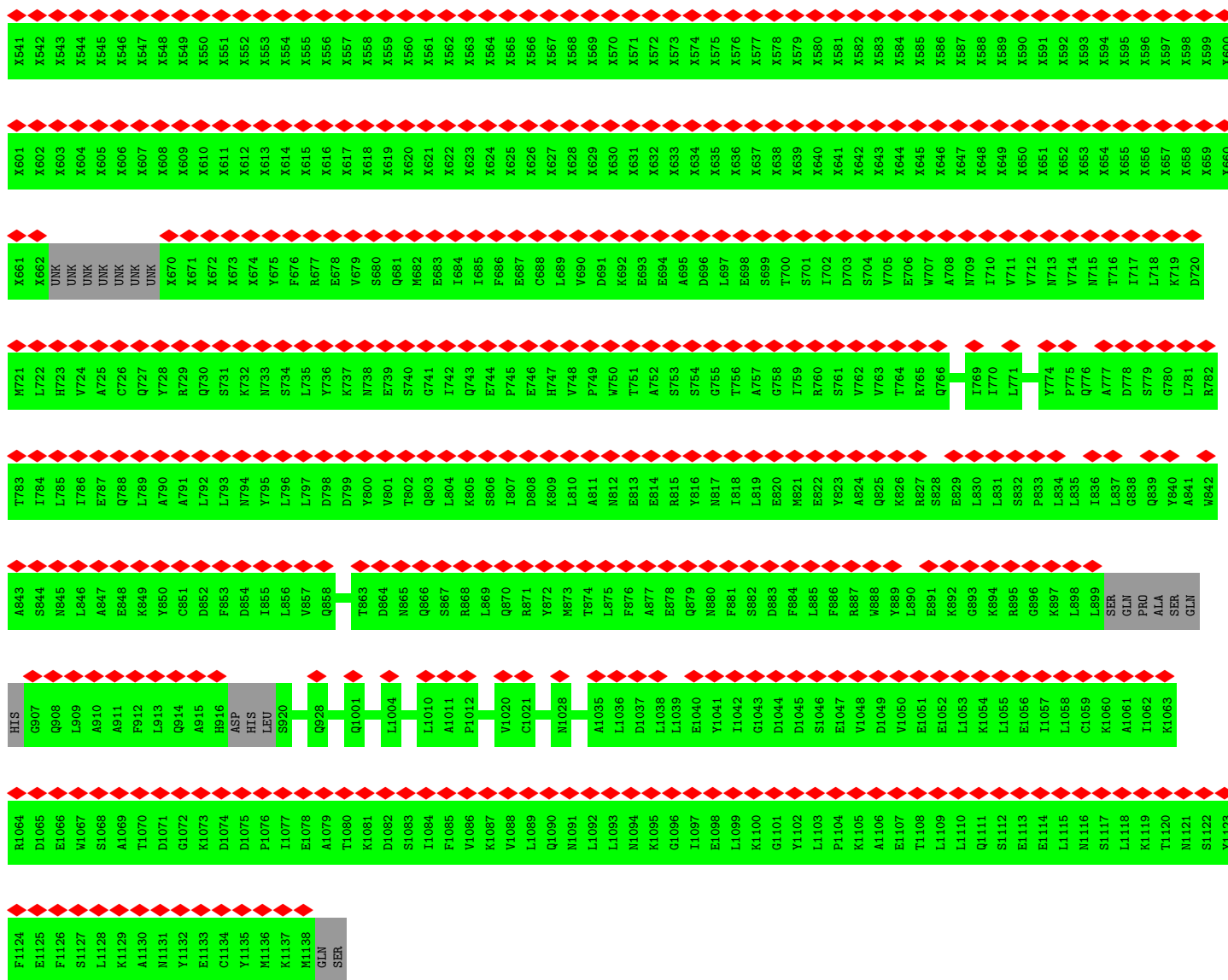


• Molecule 8: Protein SEC13 homolog

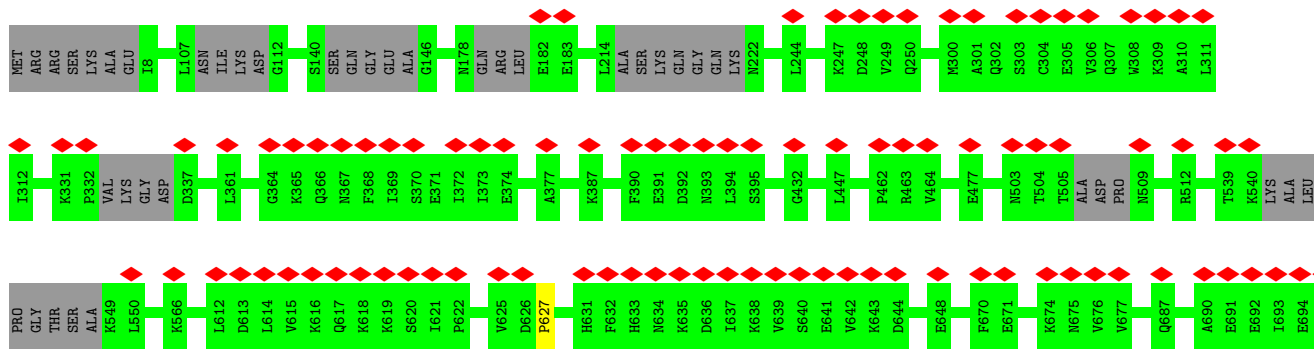


• Molecule 9: Nuclear pore complex protein





• Molecule 11: Nup358 complex, clamps





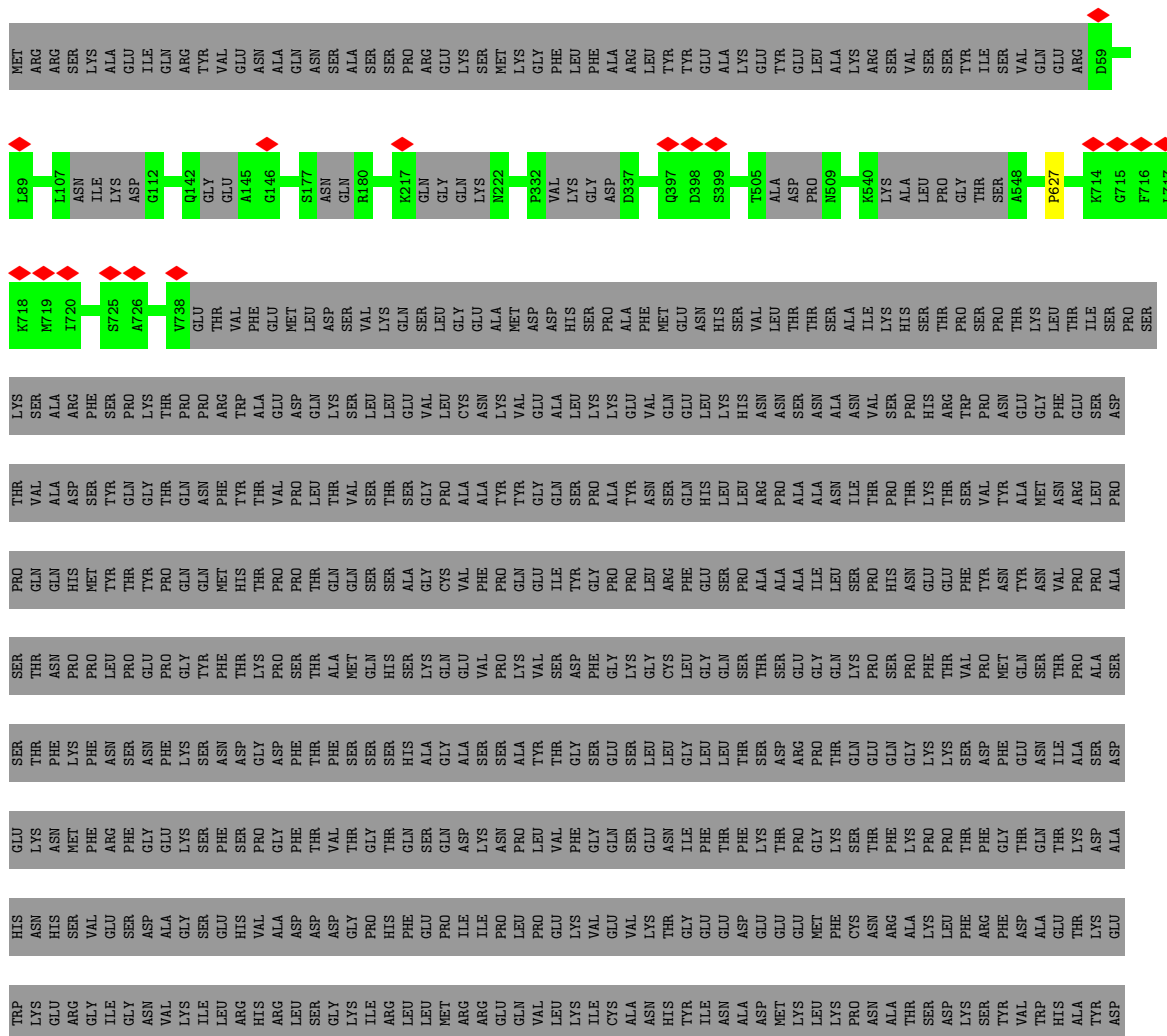
- Molecule 11: Nup358 complex, clamps

Met	Arg	Arg	S4	M14	A15	Q16	M17	S18	A19	S20	S21	P22	R23	A33	R34	L35	Y36	TYR	GLU	ALA	LYS	GLU	Y42	E43	L44	I53	SER	VAL	GLN	GLU	ARG	ASP	P60	L69	F70	E71	I72	E73	G74	N75	V76	N90	F91	T92	Q93	K94	L107	ASN	ILE	LYS	ASP	G112
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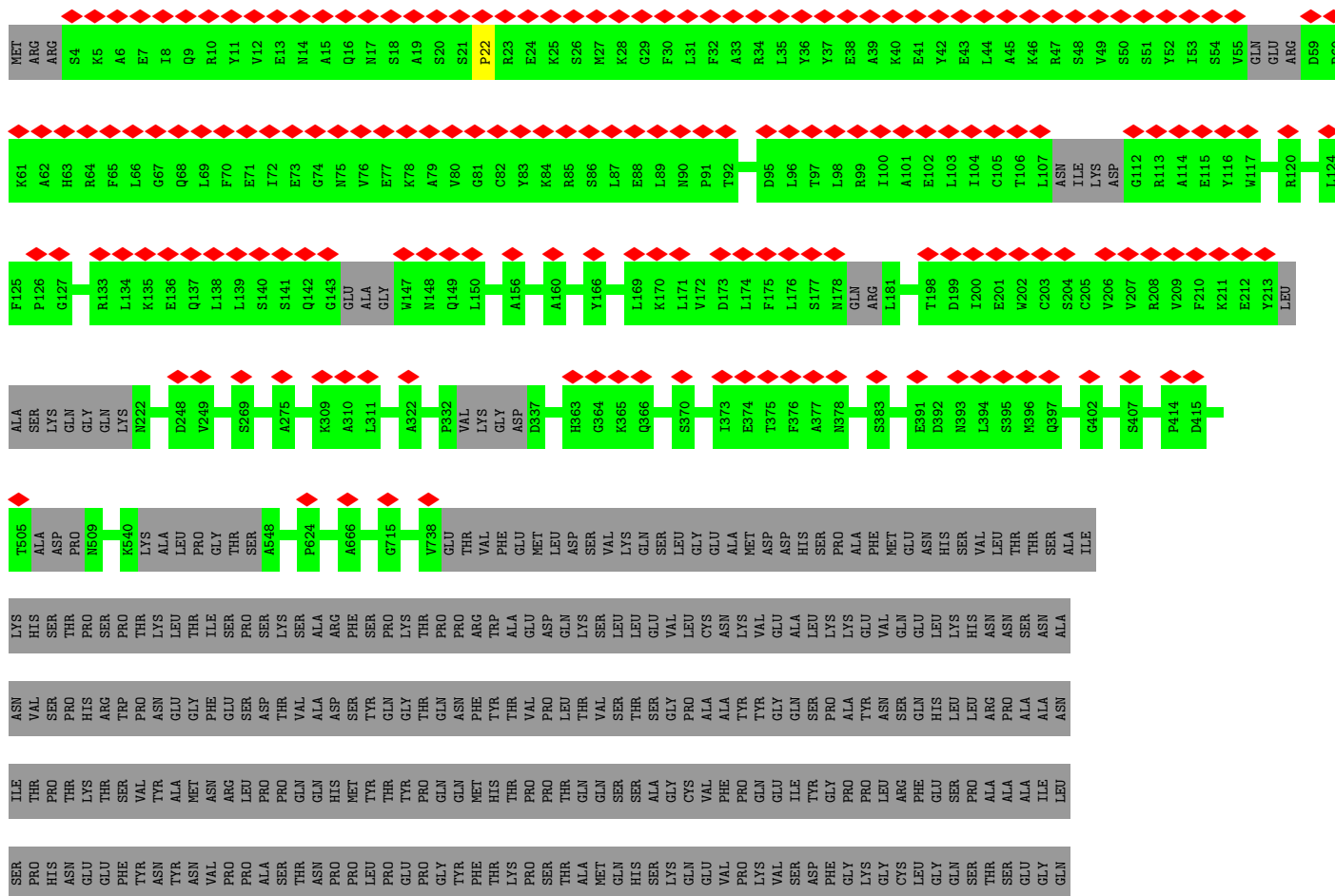


- Molecule 11: Nup358 complex, clamps





- Molecule 11: Nup358 complex, clamps



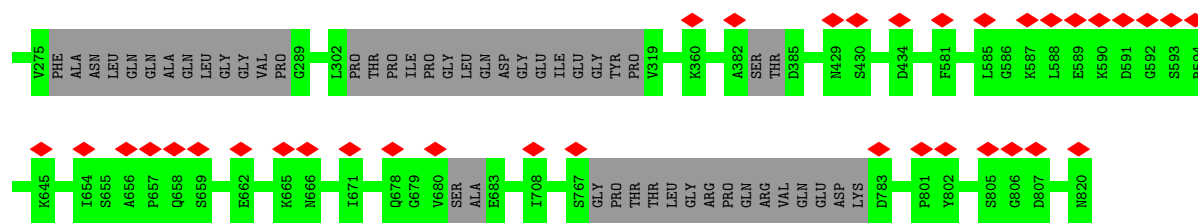






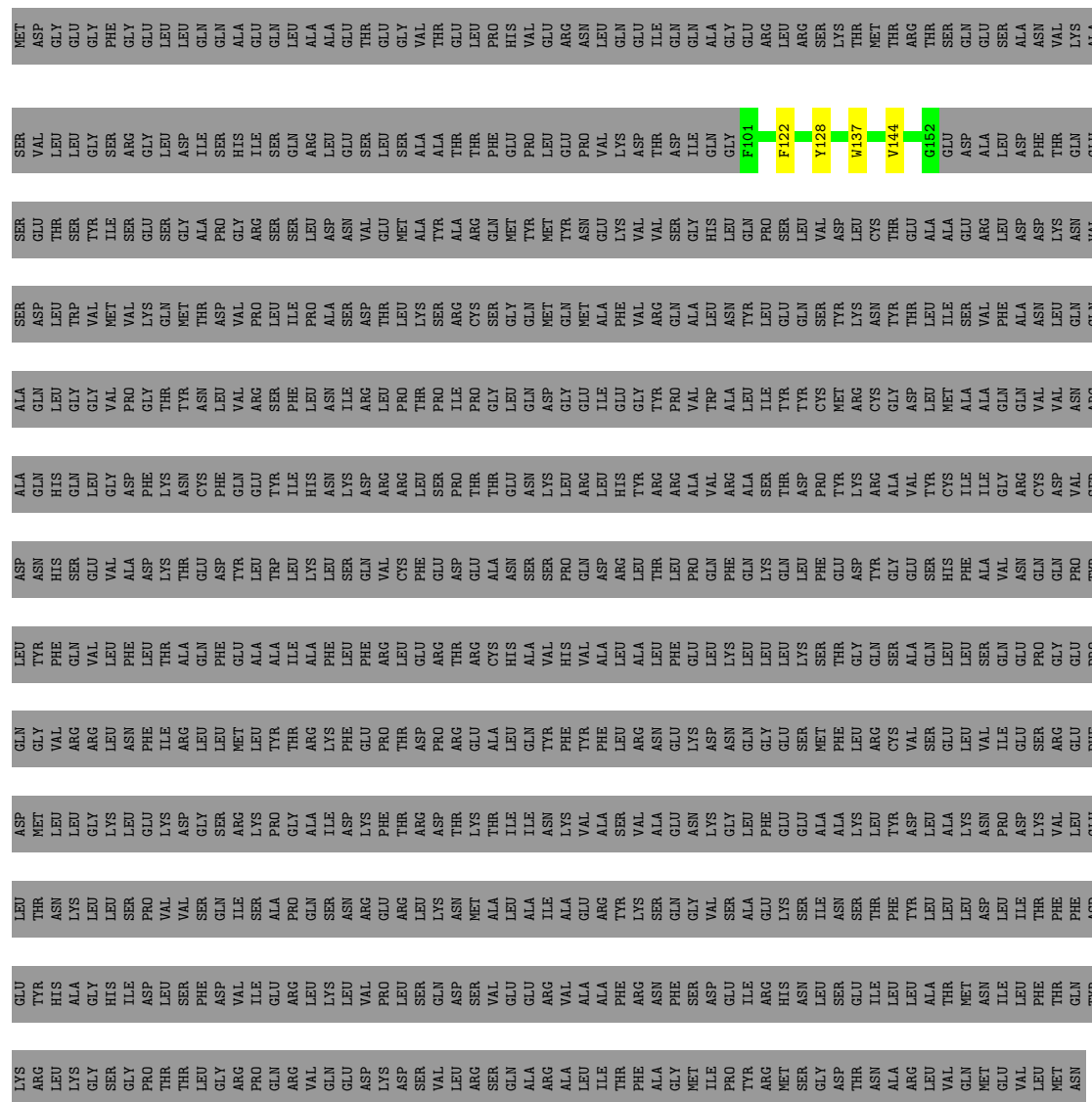
- Molecule 12: Nuclear pore complex protein Nup93

[illegible]



• Molecule 12: Nuclear pore complex protein Nup93

Chain S: 6% 94%



• Molecule 12: Nuclear pore complex protein Nup93

Chain s: 6% 94%

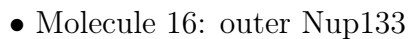


[illegible]

- Molecule 12: Nuclear pore complex protein Nup93



ASP	T242	V181	THR	SER	MET
	T243				
L244	K243	E182	VAL	LEU	GLY
	K244				
S245	R245	M183	ALA	GLY	PHE
	R246				
C247	S248	Y185	GLU	SER	GLY
	S249				
Q250	T248	A186	TYR	ARG	GLY
	T249				
M251	Q250	Q188	HIS	ASP	LEU
	Q252				
M253	Q252	Y190	VAL	SER	GLN
	M253				
A254	M253	M189	GLU	SER	ALA
	F255				
F256	A254	Q191	TRP	ARG	LEU
	F257				
R257	F256	M192	GLN	SER	THR
	Q258				
A259	R257	E194	LYS	LEU	HIS
	L260				
M261	A259	K195	ARG	ALA	VAL
	M261				
Y262	M261	V196	VAL	SER	GLY
	Y263				
L263	Y262	V197	GLN	SER	THR
	E264				
Q265	L263	S198	VAL	ALA	GLU
	Q265				
S266	Q265	G199	LEU	THR	ASN
	Y267				
K268	S266	H200	HIS	PHE	VAL
	Y268				
M269	K268	Q202	LEU	PRO	GLN
	C269				
T270	M269	P203	ALA	LEU	GLY
	T271				
L272	T270	S204	SER	GLY	ARG
	L273				
S274	L272	L205	GLU	VAL	LEU
	S274				
V275	L273	V206	ASP	LVS	GLN
	V275				
PHE	V275	D207	ALA	ASP	GLU
	ALA				
ASN	ALA	L208	LEU	THR	ILE
	ASN				
LEU	ASN	C209	PHE	ILE	GLN
	LEU				
GLN	LEU	T210	THR	GLN	GLY
	GLN				
ALA	GLN	E211	GLU	PHE	GLY
	ALA				
GLN	ALA	A212	SER	LEU	ARG
	GLN				
LEU	GLN	A213	GLU	LVS	LEU
	LEU				
GLY	LEU	E214	THR	ASN	SER
	GLY				
VAL	VAL	R215	SER	LVS	LYS
	VAL				
PRO	PRO	LEU	TYR	SER	MET
	PRO				
GLY	GLY	ASP	ILE	ASP	THR
	GLY				
THR	THR	K219	GLU	ALA	THR
	THR				
ALA	ALA	W220	SER	LEU	ARG
	ALA				
GLN	GLN	V221	ALA	SER	SER
	GLN				
LEU	LEU	Q222	GLY	LEU	GLN
	LEU				
GLY	GLY	D223	ARG	ILE	GLY
	GLY				
VAL	VAL	L224	SER	GLU	SER
	VAL				
PRO	PRO	W225	SER	ARG	ASN
	PRO				
GLY	GLY	V226	LEU	ASP	LVS
	GLY				
THR	THR	M227	THR	ASP	ALA
	THR				



K121	N181	G241	D301	T361	G421	SER	D541	L601	R661	M721	L781	A841	Q901
I122	I182	M242	M302	L362	T422	SER	E542	H602	M662	L722	R782	W842	P902
S123	L183	L243	S303	V363	G423	VAL	L543	Q603	C663	H723	T783	A843	A903
H124	H184	S244	R304	T364	R424	LYS	D544	V604	T664	V724	T784	S844	S904
S125	E185	G245	V305	V365	S425	SER	L545	G605	V665	A725	L785	N845	Q905
S126	G186	I246	L306	K366	T426	SER	A546	L606	PRO	C726	L786	L846	H906
S127	T187	G247	R307	D367	L427	ARG	V547	F607	GLN	Q727	E787	A847	G907
A128	Y188	R248	E308	E368	P428	ALA	N548	S608	ASN	Y728	Q788	E848	Q908
K129	R249	R249	I309	G369	Q429	VAL	Q549	R609	T670	R729	L789	R849	L909
L130	E190	V250	I310	Y370	E430	VAL	I550	L610	A671	Q730	A790	R850	A910
M131	S191	S251	S311	N371	K431	LYS	S551	S611	A672	S731	A791	C851	A911
V132	Y192	T252	D312	I372	I432	ASP	V552	T612	D673	K732	L792	D852	F912
C133	T193	L253	A313	S373	P433	ARG	D553	C613	V674	M733	L793	F853	L913
K134	E194	F254	I314	D374	F434	PRO	L554	Q614	V675	S734	N794	D854	Q914
E135	F195	G255	W315	E375	E435	ASP	L555	T615	F676	L735	Y795	L855	A915
L136	G196	I256	G316	I376	A436	GLN	D556	K616	R677	Y736	L796	L856	H916
P137	S197	L257	S317	T377	Q437	ILE	D557	G617	E678	K737	L797	W857	D917
L138	S198	S258	E318	V378	G438	HIS	Y558	M618	V679	N738	D798	Q858	H918
P139	L199	P259	S319	E379	D439	ASP	P559	L619	S680	E739	D799	R859	L919
L140	C200	A260	D320	V380	N440	ASP	A560	V620	Q681	S740	Y800	C860	S920
S141	A201	V261	Y321	T381	I441	K505	S561	A621	M682	G741	Y801	E861	W921
D142	F202	E262	D322	Q382	V442	K507	D562	T622	E683	I742	T802	M862	L922
S143	V203	S263	D323	F383	G443	H508	P563	R623	L684	Q743	Q803	T863	H923
E144	T204	T264	I324	N384	A444	L509	R564	L624	L685	E744	L804	D864	E924
W145	A205	T265	K325	F385	G445	K510	W565	L625	F686	P745	R805	N865	L925
S146	V206	C266	A326	V386	S446	A511	A566	L626	E687	E746	S806	Q866	N926
A147	K207	S267	G327	F387	C447	A512	E567	S627	C688	H747	I807	S867	S927
D148	G208	V268	I328	Q388	E448	F513	S568	E628	L689	V748	D808	R868	Q928
L149	N209	L269	N329	A389	G449	L514	V569	H629	V690	P749	R809	L869	E929
V150	S210	W270	I330	R390	N450	R515	P570	A630	D691	Q750	L810	Q870	F930
D151	F211	D271	N331	G391	P451	Y516	E571	E631	K692	T751	A811	R871	E931
I152	I212	K272	Y332	M392	V452	C517	E572	K632	E693	A752	N812	Y872	K932
C153	L213	G273	L333	Q393	F453	R518	A573	L633	E694	S753	E813	M873	A933
A154	S214	D274	S334	L394	F454	K519	A574	S634	A695	S754	E814	T874	H934
Q155	S215	C275	L335	C395	I455	D520	G575	A635	D696	G755	R815	L875	A935
T156	E216	F276	N336	Q396	R456	I521	F576	A636	L697	T756	Y816	F876	R936
G157	K217	Y277	Q337	L397	K457	L522	S577	L637	E698	A757	N817	A877	L937
D158	N218	T278	N338	V398	S458	G523	N578	V638	S699	G758	T818	E878	Q938
P159	Q219	L279	C339	V399	G459	A524	T579	L639	T700	I759	L819	Q879	T939
A160	L220	T280	D340	P400	N460	Q525	S580	K640	S701	R760	E820	N880	L940
A161	V221	D281	G341	M401	L461	S526	L581	N641	I702	S761	M821	F881	A941
A162	R222	S282	L342	F402	T462	M527	L582	H642	D703	V762	E822	S882	N942
Q163	L223	S283	V343	S403	V463	V528	L583	H643	S704	W763	R823	D883	M943
S164	T224	I284	I344	S404	V464	D529	L584	A644	V705	T764	A824	F884	E944
V165	P225	N285	L345	Q405	A465	S530	H585	K645	E706	R765	Q825	L885	T945
A166	D226	K286	S346	A406	R466	L531	Q586	L646	W707	Q766	K826	F886	R946
L167	A227	W287	A347	C407	GLU	F532	L587	P647	A708	H767	R827	R887	Y947
M168	S228	D288	A348	Y408	THR	S533	E588	V648	A709	G768	S828	W888	F948
A169	G229	L289	W349	L409	SER	D534	D589	L649	N709	I769	E829	Y889	C949
A170	K230	D290	H350	Y410	VAL	S535	K591	V650	I710	T770	L830	Y890	Q950
T171	M231	D291	P351	T411	PRO	D536	M591	N651	V711	L771	L831	E891	K951
P172	N232	T292	G352	Q412	GLU	M537	K592	S652	W712	K772	S832	K892	K952
E173	Q233	S293	D353	E413	HIS	E538	A593	A653	V713	V773	F833	C893	T953
G174	R234	E294	N354	M414	MET	L594	H594	T654	N714	Y774	L834	K894	L954
S175	V235	S295	P355	I415	GLU	S595	S595	Q655	T715	P775	L835	R895	L955
S176	L236	Q296	C356	F416	GLU	S596	F596	L656	T716	Q776	T836	C896	Q956
R177	P237	V297	Q357	A417	SER	F597	V597	A657	I717	A777	L837	R897	L957
Y178	Q238	L298	I358	C418	LEU	S598	V598	L658	L718	D778	L838	L898	S958
W179	G239	N299	Y359	S419		D540	D599	D659	D720	S779	K719	L899	K959
P180	Q240	W300	Y360	T420			F600	K660		G780		S900	L960

A961	A962	L963	A964	S965	D966	F967	Q968	E969	D970	V971	L972	Q973	E974	K975	V976	E977	E978	I979	A980	E981	E982	E983	H984	F985	L986	L987	H988	Q989	E990	T991	L992	P993	K994	K995	L996	L997	E998	E999	K1000	Q1001	L1002	D1003	L1004	N1005	A1006	M1007	P1008	V1009	L1010	A1011	P1012	F1013	Q1014	L1015	T1016	Q1017	L1018	Y1019	V1020
C1021	E1022	E1023	N1024	K1025	R1026	A1027	N1028	E1029	N1030	D1031	F1032	M1033	K1034	A1035	L1036	D1037	L1038	L1039	E1040	Y1041	I1042	G1043	D1044	D1045	S1046	E1047	V1048	D1049	V1050	E1051	E1052	L1053	K1054	L1055	E1056	I1057	L1058	C1059	K1060	A1061	I1062	K1063	R1064	D1065	E1066	W1067	S1068	A1069	T1070	D1071	G1072	K1073	D1074	D1075	P1076	I1077	E1078	A1079	T1080
K1081	D1082	S1083	I1084	F1085	V1086	K1087	V1088	L1089	Q1090	M1091	L1092	L1093	N1094	K1095	G1096	I1097	E1098	L1099	K1100	G1101	Y1102	L1103	P1104	K1105	A1106	E1107	T1108	L1109	L1110	Q1111	S1112	E1113	E1114	L1115	M1116	S1117	L1118	K1119	T1120	M1121	S1122	Y1123	F1124	E1125	F1126	S1127	L1128	K1129	A1130	M1131	Y1132	E1133	C1134	Y1135	M1136	K1137	M1138	GLN	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1279270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.334	Depositor
Minimum map value	-0.334	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	710.144, 710.144, 710.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.387, 1.387, 1.387	Depositor

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	0.31	0/9232	0.46	0/12806
1	a	0.27	0/8804	0.43	0/12220
2	B	0.34	0/4893	0.47	0/6602
2	b	0.36	0/4636	0.49	0/6272
3	C	0.27	0/2615	0.48	0/3550
3	c	0.28	0/2500	0.49	0/3394
4	D	0.27	0/2536	0.46	0/3442
4	d	0.27	0/2498	0.45	0/3392
5	E	0.33	0/7960	0.51	0/10948
5	e	0.34	0/8229	0.51	0/11264
6	F	0.28	0/1606	0.48	0/2231
6	f	0.27	0/2594	0.46	0/3526
7	G	0.33	0/4299	0.49	0/5856
7	g	0.38	0/4888	0.54	0/6644
8	H	0.28	0/2299	0.46	0/3139
8	h	0.28	0/2322	0.46	0/3169
9	I	0.24	0/3621	0.40	0/5050
9	i	0.23	0/3339	0.37	0/4651
10	J	0.23	0/2253	0.37	0/3141
11	K	0.25	0/3452	0.43	0/4805
11	L	0.24	0/3362	0.42	0/4677
11	M	0.26	0/3238	0.46	0/4506
11	N	0.25	0/3471	0.45	0/4830
11	O	0.24	0/3380	0.43	0/4700
12	P	0.25	0/2939	0.39	0/4093
12	S	0.35	0/438	0.46	0/586
12	p	0.44	0/2251	0.43	0/3118
12	s	0.32	0/438	0.45	0/586
13	W	0.35	0/2692	0.49	0/3638
15	Y	0.32	0/1668	0.71	0/2311
16	j	0.24	0/5091	0.41	0/7095
All	All	0.30	0/113544	0.46	0/156242

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
1	A	0	2
1	a	0	2
6	f	0	1
15	Y	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	THR	Peptide
1	A	1771	SER	Peptide
15	Y	286	TYR	Peptide
1	a	1053	THR	Peptide
1	a	1355	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	1759/2011 (88%)	1626 (92%)	129 (7%)	4 (0%)	47	78
1	a	1691/2011 (84%)	1552 (92%)	131 (8%)	8 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	584/653 (89%)	564 (97%)	19 (3%)	1 (0%)	47	78
2	b	579/653 (89%)	562 (97%)	15 (3%)	2 (0%)	41	74
3	C	315/375 (84%)	303 (96%)	12 (4%)	0	100	100
3	c	299/375 (80%)	284 (95%)	14 (5%)	1 (0%)	41	74
4	D	310/360 (86%)	298 (96%)	12 (4%)	0	100	100
4	d	306/360 (85%)	293 (96%)	13 (4%)	0	100	100
5	E	1298/1435 (90%)	1239 (96%)	56 (4%)	3 (0%)	47	78
5	e	1227/1435 (86%)	1167 (95%)	59 (5%)	1 (0%)	51	83
6	F	324/326 (99%)	312 (96%)	12 (4%)	0	100	100
6	f	320/326 (98%)	308 (96%)	11 (3%)	1 (0%)	41	74
7	G	545/1742 (31%)	508 (93%)	35 (6%)	2 (0%)	34	69
7	g	595/1742 (34%)	543 (91%)	50 (8%)	2 (0%)	41	74
8	H	284/320 (89%)	274 (96%)	9 (3%)	1 (0%)	34	69
8	h	284/320 (89%)	274 (96%)	8 (3%)	2 (1%)	22	59
9	I	719/916 (78%)	675 (94%)	43 (6%)	1 (0%)	51	83
9	i	657/916 (72%)	628 (96%)	29 (4%)	0	100	100
10	J	449/1140 (39%)	422 (94%)	27 (6%)	0	100	100
11	K	681/2905 (23%)	623 (92%)	57 (8%)	1 (0%)	51	83
11	L	659/2905 (23%)	614 (93%)	45 (7%)	0	100	100
11	M	638/2905 (22%)	575 (90%)	62 (10%)	1 (0%)	47	78
11	N	683/2905 (24%)	614 (90%)	68 (10%)	1 (0%)	51	83
11	O	661/2905 (23%)	613 (93%)	47 (7%)	1 (0%)	47	78
12	P	581/820 (71%)	539 (93%)	42 (7%)	0	100	100
12	S	50/820 (6%)	49 (98%)	1 (2%)	0	100	100
12	p	424/820 (52%)	401 (95%)	21 (5%)	2 (0%)	29	66
12	s	50/820 (6%)	46 (92%)	4 (8%)	0	100	100
13	W	318/1388 (23%)	305 (96%)	12 (4%)	1 (0%)	41	74
15	Y	323/728 (44%)	308 (95%)	11 (3%)	4 (1%)	13	48
16	j	1022/1140 (90%)	960 (94%)	62 (6%)	0	100	100
All	All	18635/38477 (48%)	17479 (94%)	1116 (6%)	40 (0%)	50	78

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	460	ILE
15	Y	271	LYS
1	a	57	PRO
1	a	58	PRO
1	a	1095	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	100/1779 (6%)	99 (99%)	1 (1%)	76	86
1	a	77/1779 (4%)	75 (97%)	2 (3%)	46	69
2	B	517/580 (89%)	501 (97%)	16 (3%)	40	65
2	b	447/580 (77%)	439 (98%)	8 (2%)	59	77
3	C	288/329 (88%)	282 (98%)	6 (2%)	53	74
3	c	276/329 (84%)	268 (97%)	8 (3%)	42	66
4	D	273/310 (88%)	269 (98%)	4 (2%)	65	81
4	d	266/310 (86%)	263 (99%)	3 (1%)	73	85
5	E	382/1256 (30%)	366 (96%)	16 (4%)	30	59
5	e	545/1256 (43%)	521 (96%)	24 (4%)	28	58
6	f	266/275 (97%)	262 (98%)	4 (2%)	65	81
7	G	384/1474 (26%)	361 (94%)	23 (6%)	19	50
7	g	490/1474 (33%)	463 (94%)	27 (6%)	21	53
8	H	236/273 (86%)	230 (98%)	6 (2%)	47	70
8	h	245/273 (90%)	240 (98%)	5 (2%)	55	74
12	S	47/721 (6%)	43 (92%)	4 (8%)	10	40
12	s	47/721 (6%)	43 (92%)	4 (8%)	10	40
13	W	295/1219 (24%)	291 (99%)	4 (1%)	67	82
All	All	5181/14938 (35%)	5016 (97%)	165 (3%)	42	65

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	972	GLU
7	g	1285	SER
5	e	1079	LEU
6	f	119	VAL
7	g	1347	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
7	g	1165	ASN
7	g	1220	ASN
7	g	1499	HIS
7	G	1431	GLN
7	G	1370	GLN

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.

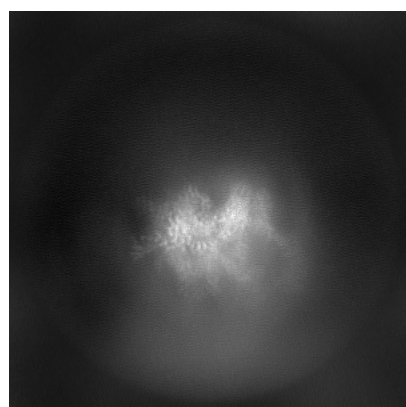
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31600. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

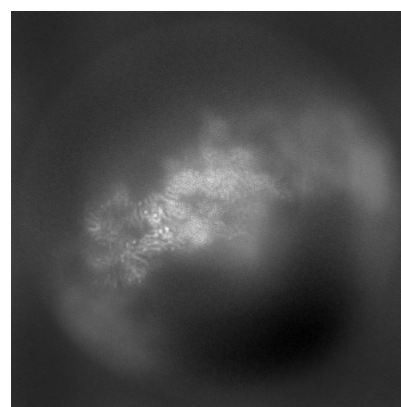
6.1.1 Primary map



X



Y

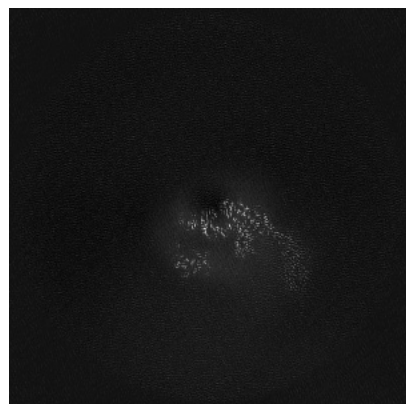


Z

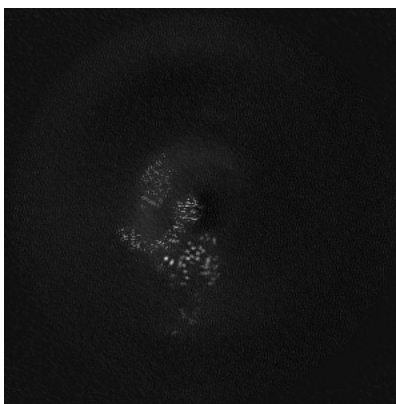
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

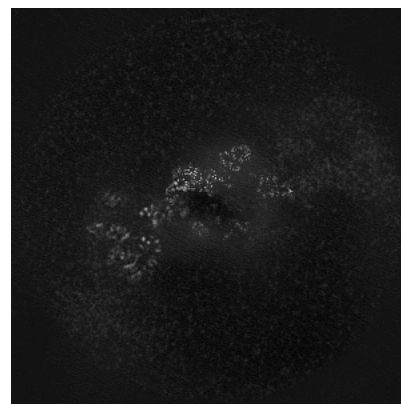
6.2.1 Primary map



X Index: 256



Y Index: 256

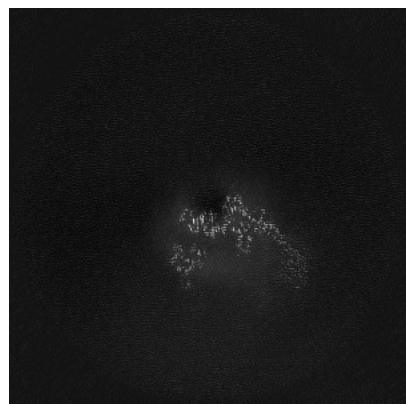


Z Index: 256

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

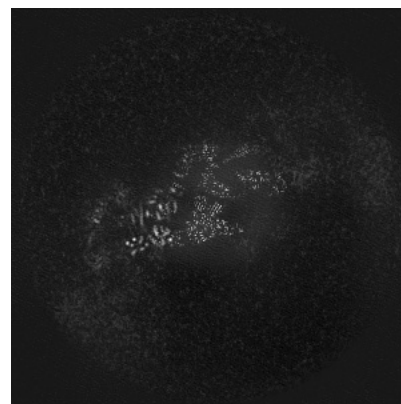
6.3.1 Primary map



X Index: 252



Y Index: 223

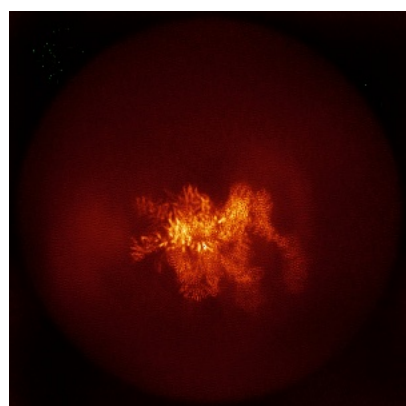


Z Index: 236

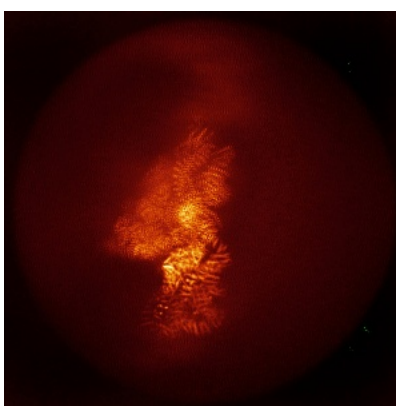
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

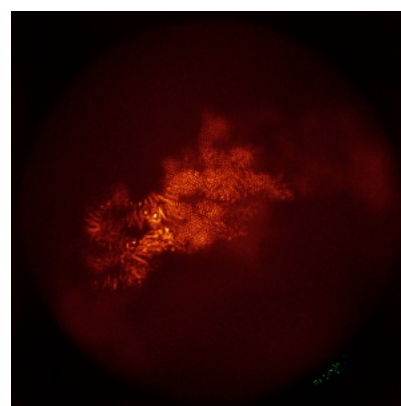
6.4.1 Primary map



X



Y

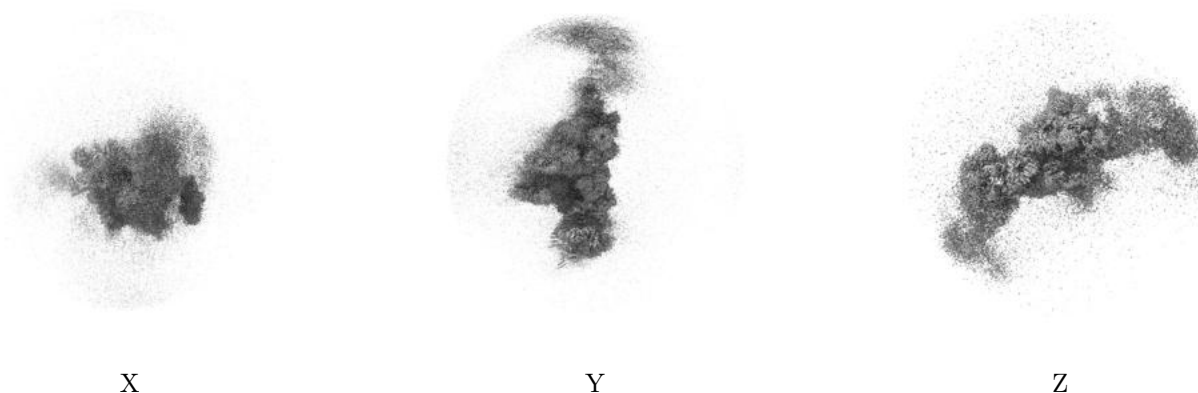


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

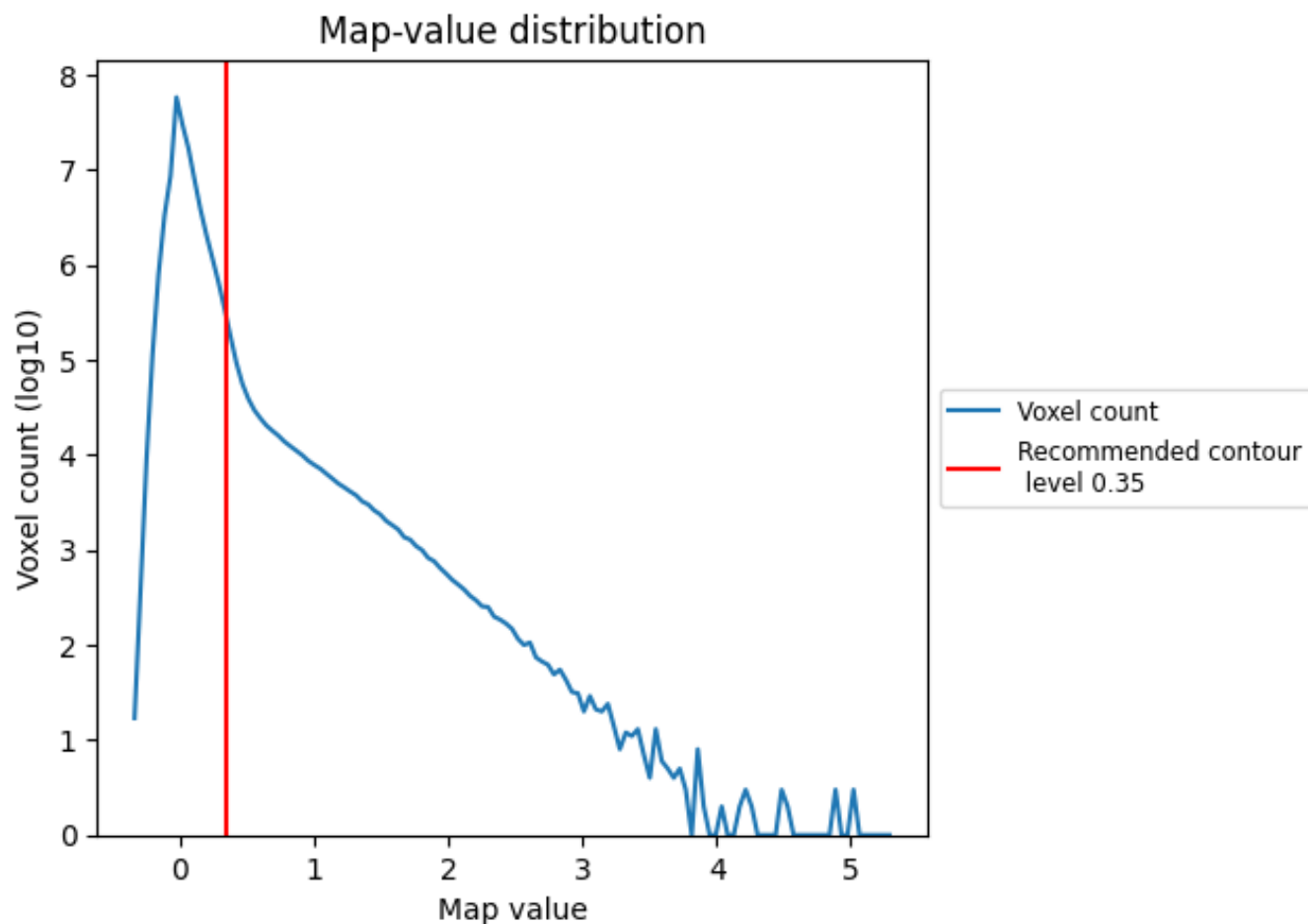
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

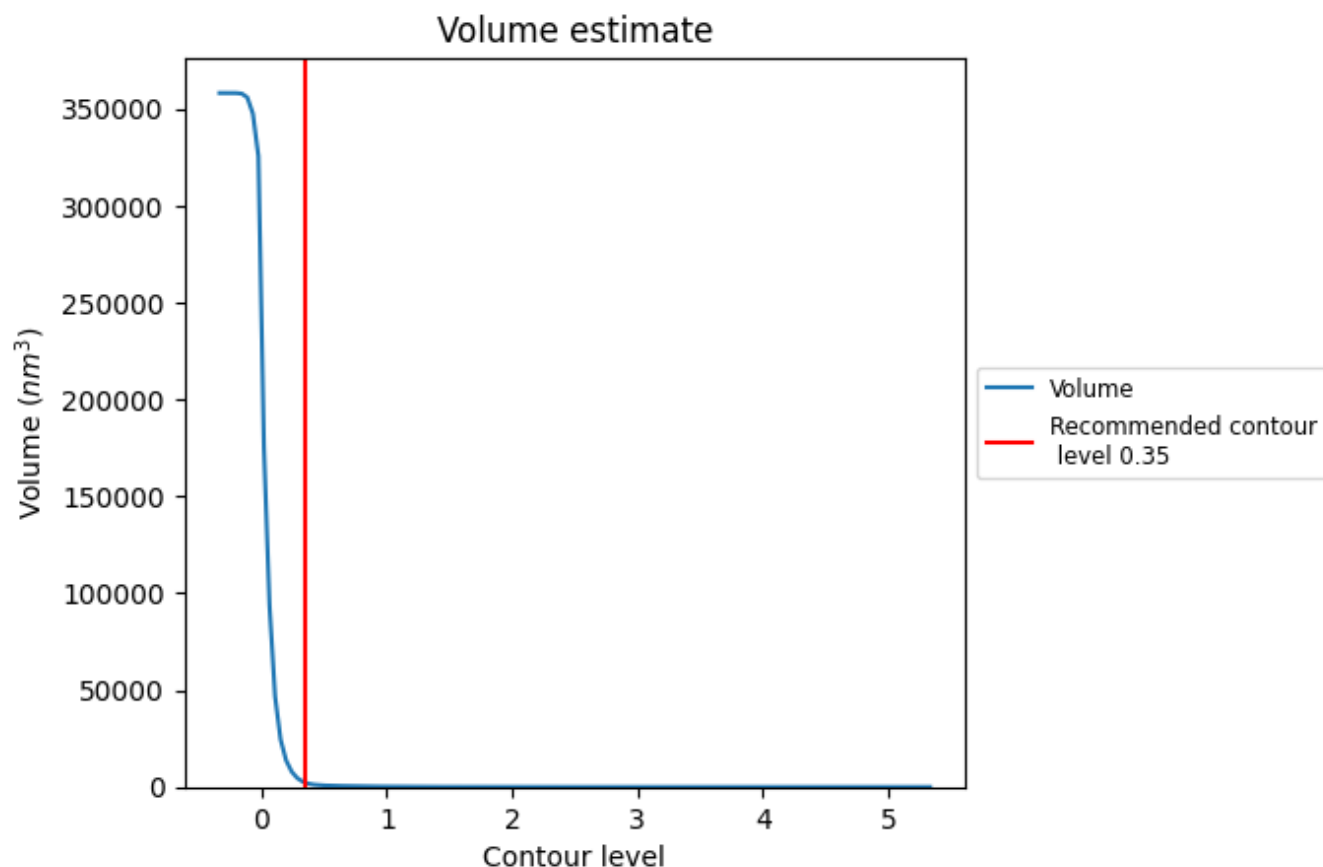
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

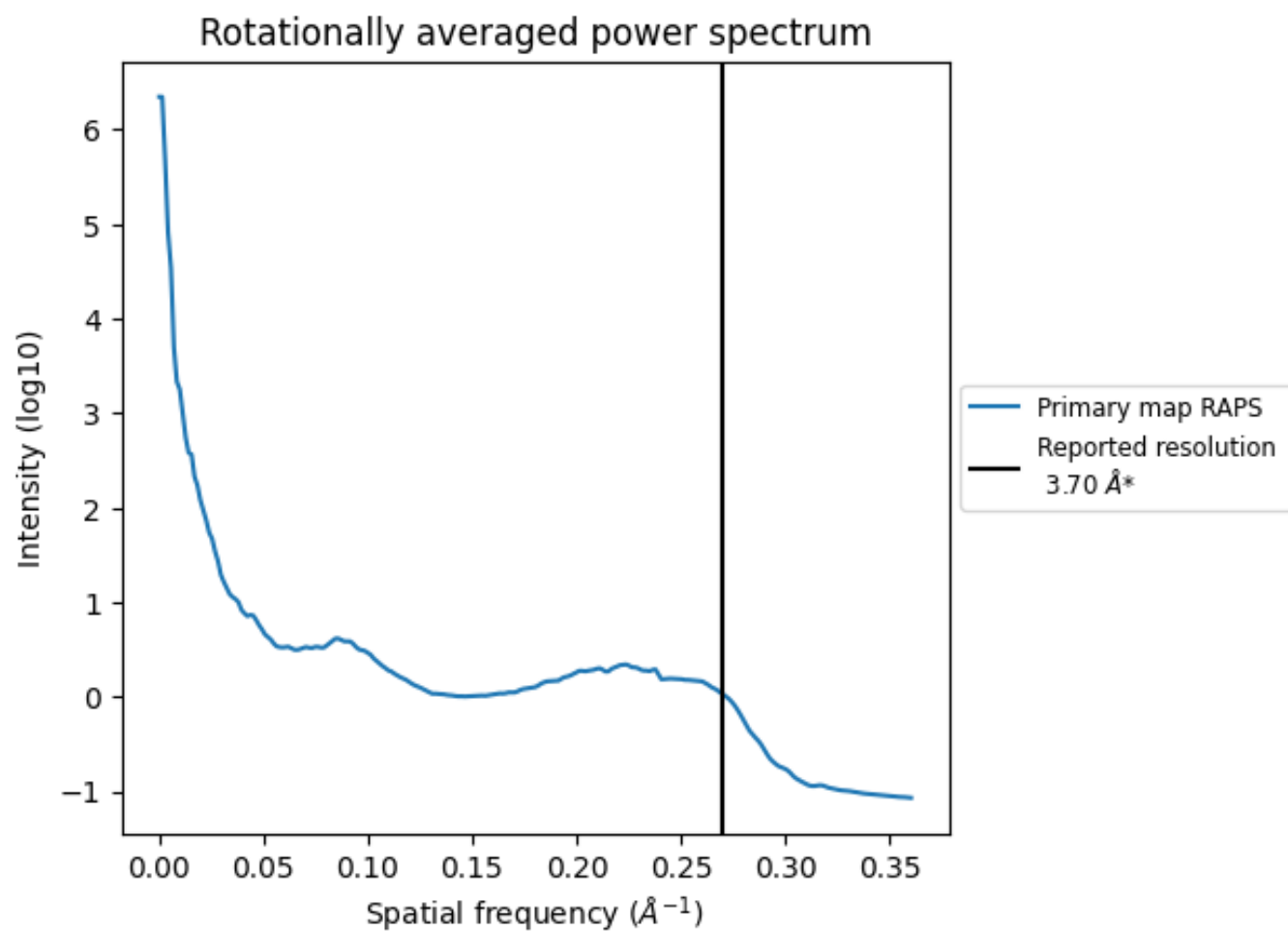
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2248 nm^3 ; this corresponds to an approximate mass of 2031 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

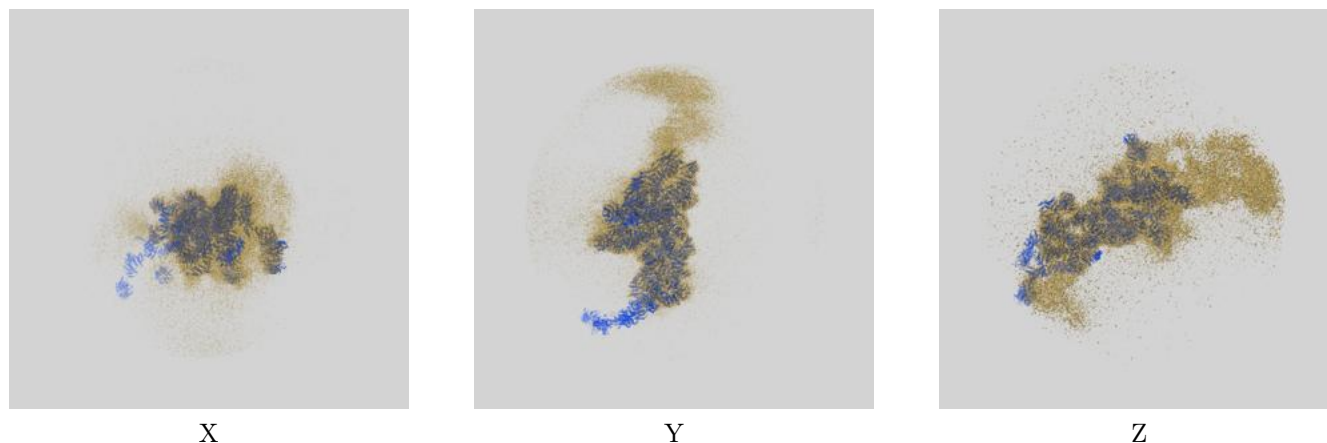
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

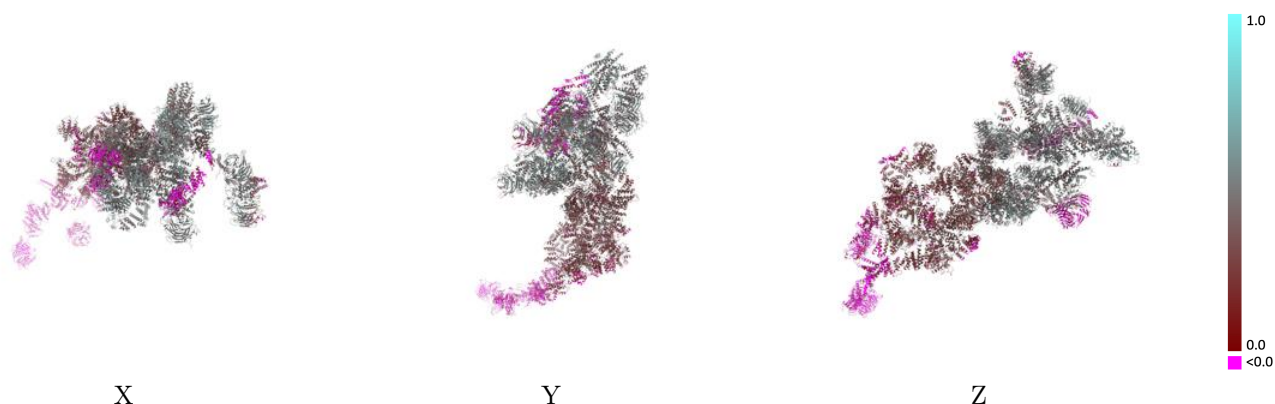
This section contains information regarding the fit between EMDB map EMD-31600 and PDB model 7FIK. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



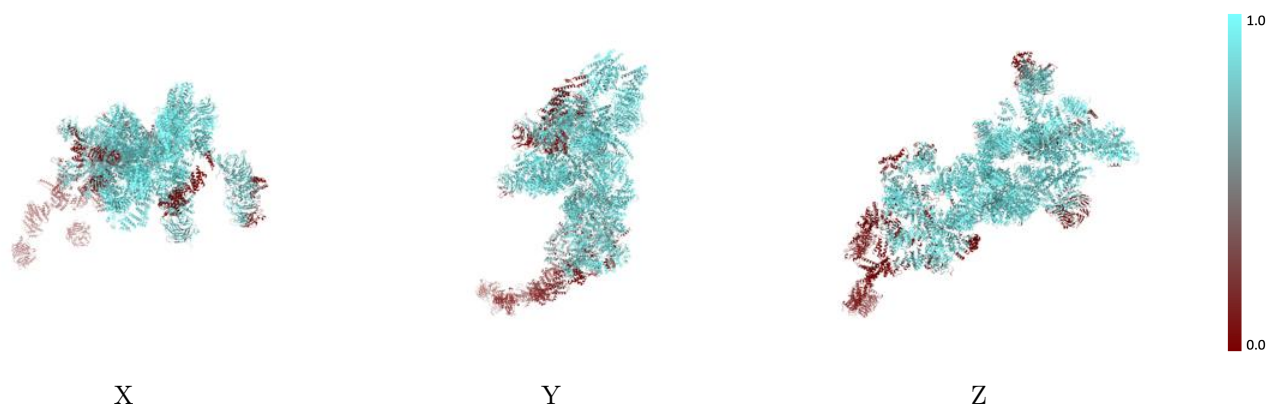
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



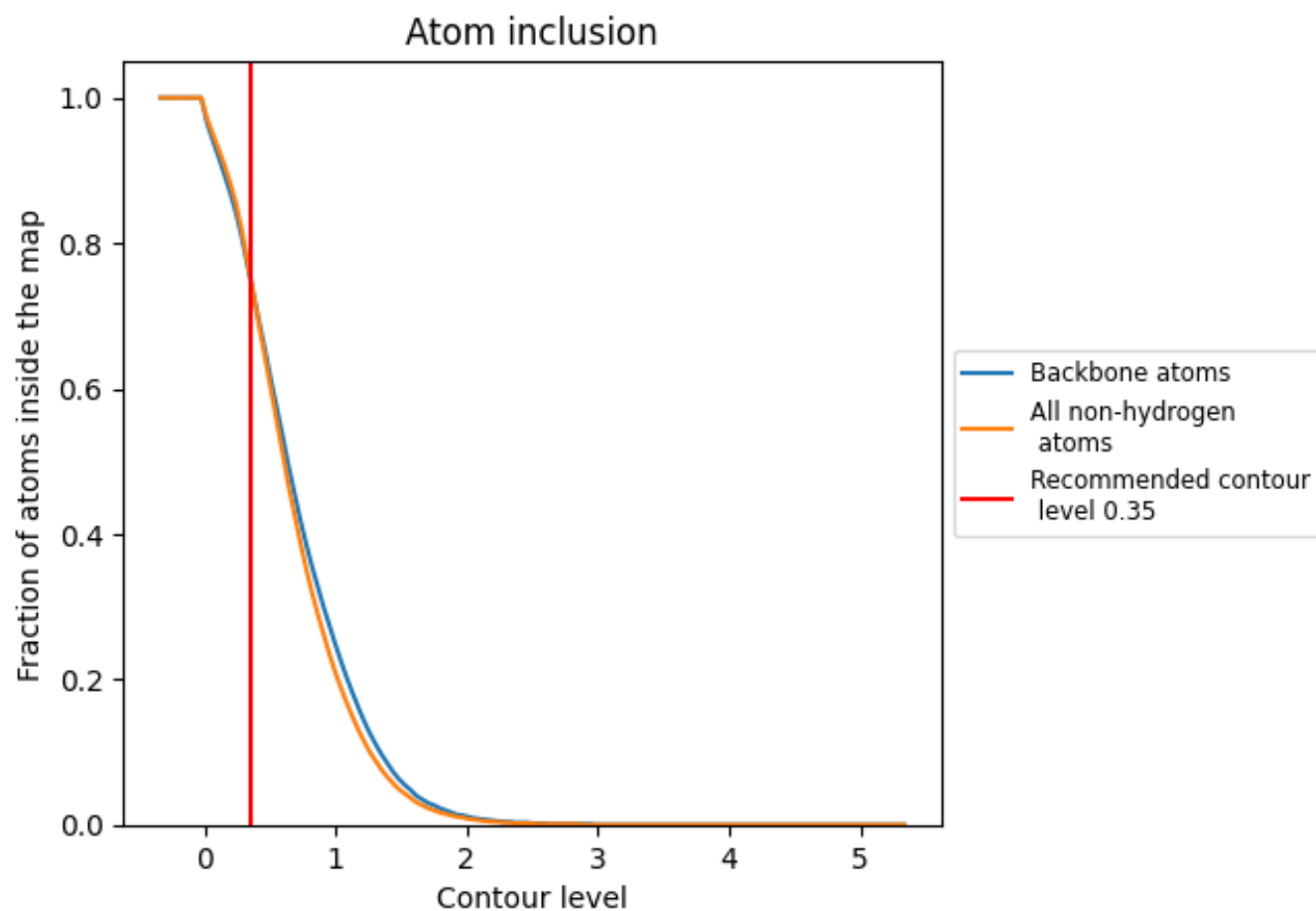
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.3460
A	 0.9580	 0.4790
B	 0.8710	 0.4340
C	 0.9490	 0.5030
D	 0.9220	 0.4710
E	 0.7110	 0.4090
F	 0.7750	 0.4700
G	 0.8890	 0.3440
H	 0.9590	 0.4710
I	 0.8330	 0.2830
J	 0.1110	 0.0820
K	 0.7490	 0.2950
L	 0.5250	 0.2780
M	 0.9400	 0.3220
N	 0.6850	 0.2870
O	 0.7840	 0.2290
P	 0.8780	 0.2830
S	 0.9190	 0.4340
W	 0.9640	 0.4950
X	 0.2370	 0.0090
Y	 0.2550	 -0.0240
a	 0.9670	 0.4830
b	 0.8760	 0.4240
c	 0.9290	 0.4670
d	 0.9660	 0.4690
e	 0.8850	 0.4500
f	 0.9850	 0.5100
g	 0.8900	 0.3330
h	 0.9510	 0.3740
i	 0.3530	 0.1570
j	 0.0000	 -0.0560
p	 0.1080	 -0.0130
s	 0.9530	 0.3980

