



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:49 AM UTC

PDB ID : 8TIE / pdb_00008tie
EMDB ID : EMD-41285
Title : Double nuclear outer ring of Nup84-complexes from the yeast NPC
Authors : Akey, C.W.; Echeverria, I.; Ouch, C.; Fernandez-Martinez, J.; Rout, M.P.
Deposited on : 2023-07-19
Resolution : 8.10 Å(reported)
Based on initial model : .

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:

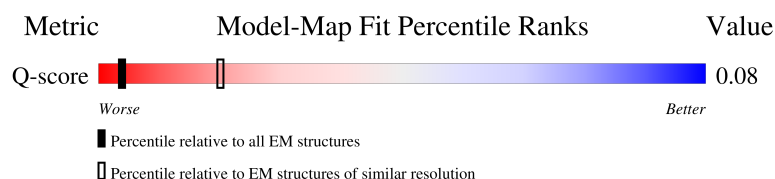
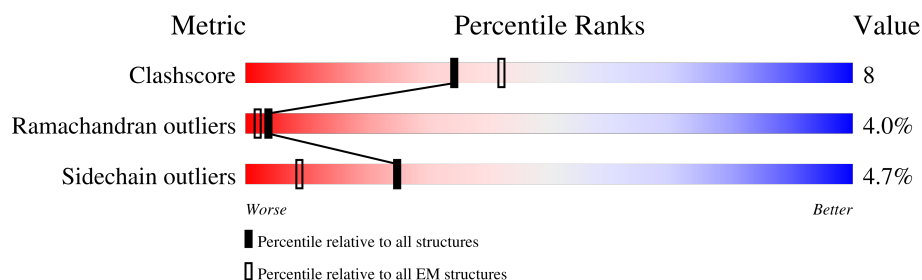
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.10 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.



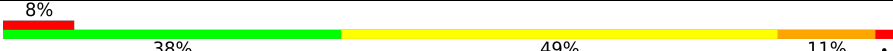
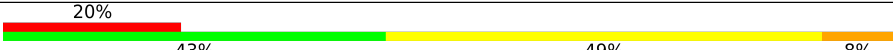
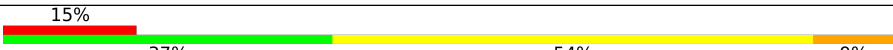
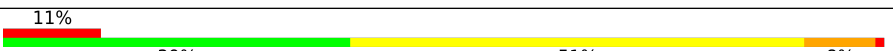
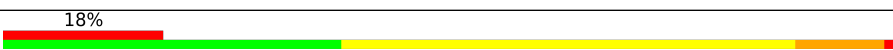
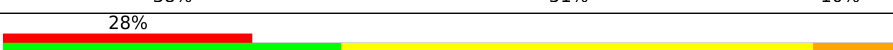
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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	1037	9% 41% 51% 5%
1	l	1037	7% 42% 48% 6%
2	b	744	5% 37% 44% 5% 13%
2	m	744	29% 35% 45% 7% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	1317	
3	n	1317	
4	d	297	
4	o	297	
5	e	307	
5	p	307	
6	f	726	
6	q	726	
7	g	1157	
7	r	1157	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 76621 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 Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1012	Total	C	N	O	S	0	0
			8321	5371	1340	1577	33		
1	l	1012	Total	C	N	O	S	0	0
			8321	5371	1340	1577	33		

- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	647	Total	C	N	O	S	0	0
			5186	3339	826	993	28		
2	m	647	Total	C	N	O	S	0	0
			5190	3343	826	993	28		

- Molecule 3 is a protein called NUP145 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	610	Total	C	N	O	S	0	0
			4877	3107	808	942	20		
3	n	599	Total	C	N	O	S	0	0
			4822	3074	797	931	20		

- Molecule 4 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	286	Total	C	N	O	S	0	0
			2216	1412	381	420	3		
4	o	286	Total	C	N	O	S	0	0
			2216	1412	381	420	3		

- Molecule 5 is a protein called Nucleoporin Seh1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	307	Total	C	N	O	S	0	0
			2439	1542	423	463	11		
5	p	307	Total	C	N	O	S	0	0
			2439	1542	423	463	11		

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	726	Total	C	N	O	S	0	0
			5895	3766	962	1149	18		
6	q	726	Total	C	N	O	S	0	0
			5895	3766	962	1149	18		

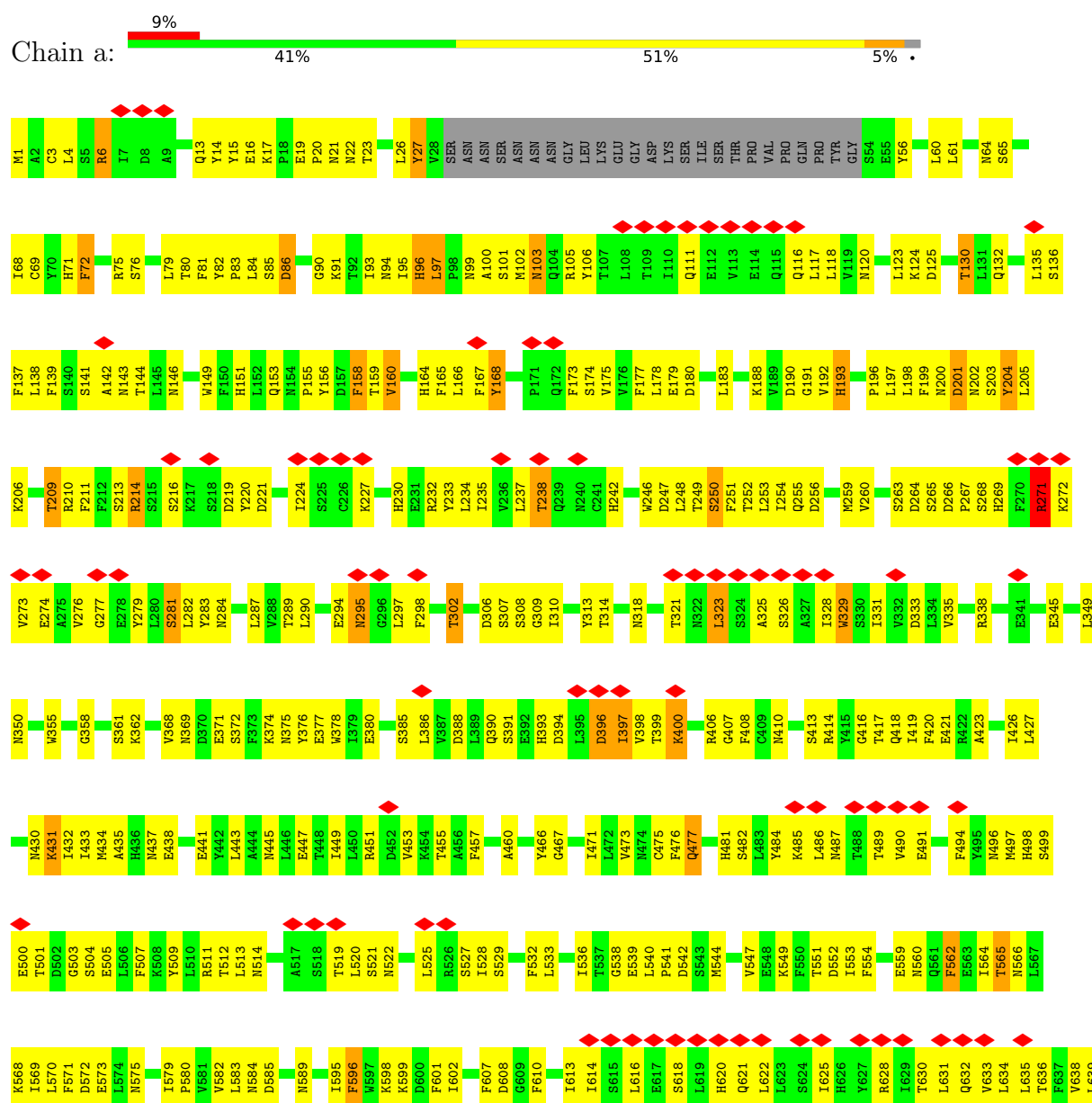
- Molecule 7 is a protein called NUP133 isoform 1.

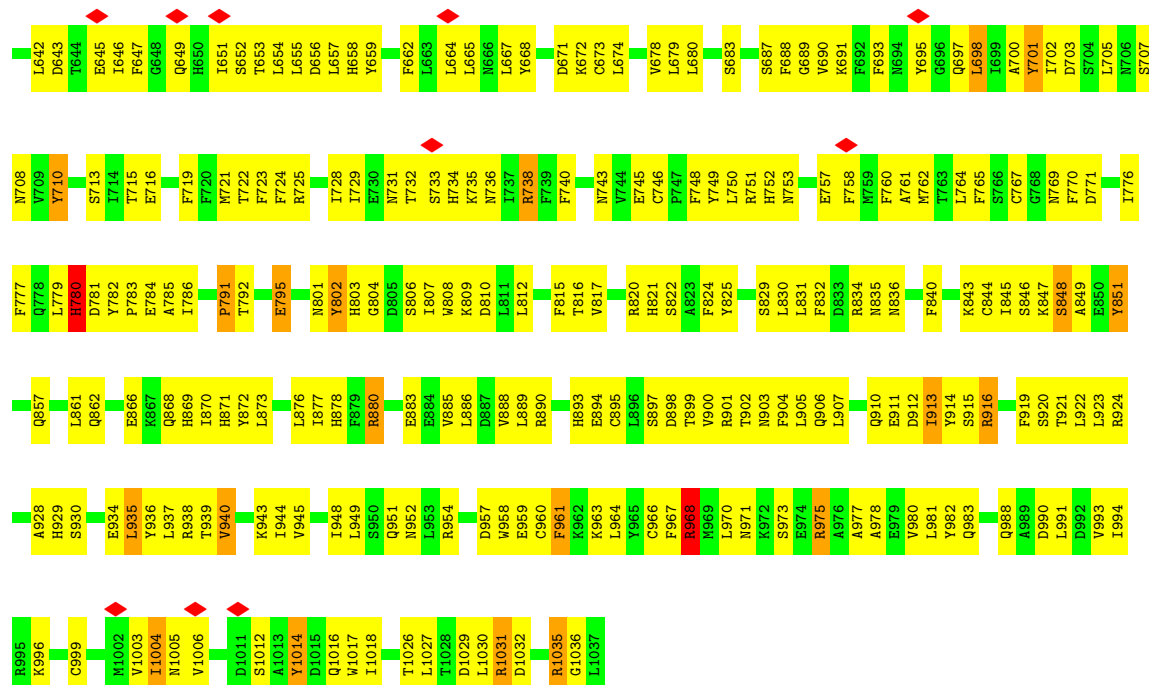
Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	1157	Total	C	N	O	S	0	0
			9403	6023	1525	1823	32		
7	r	1157	Total	C	N	O	S	0	0
			9401	6023	1525	1821	32		

3 Residue-property plots

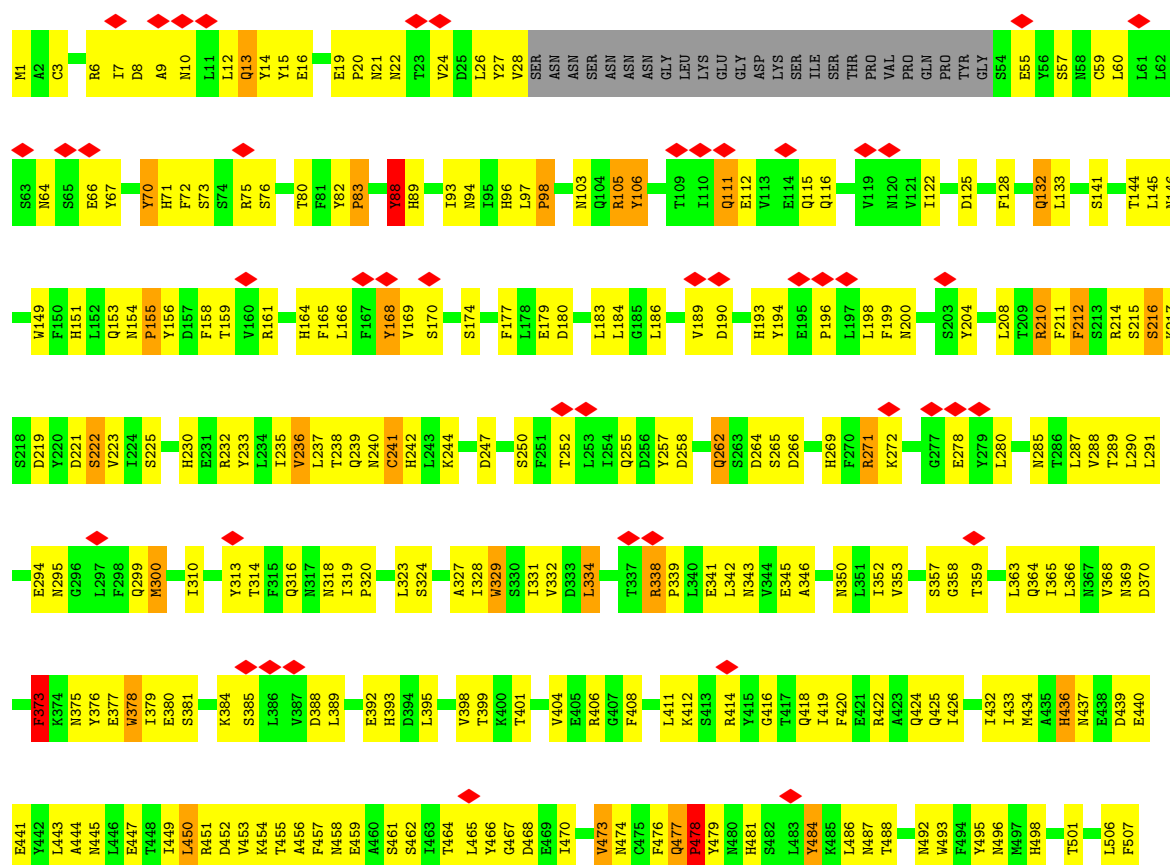
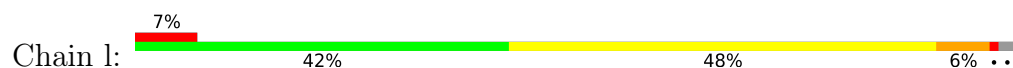
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

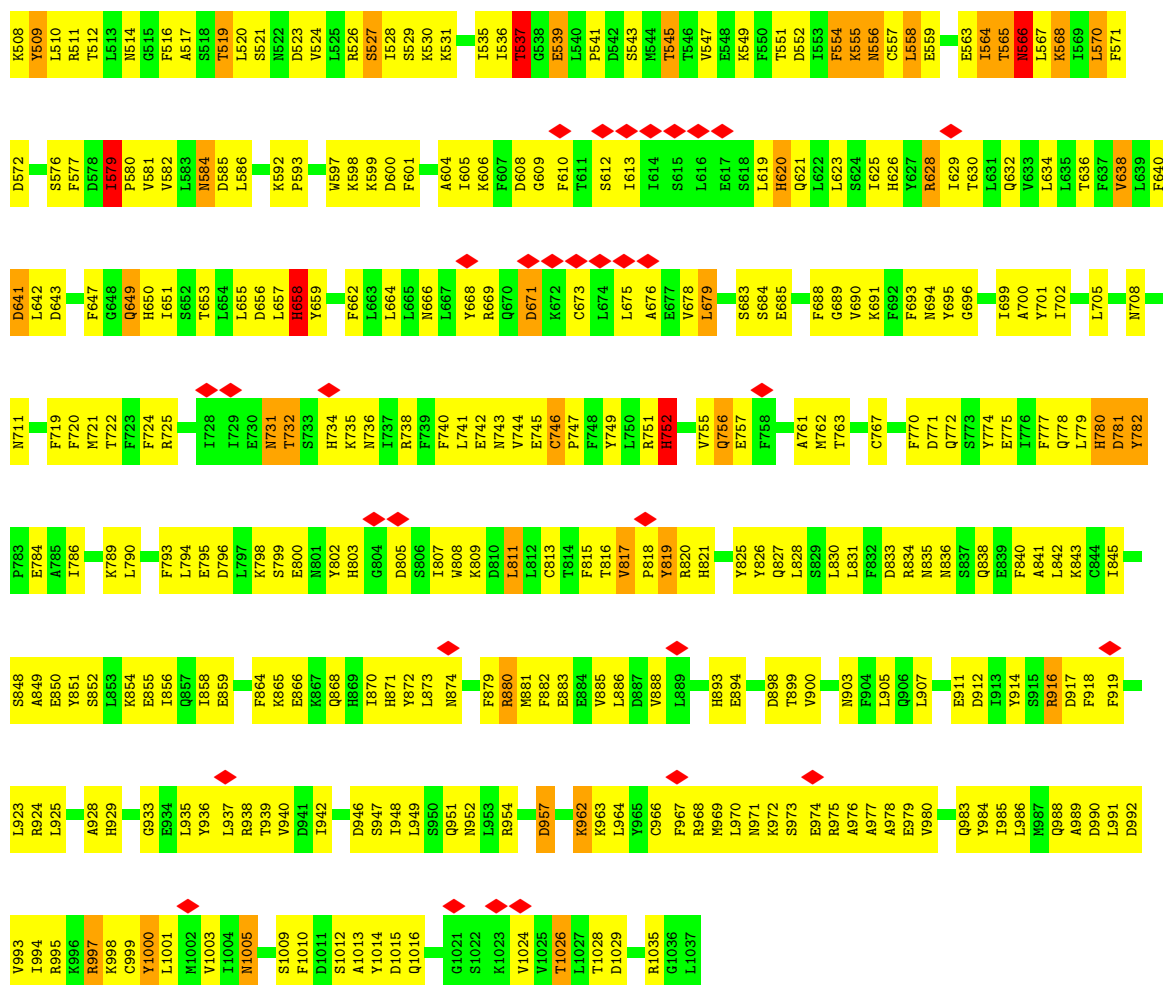
• Molecule 1: Nucleoporin NUP120



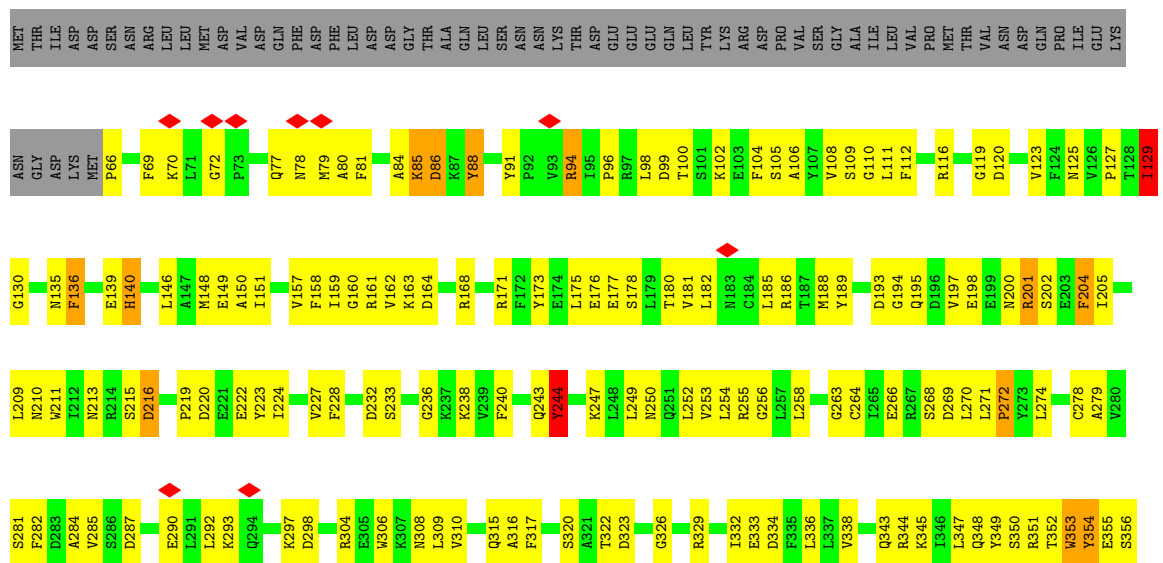


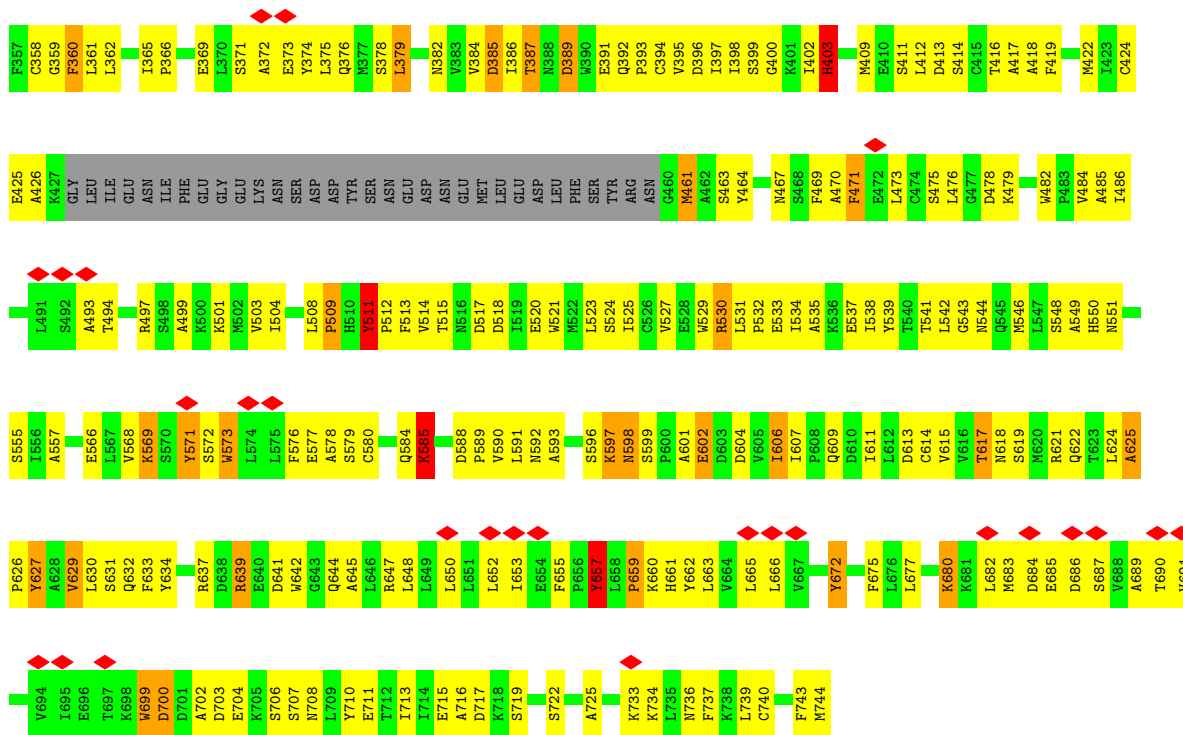
● Molecule 1: Nucleoporin NUP120



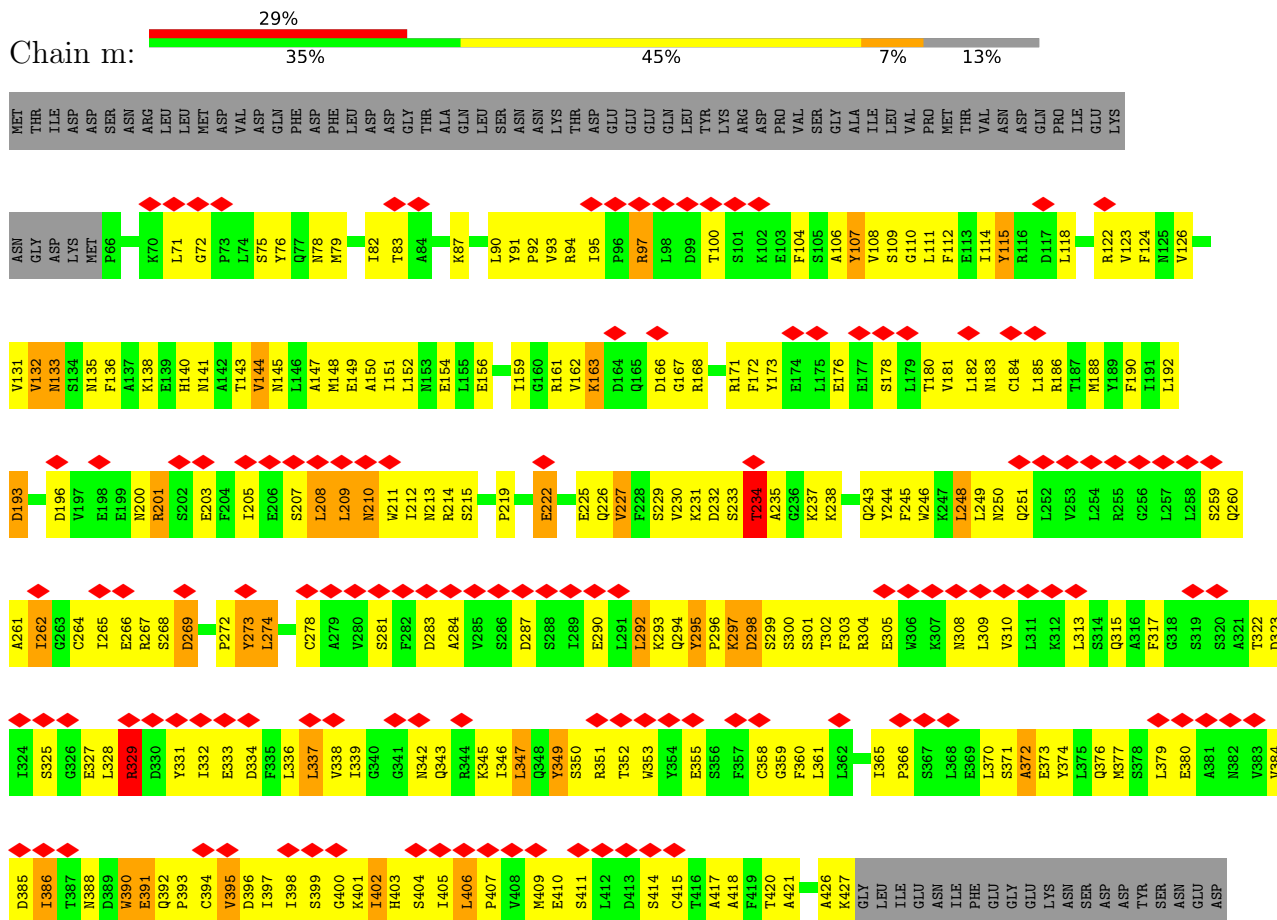


• Molecule 2: Nucleoporin NUP85

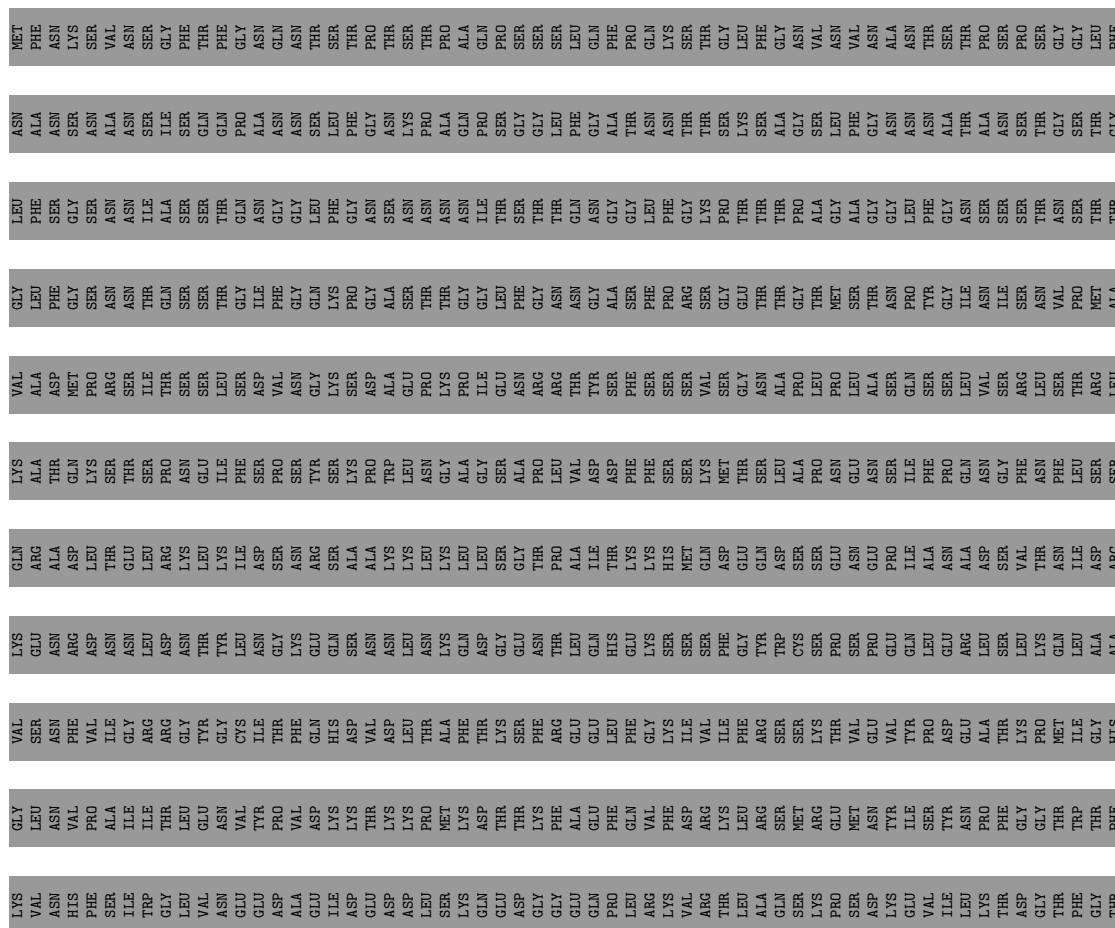




- Molecule 2: Nucleoporin NUP85

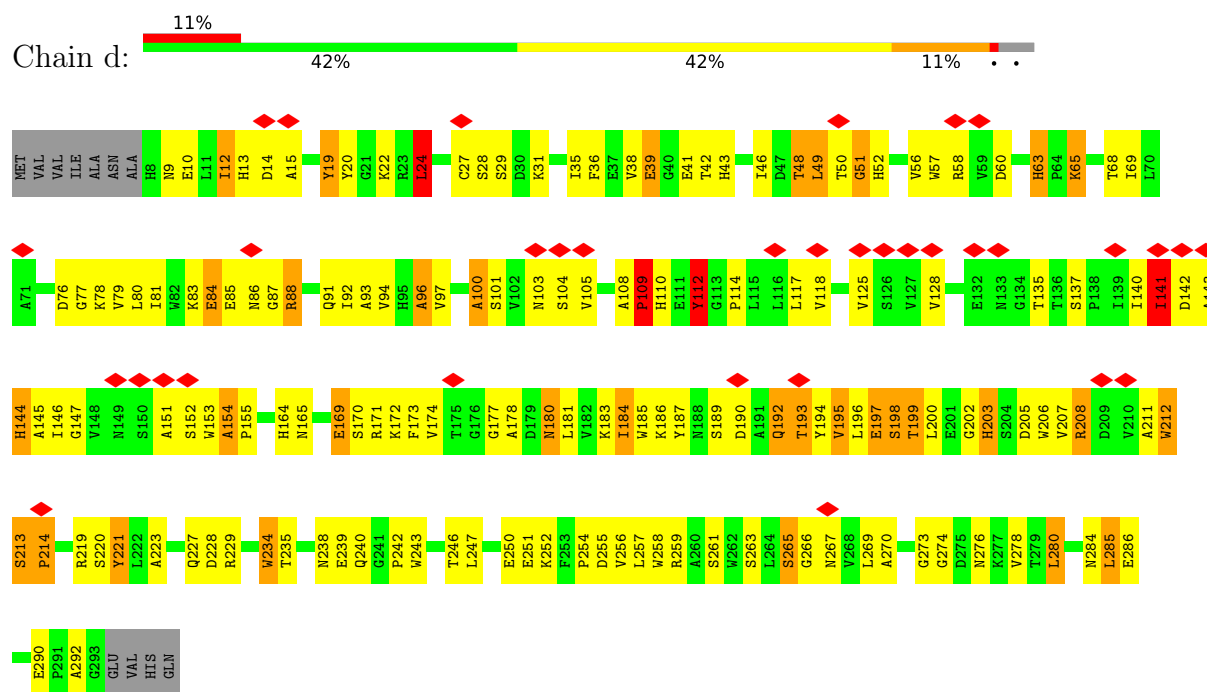


- Molecule 3: NUP145 isoform 1

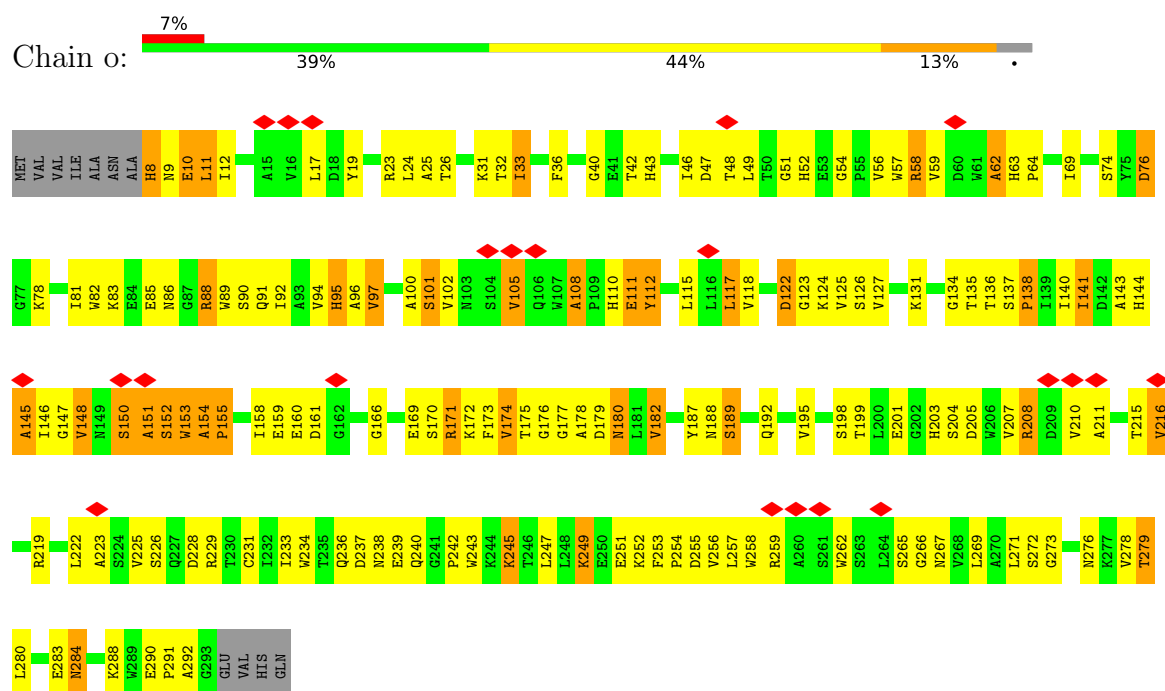


Q690	P691	I613	P633	R463	L399	P330	R264	Y189	G115	LEU	LYS	GLY	LEU	GLY	VAL	LYS	GLN	LYS	VAL
E692	N614	N615	Q534	S466	E400	R331	H265	L190	P116	SER	VAL	ASN	ASN	ASP	SER	ASN	ARG	ALA	ALA
K693	V615	L536	Q535	K467	S401	C266	C266	K192	C117	GLY	GLY	LYS	LYS	ASP	PHE	ARG	ALA	THR	THR
A694	F616	I537	I537	E468	V403	L335	R267	E195	N119	ASP	PHE	ASP	PRO	VAL	VAL	ASN	THR	LYS	PRO
Y695	E617	F538	F538	E468	Q404	A336	T269	E195	E120	SER	SER	ASP	ASP	ILE	GLY	ASN	THR	SER	ARG
L696	V618	L696	Q541	A473	S405	E337	S270	E195	E120	ILE	ILE	SER	SER	GLY	ARG	ASN	GLU	THR	ILE
R697	Y619	Y619	A542	T474	H406	Q338	V273	T198	L123	VAL	TRP	ILE	ILE	ARG	ARG	LEU	LEU	SER	SER
G698	A542	A542	L543	F477	L407	L339	S274	T199	L124	GLU	GLY	GLY	THR	ARG	ARG	ASP	ARG	PRO	THR
E699	L543	L543	D408	A478	D408	L340	Q275	A201	F125	GLU	LEU	LEU	LEU	GLY	THR	ASN	GLY	ASN	GLY
F700	K544	K544	Q341	A479	Q341	Q341	Q275	A201	F125	GLU	VAL	VAL	VAL	THR	THR	ASN	LEU	SER	SER
A701	D545	D545	K342	Q480	F410	K342	I276	R202	G128	LYS	ASN	ASN	GLY	THR	CYS	TYR	LYS	ILE	LYS
Q702	R546	R546	K343	Q480	F410	K343	I276	R202	G128	ALA	GLU	GLU	VAL	GLY	GLY	ASN	ILE	PHE	PHE
R703	Y547	Y547	S344	L481	P413	S344	G277	S204	E120	TYR	GLU	GLU	VAL	ILE	ILE	ASN	ASP	SER	ASP
L704	E548	E548	S344	L481	P413	S344	G277	S204	E120	TYR	GLU	GLU	VAL	ILE	ILE	ASN	ASP	SER	ASP
M705	S553	S553	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
K706	L553	L553	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
C707	K544	K544	Q341	A484	P417	G346	E281	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
T708	D545	D545	K342	Q480	F410	K342	I276	R202	G128	LYS	ASN	ASN	GLY	THR	CYS	TYR	LYS	ILE	LYS
Y709	R546	R546	K343	Q480	F410	K343	I276	R202	G128	ALA	GLU	GLU	VAL	GLY	GLY	ASN	ALA	ASP	ASP
K710	Y547	Y547	S344	L481	P413	S344	G277	S204	E120	TYR	GLU	GLU	VAL	ILE	ILE	ASN	ASP	SER	ASP
I711	E548	E548	S344	L481	P413	S344	G277	S204	E120	TYR	GLU	GLU	VAL	ILE	ILE	ASN	ASP	SER	ASP
G639	L560	L560	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
M640	S562	S562	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
K641	S563	S563	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
I642	Y564	Y564	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
F643	D565	D565	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
Y644	L566	L566	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
Y647	A567	A567	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
K648	S568	S568	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
H649	M569	M569	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
C650	A570	A570	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
R651	I571	I571	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
E652	S572	S572	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
V653	T573	T573	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
C657	L580	L580	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
N658	N583	N583	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
V659	N584	N584	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
P660	P585	P585	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
S661	V586	V586	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
Q662	N588	N588	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
E663	Q587	Q587	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
I664	N589	N589	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
V665	E590	E590	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
N672	T593	T593	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
N673	L594	L594	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
P674	R595	R595	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
S675	E596	E596	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
K680	I597	I597	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
L684	L598	L598	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
E685	N599	N599	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
L686	E600	E600	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
P687	F601	F601	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
L688	R629	R629	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
P687	L530	L530	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
L688	D603	D603	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
G689	R606	R606	F483	F483	D416	T345	I280	N205	I132	GLU	ASP	ASP	PRO	THR	THR	GLY	SER	PRO	VAL
F113	D114	D114	F113	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114	D114

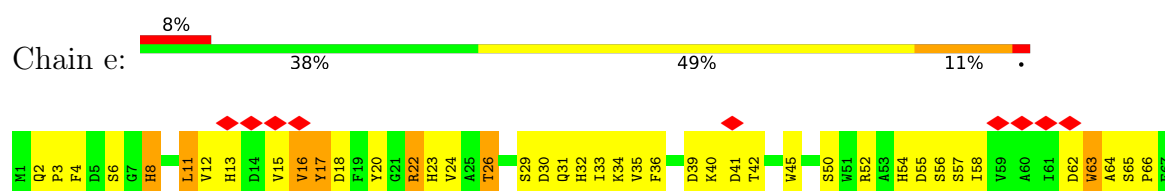
• Molecule 4: Protein transport protein SEC13

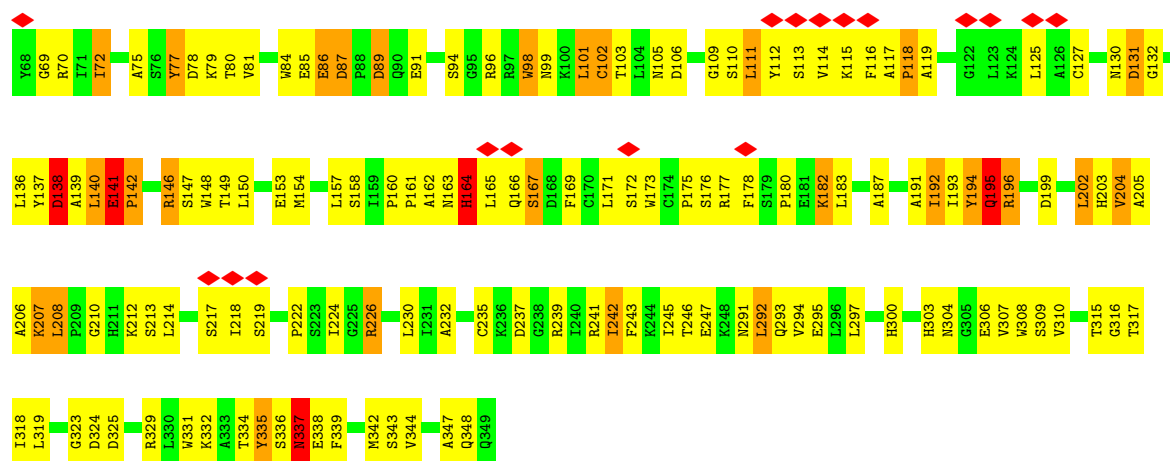


• Molecule 4: Protein transport protein SEC13

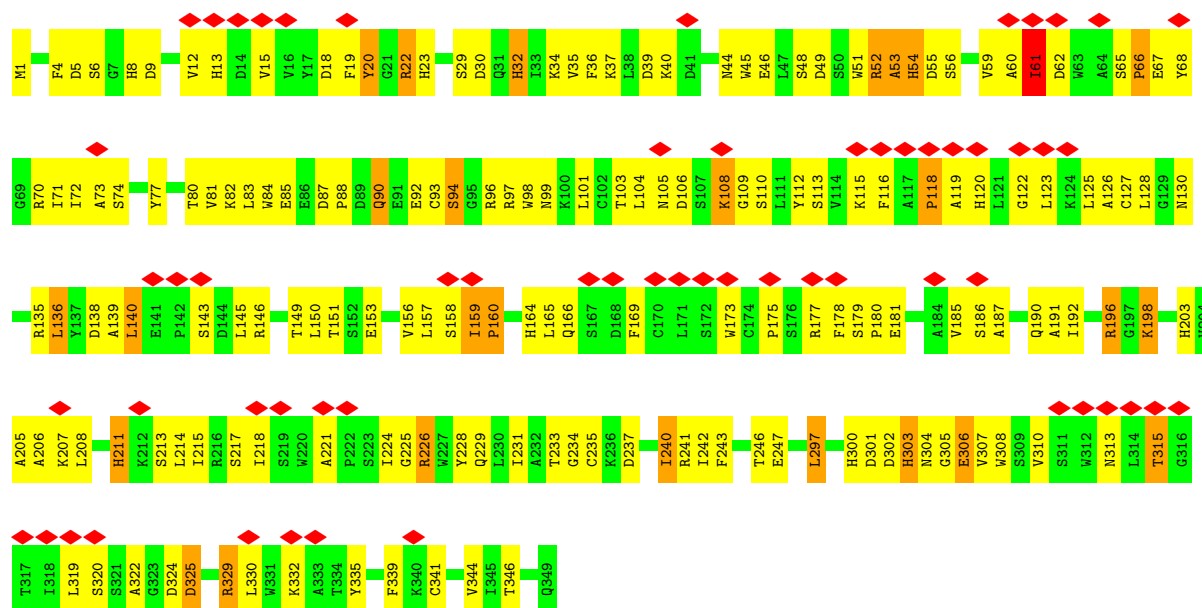


• Molecule 5: Nucleoporin Seh1

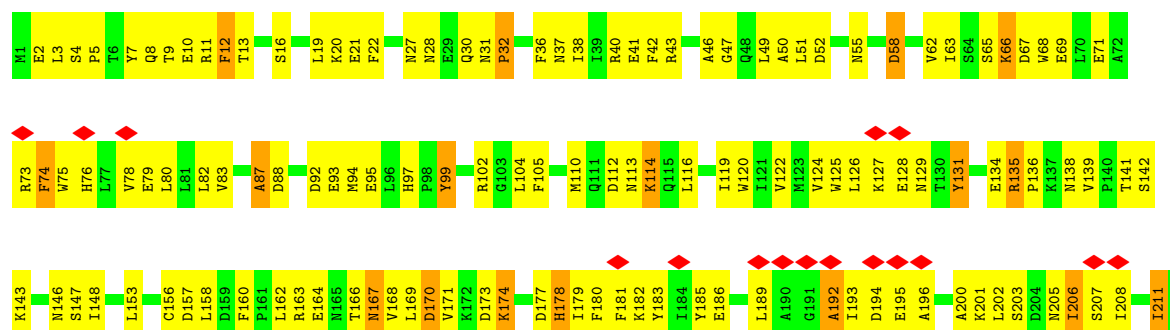


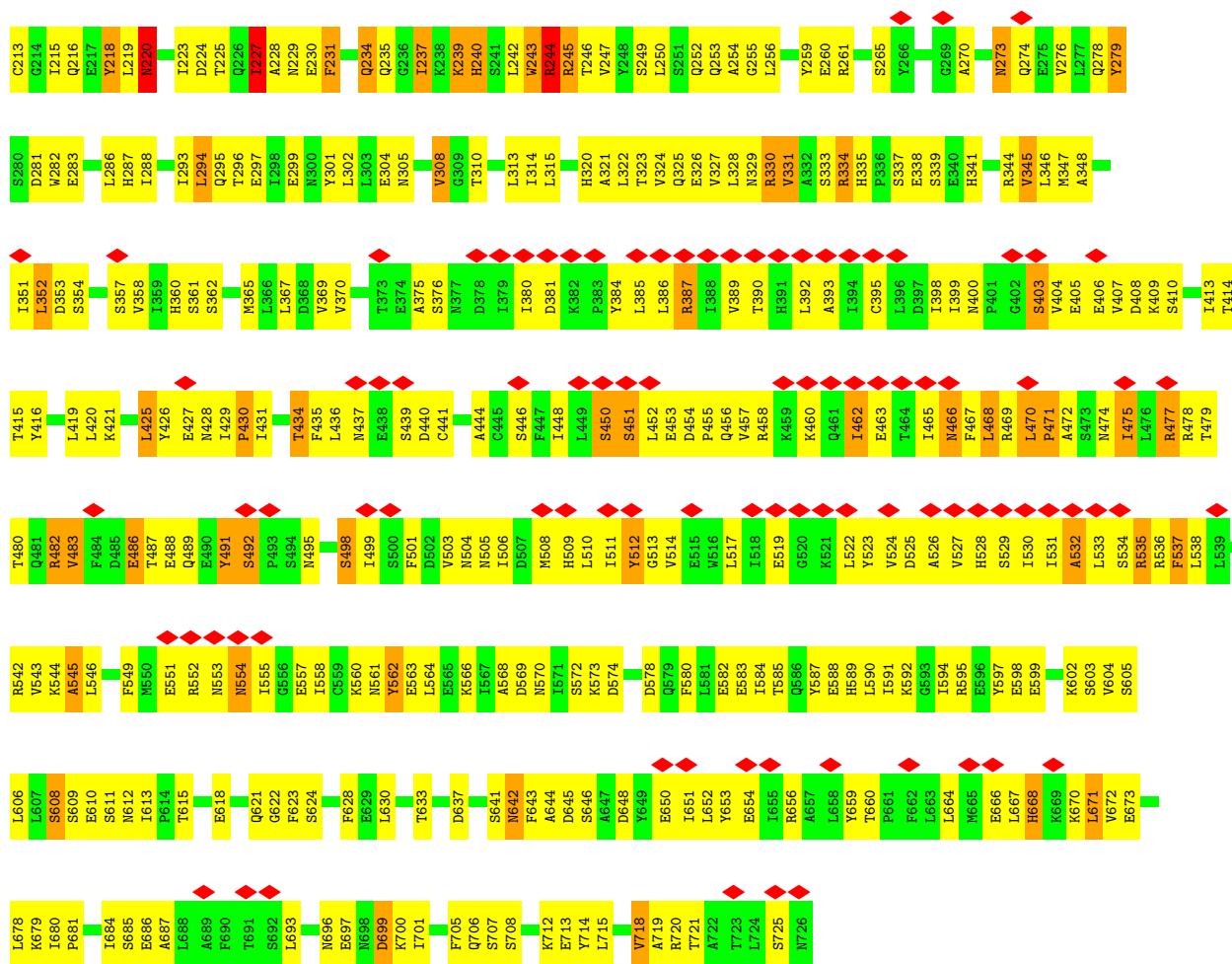


• Molecule 5: Nucleoporin Seh1

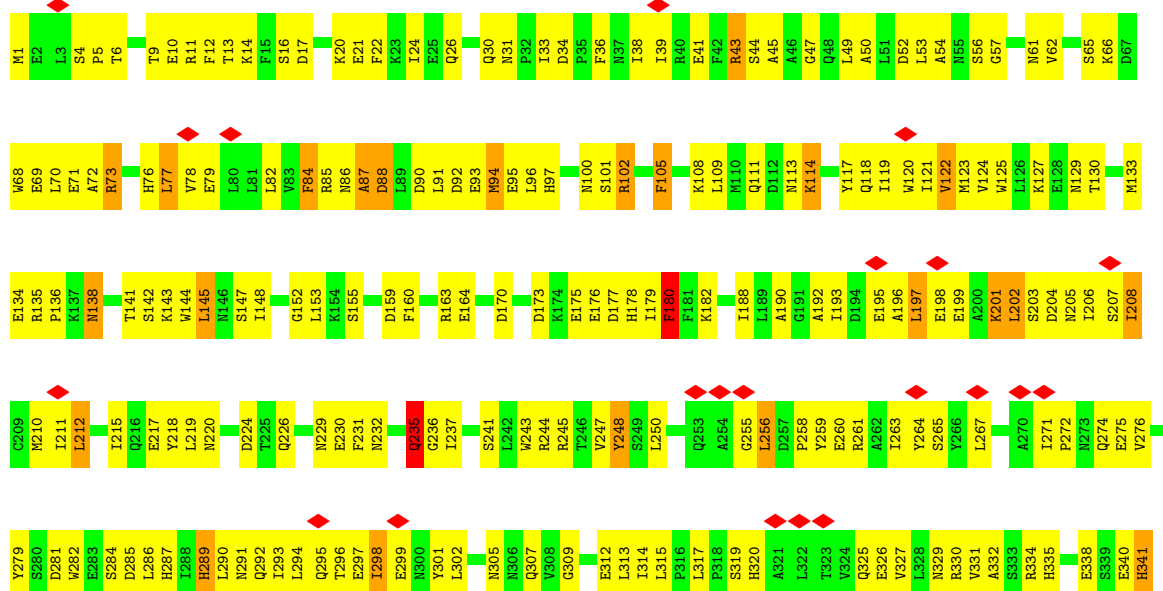


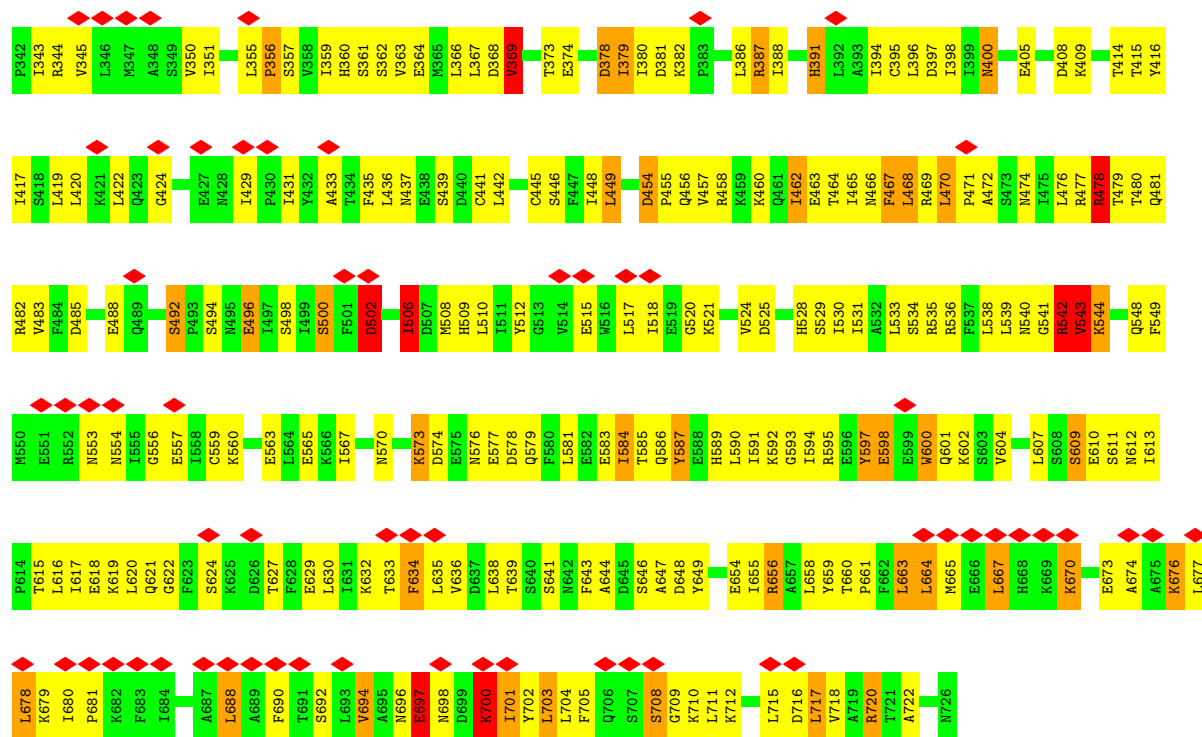
• Molecule 6: Nucleoporin NUP84



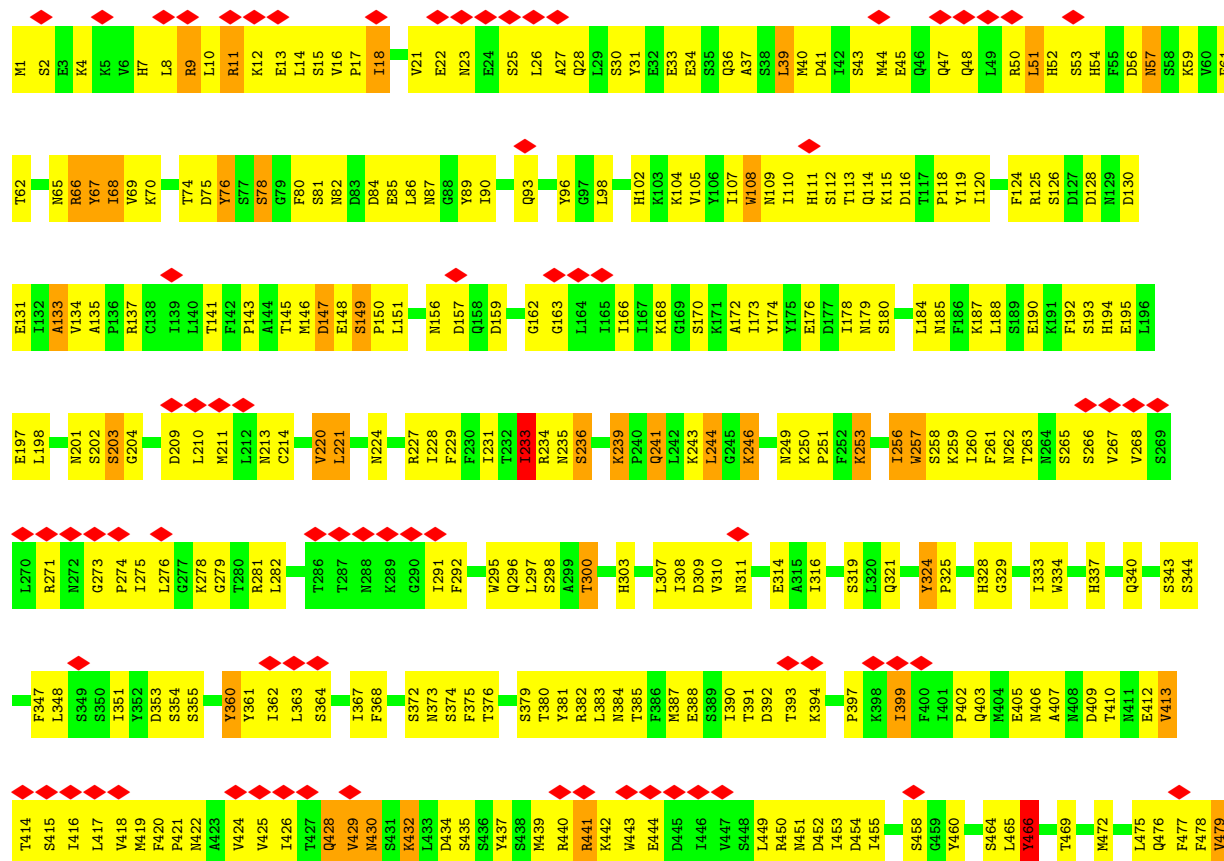


• Molecule 6: Nucleoporin NUP84





• Molecule 7: NUP133 isoform 1





V908	R66	N129	H194	I256	E318	T380	V443	I507	V571	T636	K705	N771	F843	V908
D909	Y67	D130	E197	W257	D322	Y381	E444	I508	A572	N637	F709	D772	S844	D909
D910	K70	E131	E198	K259	L323	R382	D45	N509	K573	S638	I710	M773	T846	D910
S911	T71	E132	L199	L260	Y324	N384	I446	N510	N574	P639	N711	F774	T847	S911
K912	L72	A133	P199	F261	P325	T385	V447	F511	N576	D640	F712	N776	K847	K912
G914	Q73	V134	I200	N262	A327	F386	S448	I512	K578	P641	D713	I777	F848	G914
E915	T74	A135	S202	N264	H328	E388	L449	D513	I579	F642	D714	N778	E849	E915
S916	D75	P136	S203	S265	G29	S389	R450	F514	E592	P643	L715	M779	T850	S916
L917	Y76	C138	G204	S266	L330	T390	D452	N515	K584	V644	L716	F781	L851	L917
E919	S77	I139	E205	V267	L331	D392	L463	L516	L585	I645	N718	D782	H854	E919
C920	S78	L140	E206	L270	K332	T393	D454	F517	E593	K646	C720	F783	K855	C920
H923	G79	T141	K207	N272	I333	T394	L455	E519	K590	K647	F722	N784	K856	H923
L924	F80	F142	C208	G273	D334	K394	I456	E520	F591	I646	F723	N785	L857	L924
V926	S81	M145	M211	P274	D335	F395	K396	S521	E592	I647	F724	N786	K858	V926
A927	N82	M146	L212	L275	H337	K397	Y460	L522	E593	K648	F725	N787	K859	A927
K928	D83	D147	N213	L276	P338	K398	D461	D523	L594	Q648	F726	N788	K860	K928
L929	D84	E148	C214	G277	L339	T399	S462	Q524	N595	F649	T727	N789	K861	L929
S930	E85	S149	E215	K278	Q340	F400	S463	E525	C596	L650	A728	N790	K862	S930
S931	L86	P150	E216	G279	D341	I401	S464	S526	K598	N651	C729	N791	K863	S931
L932	N87	L151	A217	T280	E342	M404	Y466	E527	K599	H652	S724	N792	K864	L932
K936	N88	A152	G219	R281	S343	E405	V467	E528	F600	H653	L735	L792	K865	K936
N937	N90	L153	L219	L282	S344	E406	L468	H529	N601	V654	D736	C793	K866	N937
N938	D91	N154	V220	L283	Q345	N408	T469	D530	S602	D461	S737	K794	K867	N938
N939	M92	P155	L221	V283	G345	D409	K470	L533	T603	V656	A738	N795	K868	N939
L944	Q93	N156	S222	T286	L346	T410	K471	L534	R605	K666	K739	N796	K869	L944
R945	I94	D157	T223	T287	F347	M411	Q471	T534	Q606	N667	E740	N797	K870	R945
K946	G95	Q158	N224	N288	L348	E412	M472	E537	S607	K668	G741	N798	K871	K946
L947	G97	Q159	M225	K289	L349	V413	G473	I538	D608	V669	L742	N799	K872	L947
N948	L98	G162	G226	G290	S350	T414	V474	F539	V609	T670	K744	N800	K873	N948
Q948	V99	G163	R227	F292	L351	T415	L475	H540	L610	N671	I745	N801	K874	Q948
Y949	N100	G166	T228	T294	Y352	S415	Q476	E543	H611	C676	V746	N802	K875	Y949
N950	D101	L164	I228	W295	D353	L416	F477	I546	D612	F677	K747	N803	K876	N950
L951	H102	L165	F229	K296	S354	L417	F478	P547	D613	N678	L748	N804	K877	L951
D952	K103	I166	F230	Q296	S355	M418	V479	P548	K616	V679	N749	N805	K878	D952
T953	Y106	G169	T231	L297	C356	N419	K480	N549	T617	D680	Y750	N806	K879	T953
I954	N109	S170	I232	A299	N357	M420	N482	L550	N620	E684	F751	N807	K880	I954
D955	H11	G170	I233	S298	T359	P421	N483	T552	N622	G685	F752	N808	K881	D955
E956	S112	Y174	N236	T300	Y360	N422	E484	L553	L623	L689	F753	N809	K882	E956
S957	T113	Y175	M237	S302	L363	A423	T485	Q554	N626	R690	F756	N810	K883	S957
K958	Q114	E176	G238	H303	S364	V425	N486	Q555	E627	L693	K757	N811	K884	K958
N959	Q115	D177	K239	P304	T365	I426	S487	H556	L628	L694	I758	N812	K885	N959
I960	K115	I178	P240	T305	T366	T427	K488	L557	L629	L695	N761	N813	K886	I960
N961	D116	N179	Q241	K306	I367	Q428	V489	S558	T630	L696	T762	N814	K887	N961
S962	T117	S180	Q241	K307	F368	V429	E490	Y559	T631	L697	Q763	N815	K888	S962
K963	P118	I181	L242	L307	D369	N430	V491	B560	K632	P698	P764	N816	K889	K963
L964	Y119	N182	K243	I308	S370	S431	G492	F563	T633	N699	V765	N817	K890	L964
Q965	I120	L184	L244	D309	S371	K432	F493	F564	V634	E700	K766	N818	K891	Q965
Q970	V121	K245	G245	N310	S372	L433	V494	F567	V635	W701	F767	N819	K892	Q970
C972	V122	K246	L247	I312	N373	D434	S435	L568	T569	E702	I768	N820	K893	C972
K973	F124	K187	L248	Y313	S374	S436	Y437	F570	F570	V501	N769	N821	K894	K973
	R125	S189	N249	E314	F375	S437	Q500			V502		N822	K895	
	S126	F192	K250	A315	T376	R440	Y437			V503		N823	K896	
	D127	S193	K251	I316	I377	R441	Y437					N824	K897	
			F252	L317	F378	K442						N825	K898	
			K253		S379							N826	K899	
			L254									N827	K900	
			Q255									N828	K901	
												N829	K902	
												N830	K903	
												N831	K904	
												N832	K905	
												N833	K906	
												N834	K907	
												N835	K908	
												N836	K909	
												N837	K910	
												N838	K911	
												N839	K912	
												N840	K913	
												N841	K914	
												N842	K915	
												N843	K916	
												N844	K917	
												N845	K918	
												N846	K919	
												N847	K920	
												N848	K921	
												N849	K922	
												N850	K923	
												N851	K924	
												N852	K925	
												N853	K926	
												N854	K927	
												N855	K928	
												N856	K929	
												N857	K930	
												N858	K931	
												N859	K932	
												N860	K933	
												N861	K934	
												N862	K935	
												N863	K936	
												N864	K937	
												N865	K938	
												N866	K939	
												N867	K940	
												N868	K941	
												N869	K942	
												N870	K943	
												N871	K944	
												N872	K945	
												N873	K946	
												N874	K947	
												N875	K948	
												N876	K949	
												N877	K950	
												N878	K951	
												N879	K952	
												N880	K953	
												N881	K954	
												N882	K955	
												N883	K956	
												N884	K957	
												N885	K958	
												N886	K959	
												N887	K960	
												N888	K961	
												N889	K962	
												N890	K963	
												N891	K964	
												N892	K965	
												N893	K966	
												N894	K967	
												N895	K968	
												N896	K969	
												N897	K970	
												N898	K971	
												N899	K972	
												N900	K973	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction applied in RELION during the alignment and reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.038	Depositor
Minimum map value	-1.569	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.66, 2.66, 2.66	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	2.24	296/8509 (3.5%)	2.49	607/11534 (5.3%)
1	l	2.21	273/8509 (3.2%)	2.45	564/11534 (4.9%)
2	b	2.20	171/5293 (3.2%)	2.48	393/7172 (5.5%)
2	m	2.26	177/5297 (3.3%)	2.51	383/7178 (5.3%)
3	c	2.19	168/4963 (3.4%)	2.45	368/6704 (5.5%)
3	n	2.21	162/4908 (3.3%)	2.51	377/6627 (5.7%)
4	d	2.07	75/2277 (3.3%)	2.22	113/3108 (3.6%)
4	o	2.24	87/2277 (3.8%)	2.39	142/3108 (4.6%)
5	e	2.19	94/2500 (3.8%)	2.30	145/3388 (4.3%)
5	p	2.31	106/2500 (4.2%)	2.42	155/3388 (4.6%)
6	f	2.24	220/6007 (3.7%)	2.55	495/8143 (6.1%)
6	q	2.16	208/6007 (3.5%)	2.43	417/8143 (5.1%)
7	g	2.15	313/9599 (3.3%)	2.41	677/13008 (5.2%)
7	r	2.25	354/9597 (3.7%)	2.50	722/13007 (5.6%)
All	All	2.21	2704/78243 (3.5%)	2.46	5558/106042 (5.2%)

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	26
1	l	0	27
2	b	0	23
2	m	0	14
3	c	0	16
3	n	0	19
4	d	0	3
4	o	0	5
5	e	0	8
5	p	0	4
6	f	0	21

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
6	q	0	20
7	g	0	20
7	r	0	31
All	All	0	237

The worst 5 of 2704 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	115	TYR	CG-CD1	23.09	1.87	1.39
2	m	115	TYR	CG-CD2	22.20	1.85	1.39
2	m	115	TYR	CE1-CZ	20.92	1.88	1.38
2	m	115	TYR	CE2-CZ	20.79	1.88	1.38
2	m	115	TYR	CD2-CE2	15.04	1.83	1.38

The worst 5 of 5558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	840	PHE	CA-CB-CG	-13.64	100.16	113.80
1	l	169	VAL	N-CA-C	-13.63	100.09	111.81
7	r	53	SER	N-CA-C	-13.09	97.05	113.55
3	n	116	PRO	N-CA-CB	12.47	116.58	103.23
1	a	137	PHE	CA-CB-CG	12.20	126.00	113.80

There are no chirality outliers.

5 of 237 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	27	TYR	Sidechain
1	a	6	ARG	Sidechain
1	a	72	PHE	Sidechain
1	a	82	TYR	Sidechain
1	a	96	HIS	Sidechain

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	8321	0	8169	27	0
1	l	8321	0	8169	46	0
2	b	5186	0	5159	41	0
2	m	5190	0	5173	73	0
3	c	4877	0	4854	67	0
3	n	4822	0	4829	31	0
4	d	2216	0	2118	132	0
4	o	2216	0	2118	62	0
5	e	2439	0	2375	78	0
5	p	2439	0	2375	14	0
6	f	5895	0	5875	53	0
6	q	5895	0	5875	147	0
7	g	9403	0	9304	459	0
7	r	9401	0	9304	64	0
All	All	76621	0	75697	1240	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 8.

The worst 5 of 1240 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:b:657:TYR:CE2	3:c:109:THR:CB	1.75	1.66
2:m:115:TYR:CE1	2:m:115:TYR:CD1	1.83	1.66
2:m:115:TYR:CE2	2:m:115:TYR:CD2	1.83	1.66
7:g:1063:LYS:HD3	7:g:1140:VAL:CG1	1.21	1.64
2:m:115:TYR:CD2	2:m:115:TYR:CG	1.86	1.62

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 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	1008/1037 (97%)	910 (90%)	69 (7%)	29 (3%)	3	23
1	l	1008/1037 (97%)	899 (89%)	67 (7%)	42 (4%)	2	17
2	b	643/744 (86%)	574 (89%)	42 (6%)	27 (4%)	2	17
2	m	643/744 (86%)	535 (83%)	73 (11%)	35 (5%)	1	15
3	c	608/1317 (46%)	540 (89%)	47 (8%)	21 (4%)	3	20
3	n	597/1317 (45%)	527 (88%)	48 (8%)	22 (4%)	2	20
4	d	284/297 (96%)	227 (80%)	42 (15%)	15 (5%)	1	15
4	o	284/297 (96%)	230 (81%)	41 (14%)	13 (5%)	2	17
5	e	303/307 (99%)	255 (84%)	35 (12%)	13 (4%)	2	17
5	p	303/307 (99%)	276 (91%)	18 (6%)	9 (3%)	3	23
6	f	724/726 (100%)	661 (91%)	42 (6%)	21 (3%)	3	23
6	q	724/726 (100%)	647 (89%)	50 (7%)	27 (4%)	2	20
7	g	1155/1157 (100%)	1022 (88%)	91 (8%)	42 (4%)	2	20
7	r	1155/1157 (100%)	994 (86%)	102 (9%)	59 (5%)	1	15
All	All	9439/11170 (84%)	8297 (88%)	767 (8%)	375 (4%)	4	18

5 of 375 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	85	SER
1	a	125	ASP
1	a	201	ASP
1	a	204	TYR
1	a	780	HIS

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	950/972 (98%)	919 (97%)	31 (3%)	33	55
1	l	950/972 (98%)	918 (97%)	32 (3%)	32	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	578/670 (86%)	557 (96%)	21 (4%)	31	52
2	m	580/670 (87%)	559 (96%)	21 (4%)	31	52
3	c	544/1161 (47%)	523 (96%)	21 (4%)	28	49
3	n	544/1161 (47%)	530 (97%)	14 (3%)	40	62
4	d	232/252 (92%)	213 (92%)	19 (8%)	10	31
4	o	232/252 (92%)	217 (94%)	15 (6%)	15	37
5	e	268/268 (100%)	249 (93%)	19 (7%)	13	35
5	p	268/268 (100%)	254 (95%)	14 (5%)	21	42
6	f	669/669 (100%)	634 (95%)	35 (5%)	21	42
6	q	669/669 (100%)	630 (94%)	39 (6%)	18	40
7	g	1088/1088 (100%)	1013 (93%)	75 (7%)	14	36
7	r	1088/1088 (100%)	1039 (96%)	49 (4%)	24	46
All	All	8660/10160 (85%)	8255 (95%)	405 (5%)	25	45

5 of 405 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	565	THR
3	n	508	LYS
7	r	973	LYS
1	l	641	ASP
2	m	399	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 293 such sidechains are listed below:

Mol	Chain	Res	Type
6	q	205	ASN
7	r	1030	ASN
6	q	360	HIS
7	r	373	ASN
7	g	93	GLN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	e	1
5	p	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	248:LYS	C	291:ASN	N	11.37
1	p	248:LYS	C	291:ASN	N	7.67

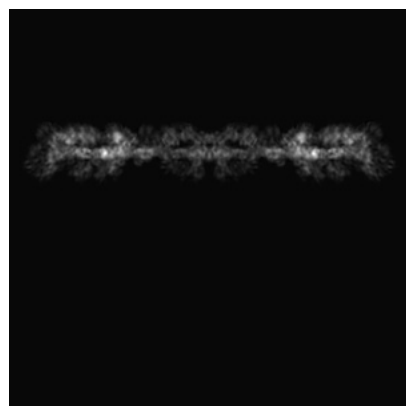
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41285. These allow visual inspection of the internal detail of the map and identification of artifacts.

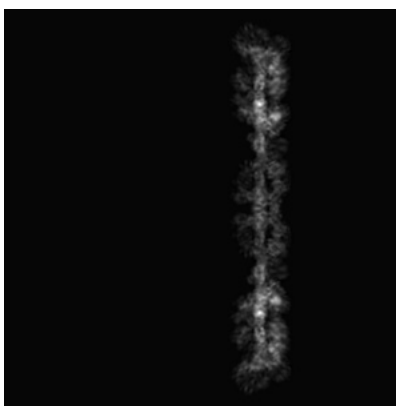
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

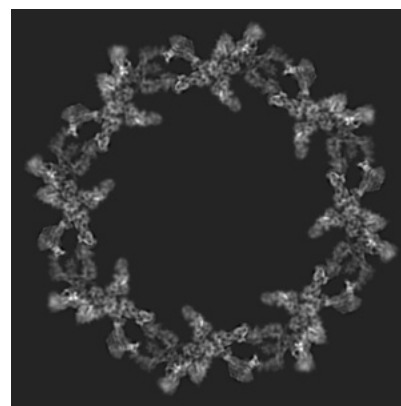
6.1.1 Primary map



X

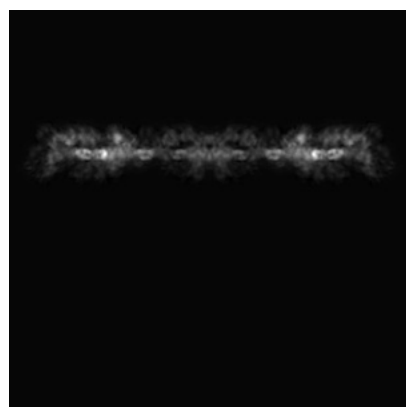


Y

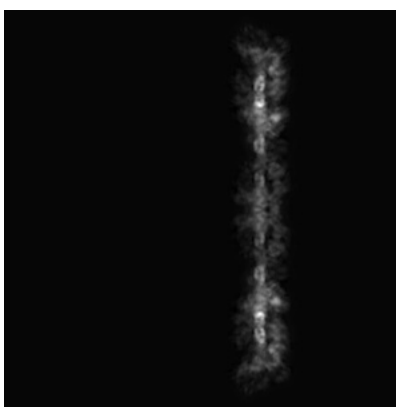


Z

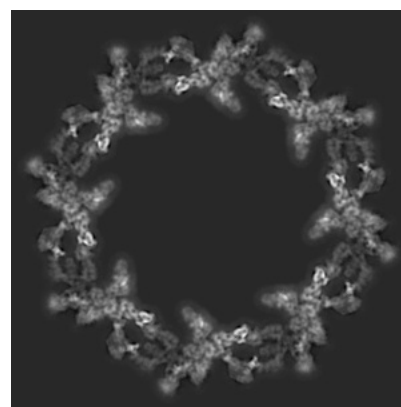
6.1.2 Raw map



X



Y

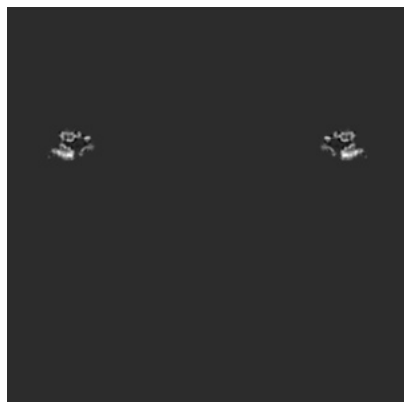


Z

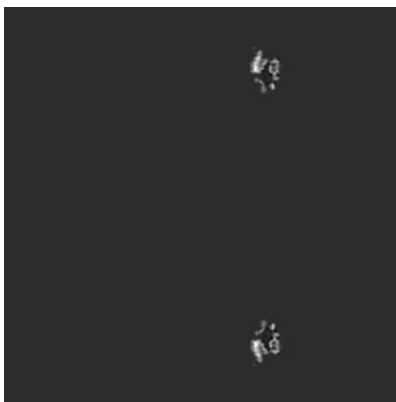
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

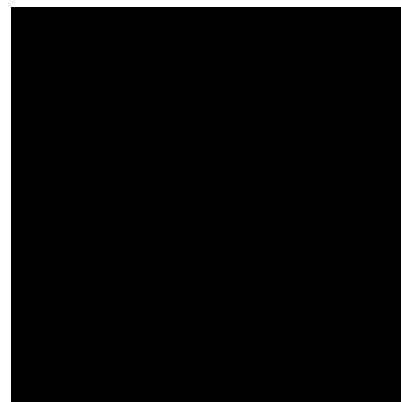
6.2.1 Primary map



X Index: 240

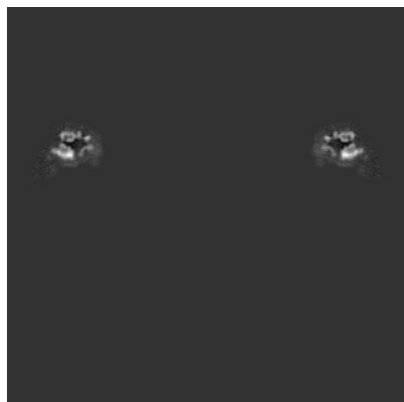


Y Index: 240

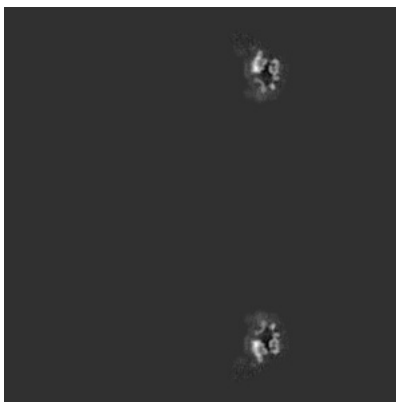


Z Index: 240

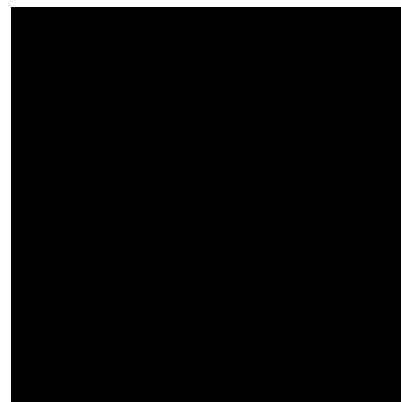
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

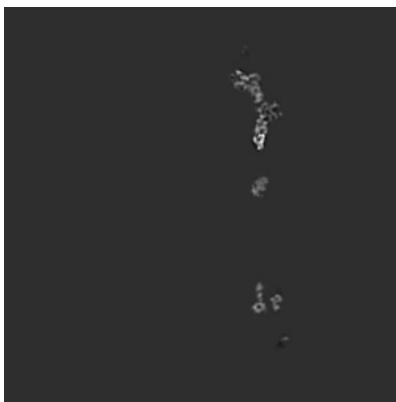
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

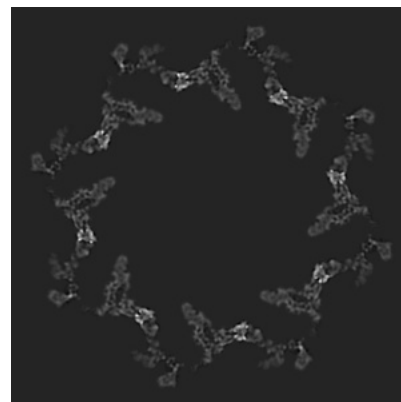
6.3.1 Primary map



X Index: 366

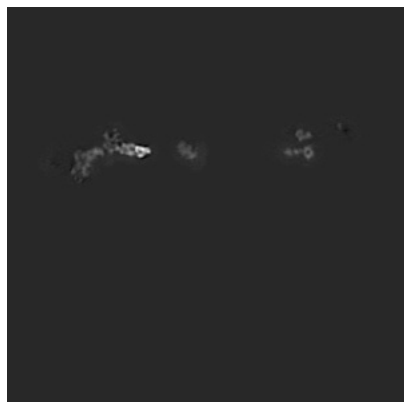


Y Index: 366

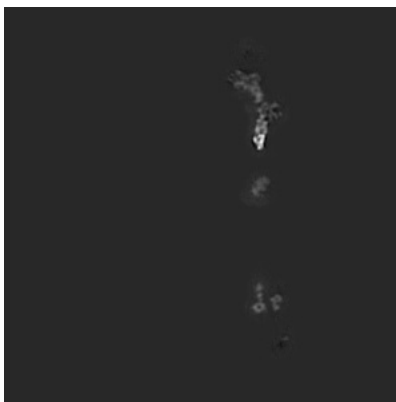


Z Index: 309

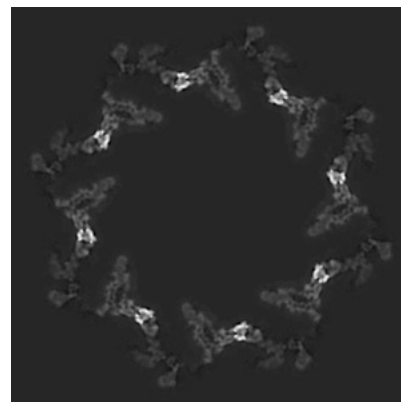
6.3.2 Raw map



X Index: 366



Y Index: 366

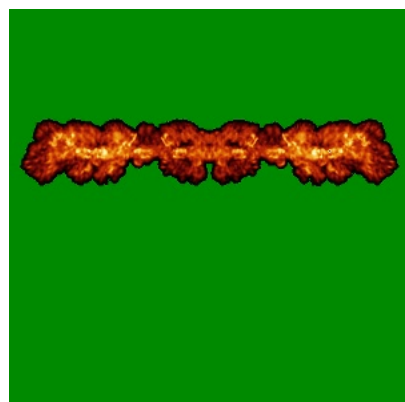


Z Index: 309

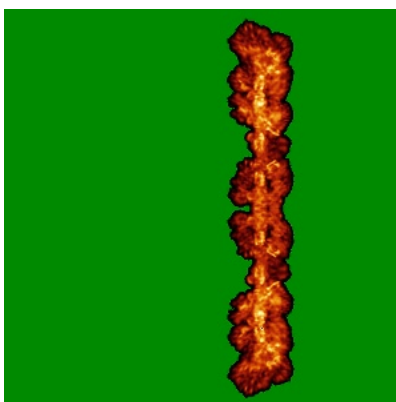
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

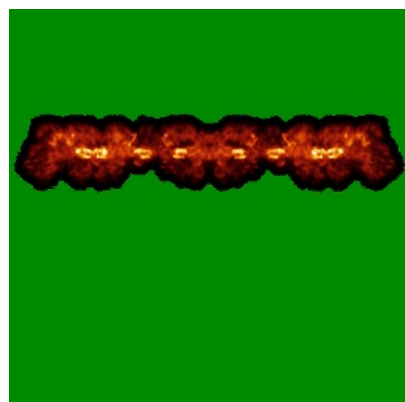


Y

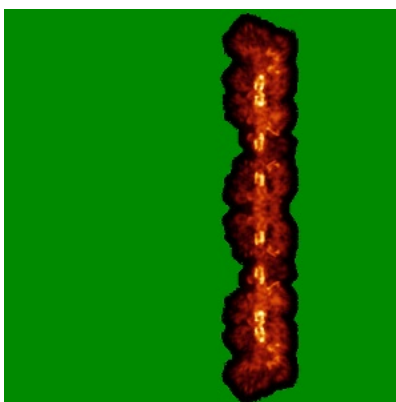


Z

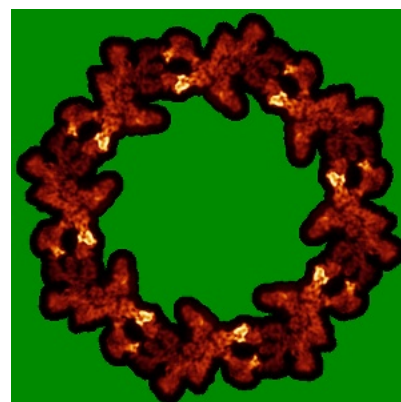
6.4.2 Raw map



X



Y

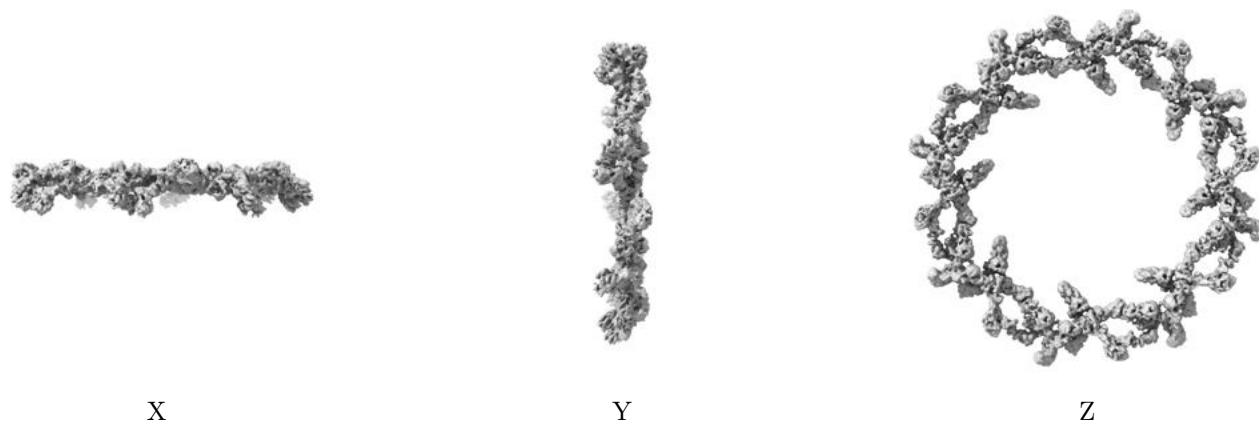


Z

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.

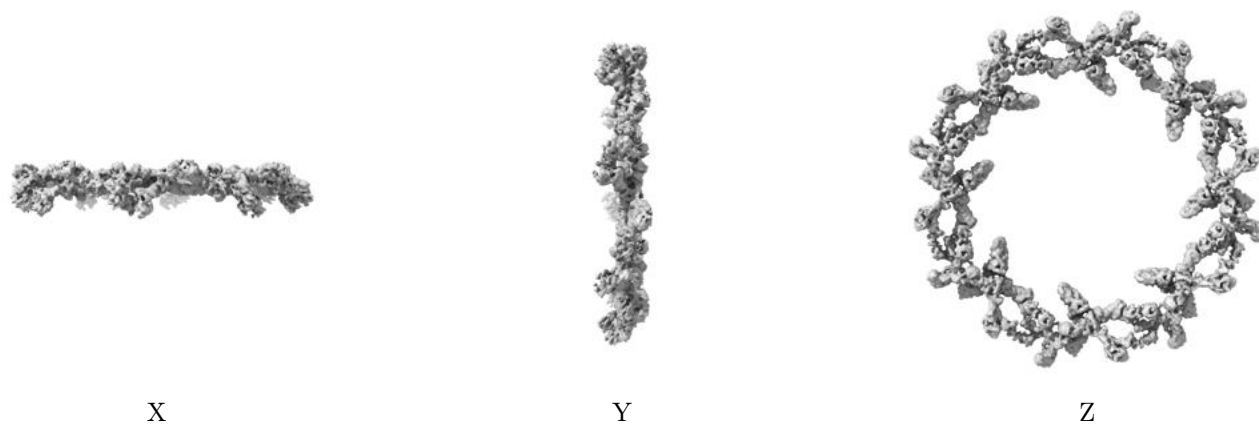
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

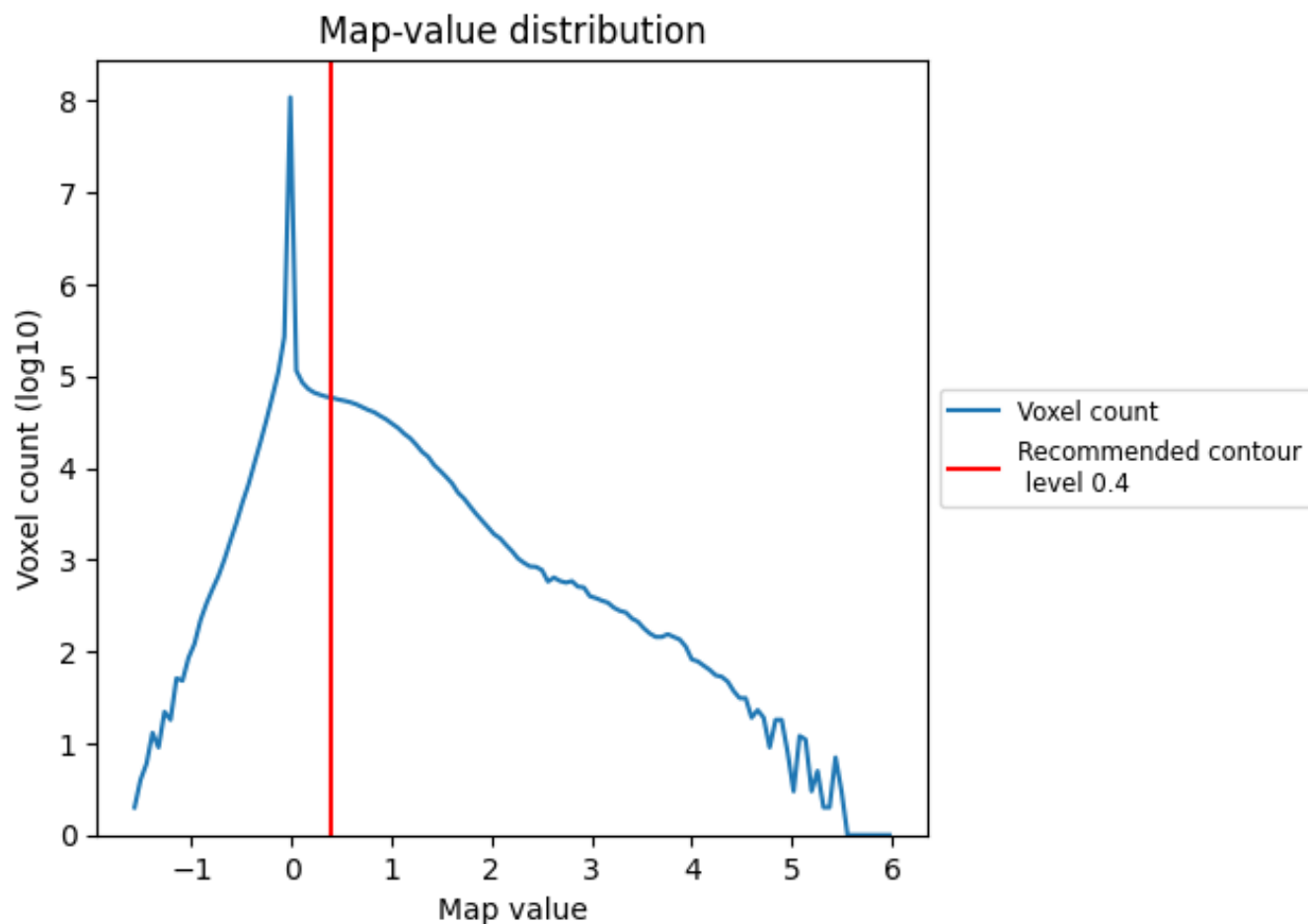
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

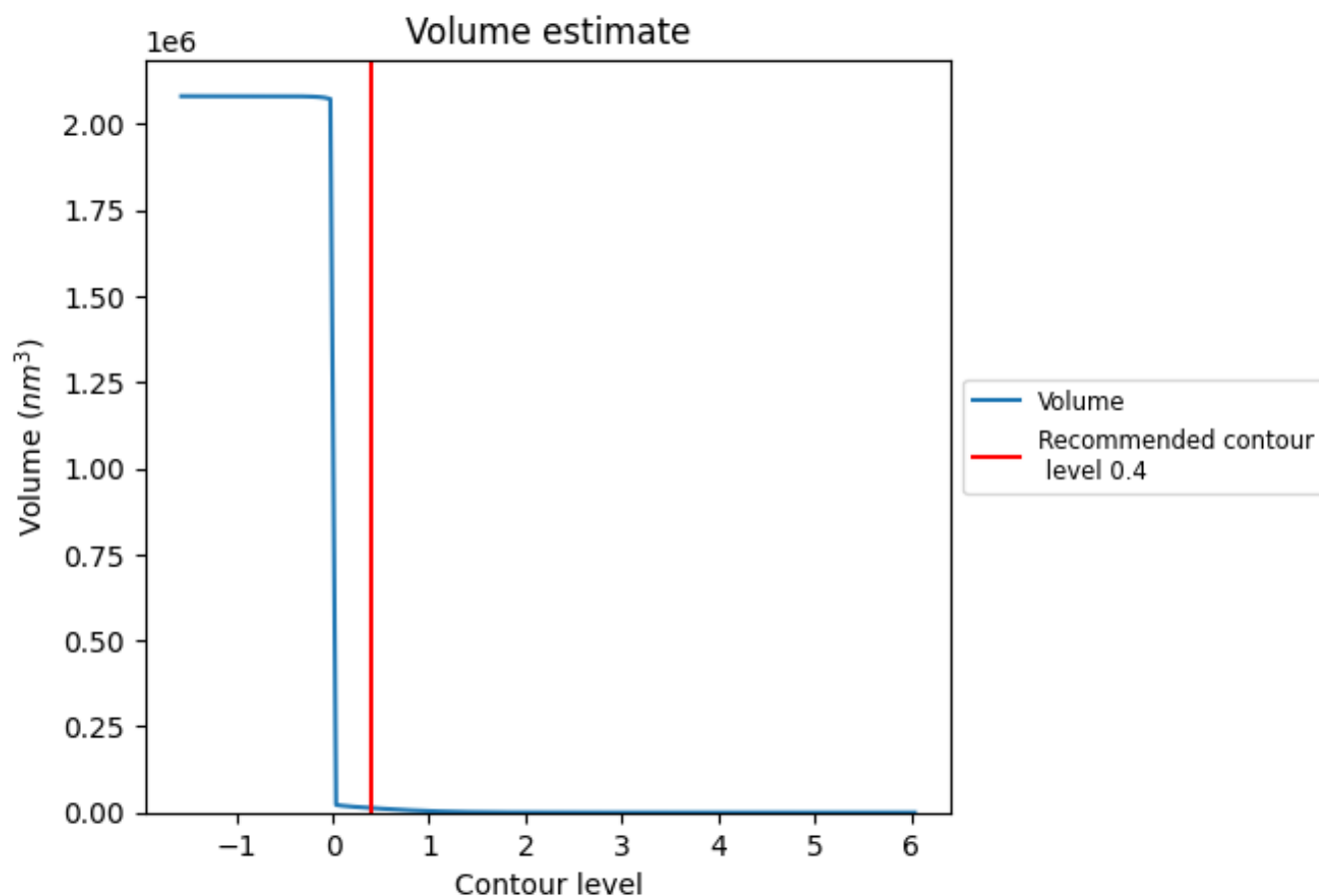
This section contains the results of statistical analysis of the map.

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.

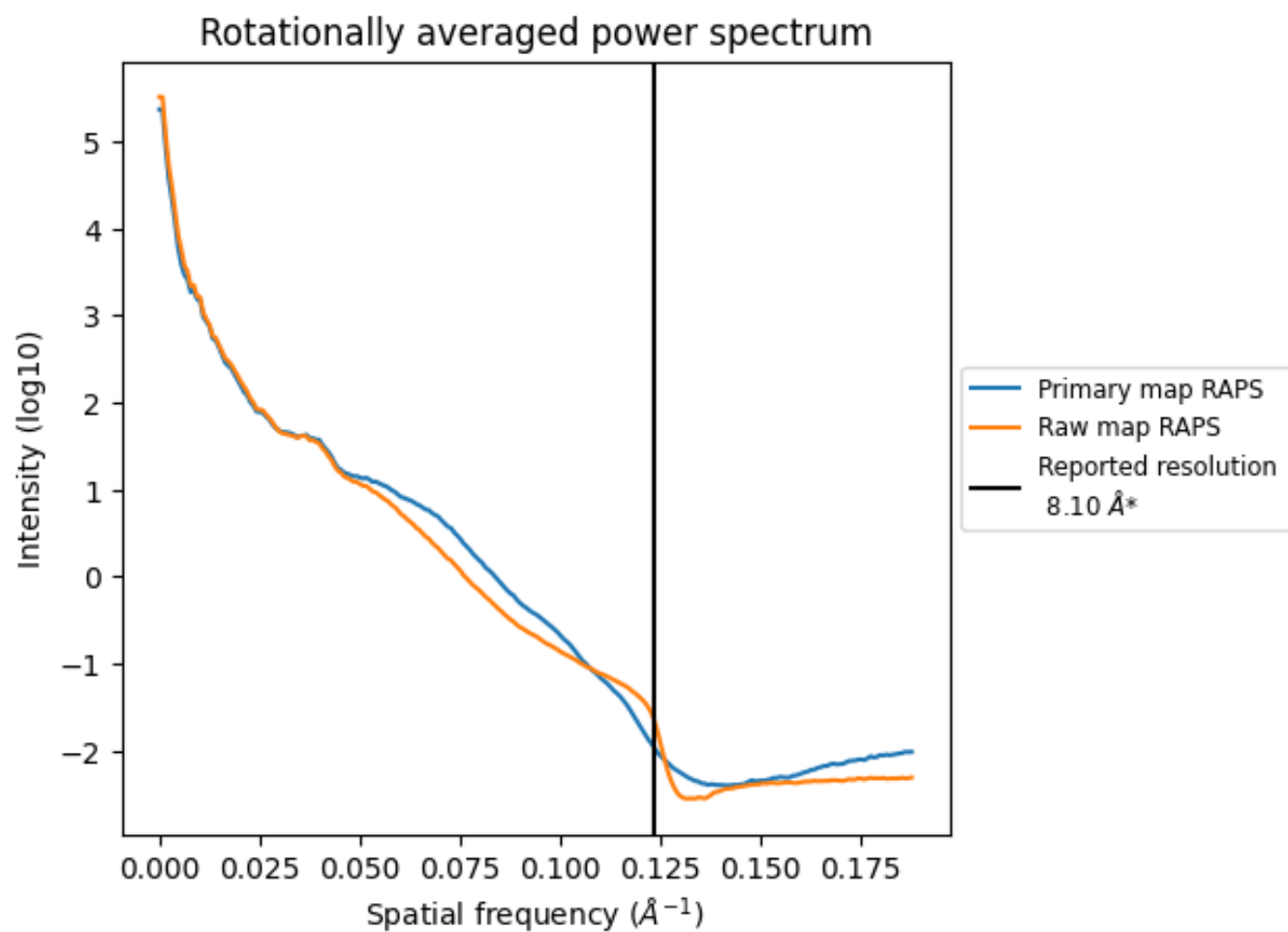
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13169 nm^3 ; this corresponds to an approximate mass of 11895 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 ⓘ

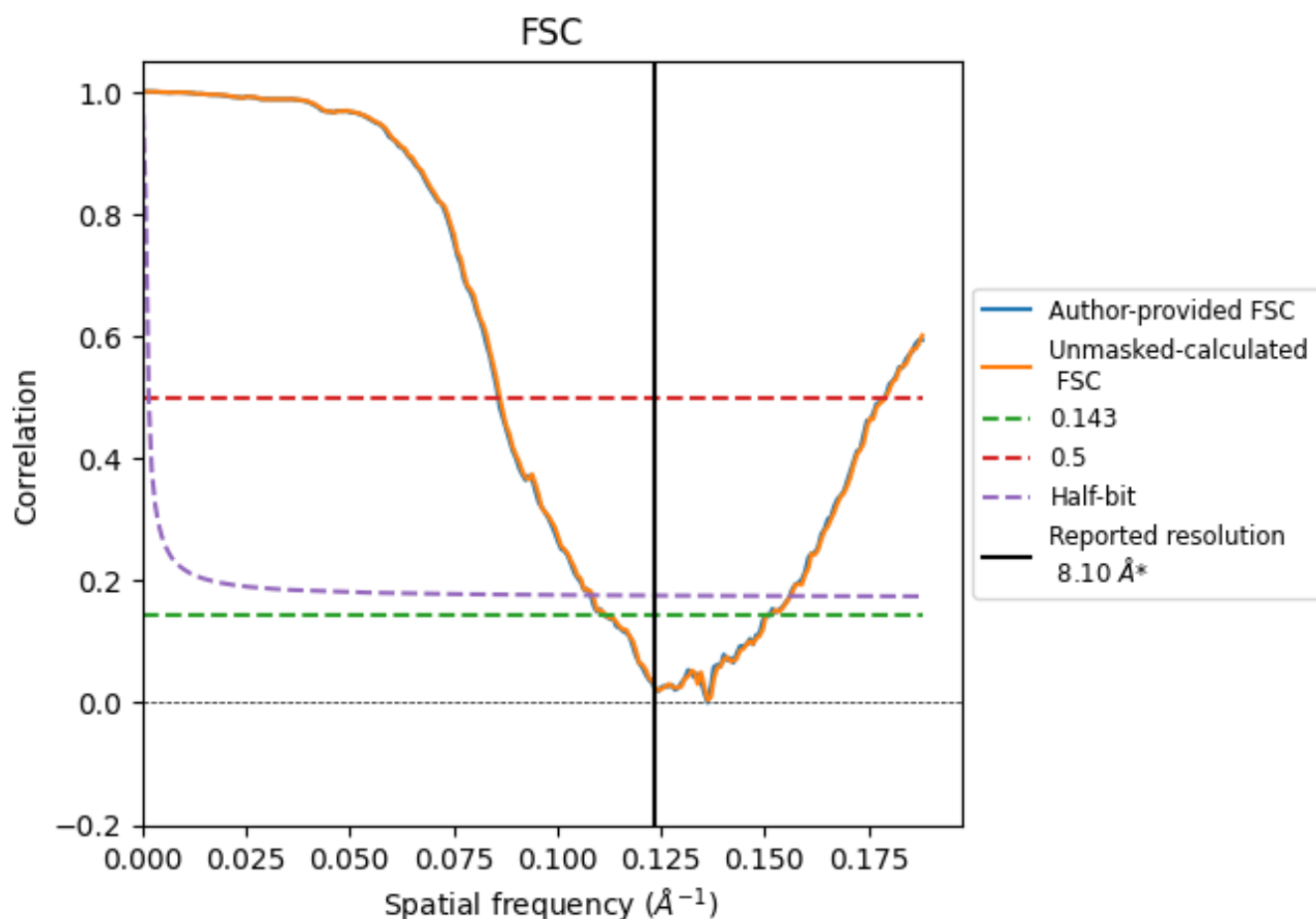


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.98	11.66	9.25
Unmasked-calculated*	8.94	11.61	9.22

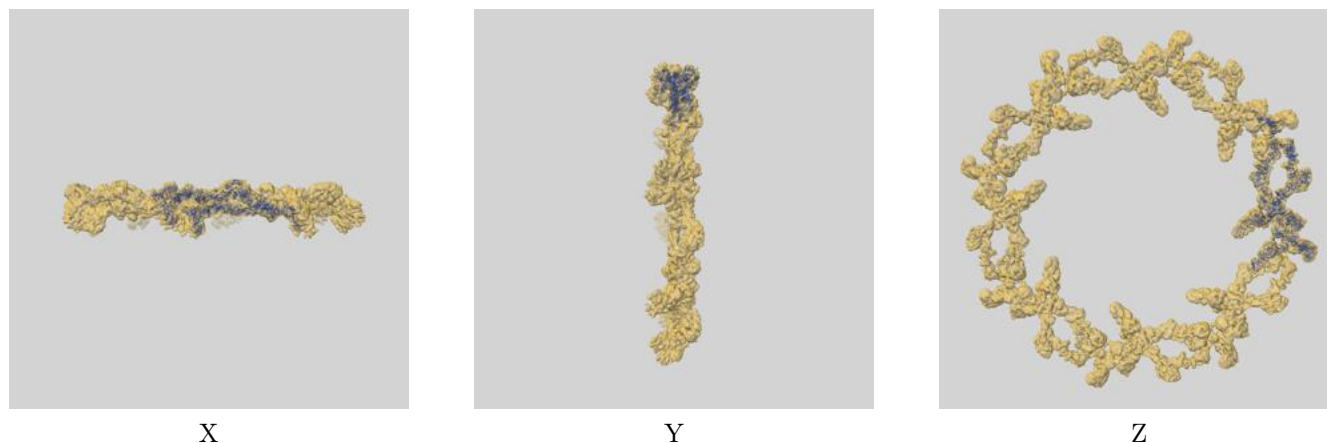
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.98 differs from the reported value 8.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.94 differs from the reported value 8.1 by more than 10 %

9 Map-model fit [i](#)

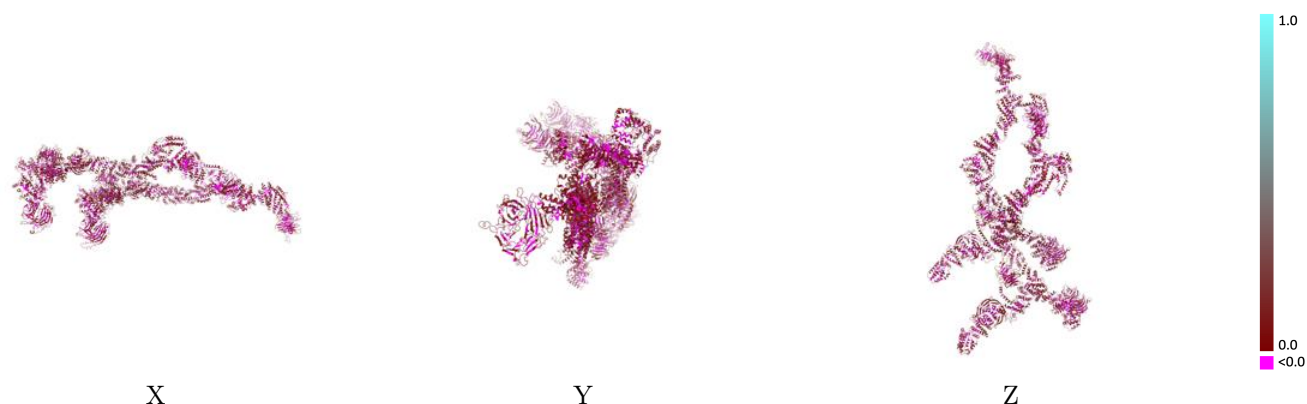
This section contains information regarding the fit between EMDB map EMD-41285 and PDB model 8TIE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



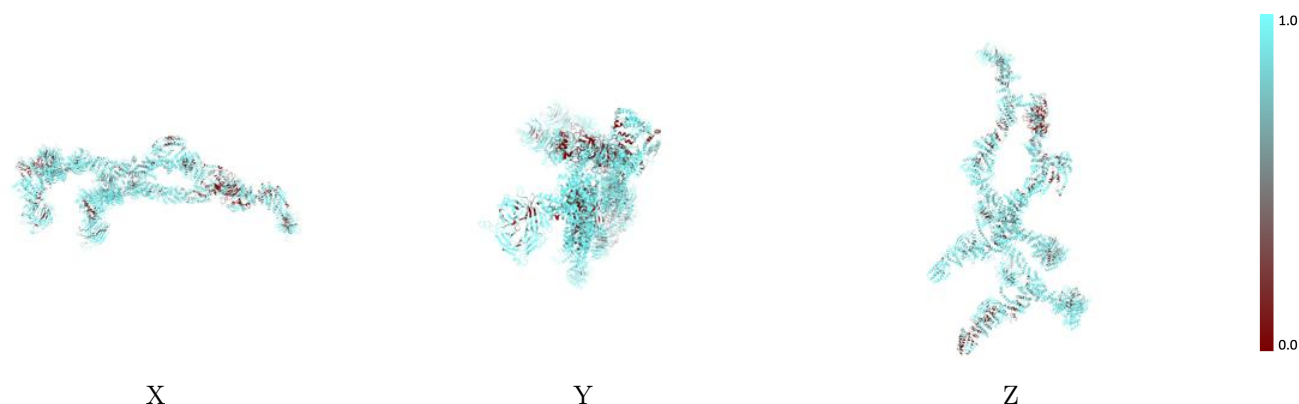
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



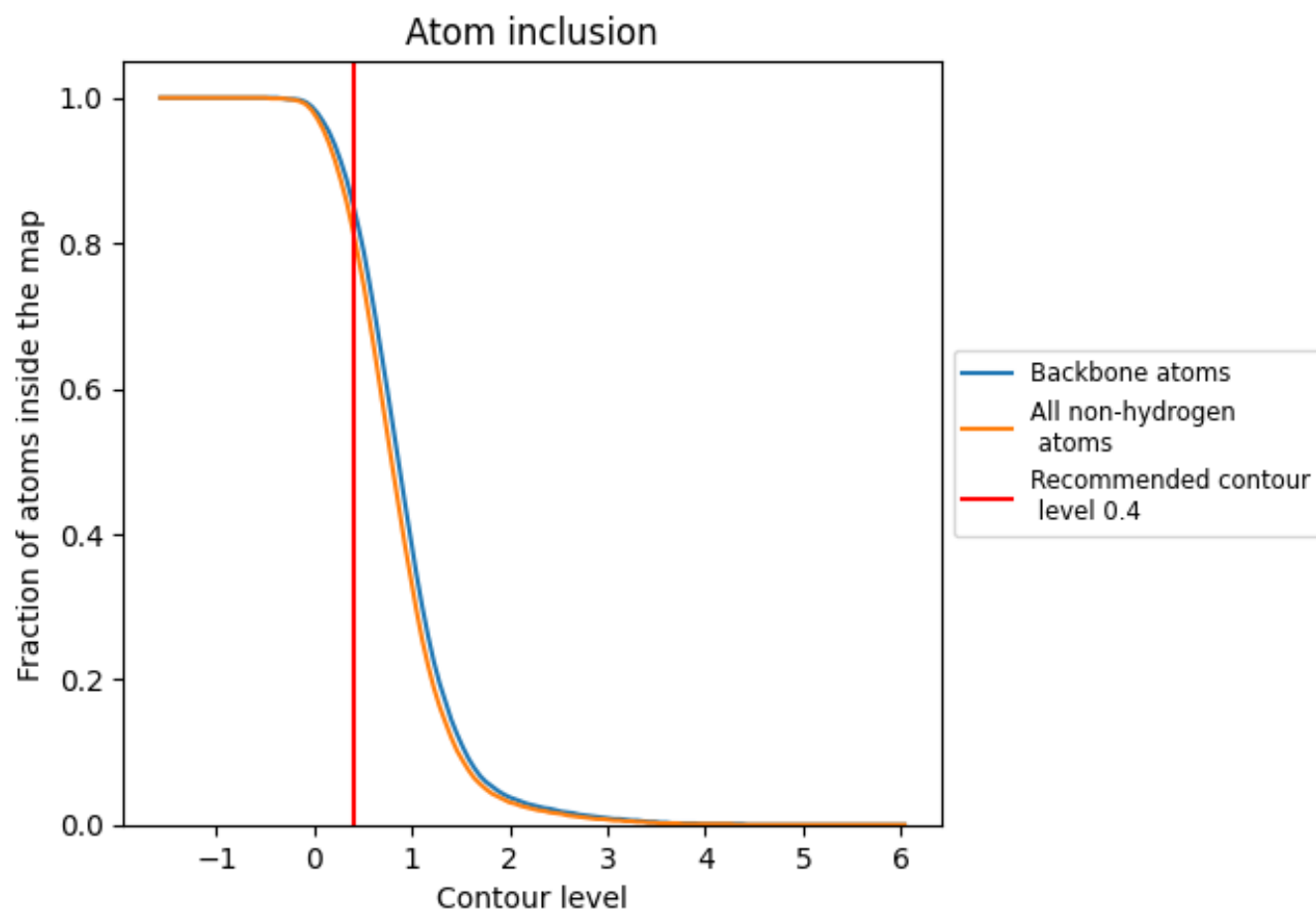
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.0800
a	0.8790	0.0790
b	0.9200	0.0820
c	0.9250	0.1050
d	0.8380	0.0730
e	0.8750	0.0860
f	0.8020	0.0840
g	0.7680	0.0720
l	0.8810	0.0810
m	0.6230	0.0780
n	0.9040	0.1040
o	0.8880	0.0840
p	0.7600	0.0720
q	0.8300	0.1000
r	0.6810	0.0490

1.0

0.0

<0.0