



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 12:12 AM JST

PDB ID : 7VCI
EMDB ID : EMD-31891
Title : Structure of *Xenopus laevis* NPC nuclear ring asymmetric unit
Authors : Tai, L.; Zhu, Y.; Sun, F.
Deposited on : 2021-09-03
Resolution : 8.10 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:

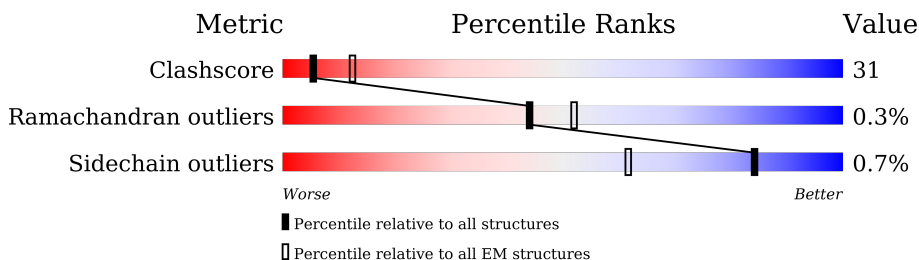
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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.





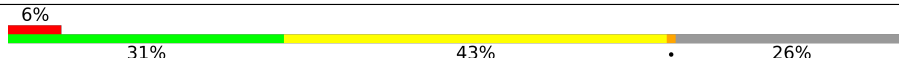
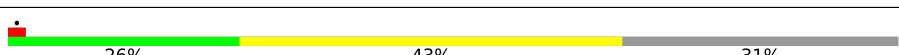
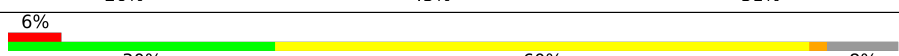
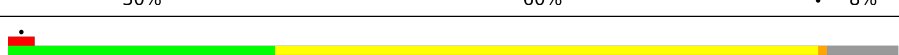
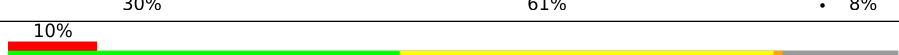
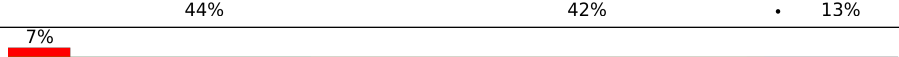



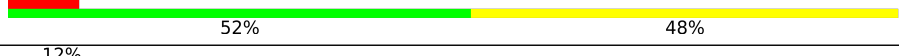

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	653	 44% 55%
1	J	653	 46% 53%
2	B	375	 14% 36% 62%
2	K	375	 11% 46% 53%
3	C	360	 33% 59% 8%
3	L	360	 33% 56% 10%
4	D	1439	 13% 58% 38%
4	M	1439	 10% 49% 47%

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Mol	Chain	Length	Quality of chain
5	E	326	 55% 45%
5	N	326	 7% 55% 45%
6	F	924	 6% 31% 43% 26%
6	O	924	 26% 43% 31%
7	G	320	 6% 30% 60% 8%
7	P	320	 30% 61% 8%
8	H	916	 10% 44% 42% 13%
8	Q	916	 7% 34% 49% 15%
9	I	1140	 24% 58% 35% 6%
9	R	1140	 69% 51% 44% 5%
10	S	2011	 8% 52% 48%
11	T	2408	 12% 28% 14% 58%
12	U	820	 48% 51%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 124700 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 Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		
1	J	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		

- Molecule 2 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		
2	K	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		

- Molecule 3 is a protein called Nucleoporin SEH1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	333	Total	C	N	O	S	0	0
			2607	1632	466	491	18		
3	L	325	Total	C	N	O	S	0	0
			2546	1592	455	482	17		

- Molecule 4 is a protein called Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		
4	M	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		

- Molecule 5 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		
5	N	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		

- Molecule 6 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	687	Total	C	N	O	S	0	0
			5560	3525	979	1024	32		
6	O	637	Total	C	N	O	S	0	0
			5168	3282	911	946	29		

- Molecule 7 is a protein called GATOR complex protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		
7	P	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		

- Molecule 8 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	798	Total	C	N	O	S	0	0
			6494	4126	1096	1240	32		
8	Q	780	Total	C	N	O	S	0	0
			6351	4034	1076	1210	31		

- Molecule 9 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1076	Total	C	N	O	S	0	0
			8482	5362	1409	1661	50		
9	R	1082	Total	C	N	O	S	0	0
			8536	5397	1420	1669	50		

- Molecule 10 is a protein called MGC83295 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	2011	Total	C	N	O	S	0	0
			15974	10112	2785	2978	99		

- Molecule 11 is a protein called Protein ELYS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	1013	8041	5095	1388	1518	40	0	0

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

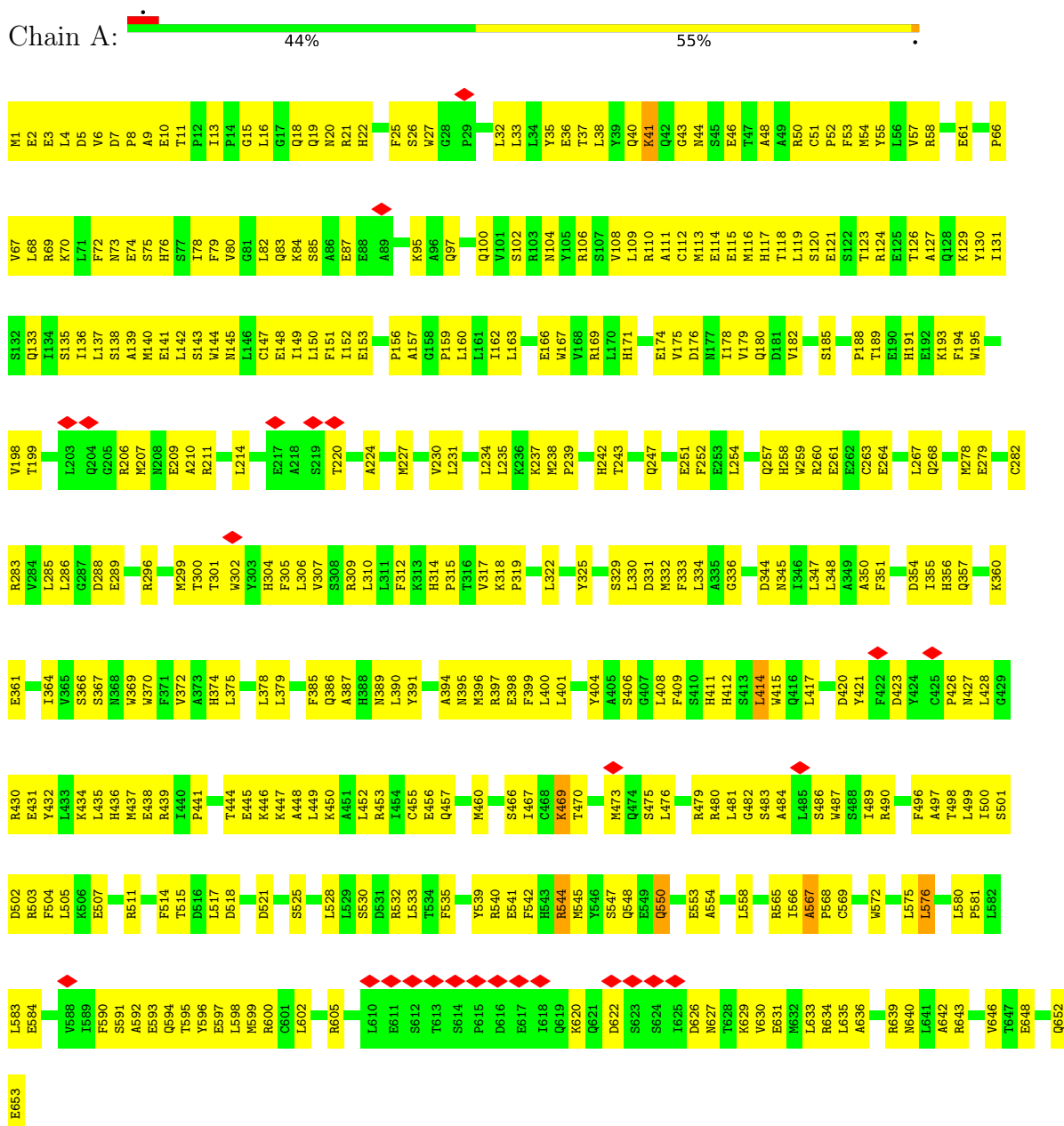
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	820	6569	4132	1146	1259	32	0	0

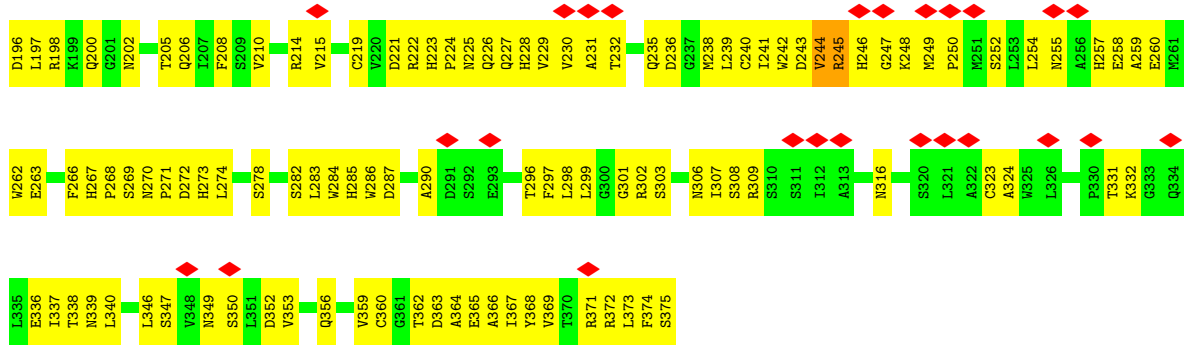
3 Residue-property plots

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.

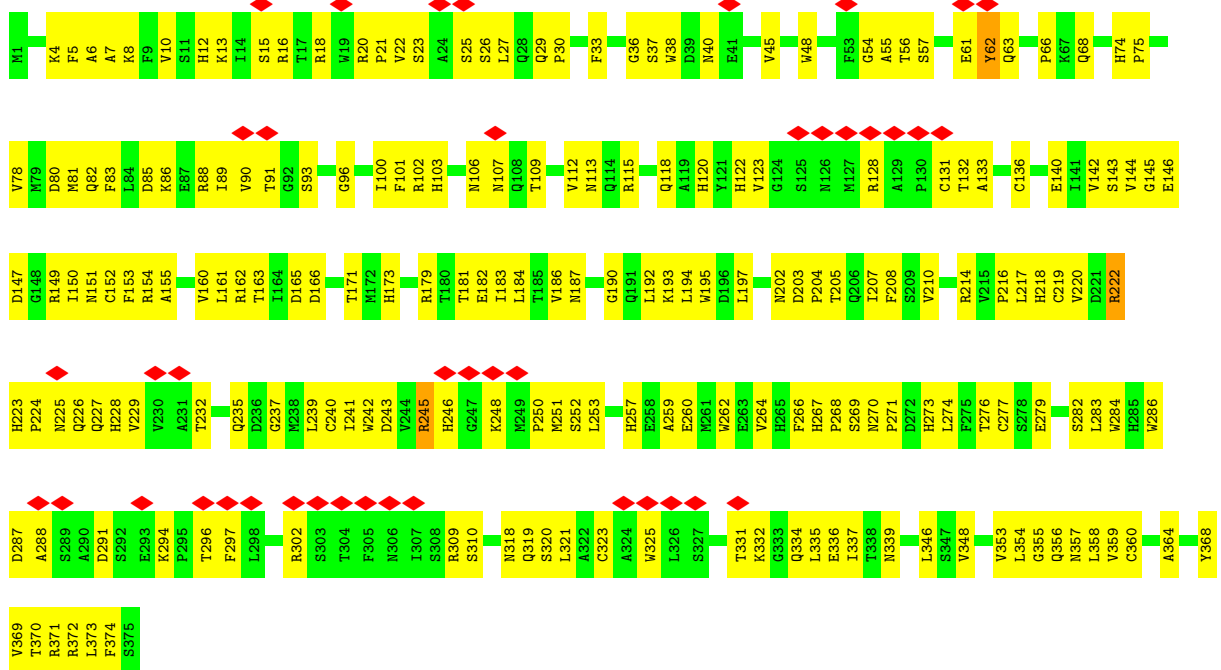
- Molecule 1: Nuclear pore complex protein Nup85

Chain A:

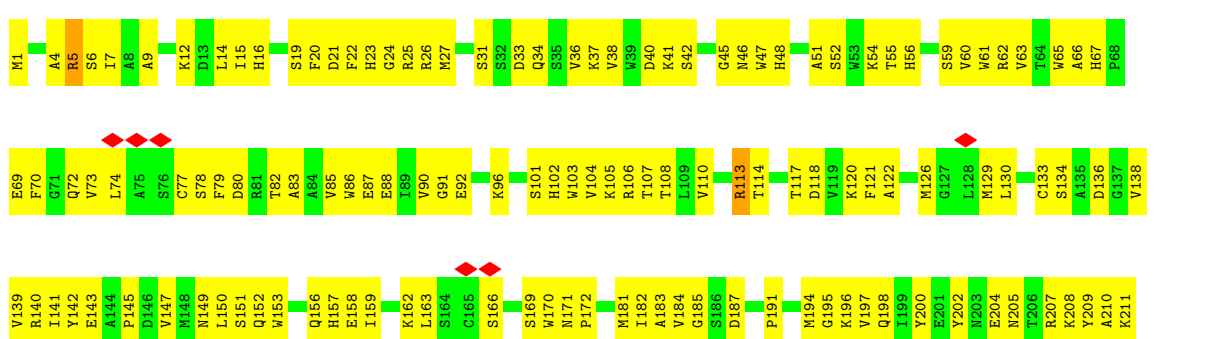




• Molecule 2: MGC154553 protein

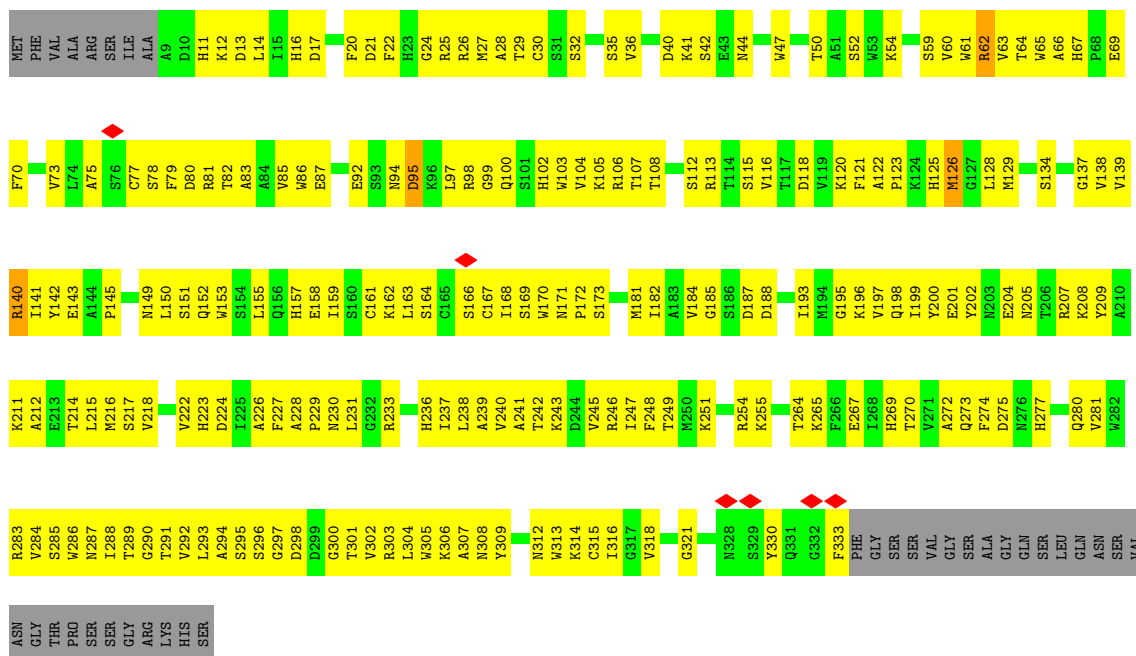


• Molecule 3: Nucleoporin SEH1-A

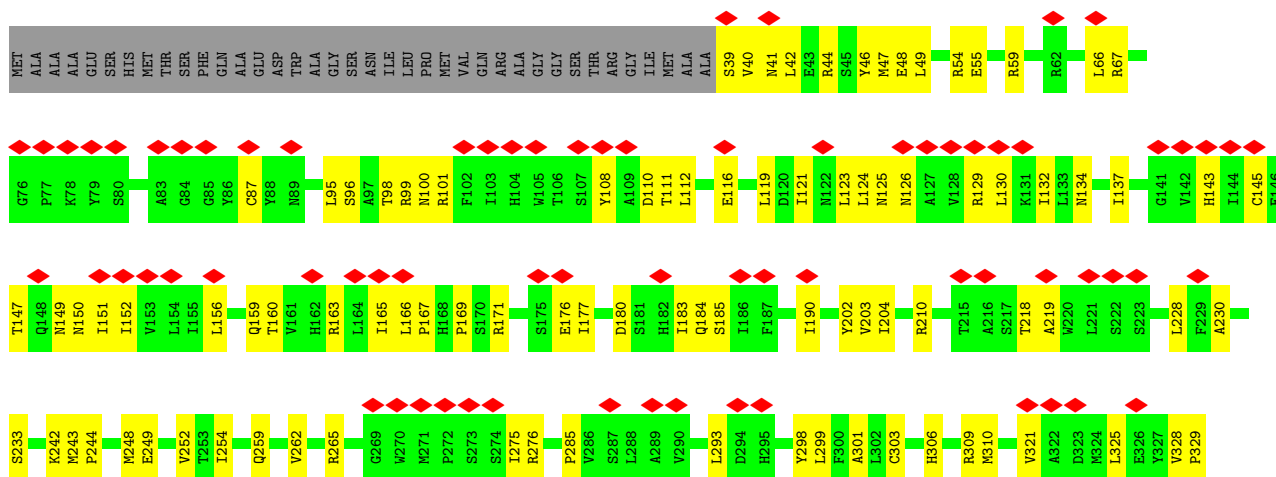




• Molecule 3: Nucleoporin SEH1-A



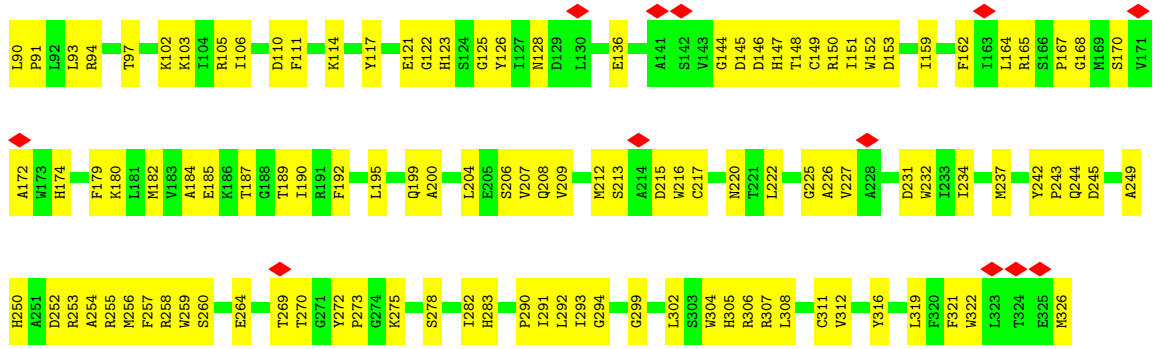
• Molecule 4: Nup160



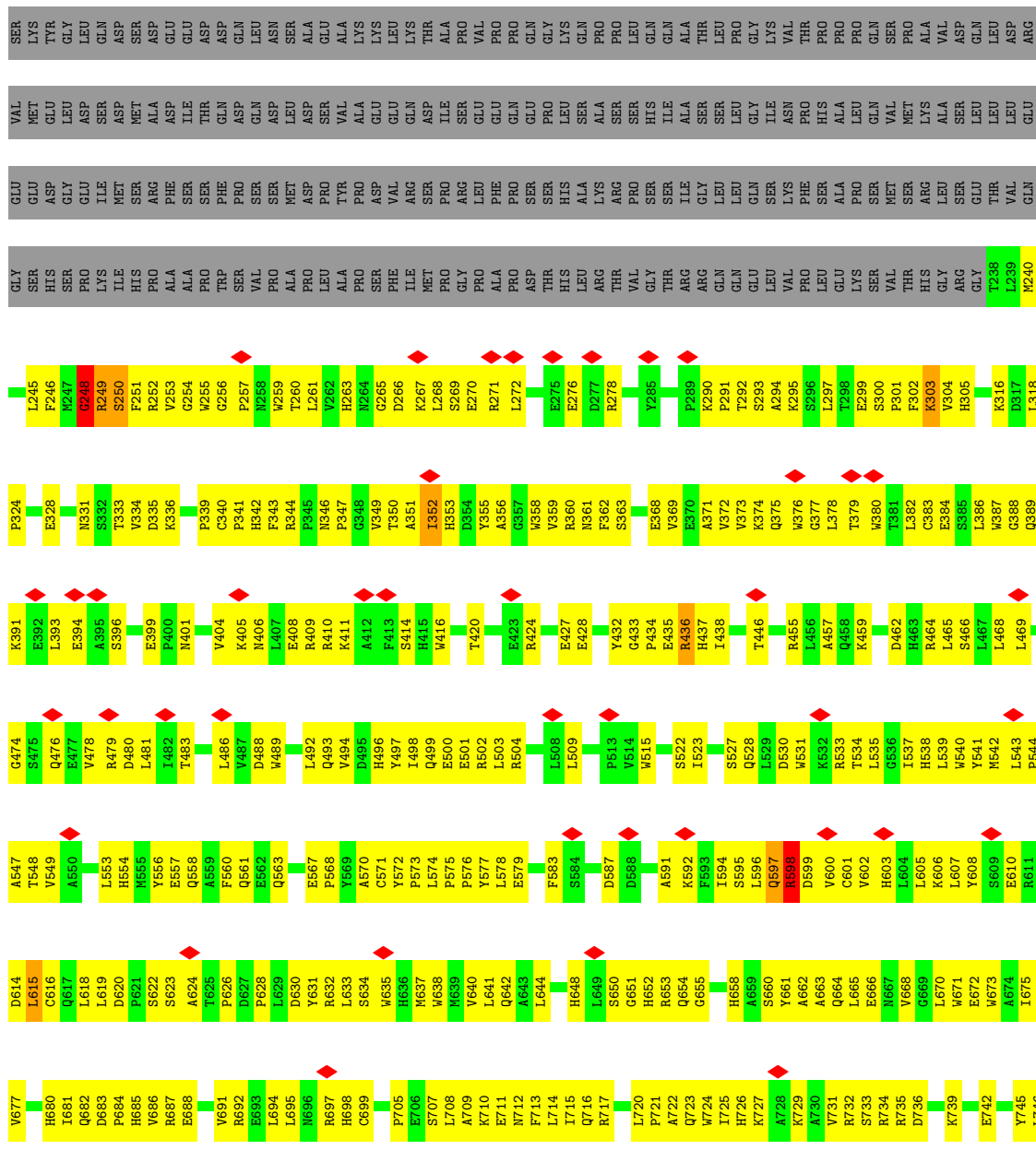
• Molecule 4: Nup160

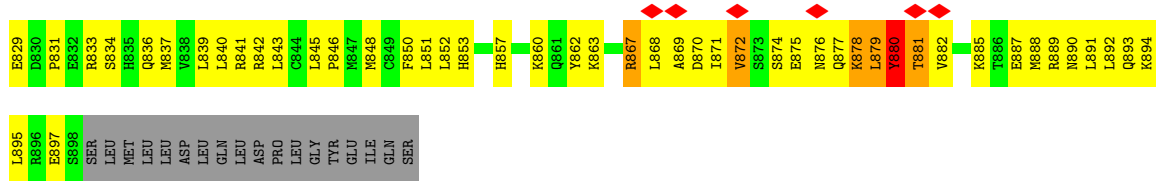


MET	ALA	ALA	ALA	ALA	GLU	SER	HIS	MET	THR	THR	PHE	GLN	ALA	GLU	ASP	TRP	ALA	GLY	SER	ASN	ILE	LEU	PRO	MET	VAL	GLN	ARG	ALA	GLY	GLY	SER	THR	ARG	GLY	ILE	ILE	MET	ALA	ALA	S39	V40	M41	S45	Y46	A52	E53	E54	E55	R59	N60	S65	L66	R67	P68	S71	L72			
V73	I74	G75	K78	Y79	S80	D81	C82	A83	G84	G85	A86	G87	Y88	M89	S93	L94	L95	S96	A97	T98	R99	M100	R101	H104	I107	M106	S107	T111	L112	E113	L114	V115	E116	L117	S118	L119	D120	I121	M122	L123	N125	L124	M126	K131	M134	C135	S136	L137	L138	D139	A211	N213	S214	T215	A216	P139	G140	G141	V142
H143	I144	C145	M149	V153	L154	I155	L156	T157	M158	V240	Q159	T160	V161	H162	R163	L164	I165	H168	R171	R174	S175	E176	I177	I178	S179	M180	S181	H182	I183	Q184	S185	E186	I187	M194	D197	P198	I199	M199	N200	P205	A206	L207	L208	A289	V290	V286	S287	L288	A289	V290	L293	L299	L299	Q304	D305	A216	H306	R309	R309
A219	W220	E226	A227	L228	F229	A230	L231	P232	I238	L239	V240	I241	M243	P244	P245	D247	M248	T253	L254	A255	E256	L257	K258	Q259	S260	Q264	R265	L266	L267	T268	G269	F272	S273	P281	A282	V286	S287	L288	A289	V290	L293	L299	L299	Q304	D305	A216	H306	R309	R309										
M310	W311	S312	Y313	K314	D315	Q316	L319	M320	V321	M324	L325	V328	P329	V330	S331	K332	D333	R335	Q336	T337	A338	G339	T340	H342	K343	L344	R345	I425	L346	A347	Y348	L352	F353	L354	L355	Y356	G358	Y360	L361	H362	T363	P364	R365	Q366	Q367	Q368	F369	C370	V371	F372	Q373	L374							
W375	C376	Y382	S383	F465	K384	E385	H386	T387	S388	T392	M393	Q394	E395	T396	L397	I398	D399	F400	W410	L412	L414	D415	D416	D417	M418	Q419	T420	K423	H424	I425	M426	P427	W435	M436	M441	P444	D445	D446	D447	L448	A449	I450	I526	N527	I528	E529	M530	E455	H614	M615	I616	A617	D618	Y619	I620	T621			
Y460	L464	A466	R469	F470	I471	I472	A473	A474	L475	Q476	K477	I479	Q480	I481	L482	R483	K484	W489	L490	S493	L497	K498	V501	V505	E506	K507	E508	I509	V514	D515	Y516	S519	Q520	E521	E522	F523	R524	Q525	I526	N527	I528	E529	M530	E455	H614	M615	I616	A617	D618	Y619	I620	T621							
C538	L539	Q540	Y541	Q542	E543	T544	L545	S546	R547	A550	L551	V552	V553	H554	P555	M559	V560	C561	R564	A572	P573	C574	H579	L580	Y581	G585	E586	H587	L588	V591	D592	I596	C597	D598	D601	S604	I610	Q611	C612	L613	H614	M615	I616	A617	D618	Y619	I620	T621											
E622	M628	C633	H634	P635	L636	S637	P638	E639	R640	V641	A642	E643	Q644	L645	L646	L649	I650	A651	D652	D653	I654	D655	L657	M658	E659	N660	I661	Q662	Q663	K664	L665	Q666	D667	I668	R669	M670	I672	Q673	L679	M682	E685	T686	M687	M688	S693	Q694	H695	N696	W700										
L701	S702	T703	L704	Y705	L794	H795	L796	L797	E801	L802	S803	D804	S805	Q806	V807	R808	K809	R810	T813	S814	G815	I816	Q817	T818	I819	L822	E825	D826	R829	K830	H831	F832	V835	F836	L839	F840	S843	G844	S845	S846	Q847	V848	H849	R850	S851	L852	N853	I858	H859	R860									
L790	E791	S792	N793	L869	W870	P871	N872	S873	P874	N875	E880	R884	N885	C886	Q887	Y888	T889	Q890	L891	Q892	Y894	V895	R896	L899	Q903	N904	N905	V906	G907	S908	C909	H910	F911	M912	L913	A914	Q915	C916	Y917	L918	V919	S943	G844	S845	S846	Q847	V848	H849	R850	S851	L852	N853	I858	H859	R860				
S863	Q867	L868	R869	W870	P871	N872	S873	P874	N875	E880	R884	N885	C886	Q887	Y888	T889	Q890	L891	Q892	Y894	V895	R896	L899	Q903	N904	N905	V906	G907	S908	C909	H910	F911	M912	L913	A914	Q915	C916	Y917	L918	V919	S943	G844	S845	S846	Q847	V848	H849	R850	S851	L852	N853	I858	H859	R860					
A934	V937	E938	R939	E940	D941	F942	L943	E944	K945	N975	E951	G952	E953	P957	R958	L959	Q960	Y961	N962	N963	R964	R967	L968	L969	E970	L974	P975	E976	L977	W978	I979	Q980	D991	L913	A914	Q915	C916	Y917	L918	V919	S943	G844	S845	S846	Q847	V848	H849	R850	S851	L852	N853	I858	H859	R860					



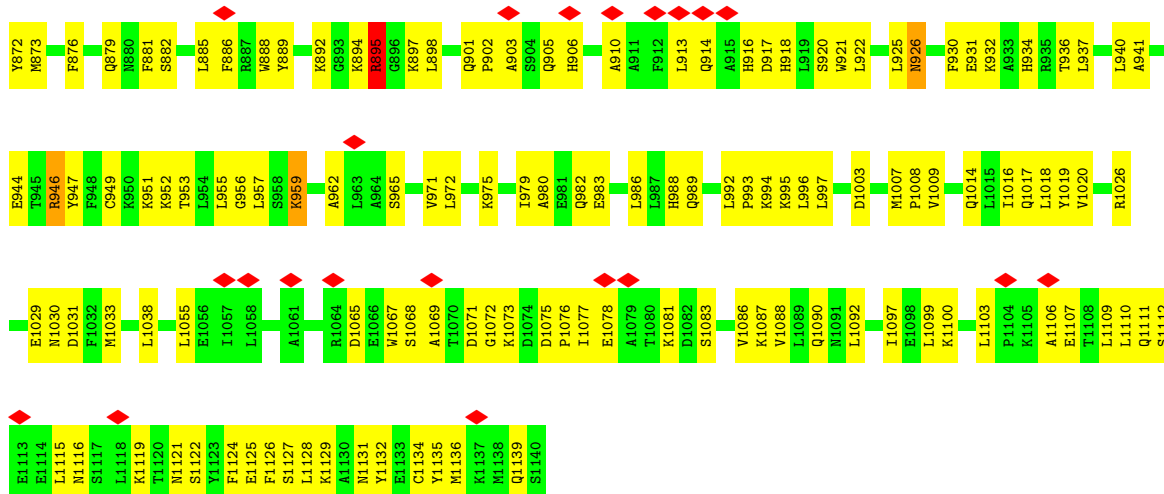
• Molecule 6: Nuclear pore complex protein Nup96



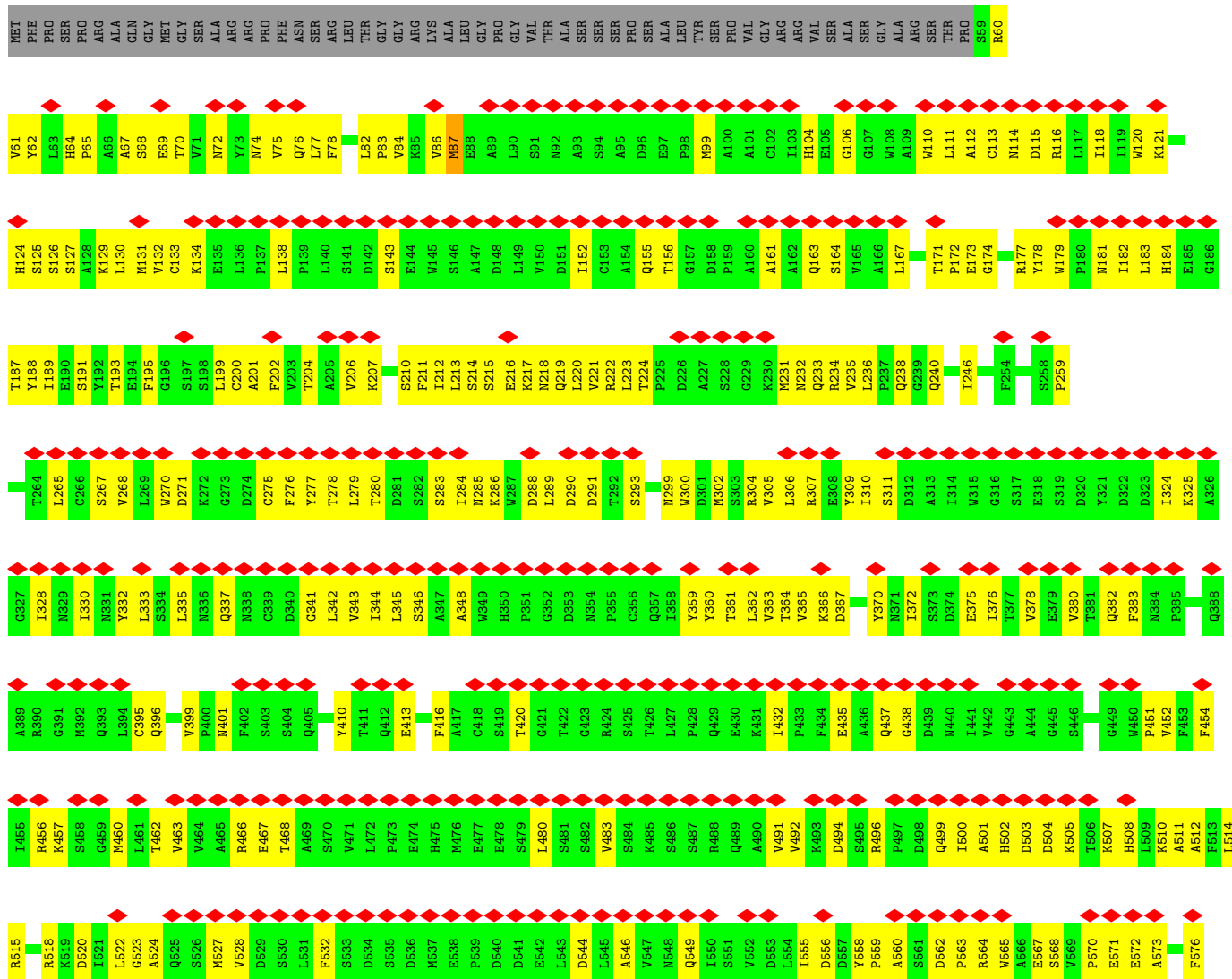


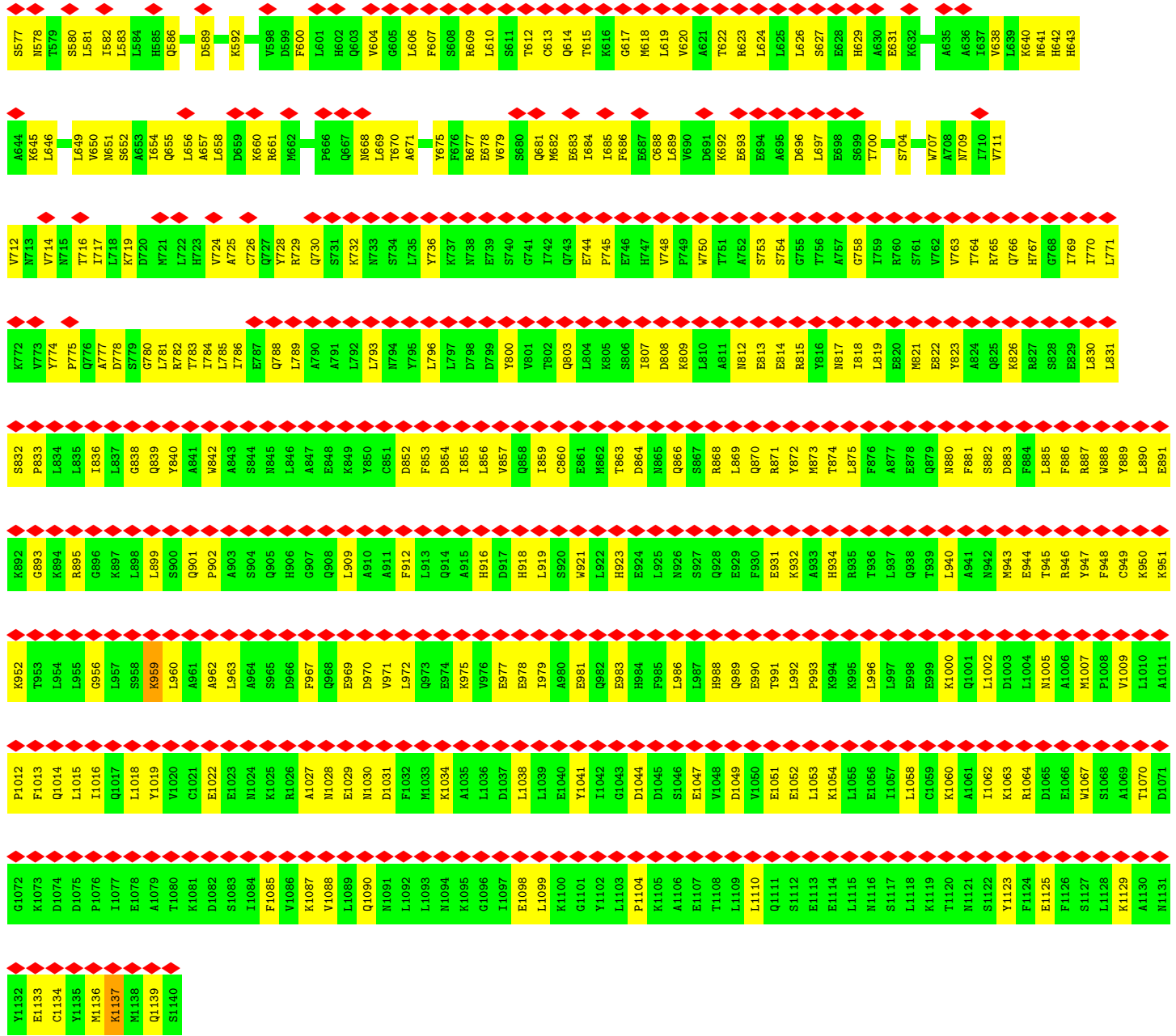
• Molecule 9: outer Nup133



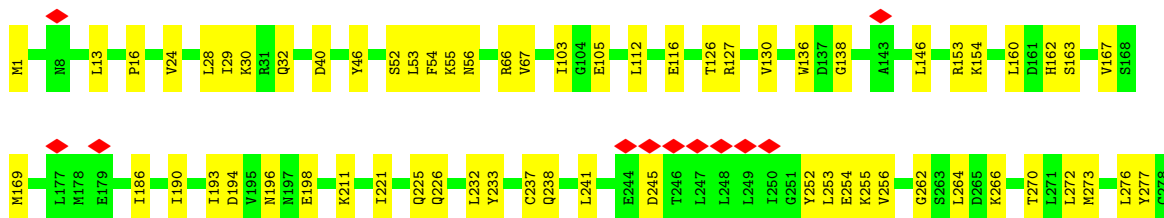


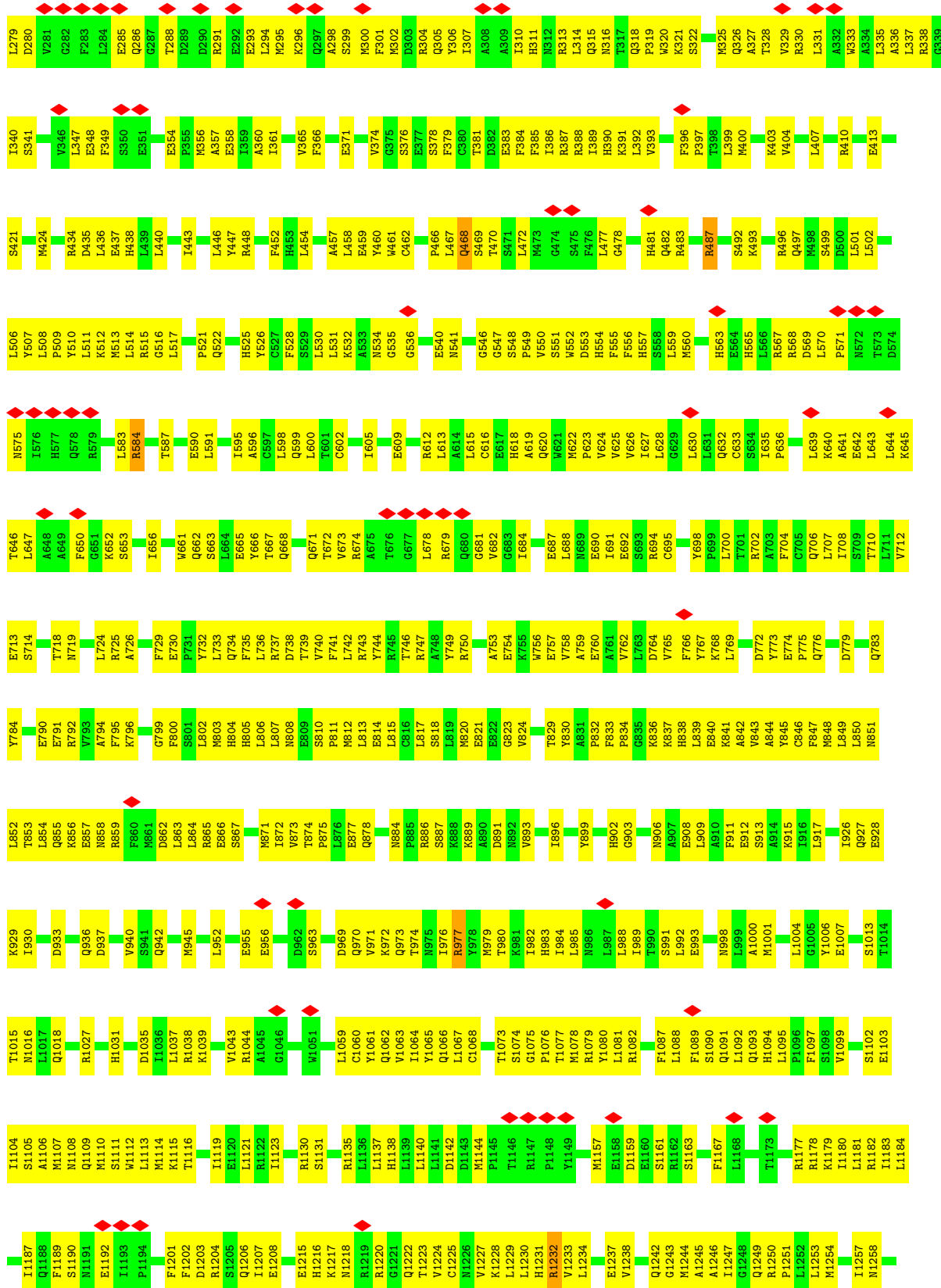
• Molecule 9: outer Nup133

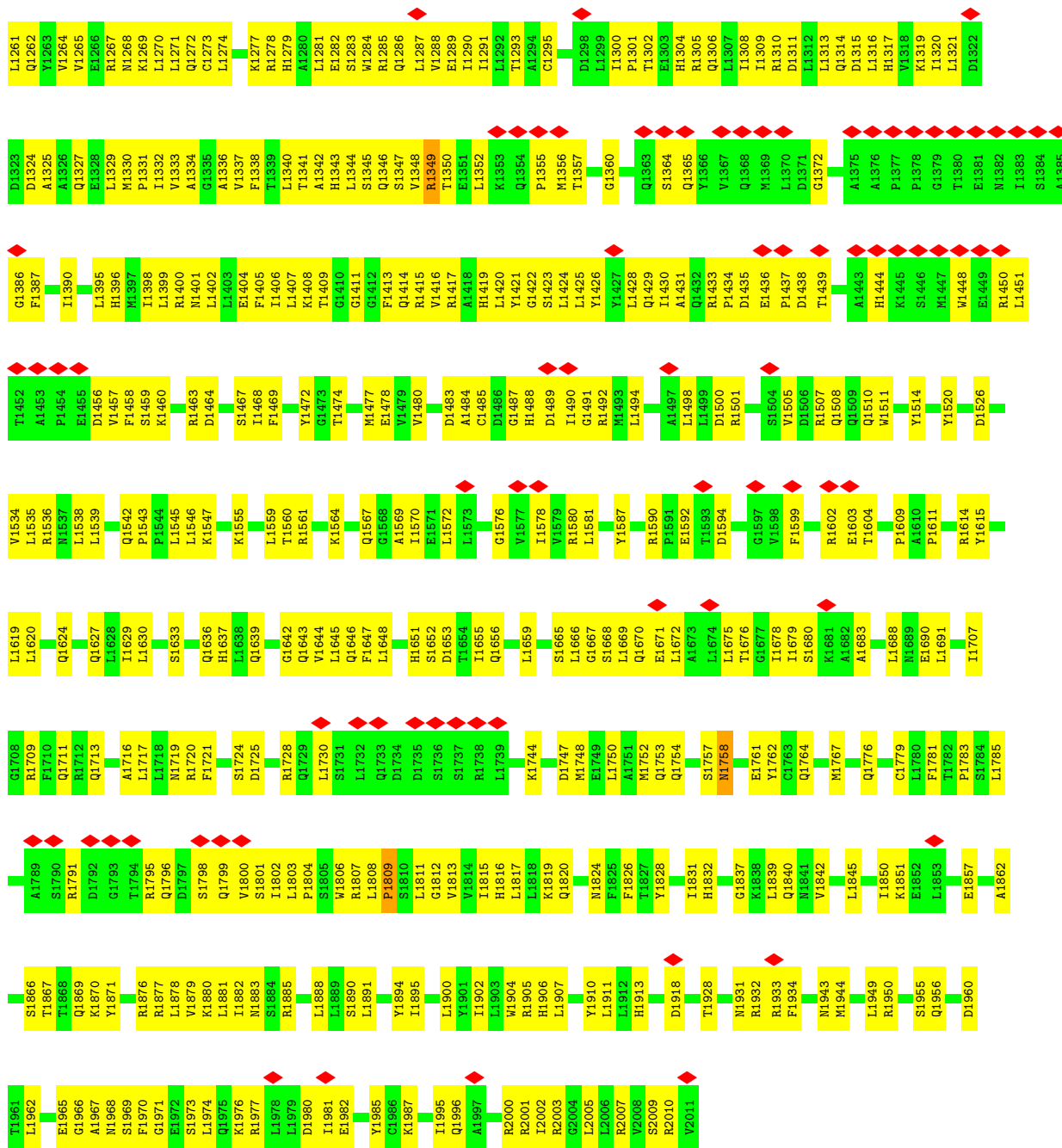




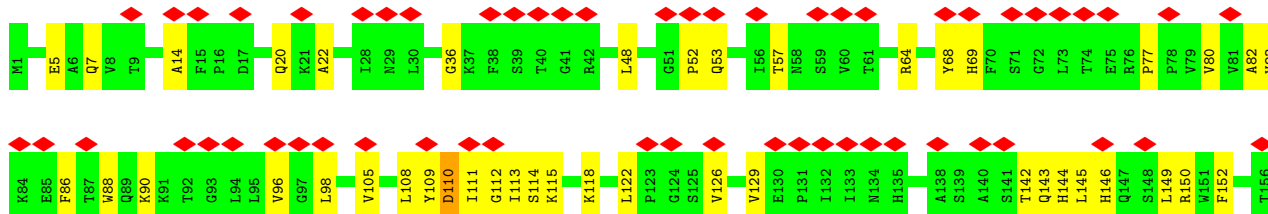
• Molecule 10: MGC83295 protein

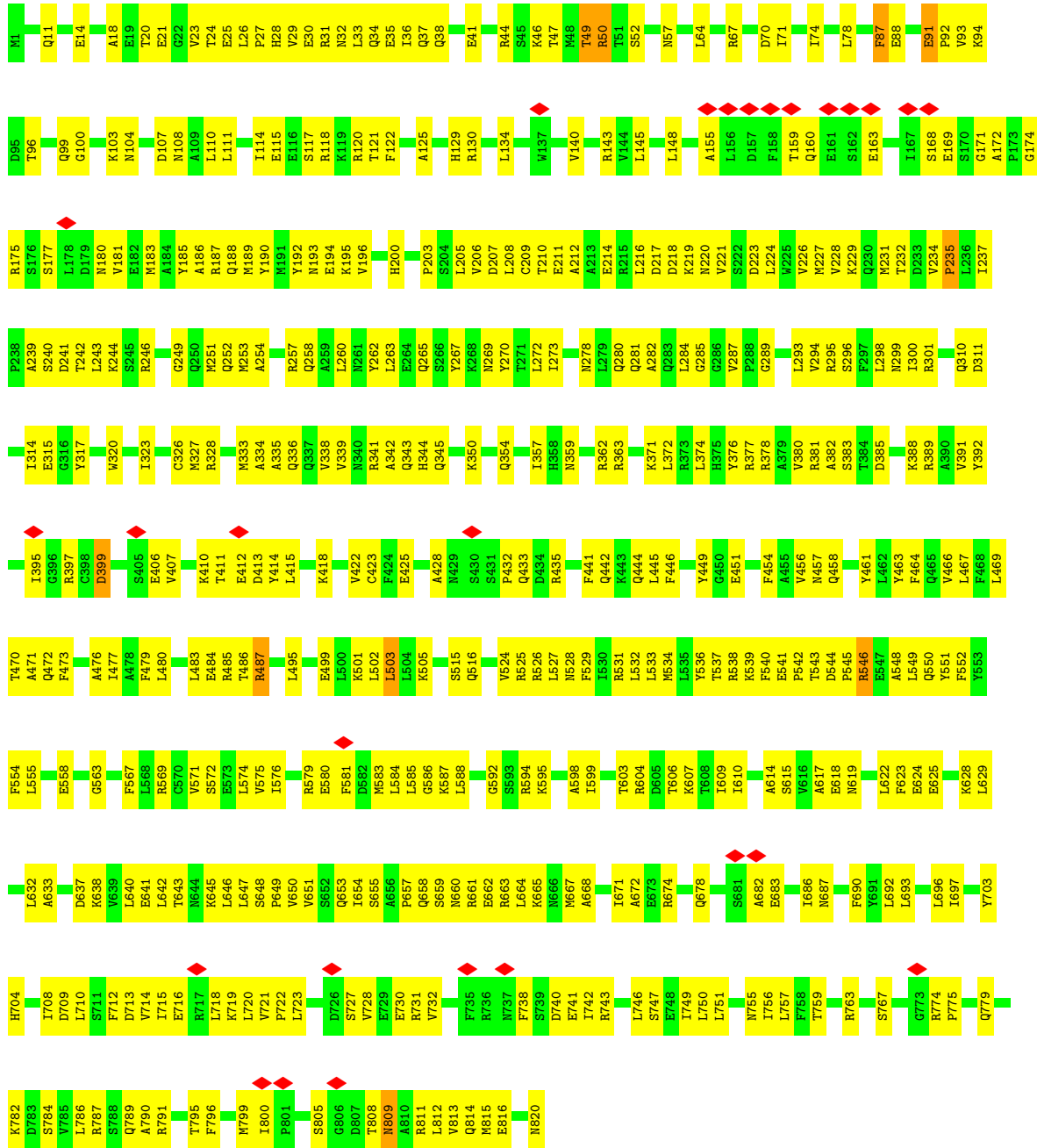






• Molecule 11: Protein ELYS





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417490	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.301	Depositor
Minimum map value	-2.133	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.24, 2.24, 2.24	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	1/5377 (0.0%)	0.65	2/7265 (0.0%)
1	J	0.31	0/5377	0.56	0/7265
2	B	0.33	0/2996	0.63	0/4074
2	K	0.28	0/2996	0.55	0/4074
3	C	0.35	0/2674	0.60	0/3628
3	L	0.31	0/2612	0.56	0/3545
4	D	0.29	0/11349	0.54	4/15414 (0.0%)
4	M	0.32	1/11349 (0.0%)	0.56	3/15414 (0.0%)
5	E	0.29	0/2643	0.53	0/3587
5	N	0.28	0/2643	0.53	0/3587
6	F	0.35	0/5699	0.60	1/7730 (0.0%)
6	O	0.35	0/5299	0.60	1/7189 (0.0%)
7	G	0.41	0/2367	0.63	1/3231 (0.0%)
7	P	0.39	0/2367	0.61	0/3231
8	H	0.32	0/6628	0.55	1/8968 (0.0%)
8	Q	0.35	0/6483	0.57	1/8772 (0.0%)
9	I	1.19	6/8647 (0.1%)	0.53	5/11720 (0.0%)
9	R	0.32	1/8703 (0.0%)	0.55	4/11797 (0.0%)
10	S	0.30	0/16272	0.54	0/22021
11	T	0.30	1/8213 (0.0%)	0.52	3/11150 (0.0%)
12	U	0.31	0/6685	0.58	1/9025 (0.0%)
All	All	0.44	10/127379 (0.0%)	0.56	27/172687 (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	1
6	F	0	4
7	G	0	2
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Q	0	1
9	I	0	2
11	T	0	1
12	U	0	1
All	All	0	13

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	576	PHE	CD2-CE2	51.58	2.42	1.39
9	I	576	PHE	CD1-CE1	51.20	2.41	1.39
9	I	576	PHE	CE1-CZ	48.40	2.29	1.37
9	I	576	PHE	CE2-CZ	46.94	2.26	1.37
9	I	576	PHE	CG-CD1	30.21	1.84	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	902	PRO	N-CD-CG	-15.00	80.70	103.20
4	M	786	PRO	N-CD-CG	-13.51	82.93	103.20
11	T	642	GLU	O-C-N	-10.30	106.22	122.70
9	R	902	PRO	CA-N-CD	-9.27	98.52	111.50
11	T	642	GLU	N-CA-CB	-9.26	93.93	110.60

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	VAL	Peptide
6	F	248	GLY	Peptide
6	F	250	SER	Peptide
6	F	409	ARG	Sidechain
6	F	598	ARG	Sidechain

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	5268	0	5226	435	0
1	J	5268	0	5226	391	0
2	B	2927	0	2800	271	0
2	K	2927	0	2800	213	0
3	C	2607	0	2513	279	0
3	L	2546	0	2444	207	0
4	D	11118	0	11035	511	0
4	M	11118	0	11035	655	0
5	E	2573	0	2503	139	0
5	N	2573	0	2503	133	0
6	F	5560	0	5469	558	0
6	O	5168	0	5080	442	0
7	G	2300	0	2180	235	0
7	P	2300	0	2180	265	0
8	H	6494	0	6413	422	0
8	Q	6351	0	6268	543	0
9	I	8482	0	8354	384	0
9	R	8536	0	8407	439	0
10	S	15974	0	16156	891	0
11	T	8041	0	7961	301	0
12	U	6569	0	6537	409	0
All	All	124700	0	123090	7598	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 31.

The worst 5 of 7598 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)
9:I:576:PHE:CD1	9:I:576:PHE:CG	1.84	1.65
9:I:576:PHE:CG	9:I:576:PHE:CD2	1.83	1.64
6:F:612:GLN:HA	12:U:183:MET:CG	1.11	1.58
8:Q:869:ALA:CB	8:Q:895:LEU:CD2	1.84	1.54
6:F:612:GLN:CA	12:U:183:MET:HG2	1.41	1.50

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	651/653 (100%)	594 (91%)	56 (9%)	1 (0%)	47	81
1	J	651/653 (100%)	607 (93%)	44 (7%)	0	100	100
2	B	373/375 (100%)	314 (84%)	57 (15%)	2 (0%)	29	69
2	K	373/375 (100%)	333 (89%)	37 (10%)	3 (1%)	19	60
3	C	331/360 (92%)	280 (85%)	50 (15%)	1 (0%)	41	77
3	L	323/360 (90%)	286 (88%)	35 (11%)	2 (1%)	25	66
4	D	1392/1439 (97%)	1294 (93%)	95 (7%)	3 (0%)	47	81
4	M	1392/1439 (97%)	1293 (93%)	95 (7%)	4 (0%)	41	77
5	E	324/326 (99%)	299 (92%)	25 (8%)	0	100	100
5	N	324/326 (99%)	299 (92%)	25 (8%)	0	100	100
6	F	685/924 (74%)	612 (89%)	69 (10%)	4 (1%)	25	66
6	O	635/924 (69%)	556 (88%)	79 (12%)	0	100	100
7	G	292/320 (91%)	262 (90%)	30 (10%)	0	100	100
7	P	292/320 (91%)	253 (87%)	38 (13%)	1 (0%)	41	77
8	H	796/916 (87%)	745 (94%)	50 (6%)	1 (0%)	51	86
8	Q	778/916 (85%)	719 (92%)	55 (7%)	4 (0%)	29	69
9	I	1074/1140 (94%)	989 (92%)	77 (7%)	8 (1%)	22	63
9	R	1080/1140 (95%)	1013 (94%)	66 (6%)	1 (0%)	51	86
10	S	2009/2011 (100%)	1874 (93%)	133 (7%)	2 (0%)	51	86
11	T	1011/2408 (42%)	960 (95%)	50 (5%)	1 (0%)	51	86
12	U	818/820 (100%)	756 (92%)	53 (6%)	9 (1%)	14	52
All	All	15604/18145 (86%)	14338 (92%)	1219 (8%)	47 (0%)	44	77

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	ALA
2	B	61	GLU
3	C	217	SER
6	F	597	GLN
6	F	615	LEU

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 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	580/580 (100%)	576 (99%)	4 (1%)	84	90
1	J	580/580 (100%)	577 (100%)	3 (0%)	88	93
2	B	329/329 (100%)	326 (99%)	3 (1%)	78	87
2	K	329/329 (100%)	327 (99%)	2 (1%)	86	92
3	C	288/309 (93%)	284 (99%)	4 (1%)	67	80
3	L	282/309 (91%)	279 (99%)	3 (1%)	73	84
4	D	1230/1262 (98%)	1220 (99%)	10 (1%)	81	89
4	M	1230/1262 (98%)	1224 (100%)	6 (0%)	88	93
5	E	275/275 (100%)	274 (100%)	1 (0%)	91	94
5	N	275/275 (100%)	274 (100%)	1 (0%)	91	94
6	F	608/816 (74%)	599 (98%)	9 (2%)	65	80
6	O	563/816 (69%)	561 (100%)	2 (0%)	91	94
7	G	250/272 (92%)	248 (99%)	2 (1%)	81	89
7	P	250/272 (92%)	249 (100%)	1 (0%)	91	94
8	H	712/816 (87%)	702 (99%)	10 (1%)	67	80
8	Q	695/816 (85%)	680 (98%)	15 (2%)	52	71
9	I	944/993 (95%)	935 (99%)	9 (1%)	76	86
9	R	950/993 (96%)	948 (100%)	2 (0%)	93	96
10	S	1779/1779 (100%)	1771 (100%)	8 (0%)	91	94
11	T	895/2166 (41%)	894 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	U	721/721 (100%)	715 (99%)	6 (1%)	81	89
All	All	13765/15970 (86%)	13663 (99%)	102 (1%)	84	90

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	62	ARG
8	Q	270	LYS
12	U	546	ARG
3	L	140	ARG
4	M	1338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
9	R	767	HIS
10	S	719	ASN
11	T	494	GLN
8	H	675	GLN
8	H	595	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

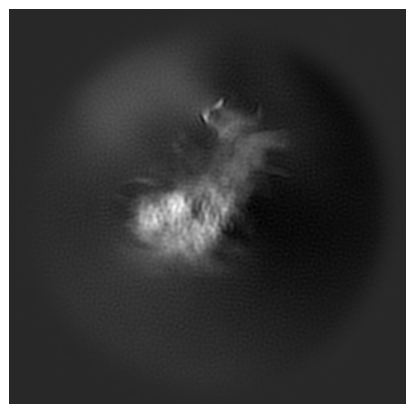
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31891. These allow visual inspection of the internal detail of the map and identification of artifacts.

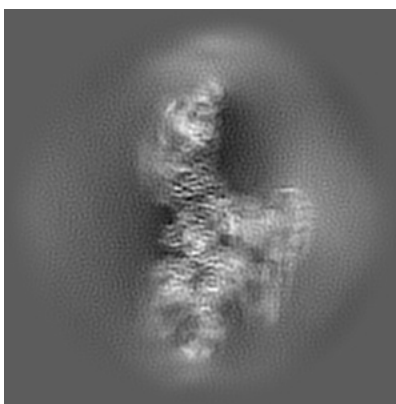
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

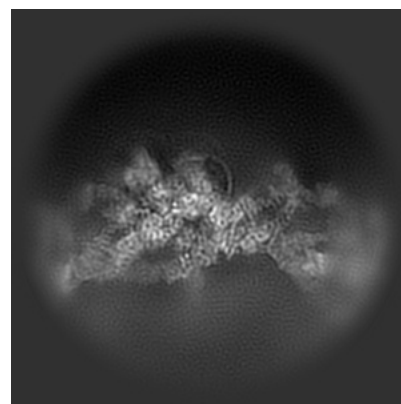
6.1.1 Primary map



X

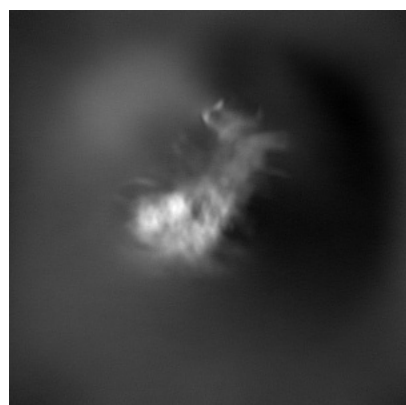


Y

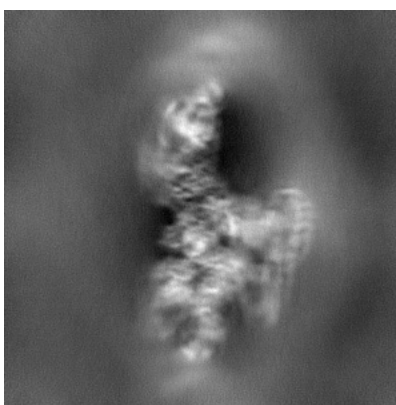


Z

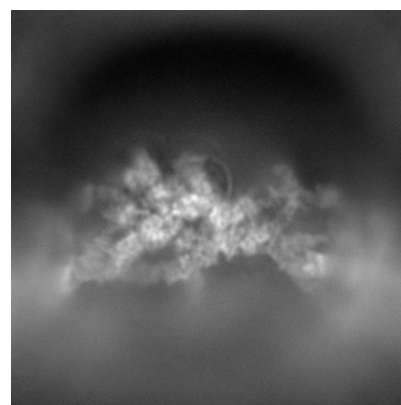
6.1.2 Raw map



X



Y

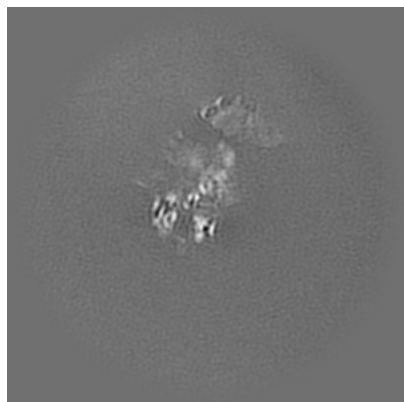


Z

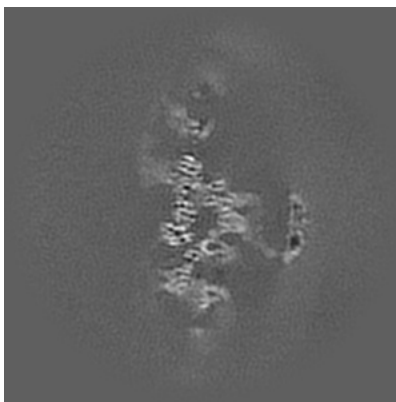
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

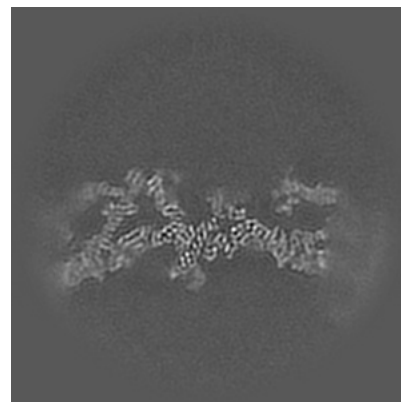
6.2.1 Primary map



X Index: 160

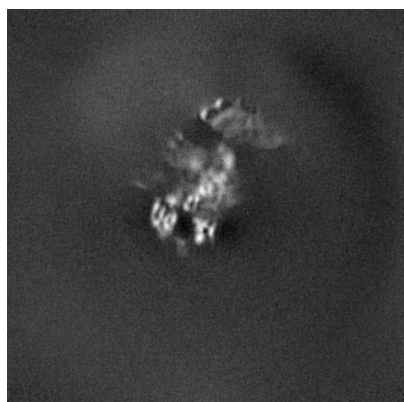


Y Index: 160

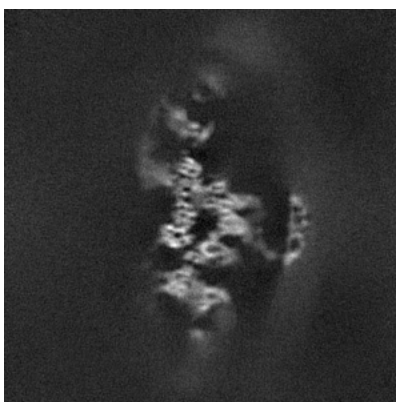


Z Index: 160

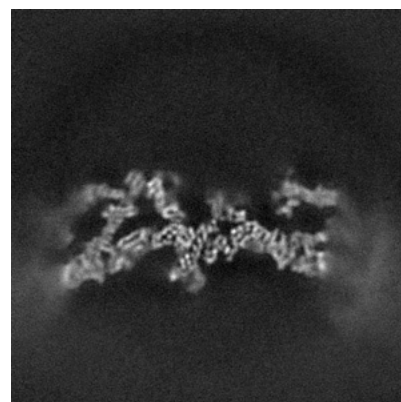
6.2.2 Raw map



X Index: 160



Y Index: 160

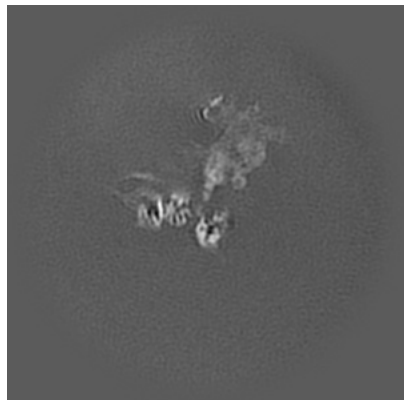


Z Index: 160

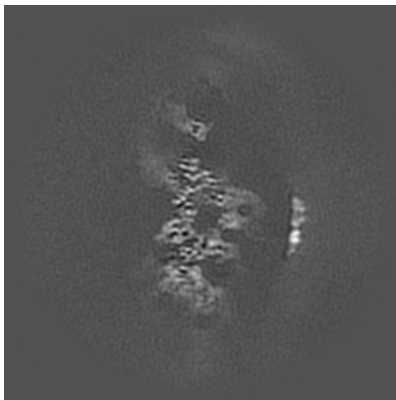
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

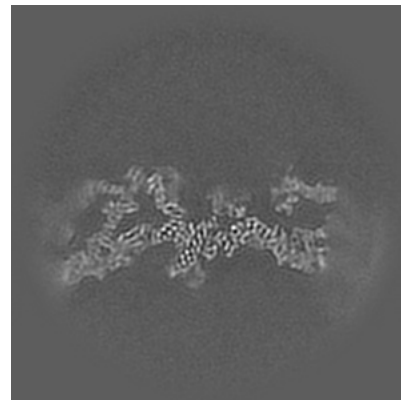
6.3.1 Primary map



X Index: 140



Y Index: 157

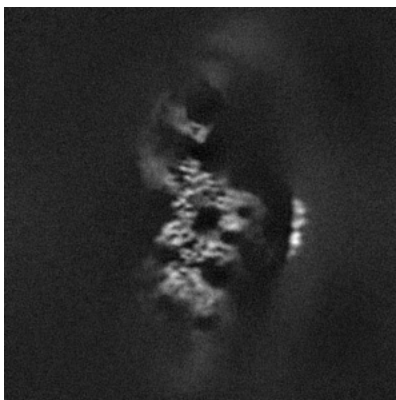


Z Index: 159

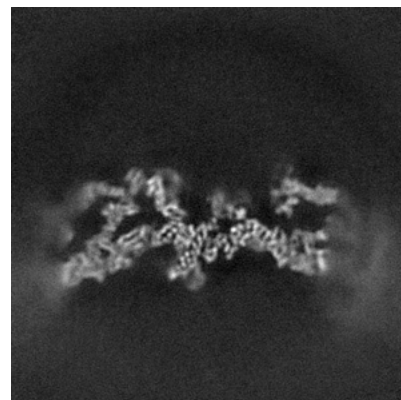
6.3.2 Raw map



X Index: 146



Y Index: 157

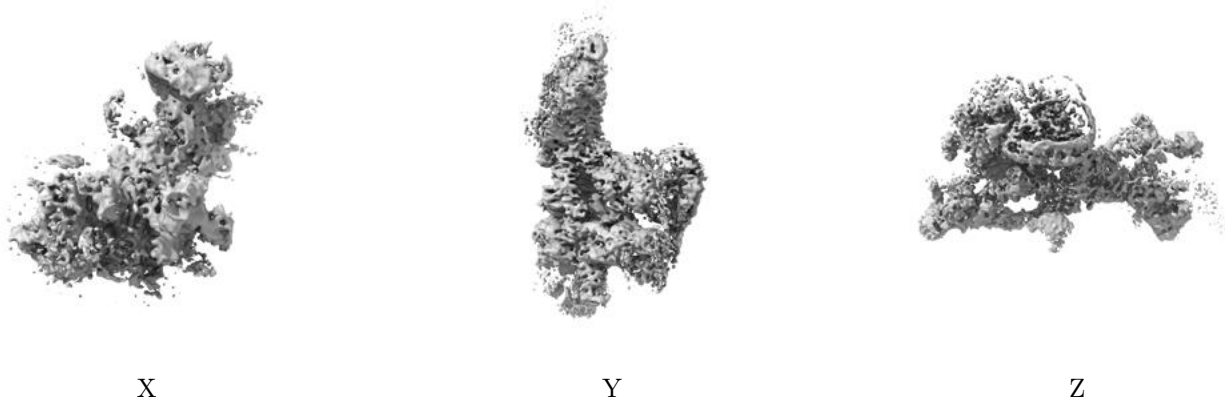


Z Index: 159

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

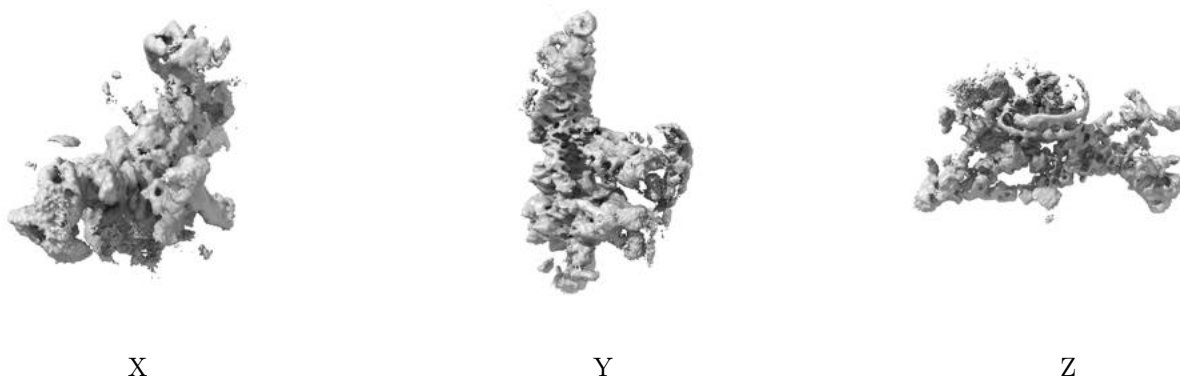
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

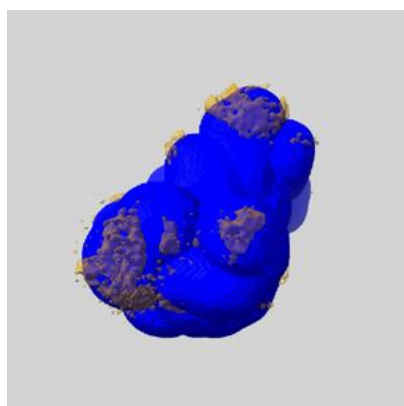
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

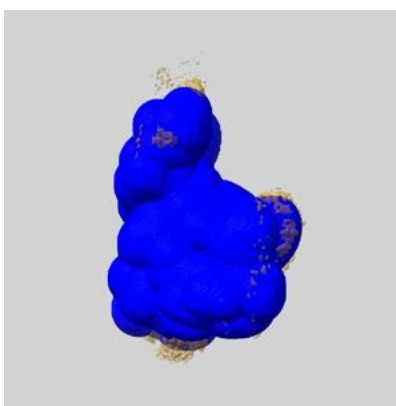
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

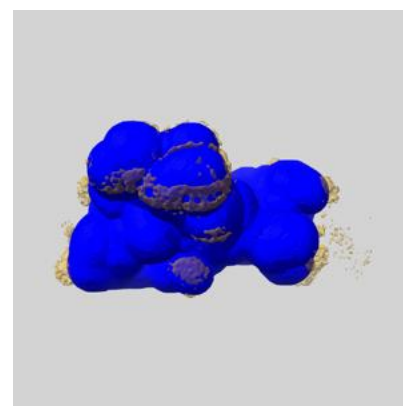
6.5.1 emd_31891_msk_1.map [i](#)



X



Y

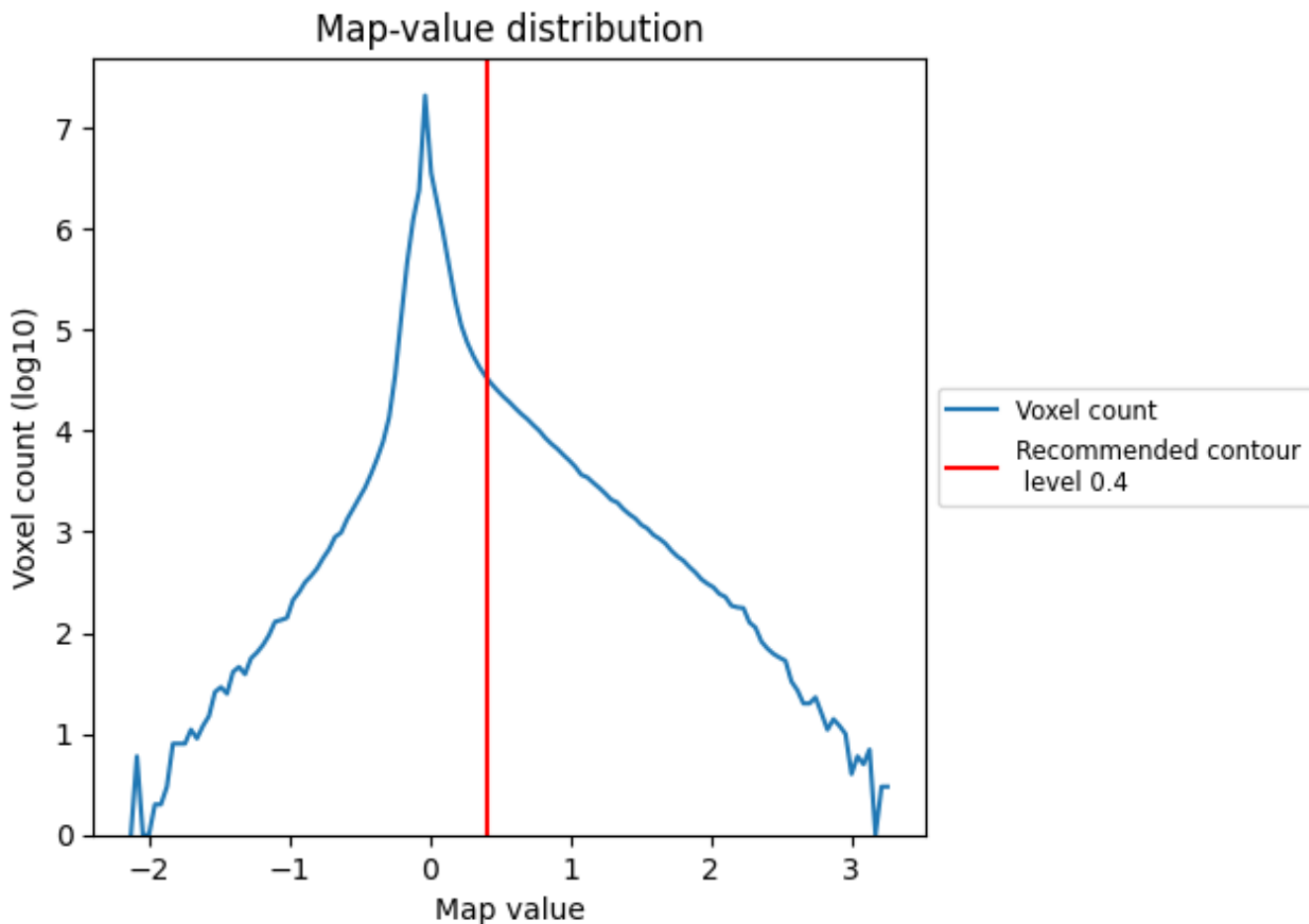


Z

7 Map analysis [i](#)

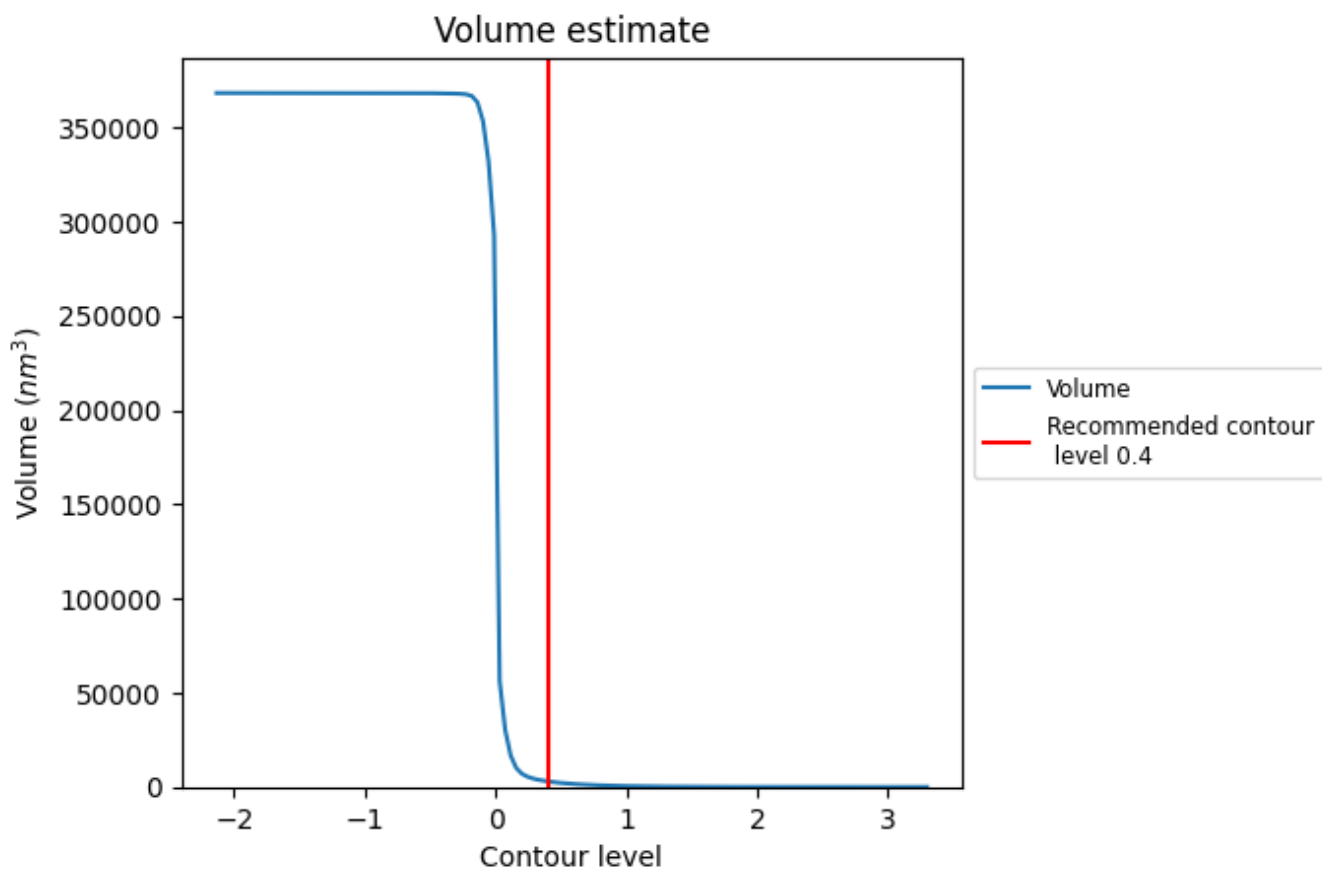
This section contains the results of statistical analysis of the map.

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.

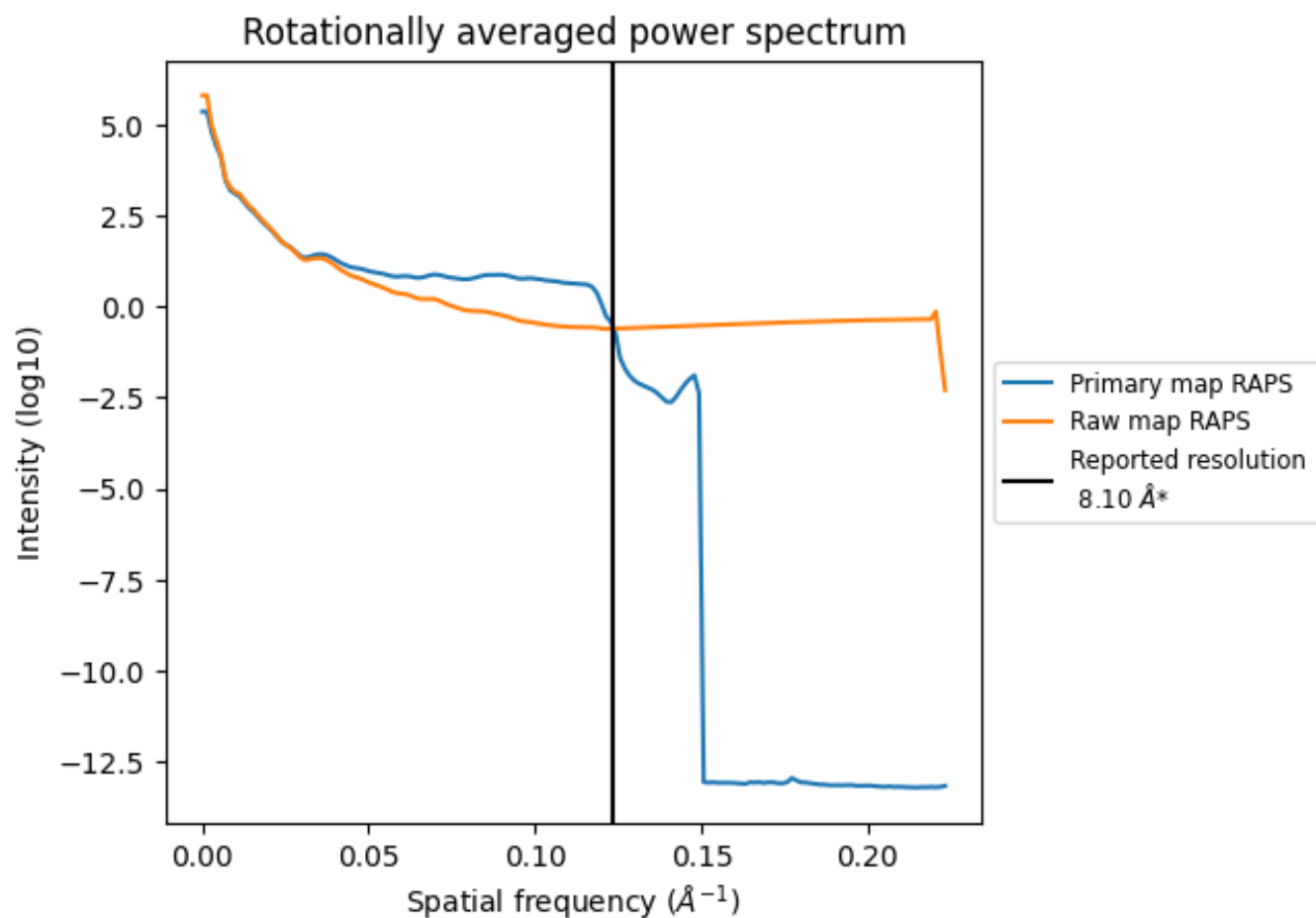
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2954 nm³; this corresponds to an approximate mass of 2669 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 [i](#)

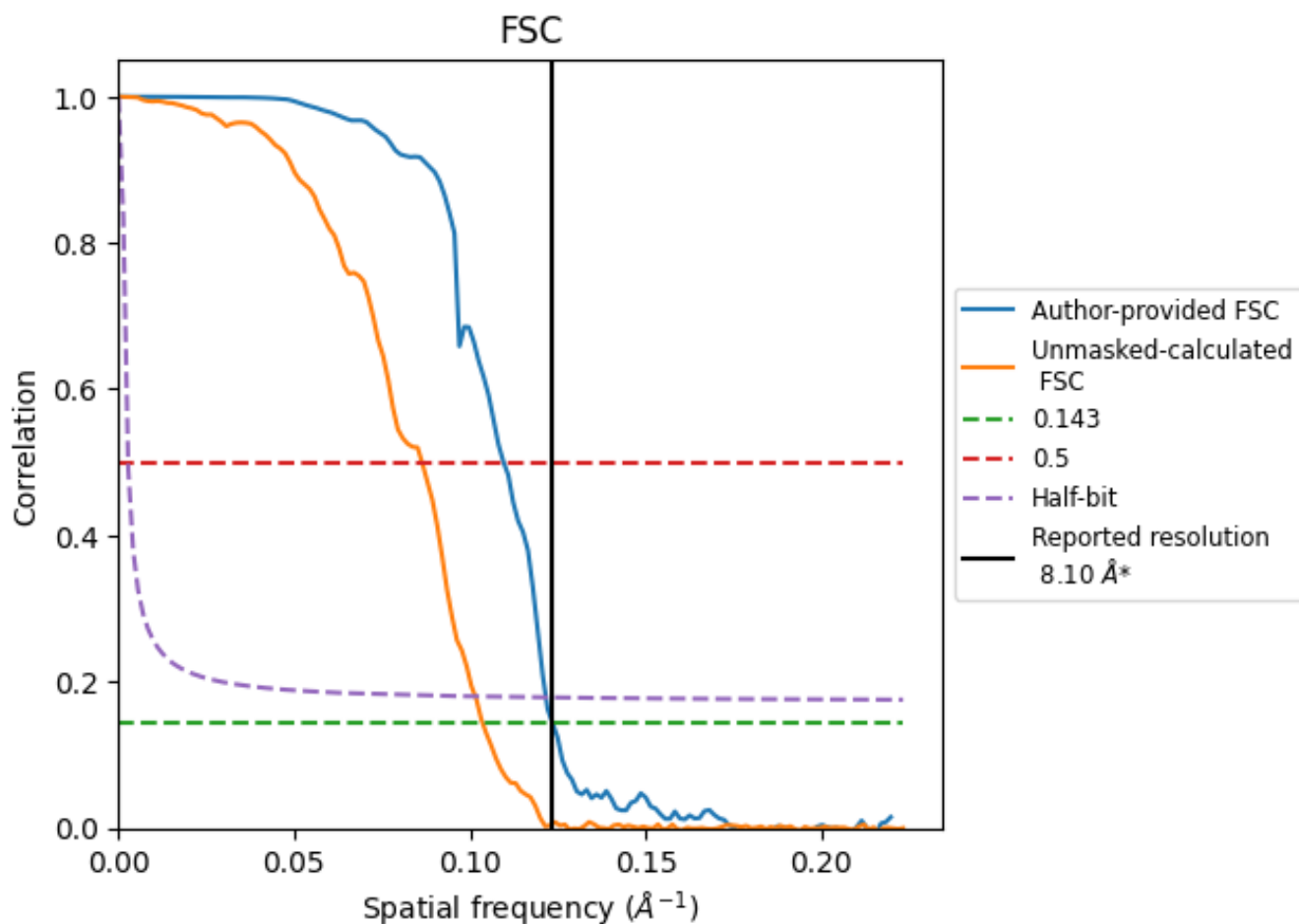


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

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 [i](#)

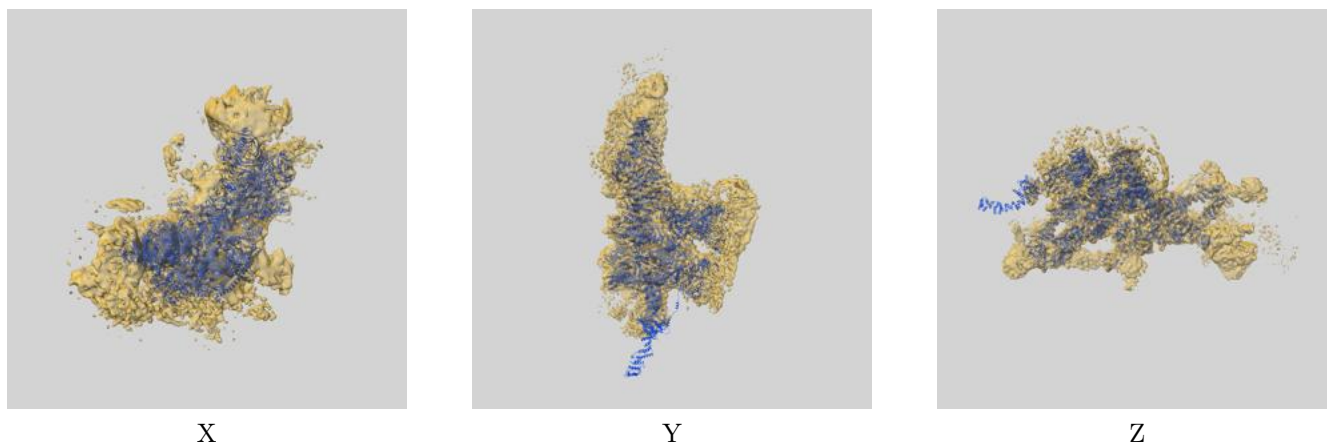
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.10	9.12	8.22
Unmasked-calculated*	9.64	11.57	9.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.64 differs from the reported value 8.1 by more than 10 %

9 Map-model fit [i](#)

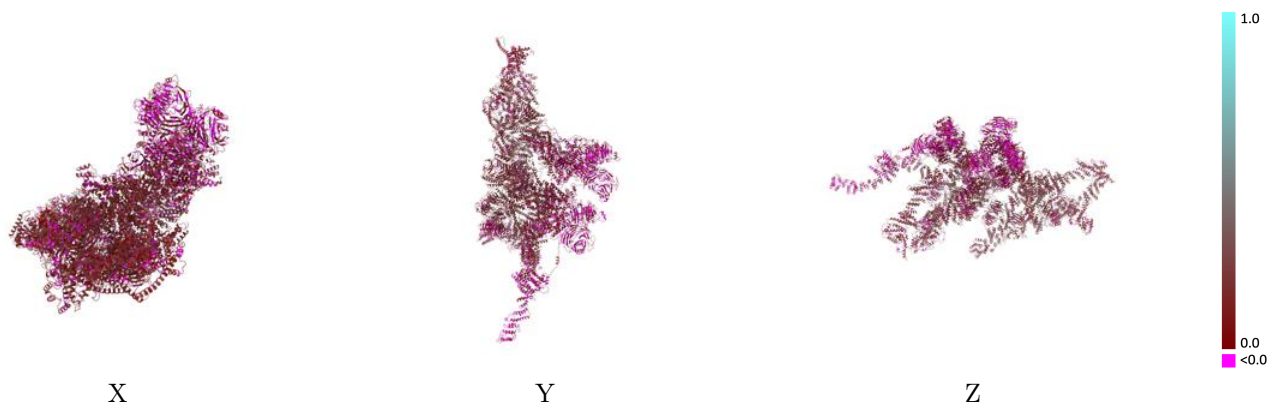
This section contains information regarding the fit between EMDB map EMD-31891 and PDB model 7VCI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



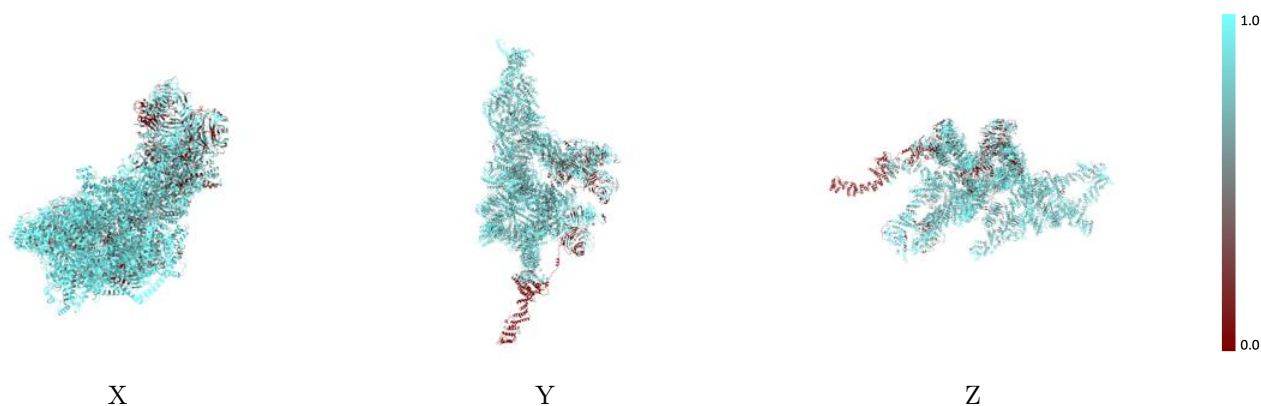
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



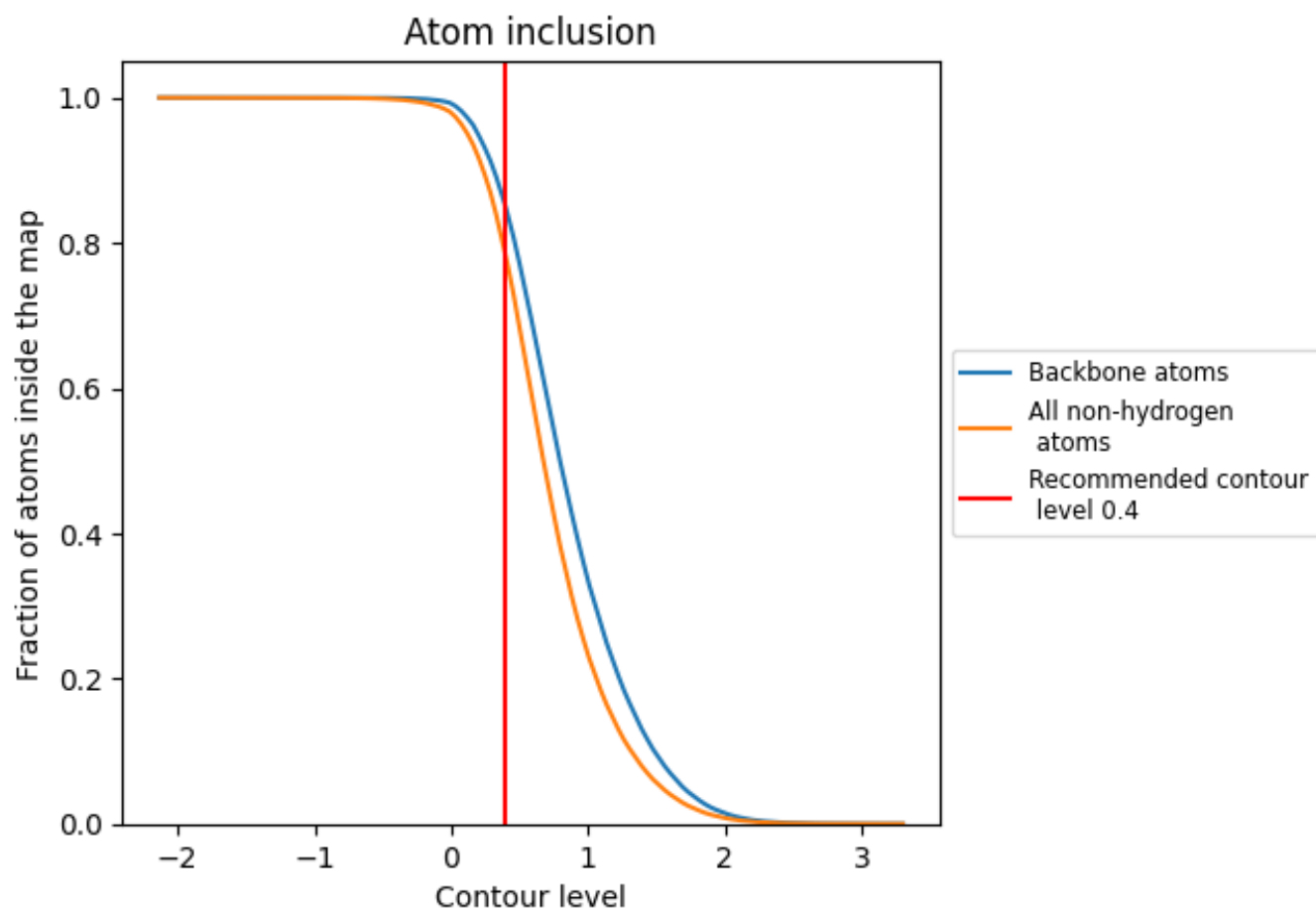
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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













































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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	 0.7813	 0.1300
A	 0.8538	 0.1760
B	 0.7864	 0.1290
C	 0.9014	 0.1700
D	 0.7970	 0.1160
E	 0.9198	 0.1150
F	 0.8319	 0.1610
G	 0.8566	 0.1570
H	 0.8033	 0.1390
I	 0.6724	 0.0990
J	 0.8920	 0.1590
K	 0.8476	 0.1030
L	 0.9235	 0.1560
M	 0.8344	 0.1070
N	 0.8671	 0.1180
O	 0.8614	 0.1840
P	 0.9084	 0.1580
Q	 0.8176	 0.1640
R	 0.2588	 0.0390
S	 0.8484	 0.1480
T	 0.6471	 0.0980
U	 0.8869	 0.1570

