



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 07:54 pm BST

PDB ID : 7PER
EMDB ID : EMD-12814
Title : Model of the inner ring of the human nuclear pore complex
Authors : Schuller, A.P.; Wojtynek, M.; Mankus, D.; Tatli, M.; Kronenberg-Tenga, R.; Regmi, S.G.; Dasso, M.; Weis, K.; Medalia, O.; Schwartz, T.U.
Deposited on : 2021-08-11
Resolution : 35.00 Å(reported)
Based on initial model : 5IJN

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

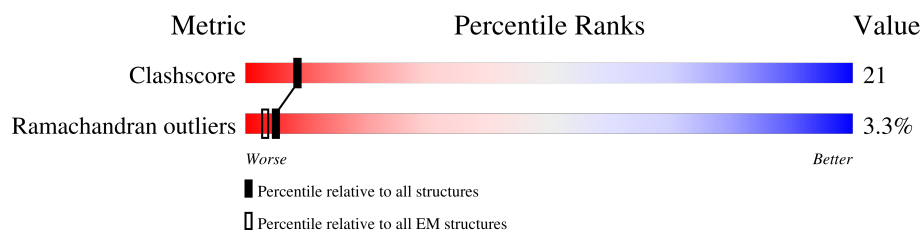
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

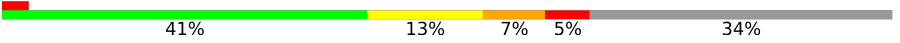
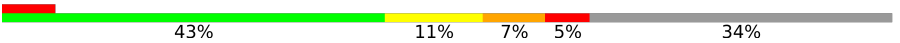
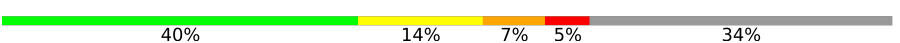
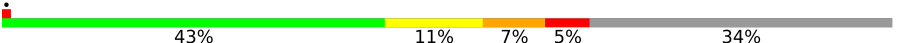





The reported resolution of this entry is 35.00 Å.

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	210492	15764
Ramachandran outliers	207382	16835

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	F	507	 41% 13% 7% 5% 34%
1	L	507	 6% 43% 11% 7% 5% 34%
1	R	507	 40% 14% 7% 5% 34%
1	X	507	 43% 11% 7% 5% 34%
2	G	599	 17% 8% . . 71%
2	M	599	 17% 7% . . 71%
2	S	599	 17% 8% . . 71%
2	Y	599	 17% 8% . . 71%
3	H	522	 18% 10% . . 68%

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Mol	Chain	Length	Quality of chain
3	N	522	
3	T	522	
3	Z	522	
4	D	2012	
4	J	2012	
4	P	2012	
4	V	2012	
5	E	1391	
5	K	1391	
5	Q	1391	
5	W	1391	
6	C	819	
6	I	819	
6	O	819	
6	U	819	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 67036 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 p54.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	335	Total	C	N	O	0	0
			1658	988	335	335		
1	X	335	Total	C	N	O	0	0
			1658	988	335	335		
1	L	335	Total	C	N	O	0	0
			1658	988	335	335		
1	R	335	Total	C	N	O	0	0
			1658	988	335	335		

- Molecule 2 is a protein called Nucleoporin p58/p45.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	171	Total	C	N	O	0	0
			853	511	171	171		
2	Y	171	Total	C	N	O	0	0
			853	511	171	171		
2	M	171	Total	C	N	O	0	0
			853	511	171	171		
2	S	171	Total	C	N	O	0	0
			853	511	171	171		

- Molecule 3 is a protein called Nuclear pore glycoprotein p62.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	169	Total	C	N	O	0	0
			842	504	169	169		
3	Z	169	Total	C	N	O	0	0
			842	504	169	169		
3	N	169	Total	C	N	O	0	0
			842	504	169	169		
3	T	169	Total	C	N	O	0	0
			842	504	169	169		

- Molecule 4 is a protein called Nuclear pore complex protein Nup205.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	1028	Total 5094	C 3038	N 1028	O 1028	0	0
4	V	1028	Total 5094	C 3038	N 1028	O 1028	0	0
4	D	1028	Total 5094	C 3038	N 1028	O 1028	0	0
4	J	1028	Total 5094	C 3038	N 1028	O 1028	0	0

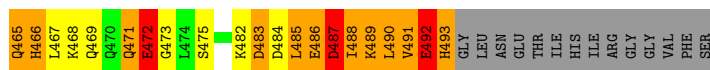
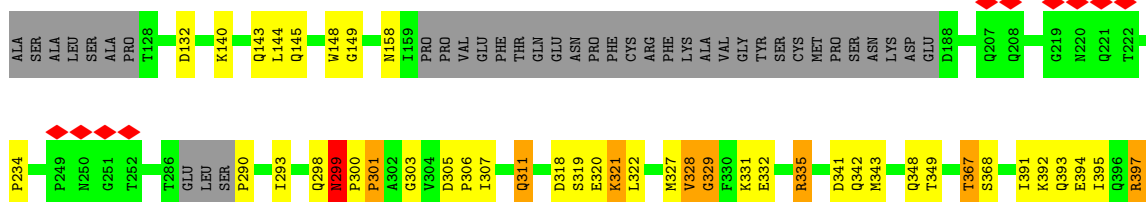
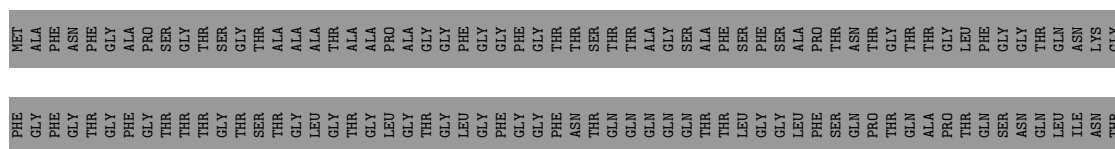
- Molecule 5 is a protein called Nuclear pore complex protein Nup155.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	W	1083	Total 5366	C 3200	N 1083	O 1083	0	0
5	K	1083	Total 5366	C 3200	N 1083	O 1083	0	0
5	E	1083	Total 5366	C 3200	N 1083	O 1083	0	0
5	Q	1083	Total 5366	C 3200	N 1083	O 1083	0	0

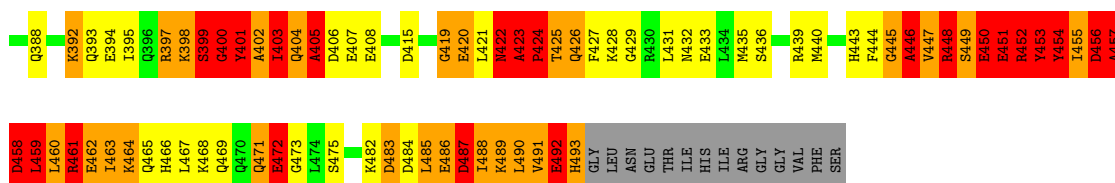
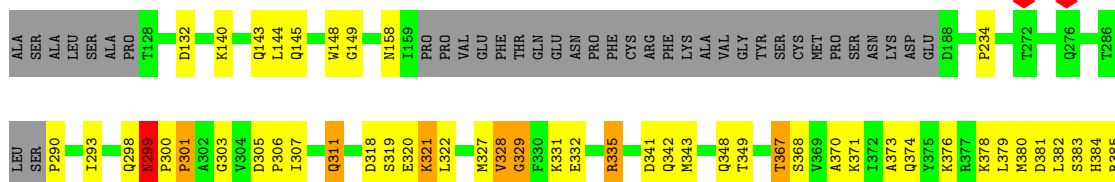
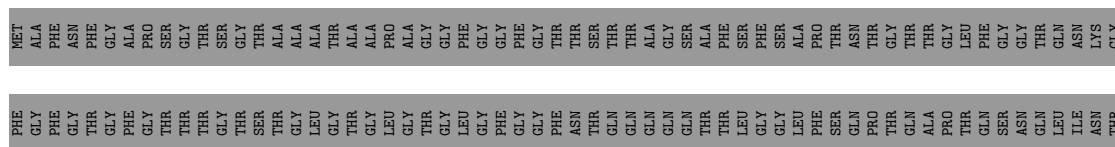
- Molecule 6 is a protein called Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	594	Total 2946	C 1758	N 594	O 594	0	0
6	I	594	Total 2946	C 1758	N 594	O 594	0	0
6	O	594	Total 2946	C 1758	N 594	O 594	0	0
6	U	594	Total 2946	C 1758	N 594	O 594	0	0

- Molecule 1: Nucleoporin p54



- Molecule 1: Nucleoporin p54



Y345	LYS	Y346	ALA	SER	PRO	SER	PRO	SER	MET
	LYS	F347	LEU	LEU	PHE	PHE	PHE	GLY	THR
	TRP	R347	LYS	PHE	GLN	GLN	ASP	GLY	GLY
	GLN	I348	ASP	GLU	SER	PRO	LEU	THR	THR
	ASN			ASN	THR	ILE	GLY	GLY	SER
	THR	Q352	LEU	ASN	THR	THR	THR	LEU	PHE
	PRO			THR	ASN	THR	THR	LEU	GLY
	ARG	R361	P248	THR	THR	SER	SER	PHE	GLY
	VAL		P249	GLY	GLY	THR	THR	GLY	GLY
	THR	E366	V250	THR	SER	SER	SER	SER	GLY
E367	THR	L367	I251	SER	ALA	LYS	THR	THR	THR
	GLY	E368	C252	GLY	SER	PRO	GLY	ALA	LEU
	PRO	N369	P253	LEU	LEU	GLY	LEU	ALA	GLY
	THR		D254	GLN	THR	THR	THR	SER	THR
	PRO	A372		ASN	THR	THR	THR	PHE	GLY
	PHE	T373		ASN	THR	THR	THR	THR	VAL
	SER	Q374	E264	ALA	SER	SER	THR	THR	VAL
	THR		R274	LEU	SER	SER	LEU	THR	ALA
	MET	R377	G275	GLY	LEU	GLY	GLY	GLY	GLY
	PRO	S378	S276	LEU	THR	THR	THR	THR	GLY
H379	ASN	H379	S277	THR	THR	THR	THR	THR	GLY
	ALA	I380		LEU	SER	ASN	THR	ASN	THR
	ALA	T381	L296	GLY	THR	THR	THR	THR	SER
	ALA			THR	PRO	GLY	THR	GLY	THR
	VAL	D384	Q302	THR	ALA	ILE	ALA	GLY	GLY
	MET	L385	R303	ALA	SER	THR	THR	VAL	GLY
	ALA		N304	THR	THR	GLY	THR	THR	PHE
	ALA	I392	K312	SER	GLY	ILE	THR	SER	THR
	THR	Y393	I313	THR	PHE	THR	THR	PHE	THR
	LEU			ALA	THR	GLY	THR	GLY	THR
A401	GLN		A316	GLY	GLY	LEU	GLY	GLY	THR
	GLM		Q317	ASN	GLU	ASN	THR	LEU	GLY
	GLN		E318	GLY	ASN	ASN	GLY	THR	ALA
	GLN		I319	LEU	GLY	LEU	LEU	SER	ALA
	PRO	A405	K320	GLY	GLY	GLY	GLY	THR	SER
	ALA	I406	N321	GLY	GLY	ASN	PRO	GLY	GLY
	THR		A322	ILE	THR	ALA	SER	THR	ALA
	GLY	L418	E323	ASP	ALA	VAL	THR	GLY	GLY
	PRO		I324	PHE	THR	THR	THR	THR	GLY
	GLN	TYR	R325	SER	THR	SER	LEU	GLY	GLY
MET	PRO	ARG	L326	SER	THR	THR	SER	THR	LEU
	PRO	LYS	R327	SER	THR	THR	ALA	PHE	ALA
	SER	MET	T328	SER	THR	THR	ALA	THR	ALA
	LEU	PHE	Q329	SER	ALA	THR	GLY	THR	ASN
	GLY	LEU	K330	ASP	SER	THR	THR	ASN	GLY
	VAL	GLY	T331	LYS	THR	THR	GLY	LEU	GLY
	SER	ASP	P332	LYS	GLY	PHE	GLY	PHE	GLY
	PHE	ALA	P333	SER	LEU	SER	SER	SER	GLY
	GLY	VAL	G334	ASP	SER	LEU	LEU	THR	THR
	THR	ASP	L335	LYS	GLY	GLY	GLY	THR	THR
PHE	PRO	VAL	Q336	THR	GLY	GLY	GLY	ASN	PRO
	PHE	PHE	H337	GLY	THR	GLY	LYS	LYS	ALA
	GLY	GLU	E338	THR	ALA	ALA	ALA	PRO	THR
	THR	THR	Y339	ARG	LEU	PRO	THR	THR	THR
	SER	GLY	A340	PRO	ALA	GLY	ALA	THR	THR
	ILE	ARG	R341	GLY	GLY	ALA	ALA	SER	ALA
	GLY	ALA	P342	ASP	LEU	SER	ALA	SER	ALA
	THR	GLU	R343	SER	GLY	THR	THR	PRO	THR
	VAL		T344	LYS	GLY	THR	ALA	THR	SER

- Molecule 2: Nucleoporin p58/p45



SR	LEU	PIE	GLN	SER	THR	ASN	GLY	GLY	THR	SER	GLY	LEU	GLN	ASN	ALA	LEU	GLY	LEU	THR	GLY	THR	THR	ALA	ASN	GLU	GLY	LEU	GLY	GLY	ILE	ASP	THR	SER	SER	SER	ASP	LYS	THR	THR	ARG	PRO	GLU	ASP	SER	THR	LYS
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ALA	LEU	LYS	ASP	GLU	ASN	LEU	P248	P249	Z250	Z251	C252	Q253	D254		E264	R274	Z275	S276	S277		L296	Q302	R303	N304		K312	L313		A316	Q317	E318	L319	K320	N321	A322	E323	E324	L324	K325	N326	R327	T328	Q329	K330	P331	P332	P333	G334	L335	G336	H337	E338	Y339	A340	A341	P342	A343		P344
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[illegible]

GLU	LYS	LYS	TRP	GLN	ASN	THR	GLY	PRO	PRO	THR	PRO	PRO	PHE	SER	THR	MET	MET	ASN	ALA	ALA	ALA	VAL	ALA	ALA	ALA	LEU	LEU	GLN	GLN	GLN	GLN	GLY	PRO	GLN	PRO	SER	PHE	GLY	THR	PRO	PHE	GLY	GLY	GLY	ILE	TYR
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THR	GLY	LEU	GLN	SER	SER	GLY	LEU	GLY	SER	SER	ASN	LEU	GLY	GLY	PHE	GLY	THR	SER	SER	GLY	PHE	GLY	CYS	SER	THR	THR	GLY	ALA	SER	THR	PHE	PHE	GLY	PHE	GLY	THR	THR	ASN	PRO	PRO	GLY	SER	SER	SER	SER	THR	SER	GLY	LEU	SER	ALA	GLY	PHE	SER	SER	SER	THR	SER	GLY	PHE	ASN	GLN
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PRO	GLY	ILE	THR	ALA	SER	ALA	GLY	LEU	THR	PHE	GLY	VAL	SER	ASN	PRO	ALA	SER	ALA	GLY	PHE	GLY	THR	GLY	GLY	GLN	LEU	LEU	GLN	LEU	LYS	PRO	PRO	ALA	ALA	GLY	ASN	LYS	ARG	GLY	LYS
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- Molecule 2: Nucleoporin p58/p45

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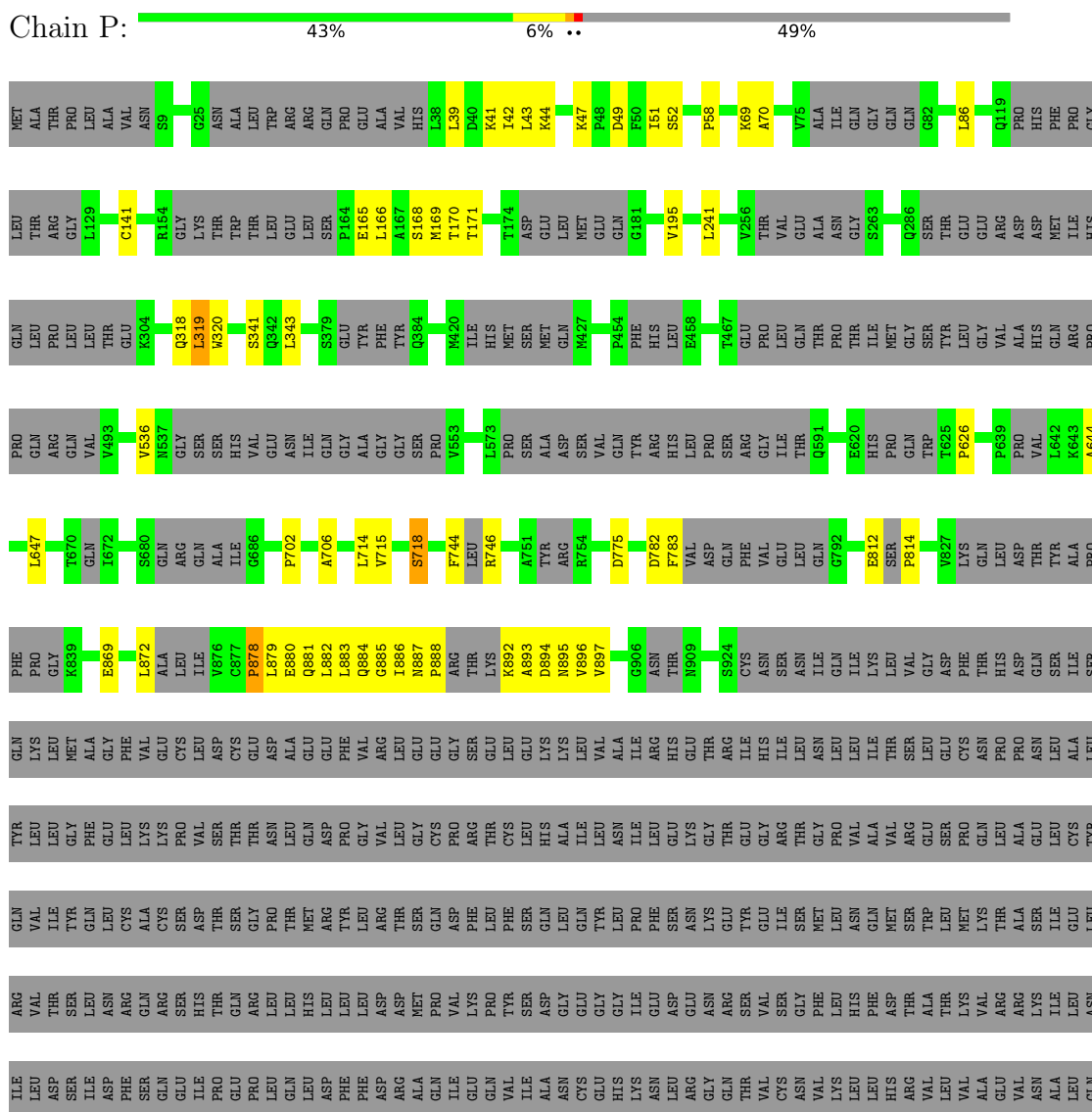
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ALA	P248	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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- Molecule 4: Nuclear pore complex protein Nup205

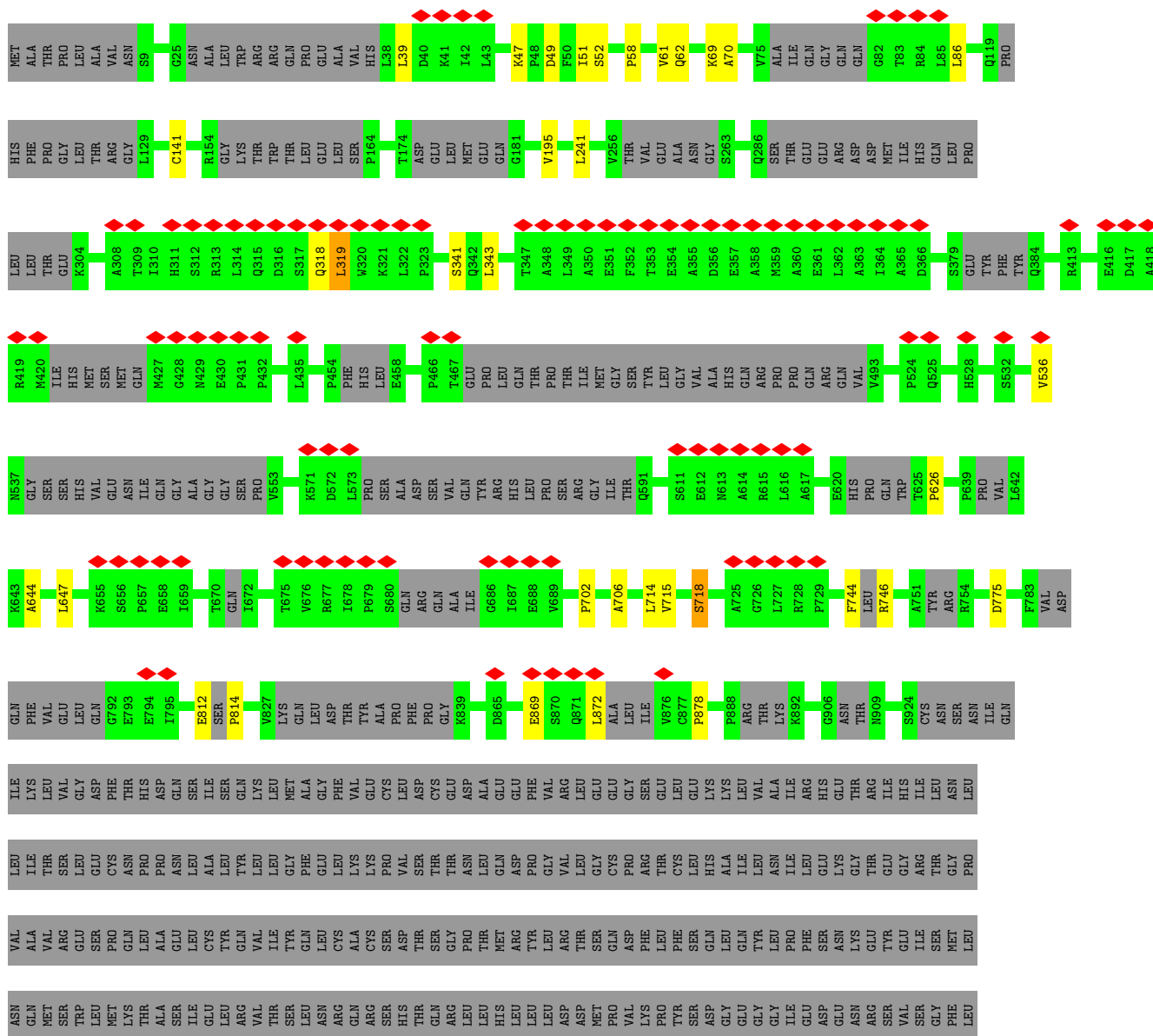


- Molecule 4: Nuclear pore complex protein Nup205

Chain D:  45% 49%

MET	ALA	THR	PRO	GLY	LEU	ALA	THR	VAL	ASN	99	G25	ASN	ALA	LEU	THR	ARG	ARG	GLN	PRO	GLU	VAL	HIS	L38	L39	K47	P48	D49	F50	I51	S52	P58	K69	A70	Y75	ALA	ILE	THR	GLU	GLY	GLN	GLN	G82	L86	G119	PRO	HIS	LEU	PRO	THR	GLY	LEU	THR	ARG	GLY	L129
																				</																																			

- Molecule 4: Nuclear pore complex protein Nup205





Frequency	Percentage
Daily	73%
Weekly	5%
Monthly	22%

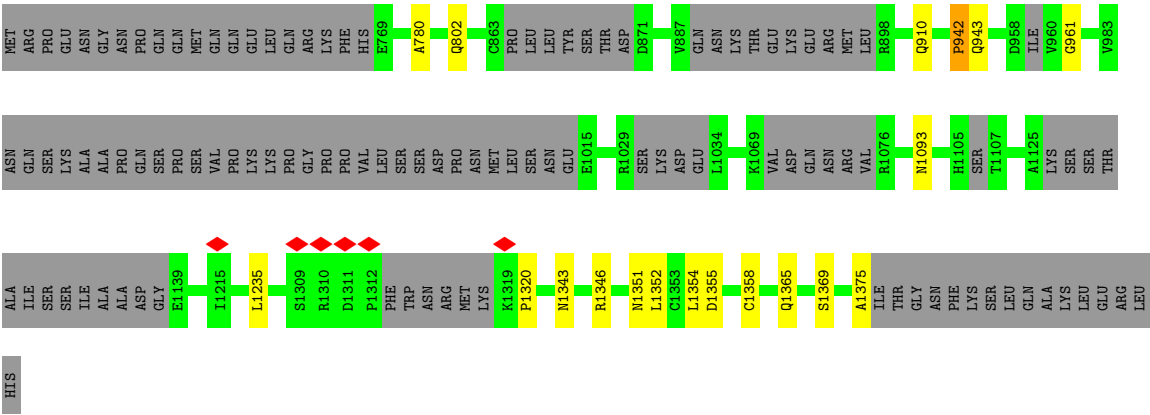


Response	Percentage
Yes, the U.S. is a democracy	73%
No, the U.S. is not a democracy	22%

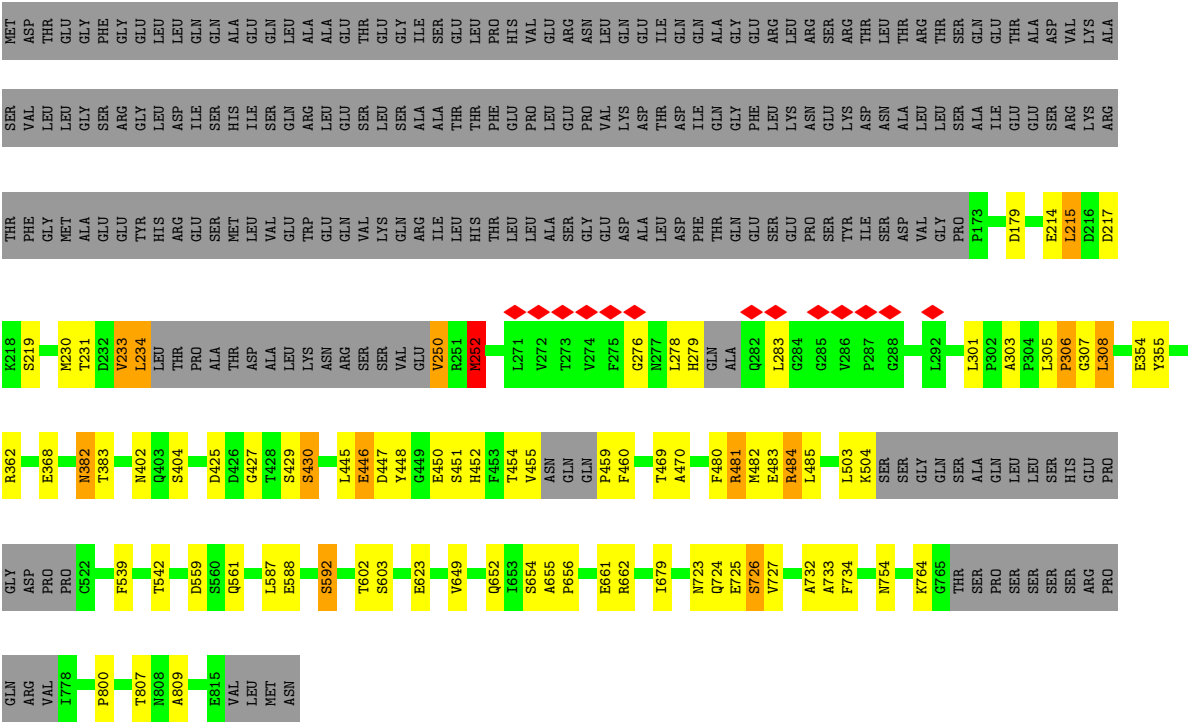


Category	Percentage
Used a mobile app to book a flight	73%
Used a mobile app to book a flight	22%
Used a mobile app to book a flight	5%



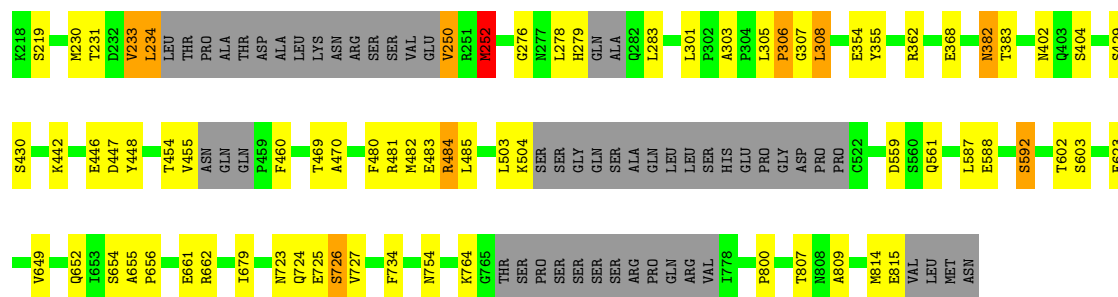


• Molecule 6: Nuclear pore complex protein Nup93



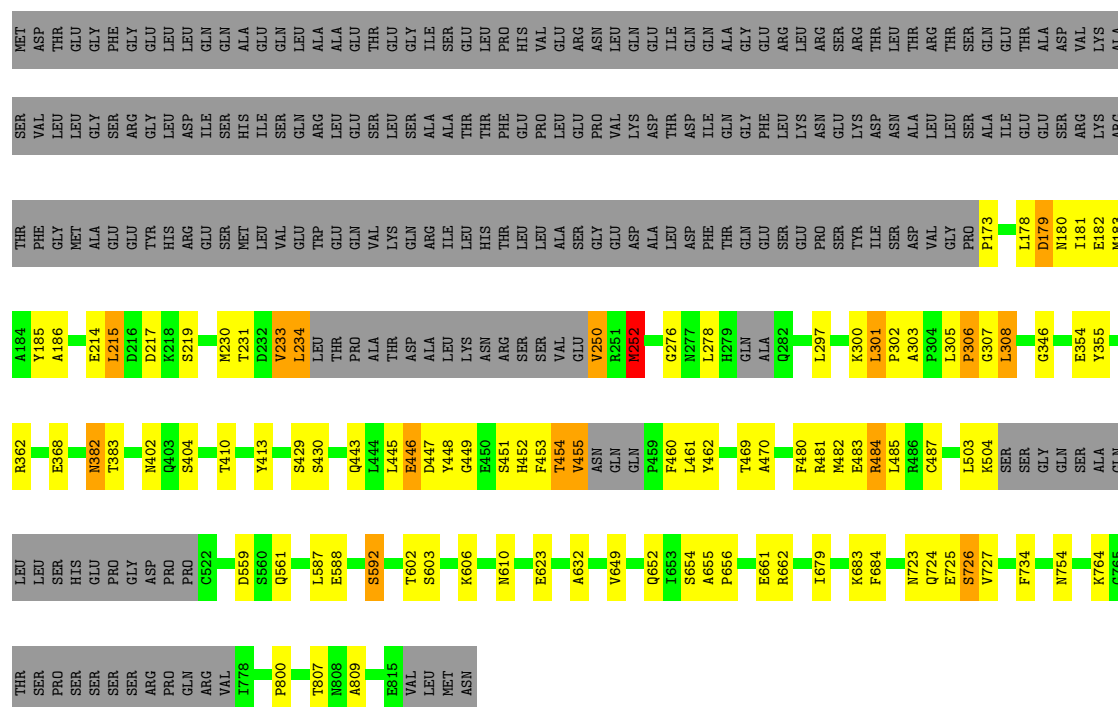
• Molecule 6: Nuclear pore complex protein Nup93





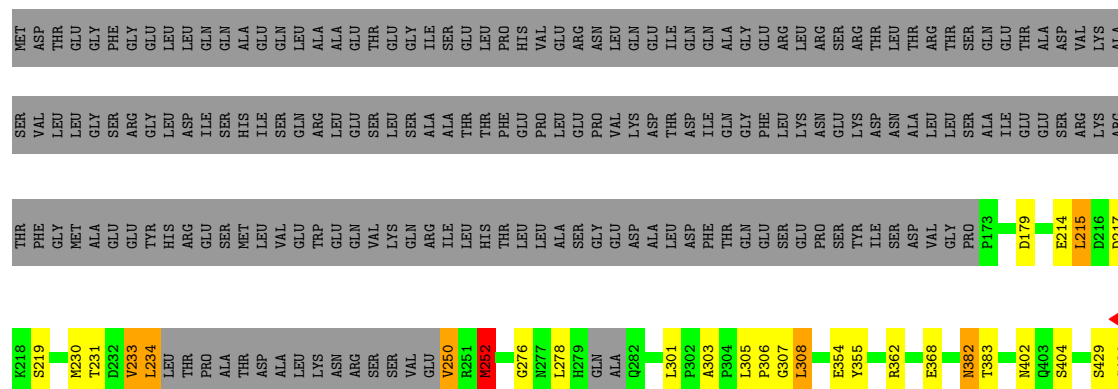
• Molecule 6: Nuclear pore complex protein Nup93

Chain O: 60% 10% 27%



• Molecule 6: Nuclear pore complex protein Nup93

Chain U: 64% 8% 27%



E446	D447	Y448	T454	V455	ASN	GLN	GLN	P459	F460	T469	A470	F480	R481	M482	E483	R484	L485	L503	K504	SER	SER	GLY	GLN	SER	SER	ALA	GLN	LEU	LEU	SER	SER	HIS	GLU	PRO	PRO	GLY	ASP	PRO	PRO	G522	D589	S590	Q561	L587	E588	S592	T602	S603	E623	V649
Q652	I653	S654	A655	P656	E661	R662	I679	N723	Q724	E725	S726	V727	F734	N754	K764	G765	THR	SER	PRO	SER	SER	SER	SER	SER	SER	ARG	ARG	PRO	GLN	ARG	VAL	I778	P800	T807	N808	A809	E815	VAL	LEU	MET	ASN									

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of subtomograms used	1252	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.000	Depositor
Minimum map value	0.000	Depositor
Average map value	0.351	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.44	Depositor
Map size (\AA)	2188.8, 2188.8, 2188.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	6.84, 6.84, 6.84	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	F	3.74	152/1655 (9.2%)	3.77	224/2302 (9.7%)
1	L	3.74	154/1655 (9.3%)	3.77	222/2302 (9.6%)
1	R	3.74	152/1655 (9.2%)	3.77	223/2302 (9.7%)
1	X	3.74	151/1655 (9.1%)	3.77	224/2302 (9.7%)
2	G	3.95	84/852 (9.9%)	3.81	122/1190 (10.3%)
2	M	3.95	85/852 (10.0%)	3.81	122/1190 (10.3%)
2	S	3.95	83/852 (9.7%)	3.81	122/1190 (10.3%)
2	Y	3.95	84/852 (9.9%)	3.81	122/1190 (10.3%)
3	H	3.44	83/841 (9.9%)	3.09	110/1174 (9.4%)
3	N	3.44	83/841 (9.9%)	3.09	110/1174 (9.4%)
3	T	3.44	83/841 (9.9%)	3.10	109/1174 (9.3%)
3	Z	3.44	84/841 (10.0%)	3.09	109/1174 (9.3%)
4	D	1.22	38/5066 (0.8%)	1.69	118/7020 (1.7%)
4	J	1.22	39/5066 (0.8%)	1.69	119/7020 (1.7%)
4	P	1.22	38/5066 (0.8%)	1.69	116/7020 (1.7%)
4	V	1.22	39/5066 (0.8%)	1.69	118/7020 (1.7%)
5	E	0.93	0/5338	1.17	10/7399 (0.1%)
5	K	0.93	0/5338	1.17	10/7399 (0.1%)
5	Q	0.93	0/5338	1.18	10/7399 (0.1%)
5	W	0.93	0/5338	1.17	10/7399 (0.1%)
6	C	0.94	1/2938 (0.0%)	1.31	20/4086 (0.5%)
6	I	0.94	1/2938 (0.0%)	1.31	20/4086 (0.5%)
6	O	0.94	1/2938 (0.0%)	1.31	20/4086 (0.5%)
6	U	0.94	1/2938 (0.0%)	1.31	19/4086 (0.5%)
All	All	1.91	1436/66760 (2.2%)	2.06	2409/92684 (2.6%)

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	F	7	31

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	7	31
1	R	7	31
1	X	7	30
2	G	9	10
2	M	9	10
2	S	9	10
2	Y	9	10
3	H	5	5
3	N	5	5
3	T	5	5
3	Z	5	5
4	D	0	19
4	J	0	20
4	P	0	21
4	V	0	20
5	E	0	1
5	K	0	1
5	Q	0	1
5	W	0	1
All	All	84	267

The worst 5 of 1436 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	380	ILE	N-CA	38.62	2.23	1.46
2	M	380	ILE	N-CA	38.57	2.23	1.46
2	G	380	ILE	N-CA	38.49	2.23	1.46
2	S	380	ILE	N-CA	38.48	2.23	1.46
2	Y	379	HIS	CA-C	37.09	2.49	1.52

The worst 5 of 2409 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	452	ARG	CA-C-N	-39.57	30.16	117.20
1	L	452	ARG	CA-C-N	-39.56	30.17	117.20
1	R	452	ARG	CA-C-N	-39.55	30.18	117.20
1	F	452	ARG	CA-C-N	-39.55	30.19	117.20
2	Y	343	ALA	CB-CA-C	-36.26	55.71	110.10

5 of 84 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	305	ASP	CA
1	F	341	ASP	CA
1	F	423	ALA	CA
1	F	454	TYR	CA
1	F	459	LEU	CA

5 of 267 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	393	GLN	Mainchain
1	F	397	ARG	Mainchain
1	F	398	LYS	Peptide,Mainchain
1	F	399	SER	Peptide
1	F	400	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1658	0	715	186	0
1	L	1658	0	715	153	0
1	R	1658	0	710	232	0
1	X	1658	0	715	153	0
2	G	853	0	384	61	0
2	M	853	0	384	56	0
2	S	853	0	384	56	0
2	Y	853	0	384	57	0
3	H	842	0	365	43	0
3	N	842	0	365	37	0
3	T	842	0	365	37	0
3	Z	842	0	365	36	0
4	D	5094	0	2272	135	0
4	J	5094	0	2271	69	0
4	P	5094	0	2253	344	0
4	V	5094	0	2258	298	0
5	E	5366	0	2365	31	0
5	K	5366	0	2362	61	0
5	Q	5366	0	2365	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	W	5366	0	2350	236	0
6	C	2946	0	1307	78	0
6	I	2946	0	1306	35	0
6	O	2946	0	1296	189	0
6	U	2946	0	1307	21	0
All	All	67036	0	29563	2028	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 21.

The worst 5 of 2028 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:G:366:GLU:CB	2:G:366:GLU:CA	1.76	1.63
1:X:451:GLU:CA	1:X:451:GLU:CB	1.77	1.61
1:F:447:VAL:CB	1:F:447:VAL:CA	1.78	1.60
1:R:447:VAL:CA	1:R:447:VAL:CB	1.78	1.60
1:L:454:TYR:CA	1:L:454:TYR:CB	1.77	1.60

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	F	329/507 (65%)	295 (90%)	16 (5%)	18 (6%)	1	15
1	L	329/507 (65%)	295 (90%)	16 (5%)	18 (6%)	1	15
1	R	329/507 (65%)	295 (90%)	16 (5%)	18 (6%)	1	15
1	X	329/507 (65%)	295 (90%)	16 (5%)	18 (6%)	1	15
2	G	169/599 (28%)	153 (90%)	11 (6%)	5 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	169/599 (28%)	153 (90%)	11 (6%)	5 (3%)	3	23
2	S	169/599 (28%)	153 (90%)	10 (6%)	6 (4%)	3	20
2	Y	169/599 (28%)	153 (90%)	10 (6%)	6 (4%)	3	20
3	H	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	2	17
3	N	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	2	17
3	T	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	2	17
3	Z	167/522 (32%)	152 (91%)	8 (5%)	7 (4%)	2	17
4	D	972/2012 (48%)	911 (94%)	46 (5%)	15 (2%)	8	40
4	J	972/2012 (48%)	911 (94%)	46 (5%)	15 (2%)	8	40
4	P	972/2012 (48%)	911 (94%)	46 (5%)	15 (2%)	8	40
4	V	972/2012 (48%)	911 (94%)	46 (5%)	15 (2%)	8	40
5	E	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	5	30
5	K	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	5	30
5	Q	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	5	30
5	W	1027/1391 (74%)	947 (92%)	58 (6%)	22 (2%)	5	30
6	C	578/819 (71%)	486 (84%)	53 (9%)	39 (7%)	1	12
6	I	578/819 (71%)	486 (84%)	53 (9%)	39 (7%)	1	12
6	O	578/819 (71%)	486 (84%)	52 (9%)	40 (7%)	1	11
6	U	578/819 (71%)	486 (84%)	53 (9%)	39 (7%)	1	12
All	All	12968/23400 (55%)	11776 (91%)	765 (6%)	427 (3%)	5	21

5 of 427 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	148	TRP
1	F	318	ASP
1	F	403	ILE
1	F	405	ALA
1	F	451	GLU

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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
1	F	5
1	X	5
1	L	5
1	R	5
2	G	3
2	S	3
2	Y	3
2	M	3
3	H	3
3	Z	3
3	N	3
3	T	3
6	C	2
6	I	2
6	O	2
6	U	2

The worst 5 of 52 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	483:GLU	C	484:ARG	N	4.02
1	I	483:GLU	C	484:ARG	N	4.02
1	O	483:GLU	C	484:ARG	N	4.02
1	U	483:GLU	C	484:ARG	N	4.02
1	C	447:ASP	C	448:TYR	N	3.63

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12814. 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](#)

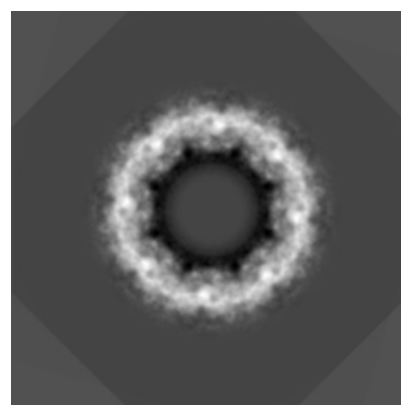
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

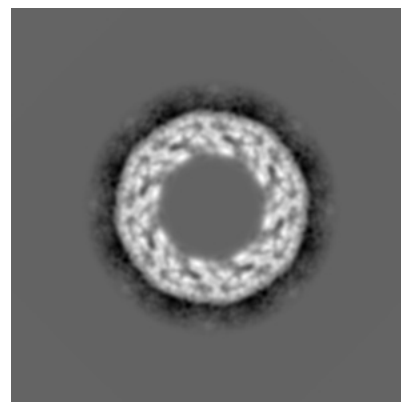
6.2.1 Primary map



X Index: 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](#)

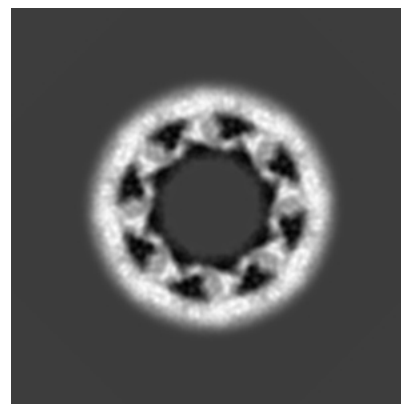
6.3.1 Primary map



X Index: 100



Y Index: 220

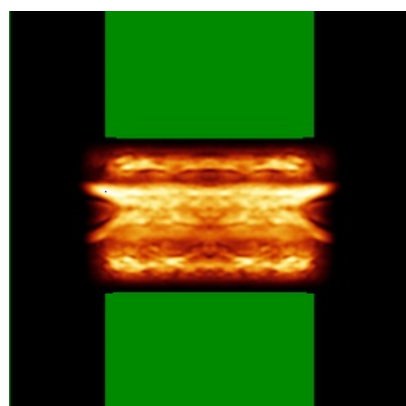


Z Index: 174

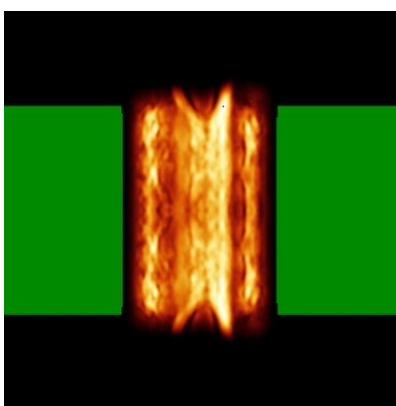
The images above show the largest variance slices of the map in three orthogonal directions.

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

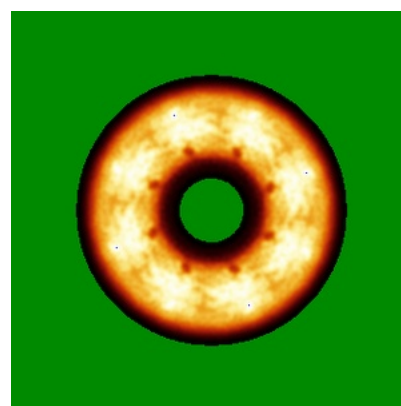
6.4.1 Primary map



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 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

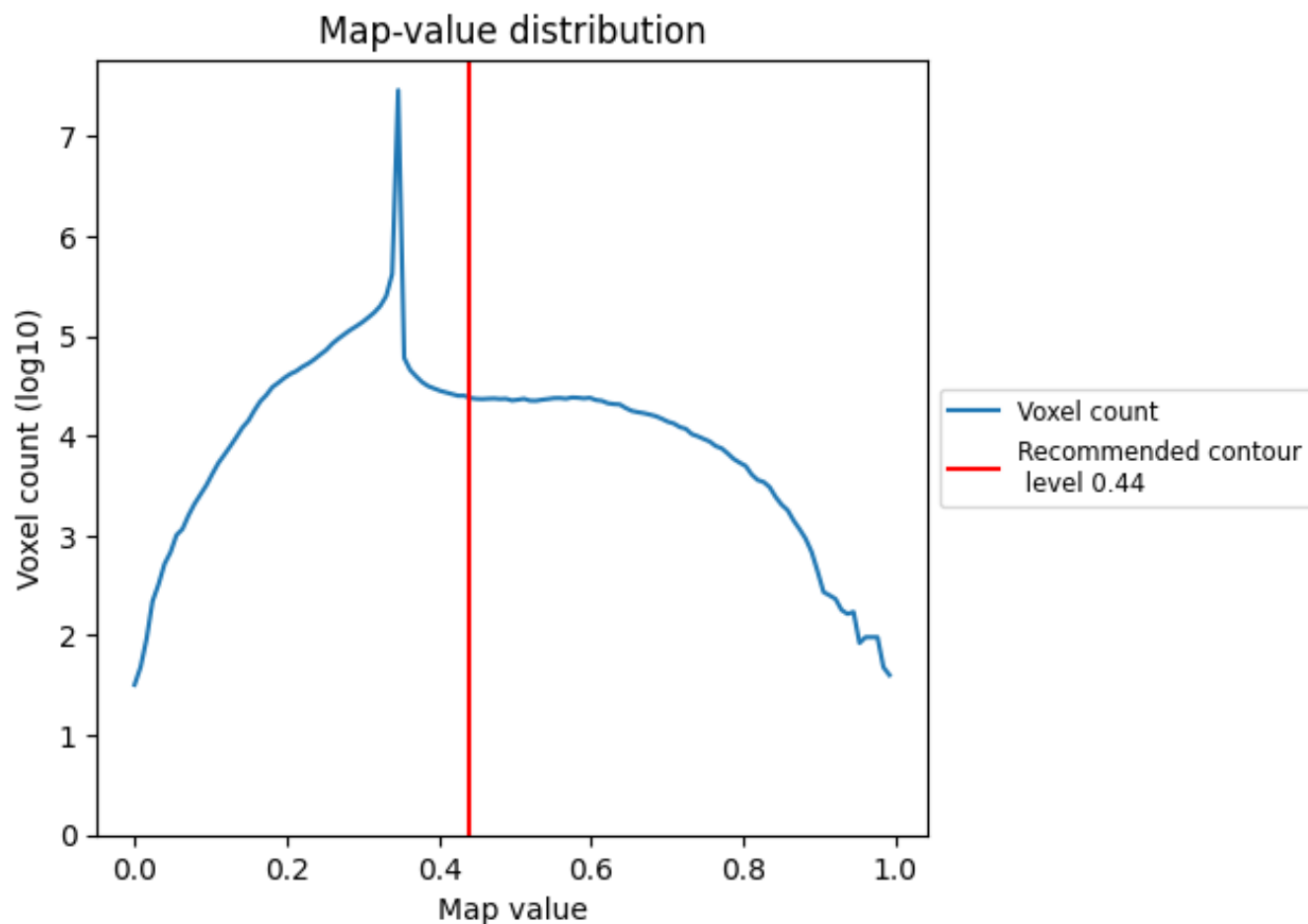
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

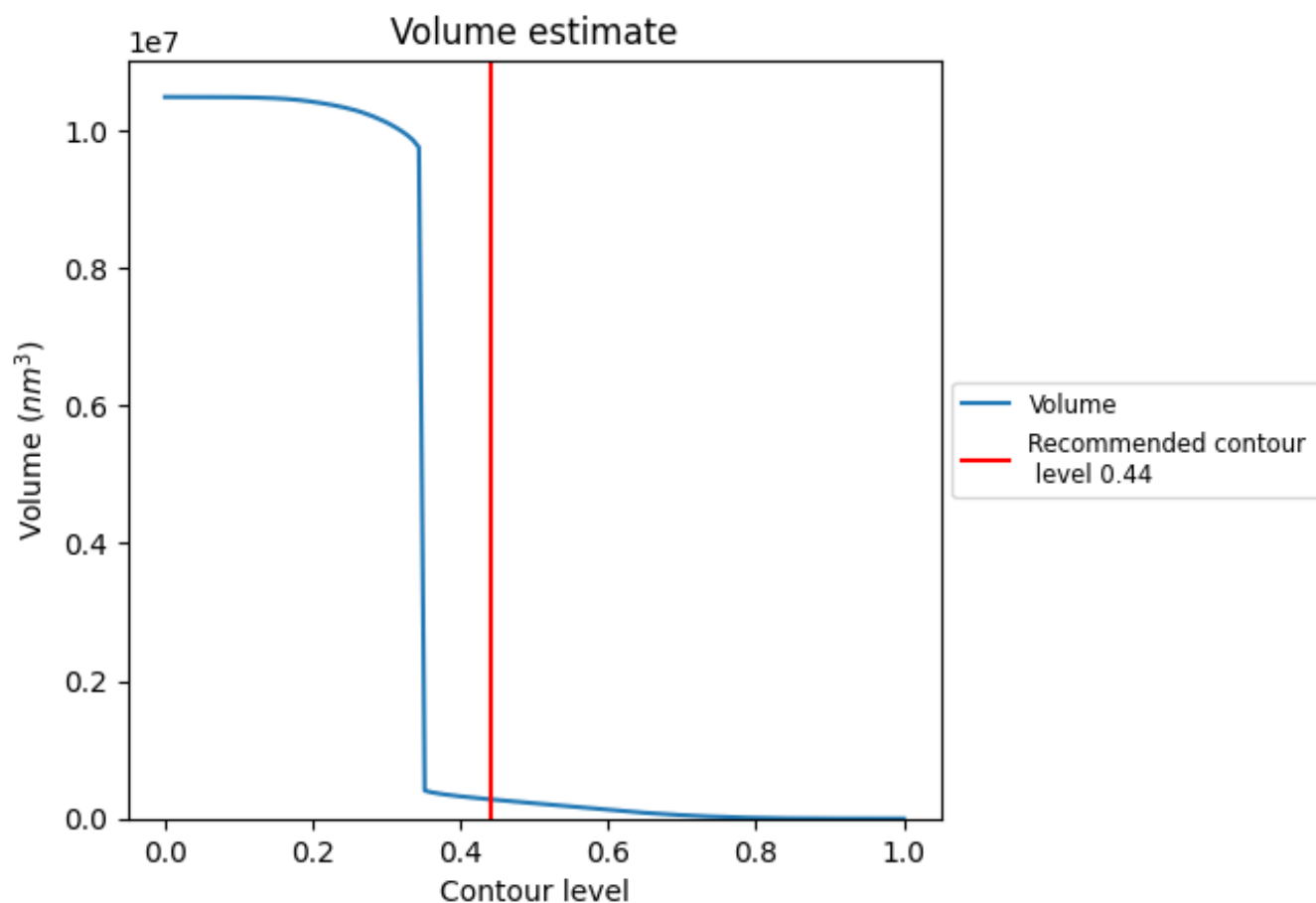
This section contains the results of statistical analysis of the map.

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.

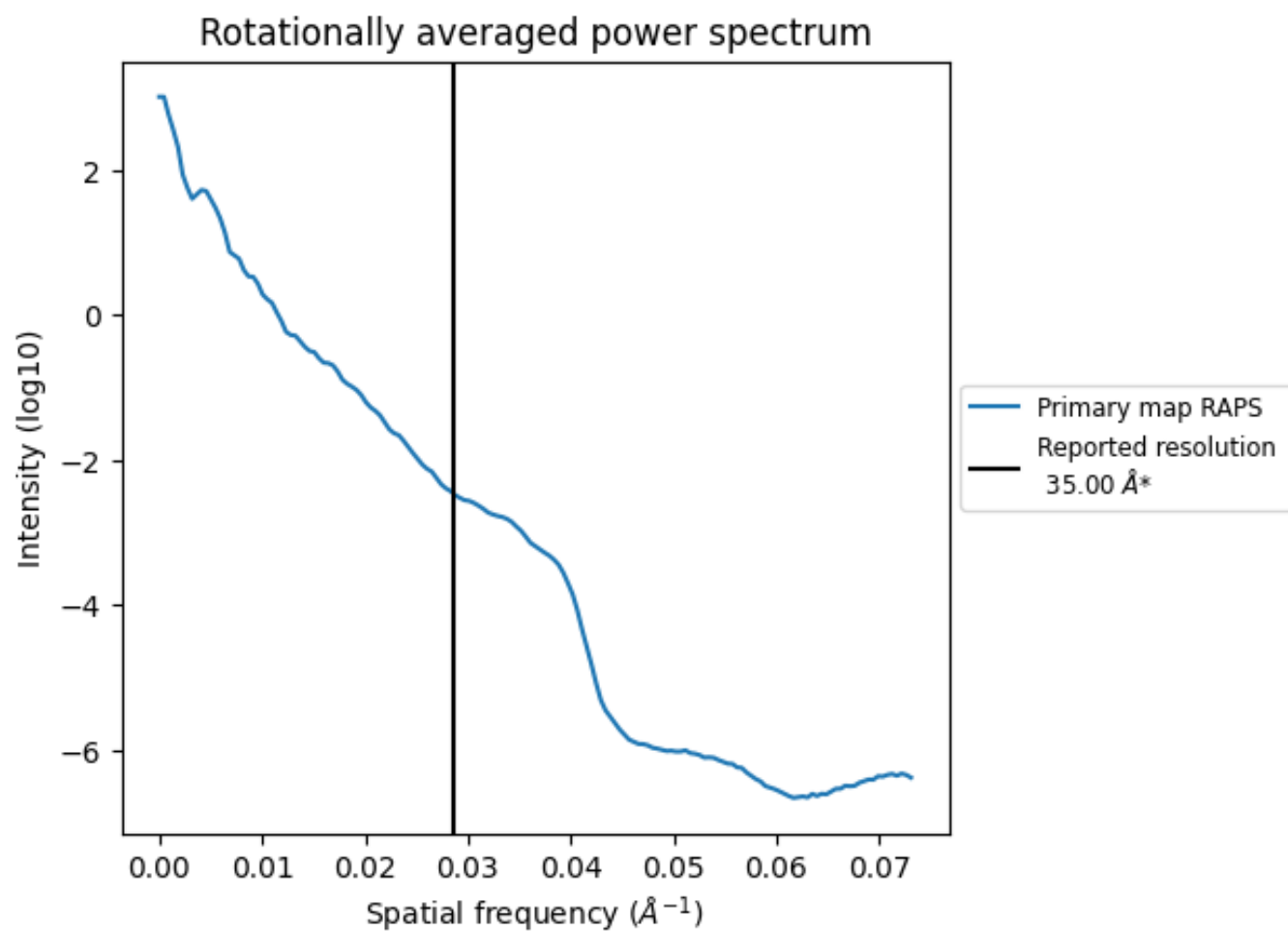
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280168 nm³; this corresponds to an approximate mass of 253083 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 0.029 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

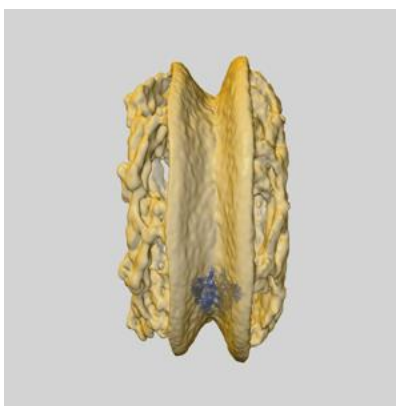
This section contains information regarding the fit between EMDB map EMD-12814 and PDB model 7PER. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

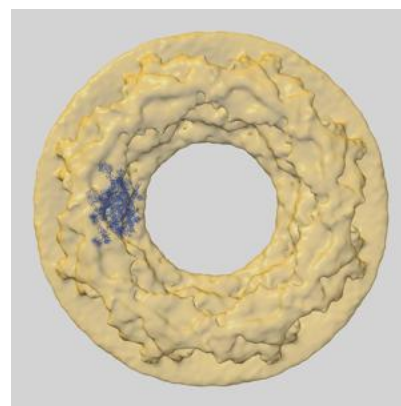
9.1.1 Map-model overlay [i](#)



X



Y

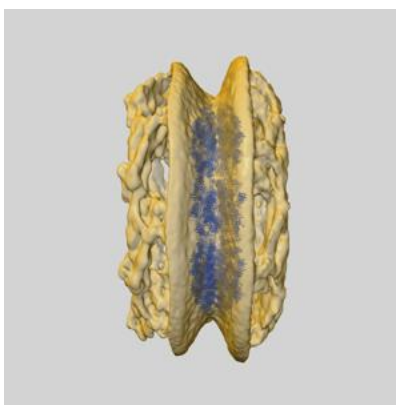


Z

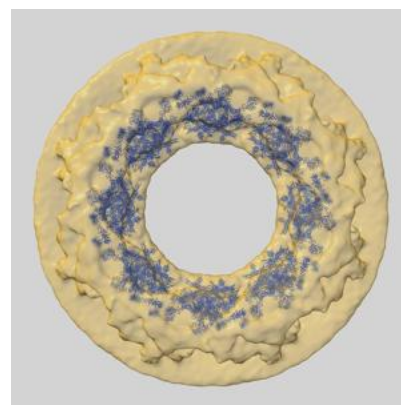
9.1.2 Map-model assembly overlay [i](#)



X



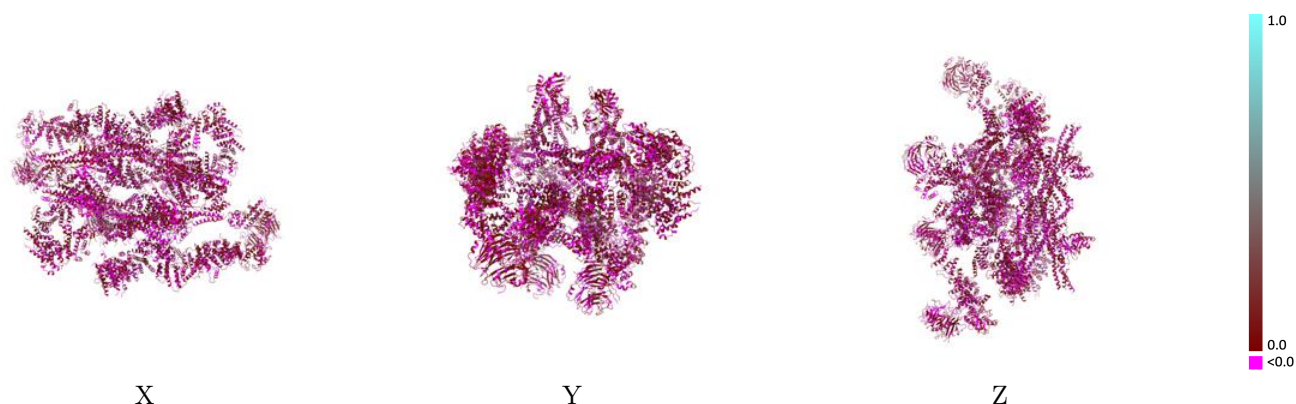
Y



Z

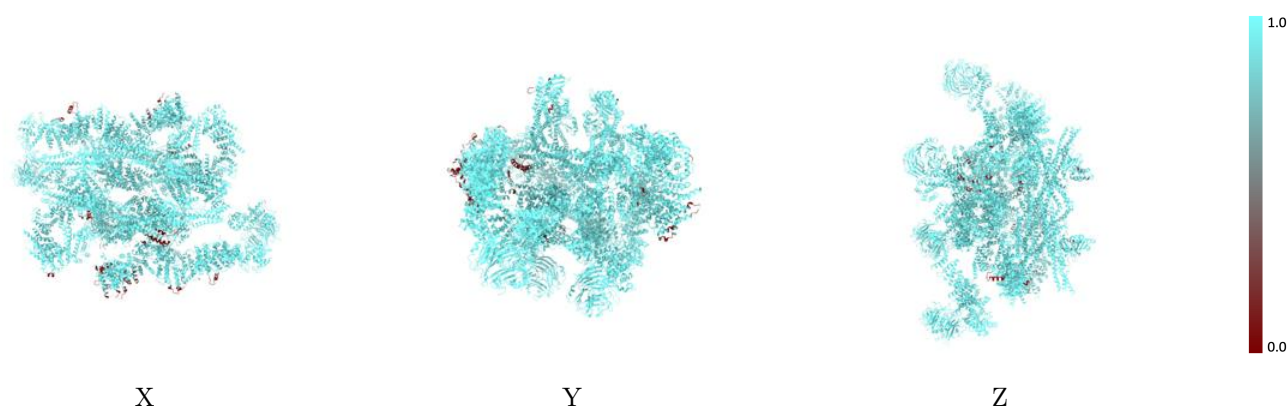
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



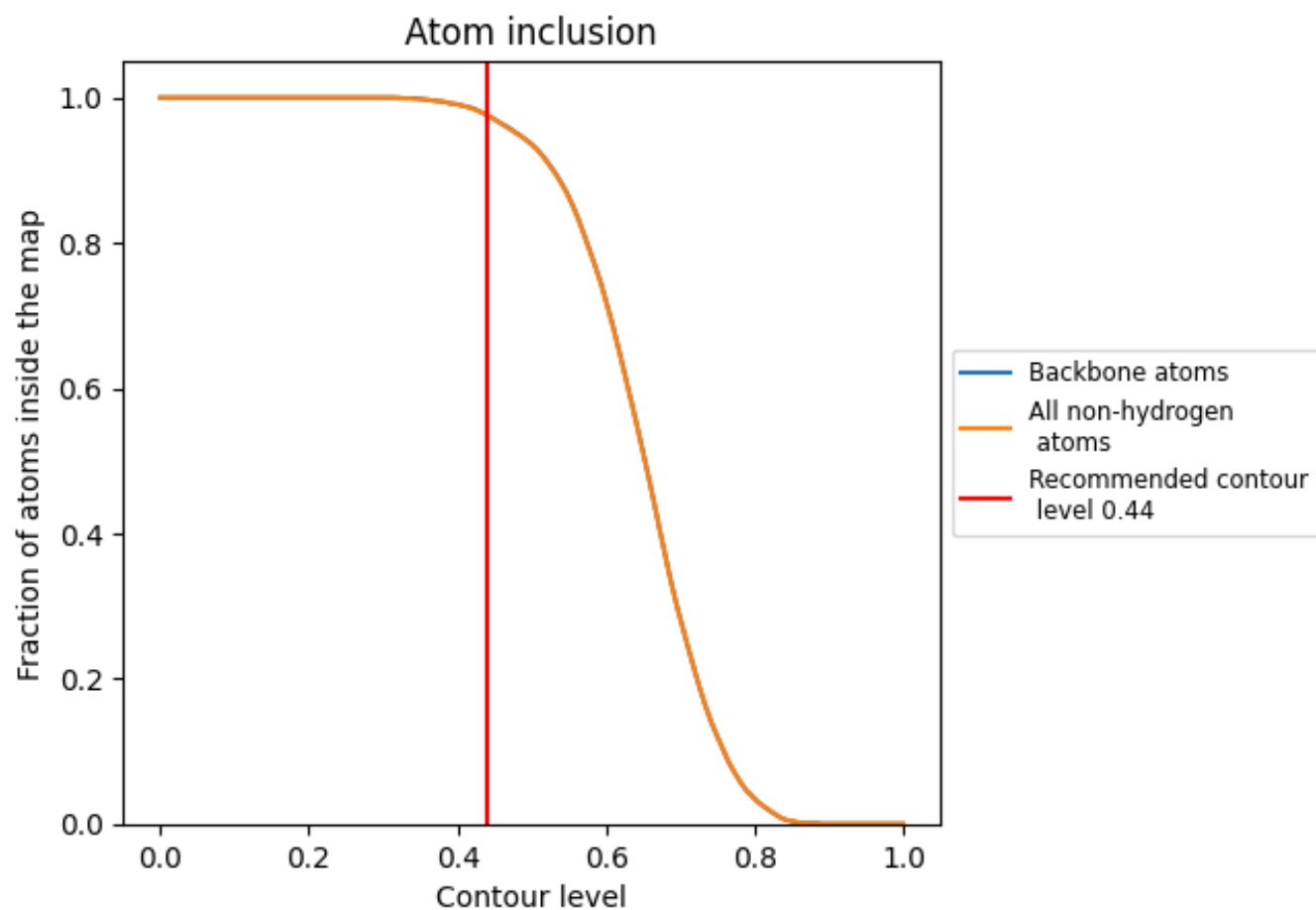
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.44).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9760	 0.0380
C	 0.9770	 0.0380
D	 0.9850	 0.0400
E	 1.0000	 0.0360
F	 0.9600	 0.0120
G	 0.9980	 0.0210
H	 1.0000	 0.0010
I	 0.9990	 0.0550
J	 0.8800	 0.0400
K	 0.9770	 0.0320
L	 0.9040	 0.0170
M	 0.9190	 -0.0010
N	 0.9810	 0.0560
O	 1.0000	 0.0270
P	 0.9990	 0.0480
Q	 0.9920	 0.0500
R	 0.9930	 0.0360
S	 1.0000	 0.0370
T	 1.0000	 0.0350
U	 0.9980	 0.0380
V	 0.9320	 0.0520
W	 0.9990	 0.0350
X	 0.9920	 0.0320
Y	 1.0000	 0.0180
Z	 1.0000	 0.0690

