



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 07:18 AM EST

PDB ID : 6UXW
EMDB ID : EMD-20934
Title : SWI/SNF nucleosome complex with ADP-BeFx
Authors : He, Y.; Han, Y.
Deposited on : 2019-11-08
Resolution : 8.96 Å(reported)
Based on initial models : 5Z3V, 4I6M

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.31.2

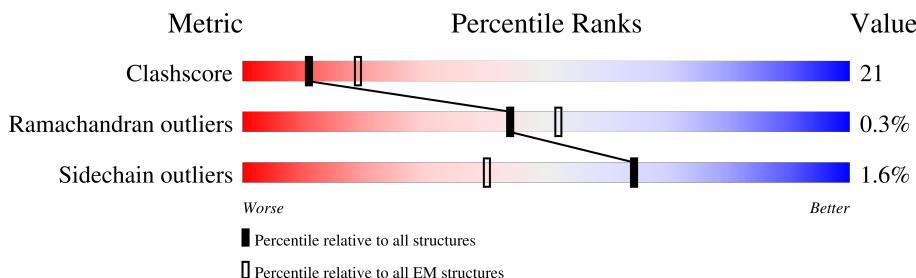
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.96 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.



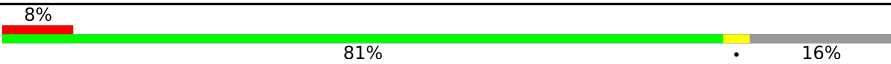

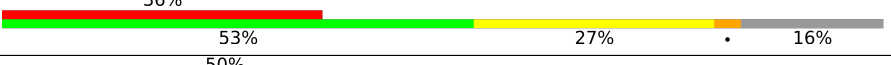
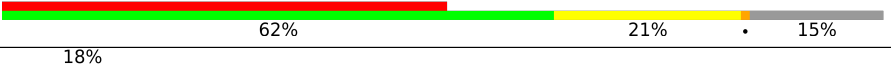



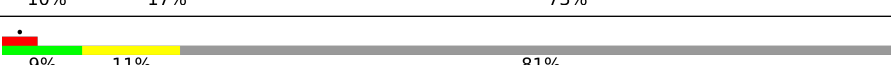
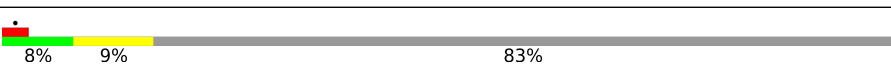



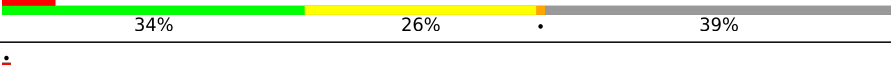


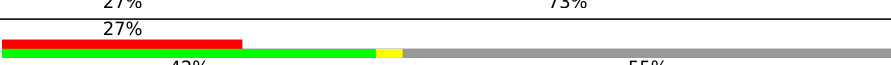

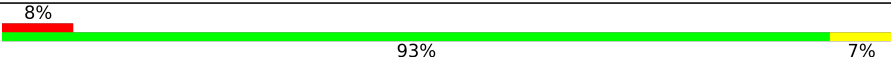
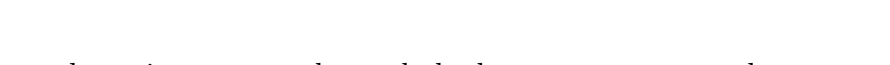
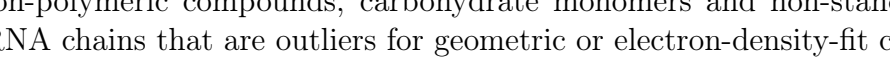
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	R	135	<div> <div>21%</div> <div>59%</div> <div>13%</div> <div>27%</div> </div>
1	V	135	<div> <div>8%</div> <div>56%</div> <div>14%</div> <div>30%</div> </div>
2	S	102	<div> <div>19%</div> <div>62%</div> <div>19%</div> <div>20%</div> </div>
2	W	102	<div> <div>11%</div> <div>62%</div> <div>16%</div> <div>23%</div> </div>
3	T	129	<div> <div>24%</div> <div>77%</div> <div>6%</div> <div>17%</div> </div>
3	X	129	<div> <div>16%</div> <div>74%</div> <div>9%</div> <div>17%</div> </div>
4	U	122	<div> <div>11%</div> <div>68%</div> <div>8%</div> <div>24%</div> </div>
4	Y	122	<div> <div>9%</div> <div>66%</div> <div>10%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
5	a	185	
6	b	200	
7	P	477	
8	Q	467	
9	Z	157	
10	A	1703	
11	B	1314	
12	C	905	
13	D	825	
13	E	825	
13	F	825	
13	G	825	
14	H	566	
15	I	179	
16	J	67	
16	K	67	
16	L	67	
16	N	67	
16	O	67	
17	M	83	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BEF	A	1803	-	-	X	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 41275 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	V	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	102	ALA	GLY	conflict	UNP P84233
V	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	W	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	T	107	Total	C	N	O	0	0
			811	510	158	143		
3	X	107	Total	C	N	O	0	0
			815	513	159	143		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	99	ARG	GLY	conflict	UNP P06897
T	123	SER	ALA	conflict	UNP P06897
X	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
X	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	Y	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	29	THR	SER	conflict	UNP P02281
Y	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called 601 sequence bottom strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	155	Total	C	N	O	P	0	0
			3160	1502	574	929	155		

- Molecule 6 is a DNA chain called 601 sequence top strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	155	Total	C	N	O	P	0	0
			3195	1514	595	931	155		

- Molecule 7 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	399	Total	C	N	O	S	3	0
			3227	2081	528	603	15		

- Molecule 8 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	396	Total	C	N	O	S	1	0
			3198	2053	523	615	7		

- Molecule 9 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 10 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	778	Total	C	N	O	S	1	0
			6385	4041	1139	1185	20		

- Molecule 11 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	482	Total	C	N	O	S	0	0
			3890	2519	637	723	11		

- Molecule 12 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	245	Total	C	N	O	S	0	0
			2005	1256	346	395	8		

- Molecule 13 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	159	Total	C	N	O	S	0	0
			1322	853	225	239	5		
13	E	139	Total	C	N	O	S	0	0
			1152	746	198	205	3		
13	F	221	Total	C	N	O	S	0	0
			1583	987	287	304	5		
13	G	197	Total	C	N	O	S	0	0
			1435	904	258	268	5		

- Molecule 14 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	257	Total	C	N	O	S	0	0
			2085	1323	355	400	7		

- Molecule 15 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	109	Total	C	N	O	S	0	0
			818	504	155	156	3		

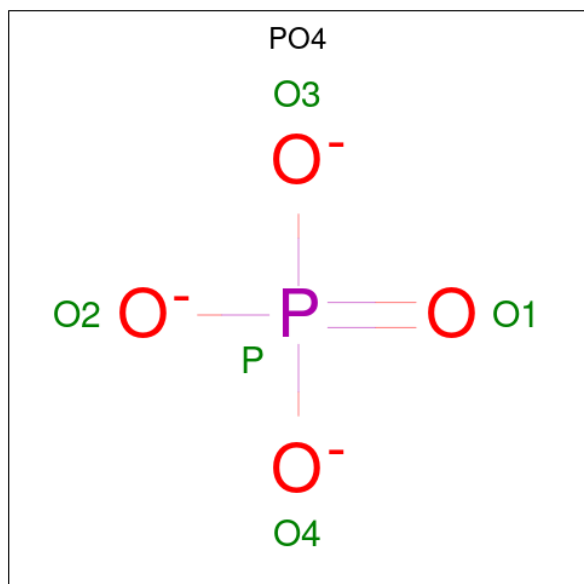
- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	67	Total	C	N	O	0	0
			336	201	67	68		
16	K	28	Total	C	N	O	0	0
			140	84	28	28		
16	L	18	Total	C	N	O	0	0
			90	54	18	18		
16	N	30	Total	C	N	O	0	0
			150	90	30	30		
16	O	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 17 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

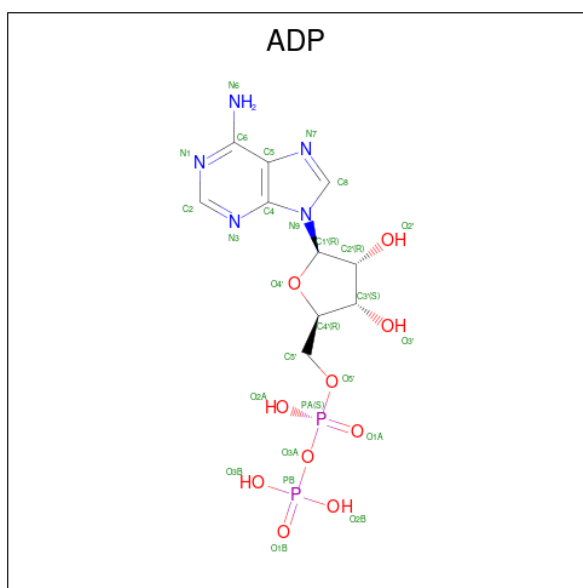
Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	83	Total	C	N	O	0	0
			416	249	83	84		

- Molecule 18 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



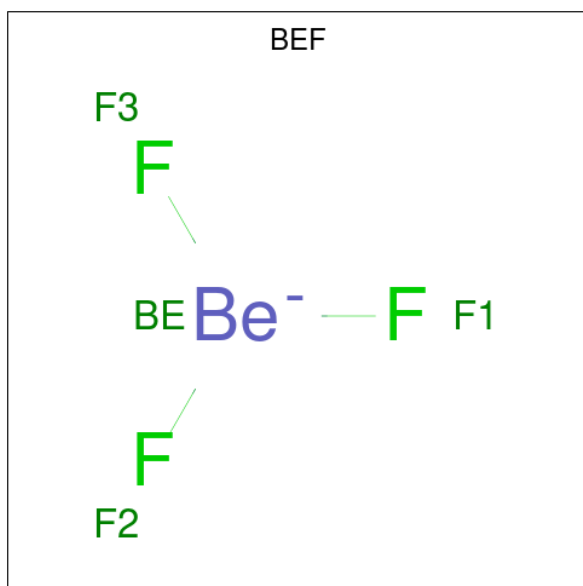
Mol	Chain	Residues	Atoms			AltConf
18	P	1	Total	O	P	0
			25	20	5	
18	P	1	Total	O	P	0
			25	20	5	
18	P	1	Total	O	P	0
			25	20	5	
18	P	1	Total	O	P	0
			25	20	5	
18	Q	1	Total	O	P	0
			30	24	6	
18	Q	1	Total	O	P	0
			30	24	6	
18	Q	1	Total	O	P	0
			30	24	6	
18	Q	1	Total	O	P	0
			30	24	6	
18	Q	1	Total	O	P	0
			30	24	6	
18	Q	1	Total	O	P	0
			30	24	6	
18	A	1	Total	O	P	0
			5	4	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	Be	F	0
			4	1	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

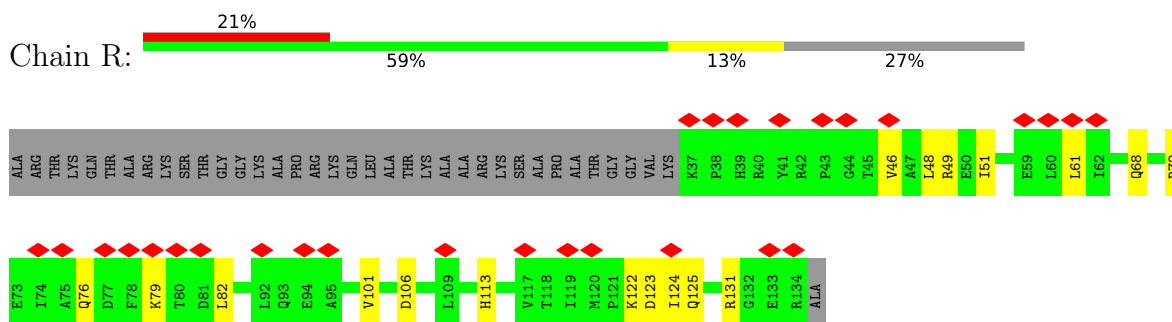
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	P	33	Total	O	0
			33	33	
22	Q	51	Total	O	0
			51	51	
22	Z	2	Total	O	0
			2	2	

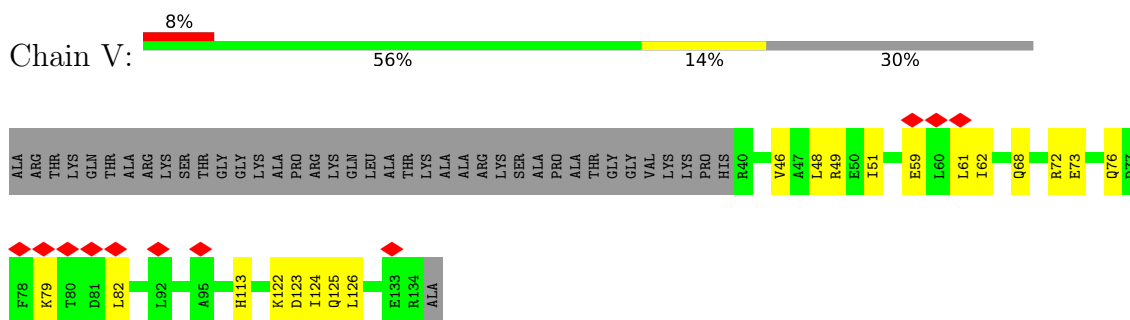
3 Residue-property plots [i](#)

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.

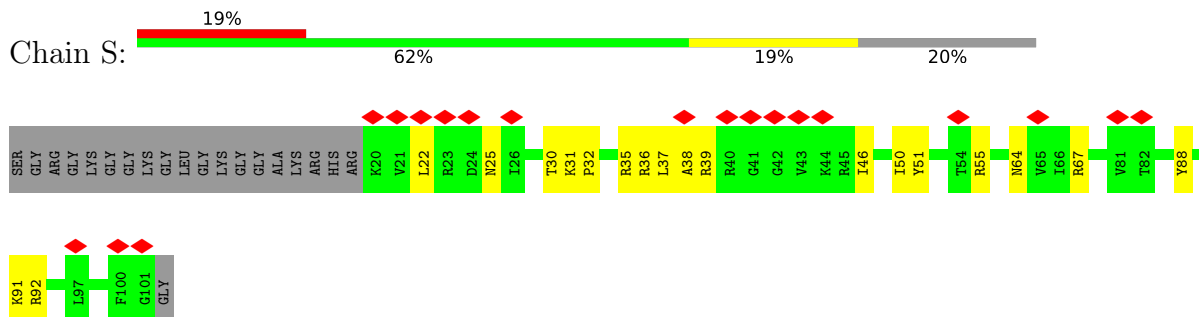
- Molecule 1: Histone H3.2



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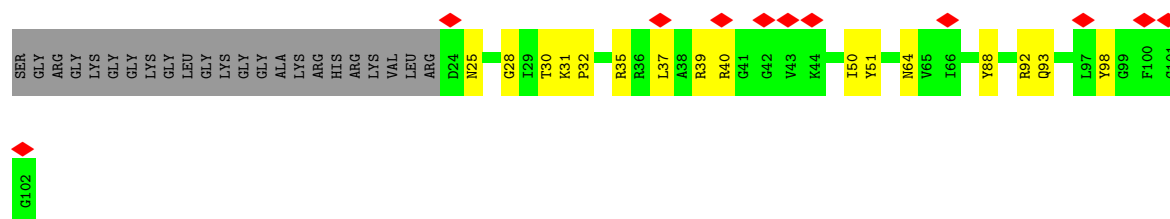


- Molecule 2: Histone H4

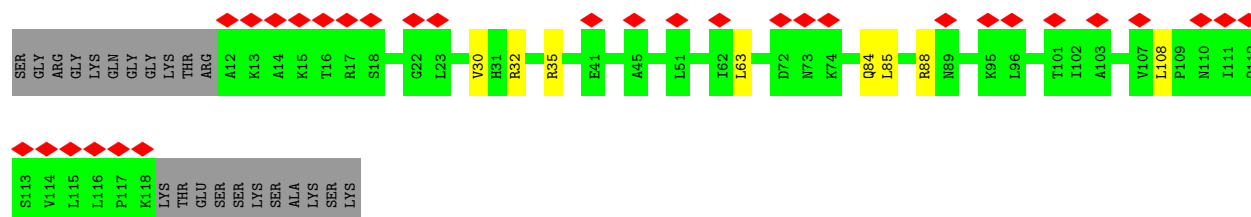
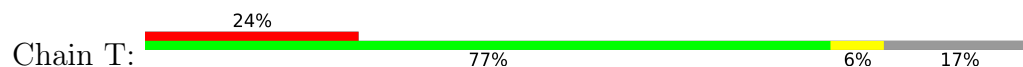


- Molecule 2: Histone H4

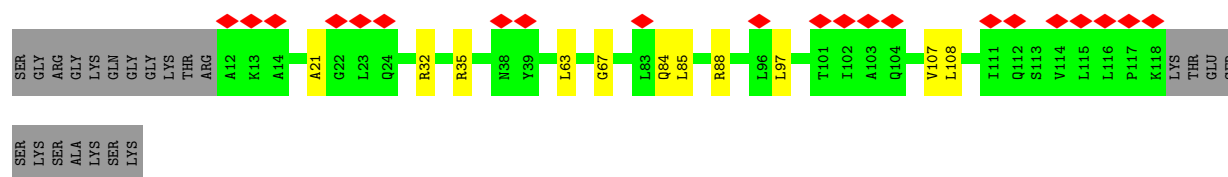
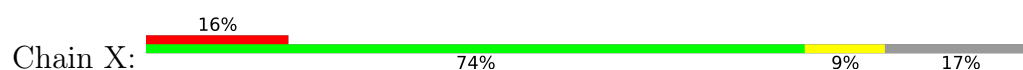




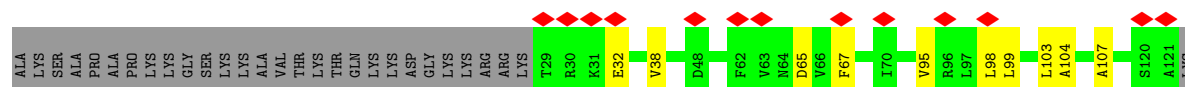
• Molecule 3: Histone H2A type 1



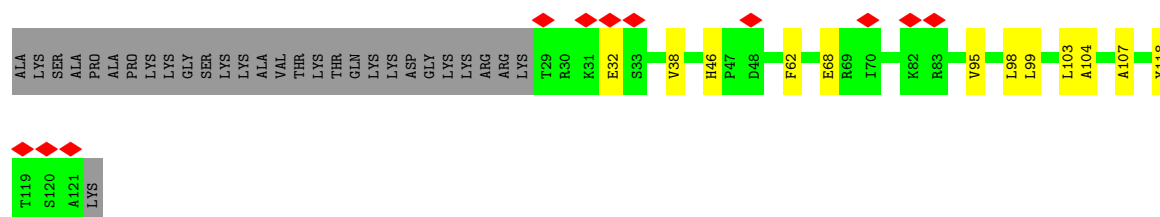
• Molecule 3: Histone H2A type 1



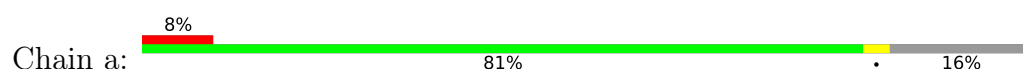
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1

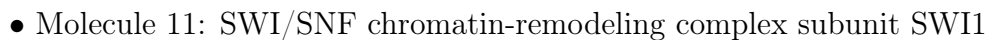


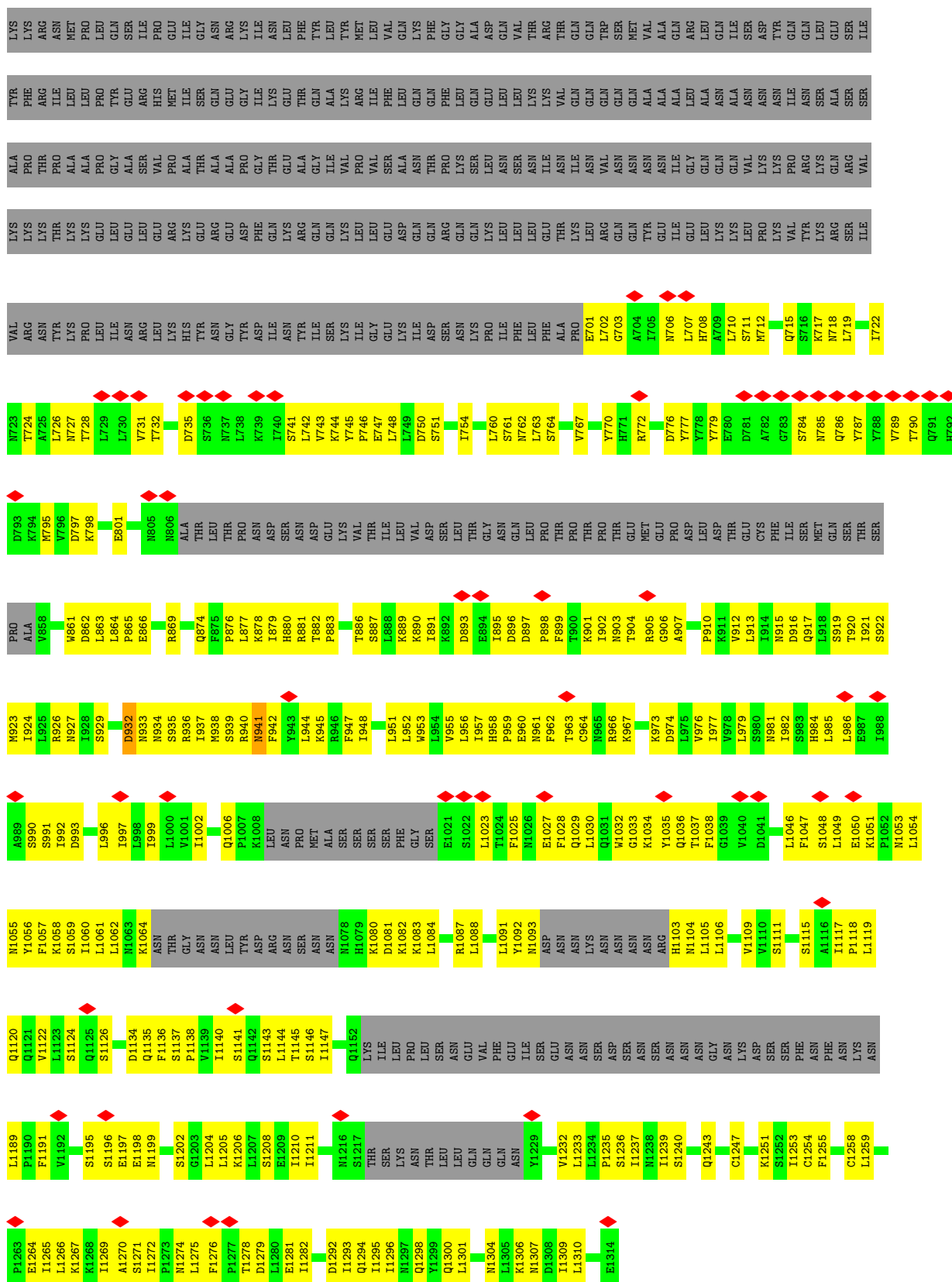
• Molecule 5: 601 sequence bottom strand





R1084	V1085	A1086	G1087	F1088	E1090	L1091	L1092	D1093	R1094	I1095	L1096	P1097	K1098	L1099	F1100	A1101	T1102	G1103	V1106	L1107	I1108	F1109	F1110	Q1111	T1113	Q1114	I1115	M1116	D1117	M1118	E1120	D1121	F1122	R1123	L1124	Y1125	I1126	N1127	I1128	K1129	L1131	R1132	L1133	G1135	H1136	T1137	K1138	S1139	D1140	E1141	R1142	S1143	E1144						
M1022	Y1023	Q1024	Q1025	M1026	L1027	K1028	Y1029	R1030	ARG	LEU	PHE	ILE	GLY	ASP	GLN	ASN	ASN	LYS	VAL	G1047	F1048	M1049	N1050	Q1054	L1055	K1056	K1057	I1058	C1059	D1060	H1061	P1062	F1063	V1064	F1065	E1066	E1067	V1068	E1069	D1070	Q1071	I1072	M1073	P1074	T1075	R1076	E1077	T1078	N1079	D1080	I1081	I1082	W1083						
F960	ALA	ASN	THR	GLY	GLN	D967	K968	I969	E970	L971	S972	E973	E974	E975	T976	L977	L978	V979	I980	R981	R982	L983	H984	K985	R988	P989	F990	R993	R994	L995	K996	K997	D998	V999	E1000	K1001	E1002	L1003	P1004	D1005	K1006	V1007	E1008	K1009	V1010	V1011	K1012	C1013	K1014	M1015	S1016	A1017	L1018	Q1019	Q1020	I1021			
E834	F835	A836	K837	W838	A839	P840	T841	L842	R843	T844	I845	S846	F847	K848	G849	S850	P851	N852	E853	R854	K855	A856	K857	Q858	A859	K860	I861	R862	A863	G864	E865	F866	D867	V868	V869	L870	T871	T872	F873	E874	Y875	I876	I877	K878	E879	R880	A881	L882	L883	S884	K885	V886	K887	W888	V889	H890	M891	I892	I893
D894	E895	G896	H897	R898	M899	K900	N901	A902	Q903	S904	K905	L906	S907	L908	N911	T912	H913	L920	I921	L922	T923	G924	T925	P926	L927	Q928	N929	N930	L931	P932	E933	L934	W935	A936	L937	L938	N939	F940	V941	L942	P943	K944	I945	F946	E947	S948	V949	K950	S951	F952	D953	E954	W955	F956	Q957	T958	P959		
T766	L767	K768	D769	Y770	Q771	I772	K773	L774	L775	Q776	W777	V779	N784	H785	L786	G787	G788	I789	A790	D792	E793	M794	G795	L796	G797	K798	Q801	T802	L805	L806	T807	E811	M812	K813	N814	I815	R816	G817	P818	L819	L820	V821	I822	L825	S826	T827	L828	S829	N830	W831	S832	S833							
LYS	GLU	MET	ILE	ASP	SER	HIS	ILE	LYS	GLU	ALA	SER	GLU	VAL	ASP	LEU	ASP	SER	MET	VAL	PRO	LYS	MET	LYS	ASP	ASP	ASN	ASN	SER	ASN	VAL	D743	Y744	Y745	N746	H749	R750	I751	K752	E753	D754	I755	K756	K757	Q758	P759	V821	I822	L761	L762	V763	G764	G765							
Q645	K646	R647	A648	E649	K650	K651	A652	K653	E654	R655	L656	Q657	A658	L659	K660	ALA	ASN	ASP	GLU	GLU	ALA	TYR	ILE	LYS	L670	L671	D672	Q673	T674	D676	T677	R678	I679	T680	H681	L682	L683	R684	Q685	T686	A687	A688	L689	ASP	SER	LEU	THR	ALA	VAL	LYS	ASP	GLN	LYS	TYR	THR				
LYS	H555	Q556	N557	S558	L559	N562	T563	H564	P565	N566	F567	L568	S569	K570	I571	R572	N573	L574	N575	D578	Q584	L585	Y586	K587	N588	H589	L592	K593	L594	R595	R596	K597	K598	T599	E600	A601	V602	L605	K606	S607	M608	S611	Q615	R619	L633	E641	R642	D643	E644										
PRO	GLN	LYS	VAL	PRO	LEU	ASN	VAL	GLN	ASP	GLN	TYR	LYS	GLU	ILE	LYS	VAL	VAL	ASP	ILE	ASP	PRO	ASP	PRO	THR	THR	GLN	PHE	MET	PRO	ASN	THR	THR	PHE	ALA	ILE	S459	H460	S461	Y465	Q466	T467	L468	L469	A470	M471	S472	D473	H474	A475	I479	E480	P481	C482	V483	L484				
ALA	ARG	ARG	GLN	THR	HIS	ASN	THR	GLN	ASP	GLN	THR	ASN	GLY	GLY	THR	VAL	GLN	THR	PRO	ILE	THR	GLN	THR	THR	GLU	GLU	GLU	THR	ASN	GLU	THR	ASP	PHE	ALA	ILE	ALA	ALA	PRO	PRO	ASN	LEU	ASP	ASP	LYS	GLU	GLU	ALA	VAL	SER	LEU	GLN	GLY	PHE						





- Molecule 12: SWI/SNF chromatin-remodeling complex subunit SNF5

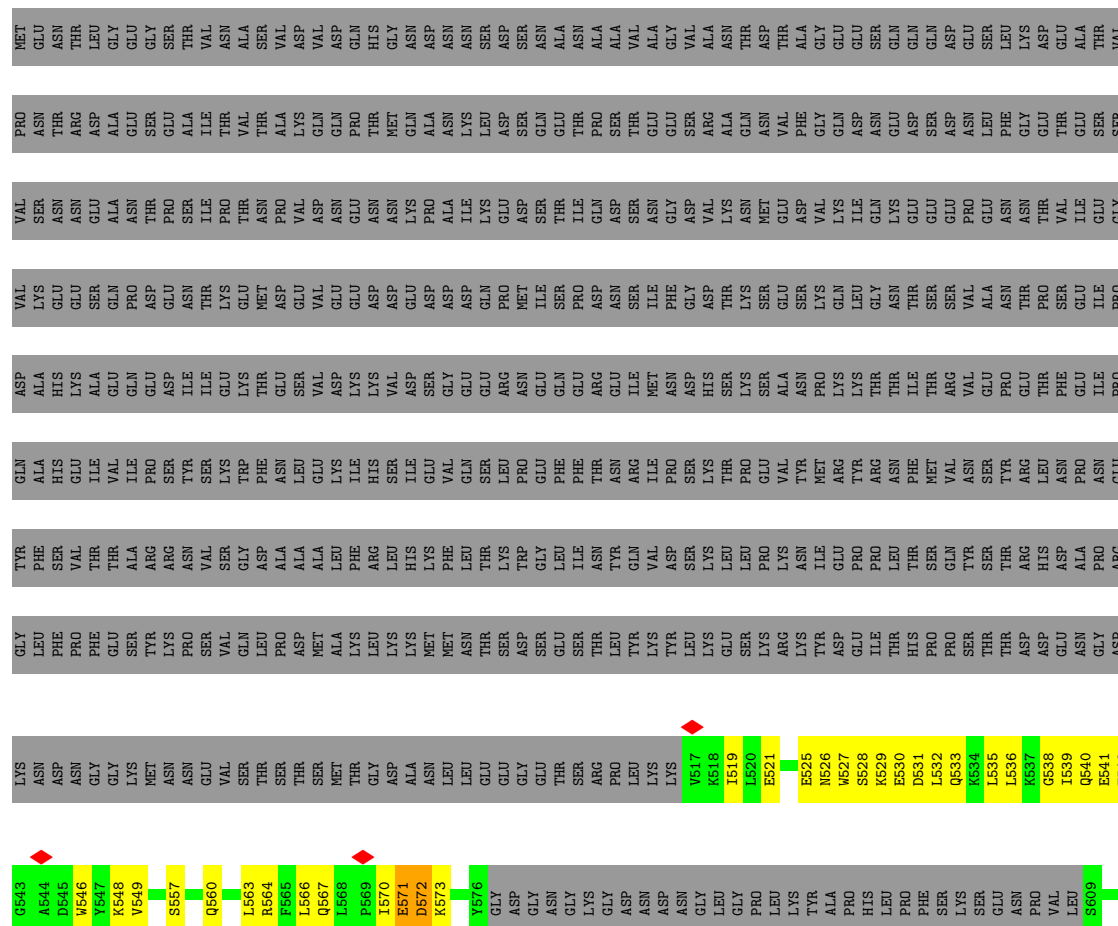


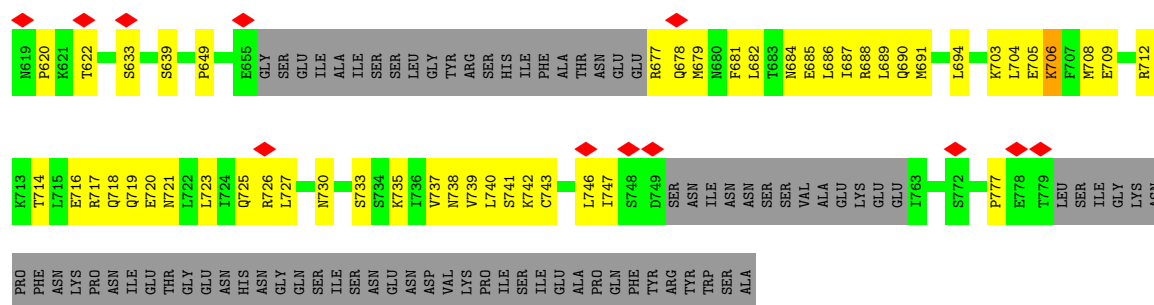
[illegible]



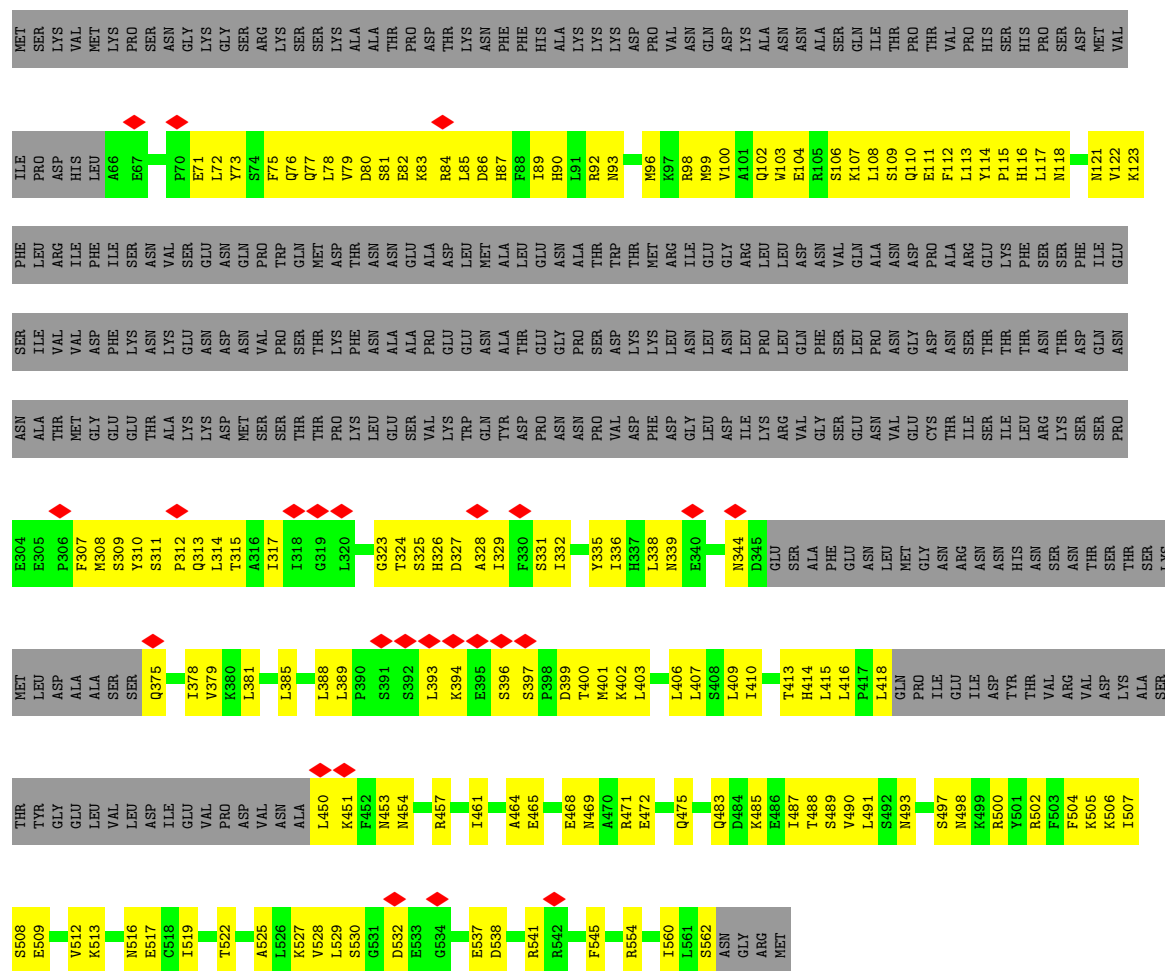


- Molecule 13: SWI/SNF complex subunit SWI3

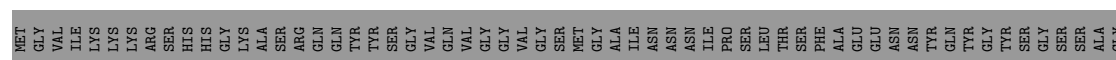
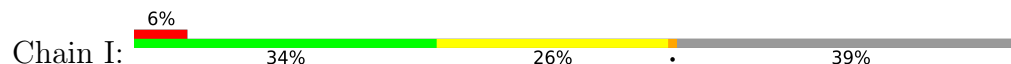


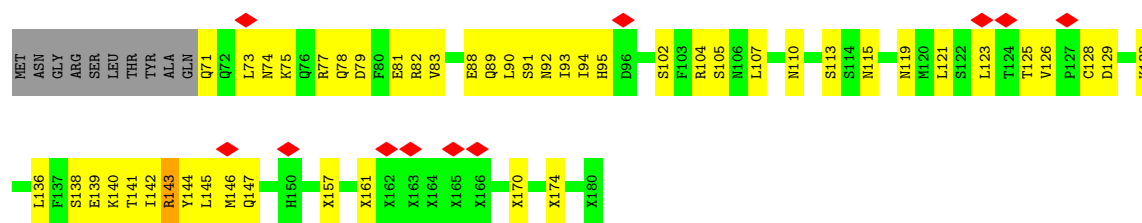


• Molecule 14: Transcription regulatory protein SNF12

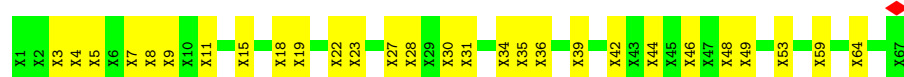


• Molecule 15: Transcription regulatory protein SNF6





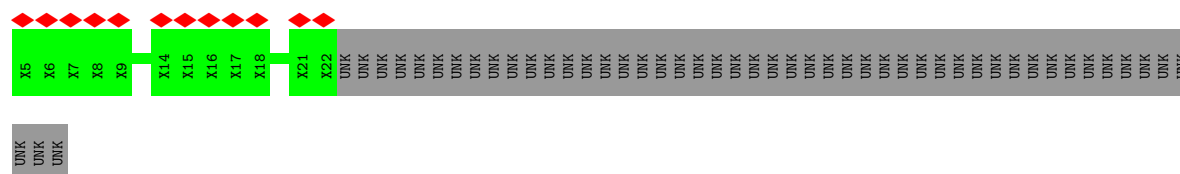
- Molecule 16: Unknown protein



- Molecule 16: Unknown protein



- Molecule 16: Unknown protein



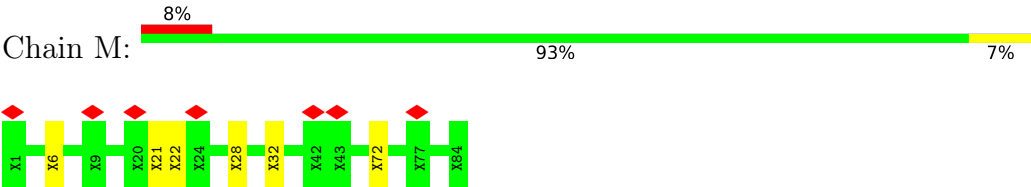
- Molecule 16: Unknown protein



- Molecule 16: Unknown protein



- Molecule 17: SWI/SNF global transcription activator complex subunit SWP82



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.24, 2.24, 2.24	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, BEF, ADP

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	R	0.24	0/813	0.38	0/1093
1	V	0.24	0/789	0.38	0/1059
2	S	0.24	0/660	0.42	0/885
2	W	0.25	0/634	0.41	0/848
3	T	0.24	0/821	0.40	0/1112
3	X	0.24	0/825	0.40	0/1116
4	U	0.24	0/729	0.37	0/985
4	Y	0.24	0/737	0.37	0/993
5	a	0.58	6/3541 (0.2%)	0.94	0/5458
6	b	0.55	4/3587 (0.1%)	0.92	0/5539
7	P	0.43	0/3303	0.61	1/4465 (0.0%)
8	Q	0.45	0/3269	0.59	0/4432
9	Z	0.41	0/501	0.57	0/669
10	A	0.28	0/6488	0.50	1/8732 (0.0%)
11	B	0.38	0/3958	0.52	0/5364
12	C	0.35	0/2040	0.54	0/2756
13	D	0.34	0/1359	0.47	0/1838
13	E	0.40	0/1189	0.51	0/1616
13	F	0.32	0/1596	0.52	5/2154 (0.2%)
13	G	0.33	0/1446	0.51	3/1949 (0.2%)
14	H	0.35	0/2119	0.47	0/2856
15	I	0.32	0/682	0.48	0/913
All	All	0.39	10/41086 (0.0%)	0.61	10/56832 (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
11	B	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	153	DG	C1'-N9	-5.53	1.39	1.47
6	b	5	DT	C1'-N1	5.24	1.56	1.49
5	a	149	DC	C1'-N1	5.22	1.56	1.49
5	a	155	DT	C1'-N1	5.19	1.55	1.49
6	b	6	DC	C1'-N1	5.17	1.55	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	606	PRO	N-CA-CB	6.96	111.65	103.30
13	G	620	PRO	N-CA-CB	6.12	110.64	103.30
13	F	649	PRO	N-CA-CB	6.05	110.56	103.30
7	P	380	SER	C-N-CD	5.93	140.86	128.40
13	F	599	PRO	N-CA-CB	5.90	110.38	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	B	776	ASP	Peptide
11	B	932	ASP	Peptide

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	R	801	0	831	15	0
1	V	779	0	815	16	0
2	S	653	0	695	13	0
2	W	627	0	663	14	0
3	T	811	0	849	6	0
3	X	815	0	860	9	0
4	U	718	0	725	8	0
4	Y	726	0	747	10	0
5	a	3160	0	1741	0	0
6	b	3195	0	1742	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	3227	0	3251	170	0
8	Q	3198	0	3187	67	0
9	Z	490	0	467	19	0
10	A	6385	0	6494	327	0
11	B	3890	0	4008	253	0
12	C	2005	0	1939	165	0
13	D	1322	0	1325	95	0
13	E	1152	0	1137	86	0
13	F	1583	0	1397	74	0
13	G	1435	0	1294	59	0
14	H	2085	0	2104	139	0
15	I	818	0	708	67	0
16	J	336	0	70	20	0
16	K	140	0	33	3	0
16	L	90	0	21	0	0
16	N	150	0	41	3	0
16	O	90	0	21	2	0
17	M	416	0	92	4	0
18	A	5	0	0	0	0
18	P	25	0	0	0	0
18	Q	30	0	0	1	0
19	A	27	0	12	6	0
20	A	4	0	0	4	0
21	A	1	0	0	0	0
22	P	33	0	0	4	0
22	Q	51	0	0	4	0
22	Z	2	0	0	0	0
All	All	41275	0	37269	1458	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 1458 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)
7:P:238:VAL:HG21	7:P:404:MET:SD	1.34	1.68
7:P:36:ILE:HD12	7:P:54:MET:CE	1.34	1.52
13:D:412:TYR:CD1	14:H:560:ILE:HG23	1.62	1.35
7:P:36:ILE:CD1	7:P:54:MET:HE3	1.58	1.33
13:D:412:TYR:CD1	14:H:560:ILE:CG2	2.12	1.33

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	R	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	V	93/135 (69%)	89 (96%)	4 (4%)	0	100	100
2	S	80/102 (78%)	76 (95%)	4 (5%)	0	100	100
2	W	77/102 (76%)	73 (95%)	4 (5%)	0	100	100
3	T	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	X	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	U	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
4	Y	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
7	P	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	12	48
8	Q	391/467 (84%)	367 (94%)	22 (6%)	2 (0%)	29	69
9	Z	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	6	35
10	A	763/1703 (45%)	667 (87%)	96 (13%)	0	100	100
11	B	468/1314 (36%)	364 (78%)	104 (22%)	0	100	100
12	C	241/905 (27%)	176 (73%)	63 (26%)	2 (1%)	19	60
13	D	157/825 (19%)	130 (83%)	27 (17%)	0	100	100
13	E	137/825 (17%)	113 (82%)	24 (18%)	0	100	100
13	F	215/825 (26%)	186 (86%)	27 (13%)	2 (1%)	17	57
13	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	29	69
14	H	249/566 (44%)	217 (87%)	32 (13%)	0	100	100
15	I	78/179 (44%)	66 (85%)	12 (15%)	0	100	100
All	All	4064/10044 (40%)	3573 (88%)	478 (12%)	13 (0%)	44	77

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Q	48	ASP
13	F	606	PRO
7	P	343	SER
12	C	614	ASN
7	P	382	GLU

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	R	84/110 (76%)	84 (100%)	0	100	100
1	V	82/110 (74%)	82 (100%)	0	100	100
2	S	67/78 (86%)	67 (100%)	0	100	100
2	W	64/78 (82%)	64 (100%)	0	100	100
3	T	81/101 (80%)	81 (100%)	0	100	100
3	X	82/101 (81%)	82 (100%)	0	100	100
4	U	77/102 (76%)	77 (100%)	0	100	100
4	Y	79/102 (78%)	79 (100%)	0	100	100
7	P	357/420 (85%)	338 (95%)	19 (5%)	22	47
8	Q	363/423 (86%)	343 (94%)	20 (6%)	21	47
9	Z	53/140 (38%)	52 (98%)	1 (2%)	57	75
10	A	705/1520 (46%)	698 (99%)	7 (1%)	76	86
11	B	460/1218 (38%)	458 (100%)	2 (0%)	91	94
12	C	222/823 (27%)	219 (99%)	3 (1%)	67	80
13	D	150/751 (20%)	150 (100%)	0	100	100
13	E	129/751 (17%)	128 (99%)	1 (1%)	81	89
13	F	138/751 (18%)	138 (100%)	0	100	100
13	G	127/751 (17%)	125 (98%)	2 (2%)	62	79
14	H	239/517 (46%)	238 (100%)	1 (0%)	91	94
15	I	79/133 (59%)	78 (99%)	1 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3638/8980 (40%)	3581 (98%)	57 (2%)	64 79

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Q	94	ARG
14	H	562	SER
8	Q	321	ASP
13	G	706	LYS
12	C	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
13	G	526	ASN
14	H	493	ASN
13	G	555	ASN
14	H	76	GLN
11	B	874	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](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	PO4	Q	504	-	4,4,4	0.88	0	6,6,6	0.41	0
18	PO4	Q	505	-	4,4,4	0.87	0	6,6,6	0.42	0
18	PO4	P	504	-	4,4,4	0.85	0	6,6,6	0.60	0
18	PO4	Q	501	-	4,4,4	0.98	0	6,6,6	0.61	0
20	BEF	A	1803	-	0,3,3	-	-	-	-	-
18	PO4	P	503	-	4,4,4	0.96	0	6,6,6	0.48	0
18	PO4	Q	502	-	4,4,4	0.83	0	6,6,6	0.46	0
18	PO4	Q	503	-	4,4,4	0.84	0	6,6,6	0.56	0
19	ADP	A	1802	21	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
18	PO4	P	502	-	4,4,4	0.80	0	6,6,6	0.54	0
18	PO4	P	501	-	4,4,4	0.90	0	6,6,6	0.65	0
18	PO4	A	1801	-	4,4,4	0.79	0	6,6,6	0.80	0
18	PO4	P	505	-	4,4,4	0.88	0	6,6,6	0.43	0
18	PO4	Q	506	-	4,4,4	0.82	0	6,6,6	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	A	1802	21	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1802	ADP	C5-C4	2.46	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1802	ADP	C3'-C2'-C1'	3.33	105.99	100.98
19	A	1802	ADP	PA-O3A-PB	-3.33	121.41	132.83
19	A	1802	ADP	N3-C2-N1	-3.14	123.77	128.68
19	A	1802	ADP	C4-C5-N7	-2.60	106.69	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

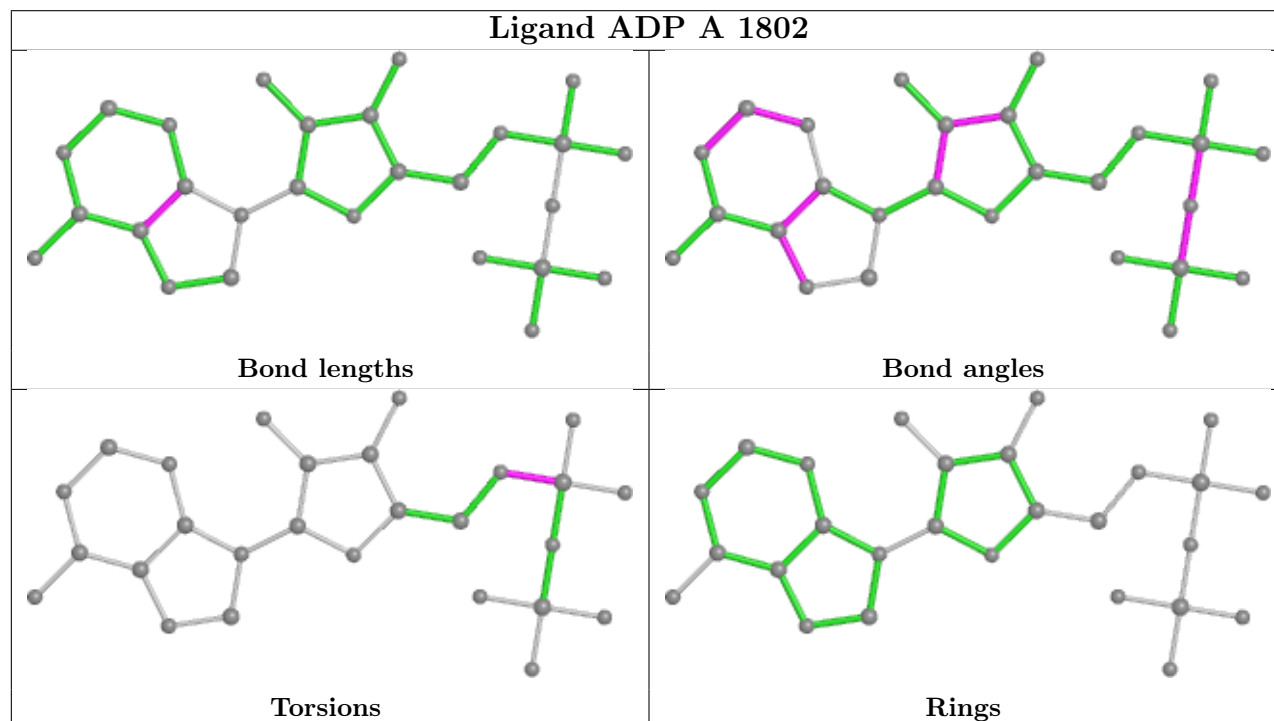
Mol	Chain	Res	Type	Atoms
19	A	1802	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Q	504	PO4	1	0
20	A	1803	BEF	4	0
19	A	1802	ADP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
15	I	1
17	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	150:HIS	C	152:UNK	N	20.17
1	M	22:UNK	C	24:UNK	N	7.86

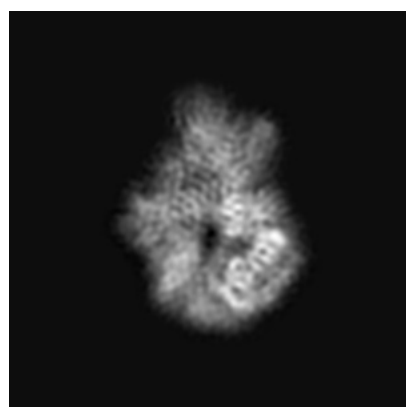
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20934. These allow visual inspection of the internal detail of the map and identification of artifacts.

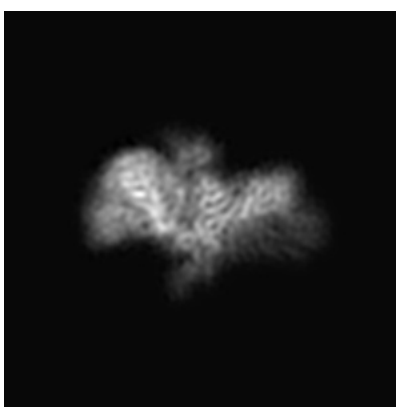
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

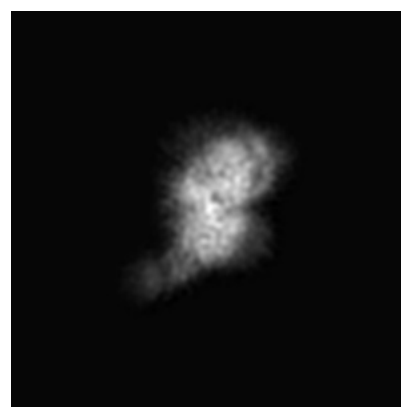
6.1.1 Primary map



X



Y

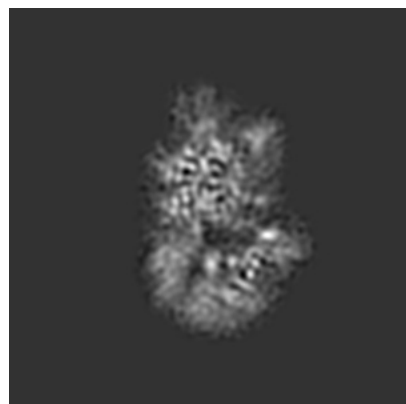


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96



Y Index: 96

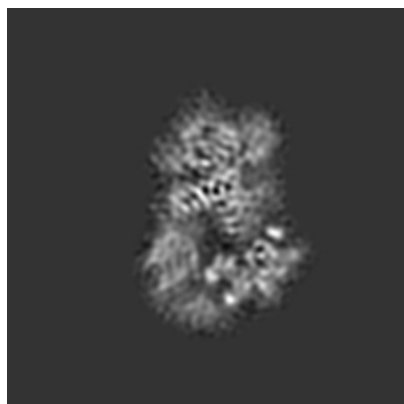


Z Index: 96

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: 102



Y Index: 107

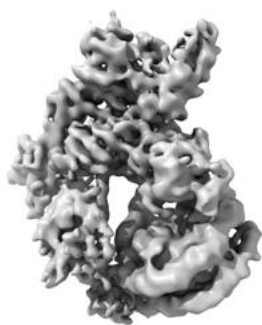


Z Index: 97

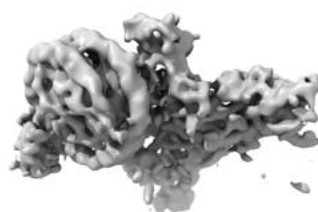
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

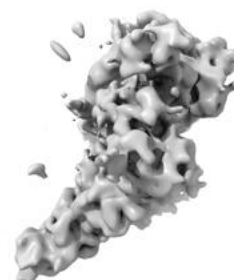
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

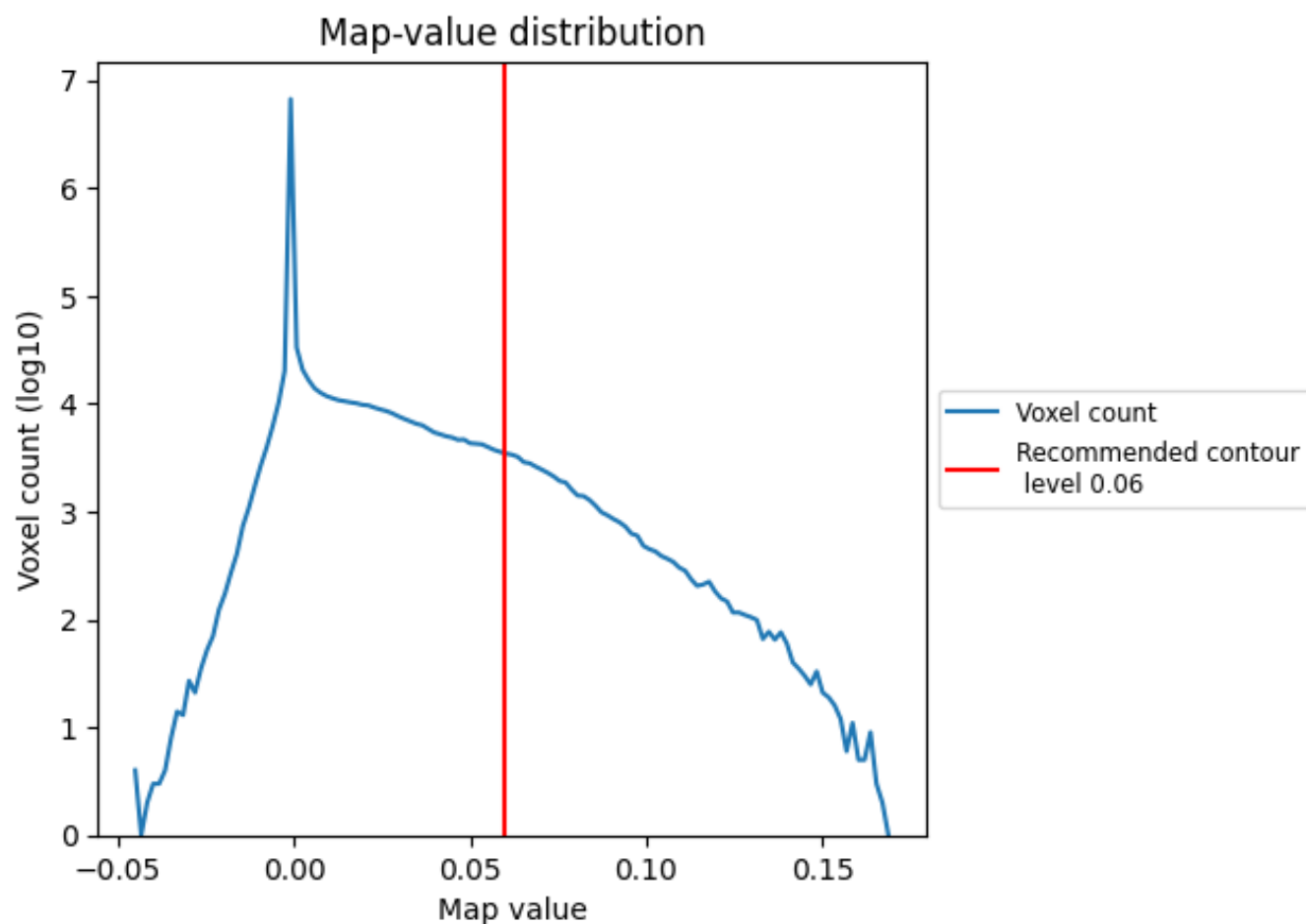
6.5 Mask visualisation

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

7 Map analysis [i](#)

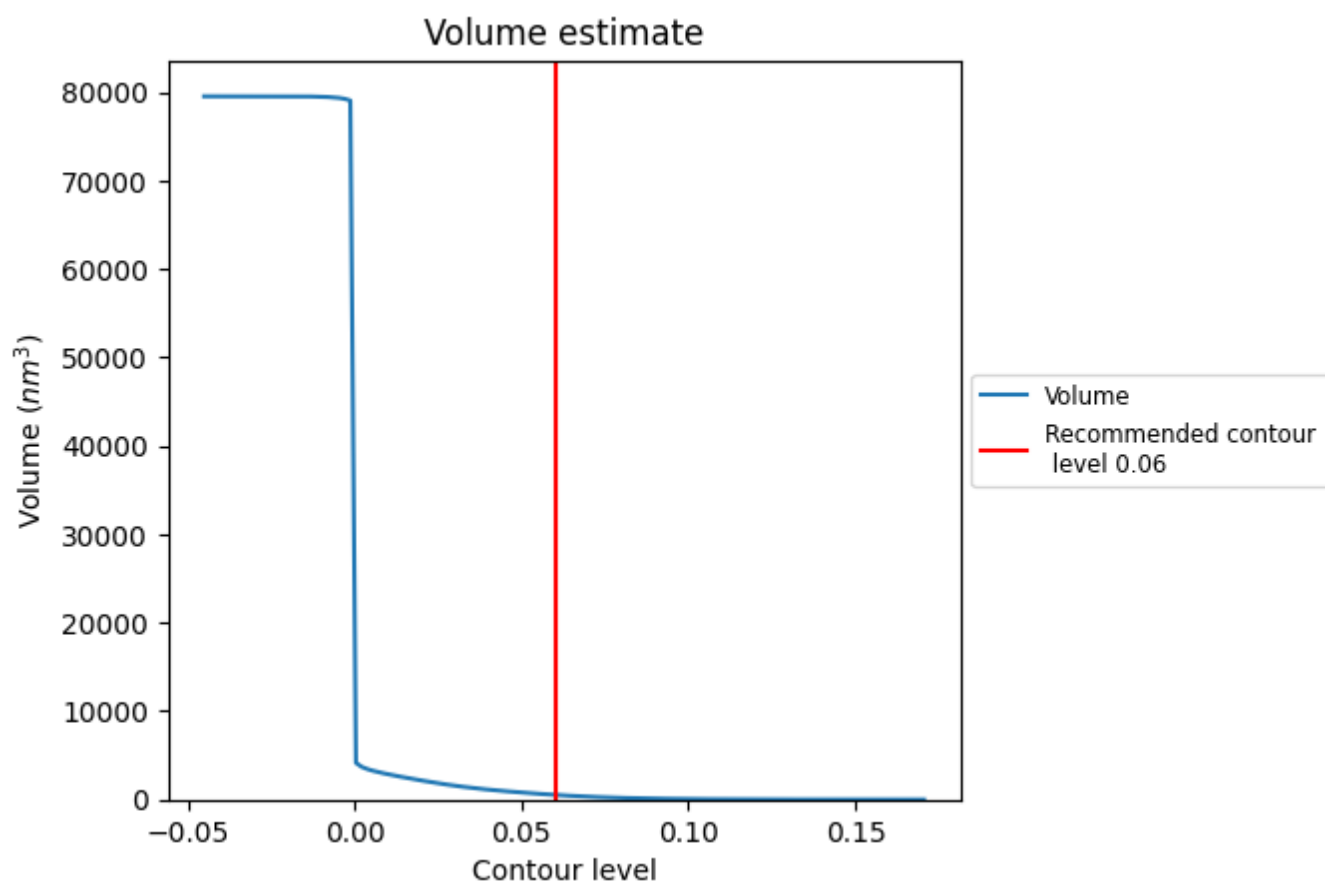
This section contains the results of statistical analysis of the map.

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.

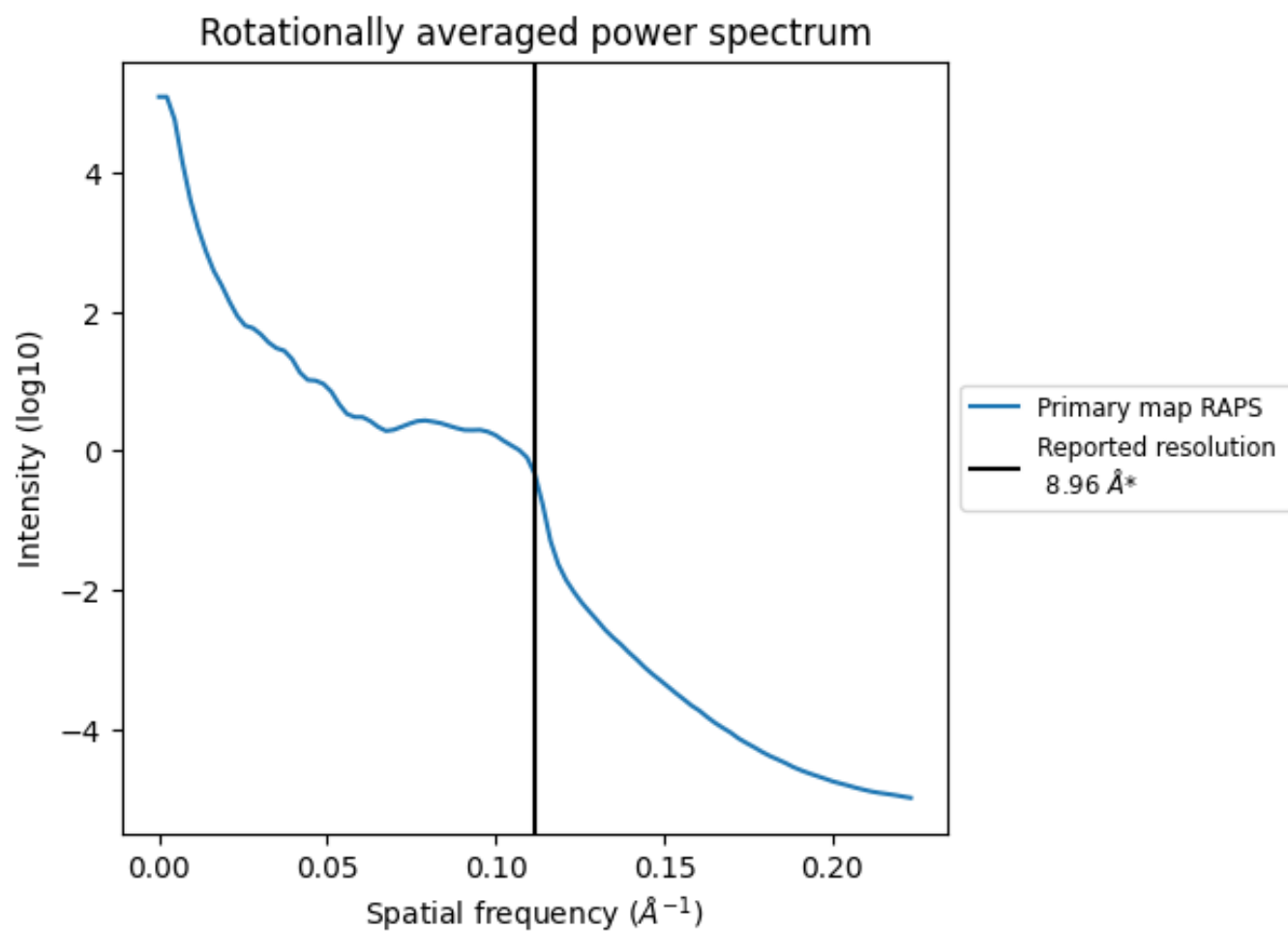
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 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 ⓘ

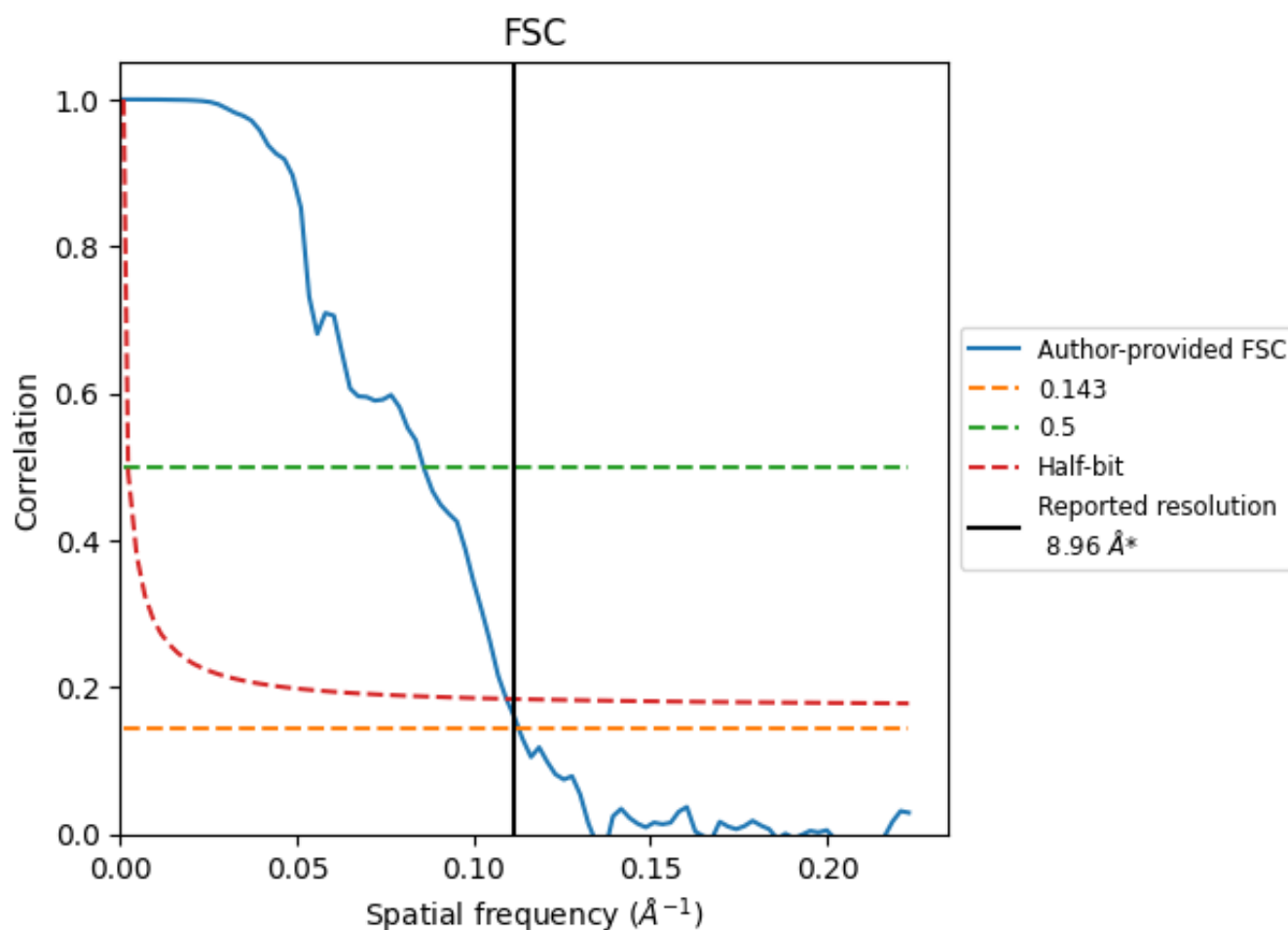


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

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 0.112 Å⁻¹

8.2 Resolution estimates [i](#)

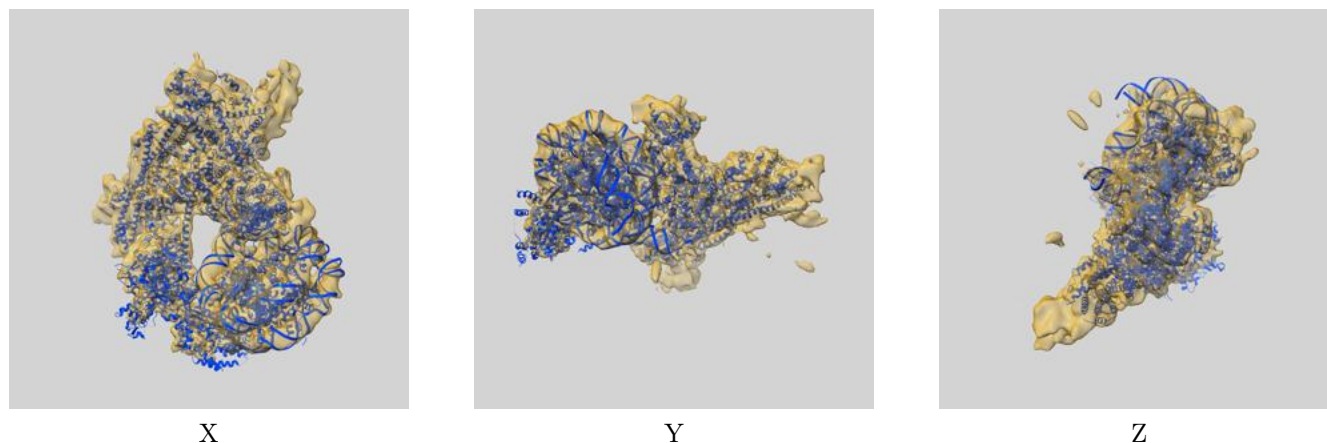
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.96	-	-
Author-provided FSC curve	8.86	11.64	9.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

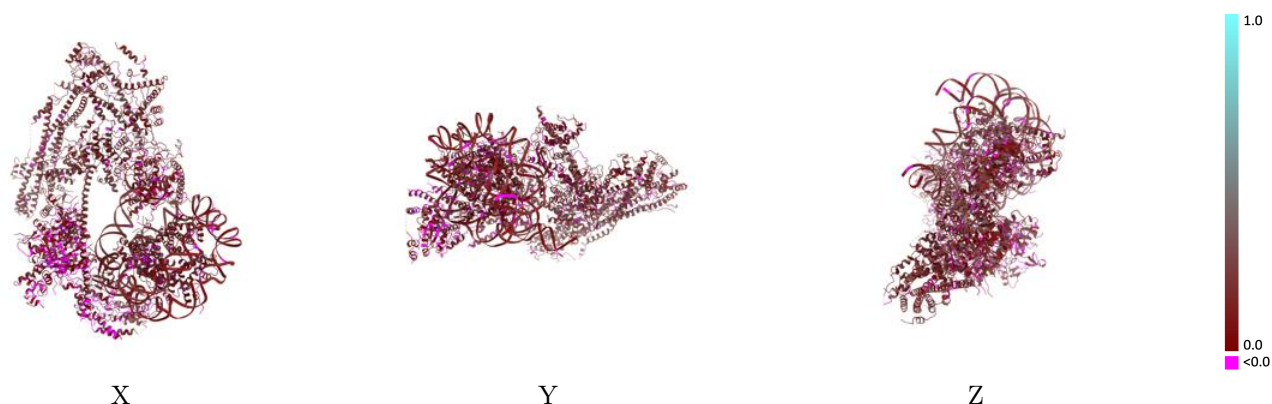
This section contains information regarding the fit between EMDB map EMD-20934 and PDB model 6UXW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



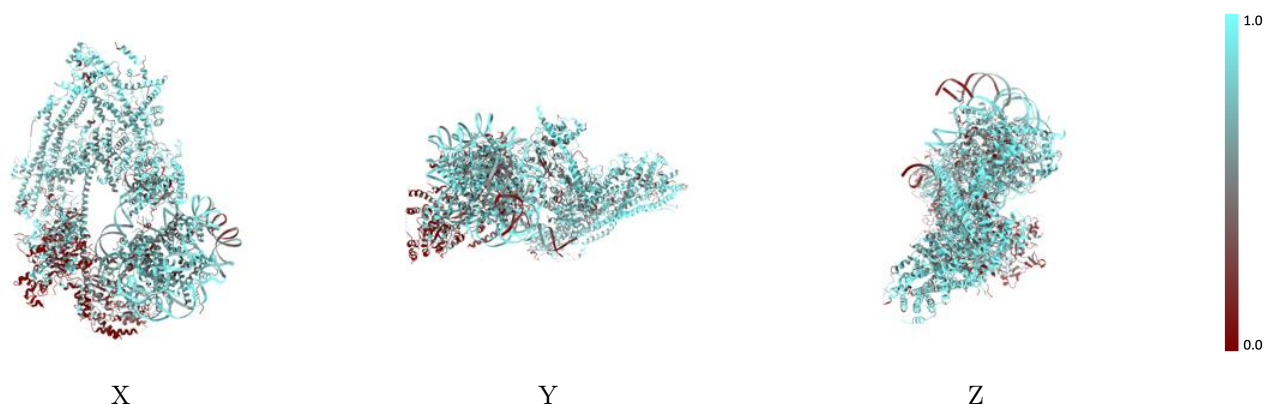
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



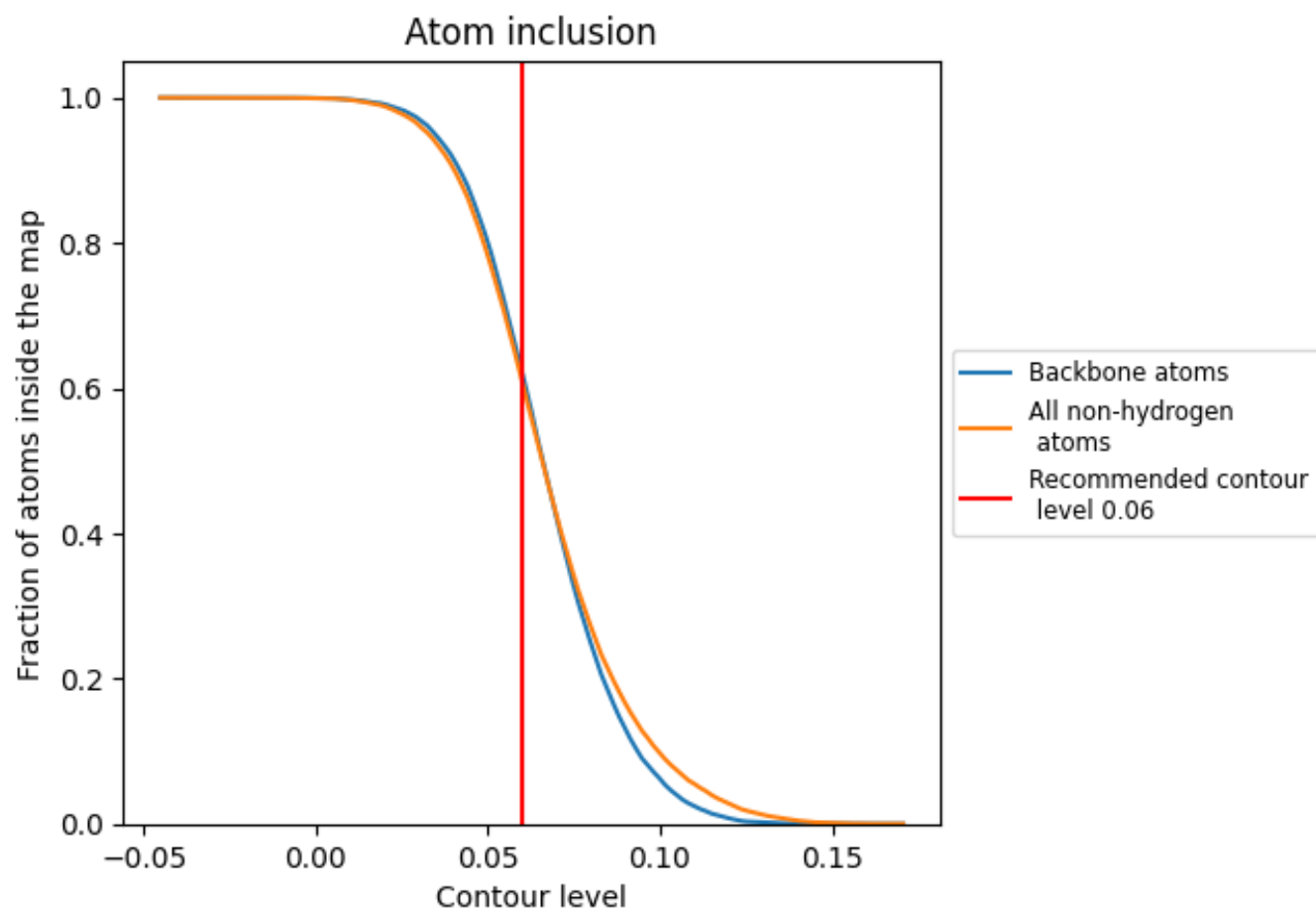
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6088	 0.1220
A	 0.3700	 0.0820
B	 0.6984	 0.1540
C	 0.6371	 0.1420
D	 0.7217	 0.1270
E	 0.7082	 0.1410
F	 0.7597	 0.1580
G	 0.7541	 0.1690
H	 0.7298	 0.1660
I	 0.7703	 0.1710
J	 0.9673	 0.2740
K	 0.8857	 0.2370
L	 0.3000	 0.1970
M	 0.8894	 0.2170
N	 0.4267	 0.0640
O	 0.7444	 0.1650
P	 0.5244	 0.0750
Q	 0.3548	 0.0520
R	 0.5816	 0.1120
S	 0.6013	 0.1060
T	 0.5802	 0.1100
U	 0.6933	 0.1590
V	 0.6587	 0.1260
W	 0.6766	 0.1050
X	 0.6734	 0.1180
Y	 0.6996	 0.1370
Z	 0.4376	 0.0930
a	 0.7288	 0.1300
b	 0.7543	 0.1380

