



wwPDB EM Validation Summary Report ⓘ

May 13, 2025 – 02:21 AM EDT

PDB ID : 6UXW / pdb_00006uxw
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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.43.1

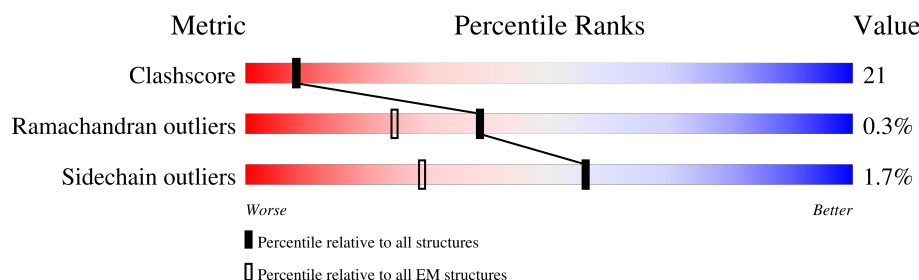
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>14%</div> <div>27%</div> </div>
1	V	135	<div> <div>8%</div> <div>56%</div> <div>15%</div> <div>30%</div> </div>
2	S	102	<div> <div>19%</div> <div>60%</div> <div>21%</div> <div>20%</div> </div>
2	W	102	<div> <div>11%</div> <div>60%</div> <div>18%</div> <div>23%</div> </div>
3	T	129	<div> <div>24%</div> <div>76%</div> <div>7%</div> <div>17%</div> </div>
3	X	129	<div> <div>16%</div> <div>73%</div> <div>10%</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		

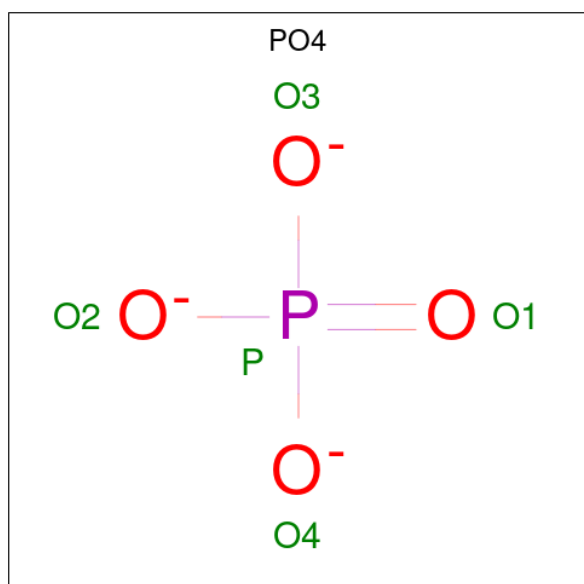
- Molecule 16 is a protein called Unknown protein.

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.

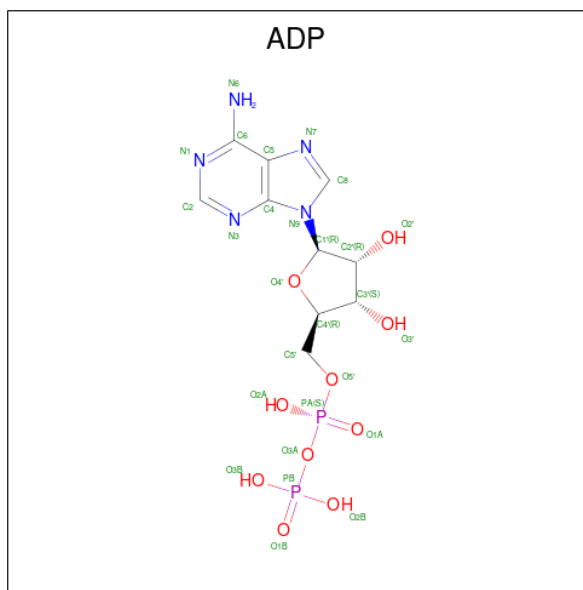
Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	83	Total	C	N	O	0	0
			416	249	83	84		

- Molecule 18 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



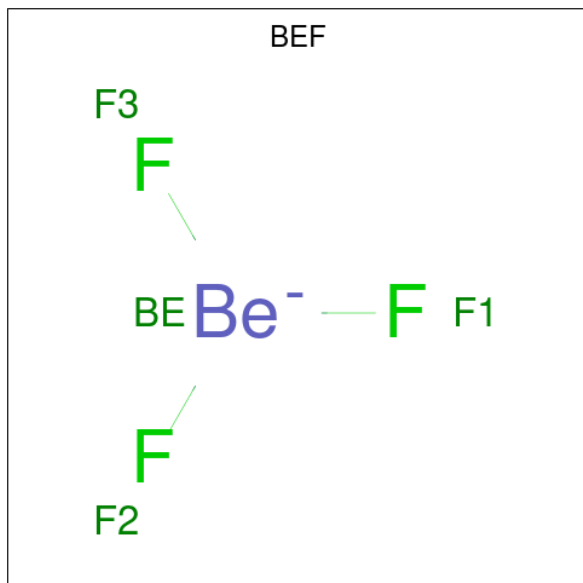
Mol	Chain	Residues	Atoms			AltConf
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	A	1	Total	O	P	0
			5	4	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

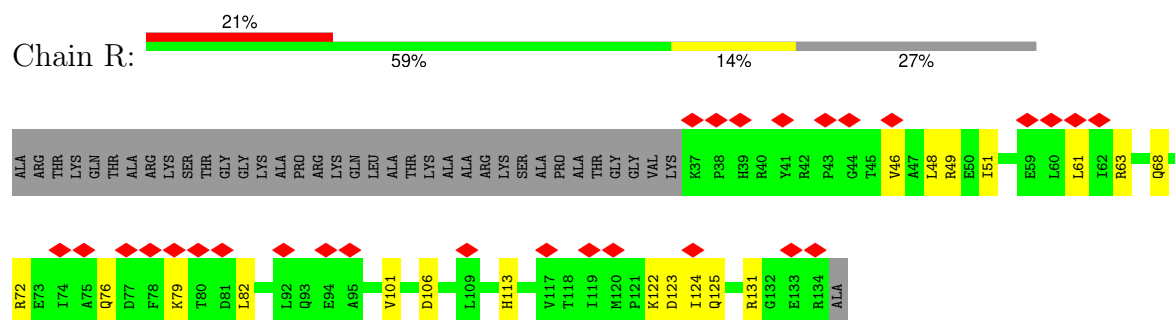
- Molecule 22 is water.

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	

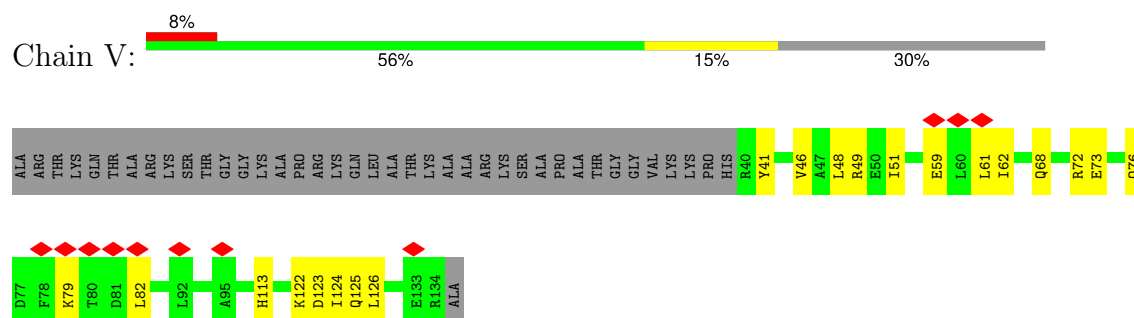
3 Residue-property plots

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.

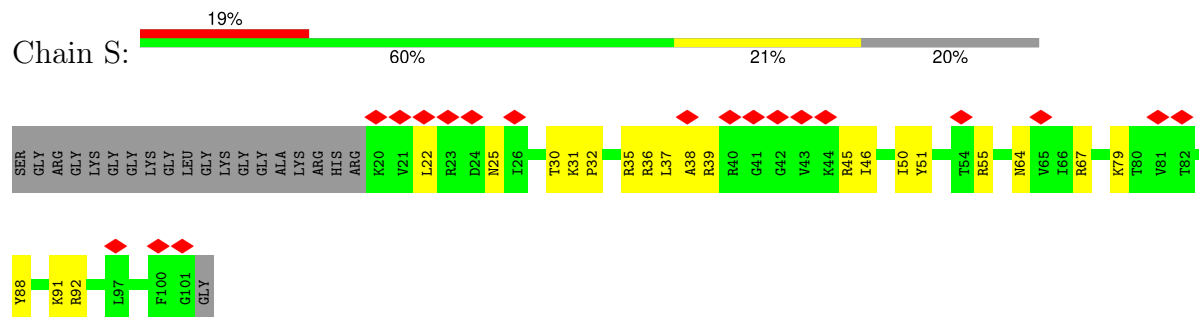
• Molecule 1: Histone H3.2



• Molecule 1: Histone H3.2

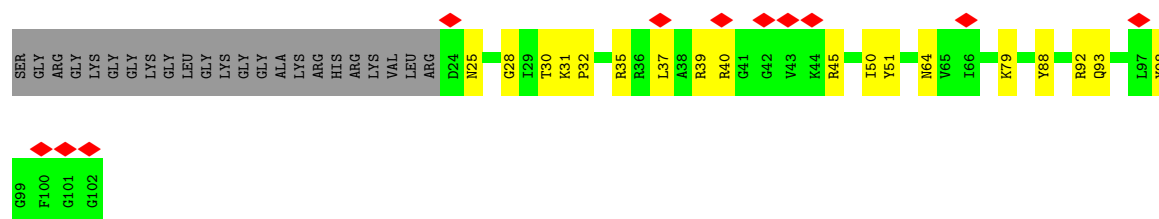


• Molecule 2: Histone H4

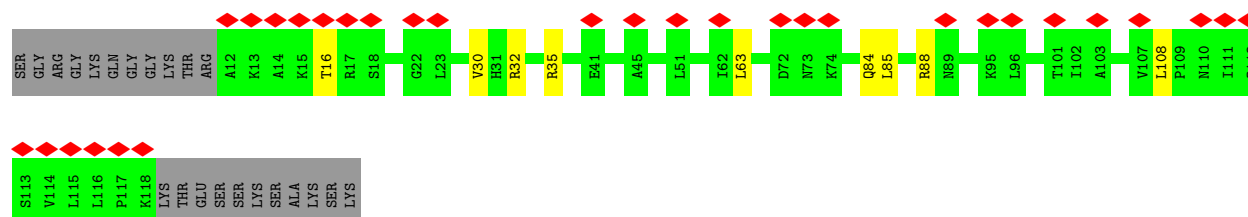
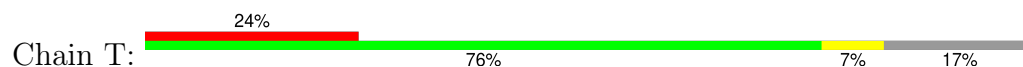


• Molecule 2: Histone H4

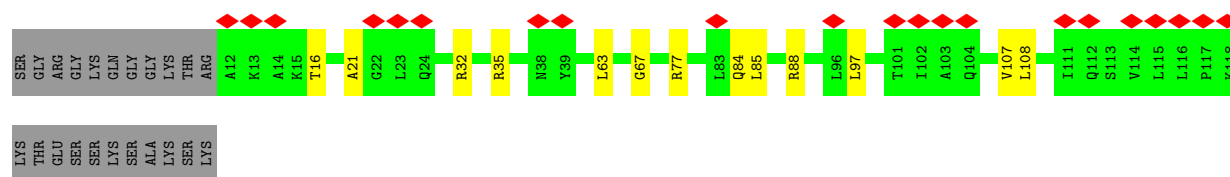
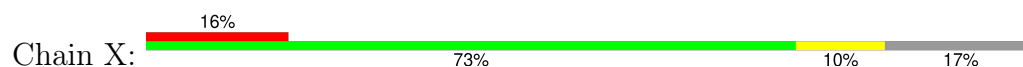




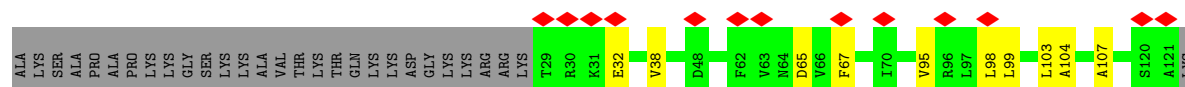
- Molecule 3: Histone H2A type 1



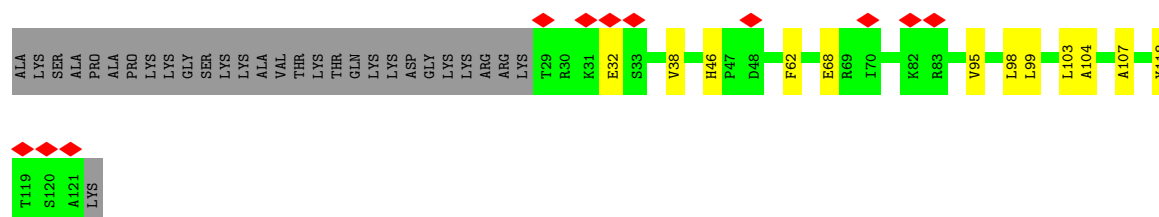
- Molecule 3: Histone H2A type 1



- Molecule 4: Histone H2B 1.1

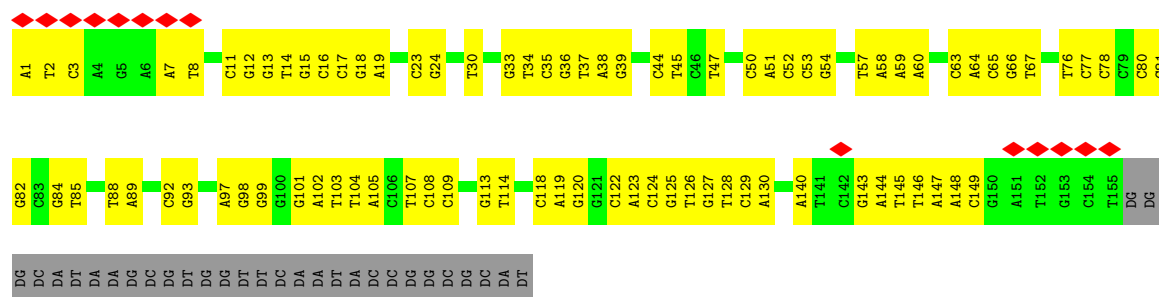


- Molecule 4: Histone H2B 1.1



- Molecule 5: 601 sequence bottom strand

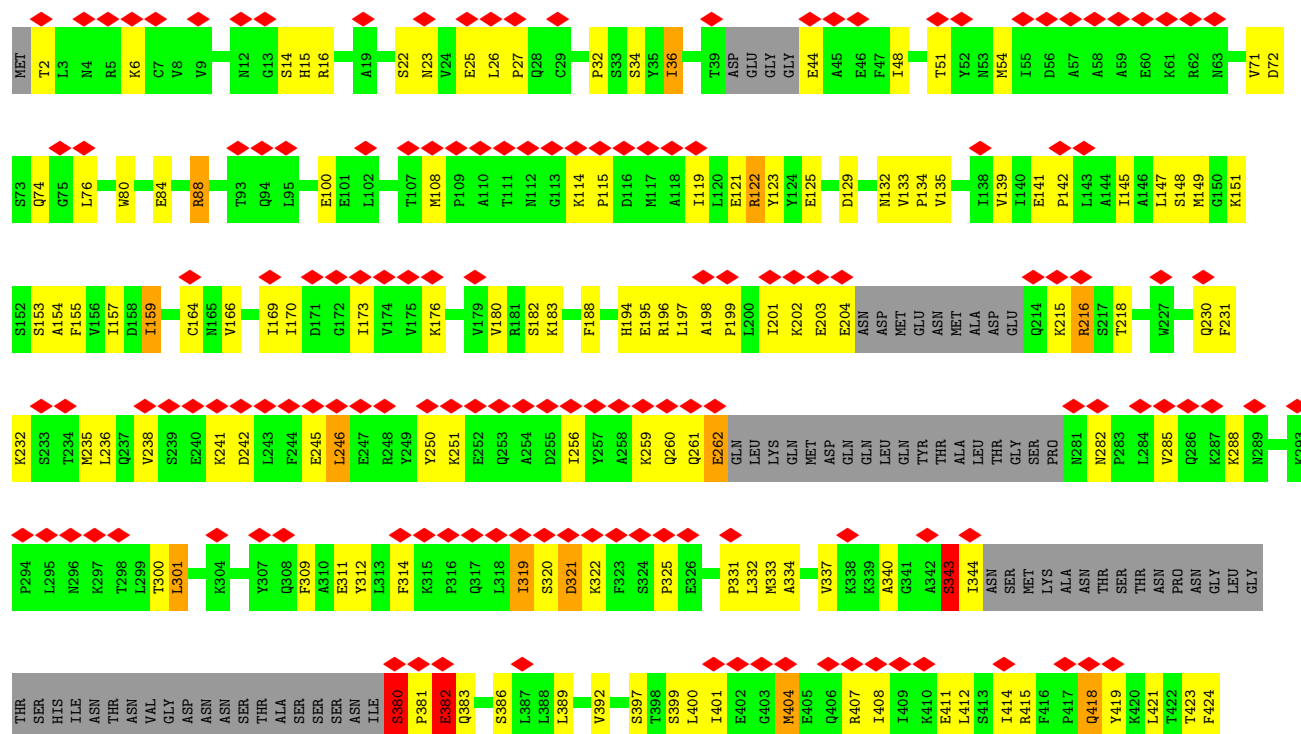


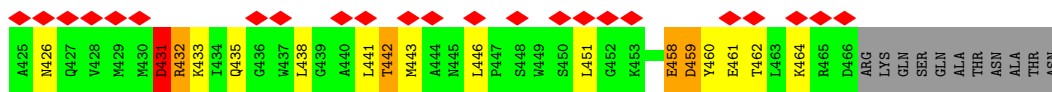


• Molecule 6: 601 sequence top strand

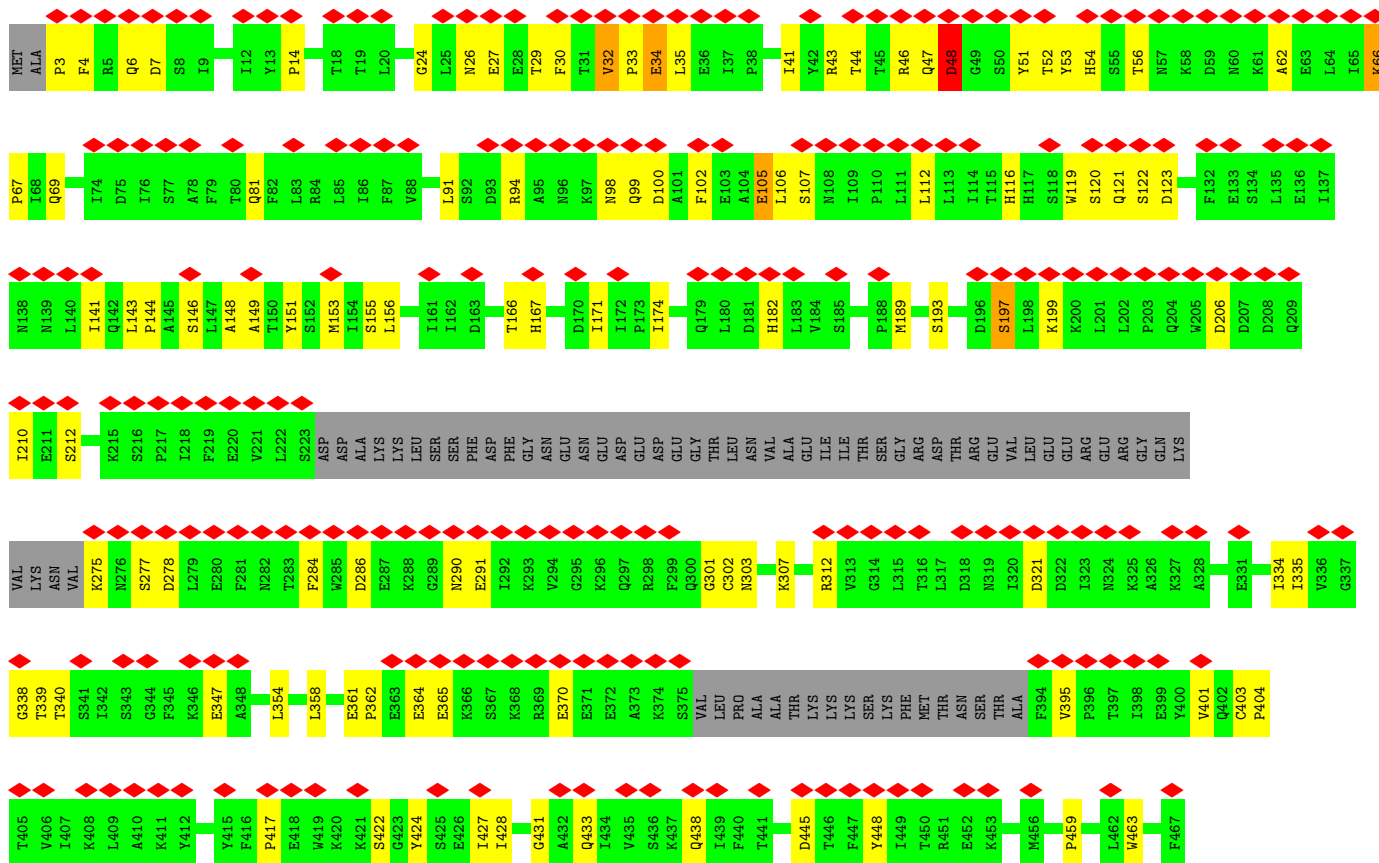


• Molecule 7: Actin-related protein 7

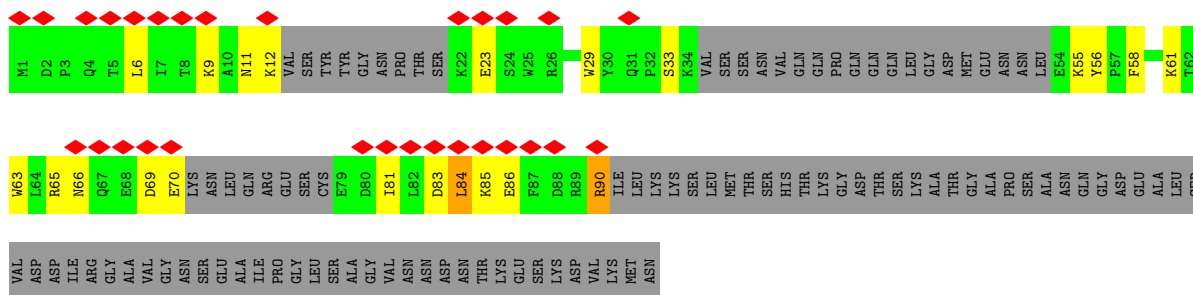




• Molecule 8: Actin-like protein ARP9



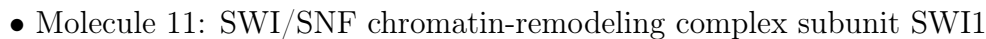
• Molecule 9: Regulator of Ty1 transposition protein 102



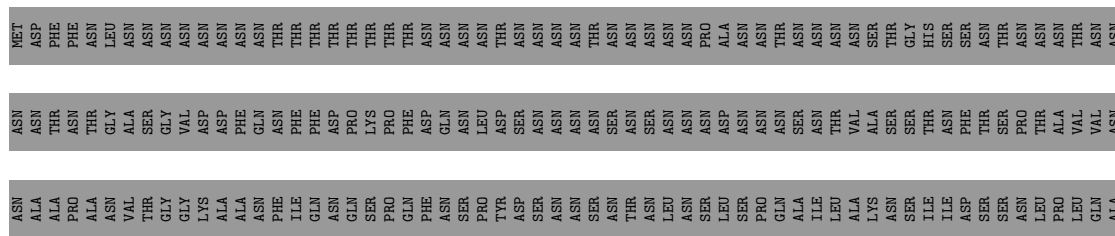
• Molecule 10: Transcription regulatory protein SNF2



[illegible]



Frequency	Percentage
Often	15%
Sometimes	21%
Rarely/Not at all	63%



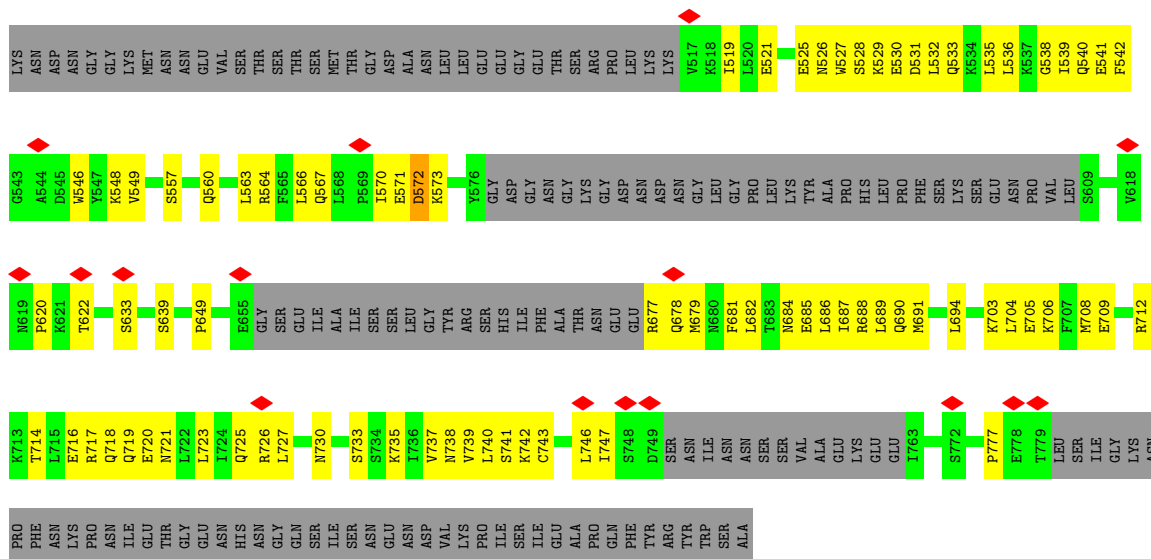


Chain D: 8% 11% 81%



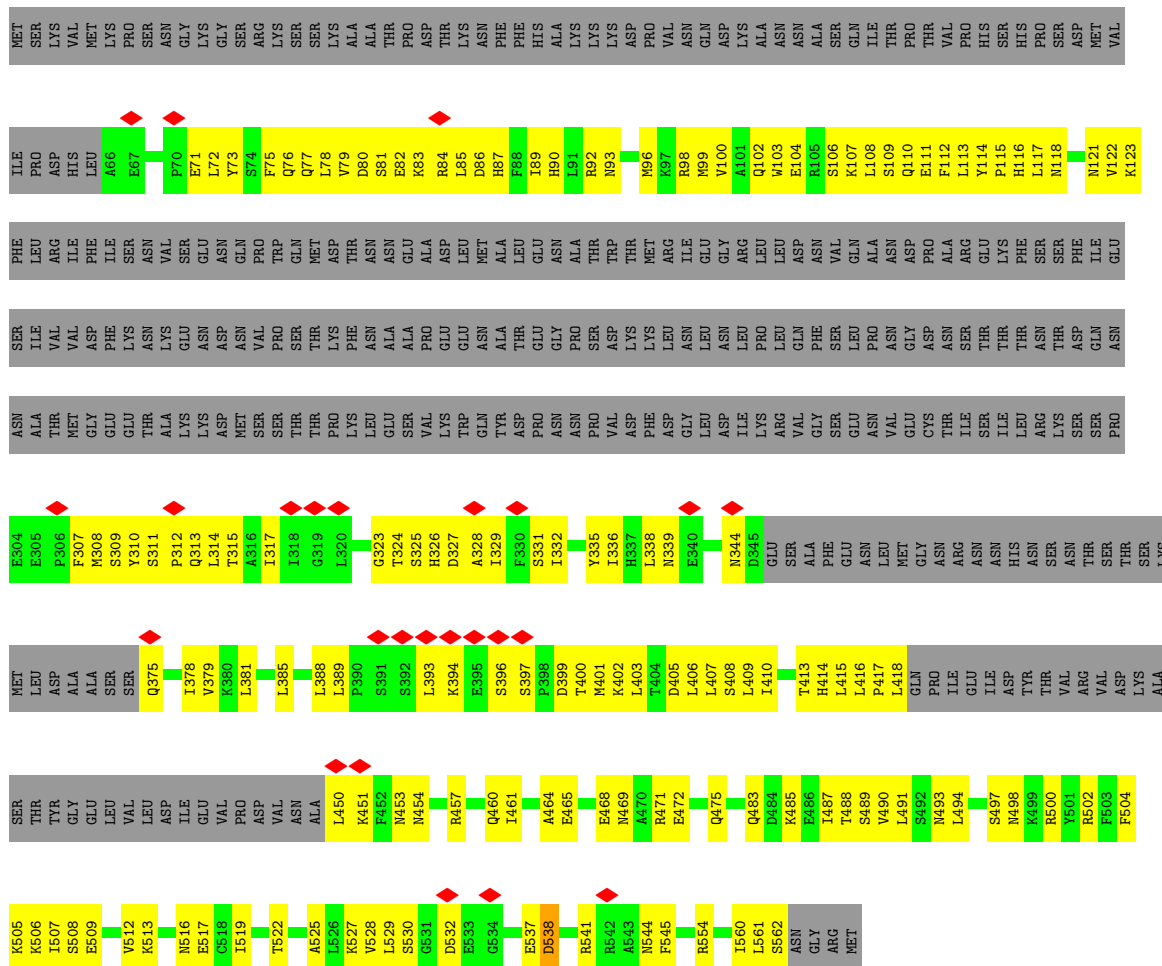






• Molecule 14: Transcription regulatory protein SNF12

Chain H: 19% 26% 55%

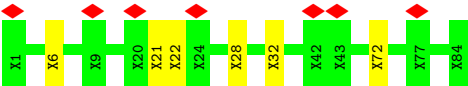
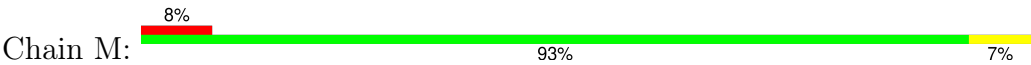


• Molecule 15: Transcription regulatory protein SNF6





- 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: PO4, ADP, MG, BEF

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	0.11	0/813	0.31	0/1093
1	V	0.11	0/789	0.31	0/1059
2	S	0.12	0/660	0.34	0/885
2	W	0.12	0/634	0.34	0/848
3	T	0.12	0/821	0.29	0/1112
3	X	0.12	0/825	0.29	0/1116
4	U	0.10	0/729	0.27	0/985
4	Y	0.10	0/737	0.27	0/993
5	a	0.23	0/3541	0.44	0/5458
6	b	0.21	0/3587	0.43	0/5539
7	P	0.56	1/3303 (0.0%)	0.90	6/4465 (0.1%)
8	Q	0.58	0/3269	0.88	2/4432 (0.0%)
9	Z	0.45	0/501	0.83	0/669
10	A	0.24	0/6488	0.49	1/8732 (0.0%)
11	B	0.35	0/3958	0.53	0/5364
12	C	0.31	0/2040	0.64	2/2756 (0.1%)
13	D	0.26	0/1359	0.45	0/1838
13	E	0.34	0/1189	0.53	0/1616
13	F	0.30	0/1596	0.58	5/2154 (0.2%)
13	G	0.32	0/1446	0.58	3/1949 (0.2%)
14	H	0.33	1/2119 (0.0%)	0.47	0/2856
15	I	0.29	0/682	0.45	0/913
All	All	0.33	2/41086 (0.0%)	0.57	19/56832 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	380	SER	C-N	5.23	1.40	1.34
14	H	544	ASN	CA-C	-5.03	1.44	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	640	ARG	CA-C-N	10.77	133.30	119.84
12	C	640	ARG	C-N-CA	10.77	133.30	119.84
13	F	649	PRO	N-CA-CB	8.29	110.56	103.35
13	F	606	PRO	N-CA-CB	8.00	111.65	103.25
13	F	599	PRO	N-CA-CB	7.19	110.38	103.19

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	18	0
1	V	779	0	815	17	0
2	S	653	0	695	16	0
2	W	627	0	663	16	0
3	T	811	0	849	7	0
3	X	815	0	860	12	0
4	U	718	0	725	8	0
4	Y	726	0	747	10	0
5	a	3160	0	1741	83	0
6	b	3195	0	1742	77	0
7	P	3227	0	3251	175	0
8	Q	3198	0	3187	71	0
9	Z	490	0	467	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	6385	0	6494	341	0
11	B	3890	0	4008	265	0
12	C	2005	0	1939	171	0
13	D	1322	0	1325	99	0
13	E	1152	0	1137	87	0
13	F	1583	0	1397	78	0
13	G	1435	0	1294	62	0
14	H	2085	0	2104	147	0
15	I	818	0	708	69	0
16	J	336	0	70	19	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	1666	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 1666 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
7:P:36:ILE:CD1	7:P:54:MET:HE3	1.52	1.39
7:P:155:PHE:CE2	7:P:333:MET:HE3	1.60	1.35
13:D:412:TYR:CD1	14:H:560:ILE:HG23	1.62	1.35

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%)	10	43
8	Q	391/467 (84%)	367 (94%)	22 (6%)	2 (0%)	25	64
9	Z	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	5	29
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%)	16	55
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%)	14	52
13	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	25	64
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%)	38	73

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Q	48	ASP

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Mol	Chain	Res	Type
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%)	331 (93%)	26 (7%)	11	31
8	Q	363/423 (86%)	344 (95%)	19 (5%)	19	40
9	Z	53/140 (38%)	51 (96%)	2 (4%)	28	49
10	A	705/1520 (46%)	698 (99%)	7 (1%)	73	82
11	B	460/1218 (38%)	459 (100%)	1 (0%)	92	94
12	C	222/823 (27%)	220 (99%)	2 (1%)	75	83
13	D	150/751 (20%)	150 (100%)	0	100	100
13	E	129/751 (17%)	129 (100%)	0	100	100
13	F	138/751 (18%)	138 (100%)	0	100	100
13	G	127/751 (17%)	126 (99%)	1 (1%)	79	85
14	H	239/517 (46%)	235 (98%)	4 (2%)	56	72
15	I	79/133 (59%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3638/8980 (40%)	3576 (98%)	62 (2%)	56 72

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Q	34	GLU
12	C	611	LEU
8	Q	94	ARG
11	B	1199	ASN
14	H	538	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
12	C	417	ASN
13	E	352	ASN
12	C	448	GLN
13	D	333	ASN
13	F	540	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	P	501	-	4,4,4	0.94	0	6,6,6	0.68	0
18	PO4	Q	504	-	4,4,4	0.93	0	6,6,6	0.44	0
20	BEF	A	1803	-	0,3,3	-	-	-		
18	PO4	Q	503	-	4,4,4	0.89	0	6,6,6	0.60	0
18	PO4	Q	505	-	4,4,4	0.91	0	6,6,6	0.45	0
18	PO4	P	505	-	4,4,4	0.93	0	6,6,6	0.46	0
18	PO4	Q	501	-	4,4,4	1.03	0	6,6,6	0.64	0
18	PO4	A	1801	-	4,4,4	0.83	0	6,6,6	0.84	0
19	ADP	A	1802	21	24,29,29	0.91	0	29,45,45	1.18	2 (6%)
18	PO4	P	504	-	4,4,4	0.89	0	6,6,6	0.64	0
18	PO4	P	503	-	4,4,4	1.01	0	6,6,6	0.51	0
18	PO4	Q	502	-	4,4,4	0.88	0	6,6,6	0.49	0
18	PO4	Q	506	-	4,4,4	0.86	0	6,6,6	0.62	0
18	PO4	P	502	-	4,4,4	0.84	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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1802	ADP	N3-C2-N1	-3.61	123.77	128.67
19	A	1802	ADP	C4-C5-N7	-2.50	106.69	109.34

There are no chirality outliers.

All (1) torsion outliers are listed below:

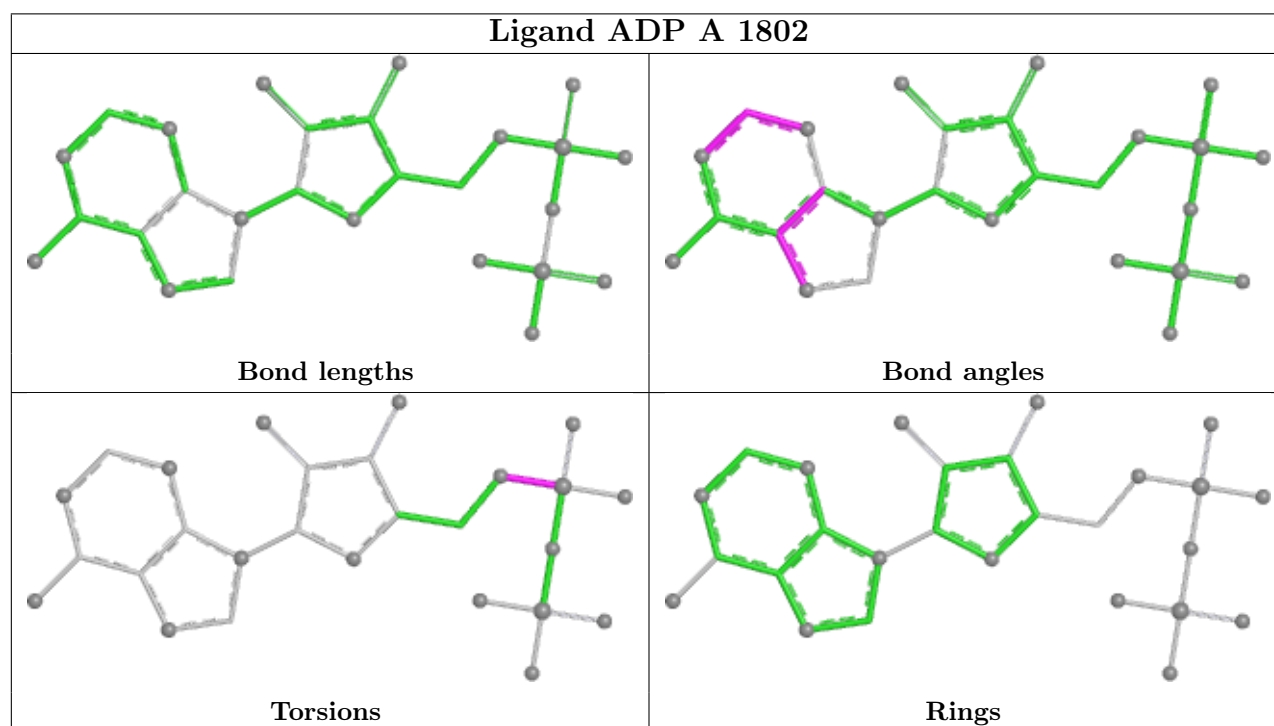
Mol	Chain	Res	Type	Atoms
19	A	1802	ADP	C5'-O5'-PA-O1A

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

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

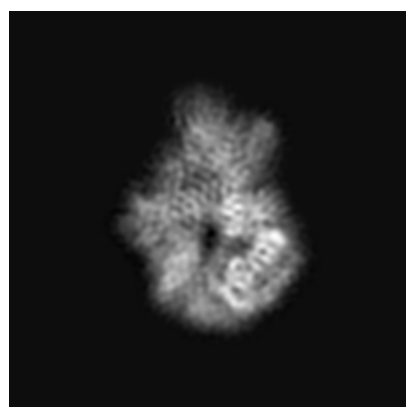
6 Map visualisation [i](#)

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.

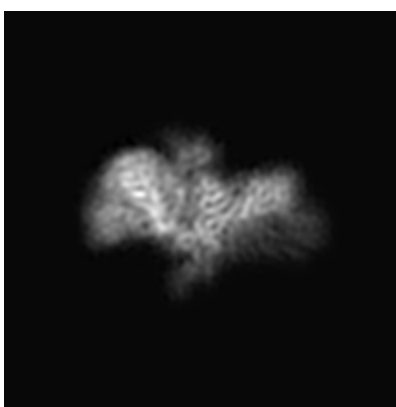
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

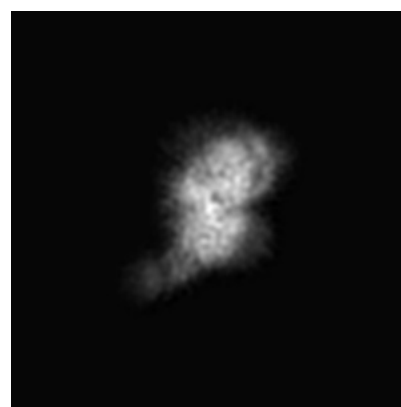
6.1.1 Primary map



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

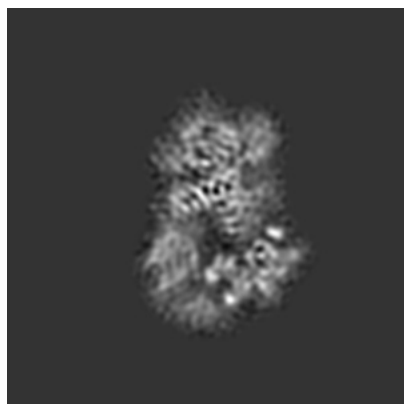


Z Index: 96

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

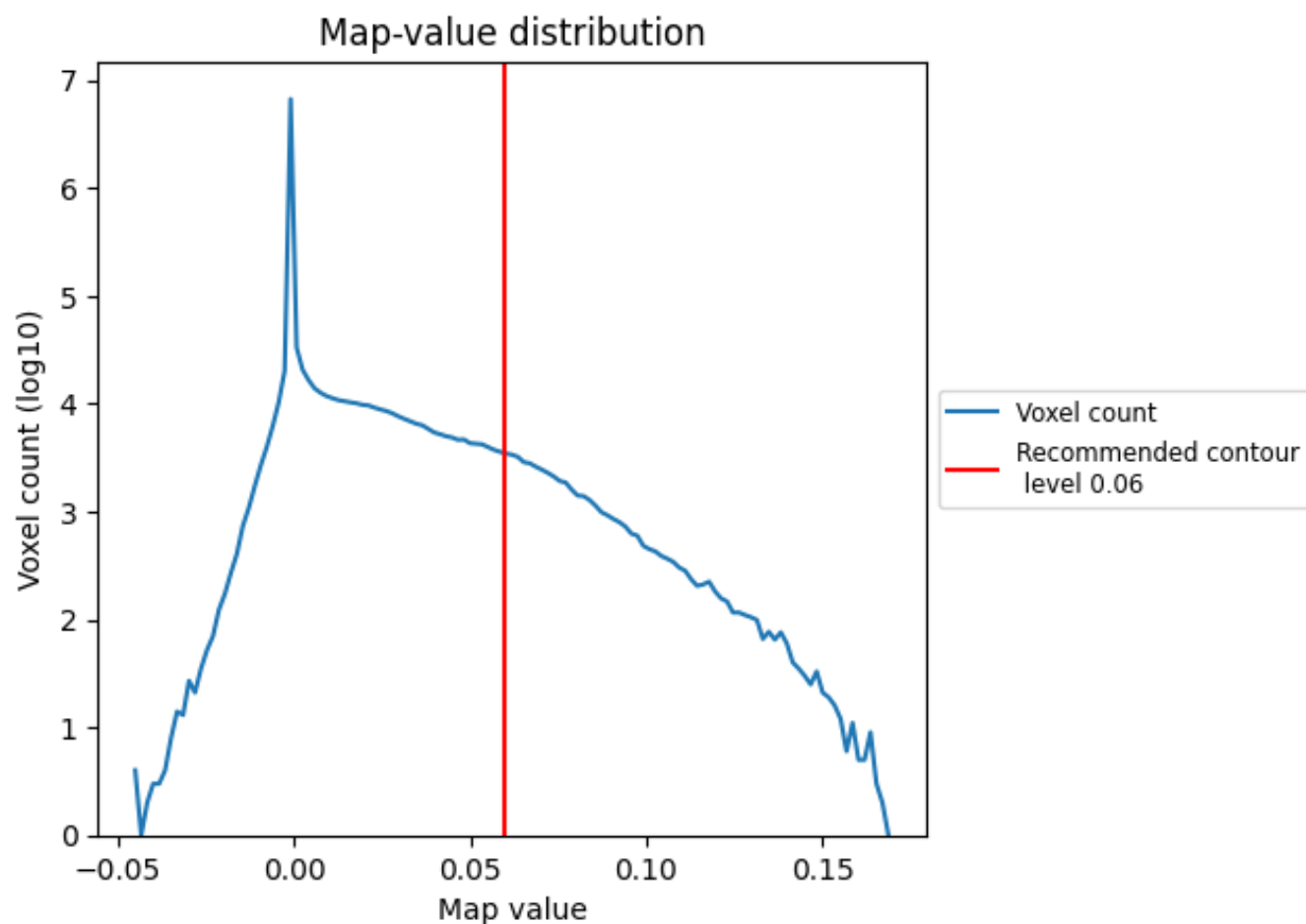
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

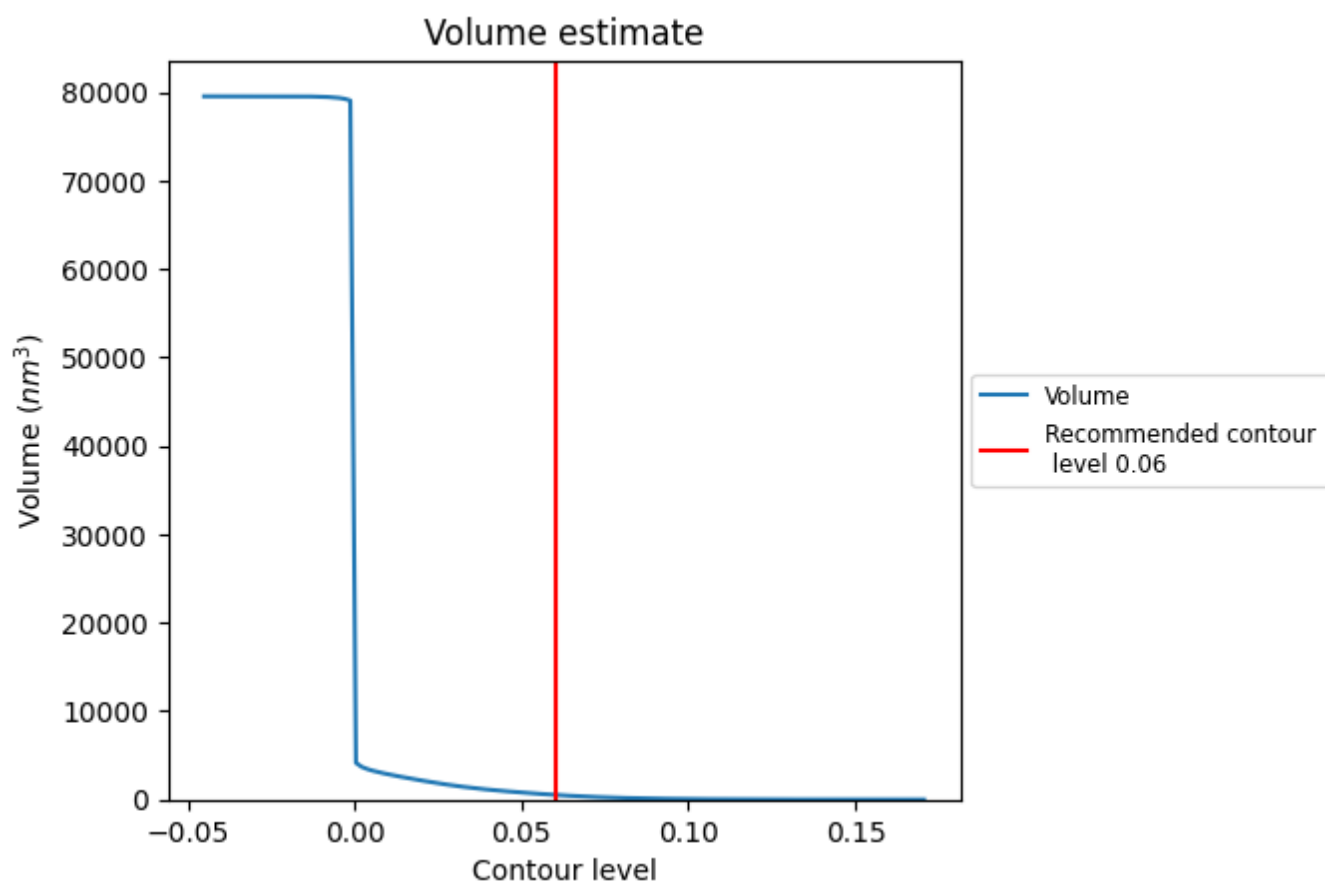
This section contains the results of statistical analysis of the map.

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.

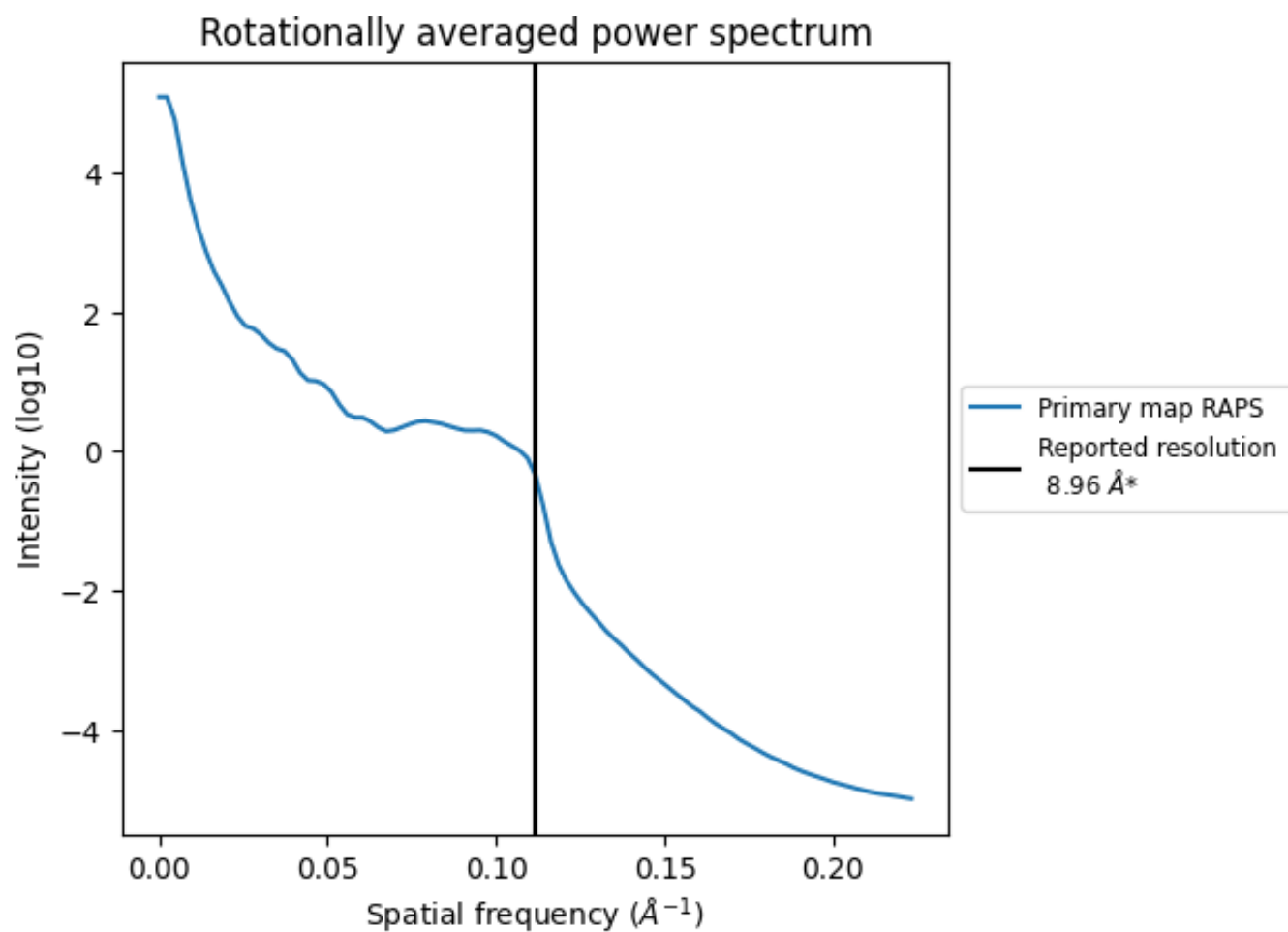
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

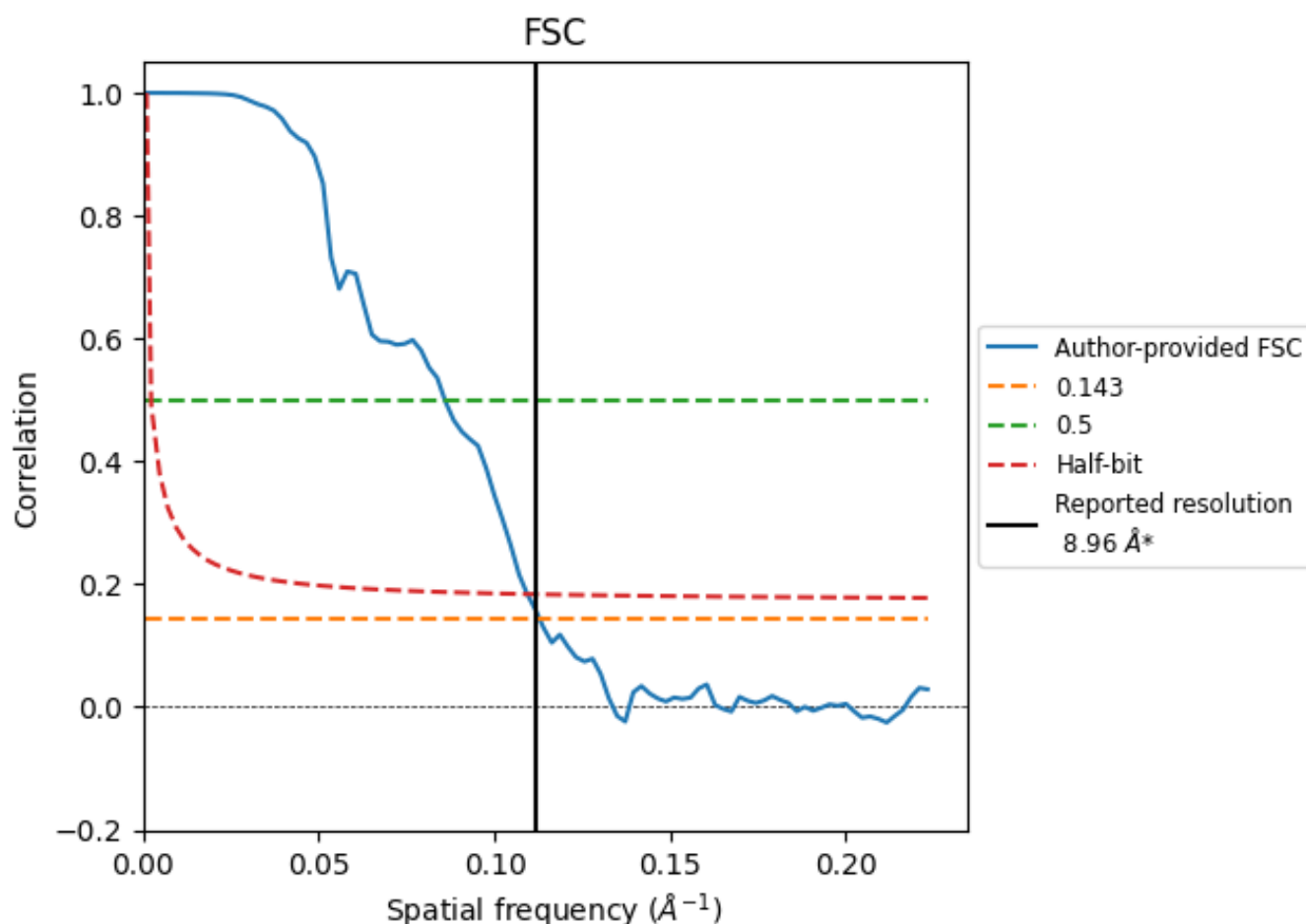


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

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](#)

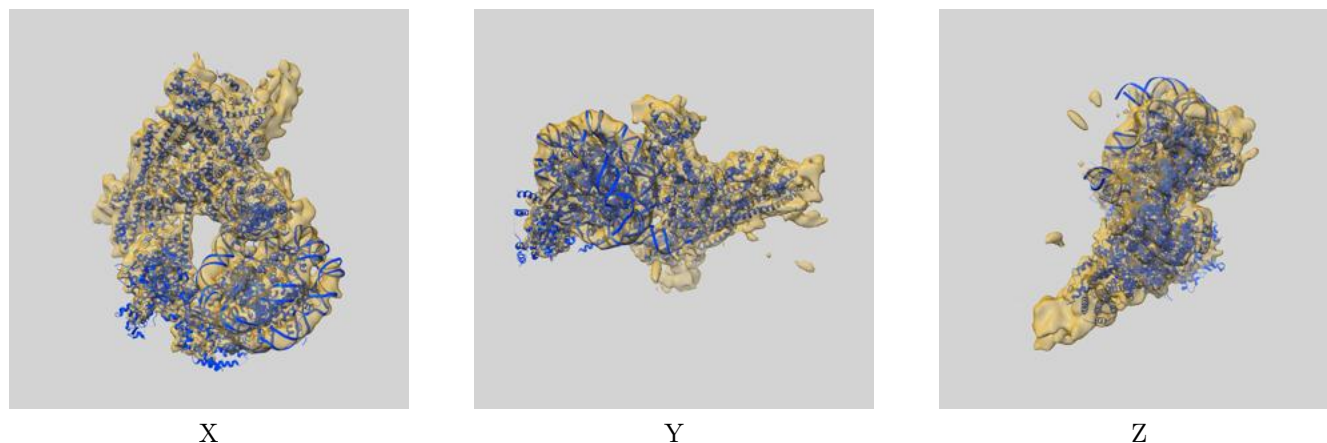
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.96	-	-
Author-provided FSC curve	8.86	11.64	9.15
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

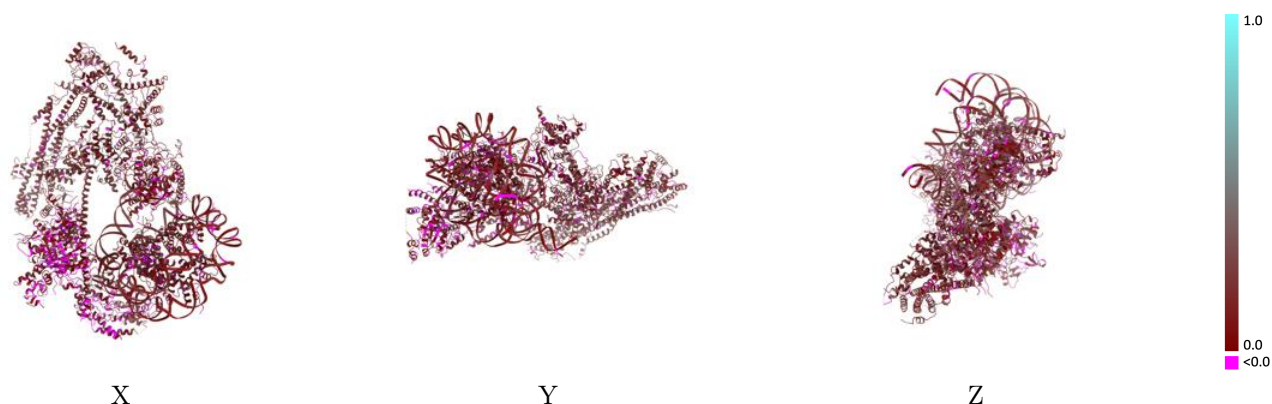
This section contains information regarding the fit between EMDB map EMD-20934 and PDB model 6UXW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



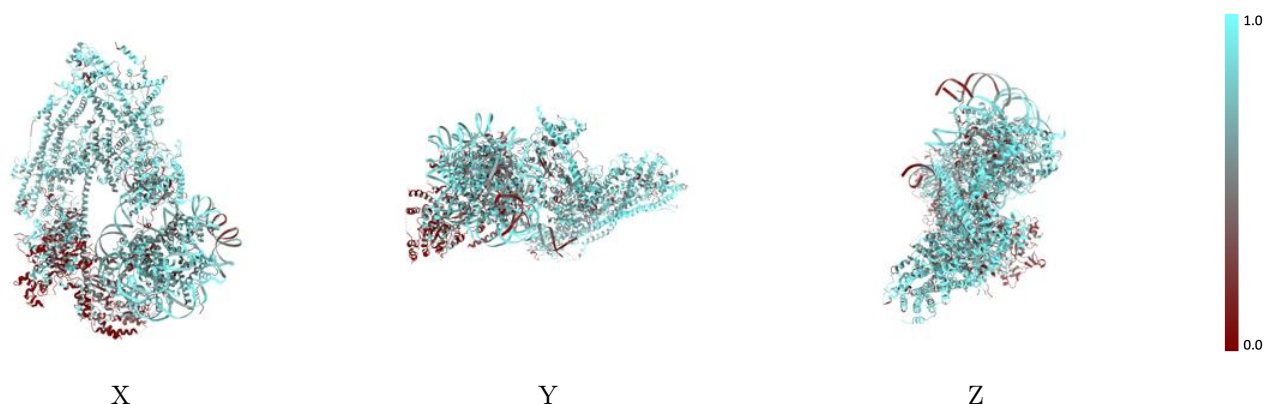
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



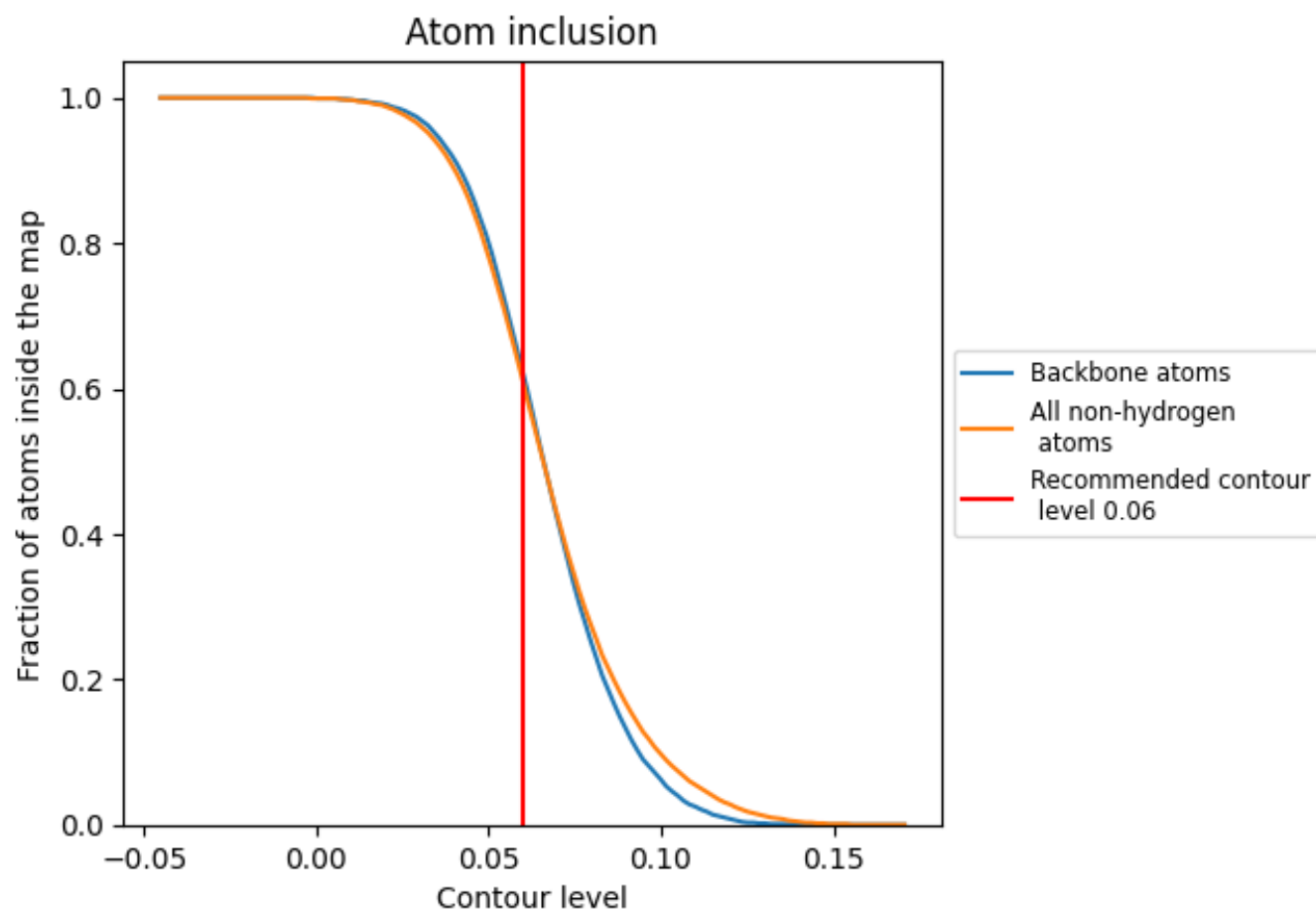
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



























































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	 0.6090	 0.1220
A	 0.3700	 0.0820
B	 0.6980	 0.1540
C	 0.6370	 0.1420
D	 0.7220	 0.1270
E	 0.7080	 0.1410
F	 0.7600	 0.1580
G	 0.7540	 0.1690
H	 0.7300	 0.1660
I	 0.7700	 0.1710
J	 0.9670	 0.2740
K	 0.8860	 0.2370
L	 0.3000	 0.1970
M	 0.8890	 0.2170
N	 0.4270	 0.0640
O	 0.7440	 0.1650
P	 0.5240	 0.0750
Q	 0.3550	 0.0520
R	 0.5820	 0.1120
S	 0.6010	 0.1060
T	 0.5800	 0.1100
U	 0.6930	 0.1590
V	 0.6590	 0.1260
W	 0.6770	 0.1050
X	 0.6730	 0.1180
Y	 0.7000	 0.1370
Z	 0.4380	 0.0930
a	 0.7290	 0.1300
b	 0.7540	 0.1380

