wwPDB EM Validation Summary Report

Nov 22, 2022 – 02:05 PM JST

PDB ID	:	7EGP
EMDB ID	:	EMD-31137
Title	:	The structure of SWI/SNF-nucleosome complex
Authors	:	Chen, Z.C.; Chen, K.J.; He, Z.Y.; Ye, Y.P.
Deposited on	:	2021-03-24
Resolution	:	6.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

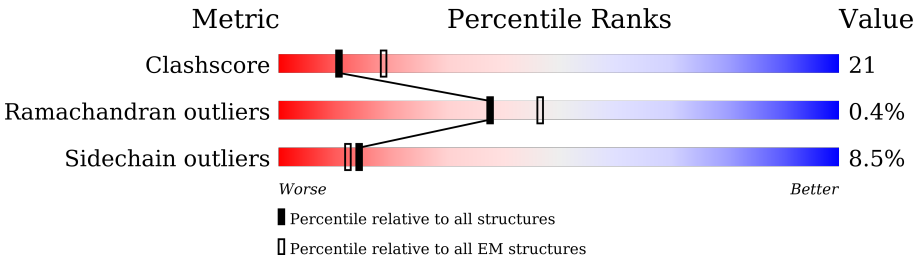
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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 <=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	B	1093	36% 9% 54%
2	C	918	5% 27% 9% 62%
3	D	836	13% 37% 9% 53%
3	E	836	14% 39% 11% 50%
4	H	566	34% 54% 12% 31%
5	I	332	9% 25% 7% 68%
6	J	634	9% 22% 74%
7	A	982	30% 46% 28% 24%

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Mol	Chain	Length	Quality of chain
8	L	157	16% 17% 66%
9	M	477	40% 38% 19%
10	N	467	5% 40% 40% 16%
11	O	135	33% 34% 5% 27%
11	S	135	27% 39% 30%
12	P	102	7% 45% 34% 6% 15%
12	T	102	5% 35% 40% 9% 16%
13	Q	129	39% 42% 17%
13	U	129	5% 36% 43% 17%
14	R	122	33% 39% 5% 24%
14	V	122	27% 42% 7% 24%
15	W	235	11% 21% 30% 20% 29%
16	X	235	14% 22% 27% 22% 29%

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
17	ADP	A	1501	-	-	X	-
18	BEF	A	1502	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 44871 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 SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	507	4098	2663	672	752	11	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1315	GLY	-	expression tag	UNP P09547
B	1316	GLY	-	expression tag	UNP P09547
B	1317	SER	-	expression tag	UNP P09547
B	1318	GLY	-	expression tag	UNP P09547
B	1319	GLY	-	expression tag	UNP P09547
B	1320	TRP	-	expression tag	UNP P09547
B	1321	SER	-	expression tag	UNP P09547
B	1322	HIS	-	expression tag	UNP P09547
B	1323	PRO	-	expression tag	UNP P09547
B	1324	GLN	-	expression tag	UNP P09547
B	1325	PHE	-	expression tag	UNP P09547
B	1326	GLU	-	expression tag	UNP P09547
B	1327	LYS	-	expression tag	UNP P09547
B	1328	TRP	-	expression tag	UNP P09547
B	1329	SER	-	expression tag	UNP P09547
B	1330	HIS	-	expression tag	UNP P09547
B	1331	PRO	-	expression tag	UNP P09547
B	1332	GLN	-	expression tag	UNP P09547
B	1333	PHE	-	expression tag	UNP P09547
B	1334	GLU	-	expression tag	UNP P09547
B	1335	LYS	-	expression tag	UNP P09547
B	1336	TRP	-	expression tag	UNP P09547
B	1337	SER	-	expression tag	UNP P09547
B	1338	HIS	-	expression tag	UNP P09547
B	1339	PRO	-	expression tag	UNP P09547
B	1340	GLN	-	expression tag	UNP P09547
B	1341	PHE	-	expression tag	UNP P09547

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1342	GLU	-	expression tag	UNP P09547
B	1343	LYS	-	expression tag	UNP P09547

- Molecule 2 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	351	Total	C	N	O	S	0	0
			2873	1794	506	563	10		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	906	GLY	-	expression tag	UNP P18480
C	907	GLY	-	expression tag	UNP P18480
C	908	SER	-	expression tag	UNP P18480
C	909	GLY	-	expression tag	UNP P18480
C	910	GLY	-	expression tag	UNP P18480
C	911	ASP	-	expression tag	UNP P18480
C	912	TYR	-	expression tag	UNP P18480
C	913	LYS	-	expression tag	UNP P18480
C	914	ASP	-	expression tag	UNP P18480
C	915	ASP	-	expression tag	UNP P18480
C	916	ASP	-	expression tag	UNP P18480
C	917	ASP	-	expression tag	UNP P18480
C	918	LYS	-	expression tag	UNP P18480

- Molecule 3 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
3	E	422	Total	C	N	O	S	0	0
			3454	2208	593	641	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	826	GLY	-	expression tag	UNP P32591
D	827	GLY	-	expression tag	UNP P32591
D	828	SER	-	expression tag	UNP P32591
D	829	GLY	-	expression tag	UNP P32591
D	830	GLY	-	expression tag	UNP P32591

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Chain	Residue	Modelled	Actual	Comment	Reference
D	831	HIS	-	expression tag	UNP P32591
D	832	HIS	-	expression tag	UNP P32591
D	833	HIS	-	expression tag	UNP P32591
D	834	HIS	-	expression tag	UNP P32591
D	835	HIS	-	expression tag	UNP P32591
D	836	HIS	-	expression tag	UNP P32591
E	826	GLY	-	expression tag	UNP P32591
E	827	GLY	-	expression tag	UNP P32591
E	828	SER	-	expression tag	UNP P32591
E	829	GLY	-	expression tag	UNP P32591
E	830	GLY	-	expression tag	UNP P32591
E	831	HIS	-	expression tag	UNP P32591
E	832	HIS	-	expression tag	UNP P32591
E	833	HIS	-	expression tag	UNP P32591
E	834	HIS	-	expression tag	UNP P32591
E	835	HIS	-	expression tag	UNP P32591
E	836	HIS	-	expression tag	UNP P32591

- Molecule 4 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	388	Total	C	N	O	S	0	0
			3145	1995	536	603	11		

- Molecule 5 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	106	Total	C	N	O	S	0	0
			888	553	158	173	4		

- Molecule 6 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	167	Total	C	N	O	S	0	0
			1360	877	241	240	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	624	GLY	-	expression tag	UNP P43554
J	625	GLY	-	expression tag	UNP P43554

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Chain	Residue	Modelled	Actual	Comment	Reference
J	626	SER	-	expression tag	UNP P43554
J	627	GLY	-	expression tag	UNP P43554
J	628	GLY	-	expression tag	UNP P43554
J	629	HIS	-	expression tag	UNP P43554
J	630	HIS	-	expression tag	UNP P43554
J	631	HIS	-	expression tag	UNP P43554
J	632	HIS	-	expression tag	UNP P43554
J	633	HIS	-	expression tag	UNP P43554
J	634	HIS	-	expression tag	UNP P43554

- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	750	Total	C	N	O	S	0	0
			6162	3900	1101	1141	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1401	GLY	-	expression tag	UNP P22082
A	1402	GLY	-	expression tag	UNP P22082
A	1403	SER	-	expression tag	UNP P22082
A	1404	GLY	-	expression tag	UNP P22082
A	1405	GLY	-	expression tag	UNP P22082
A	1406	HIS	-	expression tag	UNP P22082
A	1407	HIS	-	expression tag	UNP P22082
A	1408	HIS	-	expression tag	UNP P22082
A	1409	HIS	-	expression tag	UNP P22082
A	1410	HIS	-	expression tag	UNP P22082
A	1411	HIS	-	expression tag	UNP P22082

- Molecule 8 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	53	Total	C	N	O	0	0
			482	308	83	91		

- Molecule 9 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	387	Total	C	N	O	S	3	0
			3131	2020	516	591	4		

- Molecule 10 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	392	Total	C	N	O	S	1	0
			3167	2033	519	611	4		

- Molecule 11 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
11	S	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- Molecule 12 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
12	T	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 13 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	107	Total	C	N	O	0	0
			811	510	158	143		
13	U	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 14 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
14	V	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
R	29	THR	SER	engineered mutation	UNP P02281
V	29	THR	SER	engineered mutation	UNP P02281

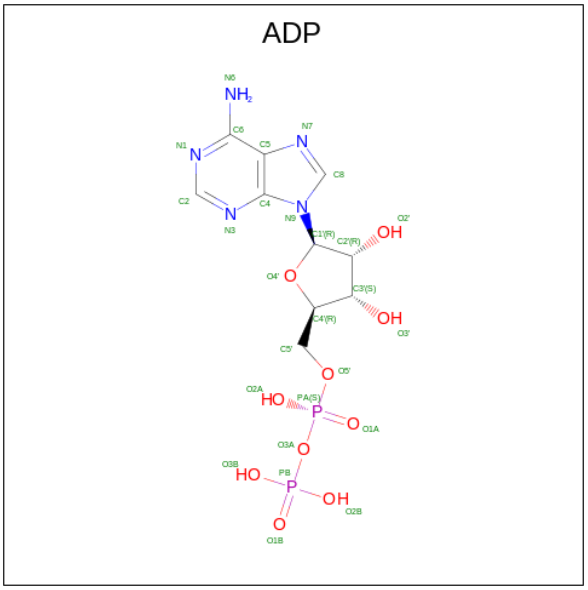
- Molecule 15 is a DNA chain called DNA (239-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	W	166	3393	1611	621	995	166	0	0

- Molecule 16 is a DNA chain called DNA (239-MER).

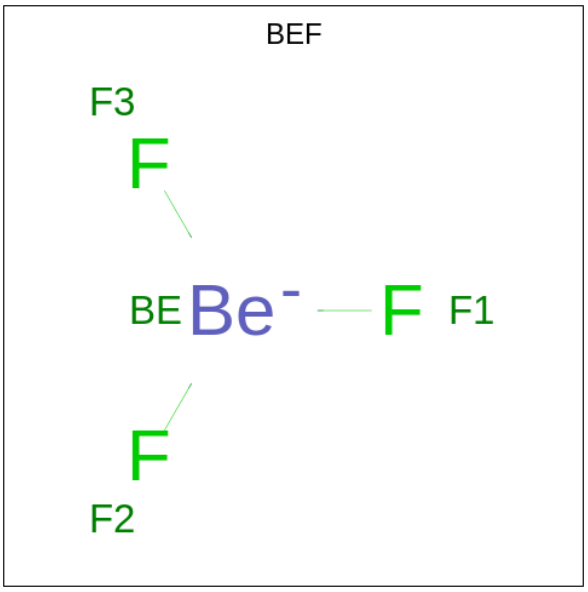
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	X	166	3413	1618	632	997	166	0	0

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

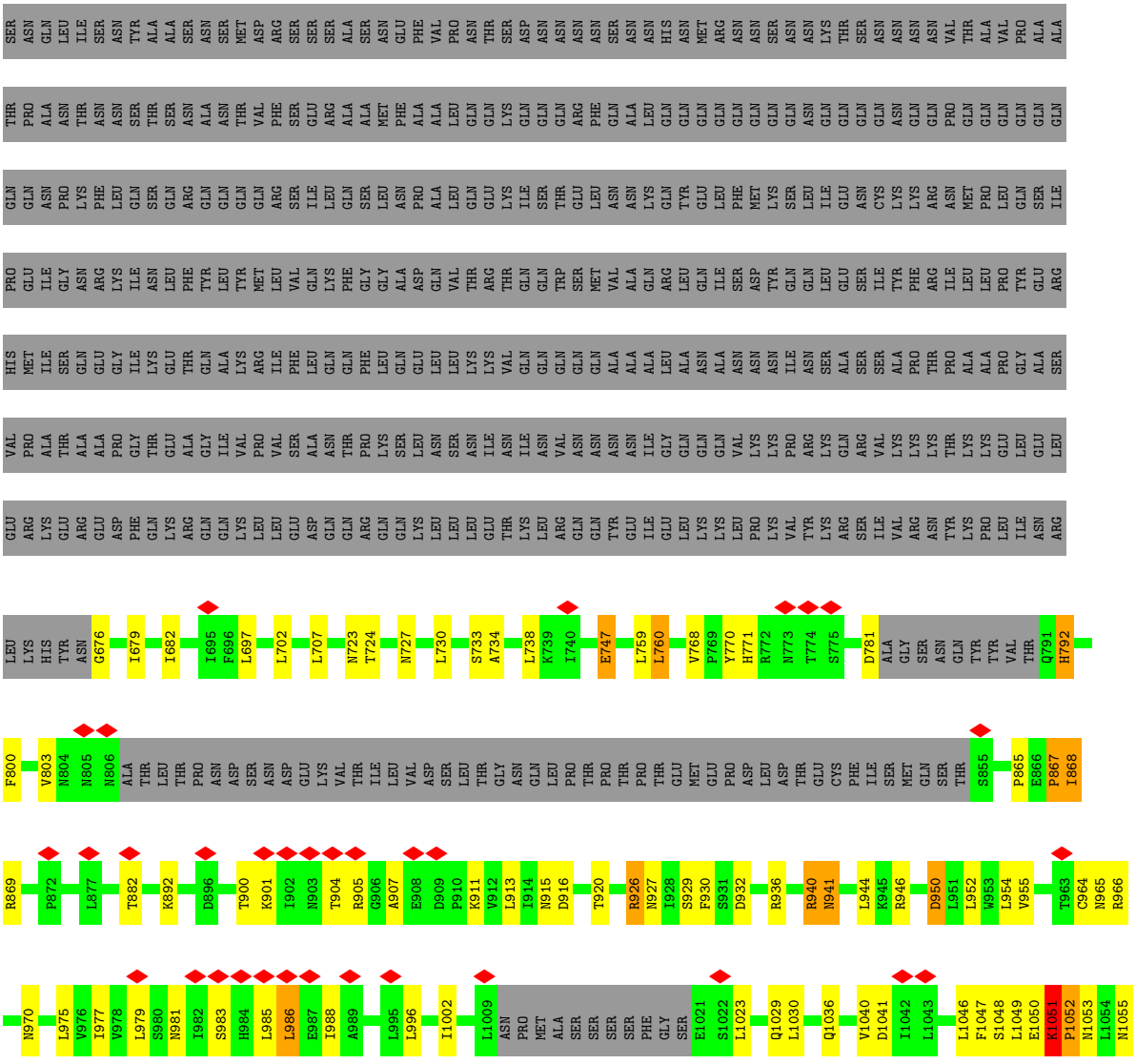
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

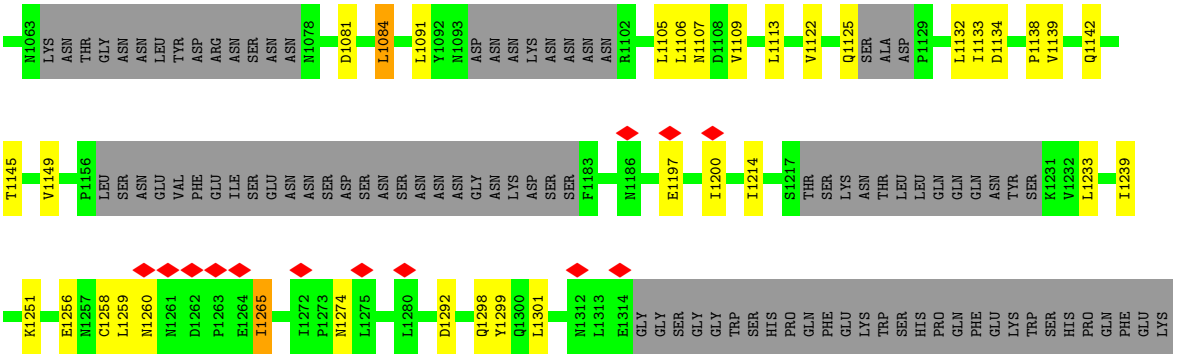
3 Residue-property plots (i)

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: SWI/SNF chromatin-remodeling complex subunit SWI1

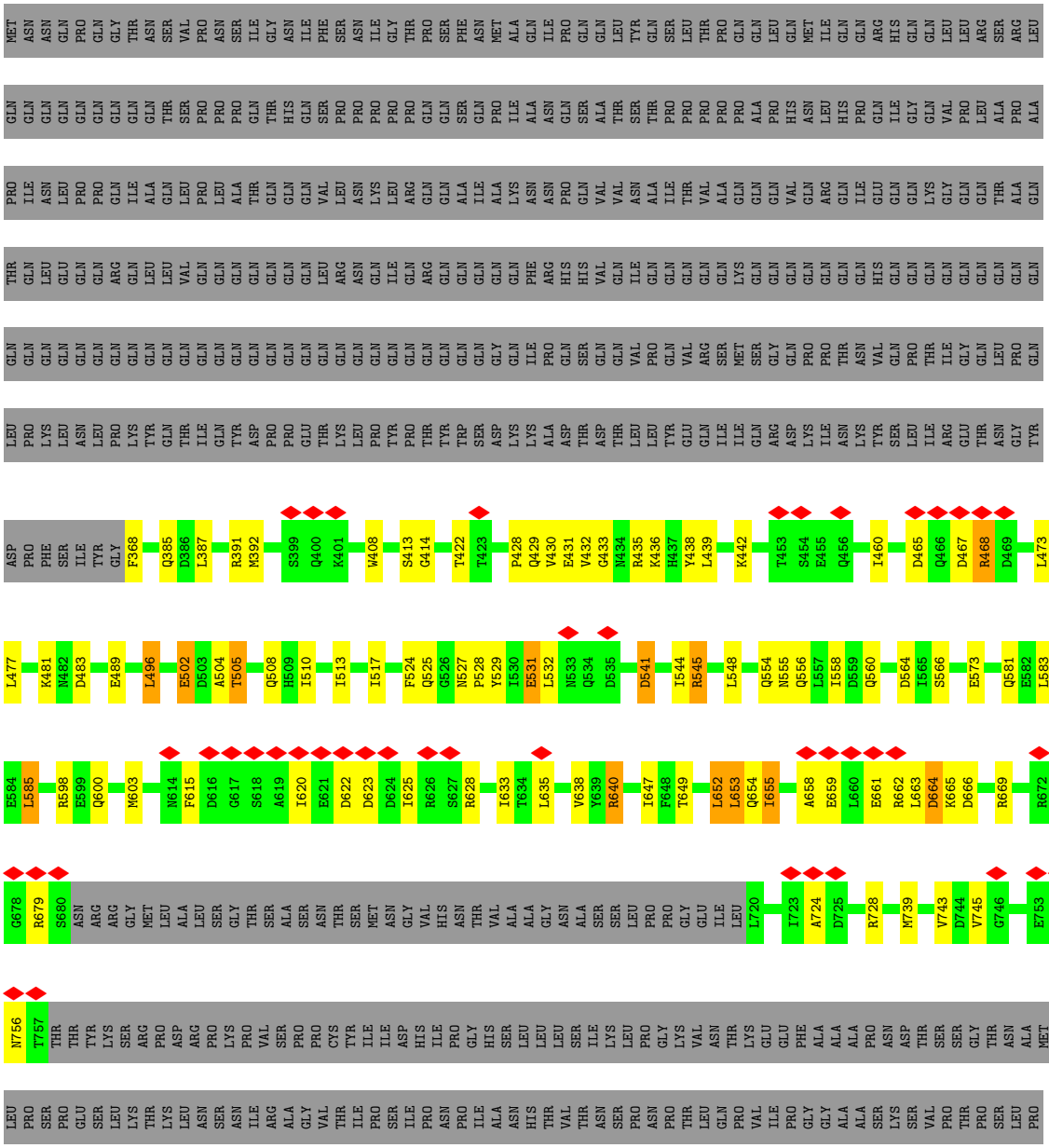
Chain B:





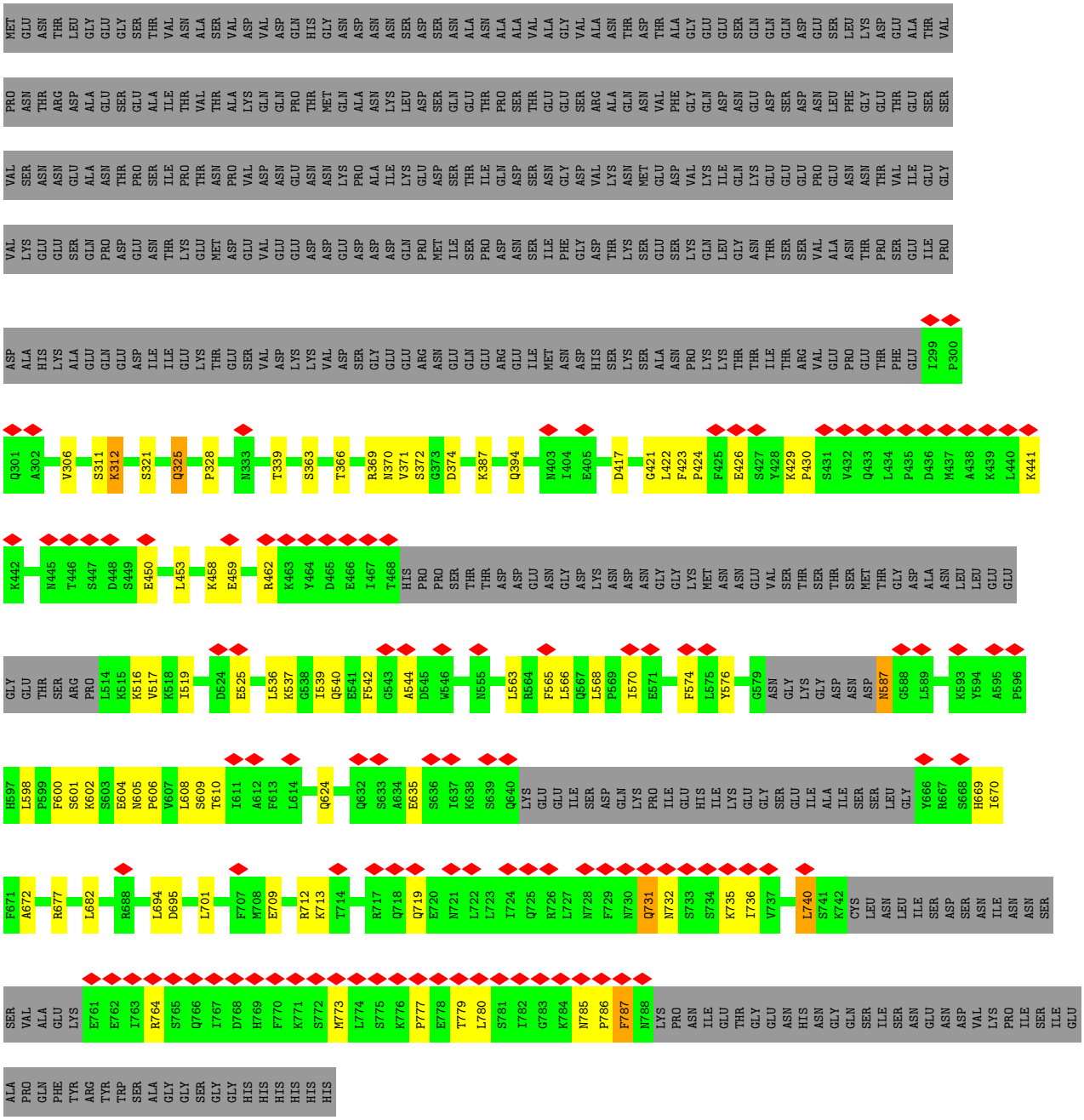
• Molecule 2: SWI/SNF chromatin-remodeling complex subunit SNF5

Chain C:



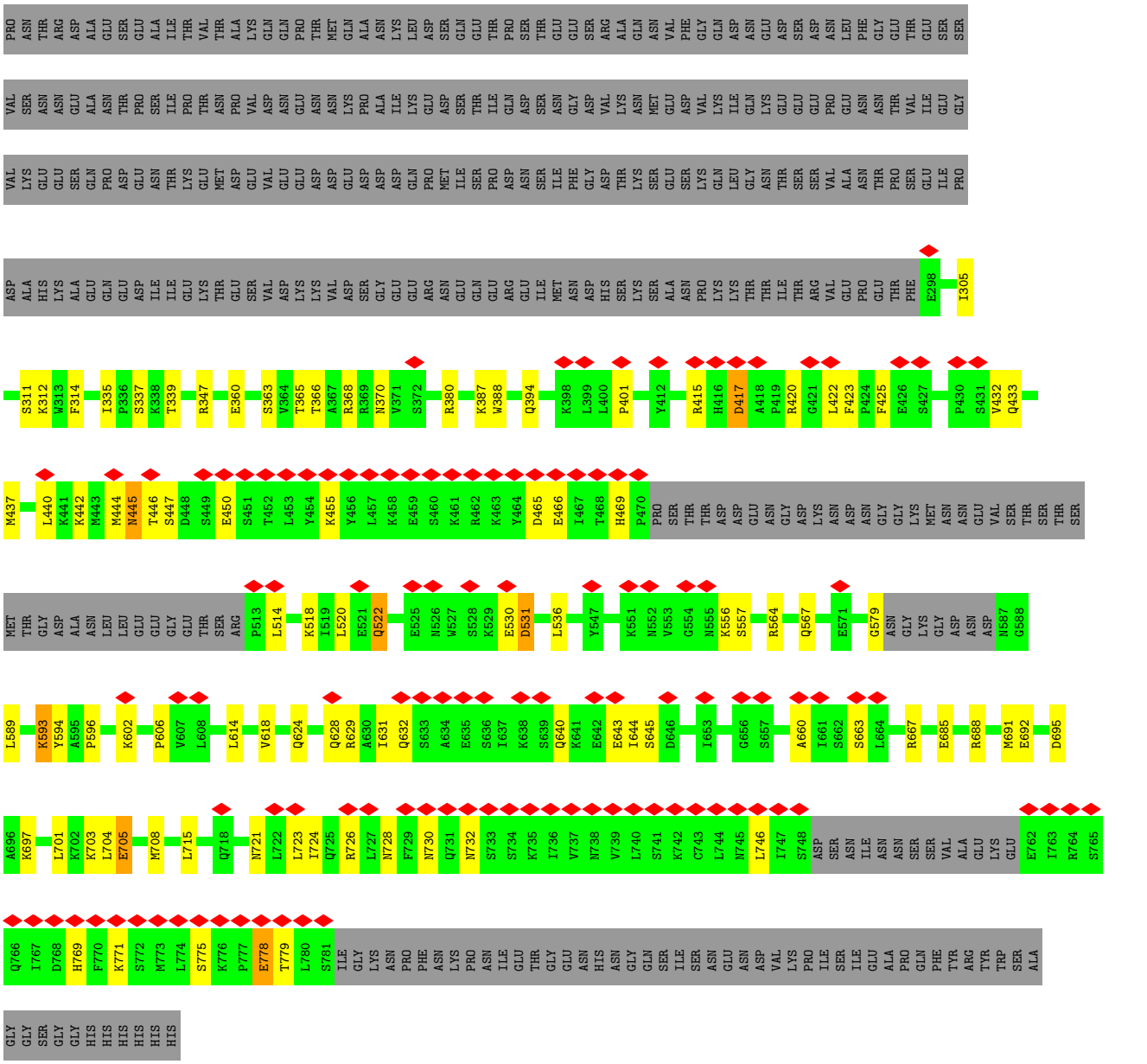
• Molecule 3: SWI/SNF complex subunit SWI3

Chain D:



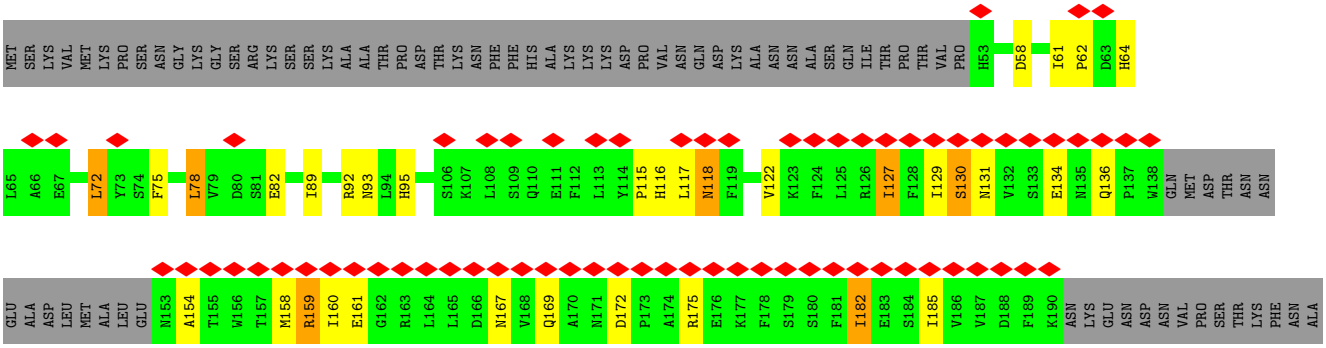
• Molecule 3: SWI/SNF complex subunit SWI3

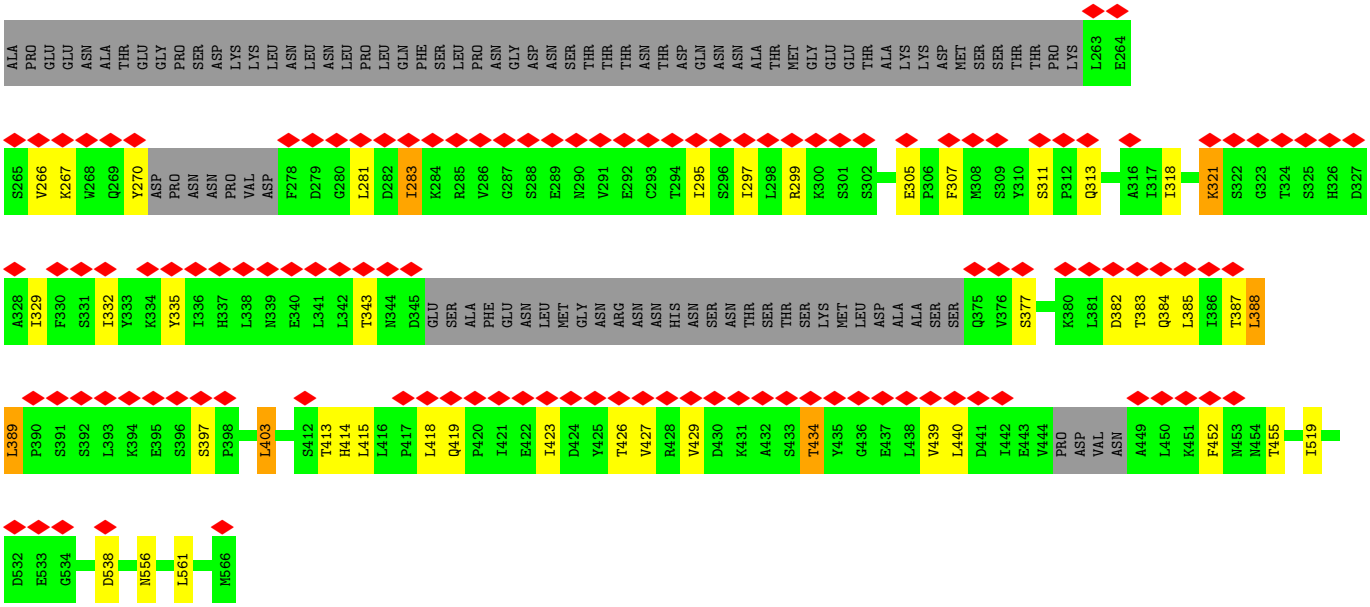
Chain E:



• Molecule 4: Transcription regulatory protein SNF12

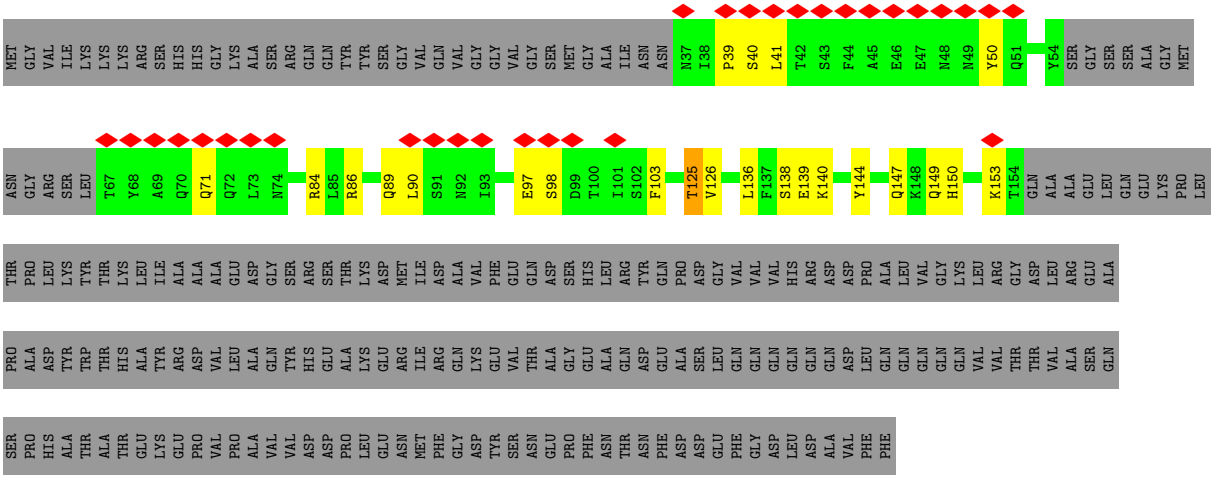
Chain H:





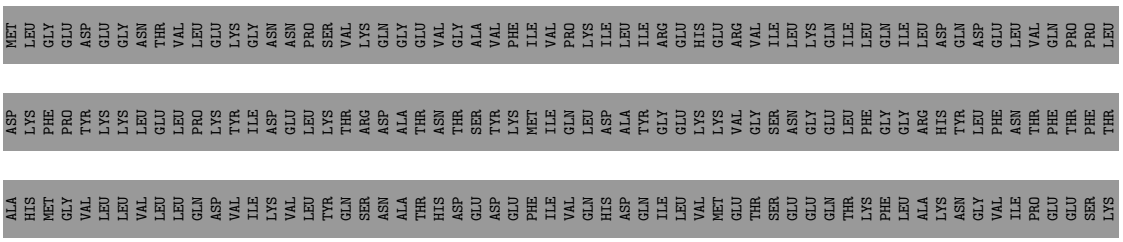
• Molecule 5: Transcription regulatory protein SNF6

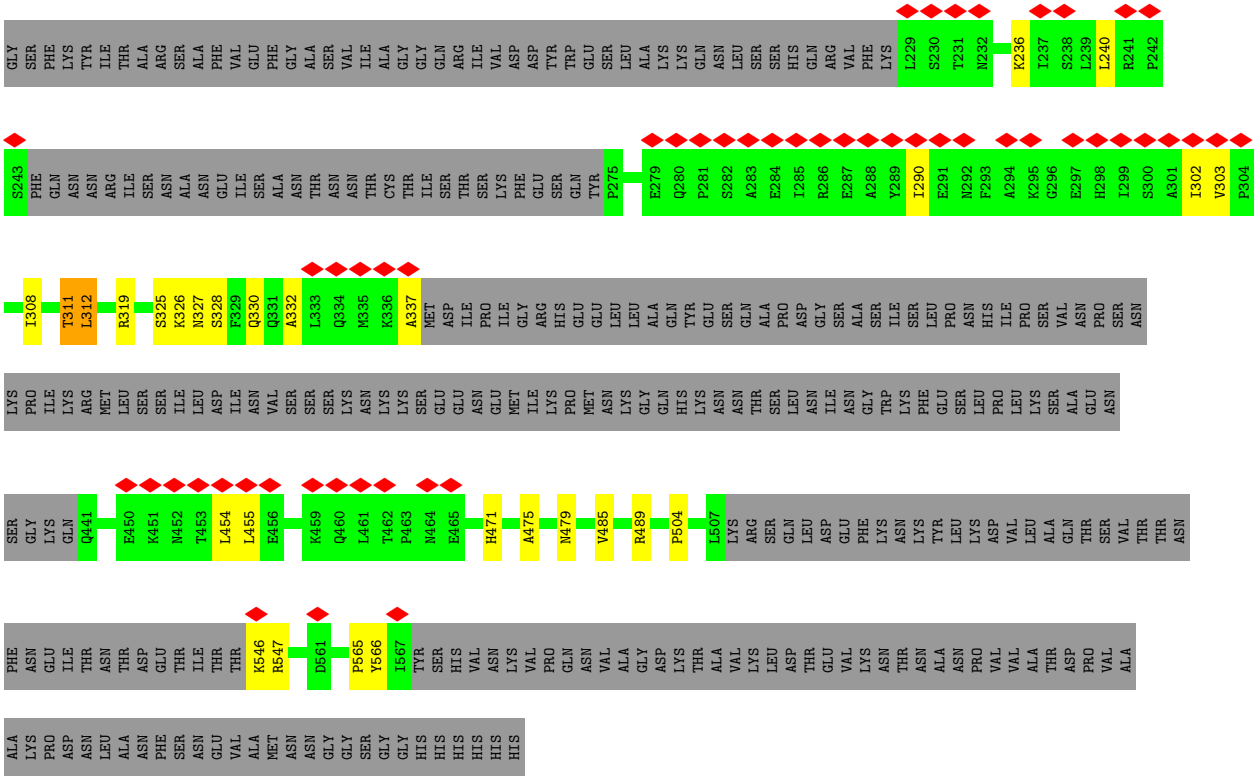
Chain I:



• Molecule 6: SWI/SNF global transcription activator complex subunit SWP82

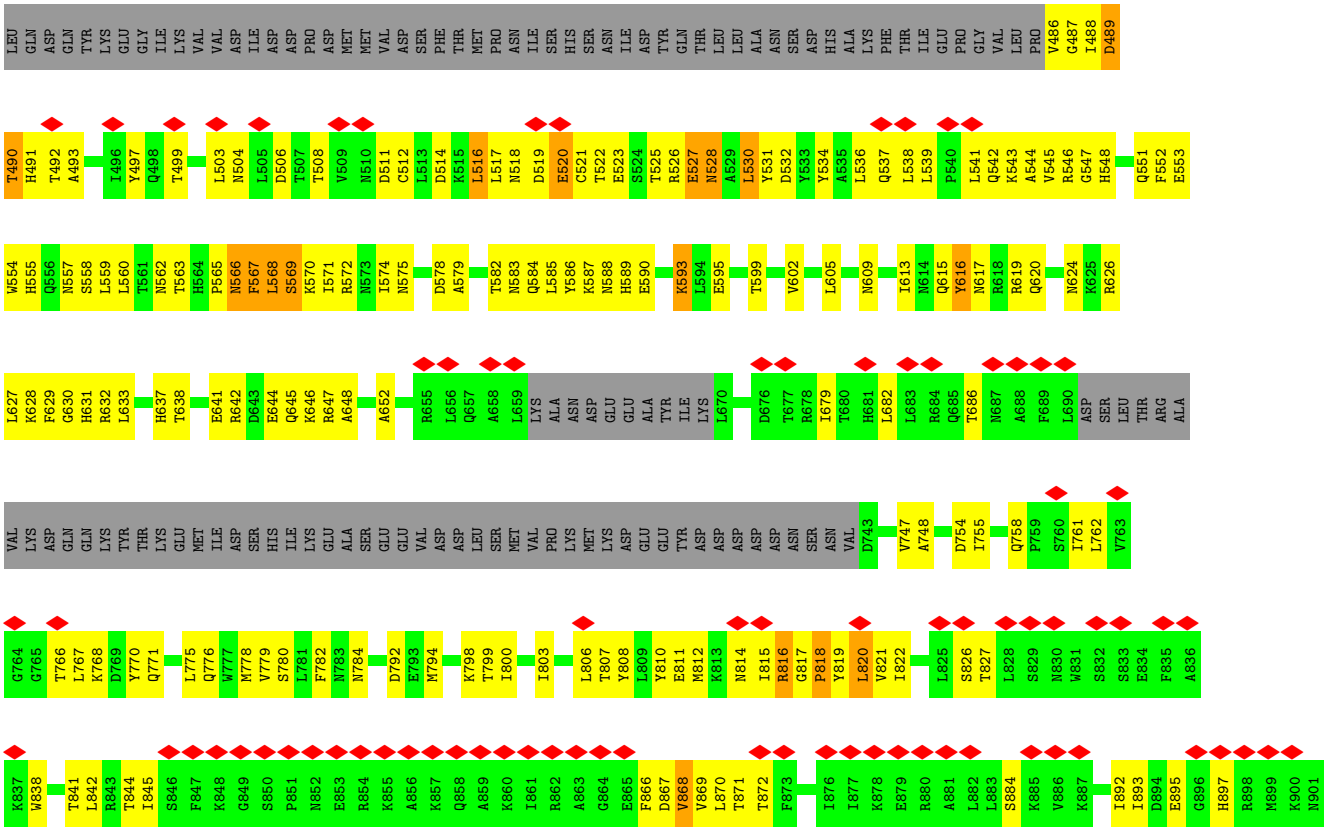
Chain J:

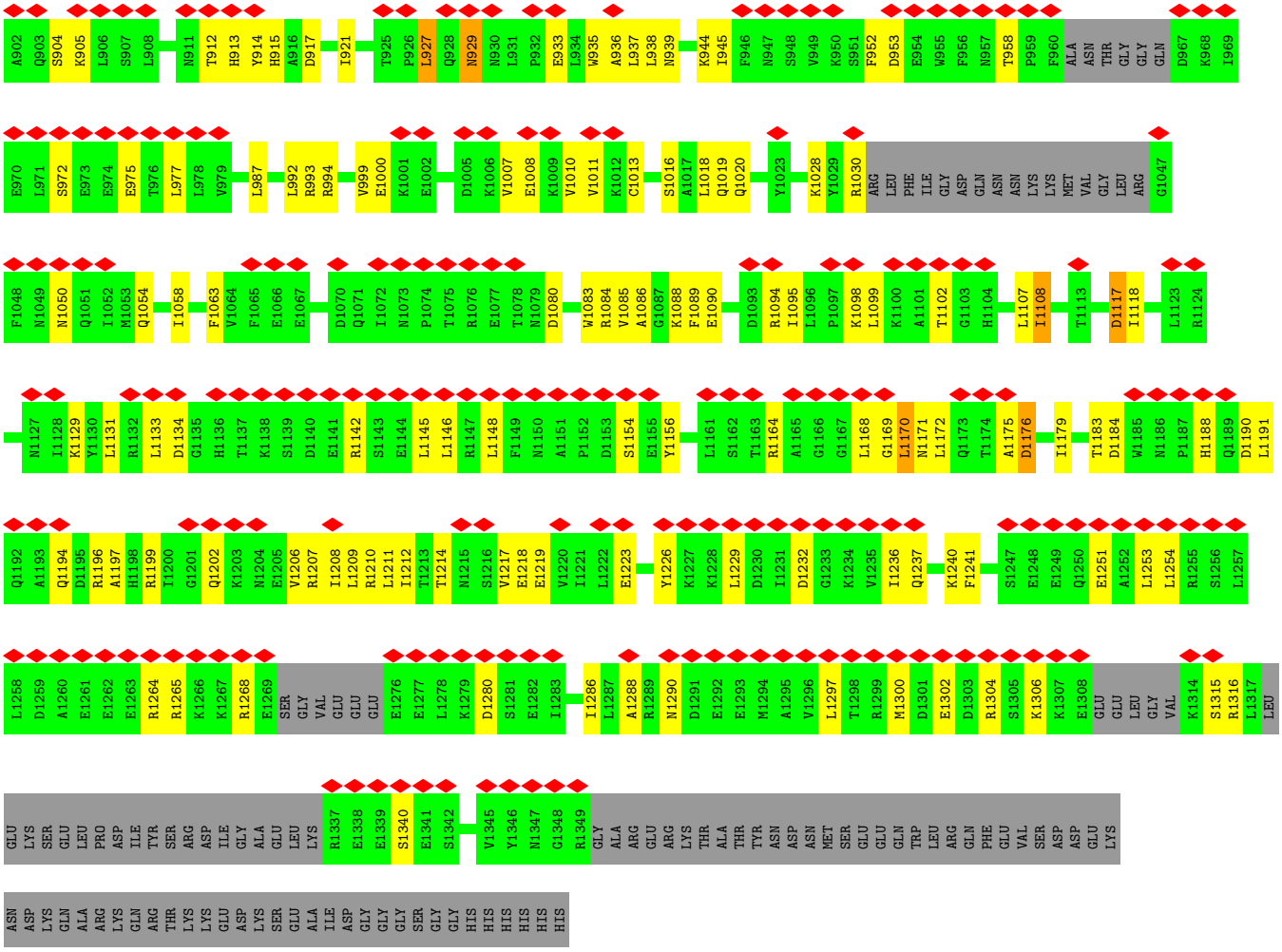




• Molecule 7: Transcription regulatory protein SNF2

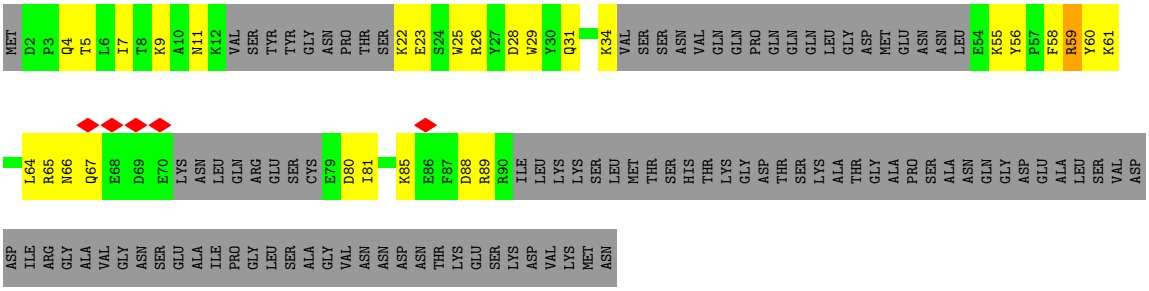
Chain A:





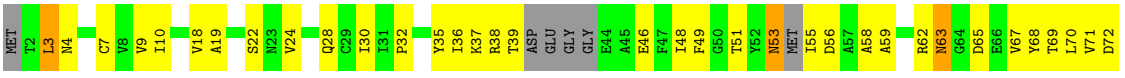
• Molecule 8: Regulator of Ty1 transposition protein 102

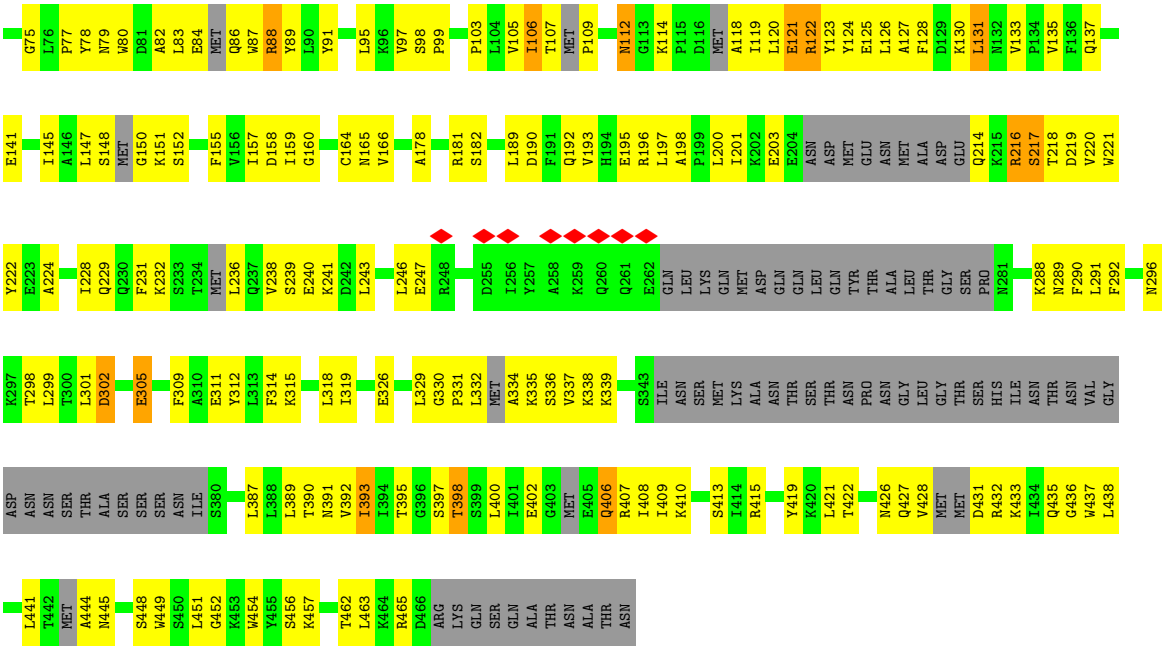
Chain L:



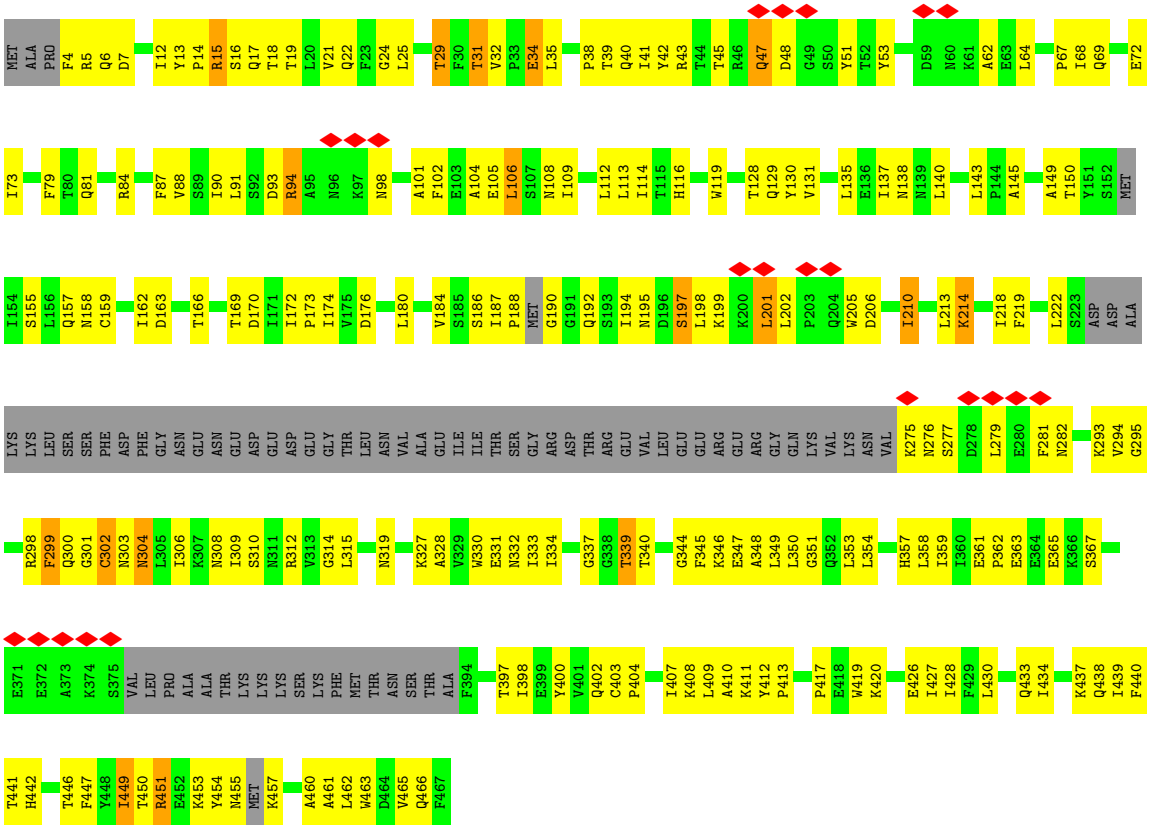
• Molecule 9: Actin-related protein 7

Chain M:



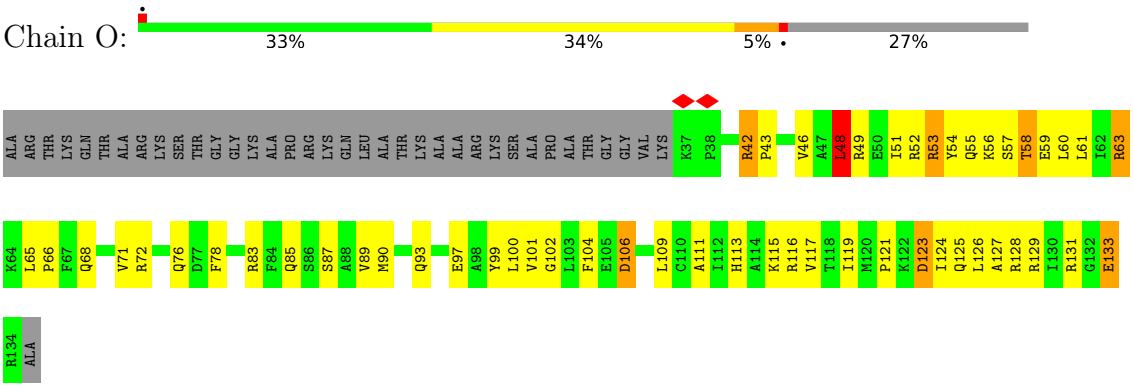


• Molecule 10: Actin-like protein ARP9



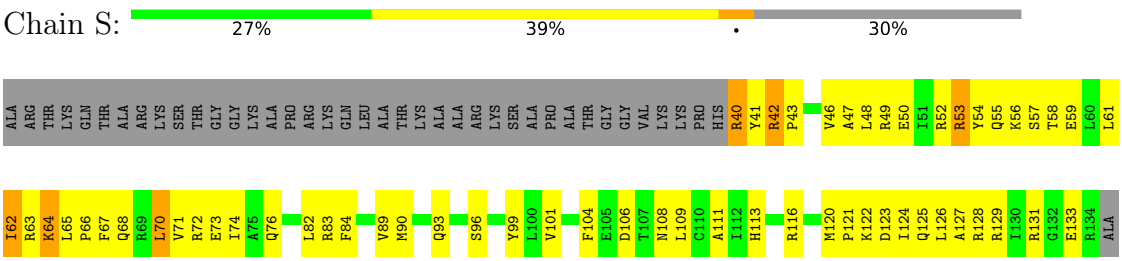
• Molecule 11: Histone H3.2

Chain O:



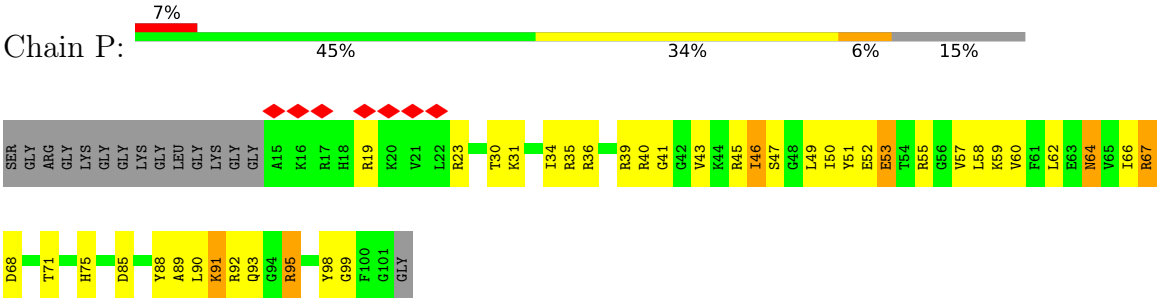
• Molecule 11: Histone H3.2

Chain S:



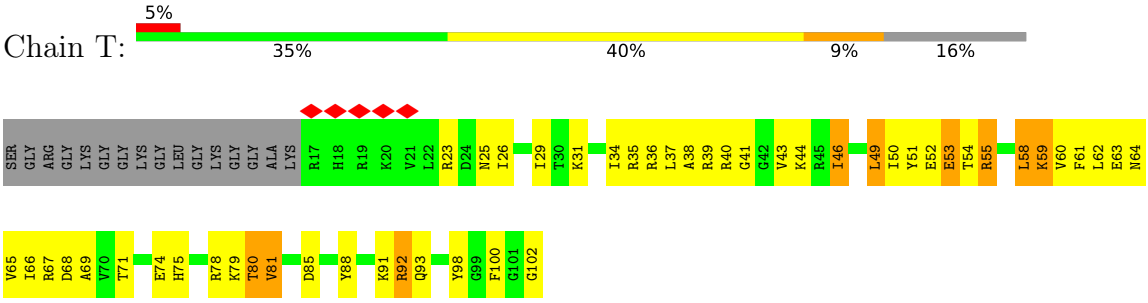
• Molecule 12: Histone H4

Chain P:



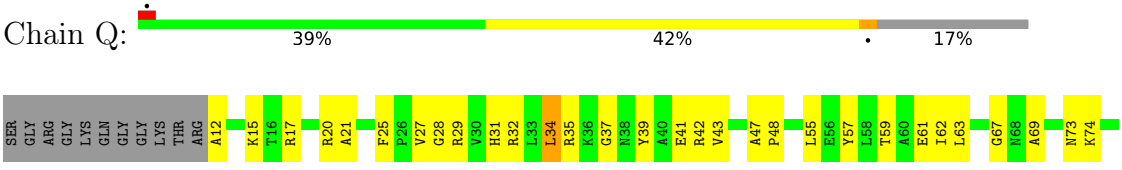
• Molecule 12: Histone H4

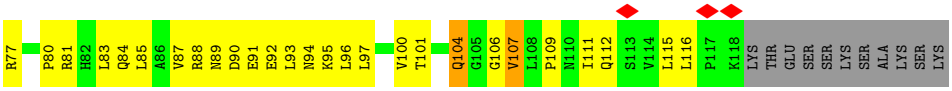
Chain T:



• Molecule 13: Histone H2A

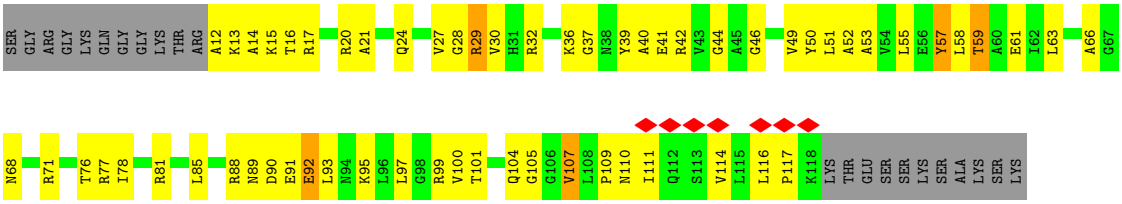
Chain Q:





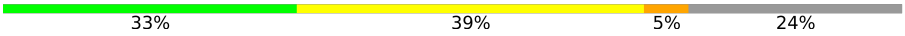
• Molecule 13: Histone H2A

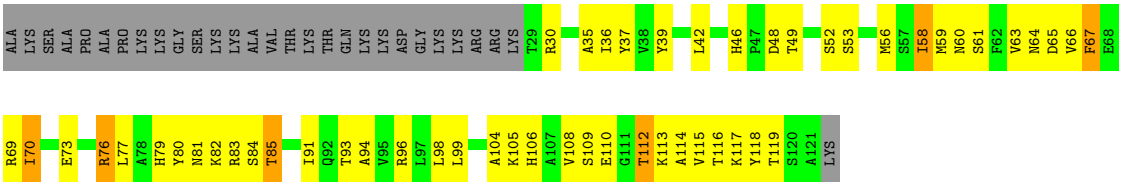
Chain U:



• Molecule 14: Histone H2B 1.1

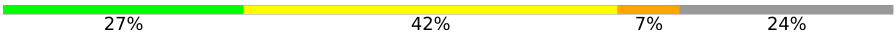
Chain R:

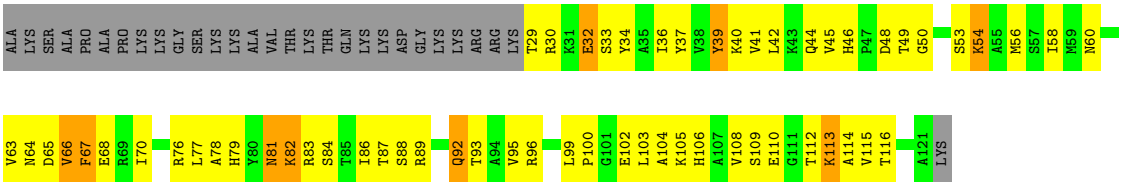




• Molecule 14: Histone H2B 1.1

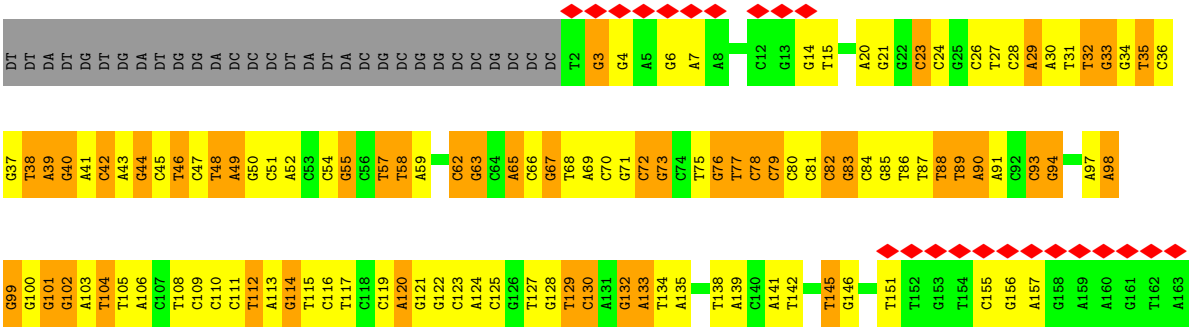
Chain V:

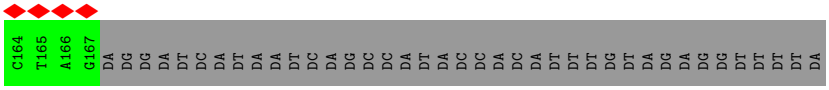




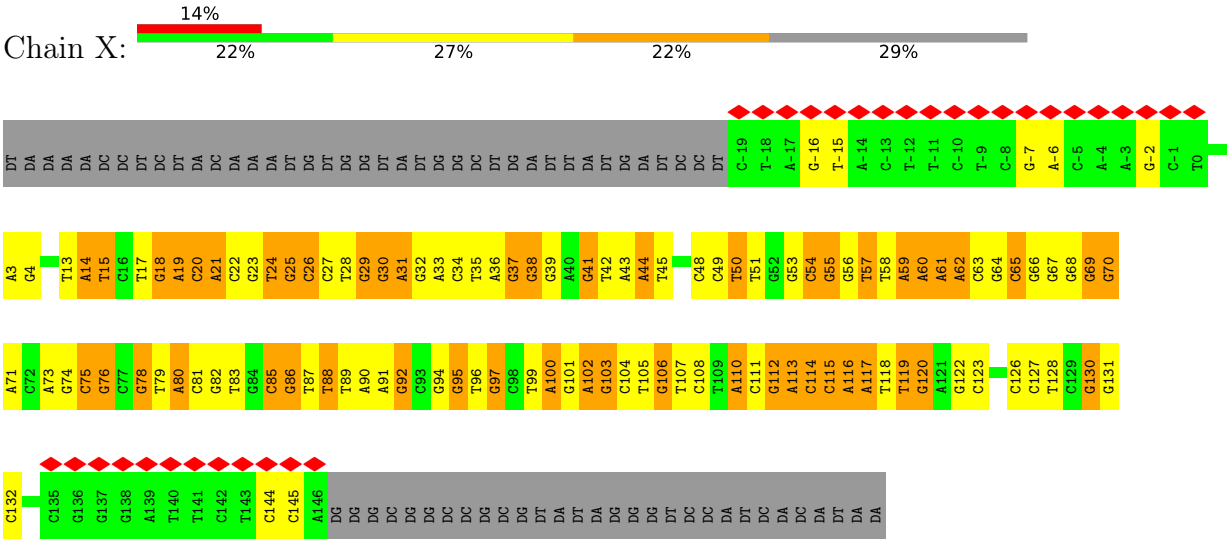
• Molecule 15: DNA (239-MER)

Chain W:





• Molecule 16: DNA (239-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	429.68002, 429.68002, 429.68002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1484, 2.1484, 2.1484	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, MG, 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	B	0.29	0/4171	0.49	1/5648 (0.0%)
2	C	0.31	0/2926	0.49	0/3953
3	D	0.30	0/3318	0.45	0/4465
3	E	0.29	0/3526	0.47	0/4747
4	H	0.26	0/3201	0.47	1/4322 (0.0%)
5	I	0.25	0/902	0.48	0/1211
6	J	0.27	0/1390	0.47	0/1874
7	A	0.32	0/6256	0.52	0/8415
8	L	0.36	0/493	0.59	0/659
9	M	0.38	0/3197	0.57	0/4313
10	N	0.35	0/3234	0.56	1/4382 (0.0%)
11	O	0.42	0/812	0.63	1/1091 (0.1%)
11	S	0.40	0/788	0.68	0/1057
12	P	0.39	0/711	0.59	0/950
12	T	0.39	0/680	0.61	0/912
13	Q	0.37	0/821	0.57	0/1112
13	U	0.41	0/825	0.60	0/1116
14	R	0.47	0/729	0.60	0/985
14	V	0.45	0/737	0.63	0/993
15	W	1.63	70/3804 (1.8%)	1.37	37/5866 (0.6%)
16	X	1.67	77/3830 (2.0%)	1.48	56/5912 (0.9%)
All	All	0.74	147/46351 (0.3%)	0.77	97/63983 (0.2%)

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	55	DG	N9-C4	-10.06	1.29	1.38
16	X	33	DA	N9-C4	-9.92	1.31	1.37
16	X	61	DA	C3'-O3'	-9.43	1.31	1.44
16	X	14	DA	N9-C4	-9.01	1.32	1.37
15	W	106	DA	N9-C4	-8.95	1.32	1.37

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	132	DG	O4'-C1'-N9	11.49	116.04	108.00
15	W	90	DA	O4'-C1'-N9	10.17	115.12	108.00
16	X	74	DG	O4'-C1'-N9	8.79	114.16	108.00
16	X	42	DT	O4'-C1'-N1	8.61	114.03	108.00
16	X	65	DC	O4'-C4'-C3'	-8.13	101.12	106.00

There are no chirality outliers.

There are no planarity outliers.

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	B	4098	0	4239	190	0
2	C	2873	0	2807	107	0
3	D	3250	0	3301	177	0
3	E	3454	0	3511	76	0
4	H	3145	0	3143	45	0
5	I	888	0	867	10	0
6	J	1360	0	1400	47	0
7	A	6162	0	6271	497	0
8	L	482	0	455	31	0
9	M	3131	0	3129	180	0
10	N	3167	0	3149	155	0
11	O	800	0	829	57	0
11	S	778	0	813	73	0
12	P	703	0	757	40	0
12	T	672	0	698	57	0
13	Q	811	0	849	54	0
13	U	815	0	860	59	0
14	R	718	0	725	51	0
14	V	726	0	747	51	0
15	W	3393	0	1863	183	0
16	X	3413	0	1865	177	0
17	A	27	0	10	27	0
18	A	4	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	1	0	0	0	0
All	All	44871	0	42288	1714	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 1714 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)
1:B:940:ARG:HH12	1:B:985:LEU:CD1	1.02	1.64
3:D:565:PHE:CZ	7:A:542:GLN:HB2	1.36	1.57
9:M:214:GLN:NE2	9:M:216:ARG:CG	1.68	1.50
3:D:565:PHE:CE1	7:A:542:GLN:HB2	1.43	1.50
3:D:540:GLN:NE2	7:A:537:GLN:HB3	1.23	1.48

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	489/1093 (45%)	460 (94%)	25 (5%)	4 (1%)	19	60
2	C	347/918 (38%)	309 (89%)	36 (10%)	2 (1%)	25	66
3	D	385/836 (46%)	372 (97%)	13 (3%)	0	100	100
3	E	414/836 (50%)	389 (94%)	24 (6%)	1 (0%)	47	81
4	H	376/566 (66%)	345 (92%)	30 (8%)	1 (0%)	41	77
5	I	102/332 (31%)	93 (91%)	8 (8%)	1 (1%)	15	54
6	J	159/634 (25%)	147 (92%)	11 (7%)	1 (1%)	25	66
7	A	734/982 (75%)	682 (93%)	46 (6%)	6 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	L	45/157 (29%)	42 (93%)	3 (7%)	0	100 100
9	M	360/477 (76%)	344 (96%)	15 (4%)	1 (0%)	41 77
10	N	381/467 (82%)	358 (94%)	22 (6%)	1 (0%)	41 77
11	O	96/135 (71%)	90 (94%)	6 (6%)	0	100 100
11	S	93/135 (69%)	84 (90%)	9 (10%)	0	100 100
12	P	85/102 (83%)	81 (95%)	4 (5%)	0	100 100
12	T	84/102 (82%)	79 (94%)	5 (6%)	0	100 100
13	Q	105/129 (81%)	102 (97%)	3 (3%)	0	100 100
13	U	105/129 (81%)	101 (96%)	4 (4%)	0	100 100
14	R	91/122 (75%)	86 (94%)	5 (6%)	0	100 100
14	V	91/122 (75%)	90 (99%)	1 (1%)	0	100 100
All	All	4542/8274 (55%)	4254 (94%)	270 (6%)	18 (0%)	38 72

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	868	ILE
1	B	1051	LYS
2	C	655	ILE
2	C	664	ASP
7	A	490	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	484/1017 (48%)	445 (92%)	39 (8%)	11 35
2	C	321/832 (39%)	291 (91%)	30 (9%)	9 28
3	D	368/758 (48%)	342 (93%)	26 (7%)	14 39
3	E	393/758 (52%)	363 (92%)	30 (8%)	13 37
4	H	360/517 (70%)	328 (91%)	32 (9%)	9 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	I	102/288 (35%)	93 (91%)	9 (9%)	10 31
6	J	150/565 (26%)	144 (96%)	6 (4%)	31 55
7	A	678/889 (76%)	639 (94%)	39 (6%)	20 45
8	L	52/140 (37%)	50 (96%)	2 (4%)	33 57
9	M	345/420 (82%)	317 (92%)	28 (8%)	11 35
10	N	359/423 (85%)	333 (93%)	26 (7%)	14 39
11	O	84/110 (76%)	71 (84%)	13 (16%)	2 14
11	S	82/110 (74%)	68 (83%)	14 (17%)	2 11
12	P	72/78 (92%)	63 (88%)	9 (12%)	4 19
12	T	67/78 (86%)	53 (79%)	14 (21%)	1 6
13	Q	81/101 (80%)	73 (90%)	8 (10%)	8 26
13	U	82/101 (81%)	73 (89%)	9 (11%)	6 22
14	R	77/102 (76%)	67 (87%)	10 (13%)	4 18
14	V	79/102 (78%)	64 (81%)	15 (19%)	1 8
All	All	4236/7389 (57%)	3877 (92%)	359 (8%)	14 33

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	216	ARG
12	P	67	ARG
9	M	402	GLU
10	N	304	ASN
14	R	65	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	614	ASN
9	M	253	GLN
7	A	637	HIS
8	L	67	GLN
10	N	139	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	BEF	A	1502	-	0,3,3	-	-	-		
17	ADP	A	1501	7,19	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)

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
17	ADP	A	1501	7,19	-	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)
17	A	1501	ADP	C5-C4	2.52	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1501	ADP	C3'-C2'-C1'	3.36	106.03	100.98
17	A	1501	ADP	PA-O3A-PB	-3.33	121.41	132.83
17	A	1501	ADP	N3-C2-N1	-3.14	123.78	128.68
17	A	1501	ADP	C4-C5-N7	-2.61	106.68	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	1501	ADP	C5'-O5'-PA-O1A

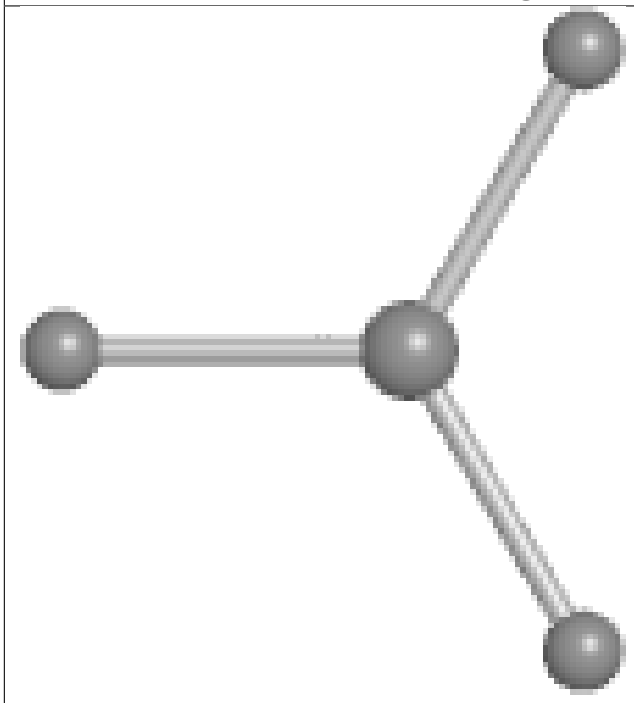
There are no ring outliers.

2 monomers are involved in 30 short contacts:

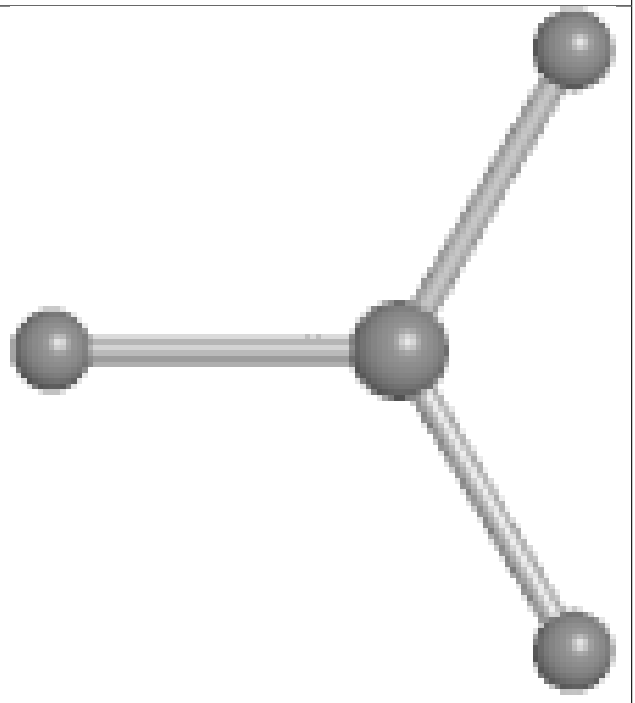
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1502	BEF	5	0
17	A	1501	ADP	27	0

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 then 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.

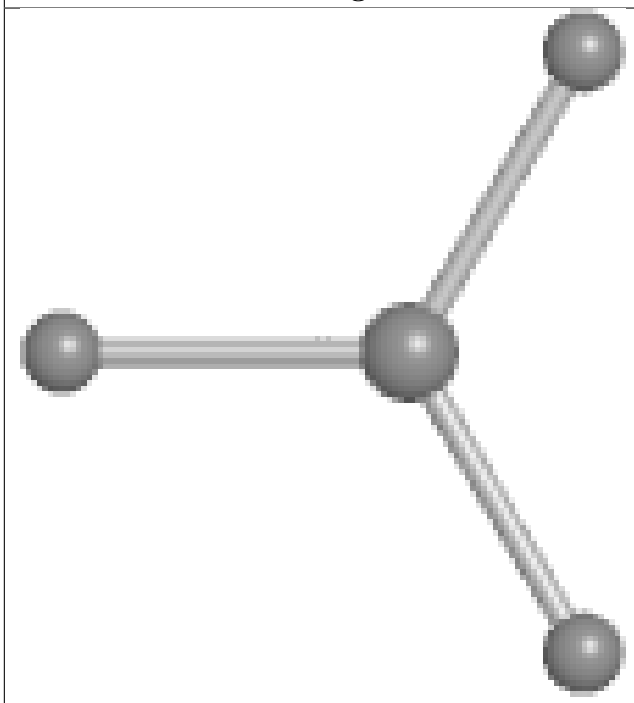
Ligand BEF A 1502



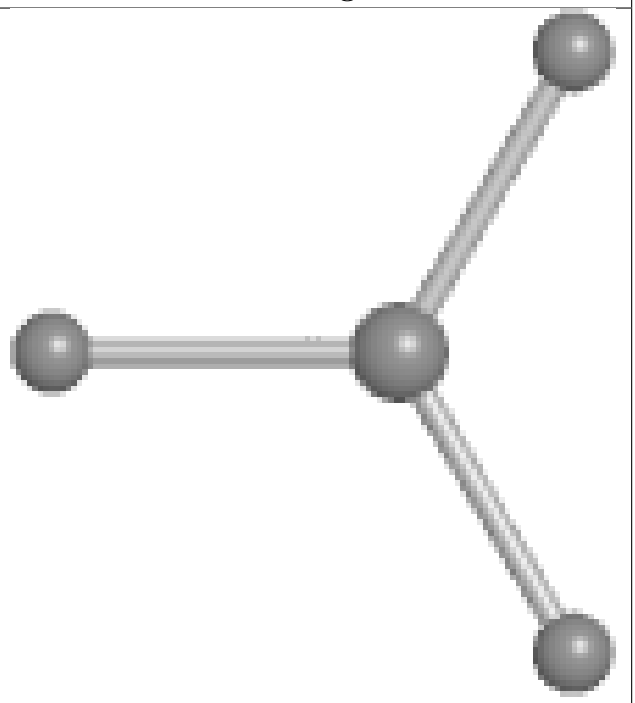
Bond lengths



Bond angles

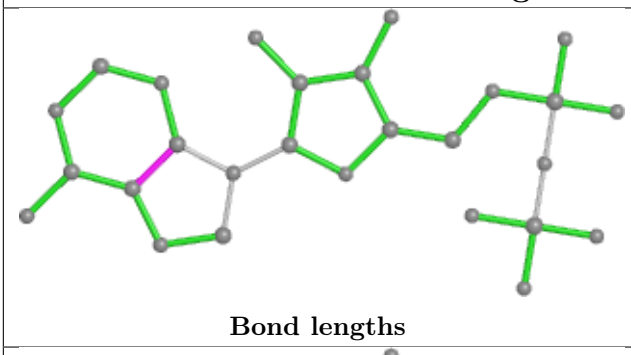


Torsions

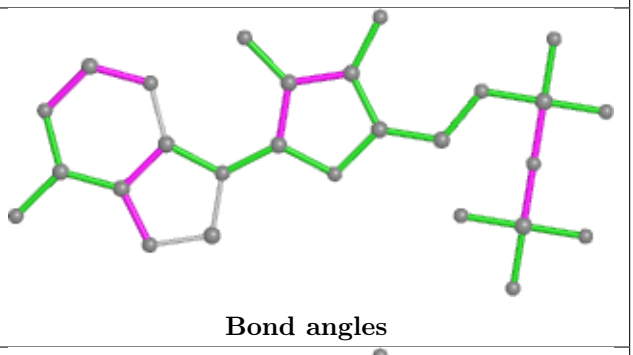


Rings

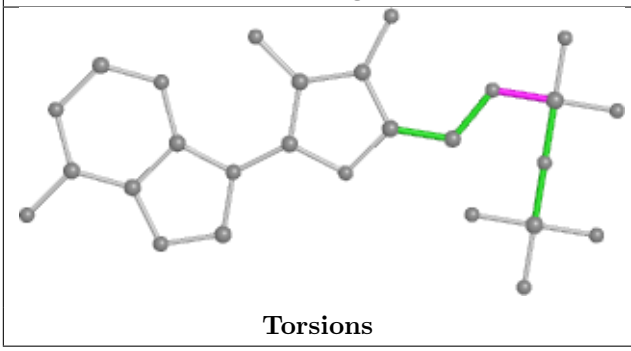
Ligand ADP A 1501



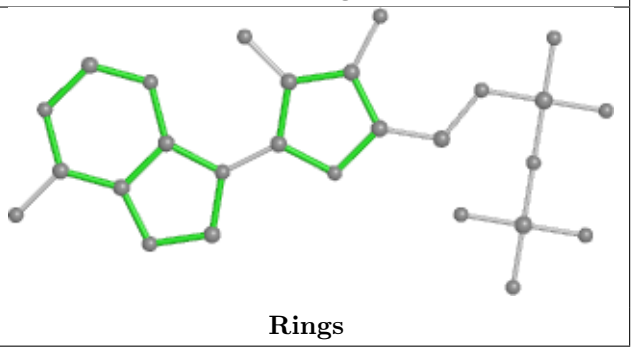
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

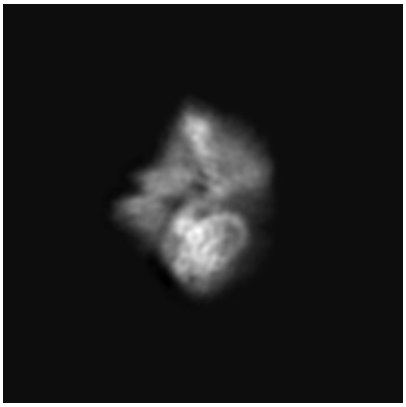
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31137. These allow visual inspection of the internal detail of the map and identification of artifacts.

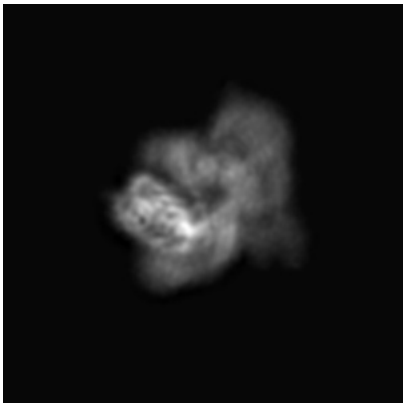
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

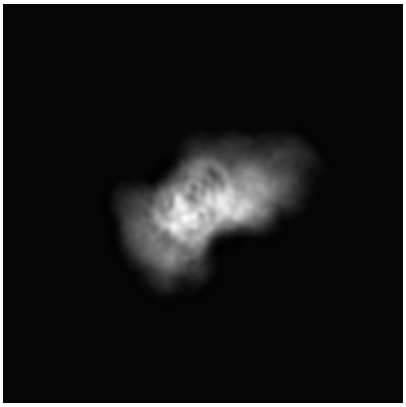
6.1.1 Primary map



X



Y

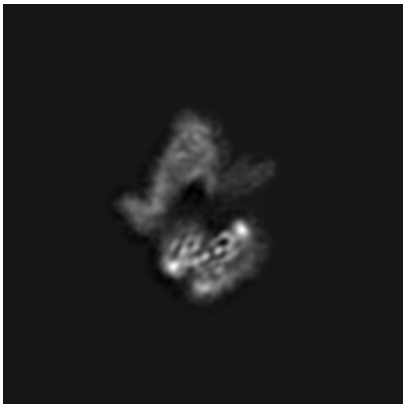


Z

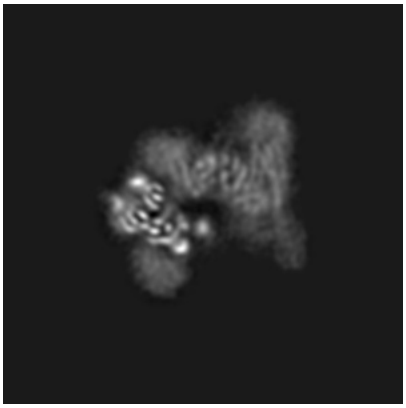
The images above show the map projected in three orthogonal directions.

6.2 Central slices

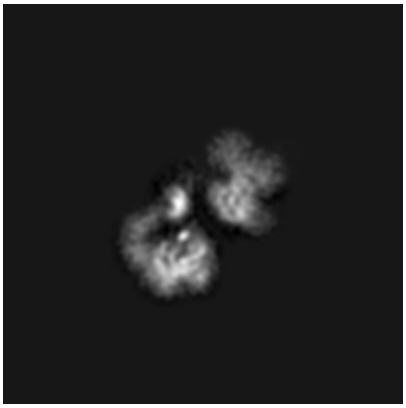
6.2.1 Primary map



X Index: 100



Y Index: 100



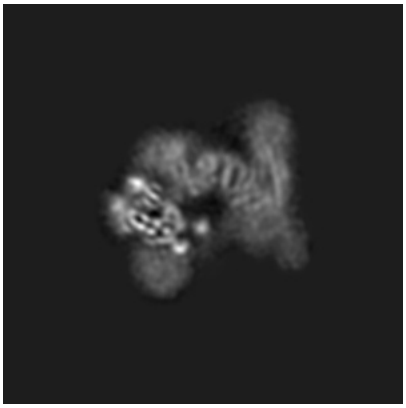
Z Index: 100

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

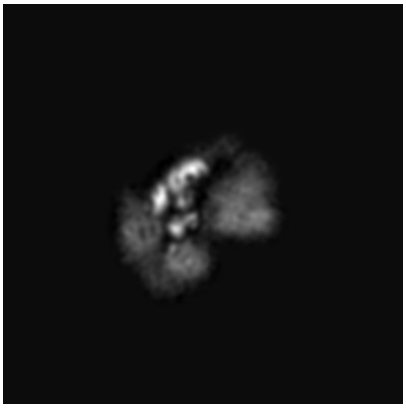
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 87



Y Index: 98

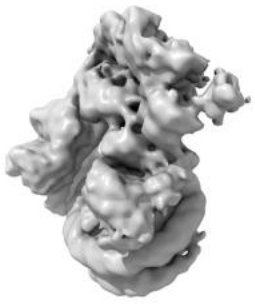


Z Index: 90

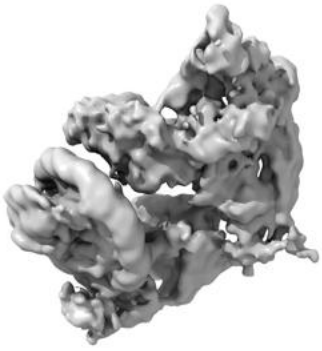
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

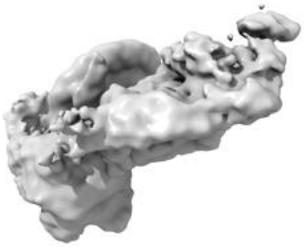
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

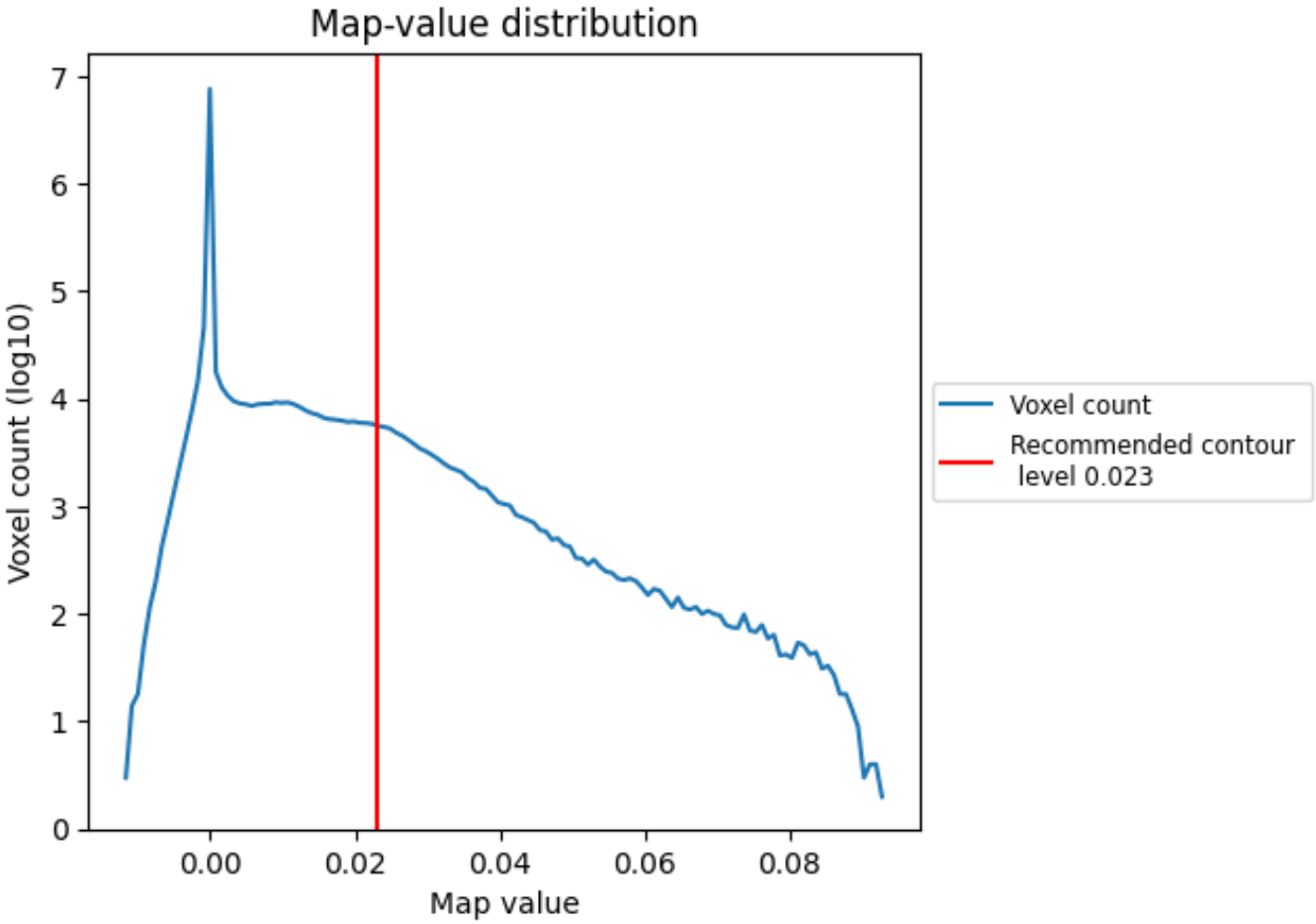
6.5 Mask visualisation (i)

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

7 Map analysis

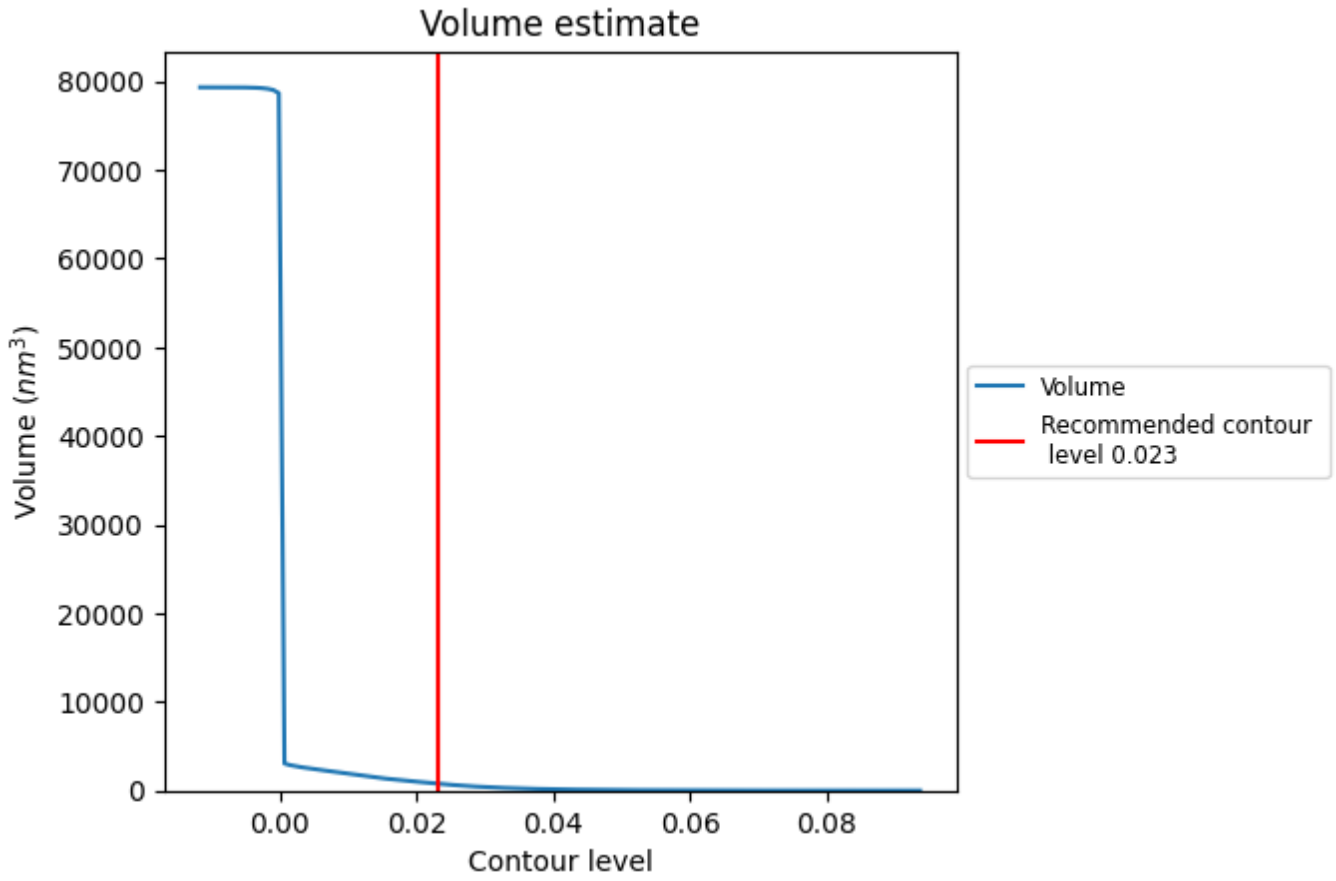
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

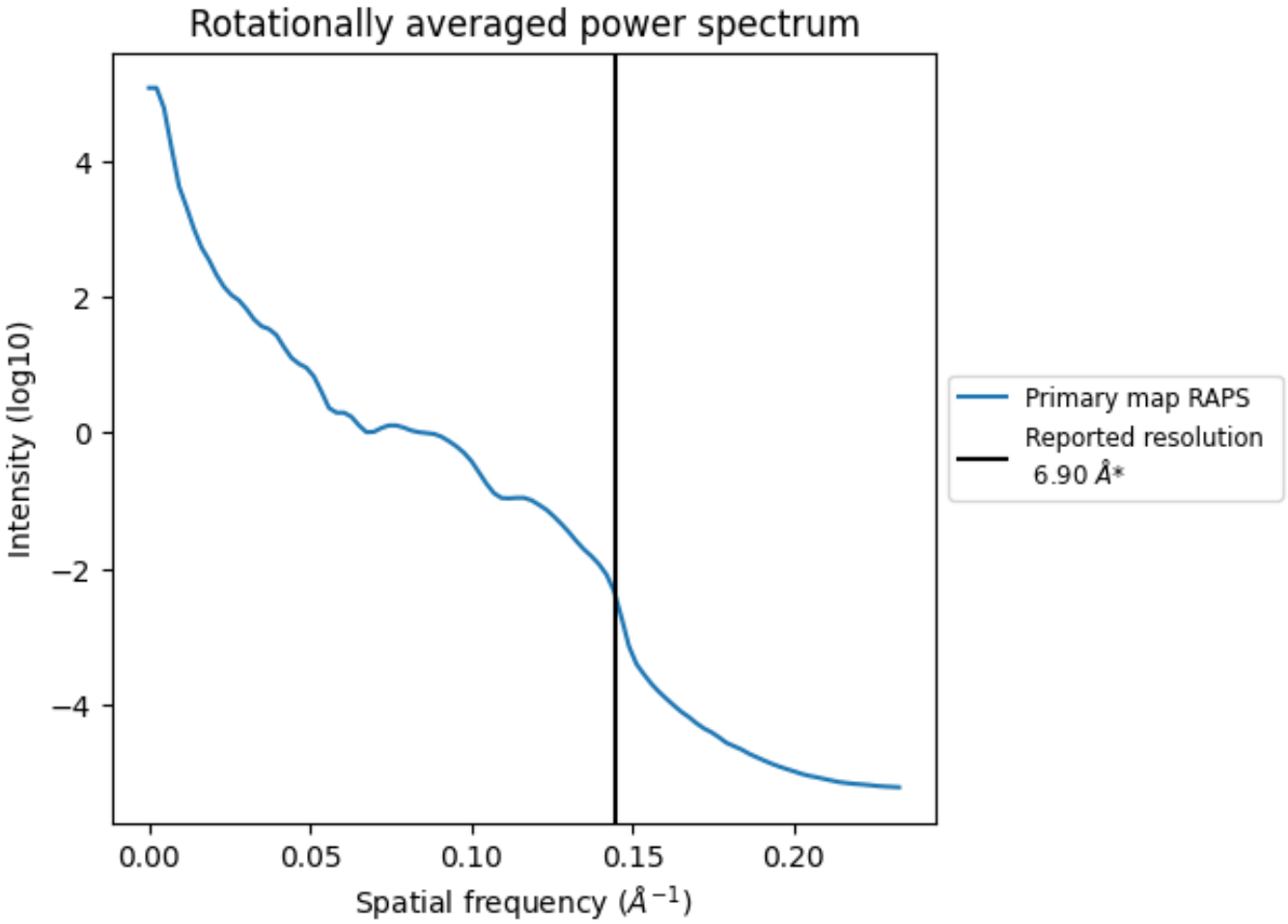
7.2 Volume estimate (i)



The volume at the recommended contour level is 786 nm^3; this corresponds to an approximate mass of 710 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.145 Å^{-1}

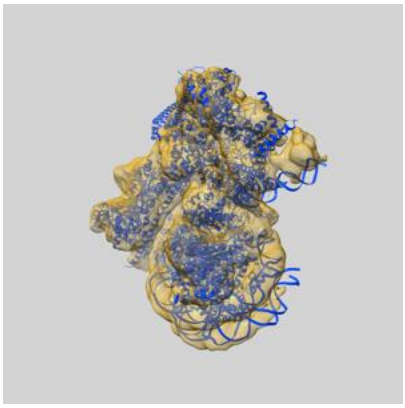
8 Fourier-Shell correlation

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

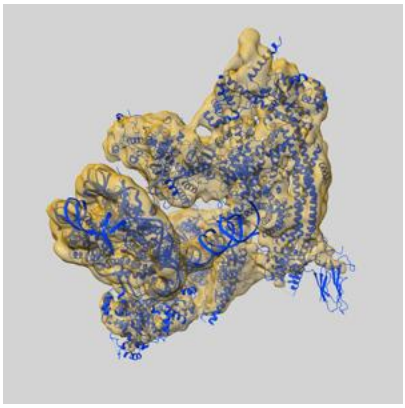
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31137 and PDB model 7EGP. Per-residue inclusion information can be found in section 3 on page 11.

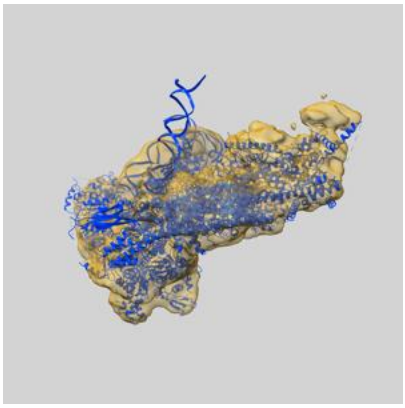
9.1 Map-model overlay



X



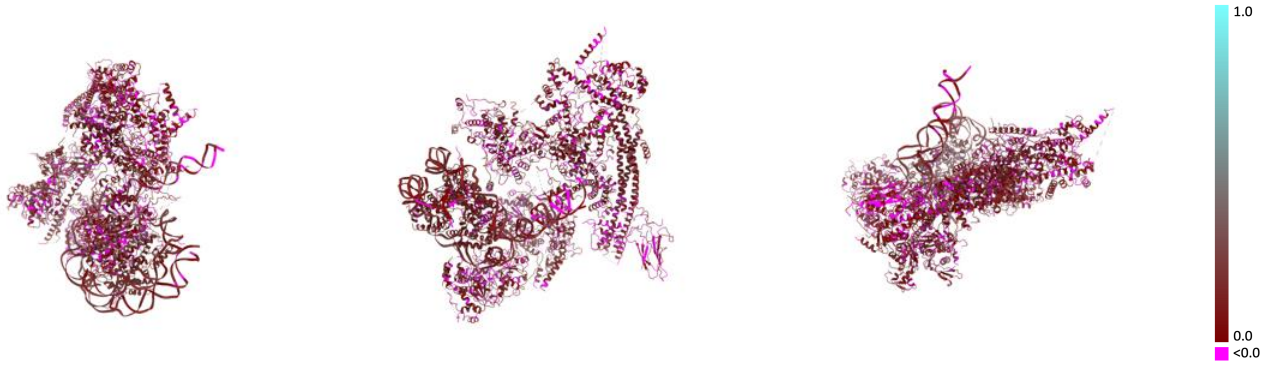
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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.

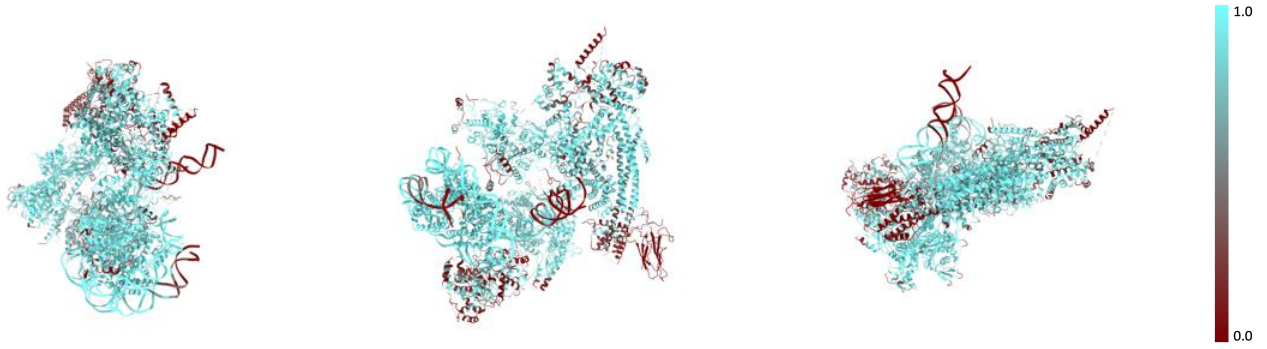
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

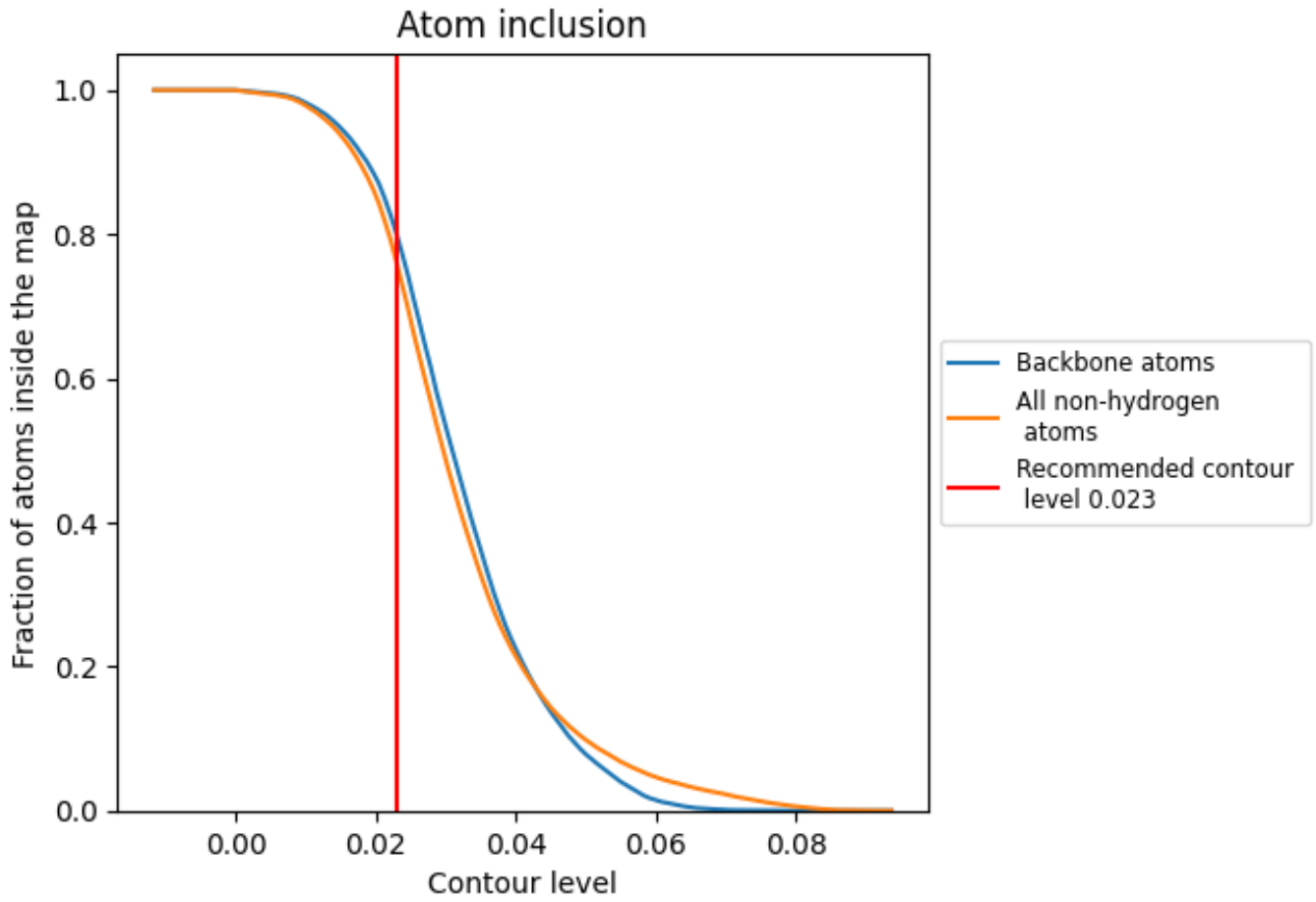
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7591	0.1050
A	0.5666	0.0840
B	0.8195	0.1060
C	0.8179	0.1010
D	0.6605	0.0800
E	0.6794	0.0780
H	0.4470	0.0690
I	0.6482	0.0950
J	0.6682	0.0770
L	0.8688	0.0480
M	0.9657	0.1100
N	0.9125	0.0950
O	0.9442	0.1280
P	0.8871	0.1410
Q	0.9504	0.1460
R	0.9929	0.1800
S	0.9773	0.1450
T	0.9167	0.1440
U	0.8949	0.1320
V	0.9619	0.1690
W	0.8087	0.1400
X	0.7981	0.1480