wwPDB EM Validation Summary Report (i)

Feb 26, 2024 – 07:21 PM EST

PDB ID	:	6VZ4
EMDB ID	:	EMD-21484
Title	:	Cryo-EM structure of Sth1-Arp7-Arp9-Rtt102 bound to the nucleosome in ADP Beryllium Fluoride state
Authors	:	Leschziner, A.E.; Baker, R.W.
Deposited on	:	2020-02-27
Resolution	:	3.90 Å(reported)
Based on initial models	:	4I6M, 5Z3U, 5TGC

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 (i) 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 (1)) were used in the production of this report:

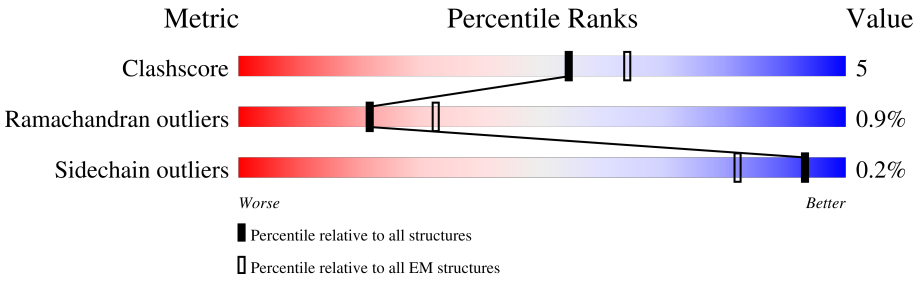
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1-A	136	70% · 28%
1	1-E	136	67% · 30%
1	10-A	136	70% · 28%
1	10-E	136	67% · 30%
1	2-A	136	70% · 28%
1	2-E	136	65% · 30%
1	3-A	136	70% · 28%
1	3-E	136	66% · 30%

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Mol	Chain	Length	Quality of chain
1	4-A	136	68% 28%
1	4-E	136	66% 30%
1	5-A	136	70% 28%
1	5-E	136	66% 30%
1	6-A	136	70% 28%
1	6-E	136	66% 30%
1	7-A	136	70% 28%
1	7-E	136	66% 30%
1	8-A	136	70% 28%
1	8-E	136	66% 30%
1	9-A	136	69% 28%
1	9-E	136	66% 30%
2	1-B	103	82% 16%
2	1-F	103	72% 5% 23%
2	10-B	103	82% 16%
2	10-F	103	72% 5% 23%
2	2-B	103	82% 16%
2	2-F	103	73% 23%
2	3-B	103	82% 16%
2	3-F	103	74% 23%
2	4-B	103	82% 16%
2	4-F	103	74% 23%
2	5-B	103	82% 16%
2	5-F	103	73% 23%
2	6-B	103	83% 16%

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Mol	Chain	Length	Quality of chain
2	6-F	103	73% · 23%
2	7-B	103	83% · 16%
2	7-F	103	72% 5% 23%
2	8-B	103	83% · 16%
2	8-F	103	73% · 23%
2	9-B	103	82% · 16%
2	9-F	103	73% · 23%
3	1-C	130	79% · 18%
3	1-G	130	75% 7% 18%
3	10-C	130	79% · 18%
3	10-G	130	75% 7% 18%
3	2-C	130	79% · 18%
3	2-G	130	75% 7% 18%
3	3-C	130	78% 5% 18%
3	3-G	130	75% 7% 18%
3	4-C	130	79% · 18%
3	4-G	130	75% 7% 18%
3	5-C	130	79% · 18%
3	5-G	130	75% 7% 18%
3	6-C	130	79% · 18%
3	6-G	130	75% 7% 18%
3	7-C	130	79% · 18%
3	7-G	130	75% 7% 18%
3	8-C	130	79% · 18%
3	8-G	130	75% 7% 18%

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Mol	Chain	Length	Quality of chain
3	9-C	130	79% · 18%
3	9-G	130	75% 7% 18%
4	1-D	125	74% 26%
4	1-H	125	72% · 26%
4	10-D	125	74% 26%
4	10-H	125	72% · 26%
4	2-D	125	74% 26%
4	2-H	125	73% · 26%
4	3-D	125	73% · 26%
4	3-H	125	73% · 26%
4	4-D	125	74% 26%
4	4-H	125	72% · 26%
4	5-D	125	74% 26%
4	5-H	125	72% · 26%
4	6-D	125	74% 26%
4	6-H	125	73% · 26%
4	7-D	125	74% 26%
4	7-H	125	73% · 26%
4	8-D	125	74% 26%
4	8-H	125	72% · 26%
4	9-D	125	74% 26%
4	9-H	125	72% · 26%
5	1-I	185	67% 12% 21%
5	10-I	185	68% 11% 21%
5	2-I	185	66% 12% 21%

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Mol	Chain	Length	Quality of chain
5	3-I	185	67% 12% 21%
5	4-I	185	67% 12% 21%
5	5-I	185	67% 12% 21%
5	6-I	185	67% 12% 21%
5	7-I	185	66% 12% 21%
5	8-I	185	67% 12% 21%
5	9-I	185	68% 11% 21%
6	1-J	185	69% 10% 21%
6	10-J	185	68% 11% 21%
6	2-J	185	69% 10% 21%
6	3-J	185	68% 11% 21%
6	4-J	185	68% 11% 21%
6	5-J	185	69% 10% 21%
6	6-J	185	68% 11% 21%
6	7-J	185	68% 11% 21%
6	8-J	185	69% 10% 21%
6	9-J	185	68% 11% 21%
7	1-K	813	67% 7% 24%
7	10-K	813	66% 9% 24%
7	2-K	813	67% 8% 24%
7	3-K	813	68% 7% 24%
7	4-K	813	65% 9% 24%
7	5-K	813	67% 8% 24%
7	6-K	813	67% 8% 24%
7	7-K	813	67% 8% 24%

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Mol	Chain	Length	Quality of chain
7	8-K	813	67% 8% 24%
7	9-K	813	66% 8% 24%
8	1-L	477	31% 79% 18%
8	10-L	477	79% 18%
8	2-L	477	79% 18%
8	3-L	477	79% 18%
8	4-L	477	79% 18%
8	5-L	477	79% 18%
8	6-L	477	79% 18%
8	7-L	477	79% 18%
8	8-L	477	79% 18%
8	9-L	477	79% 18%
9	1-M	467	19% 78% 7% 15%
9	10-M	467	78% 7% 15%
9	2-M	467	78% 7% 15%
9	3-M	467	78% 7% 15%
9	4-M	467	78% 7% 15%
9	5-M	467	78% 7% 15%
9	6-M	467	78% 7% 15%
9	7-M	467	78% 7% 15%
9	8-M	467	77% 7% 15%
9	9-M	467	78% 7% 15%
10	1-N	157	18% 31% 65%
10	10-N	157	31% 65%
10	2-N	157	31% 65%

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Mol	Chain	Length	Quality of chain
10	3-N	157	31% 65%
10	4-N	157	31% 65%
10	5-N	157	31% 65%
10	6-N	157	31% 65%
10	7-N	157	31% 65%
10	8-N	157	31% 65%
10	9-N	157	31% 65%

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
13	BEF	3-K	1503	-	-	X	-
13	BEF	9-K	1503	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 239500 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	2-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	3-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	4-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	5-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	6-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	7-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	8-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	9-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	10-A	98	Total	C	N	O	S	0	0
			809	510	157	139	3		
1	1-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	2-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	3-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	4-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	5-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	6-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	7-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	9-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		
1	10-E	95	Total	C	N	O	S	0	0
			783	493	151	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	2-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	3-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	4-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	5-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	6-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	7-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	8-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	9-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	10-B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	1-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	2-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	3-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	4-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	5-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	6-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	7-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	8-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	9-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	10-F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	2-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	3-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	4-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	5-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	6-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	7-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	8-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	9-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	10-C	107	Total	C	N	O	0	0
			823	519	161	143		
3	1-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	2-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	3-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	4-G	107	Total	C	N	O	0	0
			823	519	161	143		
3	5-G	107	Total	C	N	O	0	0
			823	519	161	143		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	6-G	107	Total 823	C 519	N 161	O 143	0	0
3	7-G	107	Total 823	C 519	N 161	O 143	0	0
3	8-G	107	Total 823	C 519	N 161	O 143	0	0
3	9-G	107	Total 823	C 519	N 161	O 143	0	0
3	10-G	107	Total 823	C 519	N 161	O 143	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	2-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	3-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	4-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	5-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	6-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	7-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	8-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	9-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	10-D	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	1-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	2-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	3-H	92	Total 719	C 453	N 129	O 135	S 2	0	0
4	4-H	92	Total 719	C 453	N 129	O 135	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	6-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	7-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	8-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	9-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
4	10-H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	THR	SER	conflict	UNP Q92130
H	33	THR	SER	conflict	UNP Q92130

- Molecule 5 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	2-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	3-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	4-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	5-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	6-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	7-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	8-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	9-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		
5	10-I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	2-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	3-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	4-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	5-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	6-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	7-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	8-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	9-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		
6	10-J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	2-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	3-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	4-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	5-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	6-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	7-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	8-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		
7	9-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	10-K	616	Total	C	N	O	S	0	0
			5055	3201	900	934	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	285	MET	-	initiating methionine	UNP P32597
K	286	GLY	-	expression tag	UNP P32597
K	287	SER	-	expression tag	UNP P32597
K	288	SER	-	expression tag	UNP P32597
K	289	HIS	-	expression tag	UNP P32597
K	290	HIS	-	expression tag	UNP P32597
K	291	HIS	-	expression tag	UNP P32597
K	292	HIS	-	expression tag	UNP P32597
K	293	HIS	-	expression tag	UNP P32597
K	294	HIS	-	expression tag	UNP P32597
K	295	SER	-	expression tag	UNP P32597
K	296	GLN	-	expression tag	UNP P32597
K	297	ASP	-	expression tag	UNP P32597
K	298	PRO	-	expression tag	UNP P32597
K	299	ASN	-	expression tag	UNP P32597
K	300	SER	-	expression tag	UNP P32597

- Molecule 8 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	2-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	3-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	4-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	5-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	6-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	7-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	8-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	9-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
8	10-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		

- Molecule 9 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	2-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	3-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	4-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	5-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	6-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	7-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	8-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	9-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
9	10-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		

- Molecule 10 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	2-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	3-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	4-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	5-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

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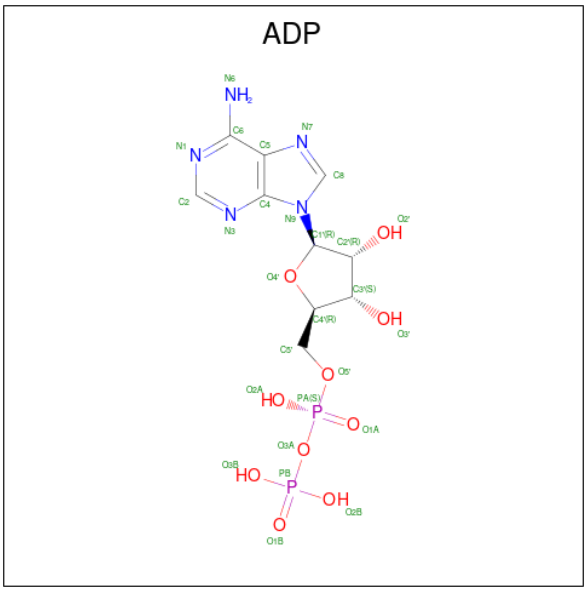
Mol	Chain	Residues	Atoms					AltConf	Trace
10	6-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	7-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	8-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	9-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
10	10-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

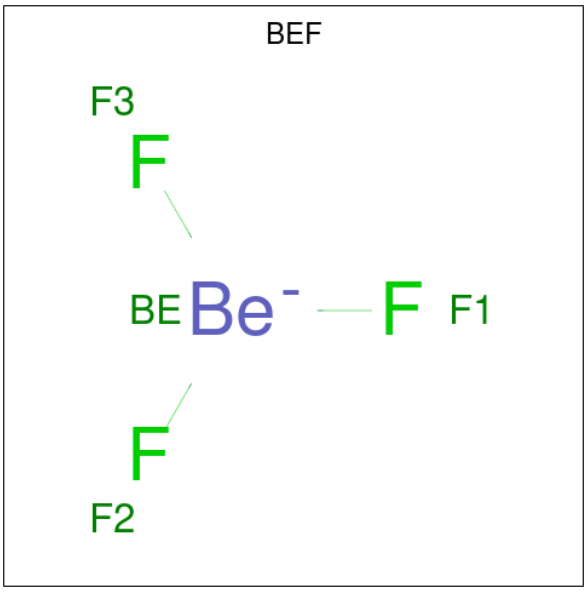
Mol	Chain	Residues	Atoms		AltConf
11	1-K	1	Total	Mg	0
			1	1	
11	2-K	1	Total	Mg	0
			1	1	
11	3-K	1	Total	Mg	0
			1	1	
11	4-K	1	Total	Mg	0
			1	1	
11	5-K	1	Total	Mg	0
			1	1	
11	6-K	1	Total	Mg	0
			1	1	
11	7-K	1	Total	Mg	0
			1	1	
11	8-K	1	Total	Mg	0
			1	1	
11	9-K	1	Total	Mg	0
			1	1	
11	10-K	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



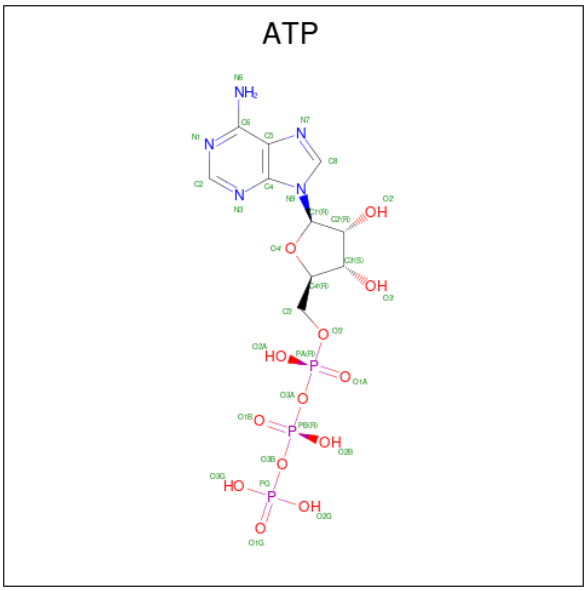
Mol	Chain	Residues	Atoms					AltConf
12	1-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	2-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	3-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	4-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	5-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	6-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	7-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	8-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	9-K	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	10-K	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	AltConf
13	1-K	1	Total Be F 4 1 3	0
13	2-K	1	Total Be F 4 1 3	0
13	3-K	1	Total Be F 4 1 3	0
13	4-K	1	Total Be F 4 1 3	0
13	5-K	1	Total Be F 4 1 3	0
13	6-K	1	Total Be F 4 1 3	0
13	7-K	1	Total Be F 4 1 3	0
13	8-K	1	Total Be F 4 1 3	0
13	9-K	1	Total Be F 4 1 3	0
13	10-K	1	Total Be F 4 1 3	0

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



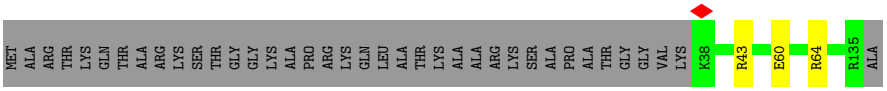
Mol	Chain	Residues	Atoms					AltConf
14	1-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	2-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	3-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	4-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	5-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	6-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	7-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	8-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	9-L	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	10-L	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

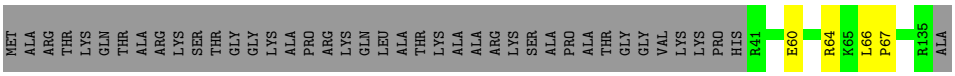
- Molecule 1: Histone H3

Chain 1-A:



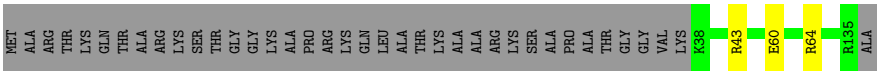
- Molecule 1: Histone H3

Chain 1-E:



- Molecule 1: Histone H3

Chain 2-A:

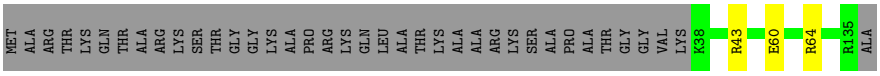


- Molecule 1: Histone H3

Chain 2-E:

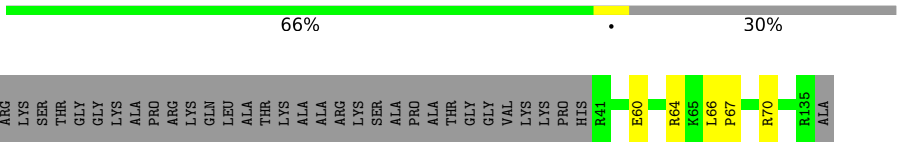
- Molecule 1: Histone H3

Chain 3-A:



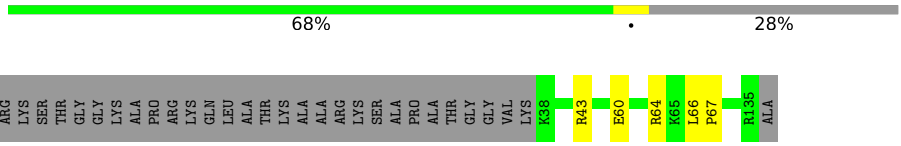
- Molecule 1: Histone H3

Chain 3-E:



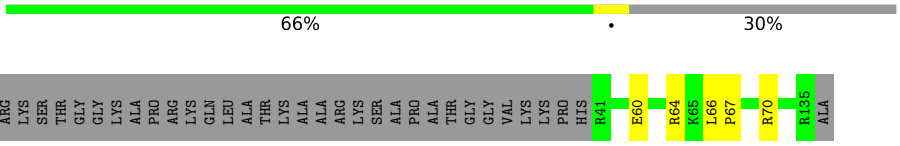
• Molecule 1: Histone H3

Chain 4-A:



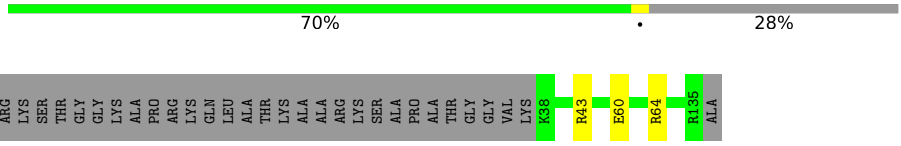
• Molecule 1: Histone H3

Chain 4-E:



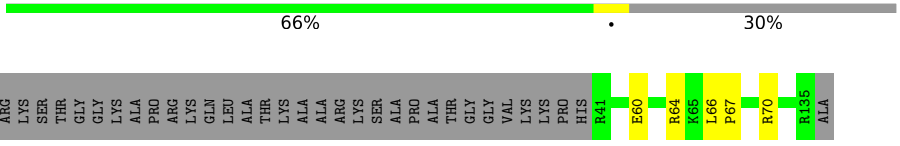
• Molecule 1: Histone H3

Chain 5-A:



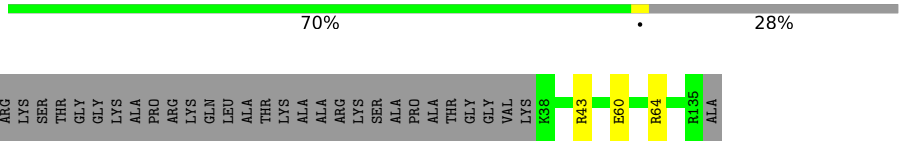
• Molecule 1: Histone H3

Chain 5-E:



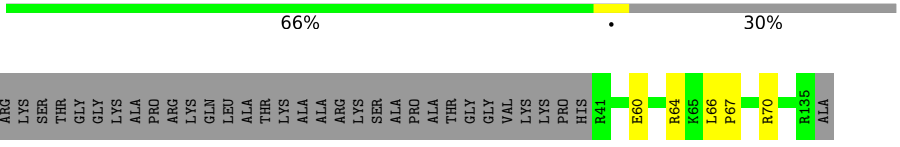
• Molecule 1: Histone H3

Chain 6-A:



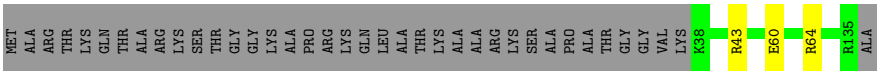
• Molecule 1: Histone H3

Chain 6-E:



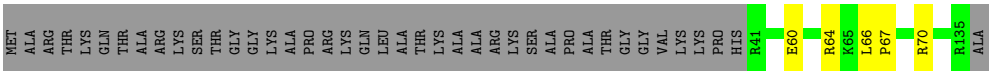
• Molecule 1: Histone H3

Chain 7-A:



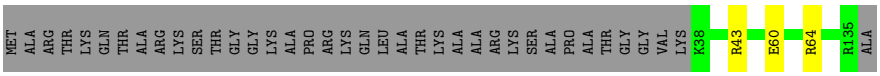
• Molecule 1: Histone H3

Chain 7-E:



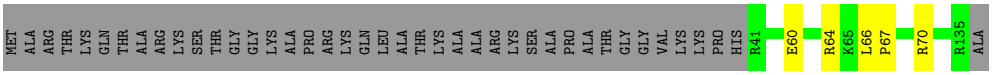
• Molecule 1: Histone H3

Chain 8-A:



• Molecule 1: Histone H3

Chain 8-E:

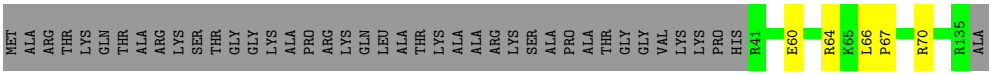


• Molecule 1: Histone H3

Chain 9-A:

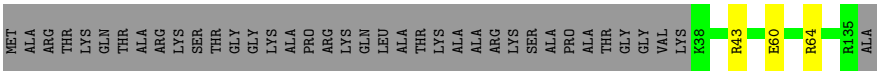
• Molecule 1: Histone H3

Chain 9-E:



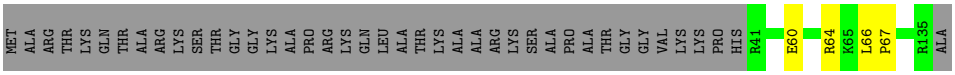
• Molecule 1: Histone H3

Chain 10-A:



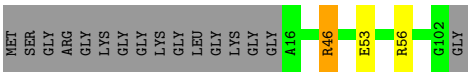
• Molecule 1: Histone H3

Chain 10-E:



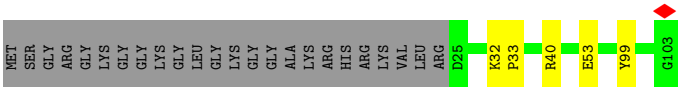
• Molecule 2: Histone H4

Chain 1-B:



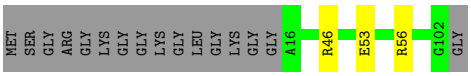
• Molecule 2: Histone H4

Chain 1-F:



• Molecule 2: Histone H4

Chain 2-B:

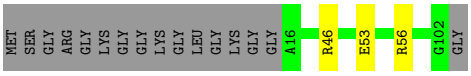


• Molecule 2: Histone H4

Chain 2-F:

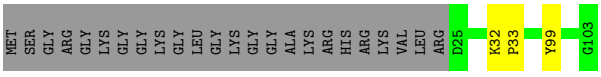
• Molecule 2: Histone H4

Chain 3-B:



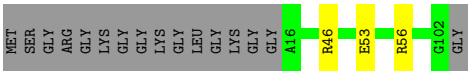
• Molecule 2: Histone H4

Chain 3-F:



• Molecule 2: Histone H4

Chain 4-B:

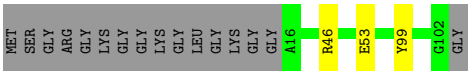


• Molecule 2: Histone H4

Chain 4-F:

• Molecule 2: Histone H4

Chain 5-B:

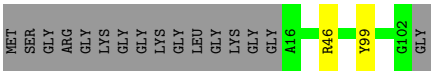


• Molecule 2: Histone H4

Chain 5-F:

• Molecule 2: Histone H4

Chain 6-B:

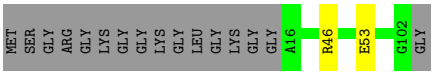


• Molecule 2: Histone H4

Chain 6-F:

• Molecule 2: Histone H4

Chain 7-B:

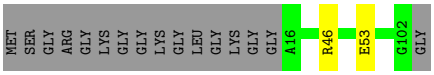


• Molecule 2: Histone H4

Chain 7-F:

• Molecule 2: Histone H4

Chain 8-B:

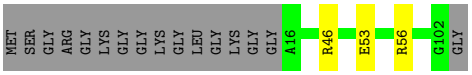


• Molecule 2: Histone H4

Chain 8-F:

• Molecule 2: Histone H4

Chain 9-B:

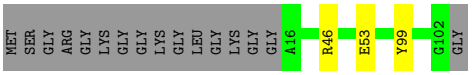


• Molecule 2: Histone H4

Chain 9-F:

• Molecule 2: Histone H4

Chain 10-B:

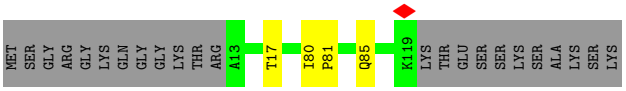


• Molecule 2: Histone H4

Chain 10-F:

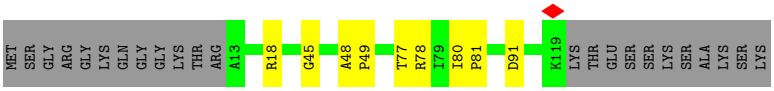
• Molecule 3: Histone H2A

Chain 1-C:



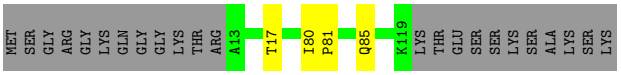
• Molecule 3: Histone H2A

Chain 1-G:



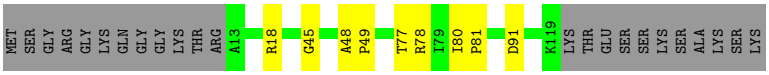
• Molecule 3: Histone H2A

Chain 2-C:



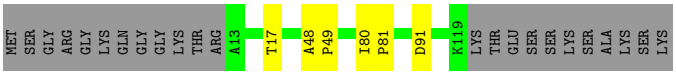
• Molecule 3: Histone H2A

Chain 2-G:



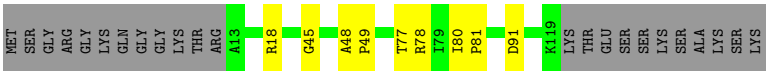
• Molecule 3: Histone H2A

Chain 3-C:



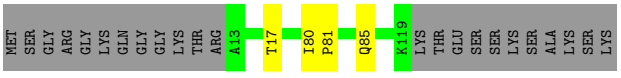
• Molecule 3: Histone H2A

Chain 3-G:



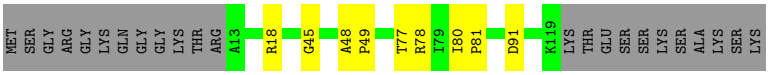
• Molecule 3: Histone H2A

Chain 4-C:



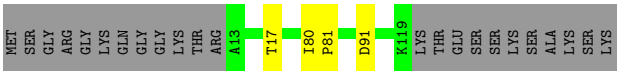
• Molecule 3: Histone H2A

Chain 4-G:



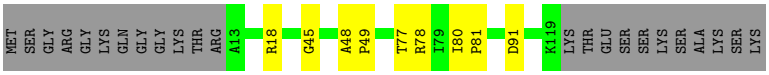
• Molecule 3: Histone H2A

Chain 5-C:



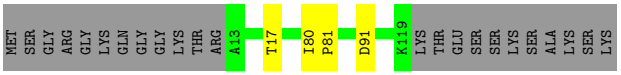
• Molecule 3: Histone H2A

Chain 5-G:



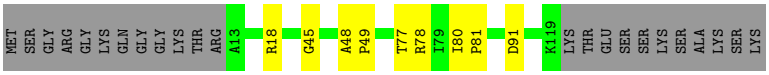
• Molecule 3: Histone H2A

Chain 6-C:



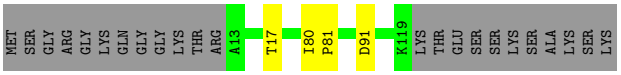
• Molecule 3: Histone H2A

Chain 6-G:



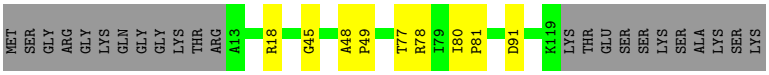
• Molecule 3: Histone H2A

Chain 7-C:



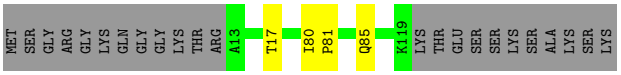
• Molecule 3: Histone H2A

Chain 7-G:



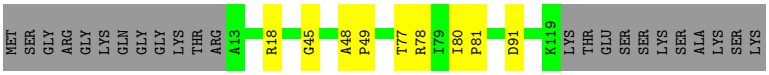
• Molecule 3: Histone H2A

Chain 8-C:



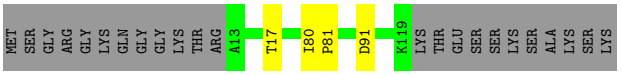
• Molecule 3: Histone H2A

Chain 8-G:



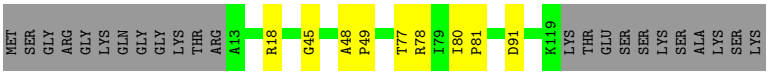
• Molecule 3: Histone H2A

Chain 9-C:



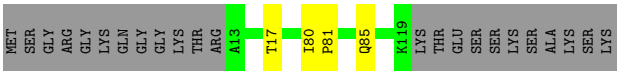
• Molecule 3: Histone H2A

Chain 9-G:



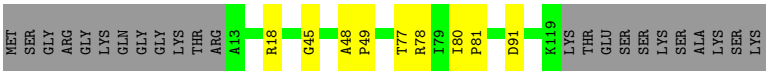
• Molecule 3: Histone H2A

Chain 10-C:



• Molecule 3: Histone H2A

Chain 10-G:



• Molecule 4: Histone H2B

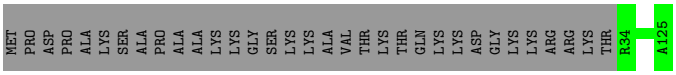
Chain 1-D:

• Molecule 4: Histone H2B

Chain 1-H:

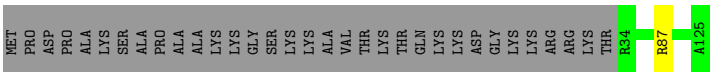
• Molecule 4: Histone H2B

Chain 2-D:



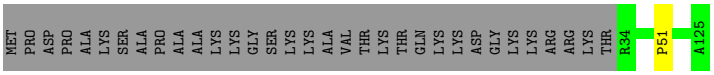
• Molecule 4: Histone H2B

Chain 2-H:



• Molecule 4: Histone H2B

Chain 3-D:

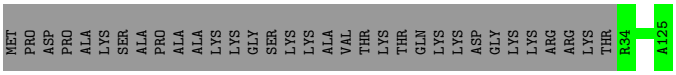


• Molecule 4: Histone H2B

Chain 3-H:

• Molecule 4: Histone H2B

Chain 4-D:

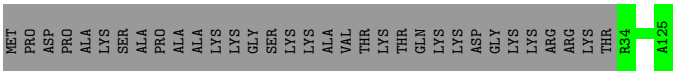


• Molecule 4: Histone H2B

Chain 4-H:

• Molecule 4: Histone H2B

Chain 5-D:

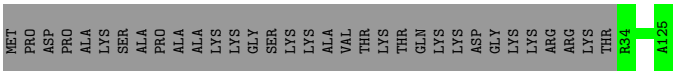


• Molecule 4: Histone H2B

Chain 5-H:

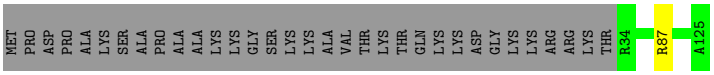
• Molecule 4: Histone H2B

Chain 6-D:



• Molecule 4: Histone H2B

Chain 6-H:

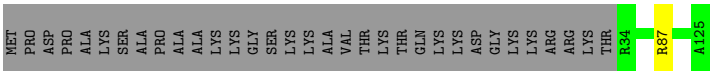


• Molecule 4: Histone H2B

Chain 7-D:

• Molecule 4: Histone H2B

Chain 7-H:



• Molecule 4: Histone H2B

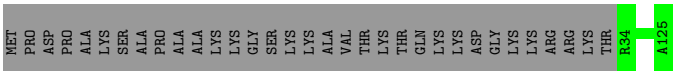
Chain 8-D:

• Molecule 4: Histone H2B

Chain 8-H:

• Molecule 4: Histone H2B

Chain 9-D:

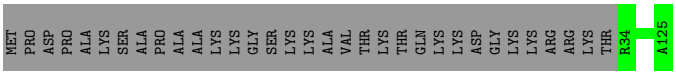


• Molecule 4: Histone H2B

Chain 9-H:

• Molecule 4: Histone H2B

Chain 10-D:

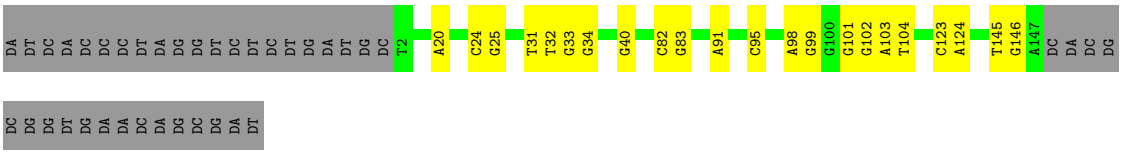


• Molecule 4: Histone H2B

Chain 10-H:

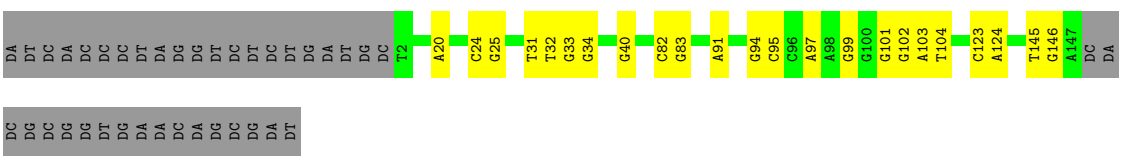
• Molecule 5: DNA (185-MER)

Chain 1-I:



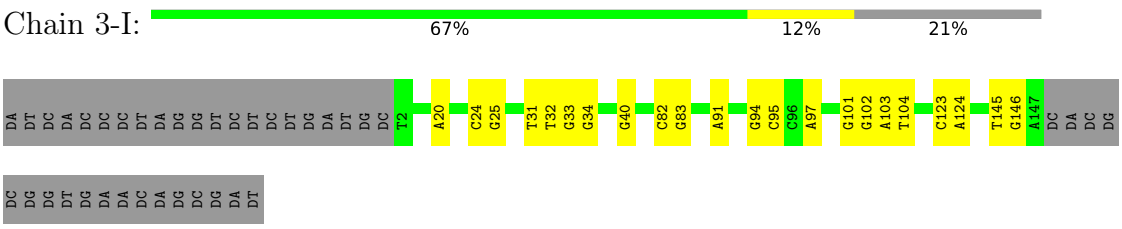
• Molecule 5: DNA (185-MER)

Chain 2-I:



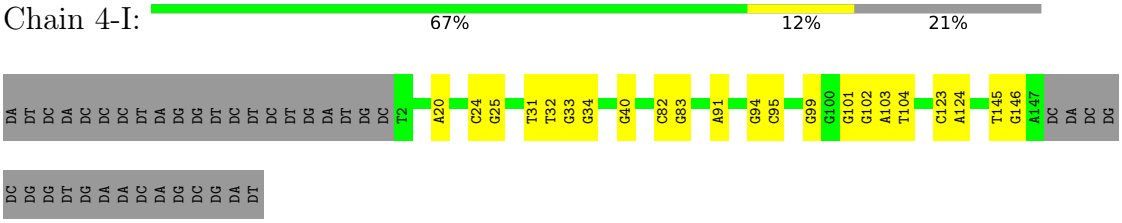
• Molecule 5: DNA (185-MER)

Chain 3-I:



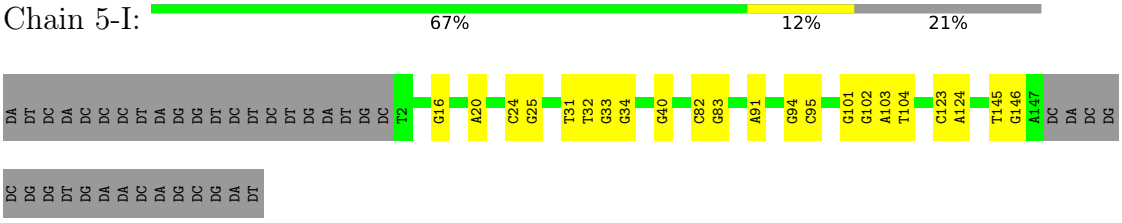
• Molecule 5: DNA (185-MER)

Chain 4-I:



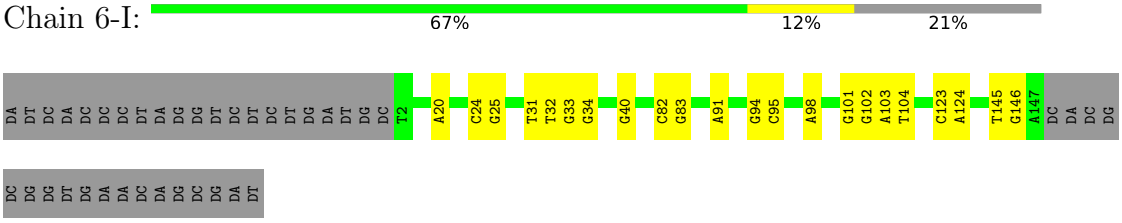
• Molecule 5: DNA (185-MER)

Chain 5-I:



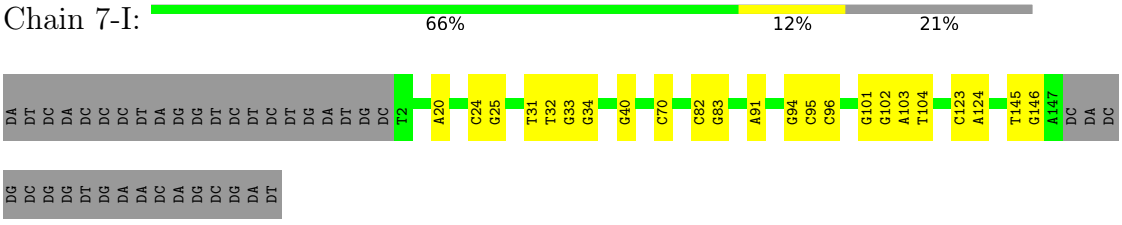
• Molecule 5: DNA (185-MER)

Chain 6-I:



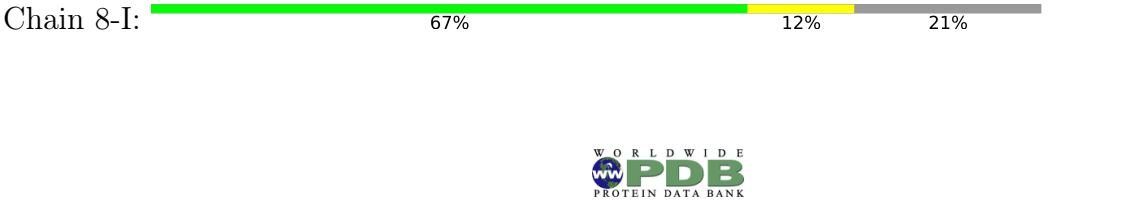
• Molecule 5: DNA (185-MER)

Chain 7-I:



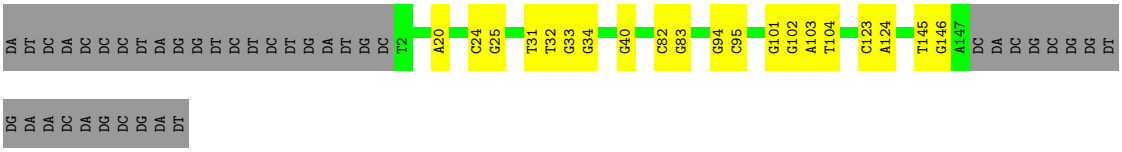
• Molecule 5: DNA (185-MER)

Chain 8-I:



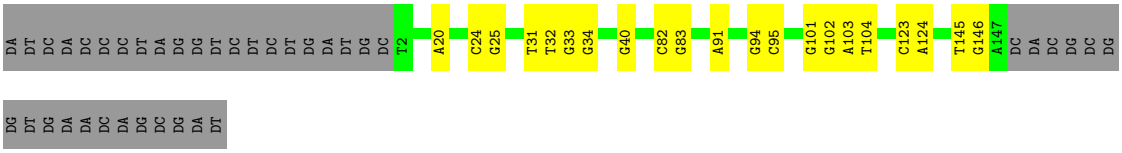
• Molecule 5: DNA (185-MER)

Chain 9-I:



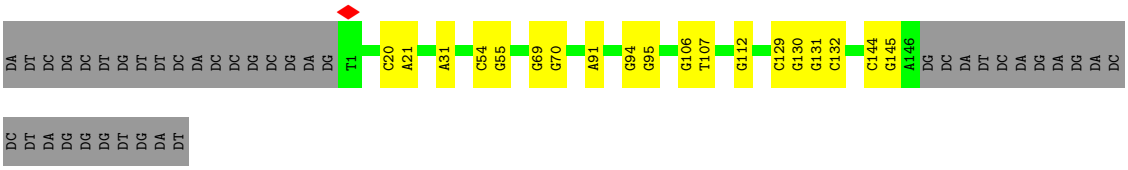
• Molecule 5: DNA (185-MER)

Chain 10-I:



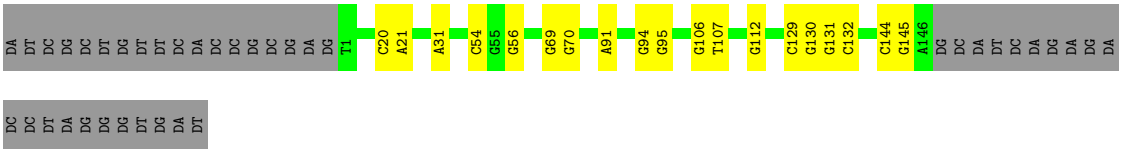
• Molecule 6: DNA (185-MER)

Chain 1-J:



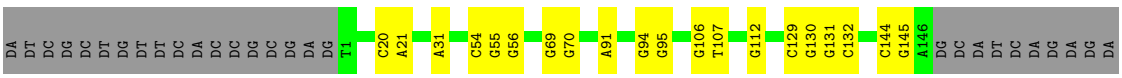
• Molecule 6: DNA (185-MER)

Chain 2-J:



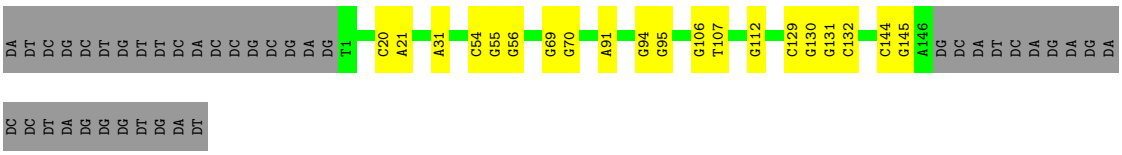
• Molecule 6: DNA (185-MER)

Chain 3-J:



• Molecule 6: DNA (185-MER)

Chain 4-J:

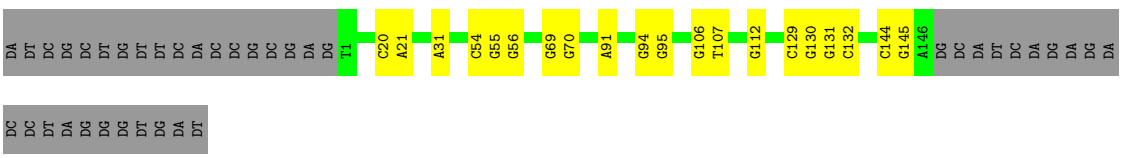


• Molecule 6: DNA (185-MER)

Chain 5-J:

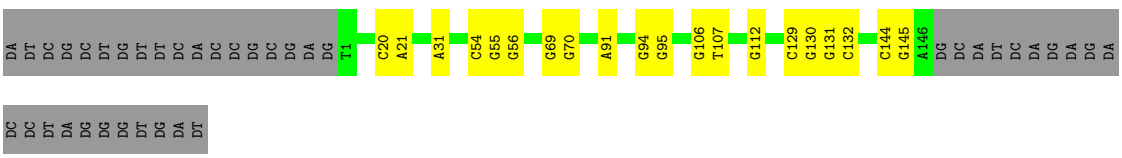
• Molecule 6: DNA (185-MER)

Chain 6-J:



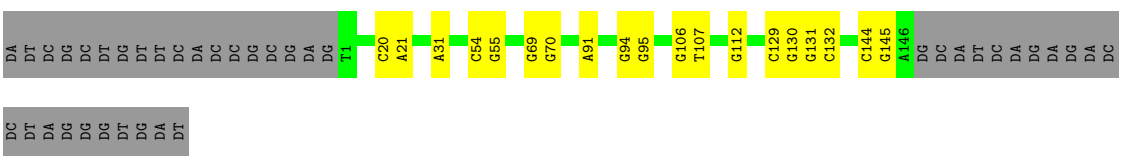
• Molecule 6: DNA (185-MER)

Chain 7-J:



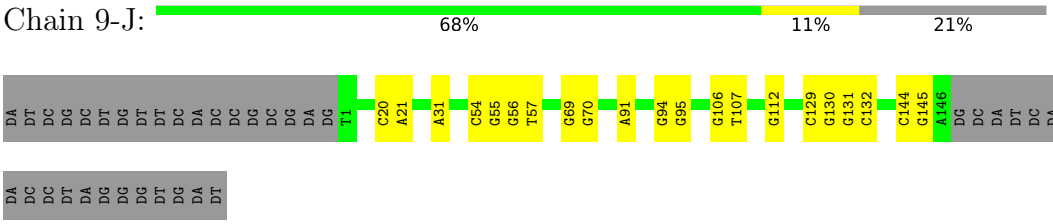
• Molecule 6: DNA (185-MER)

Chain 8-J:



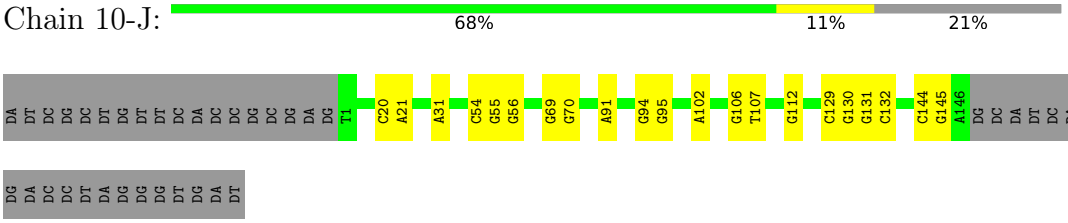
• Molecule 6: DNA (185-MER)

Chain 9-J:



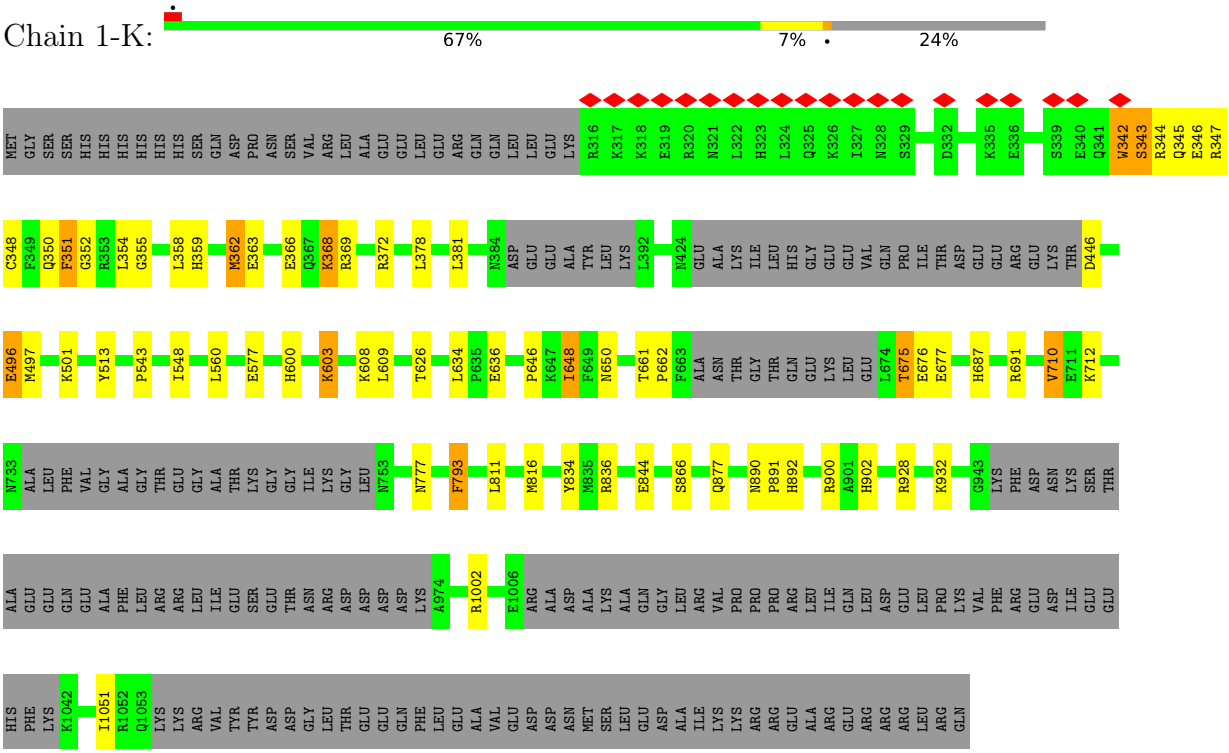
• Molecule 6: DNA (185-MER)

Chain 10-J:



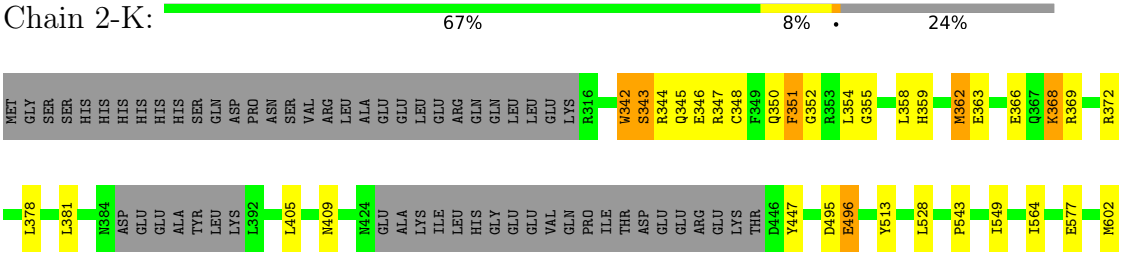
• Molecule 7: Nuclear protein STH1/NPS1

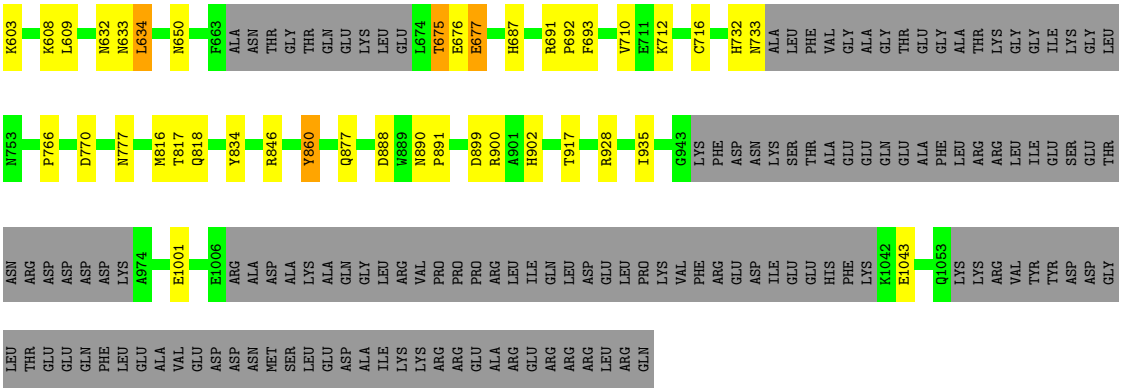
Chain 1-K:



• Molecule 7: Nuclear protein STH1/NPS1

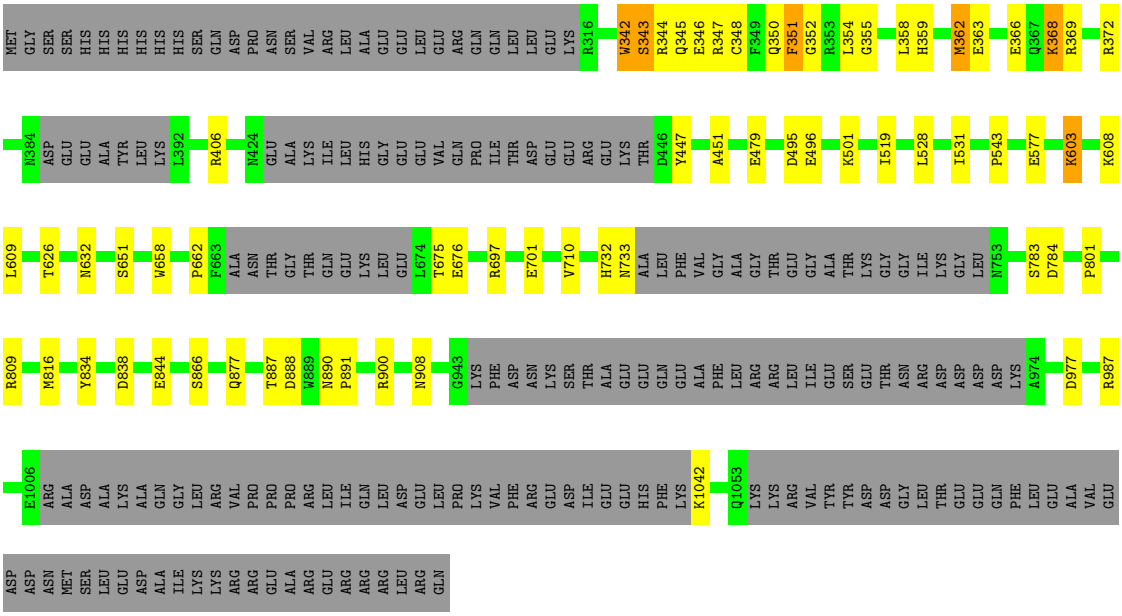
Chain 2-K:





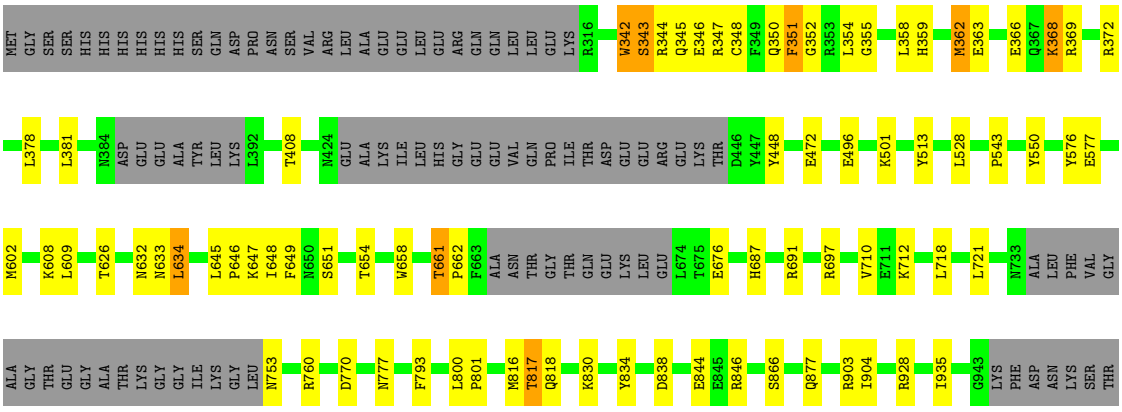
• Molecule 7: Nuclear protein STH1/NPS1

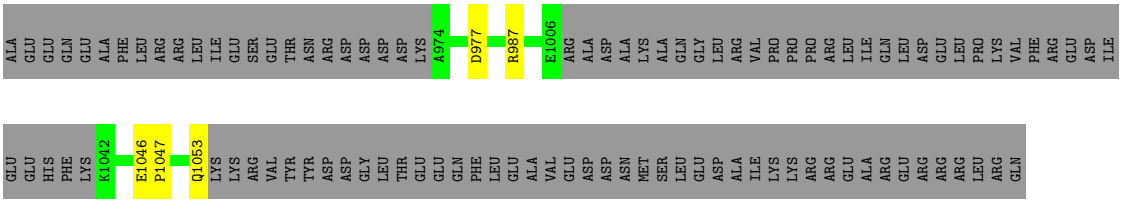
Chain 3-K:



• Molecule 7: Nuclear protein STH1/NPS1

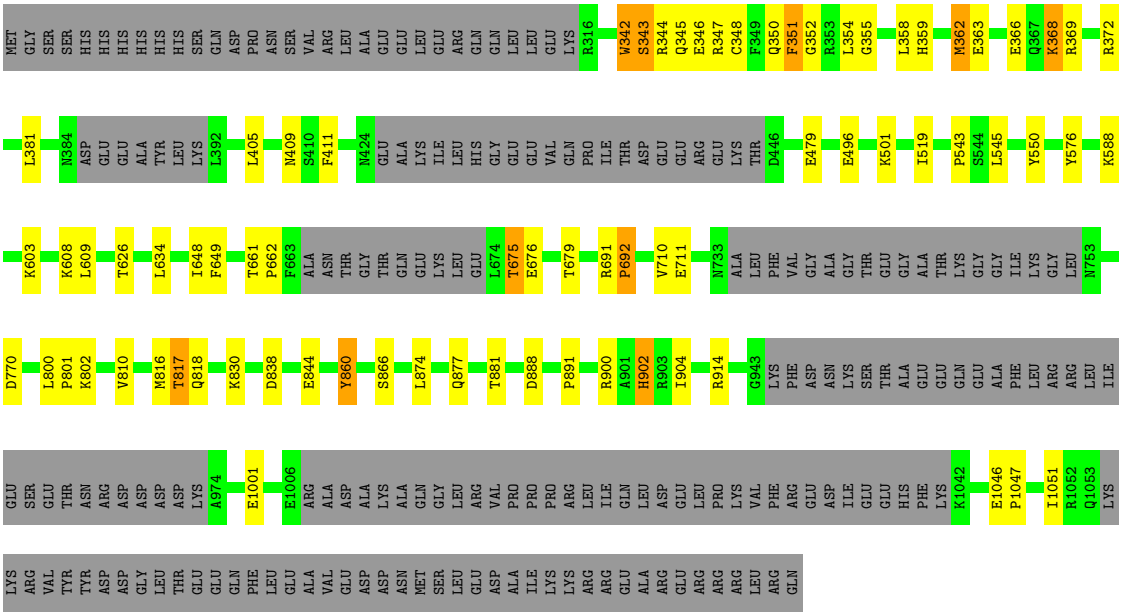
Chain 4-K:

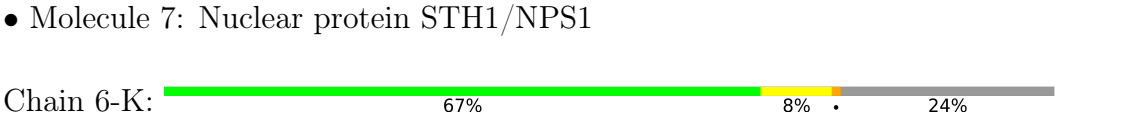


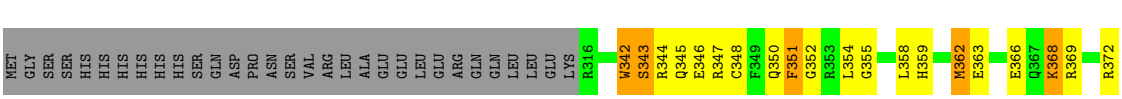


• Molecule 7: Nuclear protein STH1/NPS1

Chain 5-K:

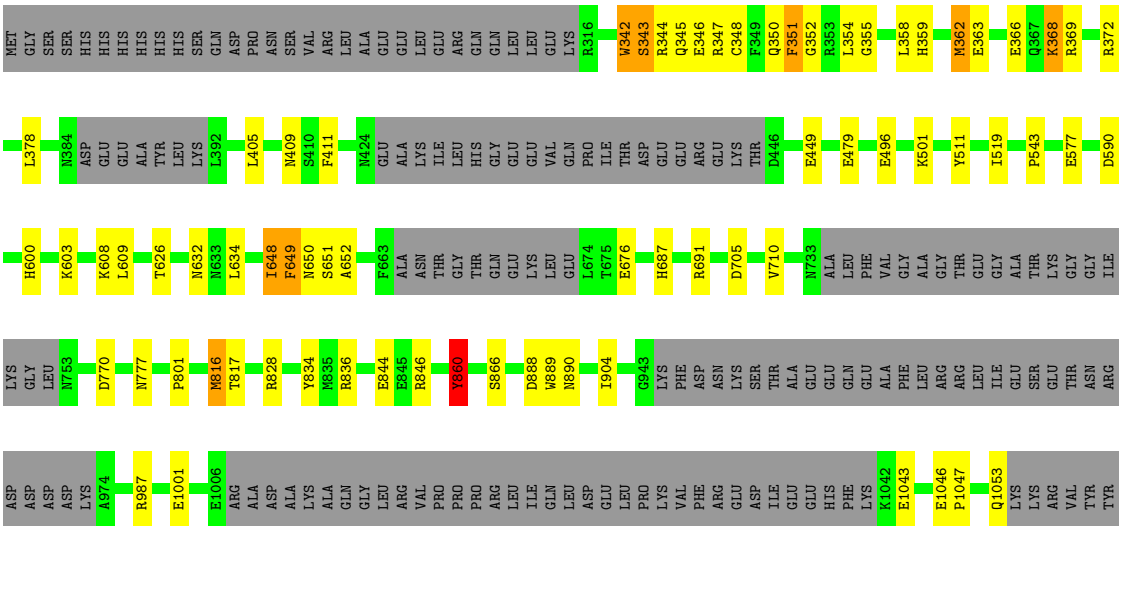


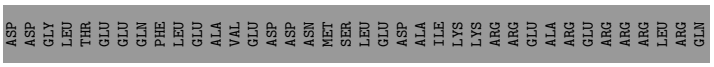




• Molecule 7: Nuclear protein STH1/NPS1

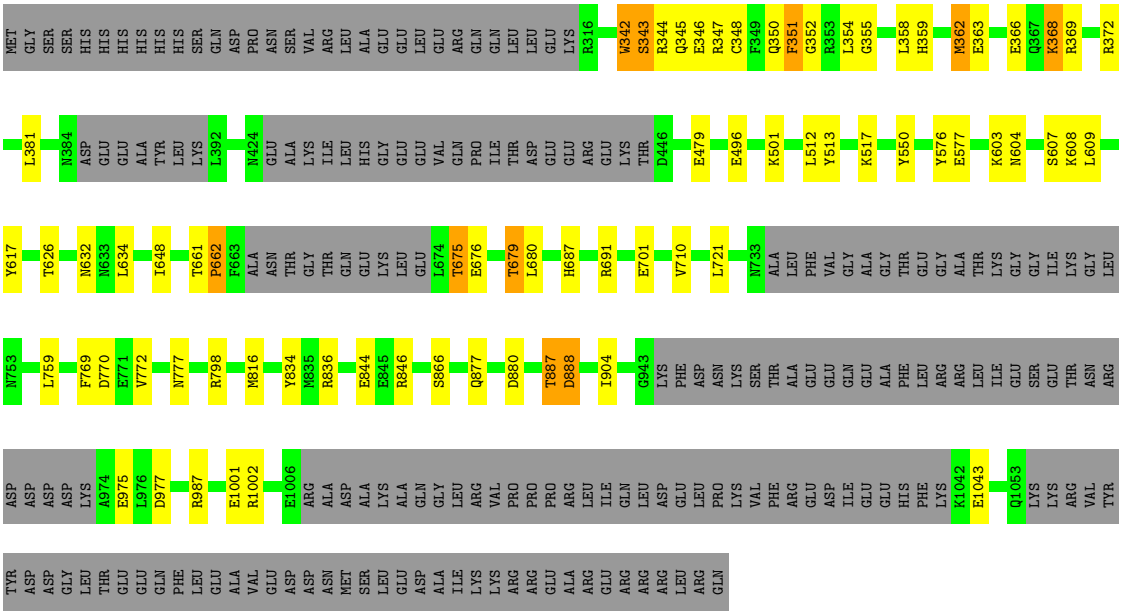
Chain 6-K:





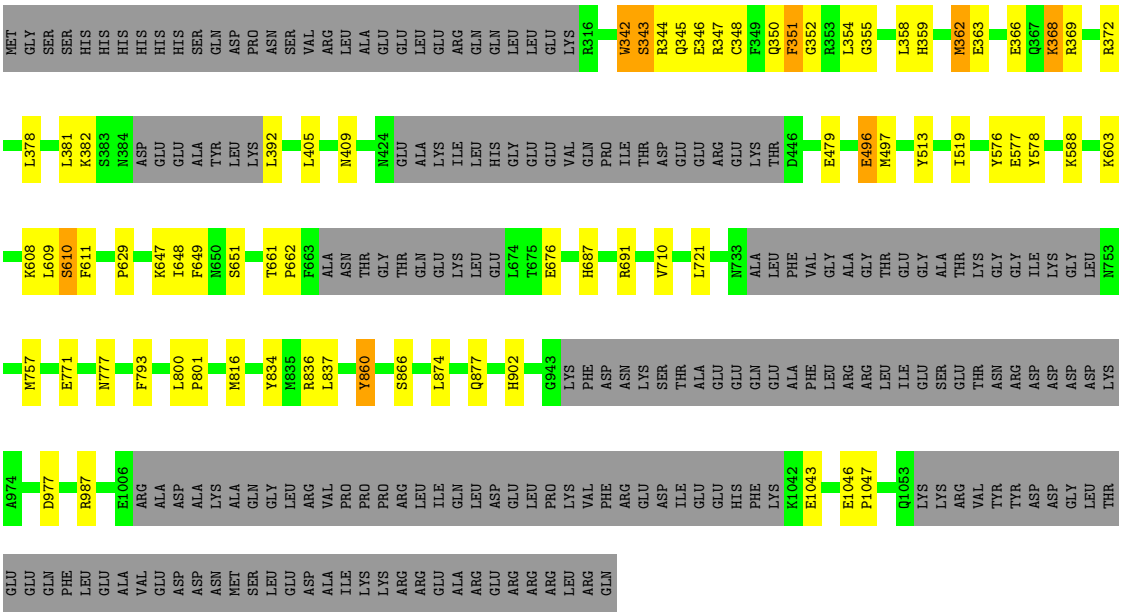
• Molecule 7: Nuclear protein STH1/NPS1

Chain 7-K:



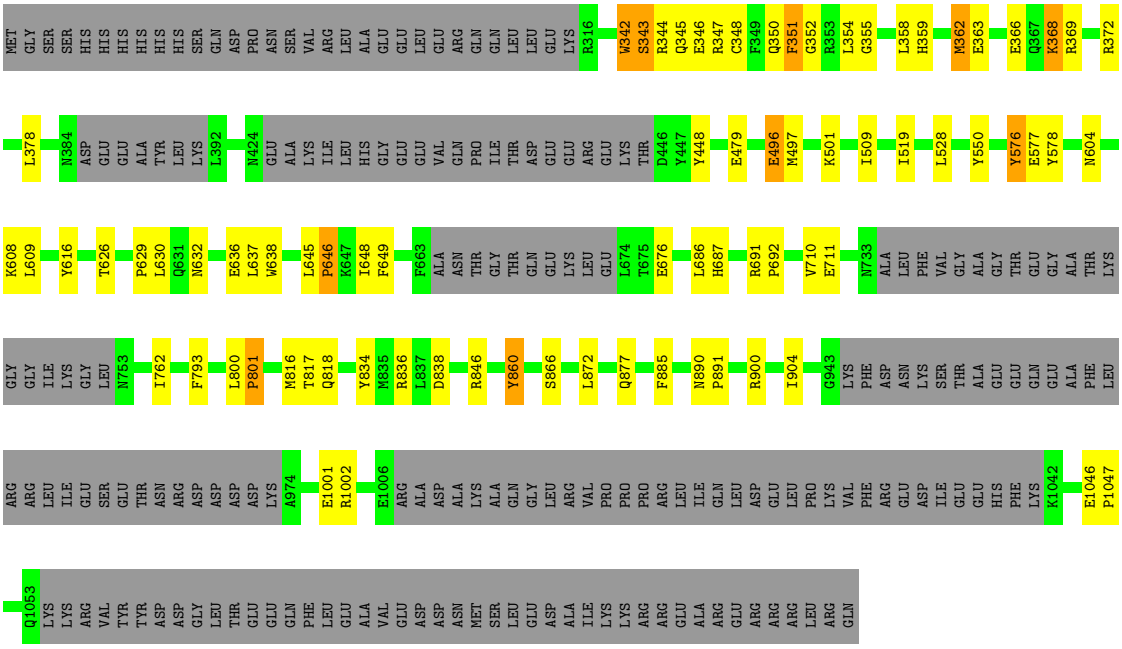
• Molecule 7: Nuclear protein STH1/NPS1

Chain 8-K:



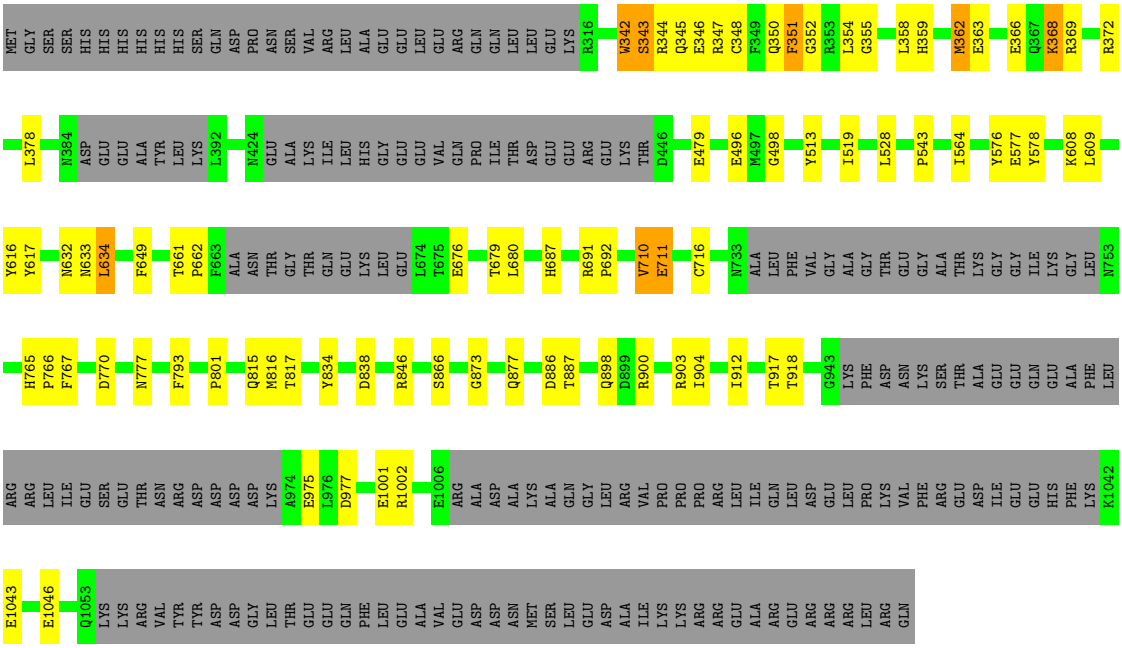
• Molecule 7: Nuclear protein STH1/NPS1

Chain 9-K:



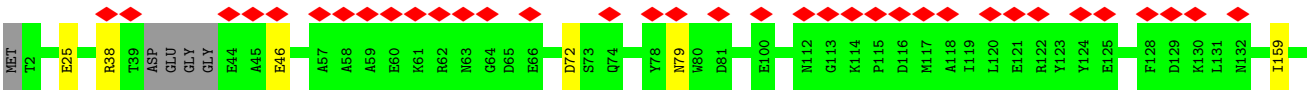
• Molecule 7: Nuclear protein STH1/NPS1

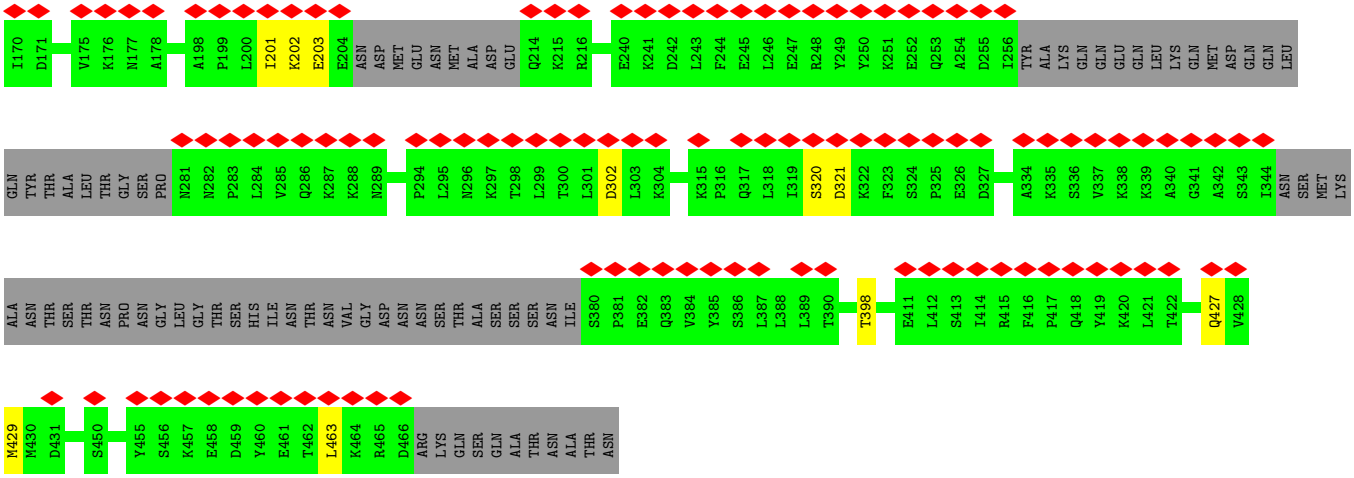
Chain 10-K:



• Molecule 8: Actin-related protein 7

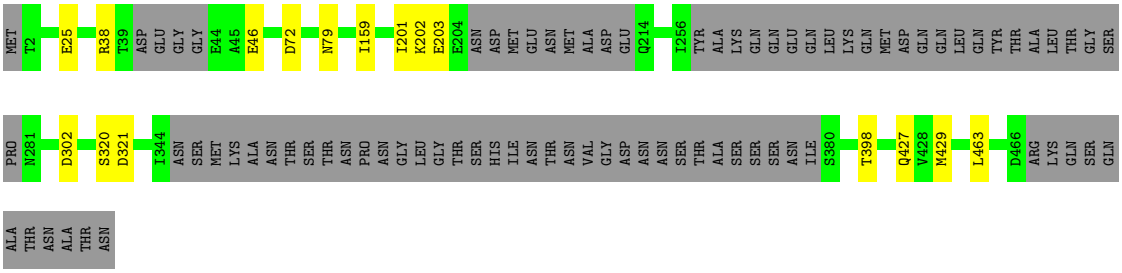
Chain 1-L:





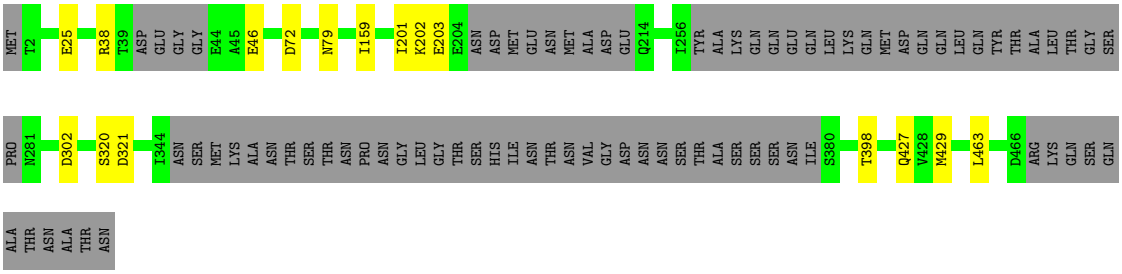
• Molecule 8: Actin-related protein 7

Chain 2-L:



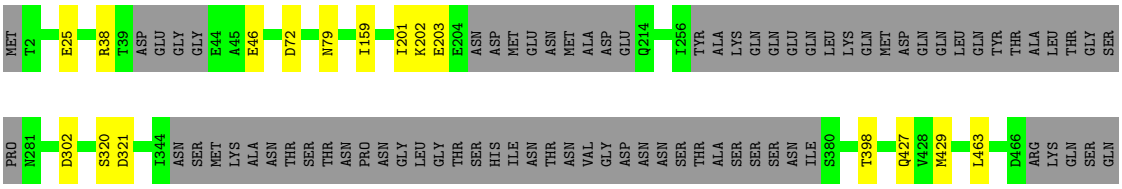
• Molecule 8: Actin-related protein 7

Chain 3-L:



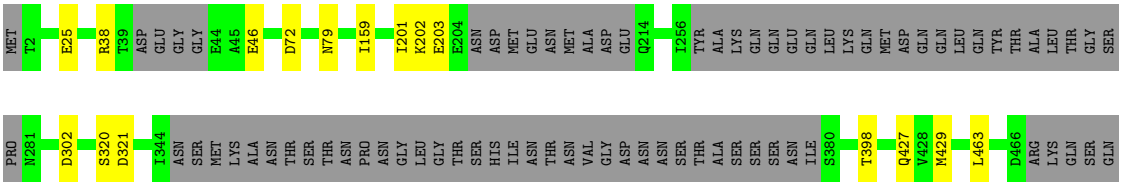
• Molecule 8: Actin-related protein 7

Chain 4-L:



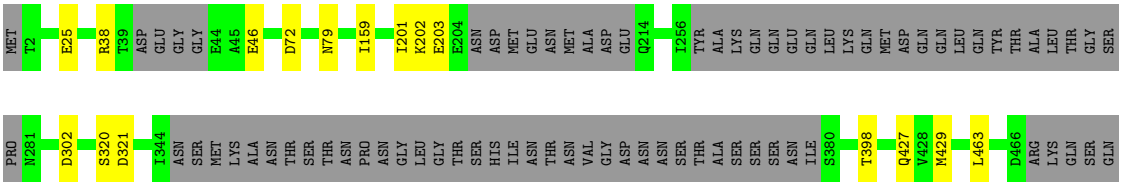
• Molecule 8: Actin-related protein 7

Chain 5-L:



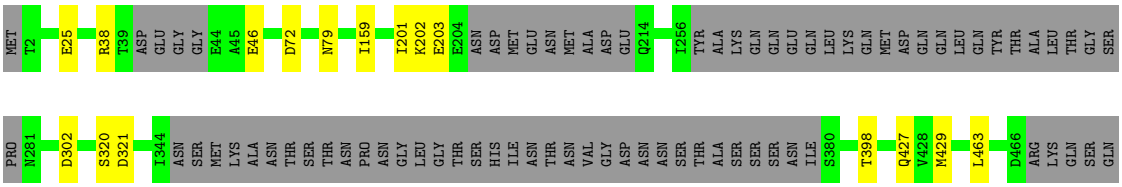
• Molecule 8: Actin-related protein 7

Chain 6-L:



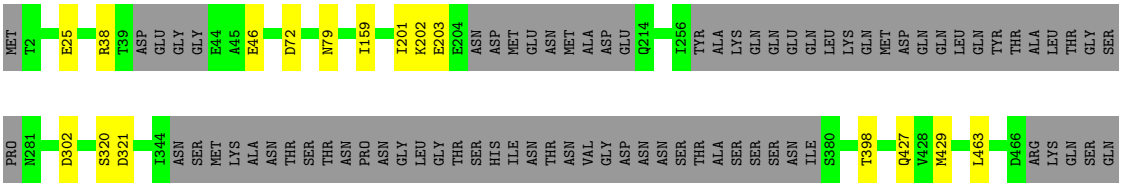
• Molecule 8: Actin-related protein 7

Chain 7-L:



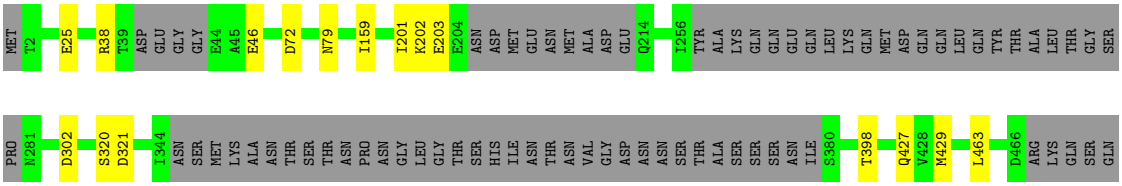
• Molecule 8: Actin-related protein 7

Chain 8-L:



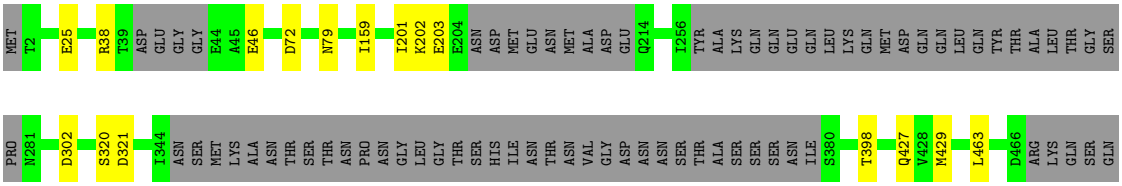
• Molecule 8: Actin-related protein 7

Chain 9-L:



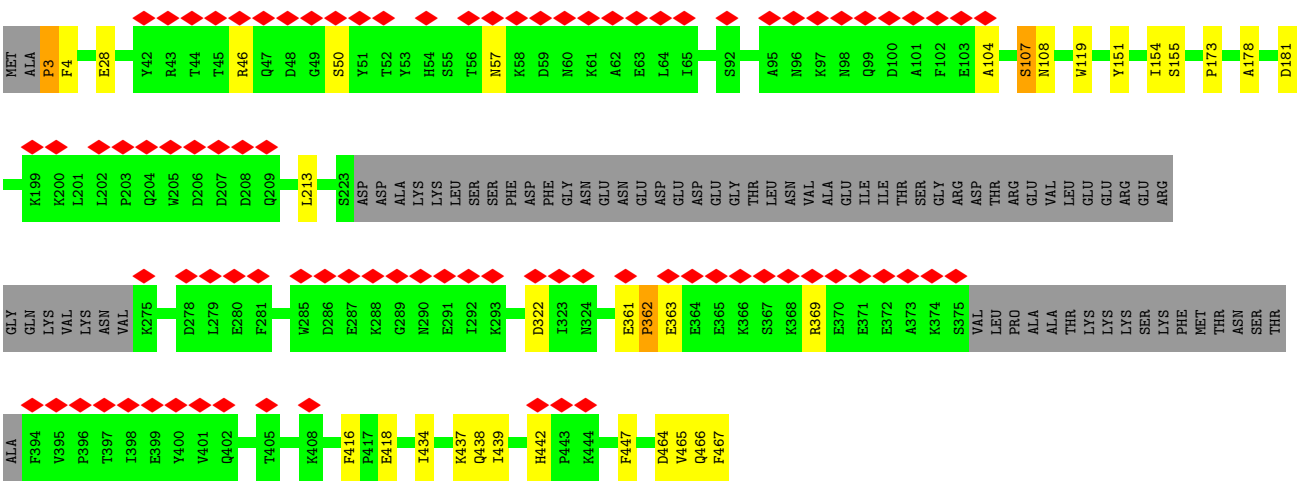
• Molecule 8: Actin-related protein 7

Chain 10-L:



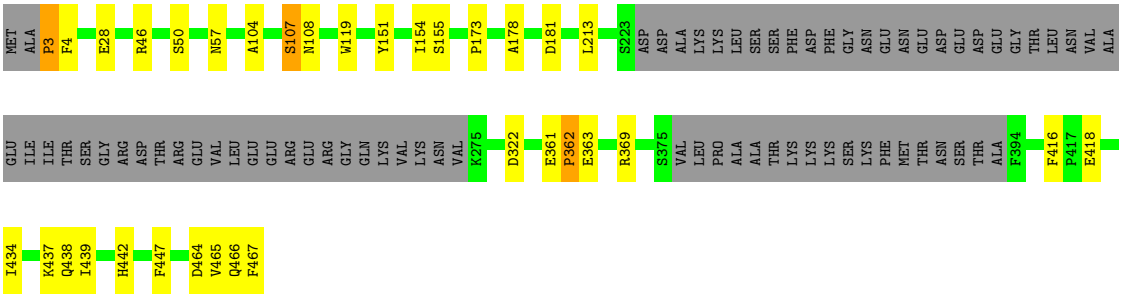
• Molecule 9: Actin-like protein ARP9

Chain 1-M:



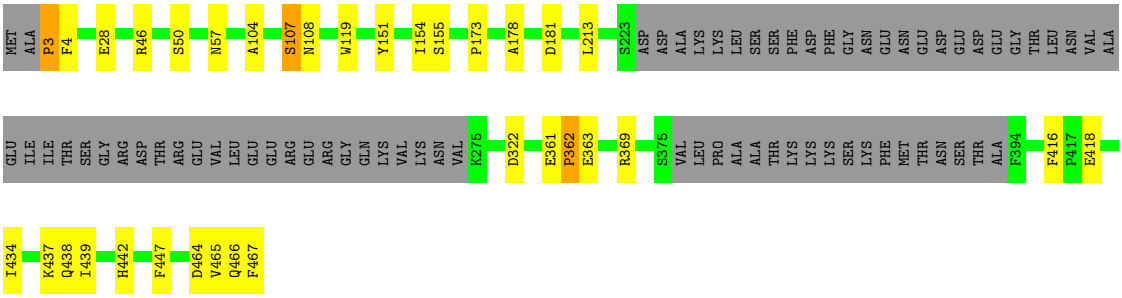
• Molecule 9: Actin-like protein ARP9

Chain 2-M:



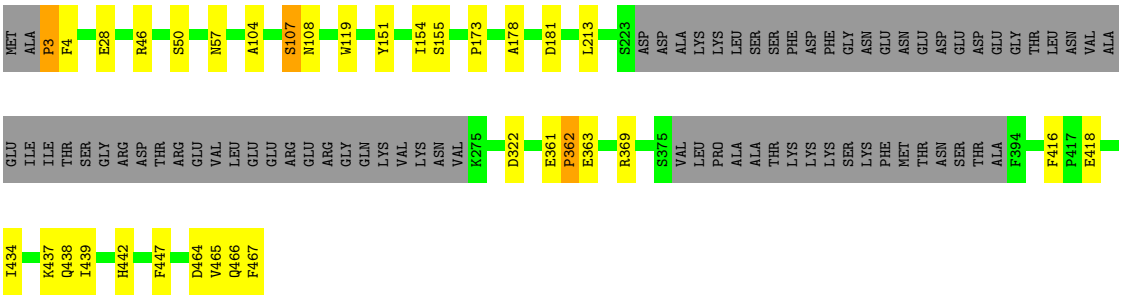
• Molecule 9: Actin-like protein ARP9

Chain 3-M:



• Molecule 9: Actin-like protein ARP9

Chain 4-M:

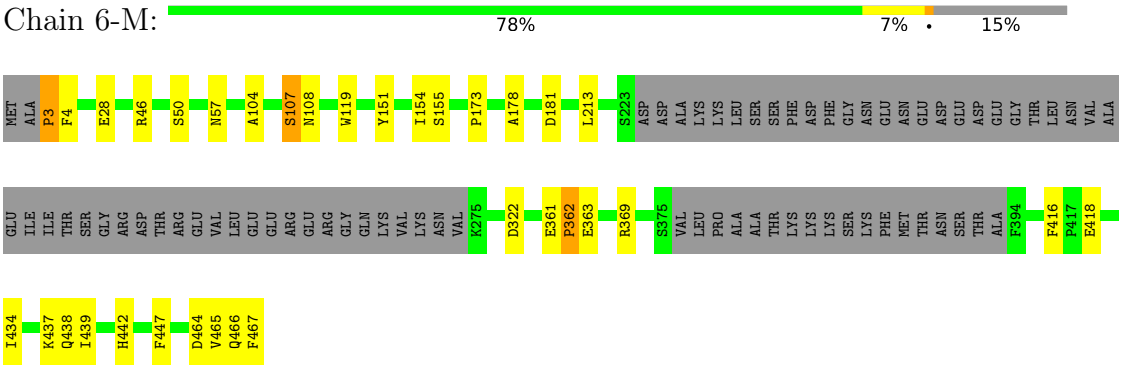


• Molecule 9: Actin-like protein ARP9

Chain 5-M:

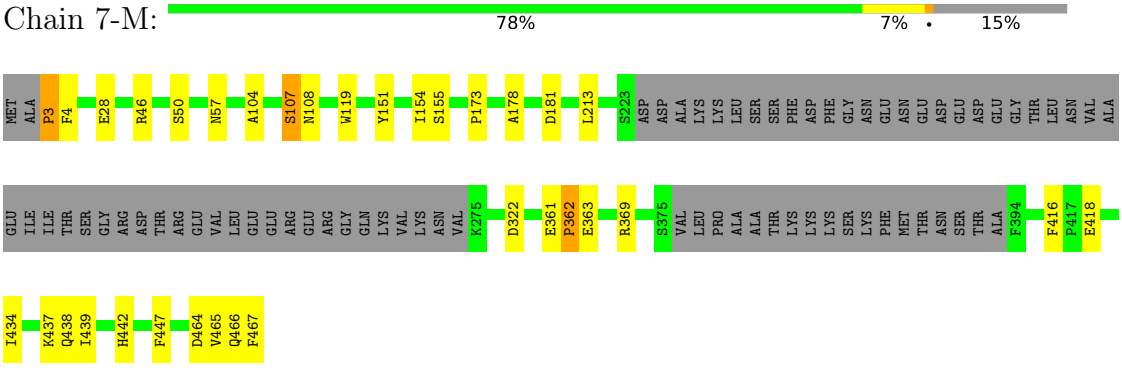
• Molecule 9: Actin-like protein ARP9

Chain 6-M:



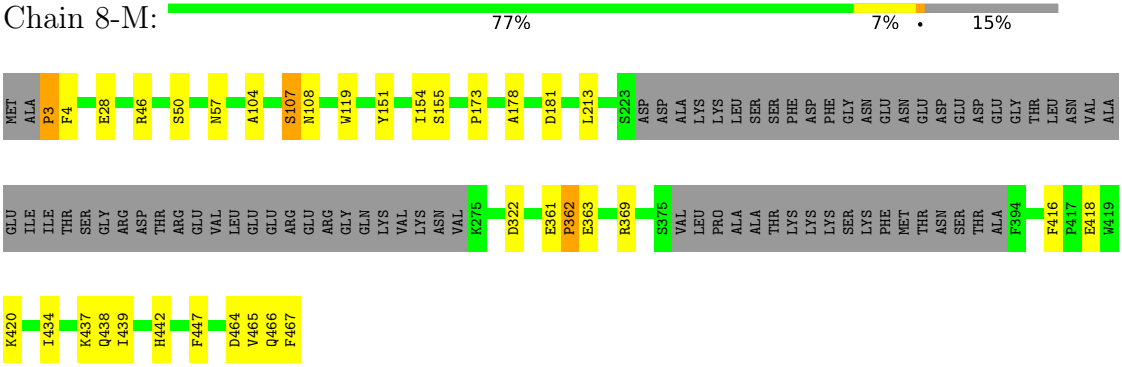
• Molecule 9: Actin-like protein ARP9

Chain 7-M:



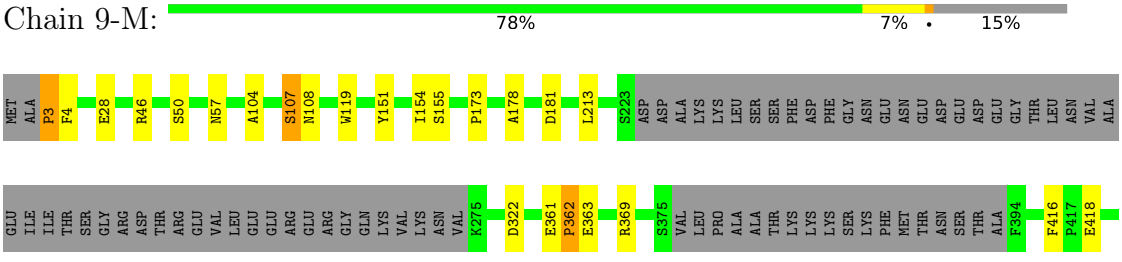
• Molecule 9: Actin-like protein ARP9

Chain 8-M:



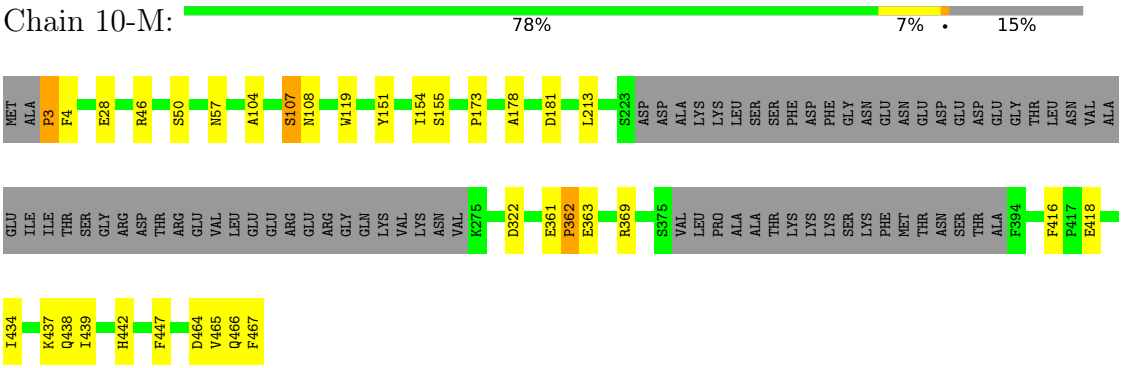
• Molecule 9: Actin-like protein ARP9

Chain 9-M:



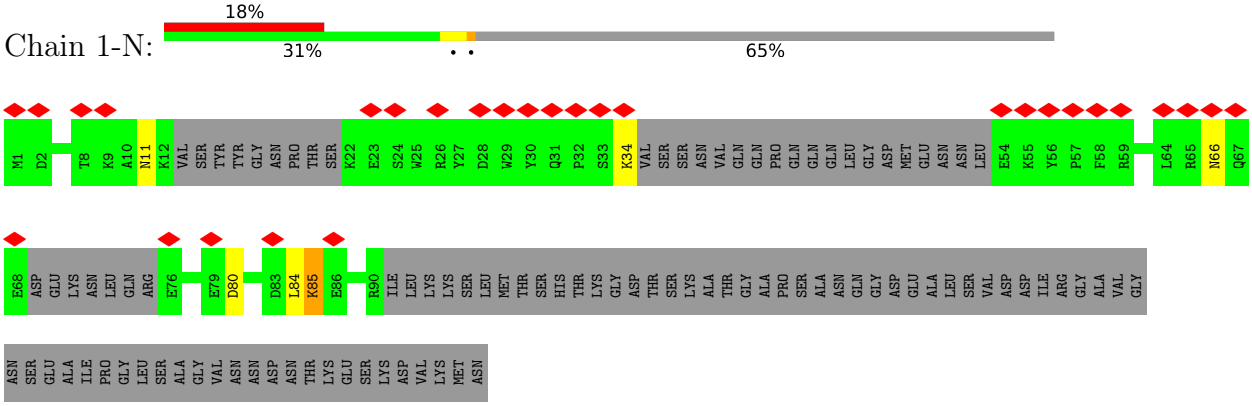
• Molecule 9: Actin-like protein ARP9

Chain 10-M:



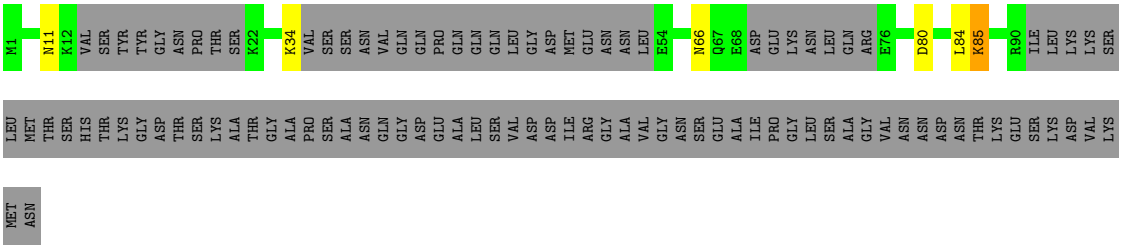
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 1-N:



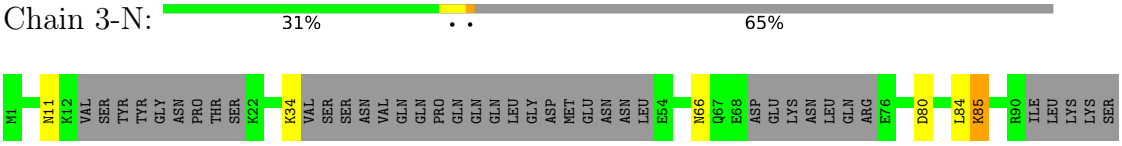
• Molecule 10: Regulator of Ty1 transposition protein 102

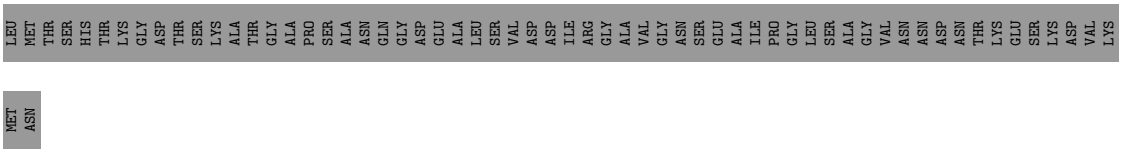
Chain 2-N:



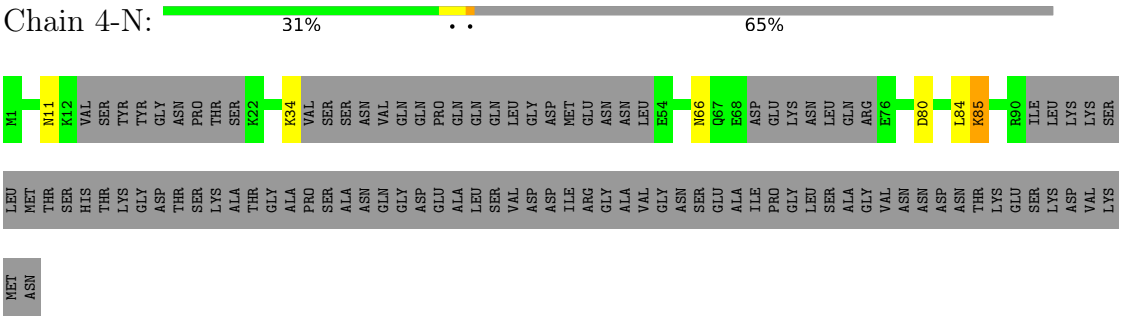
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 3-N:

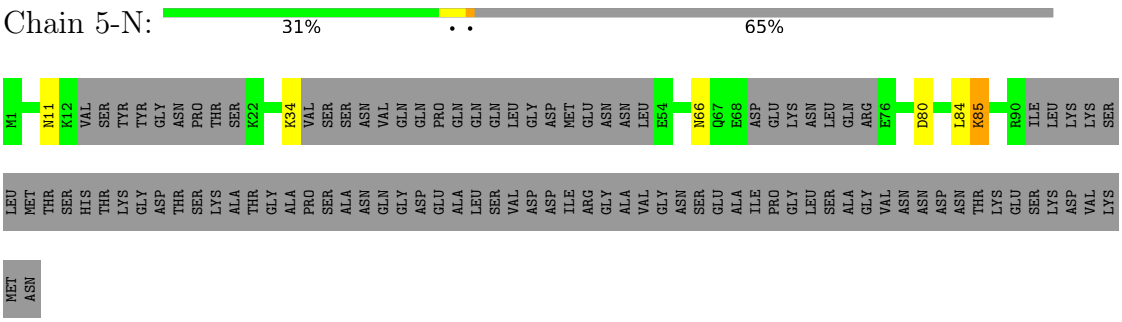




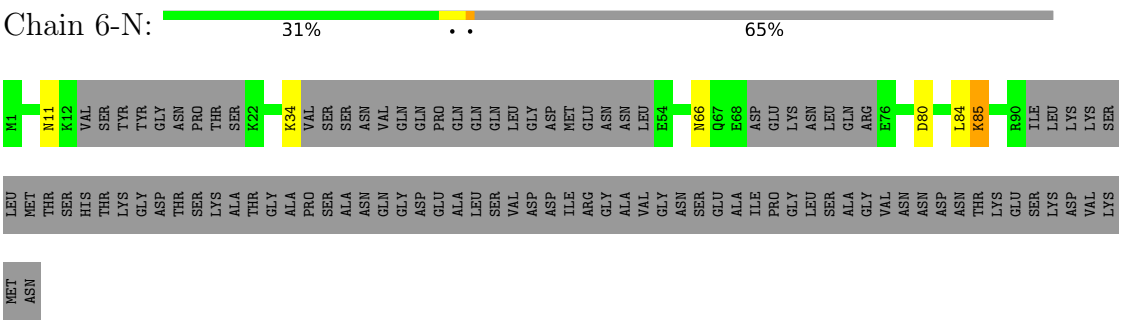
• Molecule 10: Regulator of Ty1 transposition protein 102



• Molecule 10: Regulator of Ty1 transposition protein 102



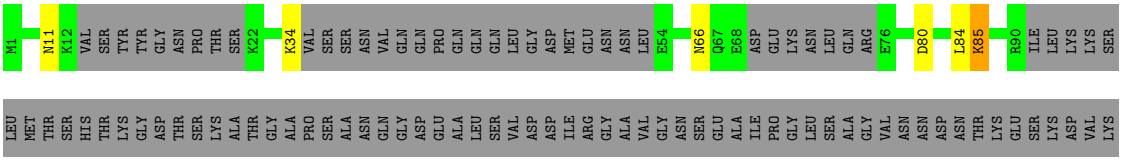
• Molecule 10: Regulator of Ty1 transposition protein 102



• Molecule 10: Regulator of Ty1 transposition protein 102

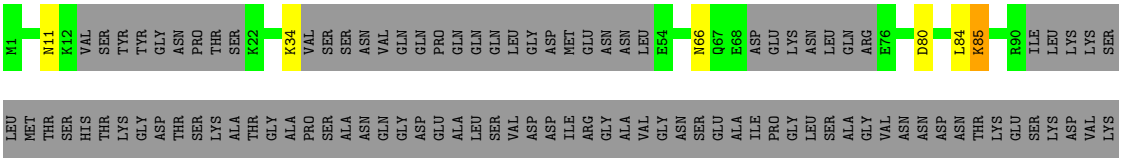
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 8-N:



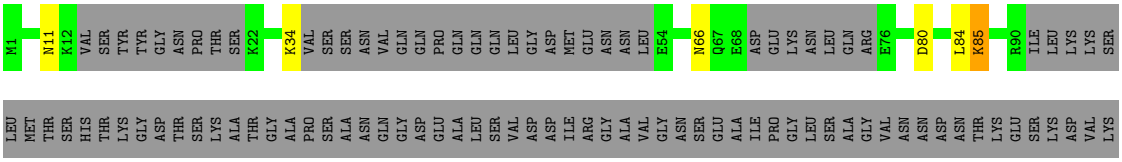
• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 9-N:



• Molecule 10: Regulator of Ty1 transposition protein 102

Chain 10-N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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, BEF, ATP, 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	1-A	0.88	0/821	0.68	0/1100
1	1-E	0.91	0/793	0.69	0/1062
1	2-A	0.88	0/821	0.67	0/1100
1	2-E	0.91	0/793	0.69	0/1062
1	3-A	0.88	0/821	0.67	0/1100
1	3-E	0.91	0/793	0.69	0/1062
1	4-A	0.88	0/821	0.67	0/1100
1	4-E	0.91	0/793	0.69	0/1062
1	5-A	0.88	0/821	0.67	0/1100
1	5-E	0.91	0/793	0.68	0/1062
1	6-A	0.88	0/821	0.68	0/1100
1	6-E	0.91	0/793	0.69	0/1062
1	7-A	0.88	0/821	0.67	0/1100
1	7-E	0.91	0/793	0.68	0/1062
1	8-A	0.88	0/821	0.68	0/1100
1	8-E	0.91	0/793	0.68	0/1062
1	9-A	0.88	0/821	0.68	0/1100
1	9-E	0.91	0/793	0.69	0/1062
1	10-A	0.88	0/821	0.68	0/1100
1	10-E	0.91	0/793	0.68	0/1062
2	1-B	0.82	0/711	0.76	2/950 (0.2%)
2	1-F	0.83	0/634	0.79	2/848 (0.2%)
2	2-B	0.82	0/711	0.76	1/950 (0.1%)
2	2-F	0.83	0/634	0.79	2/848 (0.2%)
2	3-B	0.82	0/711	0.78	1/950 (0.1%)
2	3-F	0.82	0/634	0.75	1/848 (0.1%)
2	4-B	0.82	0/711	0.76	1/950 (0.1%)
2	4-F	0.84	0/634	0.76	1/848 (0.1%)
2	5-B	0.82	0/711	0.75	1/950 (0.1%)
2	5-F	0.83	0/634	0.76	1/848 (0.1%)
2	6-B	0.82	0/711	0.75	1/950 (0.1%)
2	6-F	0.83	0/634	0.77	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	7-B	0.81	0/711	0.75	0/950
2	7-F	0.82	0/634	0.76	1/848 (0.1%)
2	8-B	0.82	0/711	0.75	0/950
2	8-F	0.82	0/634	0.76	1/848 (0.1%)
2	9-B	0.82	0/711	0.76	1/950 (0.1%)
2	9-F	0.84	0/634	0.76	1/848 (0.1%)
2	10-B	0.82	0/711	0.75	1/950 (0.1%)
2	10-F	0.83	0/634	0.77	1/848 (0.1%)
3	1-C	0.82	0/833	0.62	0/1124
3	1-G	0.83	0/833	0.69	1/1124 (0.1%)
3	2-C	0.82	0/833	0.62	0/1124
3	2-G	0.83	0/833	0.70	1/1124 (0.1%)
3	3-C	0.82	0/833	0.62	0/1124
3	3-G	0.83	0/833	0.68	1/1124 (0.1%)
3	4-C	0.82	0/833	0.62	0/1124
3	4-G	0.83	0/833	0.69	1/1124 (0.1%)
3	5-C	0.82	0/833	0.63	0/1124
3	5-G	0.83	0/833	0.69	1/1124 (0.1%)
3	6-C	0.82	0/833	0.63	0/1124
3	6-G	0.83	0/833	0.69	1/1124 (0.1%)
3	7-C	0.82	0/833	0.62	0/1124
3	7-G	0.82	0/833	0.69	1/1124 (0.1%)
3	8-C	0.82	0/833	0.62	0/1124
3	8-G	0.83	0/833	0.69	1/1124 (0.1%)
3	9-C	0.82	0/833	0.62	0/1124
3	9-G	0.82	0/833	0.69	1/1124 (0.1%)
3	10-C	0.82	0/833	0.62	0/1124
3	10-G	0.83	0/833	0.69	1/1124 (0.1%)
4	1-D	0.88	0/730	0.68	0/983
4	1-H	0.87	0/730	0.69	0/983
4	2-D	0.88	0/730	0.68	0/983
4	2-H	0.88	0/730	0.69	0/983
4	3-D	0.88	0/730	0.69	0/983
4	3-H	0.88	0/730	0.69	0/983
4	4-D	0.88	0/730	0.68	0/983
4	4-H	0.88	0/730	0.68	0/983
4	5-D	0.88	0/730	0.67	0/983
4	5-H	0.88	0/730	0.70	0/983
4	6-D	0.88	0/730	0.68	0/983
4	6-H	0.87	0/730	0.67	0/983
4	7-D	0.88	0/730	0.67	0/983
4	7-H	0.87	0/730	0.69	0/983
4	8-D	0.88	0/730	0.68	0/983

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	8-H	0.87	0/730	0.70	0/983
4	9-D	0.88	0/730	0.68	0/983
4	9-H	0.88	0/730	0.68	0/983
4	10-D	0.88	0/730	0.68	0/983
4	10-H	0.87	0/730	0.69	0/983
5	1-I	0.92	0/3333	0.98	0/5137
5	2-I	0.92	0/3333	0.98	0/5137
5	3-I	0.92	0/3333	0.98	0/5137
5	4-I	0.92	0/3333	0.98	0/5137
5	5-I	0.92	0/3333	0.98	0/5137
5	6-I	0.92	0/3333	0.98	0/5137
5	7-I	0.92	0/3333	0.98	0/5137
5	8-I	0.92	0/3333	0.98	0/5137
5	9-I	0.92	0/3333	0.98	0/5137
5	10-I	0.92	0/3333	0.98	0/5137
6	1-J	0.94	0/3381	0.97	0/5221
6	2-J	0.94	0/3381	0.97	0/5221
6	3-J	0.94	0/3381	0.97	0/5221
6	4-J	0.94	0/3381	0.97	0/5221
6	5-J	0.94	0/3381	0.97	0/5221
6	6-J	0.94	0/3381	0.97	0/5221
6	7-J	0.94	0/3381	0.97	0/5221
6	8-J	0.94	0/3381	0.97	0/5221
6	9-J	0.94	0/3381	0.97	0/5221
6	10-J	0.94	0/3381	0.97	0/5221
7	1-K	0.82	1/5138 (0.0%)	0.77	7/6910 (0.1%)
7	2-K	0.81	1/5138 (0.0%)	0.76	7/6910 (0.1%)
7	3-K	0.82	1/5138 (0.0%)	0.76	6/6910 (0.1%)
7	4-K	0.82	1/5138 (0.0%)	0.75	9/6910 (0.1%)
7	5-K	0.82	2/5138 (0.0%)	0.77	9/6910 (0.1%)
7	6-K	0.81	1/5138 (0.0%)	0.78	9/6910 (0.1%)
7	7-K	0.81	1/5138 (0.0%)	0.77	10/6910 (0.1%)
7	8-K	0.81	1/5138 (0.0%)	0.75	7/6910 (0.1%)
7	9-K	0.83	3/5138 (0.1%)	0.77	9/6910 (0.1%)
7	10-K	0.82	1/5138 (0.0%)	0.76	7/6910 (0.1%)
8	1-L	0.85	0/3220	0.70	0/4355
8	2-L	0.85	0/3220	0.70	0/4355
8	3-L	0.85	0/3220	0.70	0/4355
8	4-L	0.85	0/3220	0.70	0/4355
8	5-L	0.85	0/3220	0.70	0/4355
8	6-L	0.85	0/3220	0.70	0/4355
8	7-L	0.85	0/3220	0.70	0/4355
8	8-L	0.85	0/3220	0.70	0/4355

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	9-L	0.85	0/3220	0.70	0/4355
8	10-L	0.85	0/3220	0.70	0/4355
9	1-M	0.85	0/3259	0.70	0/4417
9	2-M	0.85	0/3259	0.70	0/4417
9	3-M	0.85	0/3259	0.70	0/4417
9	4-M	0.85	0/3259	0.70	0/4417
9	5-M	0.85	0/3259	0.70	0/4417
9	6-M	0.85	0/3259	0.70	0/4417
9	7-M	0.85	0/3259	0.70	0/4417
9	8-M	0.85	0/3259	0.70	0/4417
9	9-M	0.85	0/3259	0.70	0/4417
9	10-M	0.85	0/3259	0.70	0/4417
10	1-N	0.89	0/505	0.70	0/674
10	2-N	0.89	0/505	0.70	0/674
10	3-N	0.89	0/505	0.70	0/674
10	4-N	0.89	0/505	0.70	0/674
10	5-N	0.89	0/505	0.70	0/674
10	6-N	0.89	0/505	0.70	0/674
10	7-N	0.89	0/505	0.70	0/674
10	8-N	0.89	0/505	0.70	0/674
10	9-N	0.89	0/505	0.70	0/674
10	10-N	0.89	0/505	0.70	0/674
All	All	0.87	13/249210 (0.0%)	0.80	111/348880 (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
7	6-K	0	2
9	1-M	0	2
9	2-M	0	2
9	3-M	0	2
9	4-M	0	2
9	5-M	0	2
9	6-M	0	2
9	7-M	0	2
9	8-M	0	2
9	9-M	0	2
9	10-M	0	2
All	All	0	22

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	342	TRP	C-N	8.43	1.53	1.34
7	2-K	342	TRP	C-N	8.43	1.53	1.34
7	3-K	342	TRP	C-N	8.43	1.53	1.34
7	4-K	342	TRP	C-N	8.43	1.53	1.34
7	5-K	342	TRP	C-N	8.43	1.53	1.34

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	342	TRP	C-N-CA	13.52	155.50	121.70
7	2-K	342	TRP	C-N-CA	13.52	155.50	121.70
7	3-K	342	TRP	C-N-CA	13.52	155.50	121.70
7	4-K	342	TRP	C-N-CA	13.52	155.50	121.70
7	5-K	342	TRP	C-N-CA	13.52	155.50	121.70

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	1-M	3	PRO	Peptide,Mainchain
9	2-M	3	PRO	Peptide,Mainchain
9	3-M	3	PRO	Peptide,Mainchain
9	4-M	3	PRO	Peptide,Mainchain
9	5-M	3	PRO	Mainchain

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	1-A	809	0	849	3	0
1	1-E	783	0	822	3	0
1	2-A	809	0	849	3	0
1	2-E	783	0	822	5	0
1	3-A	809	0	849	3	0
1	3-E	783	0	822	4	0
1	4-A	809	0	849	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-E	783	0	822	4	0
1	5-A	809	0	849	3	0
1	5-E	783	0	822	4	0
1	6-A	809	0	849	3	0
1	6-E	783	0	822	4	0
1	7-A	809	0	849	4	0
1	7-E	783	0	822	4	0
1	8-A	809	0	849	3	0
1	8-E	783	0	822	4	0
1	9-A	809	0	849	3	0
1	9-E	783	0	822	4	0
1	10-A	809	0	849	3	0
1	10-E	783	0	822	3	0
2	1-B	703	0	757	3	0
2	1-F	627	0	663	2	0
2	2-B	703	0	757	2	0
2	2-F	627	0	663	1	0
2	3-B	703	0	757	2	0
2	3-F	627	0	663	1	0
2	4-B	703	0	757	3	0
2	4-F	627	0	663	1	0
2	5-B	703	0	757	3	0
2	5-F	627	0	663	2	0
2	6-B	703	0	757	2	0
2	6-F	627	0	663	2	0
2	7-B	703	0	757	3	0
2	7-F	627	0	663	3	0
2	8-B	703	0	757	2	0
2	8-F	627	0	663	2	0
2	9-B	703	0	757	2	0
2	9-F	627	0	663	2	0
2	10-B	703	0	757	2	0
2	10-F	627	0	663	3	0
3	1-C	823	0	882	3	0
3	1-G	823	0	882	8	0
3	2-C	823	0	882	3	0
3	2-G	823	0	882	8	0
3	3-C	823	0	882	4	0
3	3-G	823	0	882	8	0
3	4-C	823	0	882	3	0
3	4-G	823	0	882	8	0
3	5-C	823	0	882	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5-G	823	0	882	8	0
3	6-C	823	0	882	3	0
3	6-G	823	0	882	8	0
3	7-C	823	0	882	3	0
3	7-G	823	0	882	8	0
3	8-C	823	0	882	3	0
3	8-G	823	0	882	8	0
3	9-C	823	0	882	3	0
3	9-G	823	0	882	8	0
3	10-C	823	0	882	3	0
3	10-G	823	0	882	8	0
4	1-D	719	0	740	0	0
4	1-H	719	0	740	2	0
4	2-D	719	0	740	0	0
4	2-H	719	0	740	2	0
4	3-D	719	0	740	0	0
4	3-H	719	0	740	2	0
4	4-D	719	0	740	0	0
4	4-H	719	0	740	2	0
4	5-D	719	0	740	0	0
4	5-H	719	0	740	2	0
4	6-D	719	0	740	0	0
4	6-H	719	0	740	2	0
4	7-D	719	0	740	0	0
4	7-H	719	0	740	2	0
4	8-D	719	0	740	0	0
4	8-H	719	0	740	2	0
4	9-D	719	0	740	0	0
4	9-H	719	0	740	2	0
4	10-D	719	0	740	0	0
4	10-H	719	0	740	2	0
5	1-I	2975	0	1639	20	0
5	2-I	2975	0	1639	18	0
5	3-I	2975	0	1639	28	0
5	4-I	2975	0	1639	23	0
5	5-I	2975	0	1639	22	0
5	6-I	2975	0	1639	26	0
5	7-I	2975	0	1639	29	0
5	8-I	2975	0	1639	34	0
5	9-I	2975	0	1639	22	0
5	10-I	2975	0	1639	30	0
6	1-J	3011	0	1639	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2-J	3011	0	1639	18	0
6	3-J	3011	0	1639	18	0
6	4-J	3011	0	1639	27	0
6	5-J	3011	0	1639	19	0
6	6-J	3011	0	1639	20	0
6	7-J	3011	0	1639	21	0
6	8-J	3011	0	1639	19	0
6	9-J	3011	0	1639	23	0
6	10-J	3011	0	1639	20	0
7	1-K	5055	0	5102	167	0
7	2-K	5055	0	5102	172	0
7	3-K	5055	0	5102	167	0
7	4-K	5055	0	5102	184	0
7	5-K	5055	0	5102	169	0
7	6-K	5055	0	5102	184	0
7	7-K	5055	0	5102	179	0
7	8-K	5055	0	5102	196	0
7	9-K	5055	0	5102	183	0
7	10-K	5055	0	5102	185	0
8	1-L	3154	0	3173	11	0
8	2-L	3154	0	3173	11	0
8	3-L	3154	0	3173	11	0
8	4-L	3154	0	3173	11	0
8	5-L	3154	0	3173	11	0
8	6-L	3154	0	3173	11	0
8	7-L	3154	0	3173	11	0
8	8-L	3154	0	3173	11	0
8	9-L	3154	0	3173	11	0
8	10-L	3154	0	3173	11	0
9	1-M	3192	0	3180	124	0
9	2-M	3192	0	3180	124	0
9	3-M	3192	0	3180	124	0
9	4-M	3192	0	3180	124	0
9	5-M	3192	0	3180	124	0
9	6-M	3192	0	3180	124	0
9	7-M	3192	0	3180	124	0
9	8-M	3192	0	3180	132	0
9	9-M	3192	0	3180	124	0
9	10-M	3192	0	3180	124	0
10	1-N	494	0	473	6	0
10	2-N	494	0	473	6	0
10	3-N	494	0	473	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	4-N	494	0	473	6	0
10	5-N	494	0	473	6	0
10	6-N	494	0	473	6	0
10	7-N	494	0	473	6	0
10	8-N	494	0	473	6	0
10	9-N	494	0	473	6	0
10	10-N	494	0	473	6	0
11	1-K	1	0	0	0	0
11	2-K	1	0	0	0	0
11	3-K	1	0	0	0	0
11	4-K	1	0	0	0	0
11	5-K	1	0	0	0	0
11	6-K	1	0	0	0	0
11	7-K	1	0	0	0	0
11	8-K	1	0	0	0	0
11	9-K	1	0	0	0	0
11	10-K	1	0	0	0	0
12	1-K	27	0	12	3	0
12	2-K	27	0	12	1	0
12	3-K	27	0	12	5	0
12	4-K	27	0	12	3	0
12	5-K	27	0	12	2	0
12	6-K	27	0	12	2	0
12	7-K	27	0	12	1	0
12	8-K	27	0	12	2	0
12	9-K	27	0	12	3	0
12	10-K	27	0	12	4	0
13	1-K	4	0	0	0	0
13	2-K	4	0	0	0	0
13	3-K	4	0	0	3	0
13	4-K	4	0	0	0	0
13	5-K	4	0	0	0	0
13	6-K	4	0	0	1	0
13	7-K	4	0	0	0	0
13	8-K	4	0	0	0	0
13	9-K	4	0	0	2	0
13	10-K	4	0	0	0	0
14	1-L	31	0	12	1	0
14	2-L	31	0	12	1	0
14	3-L	31	0	12	1	0
14	4-L	31	0	12	1	0
14	5-L	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	6-L	31	0	12	1	0
14	7-L	31	0	12	1	0
14	8-L	31	0	12	1	0
14	9-L	31	0	12	1	0
14	10-L	31	0	12	1	0
All	All	239500	0	215650	2477	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 5.

The worst 5 of 2477 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:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70
7:K:351:PHE:CE1	9:M:467:PHE:CE2	1.78	1.70

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	1-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	1-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	2-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	2-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	3-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	4-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	4-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	5-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	5-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	6-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	6-E	93/136 (68%)	93 (100%)	0	0	100	100
1	7-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	7-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	8-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	8-E	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
1	9-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	9-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
1	10-A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	10-E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
2	1-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	1-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	2-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	2-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	3-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	3-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	4-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	4-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	5-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	5-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	6-B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
2	6-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	7-B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
2	7-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	8-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	8-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	9-F	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	10-B	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	10-F	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
3	1-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	1-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	2-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	2-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	3-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	3-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	4-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	4-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	5-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	5-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	6-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	6-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	7-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	7-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	8-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	8-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	9-C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	9-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	10-C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	10-G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
4	1-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100
4	1-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	14	51
4	2-D	90/125 (72%)	86 (96%)	4 (4%)	0	100	100
4	2-H	90/125 (72%)	89 (99%)	1 (1%)	0	100	100
4	3-D	90/125 (72%)	86 (96%)	3 (3%)	1 (1%)	14	51
4	3-H	90/125 (72%)	88 (98%)	2 (2%)	0	100	100
4	4-D	90/125 (72%)	85 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	4-H	90/125 (72%)	89 (99%)	0	1 (1%)	14 51
4	5-D	90/125 (72%)	85 (94%)	5 (6%)	0	100 100
4	5-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	14 51
4	6-D	90/125 (72%)	86 (96%)	4 (4%)	0	100 100
4	6-H	90/125 (72%)	89 (99%)	1 (1%)	0	100 100
4	7-D	90/125 (72%)	85 (94%)	5 (6%)	0	100 100
4	7-H	90/125 (72%)	89 (99%)	1 (1%)	0	100 100
4	8-D	90/125 (72%)	85 (94%)	5 (6%)	0	100 100
4	8-H	90/125 (72%)	89 (99%)	0	1 (1%)	14 51
4	9-D	90/125 (72%)	87 (97%)	3 (3%)	0	100 100
4	9-H	90/125 (72%)	89 (99%)	0	1 (1%)	14 51
4	10-D	90/125 (72%)	85 (94%)	5 (6%)	0	100 100
4	10-H	90/125 (72%)	88 (98%)	1 (1%)	1 (1%)	14 51
7	1-K	602/813 (74%)	566 (94%)	24 (4%)	12 (2%)	7 40
7	2-K	602/813 (74%)	564 (94%)	25 (4%)	13 (2%)	6 38
7	3-K	602/813 (74%)	560 (93%)	30 (5%)	12 (2%)	7 40
7	4-K	602/813 (74%)	566 (94%)	24 (4%)	12 (2%)	7 40
7	5-K	602/813 (74%)	560 (93%)	30 (5%)	12 (2%)	7 40
7	6-K	602/813 (74%)	558 (93%)	32 (5%)	12 (2%)	7 40
7	7-K	602/813 (74%)	560 (93%)	31 (5%)	11 (2%)	8 42
7	8-K	602/813 (74%)	558 (93%)	36 (6%)	8 (1%)	12 48
7	9-K	602/813 (74%)	559 (93%)	32 (5%)	11 (2%)	8 42
7	10-K	602/813 (74%)	561 (93%)	29 (5%)	12 (2%)	7 40
8	1-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	2-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	3-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	4-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	5-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	6-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	7-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75
8	8-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	9-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41	75
8	10-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	41	75
9	1-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	2-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	3-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	4-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	5-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	6-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	7-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	8-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	9-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
9	10-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	10	45
10	1-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	2-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	3-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	4-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	5-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	6-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	7-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	8-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	9-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
10	10-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	7	39
All	All	21630/29020 (74%)	20713 (96%)	715 (3%)	202 (1%)	21	54

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1-K	343	SER
7	1-K	496	GLU
7	1-K	634	LEU
8	1-L	202	LYS
9	1-M	155	SER

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	1-A	86/111 (78%)	86 (100%)	0	100	100
1	1-E	83/111 (75%)	83 (100%)	0	100	100
1	2-A	86/111 (78%)	86 (100%)	0	100	100
1	2-E	83/111 (75%)	83 (100%)	0	100	100
1	3-A	86/111 (78%)	86 (100%)	0	100	100
1	3-E	83/111 (75%)	83 (100%)	0	100	100
1	4-A	86/111 (78%)	86 (100%)	0	100	100
1	4-E	83/111 (75%)	83 (100%)	0	100	100
1	5-A	86/111 (78%)	86 (100%)	0	100	100
1	5-E	83/111 (75%)	83 (100%)	0	100	100
1	6-A	86/111 (78%)	86 (100%)	0	100	100
1	6-E	83/111 (75%)	83 (100%)	0	100	100
1	7-A	86/111 (78%)	86 (100%)	0	100	100
1	7-E	83/111 (75%)	83 (100%)	0	100	100
1	8-A	86/111 (78%)	86 (100%)	0	100	100
1	8-E	83/111 (75%)	83 (100%)	0	100	100
1	9-A	86/111 (78%)	86 (100%)	0	100	100
1	9-E	83/111 (75%)	83 (100%)	0	100	100
1	10-A	86/111 (78%)	86 (100%)	0	100	100
1	10-E	83/111 (75%)	83 (100%)	0	100	100
2	1-B	72/79 (91%)	72 (100%)	0	100	100
2	1-F	64/79 (81%)	64 (100%)	0	100	100
2	2-B	72/79 (91%)	72 (100%)	0	100	100
2	2-F	64/79 (81%)	64 (100%)	0	100	100
2	3-B	72/79 (91%)	72 (100%)	0	100	100
2	3-F	64/79 (81%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4-B	72/79 (91%)	72 (100%)	0	100	100
2	4-F	64/79 (81%)	64 (100%)	0	100	100
2	5-B	72/79 (91%)	72 (100%)	0	100	100
2	5-F	64/79 (81%)	64 (100%)	0	100	100
2	6-B	72/79 (91%)	72 (100%)	0	100	100
2	6-F	64/79 (81%)	64 (100%)	0	100	100
2	7-B	72/79 (91%)	72 (100%)	0	100	100
2	7-F	64/79 (81%)	64 (100%)	0	100	100
2	8-B	72/79 (91%)	72 (100%)	0	100	100
2	8-F	64/79 (81%)	64 (100%)	0	100	100
2	9-B	72/79 (91%)	72 (100%)	0	100	100
2	9-F	64/79 (81%)	64 (100%)	0	100	100
2	10-B	72/79 (91%)	72 (100%)	0	100	100
2	10-F	64/79 (81%)	64 (100%)	0	100	100
3	1-C	84/102 (82%)	84 (100%)	0	100	100
3	1-G	84/102 (82%)	84 (100%)	0	100	100
3	2-C	84/102 (82%)	84 (100%)	0	100	100
3	2-G	84/102 (82%)	84 (100%)	0	100	100
3	3-C	84/102 (82%)	84 (100%)	0	100	100
3	3-G	84/102 (82%)	84 (100%)	0	100	100
3	4-C	84/102 (82%)	84 (100%)	0	100	100
3	4-G	84/102 (82%)	84 (100%)	0	100	100
3	5-C	84/102 (82%)	84 (100%)	0	100	100
3	5-G	84/102 (82%)	84 (100%)	0	100	100
3	6-C	84/102 (82%)	84 (100%)	0	100	100
3	6-G	84/102 (82%)	84 (100%)	0	100	100
3	7-C	84/102 (82%)	84 (100%)	0	100	100
3	7-G	84/102 (82%)	84 (100%)	0	100	100
3	8-C	84/102 (82%)	84 (100%)	0	100	100
3	8-G	84/102 (82%)	84 (100%)	0	100	100
3	9-C	84/102 (82%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	9-G	84/102 (82%)	84 (100%)	0	100	100
3	10-C	84/102 (82%)	84 (100%)	0	100	100
3	10-G	84/102 (82%)	84 (100%)	0	100	100
4	1-D	78/104 (75%)	78 (100%)	0	100	100
4	1-H	78/104 (75%)	78 (100%)	0	100	100
4	2-D	78/104 (75%)	78 (100%)	0	100	100
4	2-H	78/104 (75%)	78 (100%)	0	100	100
4	3-D	78/104 (75%)	78 (100%)	0	100	100
4	3-H	78/104 (75%)	78 (100%)	0	100	100
4	4-D	78/104 (75%)	78 (100%)	0	100	100
4	4-H	78/104 (75%)	78 (100%)	0	100	100
4	5-D	78/104 (75%)	78 (100%)	0	100	100
4	5-H	78/104 (75%)	78 (100%)	0	100	100
4	6-D	78/104 (75%)	78 (100%)	0	100	100
4	6-H	78/104 (75%)	78 (100%)	0	100	100
4	7-D	78/104 (75%)	78 (100%)	0	100	100
4	7-H	78/104 (75%)	78 (100%)	0	100	100
4	8-D	78/104 (75%)	78 (100%)	0	100	100
4	8-H	78/104 (75%)	78 (100%)	0	100	100
4	9-D	78/104 (75%)	78 (100%)	0	100	100
4	9-H	78/104 (75%)	78 (100%)	0	100	100
4	10-D	78/104 (75%)	78 (100%)	0	100	100
4	10-H	78/104 (75%)	78 (100%)	0	100	100
7	1-K	558/735 (76%)	554 (99%)	4 (1%)	84	90
7	2-K	558/735 (76%)	554 (99%)	4 (1%)	84	90
7	3-K	558/735 (76%)	554 (99%)	4 (1%)	84	90
7	4-K	558/735 (76%)	552 (99%)	6 (1%)	73	84
7	5-K	558/735 (76%)	554 (99%)	4 (1%)	84	90
7	6-K	558/735 (76%)	552 (99%)	6 (1%)	73	84
7	7-K	558/735 (76%)	554 (99%)	4 (1%)	84	90
7	8-K	558/735 (76%)	553 (99%)	5 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	9-K	558/735 (76%)	552 (99%)	6 (1%)	73	84
7	10-K	558/735 (76%)	555 (100%)	3 (0%)	88	93
8	1-L	349/420 (83%)	349 (100%)	0	100	100
8	2-L	349/420 (83%)	349 (100%)	0	100	100
8	3-L	349/420 (83%)	349 (100%)	0	100	100
8	4-L	349/420 (83%)	349 (100%)	0	100	100
8	5-L	349/420 (83%)	349 (100%)	0	100	100
8	6-L	349/420 (83%)	349 (100%)	0	100	100
8	7-L	349/420 (83%)	349 (100%)	0	100	100
8	8-L	349/420 (83%)	349 (100%)	0	100	100
8	9-L	349/420 (83%)	349 (100%)	0	100	100
8	10-L	349/420 (83%)	349 (100%)	0	100	100
9	1-M	362/423 (86%)	362 (100%)	0	100	100
9	2-M	362/423 (86%)	362 (100%)	0	100	100
9	3-M	362/423 (86%)	362 (100%)	0	100	100
9	4-M	362/423 (86%)	362 (100%)	0	100	100
9	5-M	362/423 (86%)	362 (100%)	0	100	100
9	6-M	362/423 (86%)	362 (100%)	0	100	100
9	7-M	362/423 (86%)	362 (100%)	0	100	100
9	8-M	362/423 (86%)	362 (100%)	0	100	100
9	9-M	362/423 (86%)	362 (100%)	0	100	100
9	10-M	362/423 (86%)	362 (100%)	0	100	100
10	1-N	54/140 (39%)	54 (100%)	0	100	100
10	2-N	54/140 (39%)	54 (100%)	0	100	100
10	3-N	54/140 (39%)	54 (100%)	0	100	100
10	4-N	54/140 (39%)	54 (100%)	0	100	100
10	5-N	54/140 (39%)	54 (100%)	0	100	100
10	6-N	54/140 (39%)	54 (100%)	0	100	100
10	7-N	54/140 (39%)	54 (100%)	0	100	100
10	8-N	54/140 (39%)	54 (100%)	0	100	100
10	9-N	54/140 (39%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	10-N	54/140 (39%)	54 (100%)	0	100 100
All	All	19520/25100 (78%)	19474 (100%)	46 (0%)	93 96

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	7-K	351	PHE
7	8-K	836	ARG
7	7-K	362	MET
7	8-K	351	PHE
7	9-K	351	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
7	9-K	361	GLN
8	9-L	11	HIS
8	10-L	11	HIS
8	4-L	11	HIS
7	4-K	361	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 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
12	ADP	8-K	1502	13	24,29,29	1.01	0	29,45,45	1.80	4 (13%)
14	ATP	8-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
12	ADP	6-K	1502	13	24,29,29	1.03	2 (8%)	29,45,45	1.59	4 (13%)
14	ATP	3-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
12	ADP	10-K	1502	13	24,29,29	1.08	2 (8%)	29,45,45	1.57	3 (10%)
13	BEF	4-K	1503	12	0,3,3	-	-	-		
14	ATP	5-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
13	BEF	10-K	1503	12	0,3,3	-	-	-		
13	BEF	6-K	1503	12	0,3,3	-	-	-		
14	ATP	9-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
12	ADP	7-K	1502	13	24,29,29	1.03	2 (8%)	29,45,45	1.49	3 (10%)
14	ATP	10-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
14	ATP	6-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
13	BEF	8-K	1503	12	0,3,3	-	-	-		
12	ADP	5-K	1502	13	24,29,29	1.10	2 (8%)	29,45,45	1.64	4 (13%)
13	BEF	3-K	1503	12	0,3,3	-	-	-		
13	BEF	7-K	1503	12	0,3,3	-	-	-		
12	ADP	9-K	1502	13	24,29,29	0.98	2 (8%)	29,45,45	1.64	4 (13%)
13	BEF	9-K	1503	12	0,3,3	-	-	-		
13	BEF	5-K	1503	12	0,3,3	-	-	-		
12	ADP	1-K	1502	13	24,29,29	1.03	1 (4%)	29,45,45	1.67	4 (13%)
13	BEF	1-K	1503	12	0,3,3	-	-	-		
14	ATP	1-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
14	ATP	7-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
12	ADP	3-K	1502	13	24,29,29	1.03	2 (8%)	29,45,45	1.54	4 (13%)
14	ATP	2-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
12	ADP	4-K	1502	13	24,29,29	0.99	1 (4%)	29,45,45	1.55	5 (17%)
14	ATP	4-L	501	-	26,33,33	1.00	0	31,52,52	2.15	6 (19%)
13	BEF	2-K	1503	12	0,3,3	-	-	-		
12	ADP	2-K	1502	13	24,29,29	0.99	1 (4%)	29,45,45	1.73	6 (20%)

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
12	ADP	8-K	1502	13	-	3/12/32/32	0/3/3/3
14	ATP	8-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	6-K	1502	13	-	4/12/32/32	0/3/3/3
14	ATP	3-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	10-K	1502	13	-	5/12/32/32	0/3/3/3
14	ATP	5-L	501	-	-	1/18/38/38	0/3/3/3
14	ATP	9-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	7-K	1502	13	-	3/12/32/32	0/3/3/3
14	ATP	10-L	501	-	-	1/18/38/38	0/3/3/3
14	ATP	6-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	5-K	1502	13	-	3/12/32/32	0/3/3/3
12	ADP	9-K	1502	13	-	4/12/32/32	0/3/3/3
12	ADP	1-K	1502	13	-	3/12/32/32	0/3/3/3
14	ATP	1-L	501	-	-	1/18/38/38	0/3/3/3
14	ATP	7-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	3-K	1502	13	-	7/12/32/32	0/3/3/3
14	ATP	2-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	4-K	1502	13	-	3/12/32/32	0/3/3/3
14	ATP	4-L	501	-	-	1/18/38/38	0/3/3/3
12	ADP	2-K	1502	13	-	2/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	10-K	1502	ADP	C2'-C1'	-2.42	1.50	1.53
12	4-K	1502	ADP	C2'-C1'	-2.36	1.50	1.53
12	6-K	1502	ADP	C2'-C1'	-2.33	1.50	1.53
12	7-K	1502	ADP	C2'-C1'	-2.28	1.50	1.53
12	5-K	1502	ADP	C2'-C1'	-2.26	1.50	1.53

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1-L	501	ATP	PA-O3A-PB	-6.87	109.25	132.83
14	2-L	501	ATP	PA-O3A-PB	-6.87	109.25	132.83
14	3-L	501	ATP	PA-O3A-PB	-6.87	109.25	132.83
14	4-L	501	ATP	PA-O3A-PB	-6.87	109.25	132.83
14	5-L	501	ATP	PA-O3A-PB	-6.87	109.25	132.83

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1-K	1502	ADP	C5'-O5'-PA-O1A
12	1-K	1502	ADP	C4'-C5'-O5'-PA
12	2-K	1502	ADP	C5'-O5'-PA-O1A
12	3-K	1502	ADP	PA-O3A-PB-O2B
12	3-K	1502	ADP	PA-O3A-PB-O3B

There are no ring outliers.

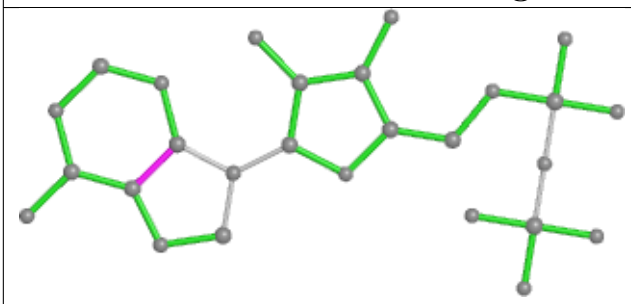
23 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	8-K	1502	ADP	2	0
14	8-L	501	ATP	1	0
12	6-K	1502	ADP	2	0
14	3-L	501	ATP	1	0
12	10-K	1502	ADP	4	0
14	5-L	501	ATP	1	0
13	6-K	1503	BEF	1	0
14	9-L	501	ATP	1	0
12	7-K	1502	ADP	1	0
14	10-L	501	ATP	1	0
14	6-L	501	ATP	1	0
12	5-K	1502	ADP	2	0
13	3-K	1503	BEF	3	0
12	9-K	1502	ADP	3	0
13	9-K	1503	BEF	2	0
12	1-K	1502	ADP	3	0
14	1-L	501	ATP	1	0
14	7-L	501	ATP	1	0
12	3-K	1502	ADP	5	0
14	2-L	501	ATP	1	0
12	4-K	1502	ADP	3	0
14	4-L	501	ATP	1	0
12	2-K	1502	ADP	1	0

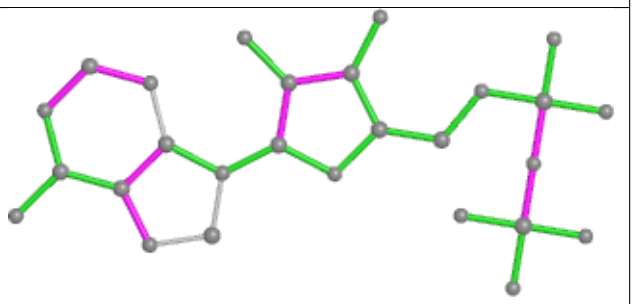
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

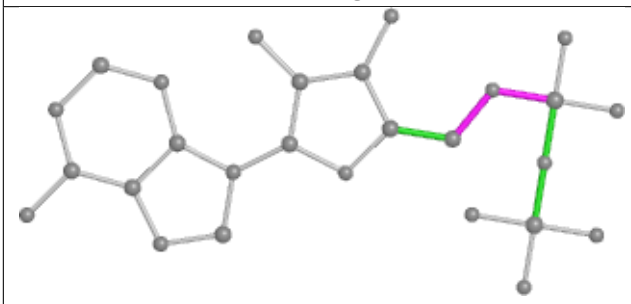
Ligand ADP K 1502



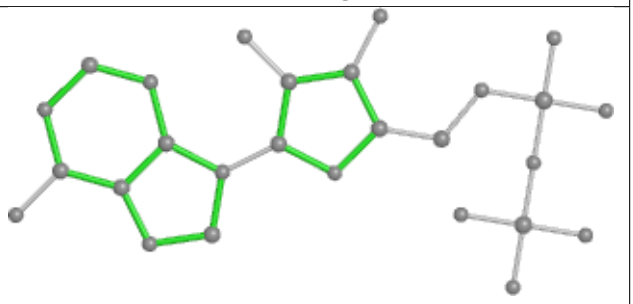
Bond lengths



Bond angles

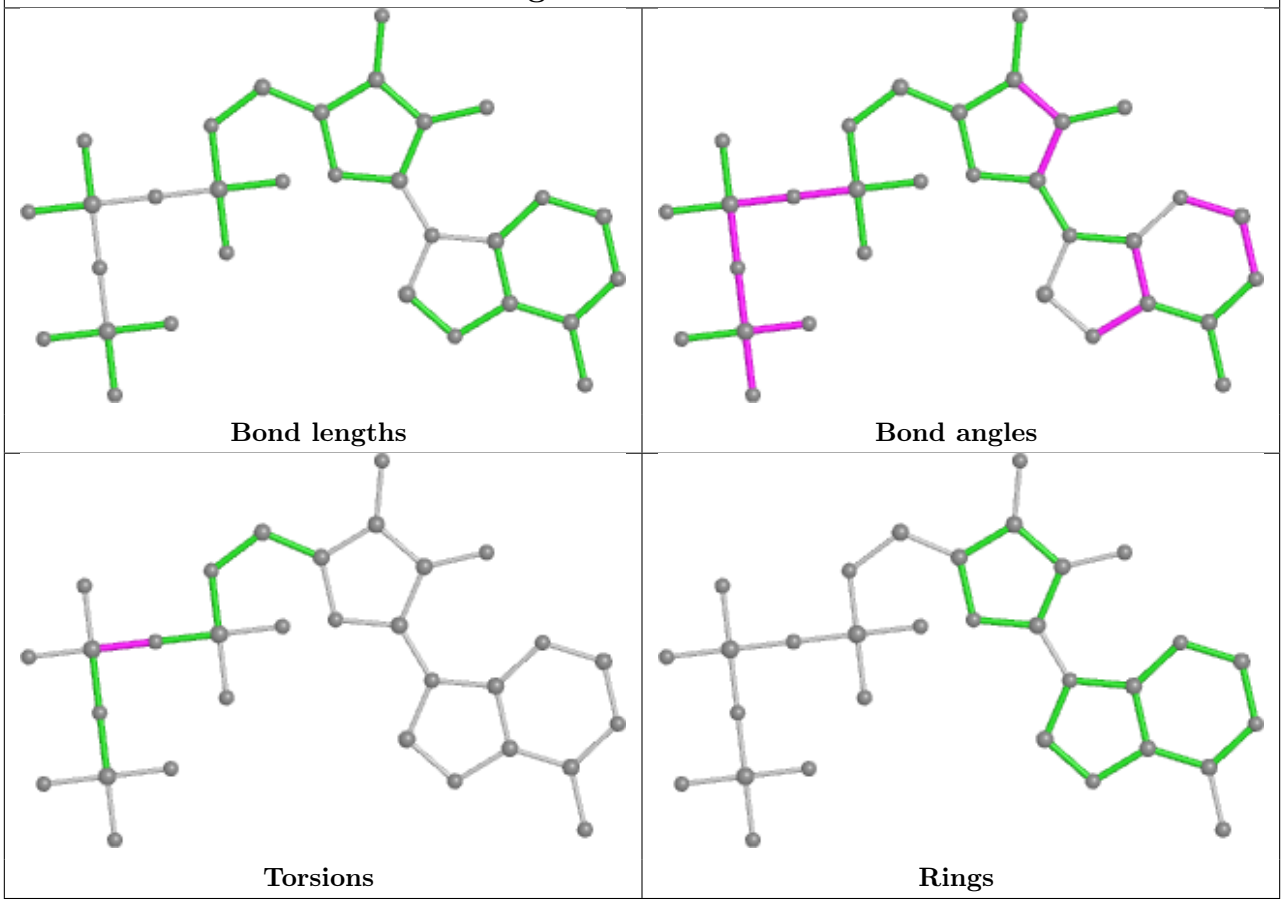


Torsions



Rings

Ligand ATP L 501



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.

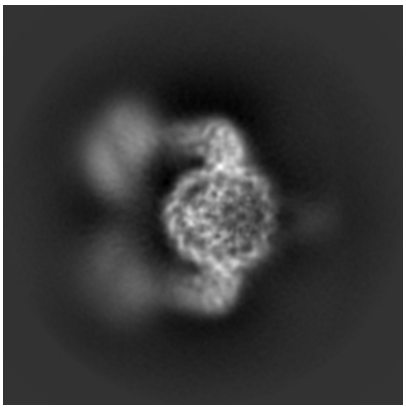
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21484. These allow visual inspection of the internal detail of the map and identification of artifacts.

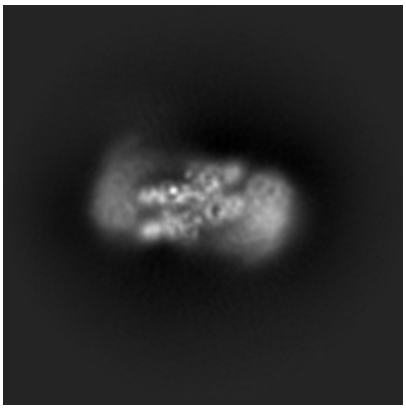
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

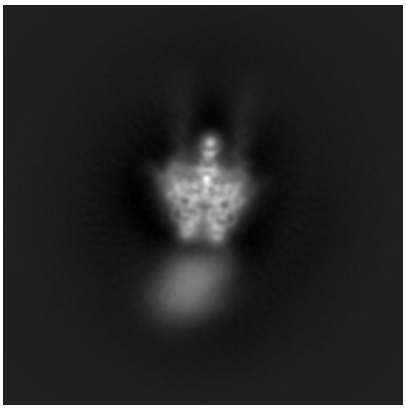
6.1.1 Primary map



X

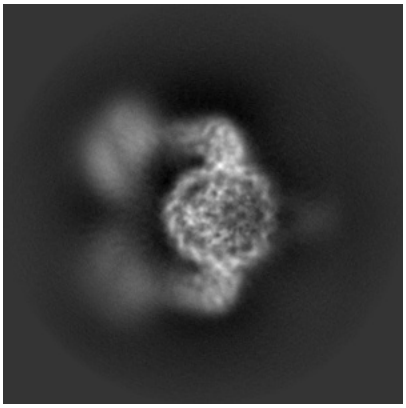


Y

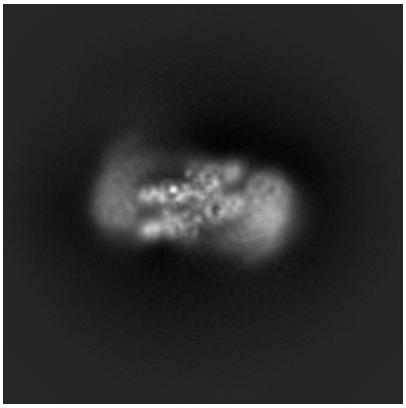


Z

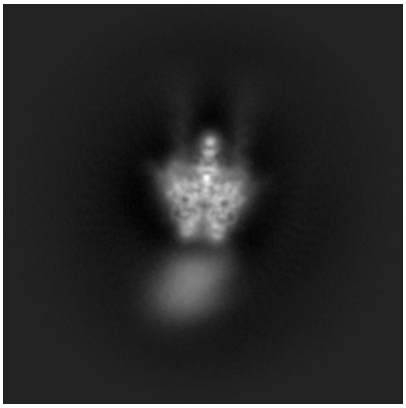
6.1.2 Raw map



X



Y

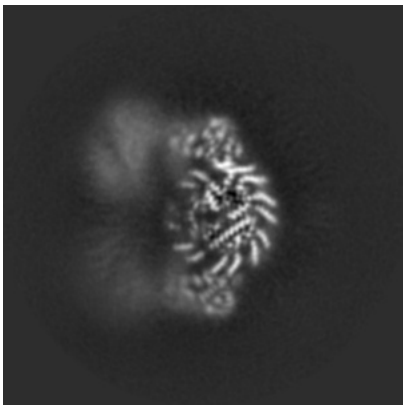


Z

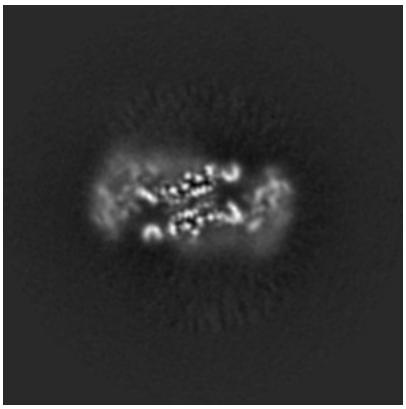
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

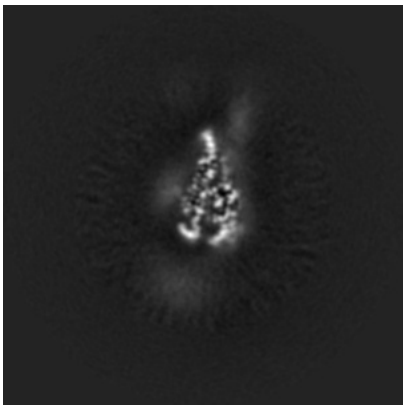
6.2.1 Primary map



X Index: 150

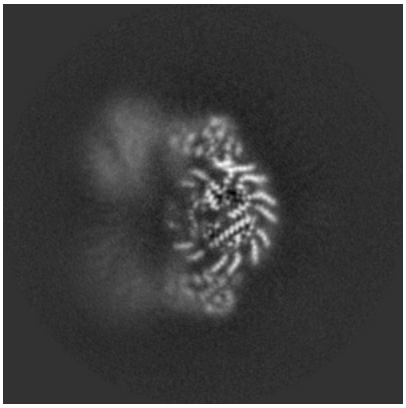


Y Index: 150

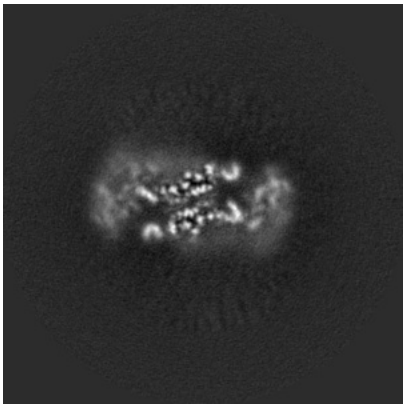


Z Index: 150

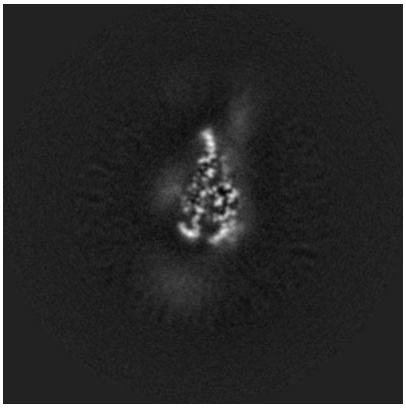
6.2.2 Raw map



X Index: 150



Y Index: 150

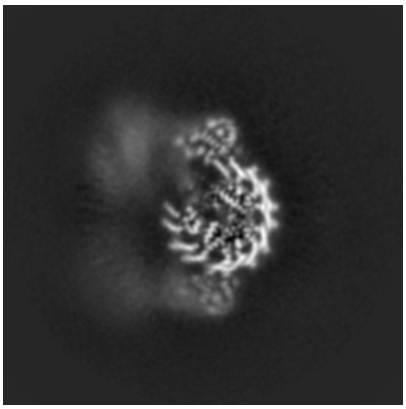


Z Index: 150

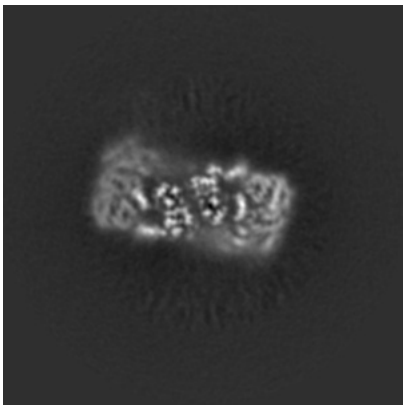
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

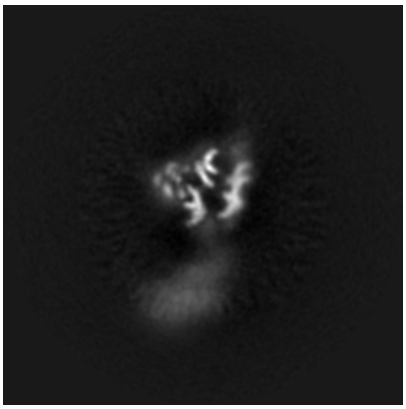
6.3.1 Primary map



X Index: 154

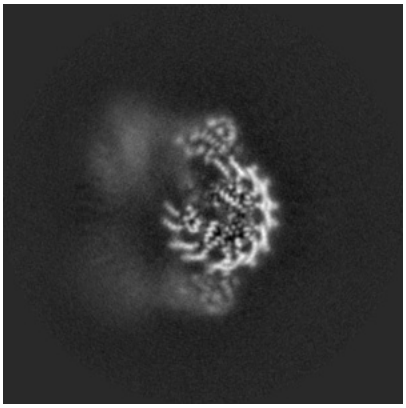


Y Index: 163

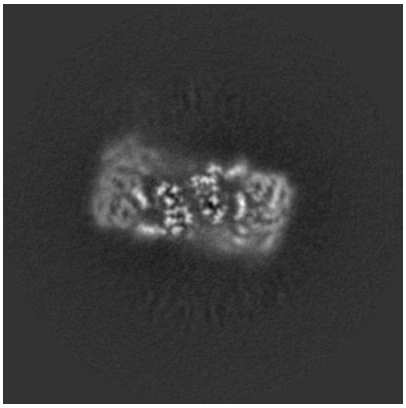


Z Index: 174

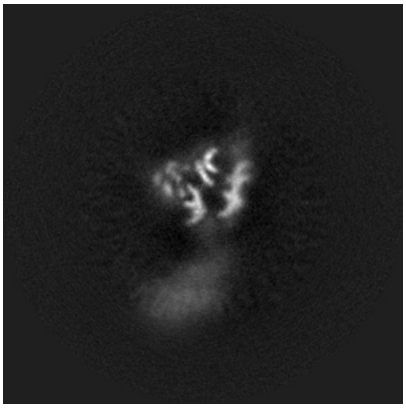
6.3.2 Raw map



X Index: 154



Y Index: 163

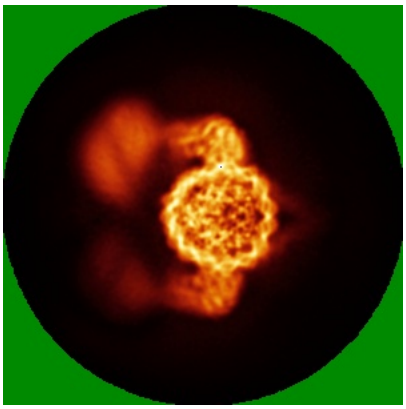


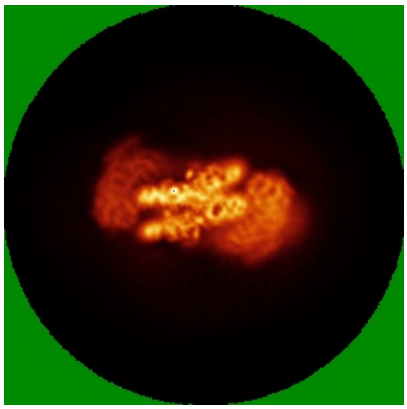
Z Index: 174

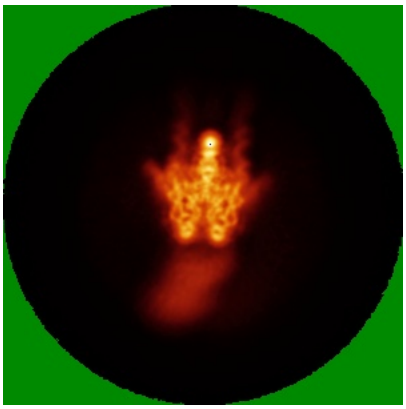
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

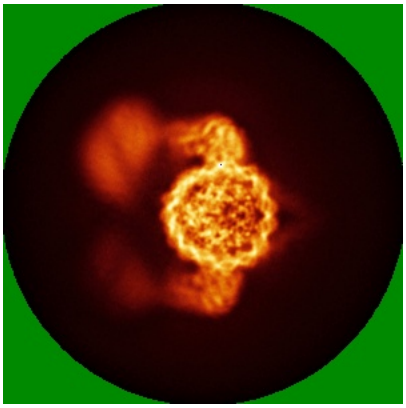
6.4.1 Primary map

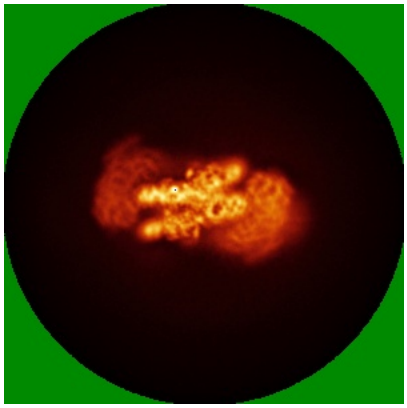

X

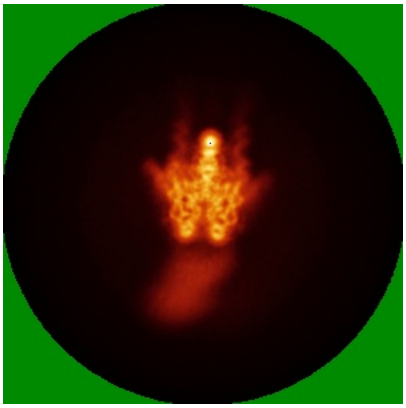

Y


Z

6.4.2 Raw map


X

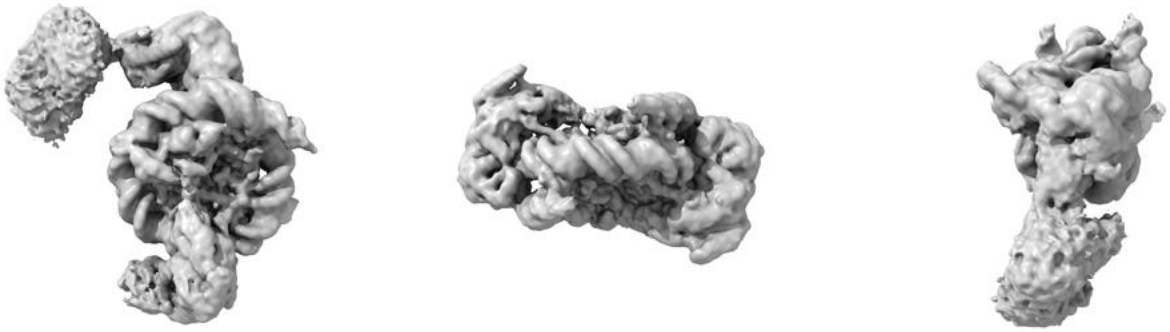

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

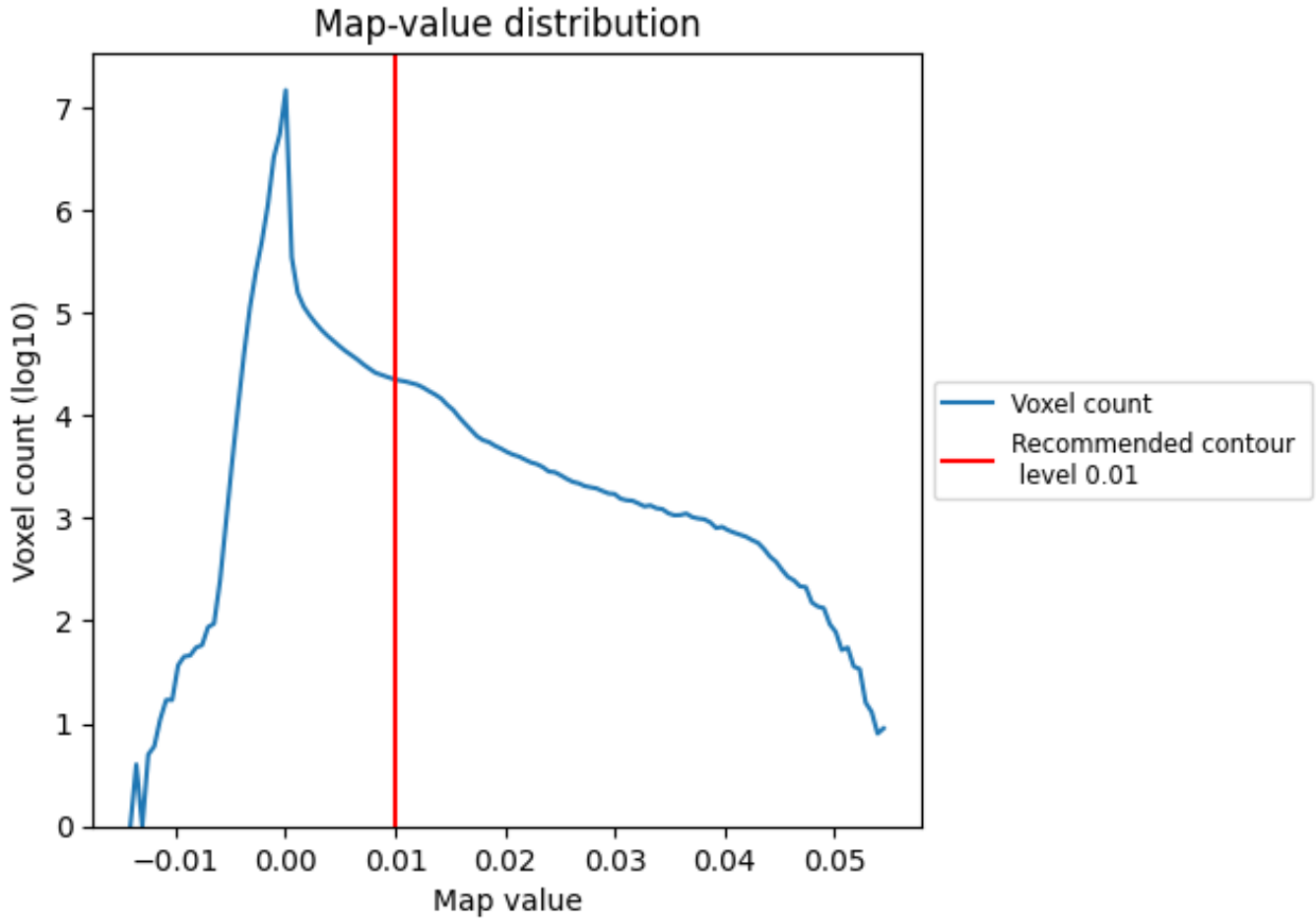
6.6 Mask visualisation (i)

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

7 Map analysis

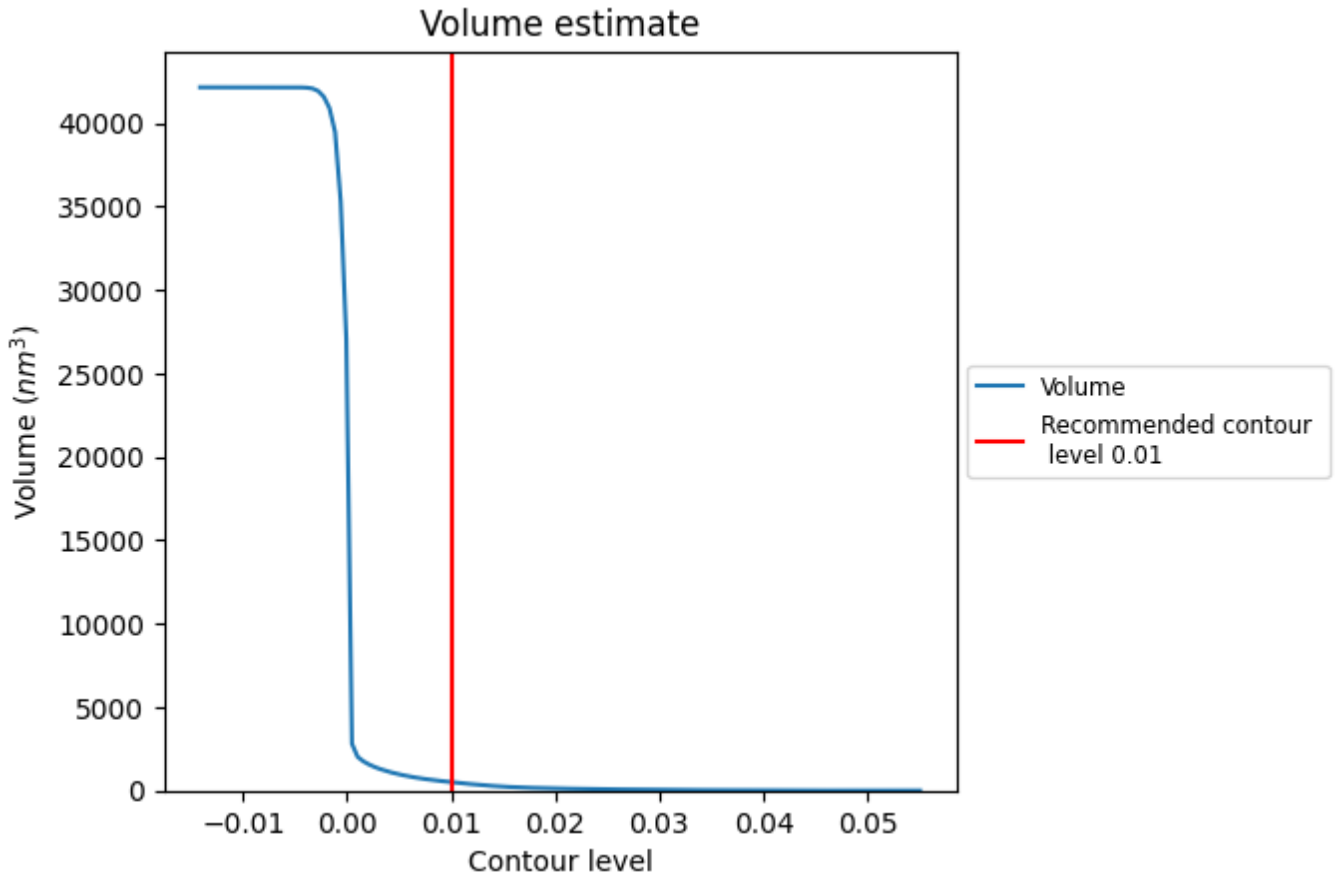
This section contains the results of statistical analysis of the map.

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.

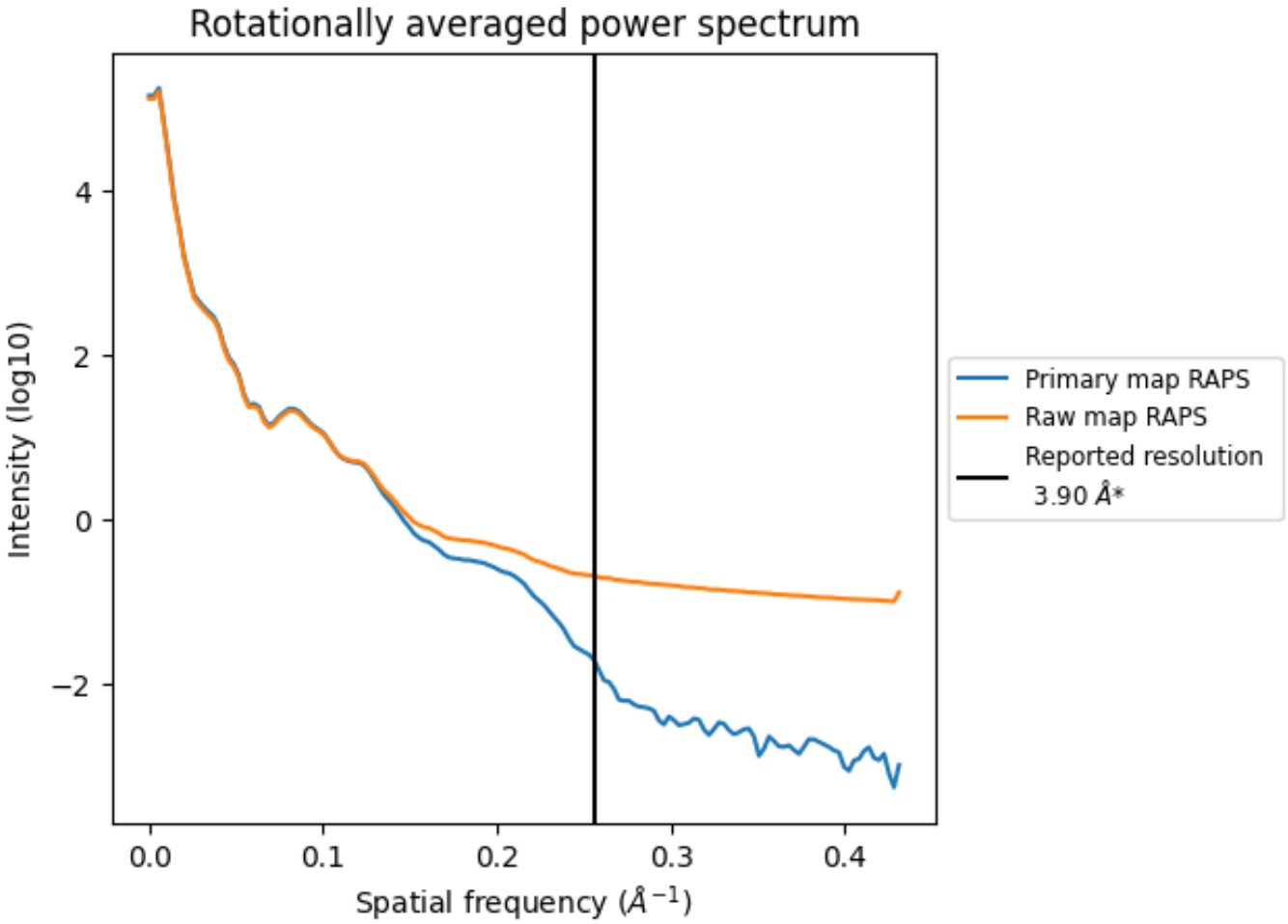
7.2 Volume estimate (i)



The volume at the recommended contour level is 505 nm^3; this corresponds to an approximate mass of 456 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)

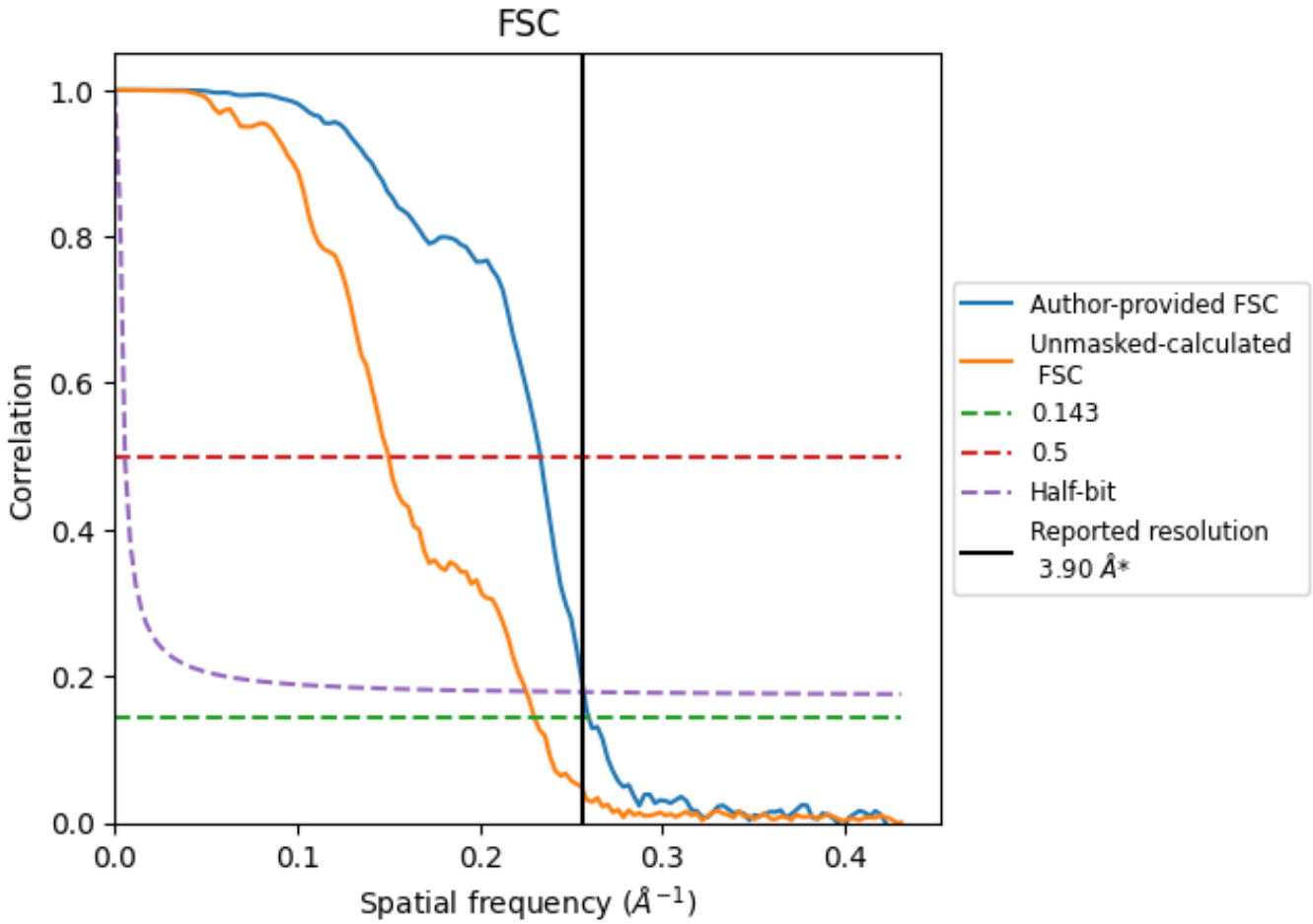


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

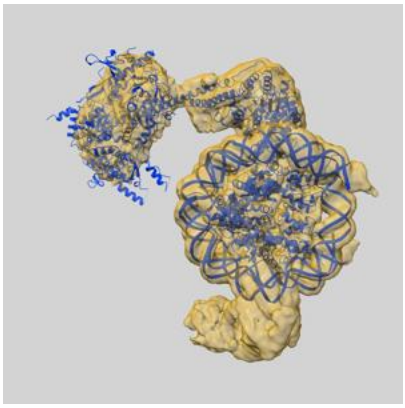
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.29	3.89
Unmasked-calculated*	4.35	6.67	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.9 by more than 10 %

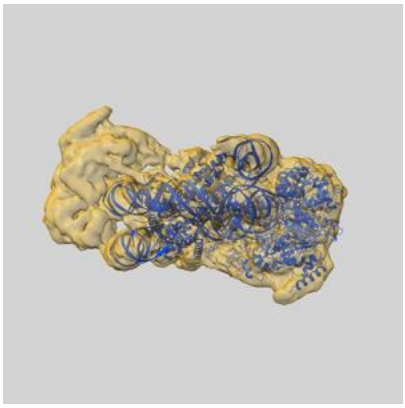
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21484 and PDB model 6VZ4. Per-residue inclusion information can be found in section 3 on page 21.

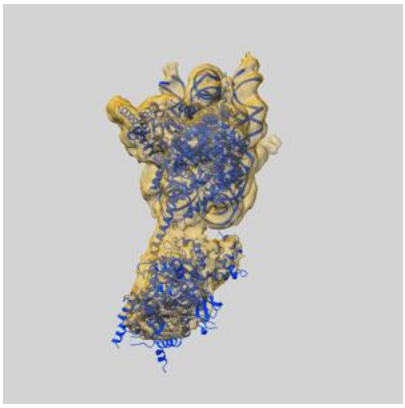
9.1 Map-model overlay



X



Y



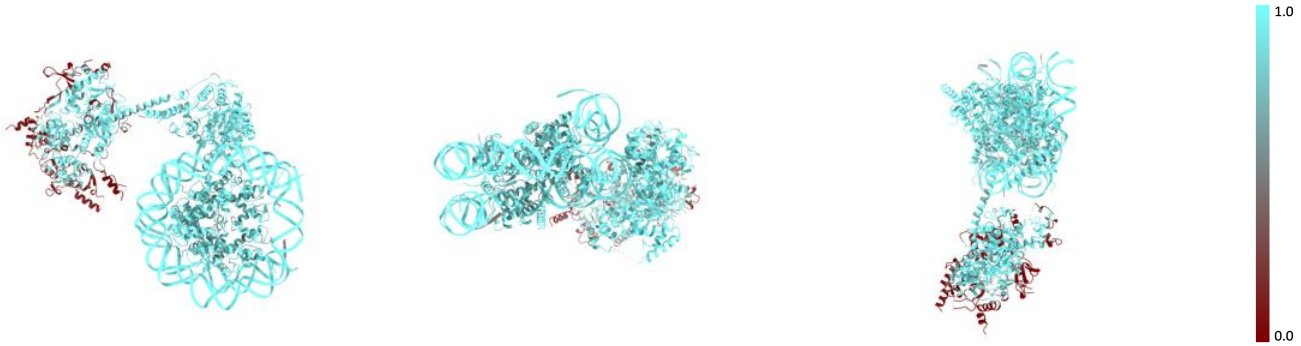
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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)

This section was not generated.

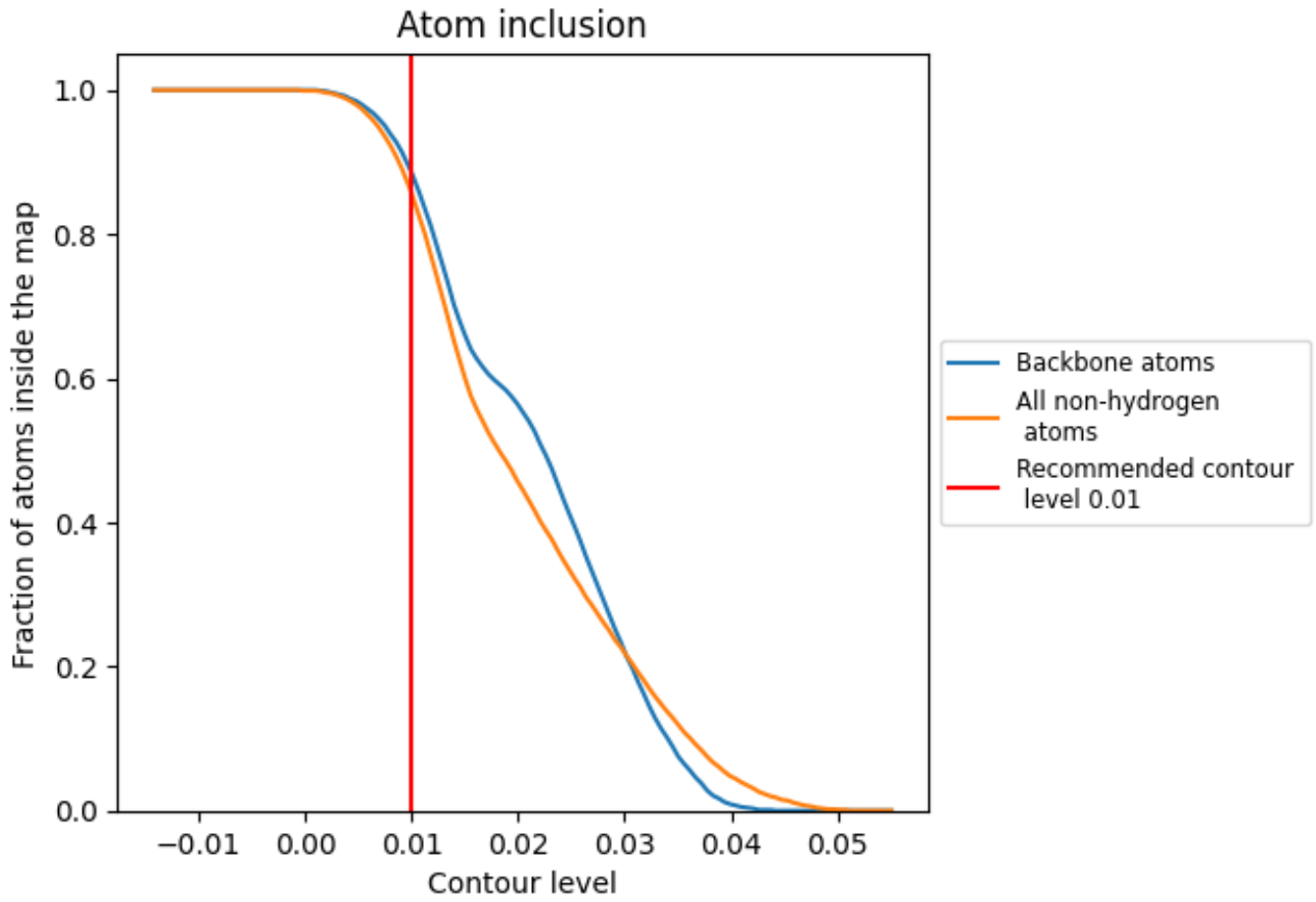
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8580
A	0.9150
B	0.9170
C	0.8930
D	0.9330
E	0.9120
F	0.9140
G	0.9100
H	0.9300
I	0.9930
J	0.9910
K	0.9210
L	0.5700
M	0.7540
N	0.4050