



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 04:55 pm GMT

PDB ID : 8C6J
EMDB ID : EMD-16452
Title : Human spliceosomal PM5 C* complex
Authors : Dybkov, O.; Kastner, B.; Luehrmann, R.
Deposited on : 2023-01-12
Resolution : 2.80 Å (reported)
Based on initial models : 5HLY, 6HYU, 7OS2, 2OK3, 6BK8, 4PJ3, 5MQF, ., 3MDF, 6QDV

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

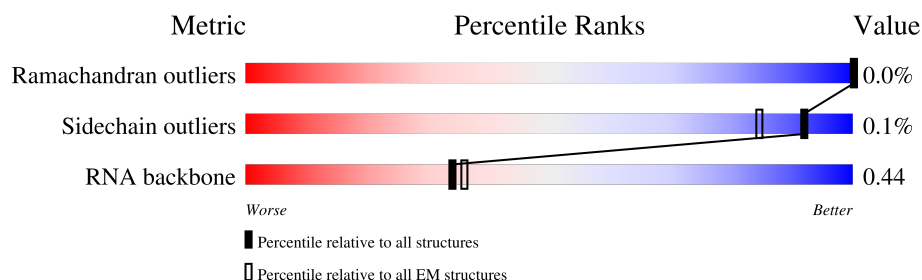
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.


















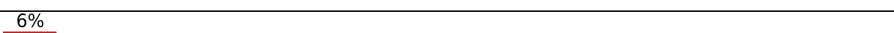
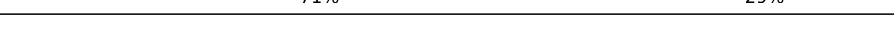

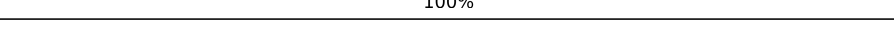




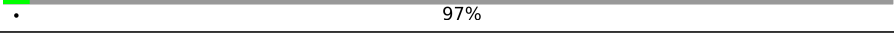

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	188	
2	4	476	
3	5	116	
4	6	106	
5	7	411	
6	8	174	
7	9	146	
8	A	2335	

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Mol	Chain	Length	Quality of chain
9	B	2136	
10	C	972	
11	C3	161	
12	CD	622	
13	CE	301	
14	CF	339	
15	CI	285	
16	CN	301	
17	CT	289	
18	D	184	
19	E	242	
20	F	758	
21	G	112	
22	H	500	
23	I	235	
24	J	514	
25	K	536	
26	L	144	
27	M	420	
28	N	357	
29	O	802	
30	P	229	
31	R	2752	
32	S	687	
33	T	855	

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Mol	Chain	Length	Quality of chain
34	U	1485	
35	V	1220	
36	W	255	
37	Y	225	
38	Z	415	
39	a	118	
39	m	118	
40	b	240	
40	k	240	
41	c	119	
41	l	119	
42	d	126	
42	n	126	
43	e	92	
43	p	92	
44	f	86	
44	q	86	
45	g	76	
45	r	76	
46	h	586	
47	i	166	
48	j	222	
49	o	579	
50	s	225	
51	t	504	

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Mol	Chain	Length	Quality of chain
51	u	504	<div><div>18%</div><div>26%</div><div>74%</div></div>
51	v	504	<div><div>14%</div><div>27%</div><div>73%</div></div>
51	w	504	<div><div>21%</div><div>26%</div><div>74%</div></div>
52	y	243	<div><div>12%</div><div>89%</div><div>11%</div></div>
53	z	451	<div><div>14%</div><div>23%</div><div>77%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 111233 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	142	Total	C	N	O	P	0	0
			3010	1346	517	1005	142		

- Molecule 2 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	77	Total	C	N	O	S	0	0
			636	395	107	133	1		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	113	Total	C	N	O	P	0	0
			2371	1064	394	801	112		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 5 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	390	Total	C	N	O	S	0	0
			3130	1976	546	589	19		

- Molecule 6 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 7 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	144	Total	C	N	O	0	0
			595	306	144	145		

- Molecule 8 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2261	Total	C	N	O	S	0	0
			17716	11283	3167	3195	71		

- Molecule 9 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	1726	Total	C	N	O	0	0
			7141	3689	1726	1726		

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	899	Total	C	N	O	S	0	0
			7114	4552	1184	1344	34		

- Molecule 11 is a protein called Peptidyl-prolyl cis-trans isomerase-like 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	C3	160	Total	C	N	O	2	0
			669	345	162	162		

- Molecule 12 is a protein called Probable ATP-dependent RNA helicase DDX41.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	CD	245	Total	C	N	O	0	0
			1025	535	245	245		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	CE	79	Total	C	N	O	0	0
			322	164	79	79		

- Molecule 14 is a protein called Protein FAM50A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CF	185	Total	C	N	O	0	0
			746	376	185	185		

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	CI	70	Total	C	N	O	0	0
			283	143	70	70		

- Molecule 16 is a protein called Nitric oxide synthase-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	250	Total	C	N	O	S	0	0
			1643	991	313	327	12		

- Molecule 17 is a protein called Splicing factor C9orf78.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	CT	102	Total	C	N	O	0	0
			414	210	102	102		

- Molecule 18 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 19 is a RNA chain called PM5 5' Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	24	Total	C	N	O	P	0	0
			511	229	97	162	23		

- Molecule 20 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	122	Total	C	N	O	S	0	0
			1088	714	197	175	2		

- Molecule 21 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	59	Total	C	N	O	S	0	0
			494	308	94	90	2		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	459	Total	C	N	O	S	0	0
			3321	2079	603	621	18		

- Molecule 23 is a RNA chain called PM5 Intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	84	Total	C	N	O	P	0	0
			1727	775	254	614	84		

- Molecule 24 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	367	Total	C	N	O	S	0	0
			2720	1697	504	511	8		

- Molecule 25 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	K	295	Total	C	N	O	P	S	0	0
			2360	1479	431	435	2	13		

- Molecule 26 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	144	Total	C	N	O	S	0	0
			1188	748	218	210	12		

- Molecule 27 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	289	Total	C	N	O	S	0	0
			2327	1459	416	432	20		

- Molecule 28 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	306	Total	C	N	O	S	0	0
			2388	1498	419	457	14		

- Molecule 29 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	O	548	Total	C	N	O	S	0	0
			3321	1939	693	682	7		

- Molecule 30 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P	117	Total	C	N	O	S	0	0
			973	595	190	186	2		

- Molecule 31 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	76	Total	C	N	O	S	0	0
			399	226	86	86	1		

- Molecule 32 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	635	Total	C	N	O	S	0	0
			3835	2264	784	781	6		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	689	Total	C	N	O	S	0	0
			4273	2649	798	813	13		

- Molecule 34 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	1330	Total	C	N	O		6	0
			5548	2884	1332	1332			

- Molecule 35 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	934	Total	C	N	O	S	0	0
			4167	2221	962	983	1		

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	W	176	Total	C	N	O	0	0
			722	370	176	176		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	Y	92	Total	C	N	O	0	0
			377	193	92	92		

- Molecule 38 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z	87	Total	C	N	O	S	0	0
			454	250	99	103	2		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	a	103	Total	C	N	O	0	0
			520	314	103	103		
39	m	95	Total	C	N	O	0	0
			395	205	95	95		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	82	Total	C	N	O	0	0
			413	249	82	82		
40	k	82	Total	C	N	O	0	0
			340	176	82	82		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	c	80	Total	C	N	O	0	0
			402	242	80	80		
41	l	80	Total	C	N	O	0	0
			329	169	80	80		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	d	84	Total	C	N	O	0	0
			420	252	84	84		
42	n	83	Total	C	N	O	0	0
			341	175	83	83		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	e	79	Total	C	N	O	0	0
			393	235	79	79		
43	p	81	Total	C	N	O	0	0
			327	165	81	81		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	f	72	Total	C	N	O	0	0
			359	215	72	72		
44	q	72	Total	C	N	O	0	0
			300	156	72	72		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	g	73	Total	C	N	O	0	0
			365	218	73	74		
45	r	73	Total	C	N	O	0	0
			302	155	73	74		

- Molecule 46 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	h	276	Total	C	N	O	S	0	0
			2280	1433	408	431	8		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	i	164	Total	C	N	O	S	0	0
			1270	810	220	233	7		

- Molecule 48 is a protein called STING ER exit protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	j	95	Total	C	N	O	0	0
			398	208	95	95		

- Molecule 49 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	513	Total	C	N	O	S	0	0
			3918	2478	692	724	24		

- Molecule 50 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	s	225	Total	C	N	O	0	0
			922	471	225	226		

- Molecule 51 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	t	137	Total	C	N	O	0	0
			581	307	137	137		
51	u	130	Total	C	N	O	0	0
			550	290	130	130		
51	v	138	Total	C	N	O	0	0
			585	309	138	138		
51	w	131	Total	C	N	O	0	0
			554	292	131	131		

- Molecule 52 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	216	Total	C	N	O	S	0	0
			1423	843	284	294	2		

- Molecule 53 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	103	Total	C	N	O	S	0	0
			606	346	133	124	3		

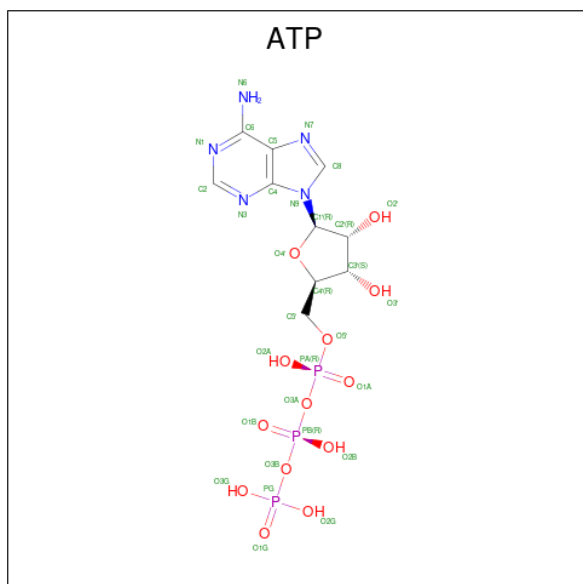
- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	6	2	Total	K	0
			2	2	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

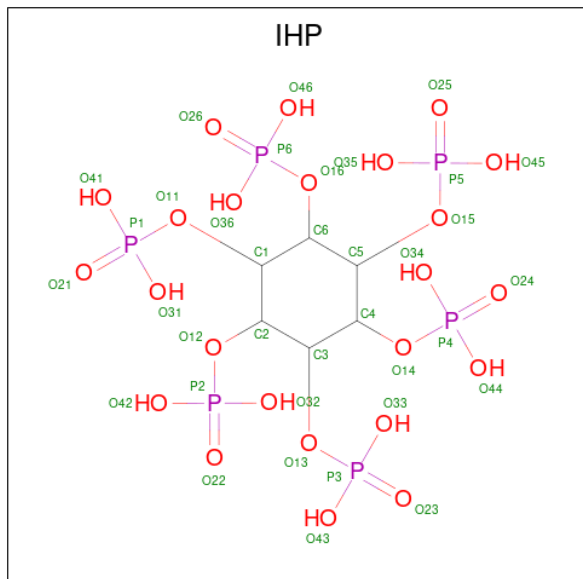
Mol	Chain	Residues	Atoms		AltConf
55	6	5	Total	Mg	0
			5	5	
55	7	1	Total	Mg	0
			1	1	
55	C	1	Total	Mg	0
			1	1	

- Molecule 56 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



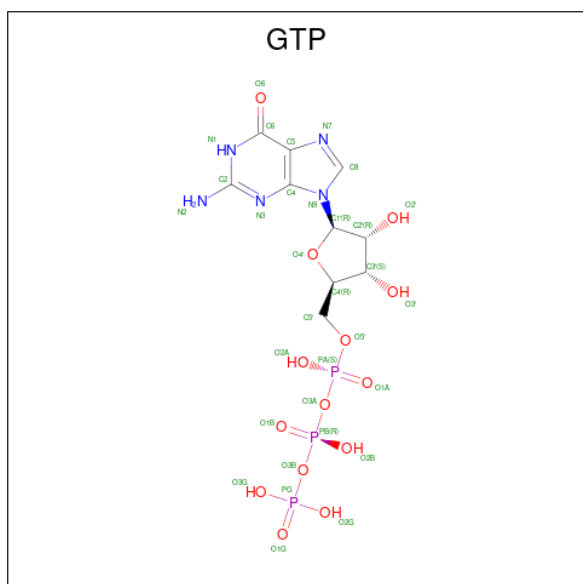
Mol	Chain	Residues	Atoms					AltConf
56	7	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 57 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 58 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

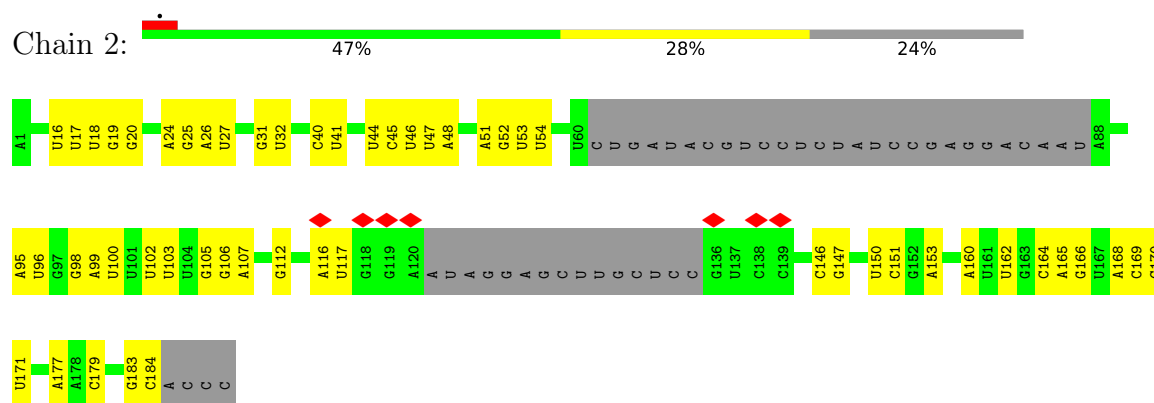
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
59	L	3	Total 3	Zn 3	0
59	M	3	Total 3	Zn 3	0

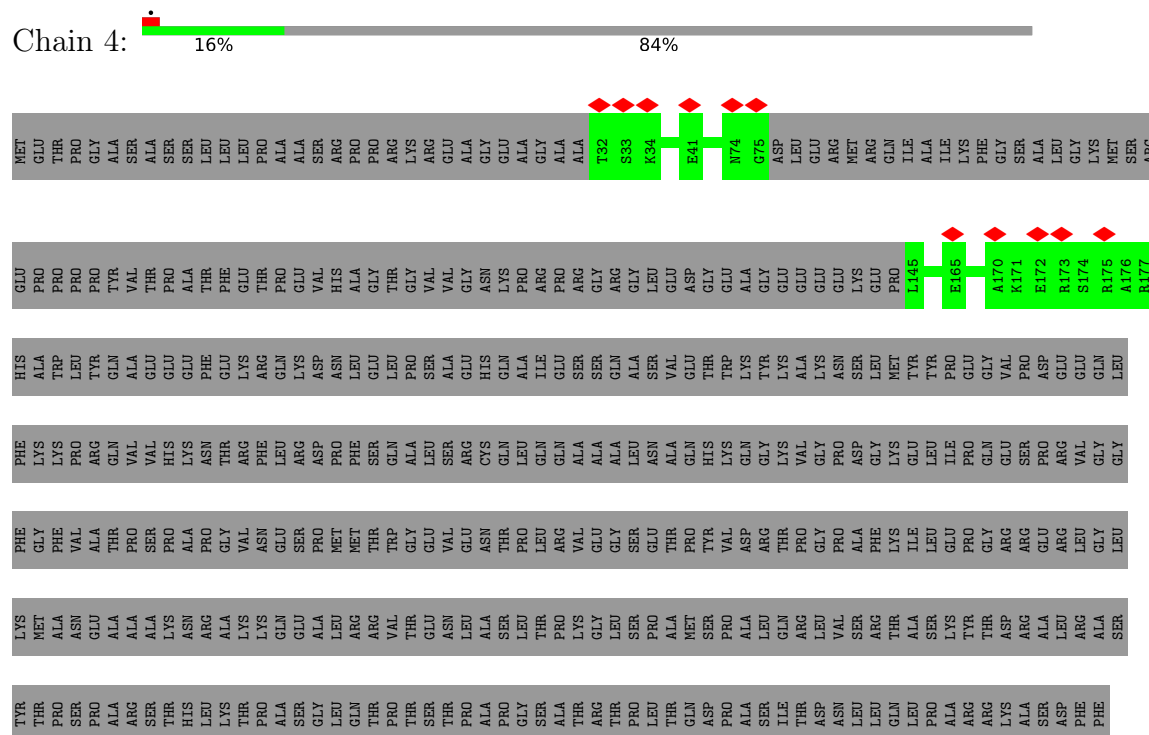
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

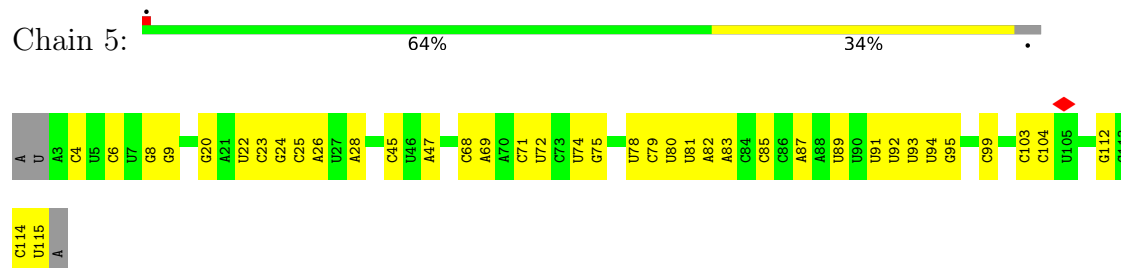
• Molecule 1: U2 snRNA



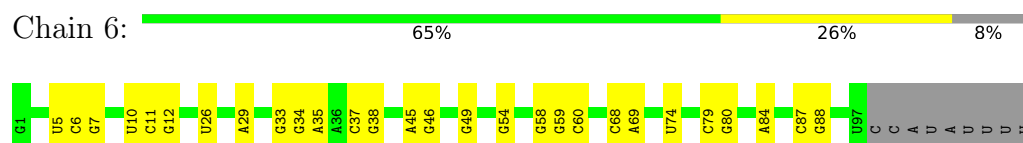
• Molecule 2: Splicing factor ESS-2 homolog



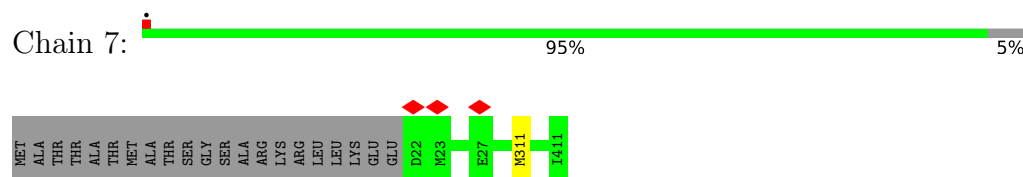
- Molecule 3: U5 snRNA



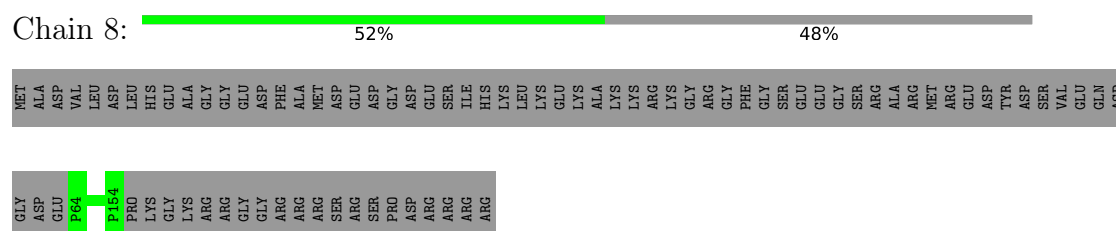
- Molecule 4: U6 snRNA



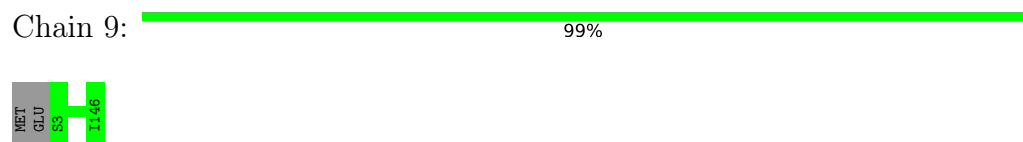
- Molecule 5: Eukaryotic initiation factor 4A-III



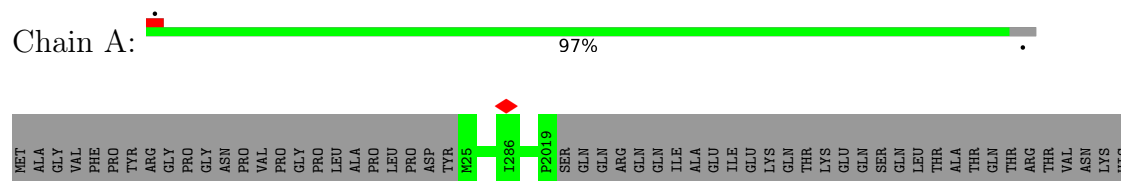
- Molecule 6: RNA-binding protein 8A



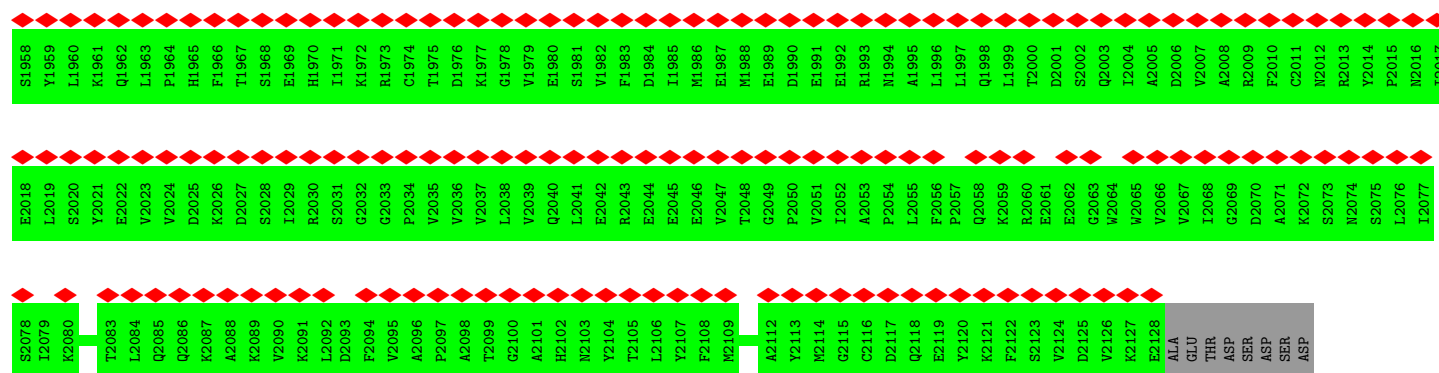
- Molecule 7: Protein mago nashi homolog



- Molecule 8: Pre-mRNA-processing-splicing factor 8

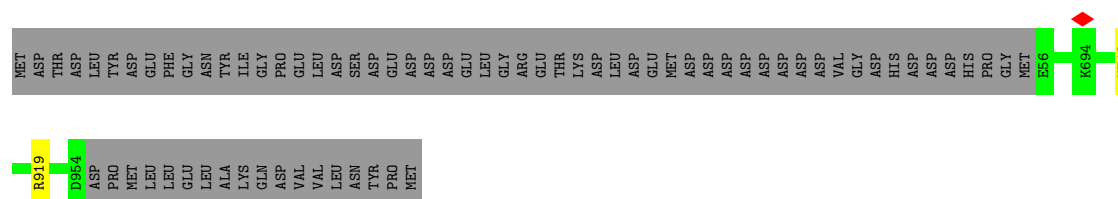






- Molecule 10: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C: 92% 8%



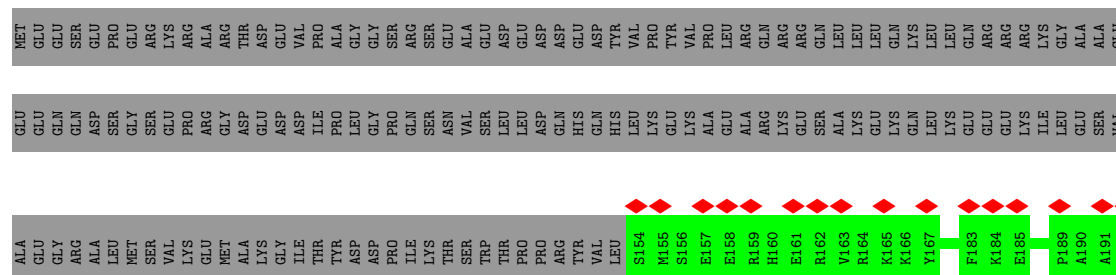
- Molecule 11: Peptidyl-prolyl cis-trans isomerase-like 3

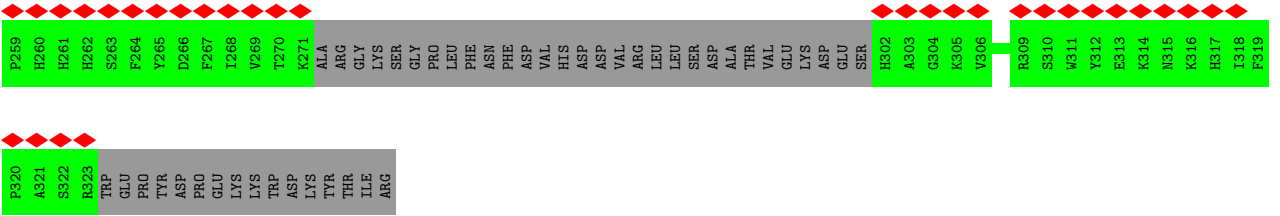
Chain C3: 61% 99%



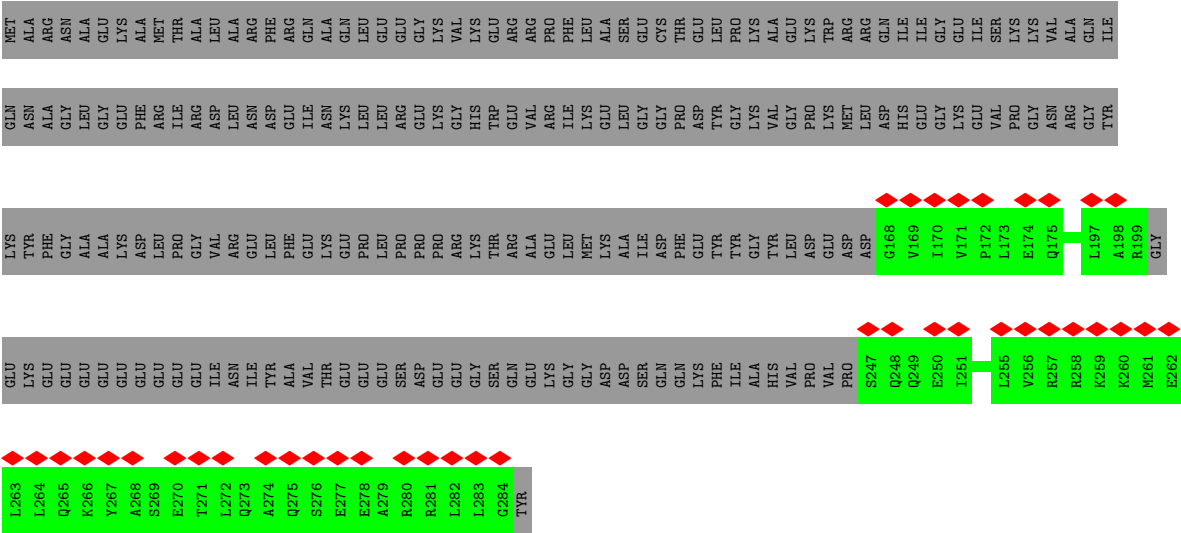
- Molecule 12: Probable ATP-dependent RNA helicase DDX41

Chain CD: 9% 39% 61%

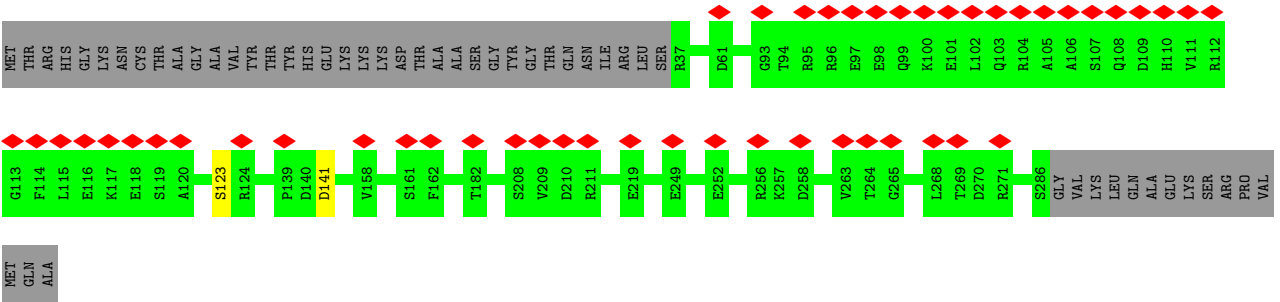
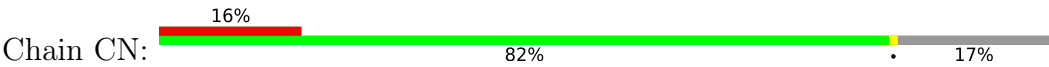




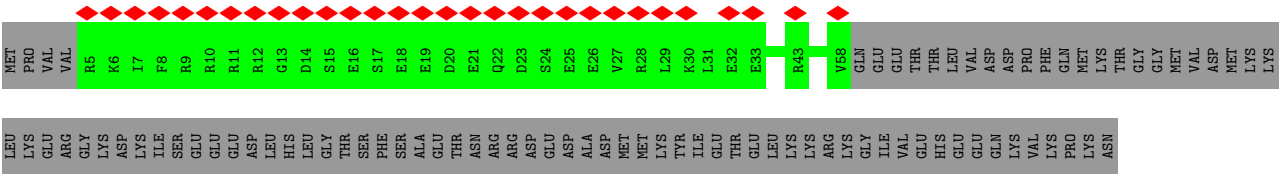
• Molecule 15: Pre-mRNA-splicing factor ISY1 homolog

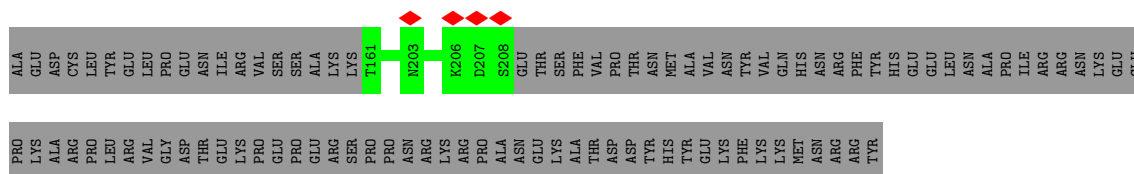


• Molecule 16: Nitric oxide synthase-interacting protein

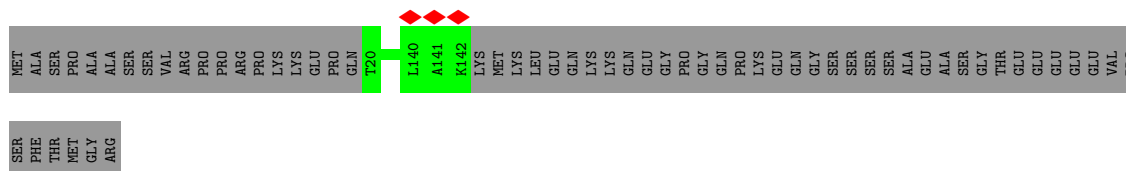


• Molecule 17: Splicing factor C9orf78

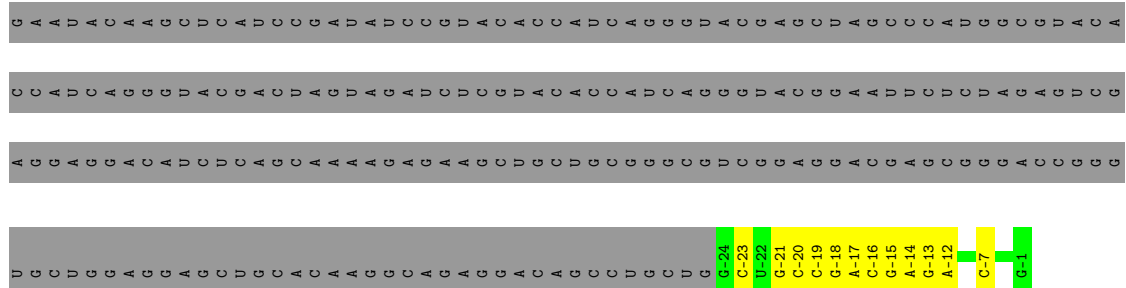




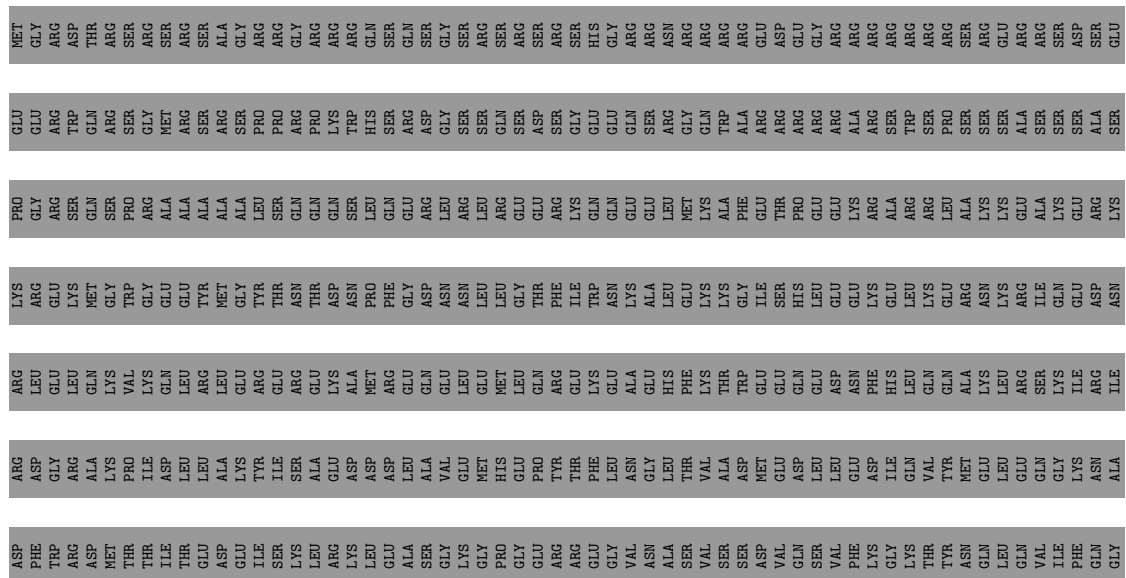
- Molecule 18: PRKR-interacting protein 1



- Molecule 19: PM5 5' Exon

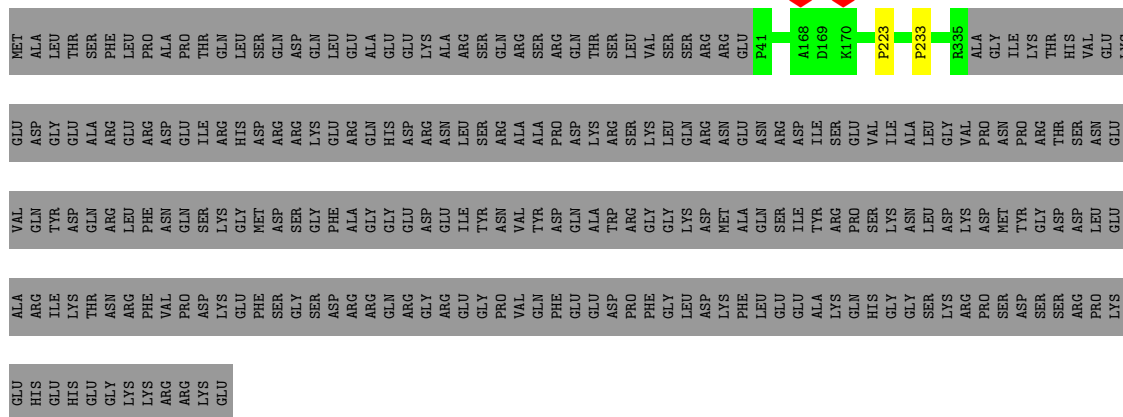


- Molecule 20: Splicing factor Cactin



- Molecule 25: SNW domain-containing protein 1

Chain K:  55% 45%



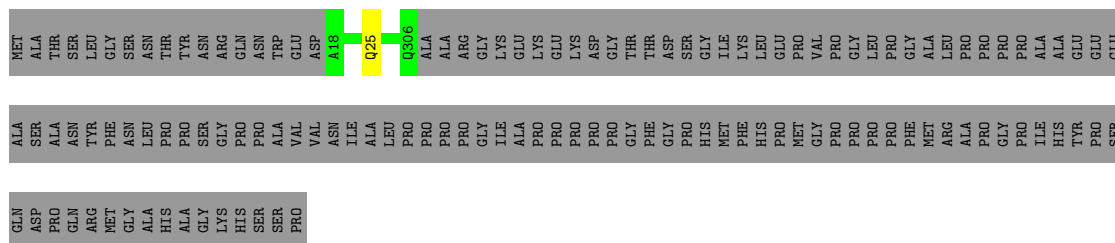
- Molecule 26: Protein BUD31 homolog

Chain L: 100%

There are no outlier residues recorded for this chain.

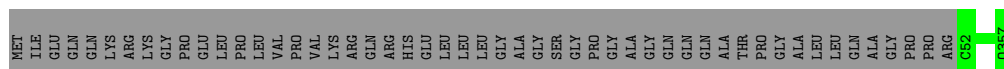
- Molecule 27: Pre-mRNA-splicing factor RBM22

Chain M: 69% 31%



- Molecule 28: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain N: 86% 14%



- Molecule 29: Cell division cycle 5-like protein

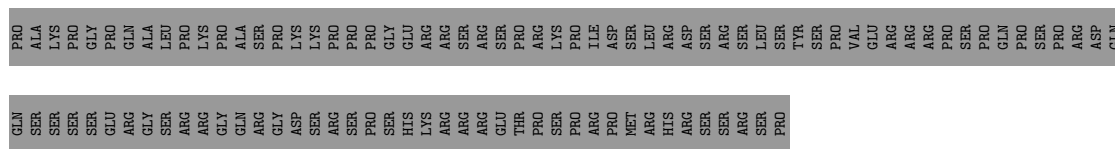
Chain 0:

Chain P:

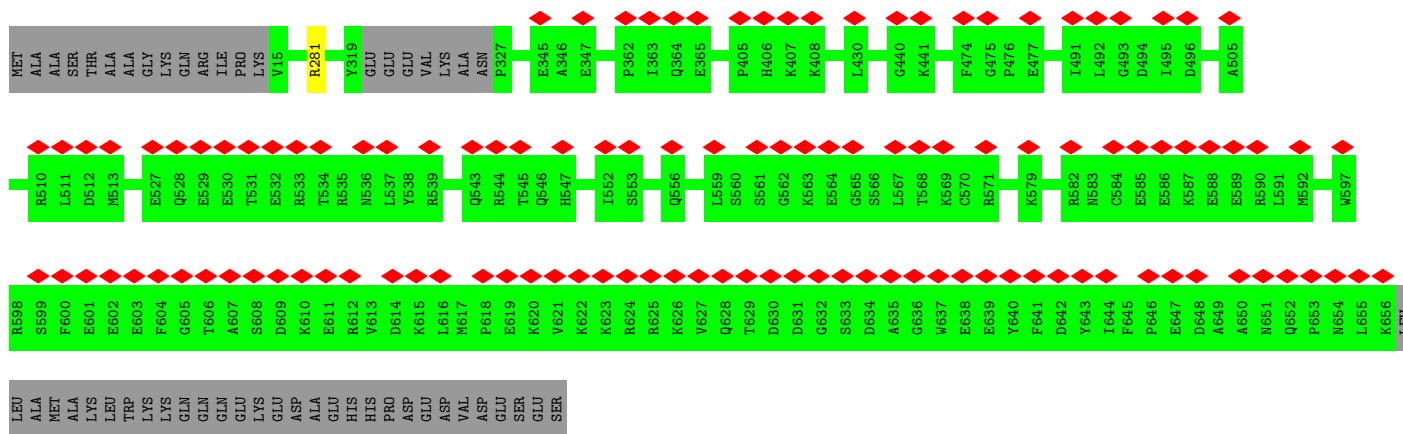
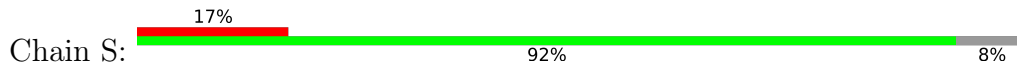
Chain R:



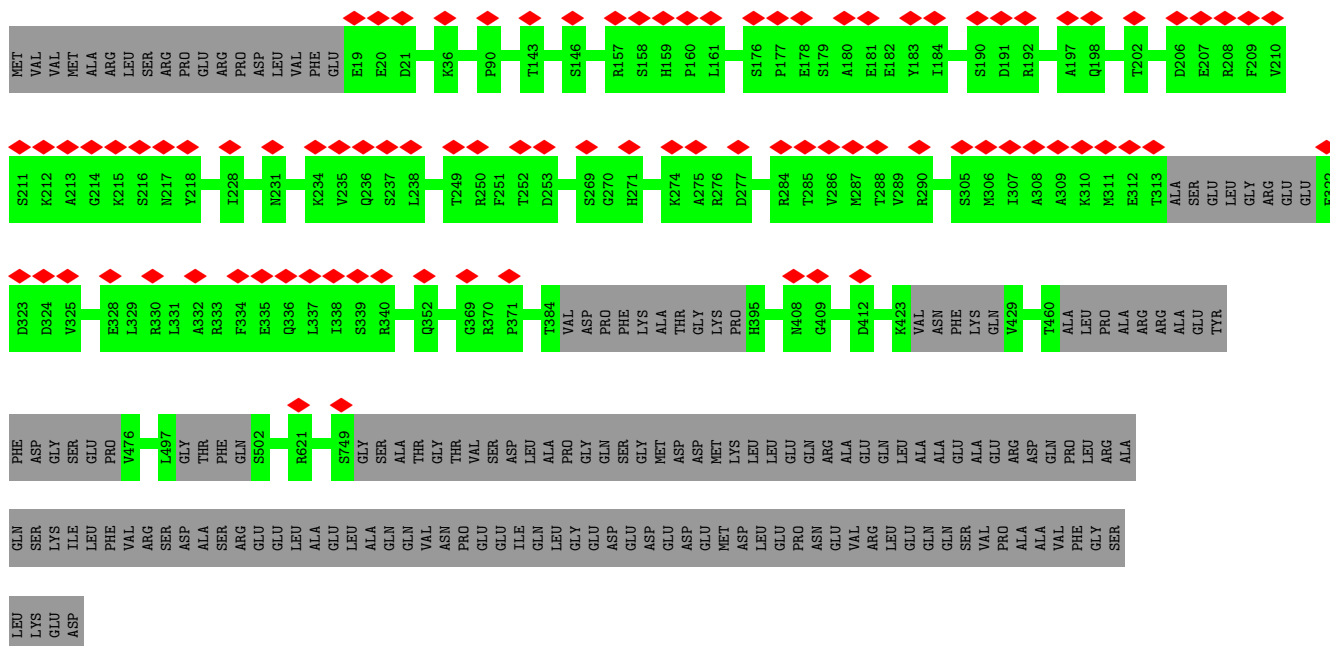
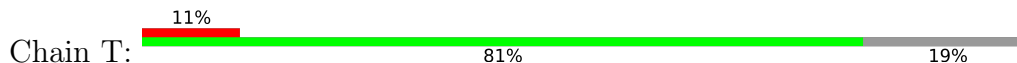




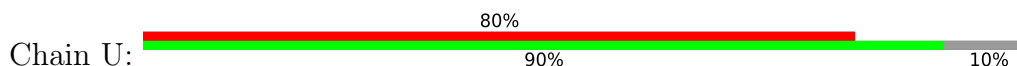
- Molecule 32: Crooked neck-like protein 1



- Molecule 33: Pre-mRNA-splicing factor SYF1



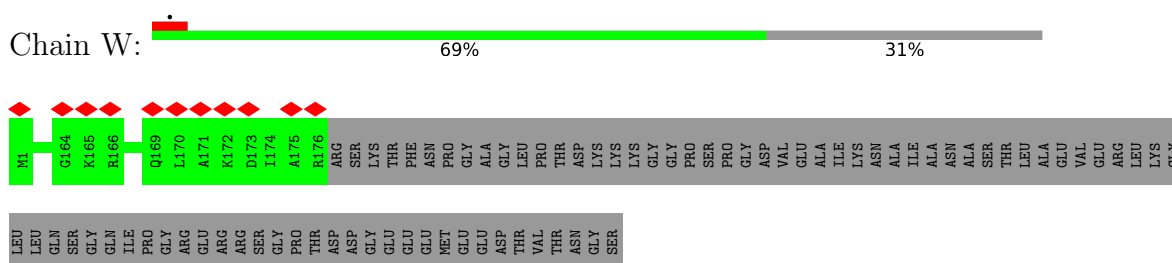
- Molecule 34: Intron-binding protein aquarium



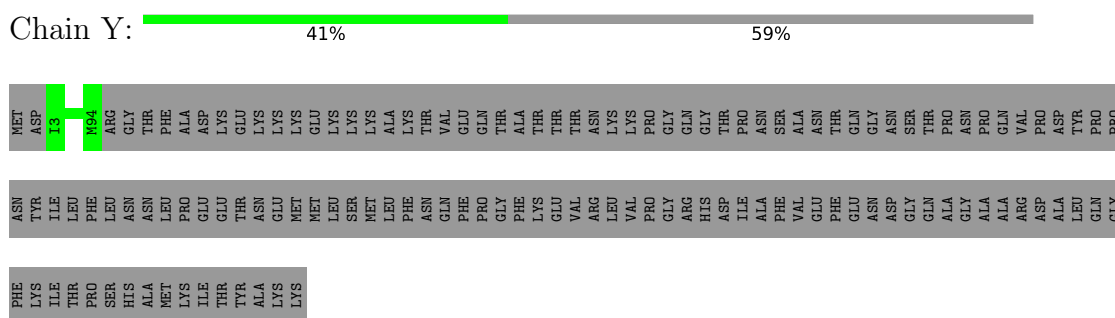


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D924	A925	S926	Y927	T928	C929	A932	V940	M941	S942	R943	W944	E945	E946	Y947	I948	S949	K950	V951	K952	N953	LYS	GLY	SER	THR	LEU	P959	D960	V961	T962	E963	V964	S965	T966	F967	F968	P969	F970	H971	E972	Y973	F974	A975	N976	A977	Q978	P980	I981	F982	K983	G984	R985	S986	Y987	E988	E989	D990			
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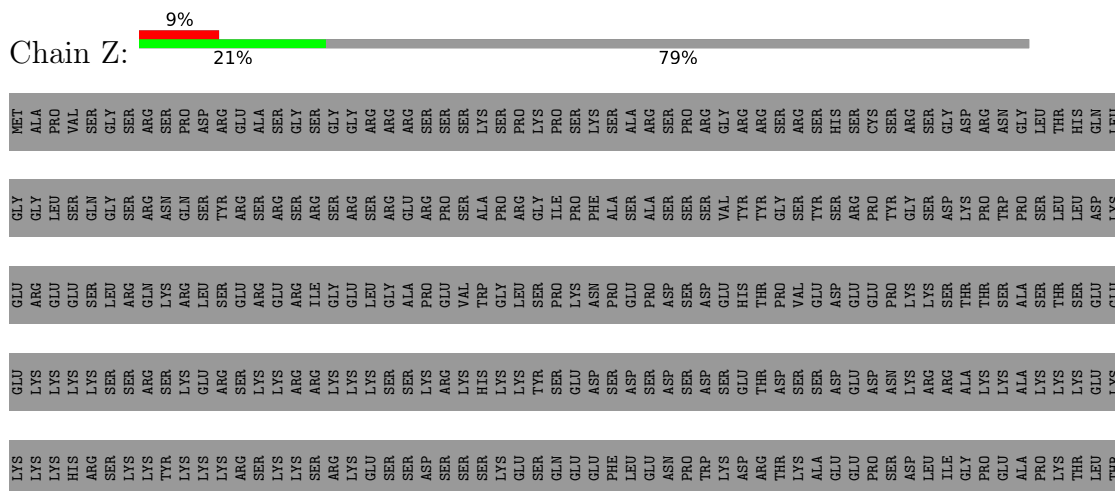
- Molecule 36: U2 small nuclear ribonucleoprotein A'



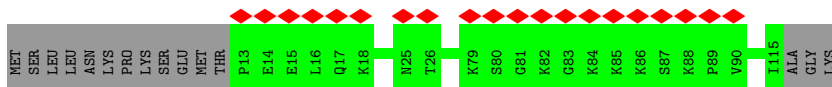
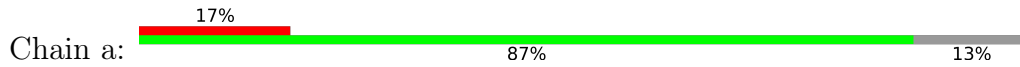
- Molecule 37: U2 small nuclear ribonucleoprotein B''



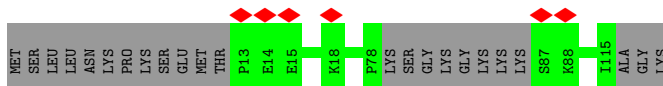
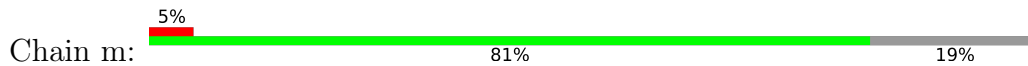
- Molecule 38: NF-kappa-B-activating protein



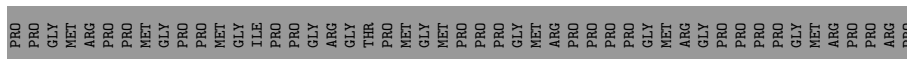
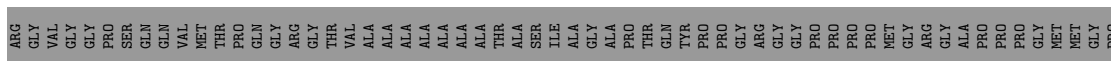
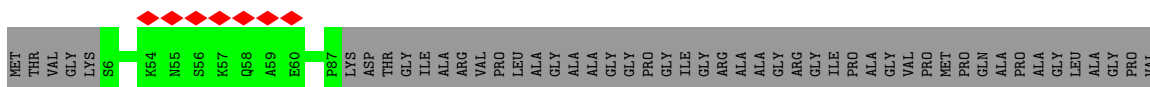
- Molecule 39: Small nuclear ribonucleoprotein Sm D2



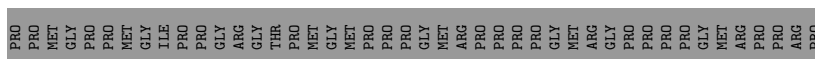
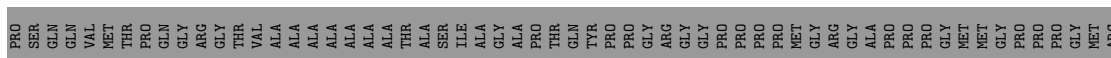
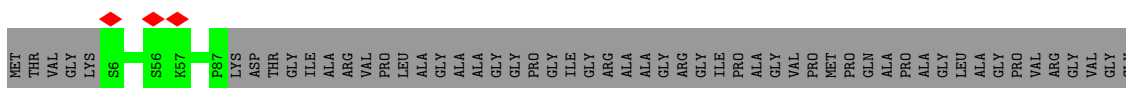
- Molecule 39: Small nuclear ribonucleoprotein Sm D2



- Molecule 40: Small nuclear ribonucleoprotein-associated proteins B and B'




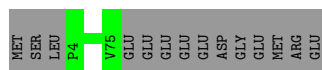
- Molecule 40: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 41: Small nuclear ribonucleoprotein Sm D1

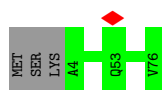


Chain q:  84% 16%



- Molecule 45: Small nuclear ribonucleoprotein G

Chain g:  96%



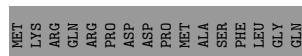
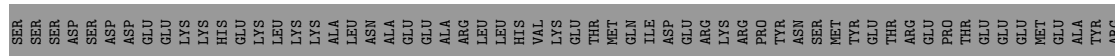
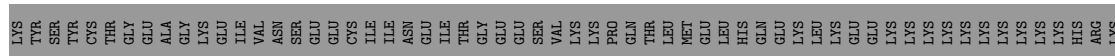
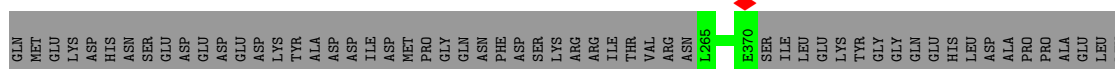
- Molecule 45: Small nuclear ribonucleoprotein G

Chain r:  96%



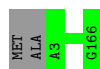
- Molecule 46: Pre-mRNA-splicing factor SLU7

Chain h:  47% 53%

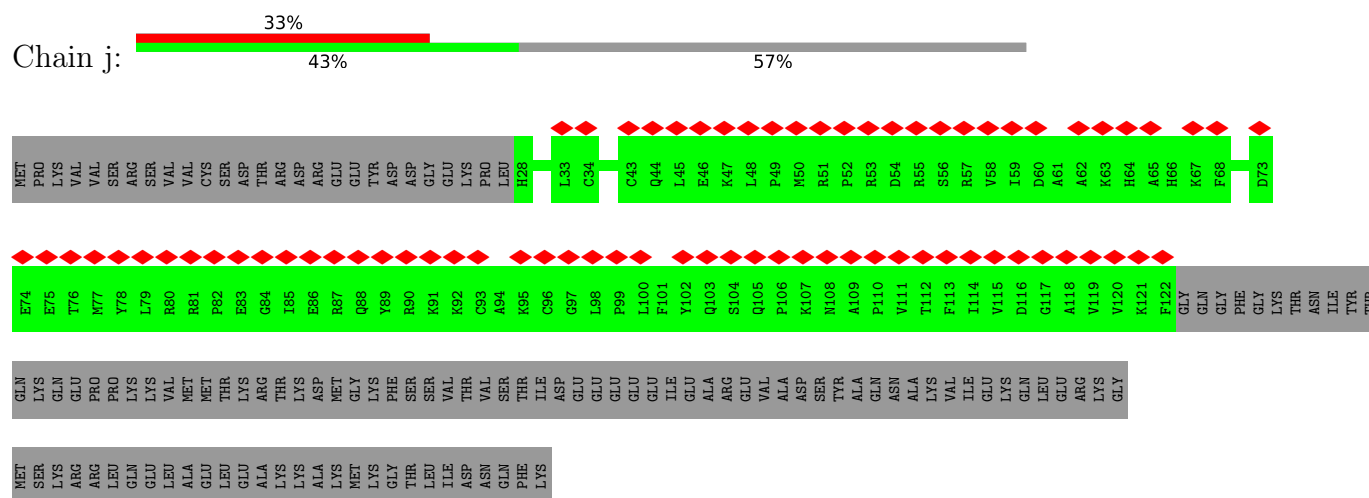


- Molecule 47: Peptidyl-prolyl cis-trans isomerase-like 1

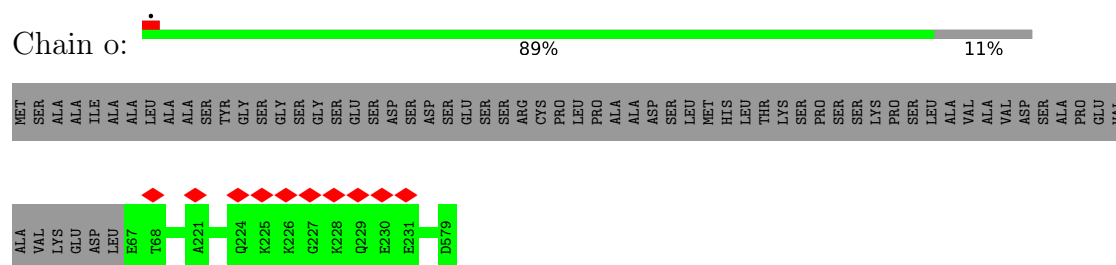
Chain i:  99%



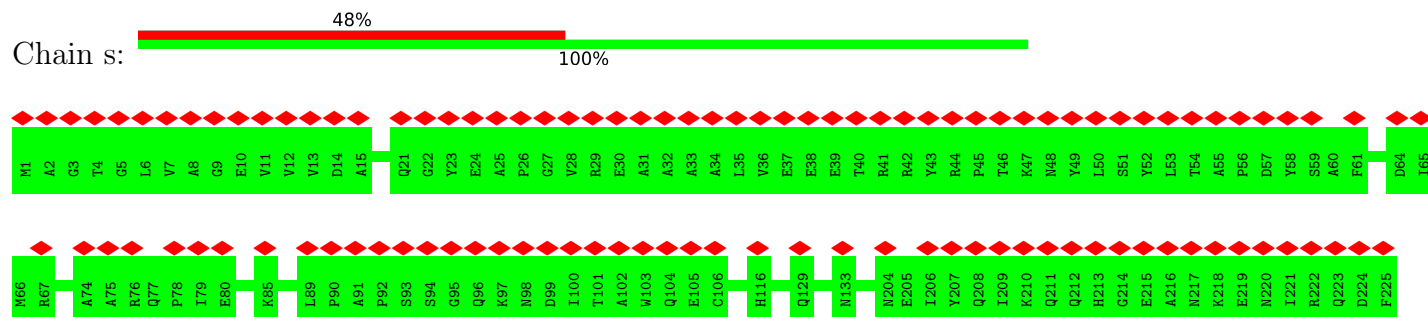
- Molecule 48: STING ER exit protein



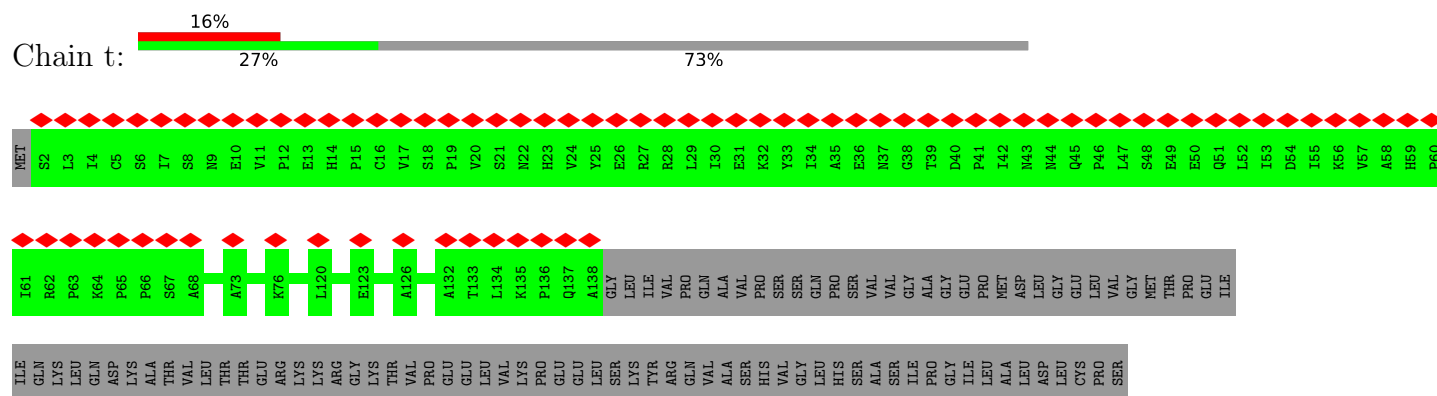
- Molecule 49: Pre-mRNA-processing factor 17

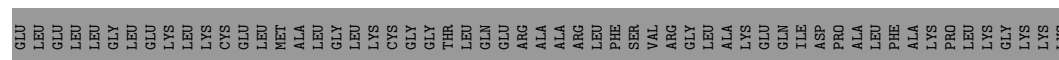


- Molecule 50: Pre-mRNA-splicing factor SPF27



- Molecule 51: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1150057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.24	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.260	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.115	Depositor
Map size (Å)	609.0, 609.0, 609.0	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IHP, ATP, GTP, SEP, K, ZN

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	2	0.21	0/3359	0.77	0/5224
2	4	0.24	0/643	0.48	0/862
3	5	0.28	0/2643	0.82	0/4110
4	6	0.28	0/2323	0.74	0/3619
5	7	0.25	0/3179	0.50	0/4291
6	8	0.25	0/748	0.50	0/1012
7	9	0.22	0/600	0.45	0/759
8	A	0.27	0/18188	0.47	0/24579
9	B	0.22	0/7219	0.43	0/9180
10	C	0.27	0/7275	0.49	0/9884
11	C3	0.23	0/675	0.50	0/856
12	CD	0.23	0/1039	0.43	0/1327
13	CE	0.24	0/323	0.48	0/406
14	CF	0.21	0/745	0.39	0/930
15	CI	0.21	0/282	0.31	0/351
16	CN	0.27	0/1674	0.50	0/2247
17	CT	0.21	0/414	0.39	0/518
18	D	0.25	0/1030	0.49	0/1371
19	E	0.25	0/571	0.80	0/889
20	F	0.27	0/1133	0.52	0/1530
21	G	0.24	0/503	0.48	0/672
22	H	0.25	0/3378	0.44	0/4509
23	I	0.22	0/1915	0.82	0/2967
24	J	0.28	0/2791	0.52	0/3788
25	K	0.28	0/2387	0.52	0/3205
26	L	0.26	0/1214	0.50	0/1627
27	M	0.26	0/2375	0.51	0/3204
28	N	0.25	0/2442	0.50	0/3309
29	O	0.23	0/3365	0.45	0/4411
30	P	0.26	0/988	0.53	0/1315
31	R	0.25	0/403	0.43	0/526
32	S	0.24	0/3907	0.44	0/5142

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	T	0.24	0/4328	0.42	0/5947
34	U	0.22	0/5628	0.43	0/7170
35	V	0.23	0/4217	0.42	0/5405
36	W	0.22	0/727	0.43	0/919
37	Y	0.22	0/379	0.43	0/478
38	Z	0.25	0/456	0.45	0/586
39	a	0.23	0/524	0.43	0/732
39	m	0.23	0/398	0.46	0/503
40	b	0.24	0/416	0.44	0/581
40	k	0.23	0/343	0.50	0/435
41	c	0.23	0/404	0.44	0/564
41	l	0.22	0/331	0.49	0/418
42	d	0.24	0/422	0.44	0/588
42	n	0.23	0/343	0.48	0/433
43	e	0.23	0/393	0.44	0/547
43	p	0.22	0/327	0.47	0/409
44	f	0.24	0/362	0.45	0/502
44	q	0.23	0/303	0.48	0/384
45	g	0.23	0/367	0.46	0/509
45	r	0.23	0/304	0.51	0/383
46	h	0.27	0/2334	0.46	0/3138
47	i	0.26	0/1304	0.48	0/1767
48	j	0.23	0/403	0.48	0/514
49	o	0.26	0/4024	0.49	0/5426
50	s	0.23	0/928	0.41	0/1171
51	t	0.23	0/591	0.40	0/759
51	u	0.23	0/559	0.41	0/717
51	v	0.22	0/595	0.37	0/764
51	w	0.22	0/563	0.40	0/722
52	y	0.25	0/1444	0.45	0/1904
53	z	0.23	0/611	0.47	0/797
All	All	0.25	0/114059	0.51	0/153792

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	73/476 (15%)	71 (97%)	2 (3%)	0	100	100
5	7	388/411 (94%)	380 (98%)	8 (2%)	0	100	100
6	8	89/174 (51%)	86 (97%)	3 (3%)	0	100	100
7	9	142/146 (97%)	141 (99%)	1 (1%)	0	100	100
8	A	2257/2335 (97%)	2206 (98%)	51 (2%)	0	100	100
9	B	1724/2136 (81%)	1702 (99%)	22 (1%)	0	100	100
10	C	897/972 (92%)	842 (94%)	55 (6%)	0	100	100
11	C3	160/161 (99%)	159 (99%)	1 (1%)	0	100	100
12	CD	243/622 (39%)	241 (99%)	2 (1%)	0	100	100
13	CE	77/301 (26%)	77 (100%)	0	0	100	100
14	CF	179/339 (53%)	177 (99%)	1 (1%)	1 (1%)	22	51
15	CI	66/285 (23%)	66 (100%)	0	0	100	100
16	CN	248/301 (82%)	230 (93%)	16 (6%)	2 (1%)	16	44
17	CT	98/289 (34%)	96 (98%)	2 (2%)	0	100	100
18	D	121/184 (66%)	119 (98%)	2 (2%)	0	100	100
20	F	120/758 (16%)	112 (93%)	8 (7%)	0	100	100
21	G	57/112 (51%)	55 (96%)	2 (4%)	0	100	100
22	H	455/500 (91%)	443 (97%)	12 (3%)	0	100	100
24	J	363/514 (71%)	348 (96%)	15 (4%)	0	100	100
25	K	291/536 (54%)	272 (94%)	18 (6%)	1 (0%)	37	67
26	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
27	M	287/420 (68%)	280 (98%)	7 (2%)	0	100	100
28	N	304/357 (85%)	286 (94%)	18 (6%)	0	100	100
29	O	542/802 (68%)	533 (98%)	9 (2%)	0	100	100
30	P	113/229 (49%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	R	72/2752 (3%)	70 (97%)	2 (3%)	0	100	100
32	S	631/687 (92%)	615 (98%)	16 (2%)	0	100	100
33	T	677/855 (79%)	655 (97%)	22 (3%)	0	100	100
34	U	1328/1485 (89%)	1320 (99%)	8 (1%)	0	100	100
35	V	924/1220 (76%)	893 (97%)	27 (3%)	4 (0%)	30	61
36	W	174/255 (68%)	170 (98%)	4 (2%)	0	100	100
37	Y	90/225 (40%)	90 (100%)	0	0	100	100
38	Z	85/415 (20%)	83 (98%)	2 (2%)	0	100	100
39	a	101/118 (86%)	100 (99%)	1 (1%)	0	100	100
39	m	91/118 (77%)	89 (98%)	2 (2%)	0	100	100
40	b	80/240 (33%)	79 (99%)	1 (1%)	0	100	100
40	k	80/240 (33%)	77 (96%)	3 (4%)	0	100	100
41	c	78/119 (66%)	77 (99%)	1 (1%)	0	100	100
41	l	78/119 (66%)	78 (100%)	0	0	100	100
42	d	82/126 (65%)	80 (98%)	2 (2%)	0	100	100
42	n	81/126 (64%)	79 (98%)	2 (2%)	0	100	100
43	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
43	p	79/92 (86%)	79 (100%)	0	0	100	100
44	f	70/86 (81%)	70 (100%)	0	0	100	100
44	q	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
45	g	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
45	r	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
46	h	272/586 (46%)	263 (97%)	9 (3%)	0	100	100
47	i	162/166 (98%)	155 (96%)	7 (4%)	0	100	100
48	j	93/222 (42%)	93 (100%)	0	0	100	100
49	o	511/579 (88%)	476 (93%)	35 (7%)	0	100	100
50	s	223/225 (99%)	220 (99%)	3 (1%)	0	100	100
51	t	135/504 (27%)	133 (98%)	2 (2%)	0	100	100
51	u	128/504 (25%)	123 (96%)	5 (4%)	0	100	100
51	v	136/504 (27%)	136 (100%)	0	0	100	100
51	w	129/504 (26%)	127 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	y	212/243 (87%)	209 (99%)	3 (1%)	0	100	100
53	z	101/451 (22%)	98 (97%)	3 (3%)	0	100	100
All	All	16628/27600 (60%)	16191 (97%)	429 (3%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	CF	201	ILE
16	CN	123	SER
35	V	987	PRO
35	V	1049	TYR
16	CN	141	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	4	70/395 (18%)	70 (100%)	0	100	100
5	7	345/361 (96%)	344 (100%)	1 (0%)	91	97
6	8	76/143 (53%)	76 (100%)	0	100	100
7	9	6/134 (4%)	6 (100%)	0	100	100
8	A	1825/2108 (87%)	1825 (100%)	0	100	100
9	B	79/1908 (4%)	79 (100%)	0	100	100
10	C	799/866 (92%)	797 (100%)	2 (0%)	91	97
11	C3	7/141 (5%)	7 (100%)	0	100	100
12	CD	15/533 (3%)	15 (100%)	0	100	100
13	CE	2/252 (1%)	2 (100%)	0	100	100
14	CF	2/304 (1%)	2 (100%)	0	100	100
15	CI	1/240 (0%)	1 (100%)	0	100	100
16	CN	155/260 (60%)	155 (100%)	0	100	100
17	CT	2/263 (1%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	D	106/157 (68%)	106 (100%)	0	100	100
20	F	111/655 (17%)	110 (99%)	1 (1%)	75	92
21	G	53/99 (54%)	53 (100%)	0	100	100
22	H	324/455 (71%)	324 (100%)	0	100	100
24	J	279/441 (63%)	279 (100%)	0	100	100
25	K	246/457 (54%)	245 (100%)	1 (0%)	89	96
26	L	130/130 (100%)	130 (100%)	0	100	100
27	M	258/361 (72%)	257 (100%)	1 (0%)	89	96
28	N	262/300 (87%)	262 (100%)	0	100	100
29	O	232/709 (33%)	232 (100%)	0	100	100
30	P	103/203 (51%)	103 (100%)	0	100	100
31	R	23/2432 (1%)	23 (100%)	0	100	100
32	S	252/617 (41%)	251 (100%)	1 (0%)	89	96
33	T	225/749 (30%)	225 (100%)	0	100	100
34	U	72/1336 (5%)	72 (100%)	0	100	100
35	V	104/1085 (10%)	104 (100%)	0	100	100
36	W	6/218 (3%)	6 (100%)	0	100	100
37	Y	3/195 (2%)	3 (100%)	0	100	100
38	Z	24/366 (7%)	24 (100%)	0	100	100
39	a	5/110 (4%)	5 (100%)	0	100	100
39	m	5/110 (4%)	5 (100%)	0	100	100
40	b	4/177 (2%)	4 (100%)	0	100	100
40	k	4/177 (2%)	4 (100%)	0	100	100
41	c	3/101 (3%)	3 (100%)	0	100	100
41	l	3/101 (3%)	3 (100%)	0	100	100
42	d	3/101 (3%)	3 (100%)	0	100	100
42	n	3/101 (3%)	3 (100%)	0	100	100
43	e	1/84 (1%)	1 (100%)	0	100	100
43	p	1/84 (1%)	1 (100%)	0	100	100
44	f	4/74 (5%)	4 (100%)	0	100	100
44	q	4/74 (5%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	g	3/66 (4%)	3 (100%)	0	100	100
45	r	3/66 (4%)	3 (100%)	0	100	100
46	h	243/520 (47%)	243 (100%)	0	100	100
47	i	133/134 (99%)	133 (100%)	0	100	100
48	j	6/198 (3%)	6 (100%)	0	100	100
49	o	400/502 (80%)	400 (100%)	0	100	100
50	s	7/196 (4%)	7 (100%)	0	100	100
51	t	11/435 (2%)	11 (100%)	0	100	100
51	u	10/435 (2%)	10 (100%)	0	100	100
51	v	11/435 (2%)	11 (100%)	0	100	100
51	w	10/435 (2%)	10 (100%)	0	100	100
52	y	114/209 (54%)	114 (100%)	0	100	100
53	z	40/371 (11%)	40 (100%)	0	100	100
All	All	7228/24169 (30%)	7221 (100%)	7 (0%)	92	98

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	F	641	ARG
25	K	233	PRO
32	S	281	ARG
27	M	25	GLN
10	C	919	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
52	y	219	ASN
52	y	215	ASN
47	i	120	GLN
28	N	101	ASN
52	y	203	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	139/188 (73%)	51 (36%)	3 (2%)
19	E	23/242 (9%)	11 (47%)	2 (8%)
23	I	82/235 (34%)	47 (57%)	3 (3%)
3	5	112/116 (96%)	39 (34%)	3 (2%)
4	6	96/106 (90%)	27 (28%)	2 (2%)
All	All	452/887 (50%)	175 (38%)	13 (2%)

5 of 175 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	U
1	2	18	U
1	2	19	G
1	2	20	G
1	2	24	A

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	6	58	G
19	E	-19	C
23	I	183	C
23	I	150	U
23	I	181	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
25	SEP	K	232	25	8,9,10	0.63	0	8,12,14	0.66	0
25	SEP	K	224	25	8,9,10	0.61	0	8,12,14	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SEP	K	232	25	-	0/5/8/10	-
25	SEP	K	224	25	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	K	224	SEP	CB-OG-P-O2P
25	K	224	SEP	CB-OG-P-O3P
25	K	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z > 2$
57	IHP	A	3000	-	36,36,36	0.72	0	54,60,60	0.91	3 (5%)
56	ATP	7	502	55	26,33,33	0.66	0	31,52,52	0.88	1 (3%)
58	GTP	C	1502	55	26,34,34	1.03	3 (11%)	32,54,54	0.80	1 (3%)

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
57	IHP	A	3000	-	-	2/30/54/54	0/1/1/1
56	ATP	7	502	55	-	4/18/38/38	0/3/3/3
58	GTP	C	1502	55	-	1/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C	1502	GTP	C5-C6	-2.76	1.41	1.47
58	C	1502	GTP	C8-N7	-2.24	1.31	1.35
58	C	1502	GTP	C5-C4	-2.04	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	3000	IHP	C6-C1-C2	2.79	116.51	110.41
57	A	3000	IHP	C5-C4-C3	-2.41	105.14	110.41
56	7	502	ATP	C5-C6-N6	2.32	123.87	120.35
57	A	3000	IHP	C6-C5-C4	-2.30	105.37	110.41
58	C	1502	GTP	O6-C6-C5	2.01	128.29	124.37

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

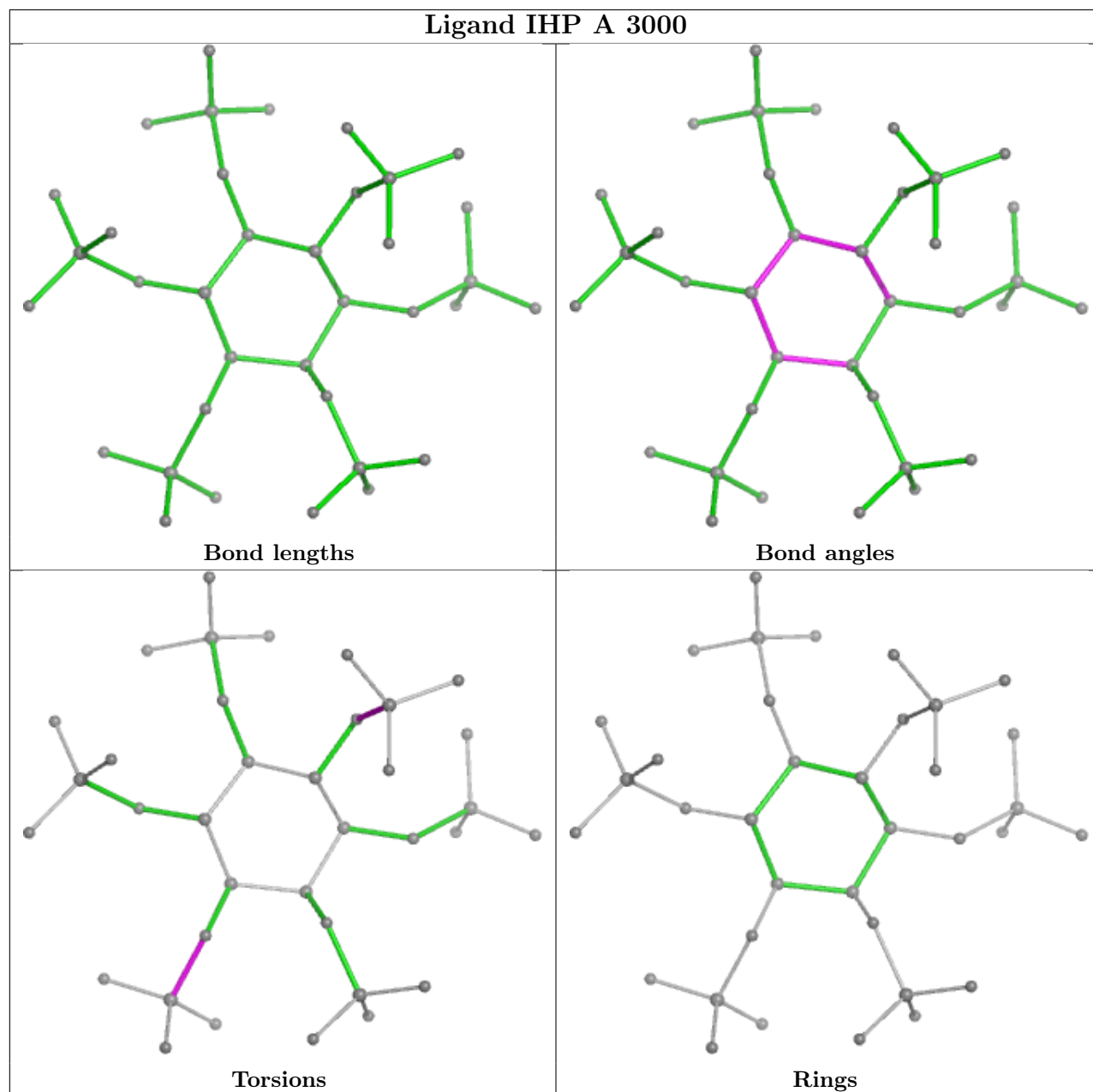
Mol	Chain	Res	Type	Atoms
56	7	502	ATP	C5'-O5'-PA-O1A
56	7	502	ATP	PB-O3A-PA-O5'
57	A	3000	IHP	C4-O14-P4-O24
56	7	502	ATP	O4'-C4'-C5'-O5'
56	7	502	ATP	C3'-C4'-C5'-O5'

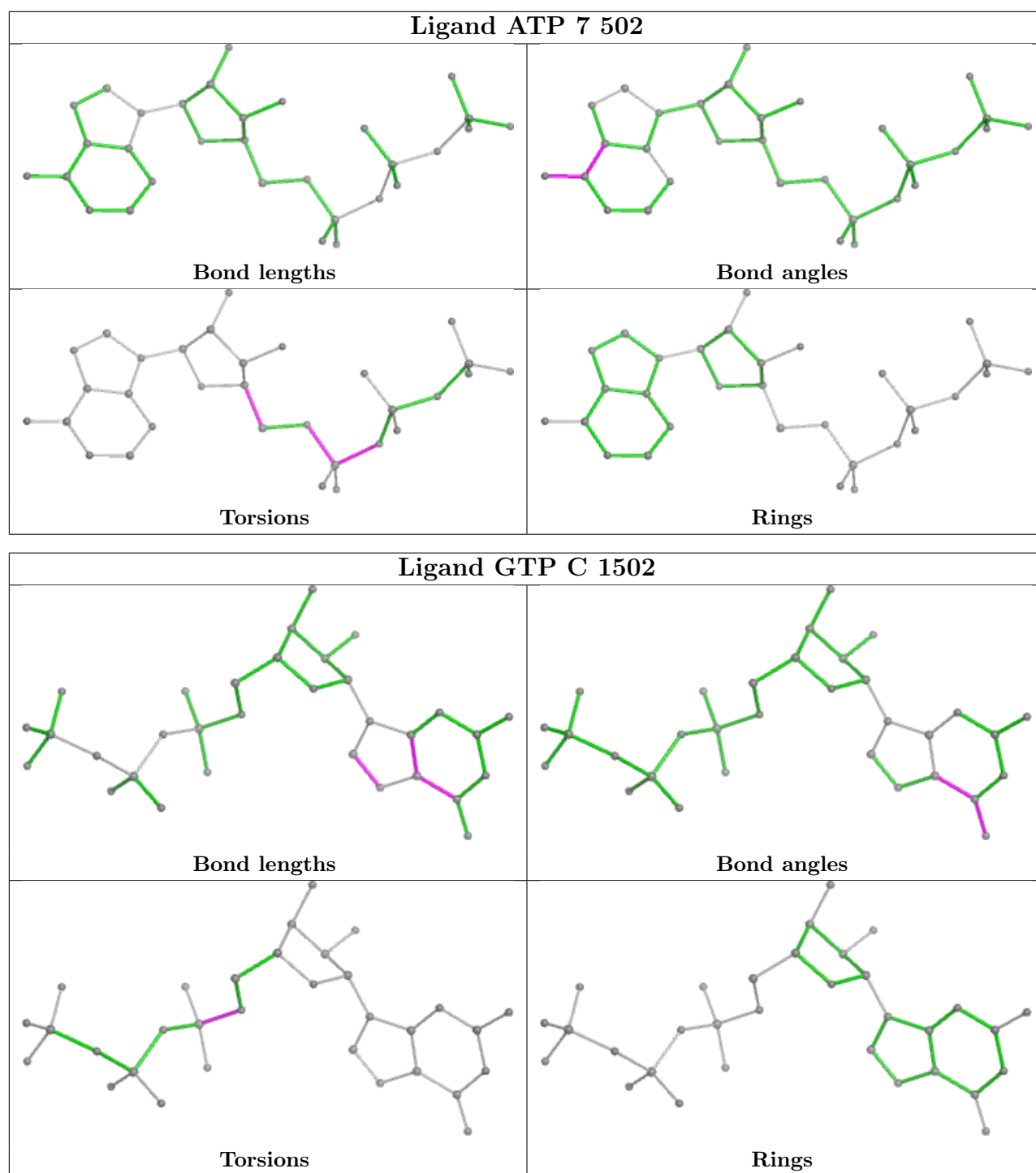
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

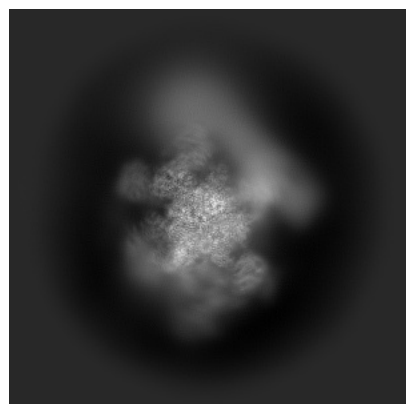
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16452. These allow visual inspection of the internal detail of the map and identification of artifacts.

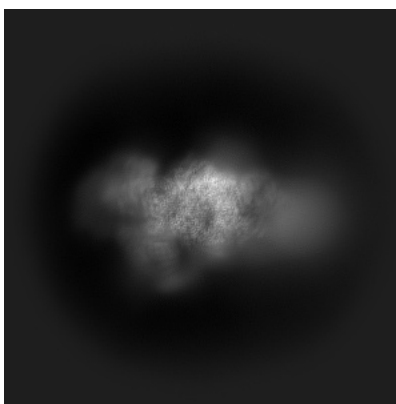
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

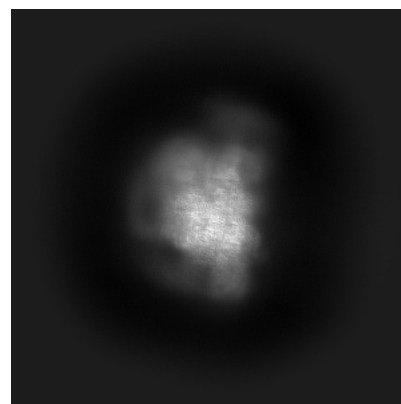
6.1.1 Primary map



X

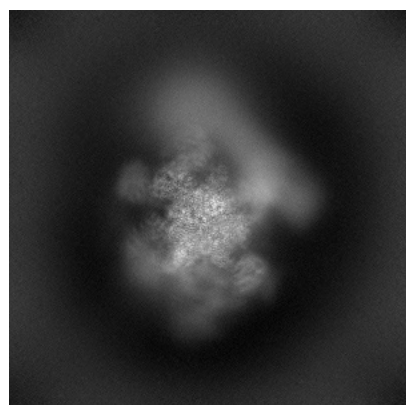


Y

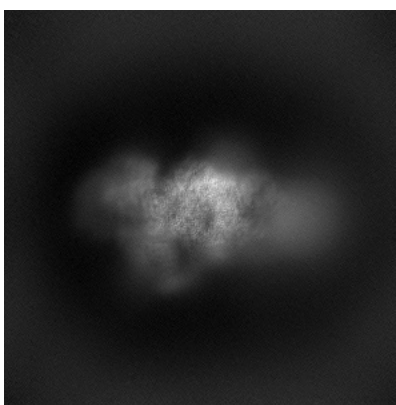


Z

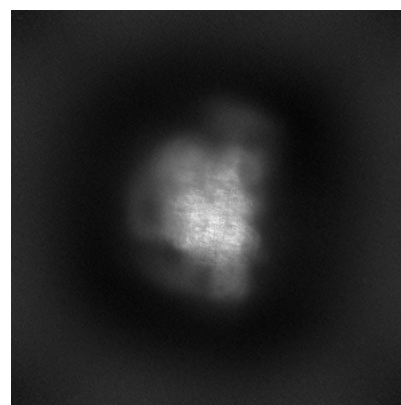
6.1.2 Raw map



X



Y

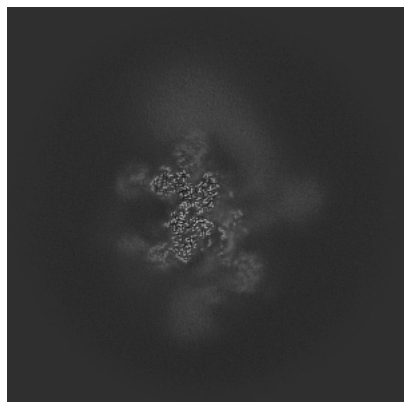


Z

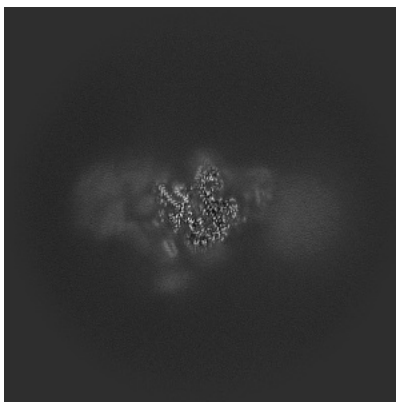
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

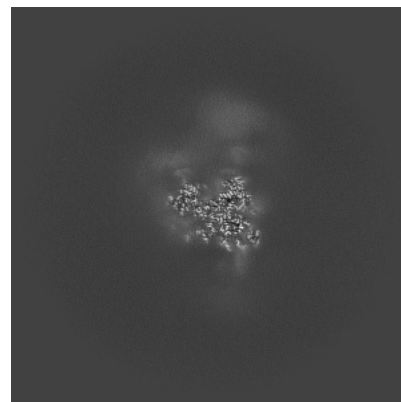
6.2.1 Primary map



X Index: 290

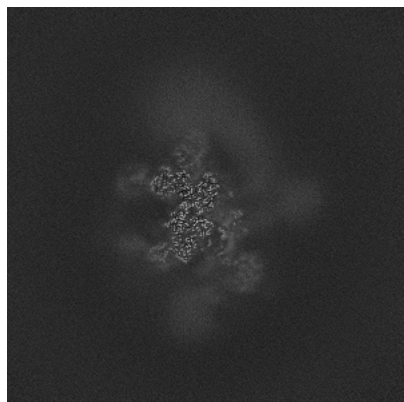


Y Index: 290

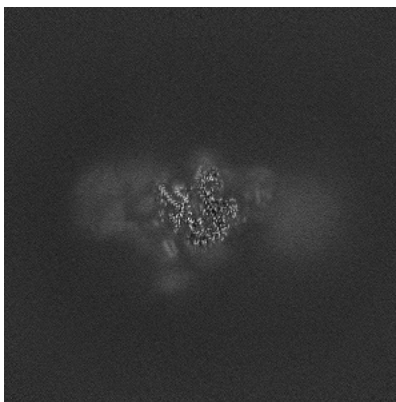


Z Index: 290

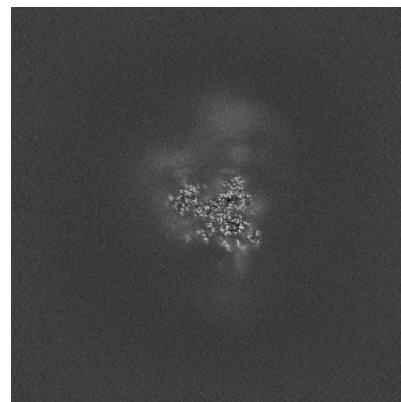
6.2.2 Raw map



X Index: 290



Y Index: 290

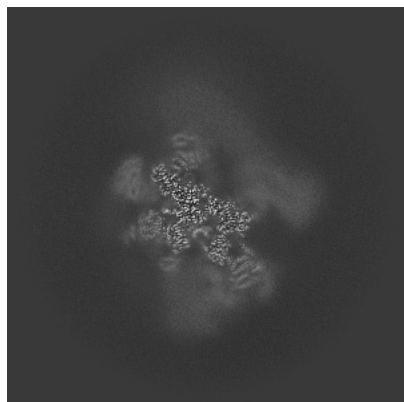


Z Index: 290

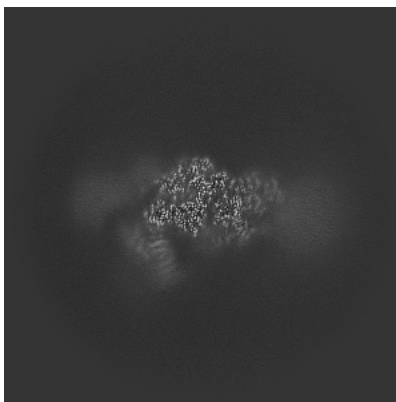
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

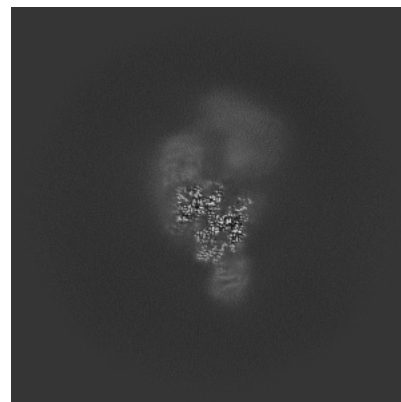
6.3.1 Primary map



X Index: 321

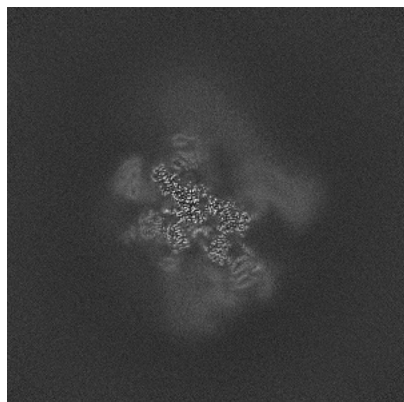


Y Index: 251

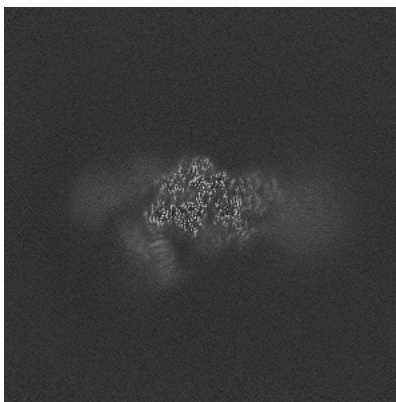


Z Index: 310

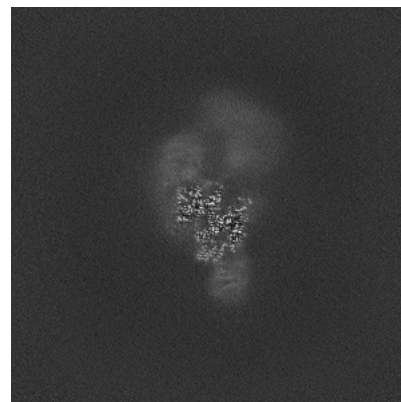
6.3.2 Raw map



X Index: 321



Y Index: 251

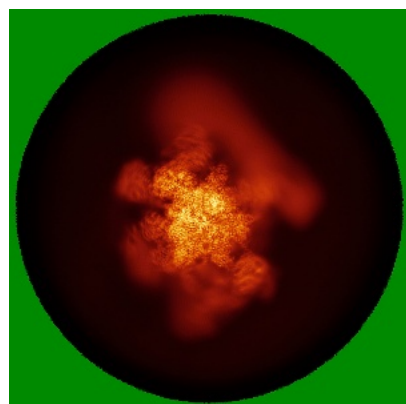


Z Index: 310

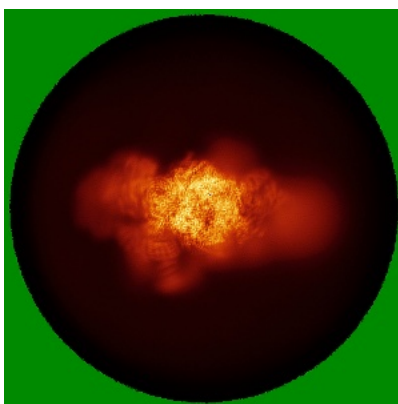
The images above show the largest variance slices of the map in three orthogonal directions.

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

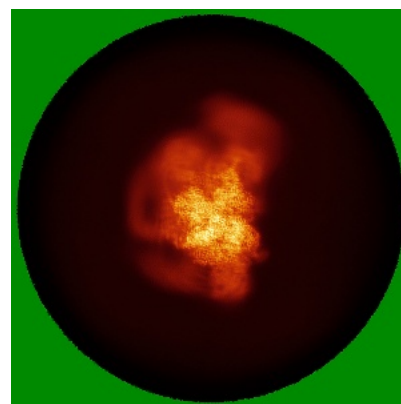
6.4.1 Primary map



X

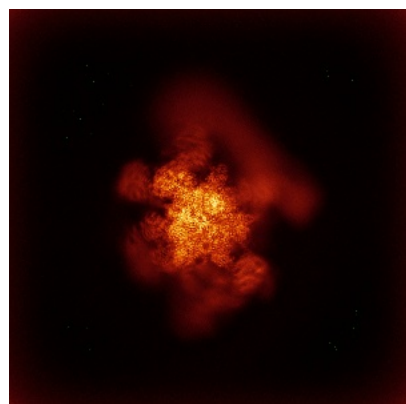


Y

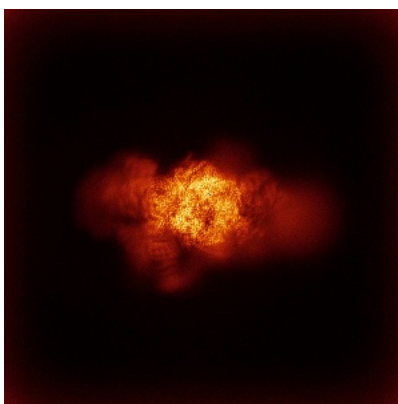


Z

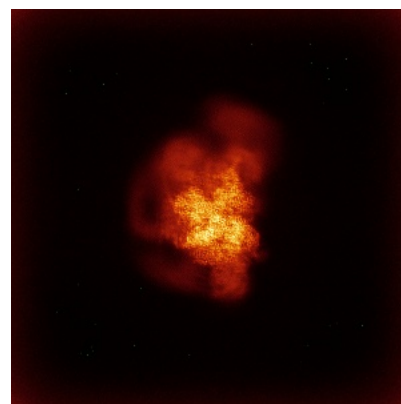
6.4.2 Raw map



X



Y

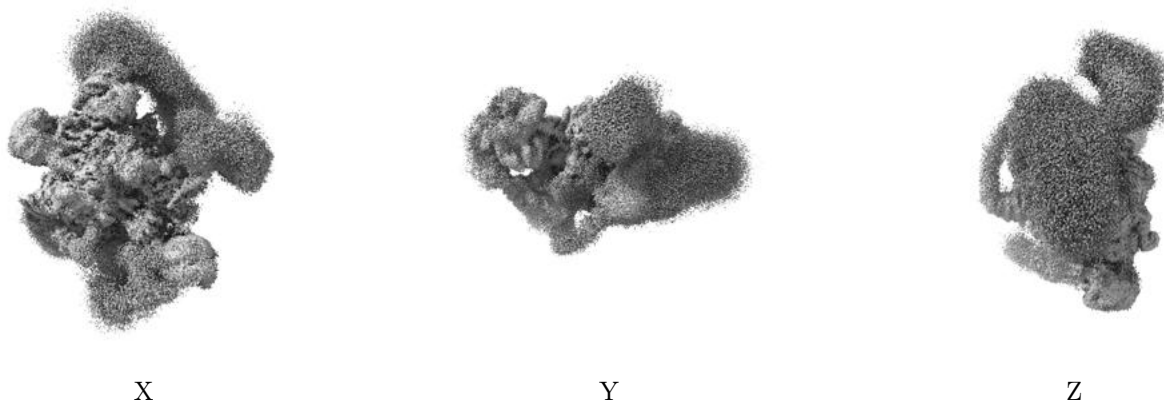


Z

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.

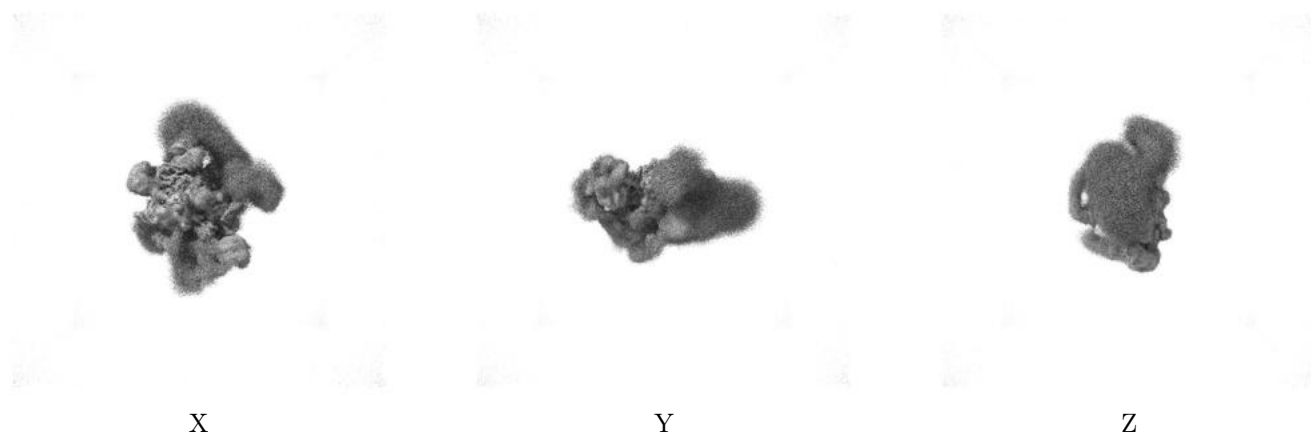
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.115. 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



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.

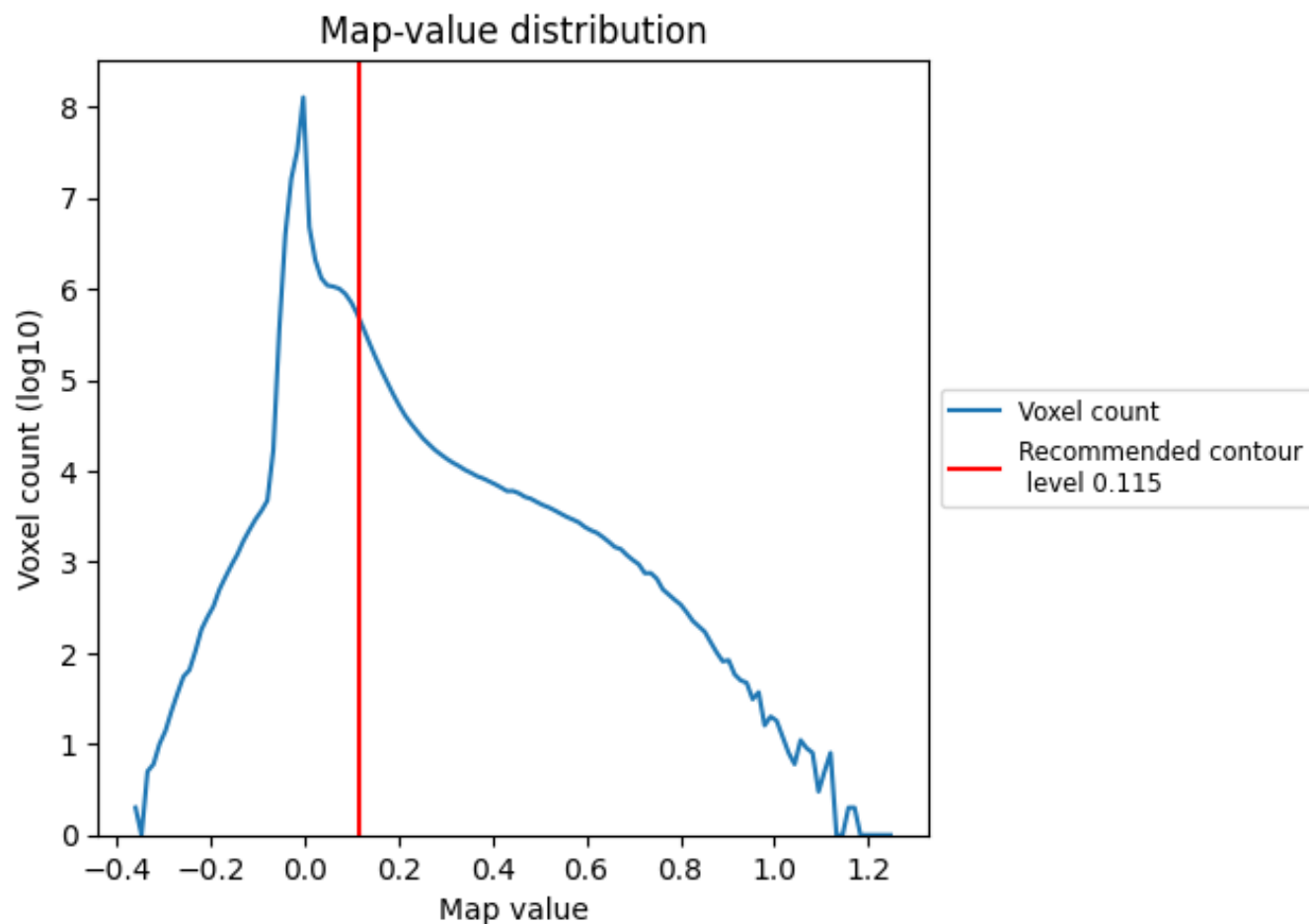
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

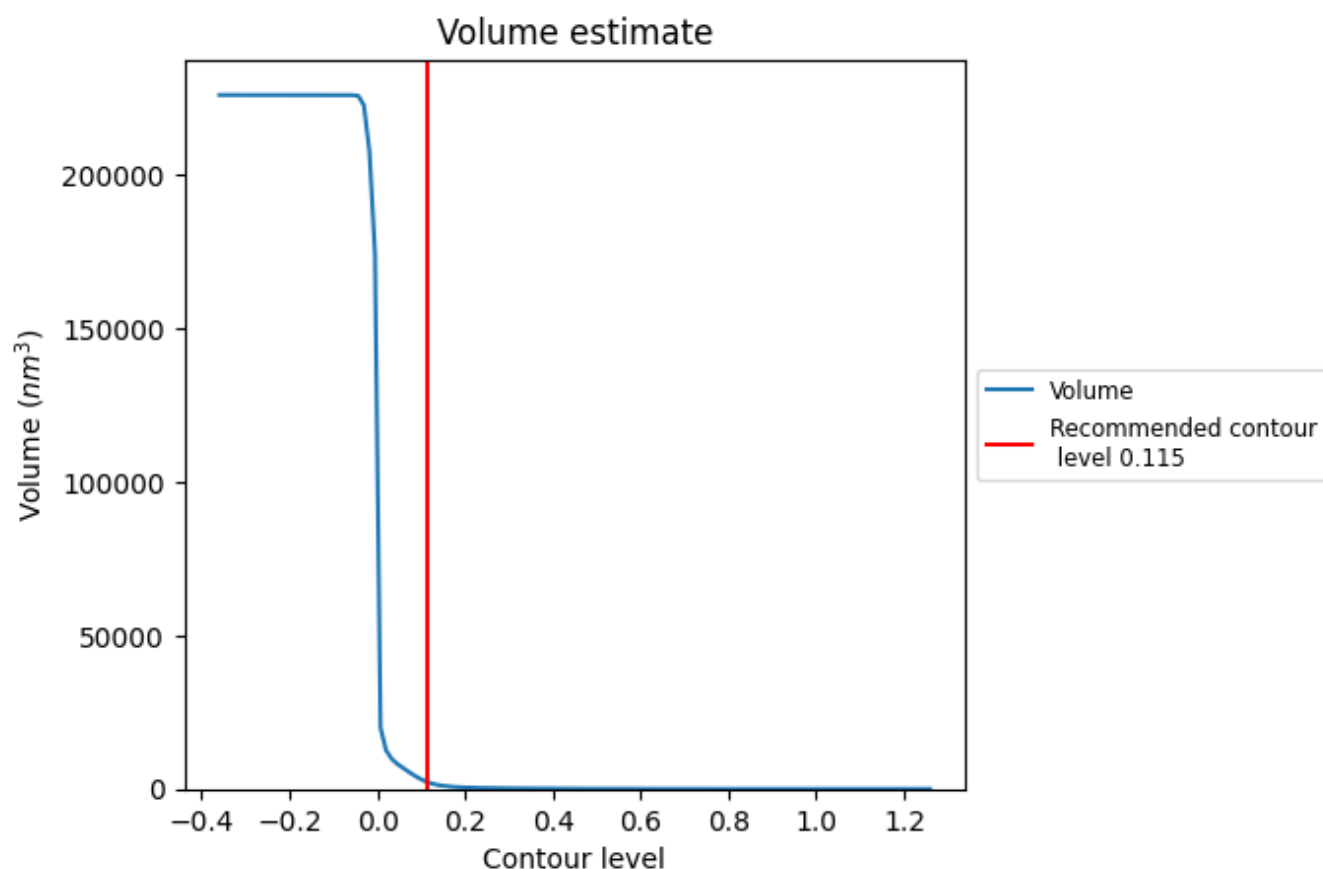
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

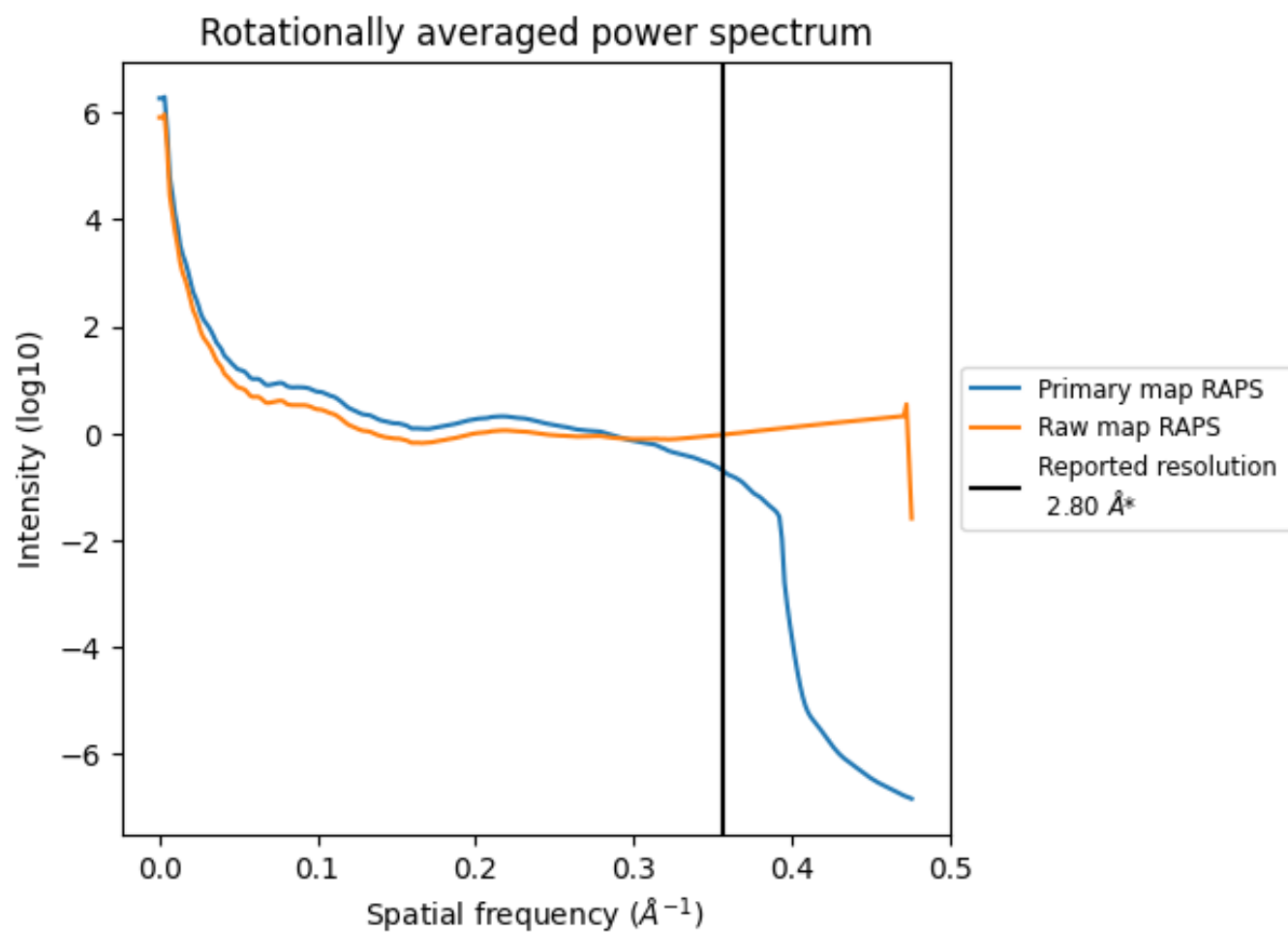
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2235 nm^3 ; this corresponds to an approximate mass of 2019 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

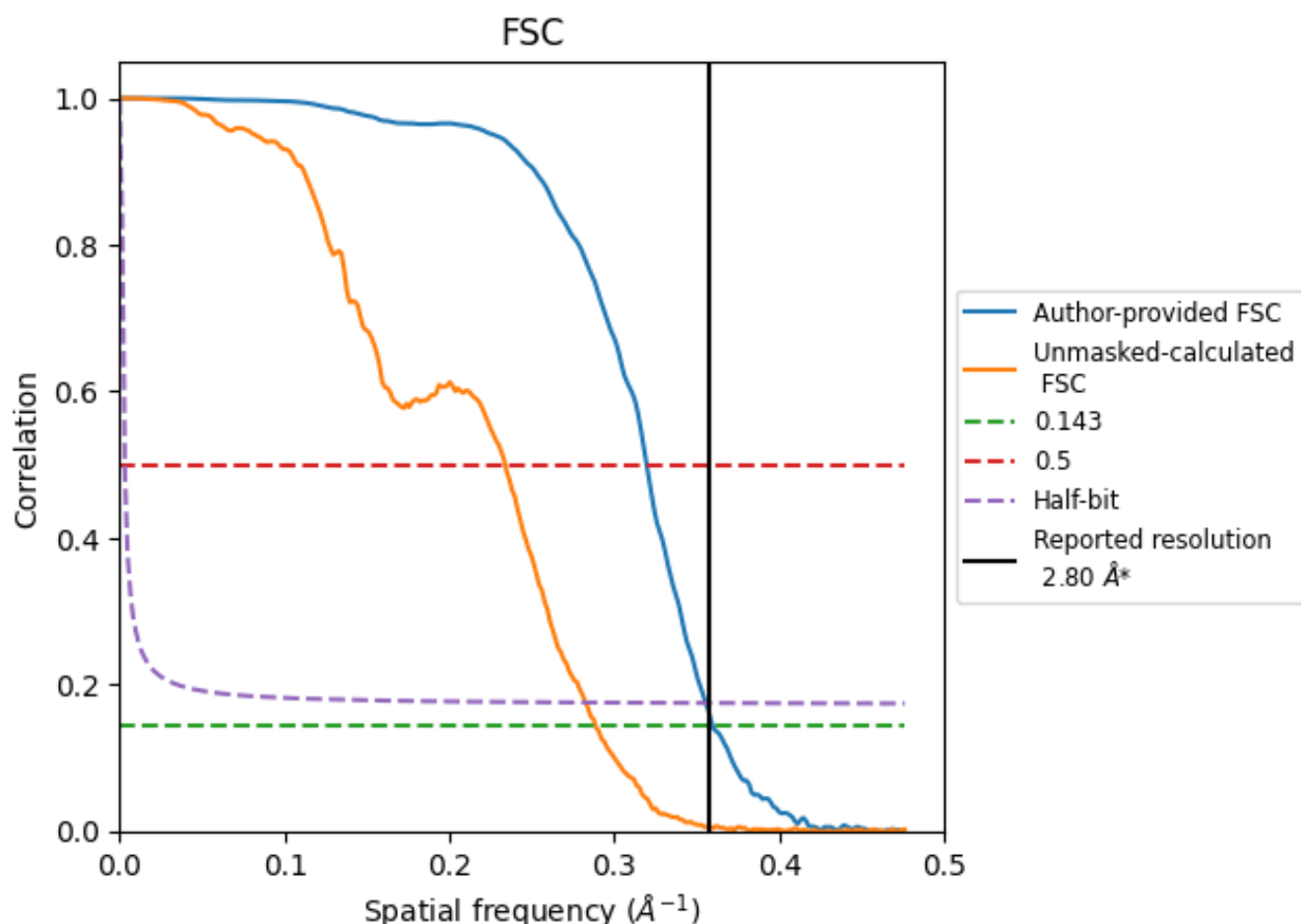


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

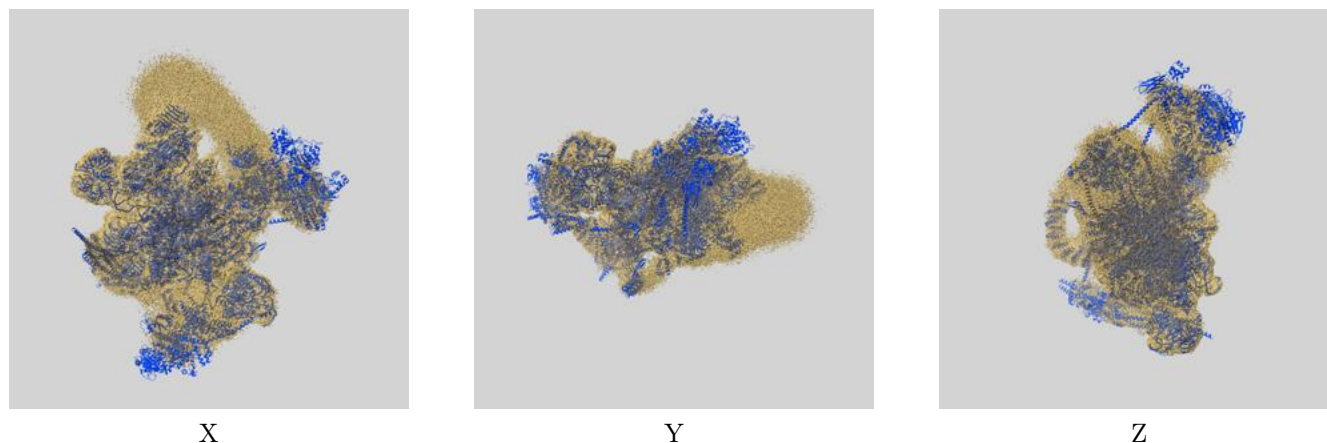
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.78	3.13	2.81
Unmasked-calculated*	3.46	4.28	3.54

*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 3.46 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

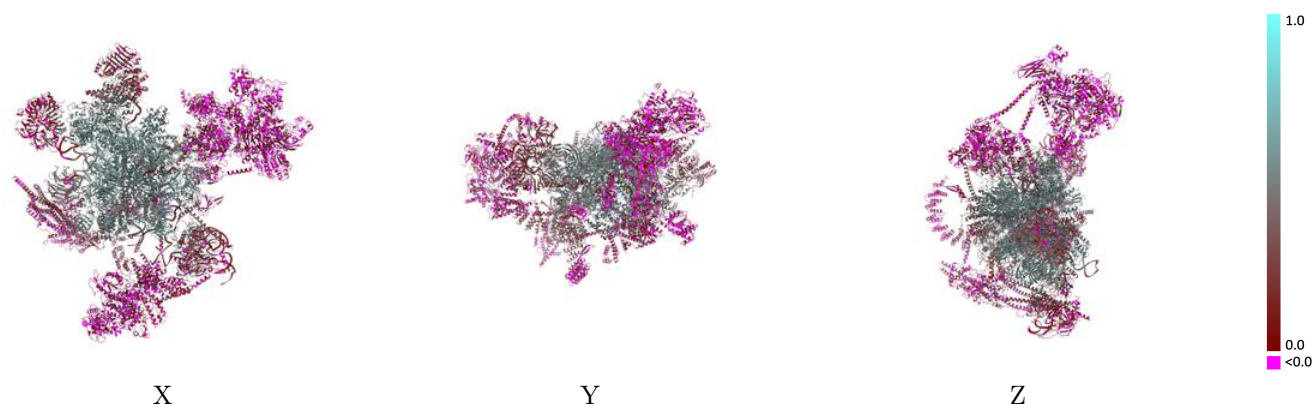
This section contains information regarding the fit between EMDB map EMD-16452 and PDB model 8C6J. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



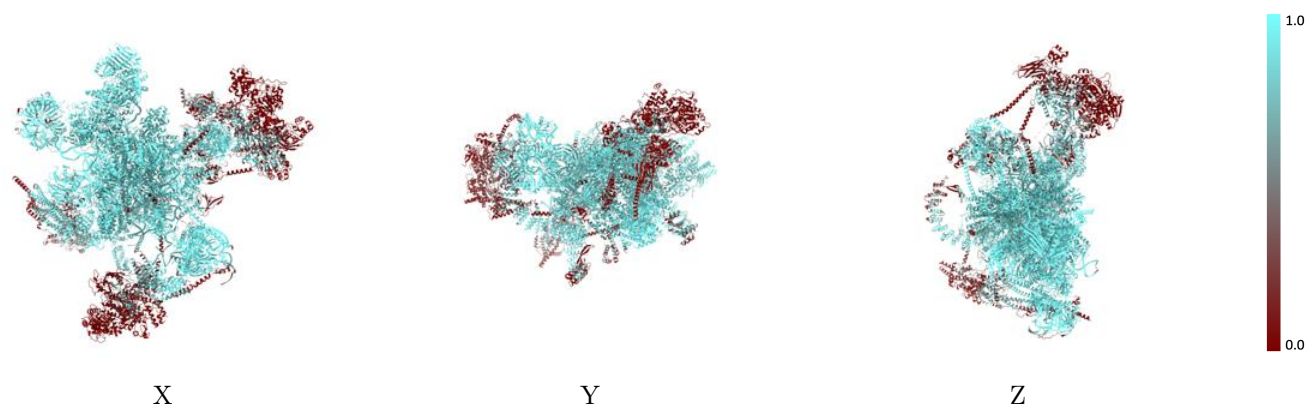
The images above show the 3D surface view of the map at the recommended contour level 0.115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



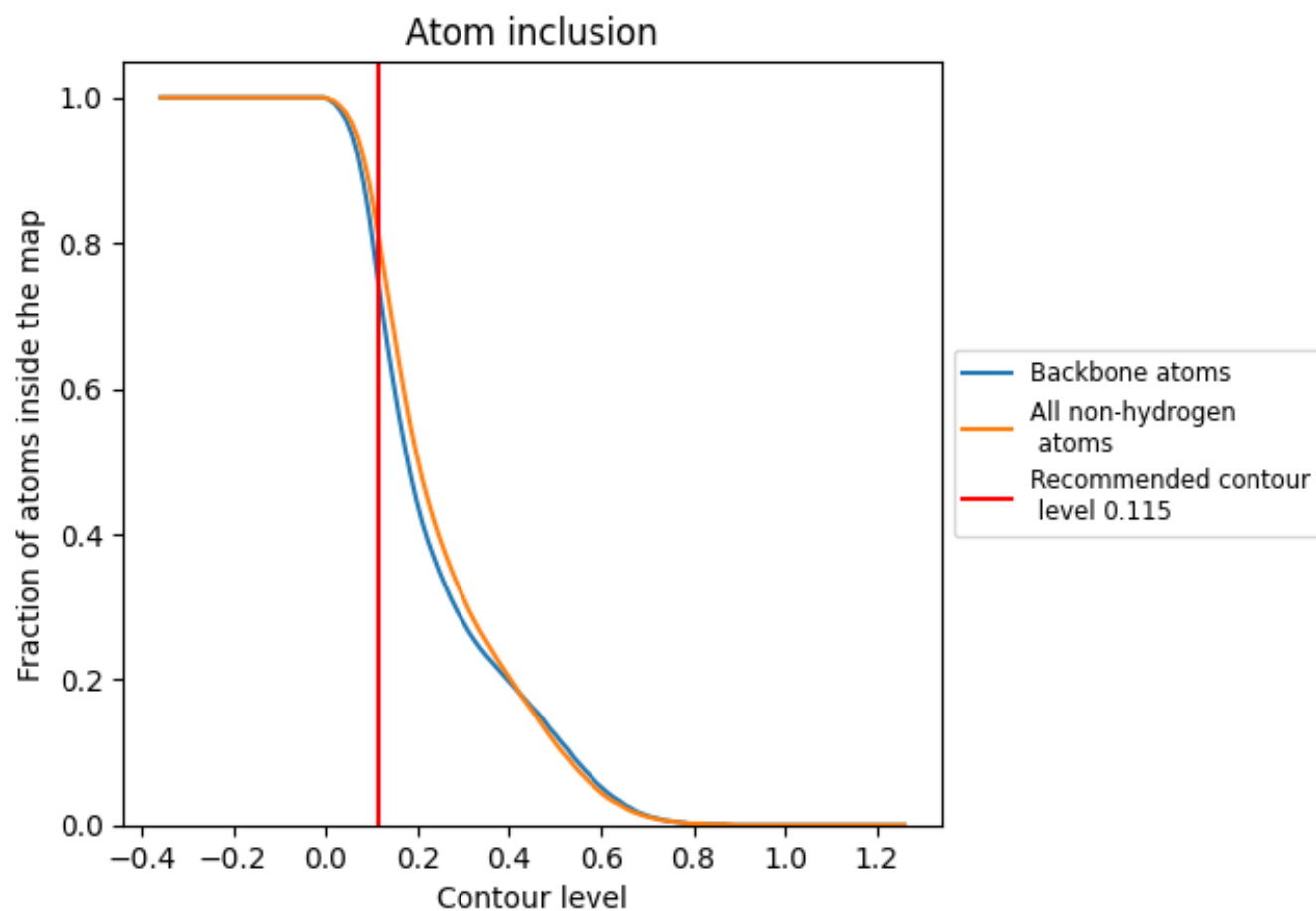
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.115).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 81% 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 (0.115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.3530
2	 0.9200	 0.2840
4	 0.7600	 0.3000
5	 0.9690	 0.3520
6	 0.9820	 0.5100
7	 0.9160	 0.3370
8	 0.9360	 0.2000
9	 0.9880	 0.2160
A	 0.9740	 0.5440
B	 0.2780	 0.0280
C	 0.9810	 0.5270
C3	 0.3120	 0.0080
CD	 0.5880	 0.0220
CE	 0.7300	 0.0950
CF	 0.1770	 0.0210
CI	 0.3850	 0.0970
CN	 0.7090	 0.3600
CT	 0.6160	 0.1320
D	 0.9090	 0.3710
E	 0.9470	 0.4160
F	 0.9870	 0.4740
G	 0.9750	 0.5220
H	 0.9670	 0.4580
I	 0.9750	 0.3200
J	 0.9410	 0.5700
K	 0.9720	 0.4900
L	 0.9920	 0.5540
M	 0.9720	 0.4470
N	 0.9770	 0.4390
O	 0.7810	 0.3740
P	 0.9770	 0.5110
R	 0.9800	 0.4340
S	 0.8460	 0.3780
T	 0.8510	 0.1920
U	 0.0940	 0.0450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
V	 0.8880	 0.1930
W	 0.9100	 0.1570
Y	 0.9970	 0.1890
Z	 0.6340	 0.3110
a	 0.8040	 0.0890
b	 0.8810	 0.2130
c	 0.9730	 0.1580
d	 0.9930	 0.3670
e	 0.9360	 0.1530
f	 0.8720	 0.1110
g	 0.9530	 0.2470
h	 0.9650	 0.5140
i	 0.9810	 0.4600
j	 0.1960	 0.0310
k	 0.9680	 0.3560
l	 0.9760	 0.2870
m	 0.8960	 0.2140
n	 0.9970	 0.4490
o	 0.9640	 0.5220
p	 0.9850	 0.3340
q	 0.9870	 0.2370
r	 0.9870	 0.4340
s	 0.4790	 0.1230
t	 0.3100	 0.0810
u	 0.2360	 0.0890
v	 0.4390	 0.0880
w	 0.1990	 0.0470
y	 0.8900	 0.4500
z	 0.4650	 0.2450