



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:43 PM EST

PDB ID : 3JAP
EMDB ID : EMD-3048
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 4.90 Å(reported)
Based on initial models : 3CW2, 2D74, 4U1E, 3J81, 4U1C, 4U1D

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

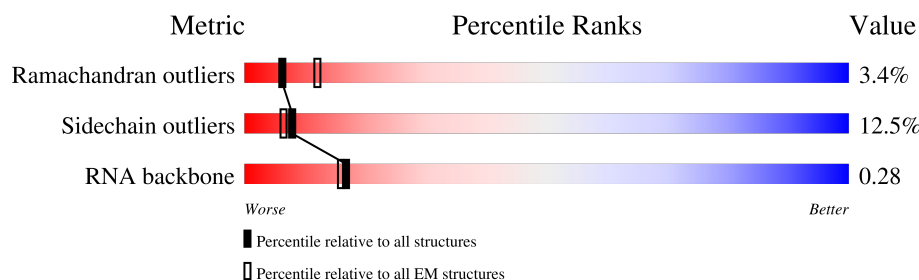
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	75	<div> <div>28%</div> <div>51%</div> <div>49%</div> </div>
2	2	1781	<div> <div>6%</div> <div>49%</div> <div>50%</div> </div>
3	3	25	<div> <div>20%</div> <div>12%</div> <div>44%</div> <div>44%</div> </div>
4	A	254	<div> <div>68%</div> <div>13%</div> <div>18%</div> </div>
5	B	255	<div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
6	C	259	<div> <div>73%</div> <div>11%</div> <div>16%</div> </div>
7	D	237	<div> <div>5%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
8	E	261	<div> <div>84%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	588	
44	p	652	
45	q	347	
46	r	31	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 98333 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 Met-tRNAi (U31:A39 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 20 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S		
			433	271	88	73	1	0	0

- Molecule 35 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 36 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	550	Total	C	N	O	S	0	0
			4189	2667	721	794	7		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	634	Total	C	N	O	S	0	0
			4899	3121	826	940	12		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	31	Total	C	N	O	S	0	0
			277	177	48	50	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

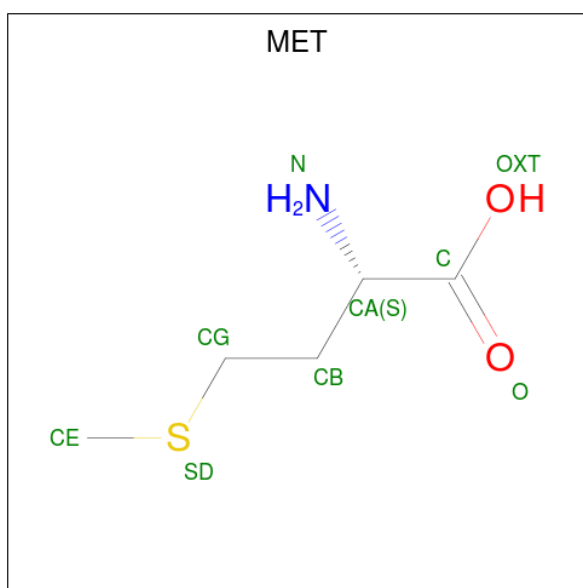
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	80	Total	Mg	0
			80	80	
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

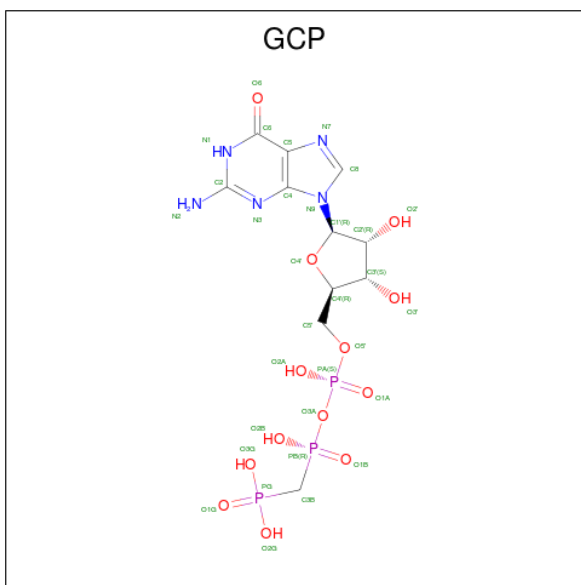
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

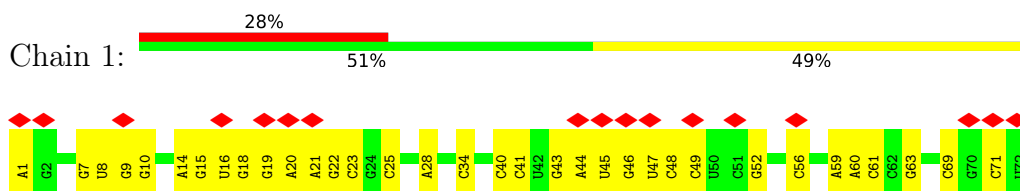


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

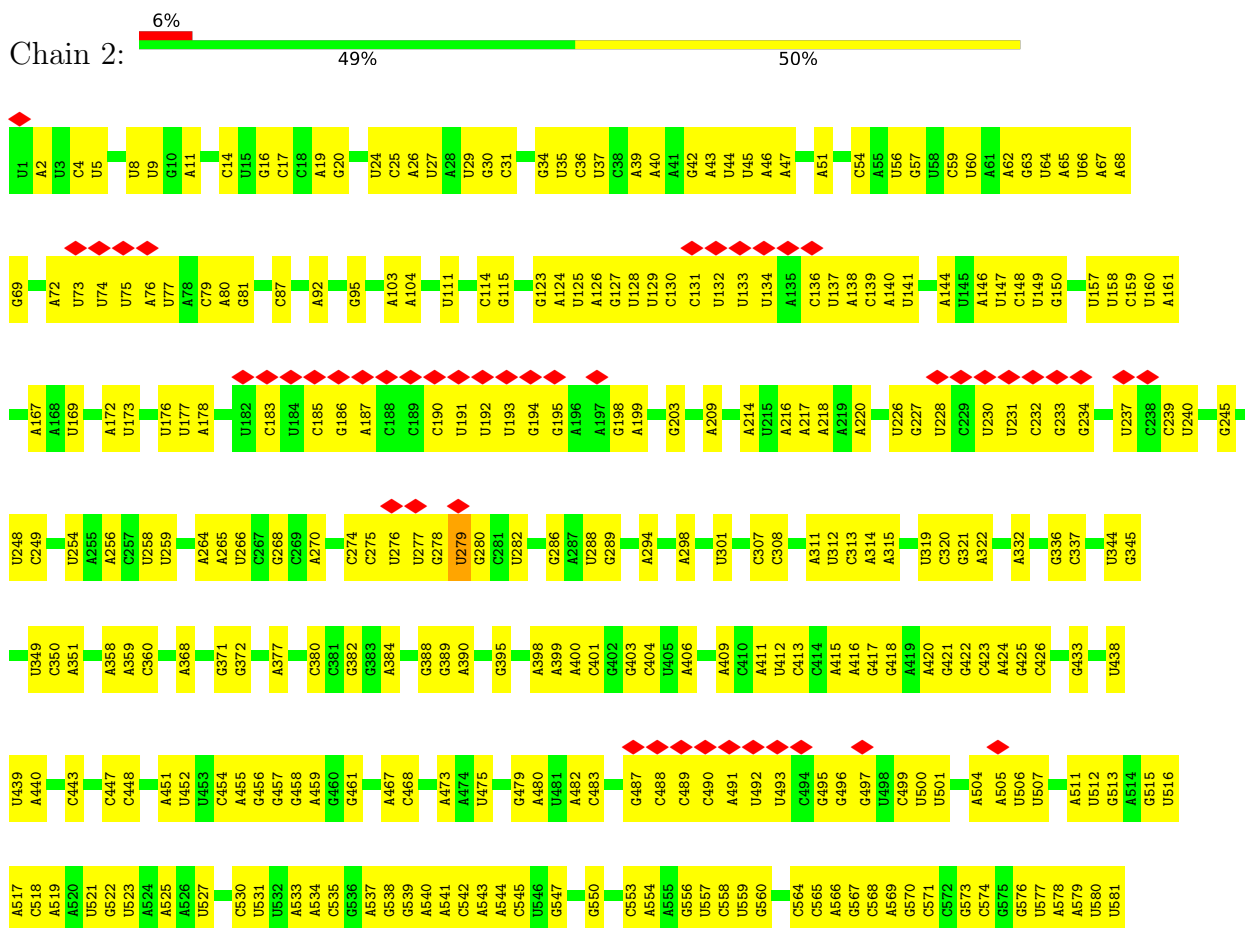
3 Residue-property plots

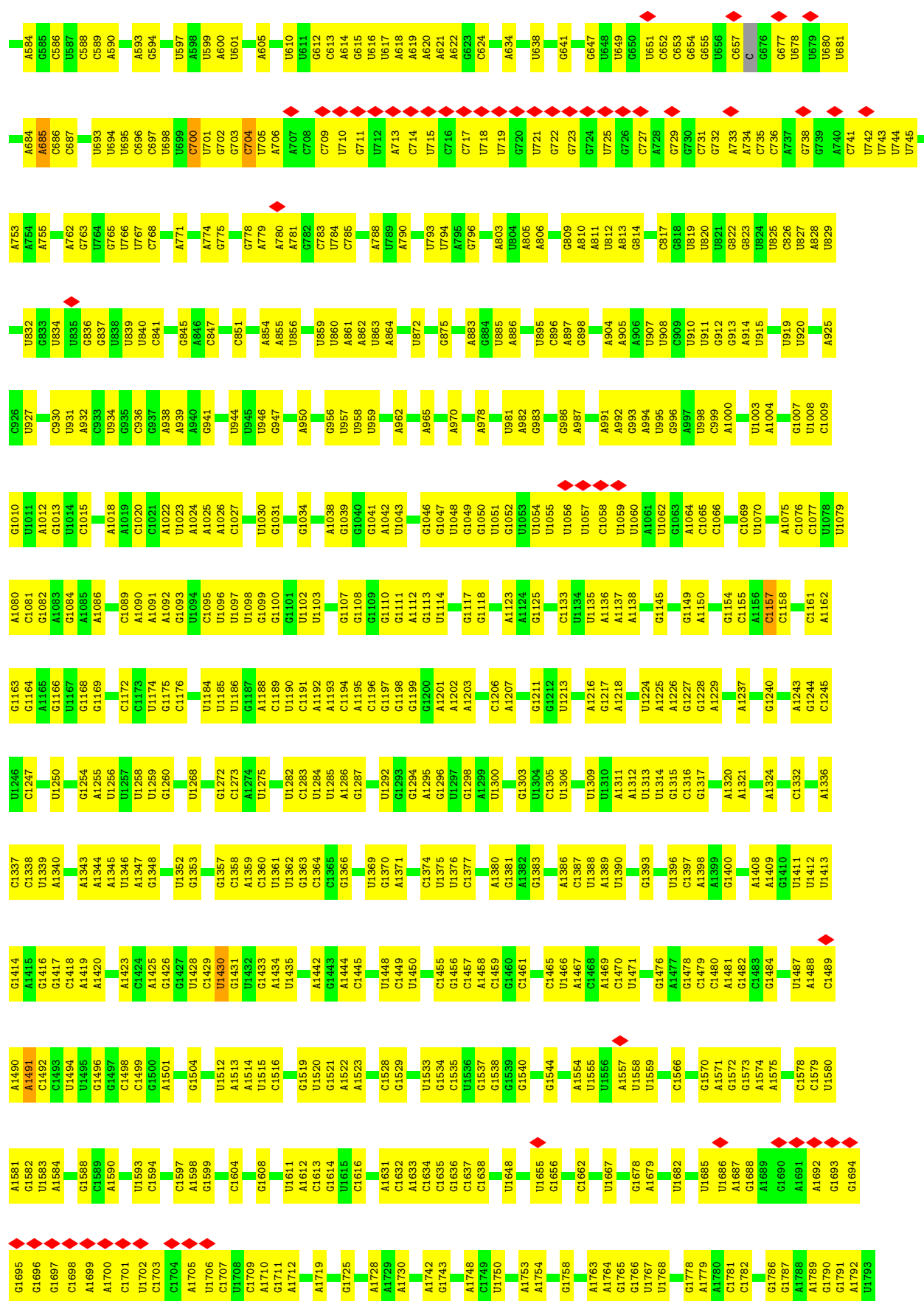
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Met-tRNAi (U31:A39 variant)



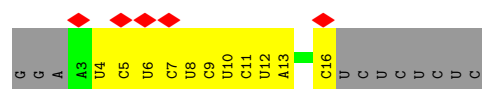
- Molecule 2: 18S rRNA



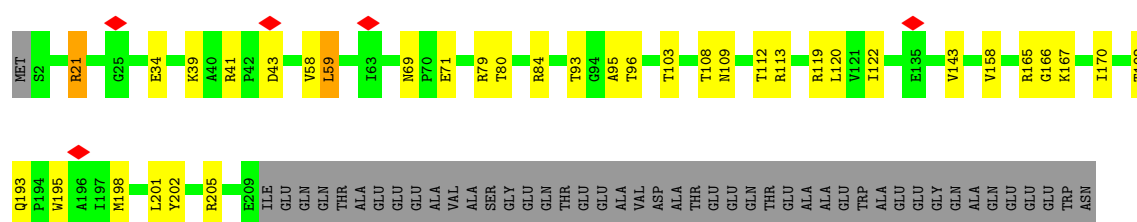


C1794
A1795
U1796
U1797
A1798

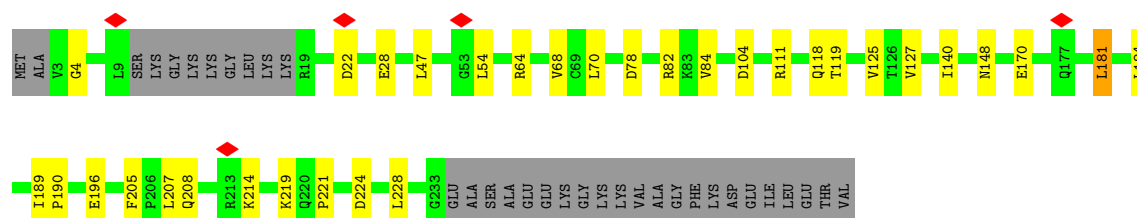
• Molecule 3: mRNA



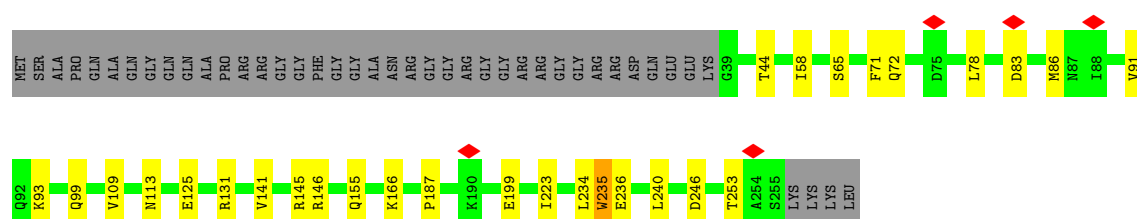
• Molecule 4: uS2



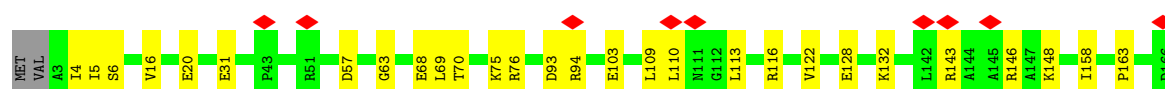
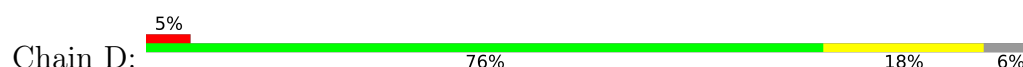
• Molecule 5: eS1



• Molecule 6: uS5

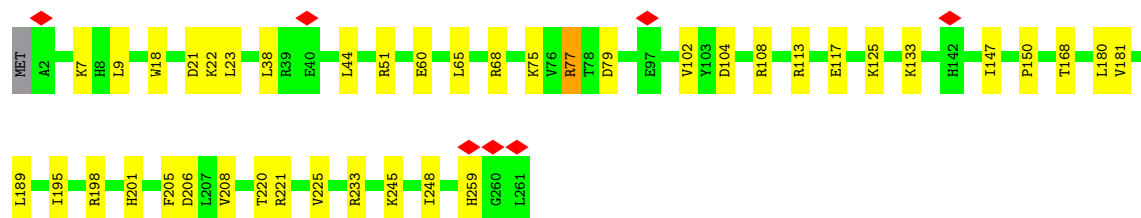
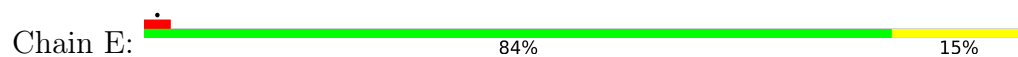


• Molecule 7: uS3

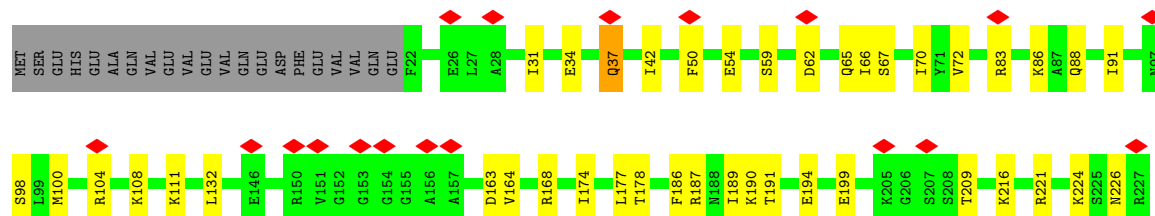
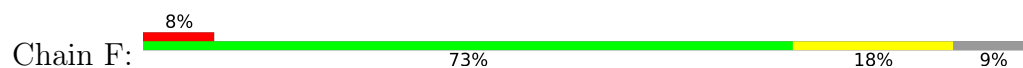




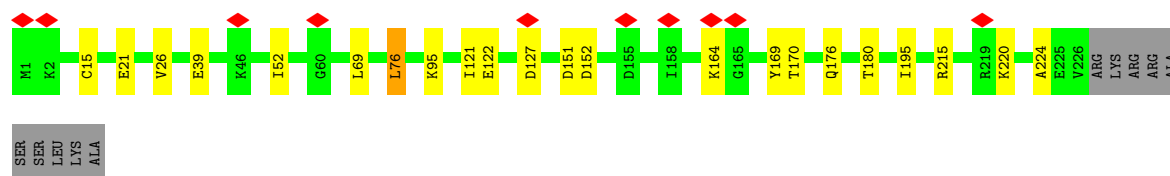
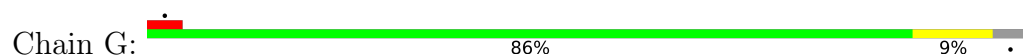
• Molecule 8: eS4



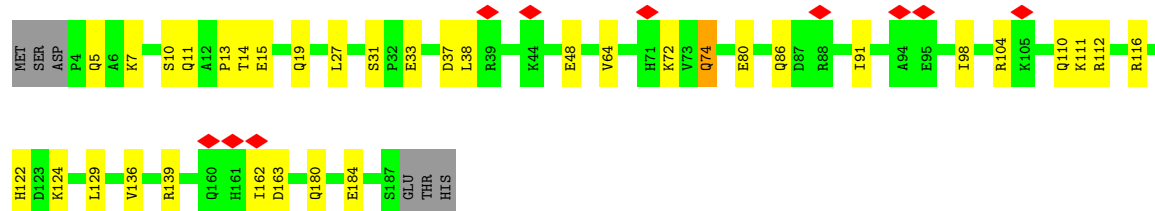
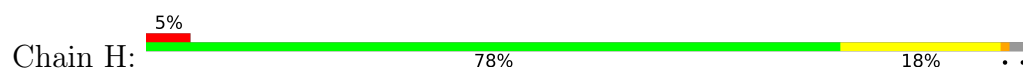
• Molecule 9: uS7



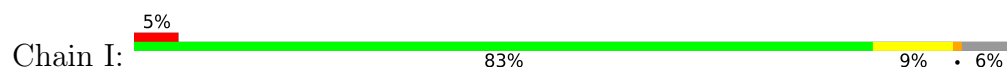
• Molecule 10: eS6

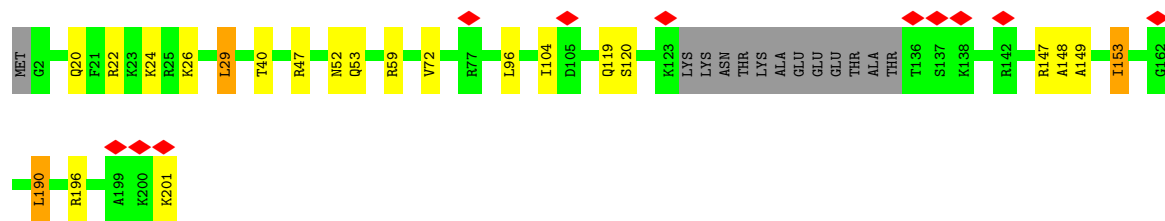


• Molecule 11: eS7

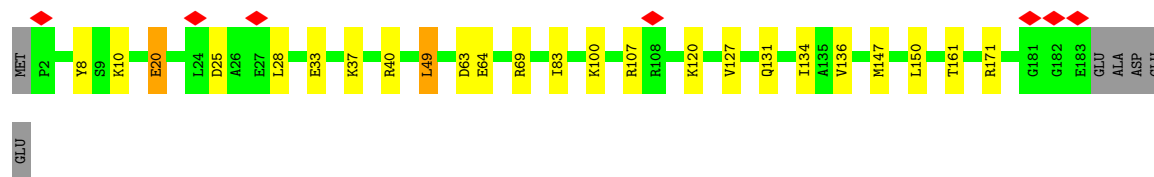
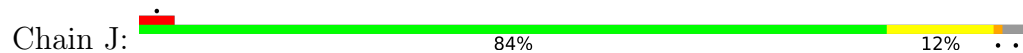


• Molecule 12: eS8





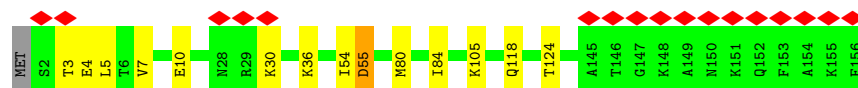
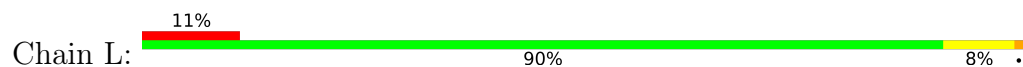
• Molecule 13: uS4



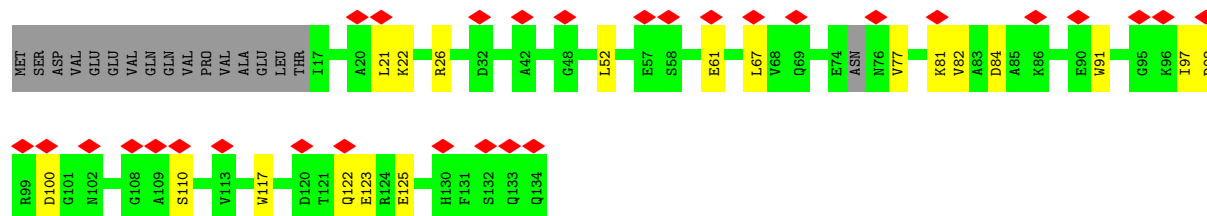
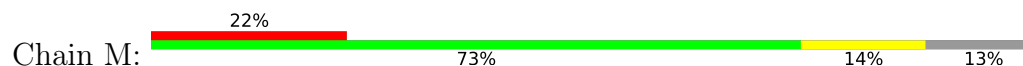
• Molecule 14: eS10



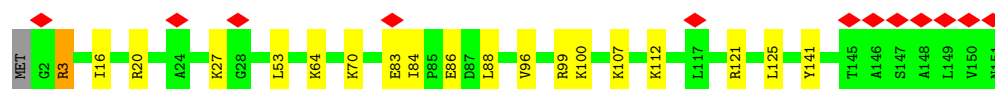
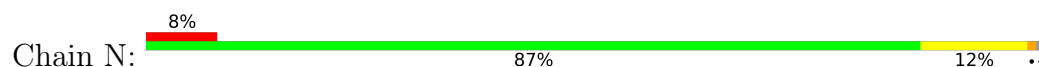
• Molecule 15: uS17




• Molecule 16: eS12



• Molecule 17: uS15



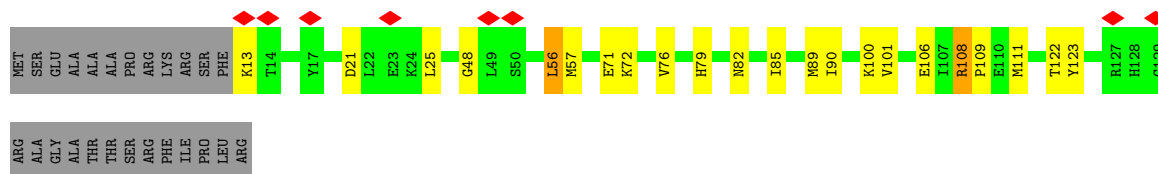
- Molecule 18: uS11

Chain O: 




- Molecule 19: uS19

Chain P: 




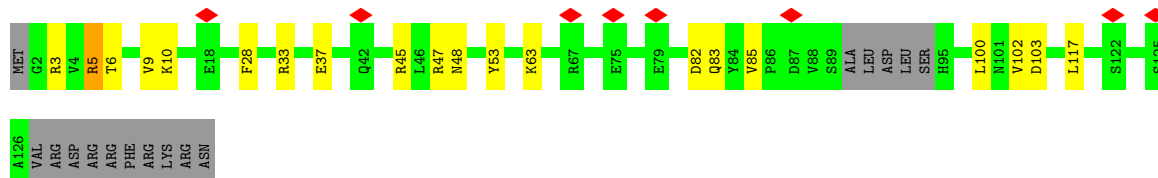
- Molecule 20: uS9

Chain Q: 




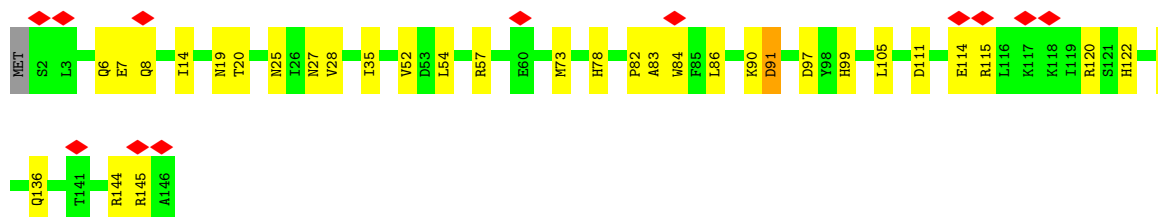
- Molecule 21: eS17

Chain R: 




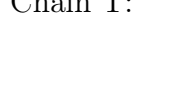
- Molecule 22: uS13

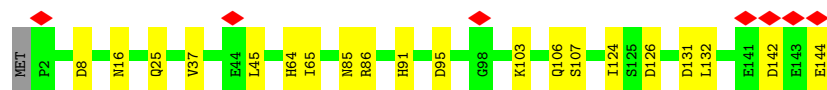
Chain S: 



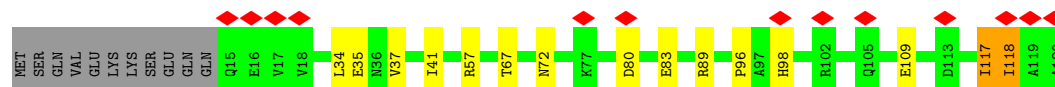
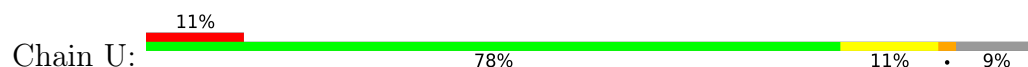
- Molecule 23: eS19

Chain T: 

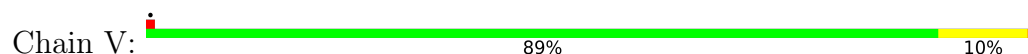




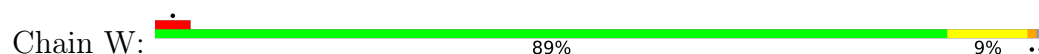
- Molecule 24: uS10



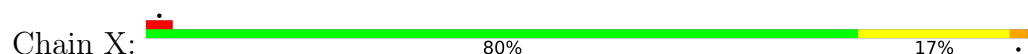
- Molecule 25: eS21



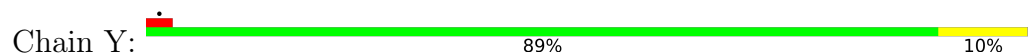
- Molecule 26: uS8



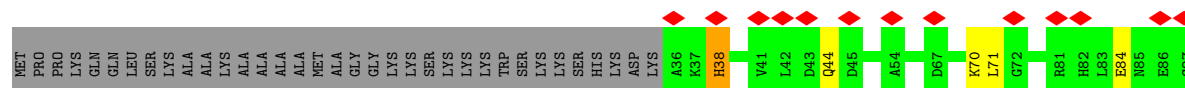
- Molecule 27: uS12



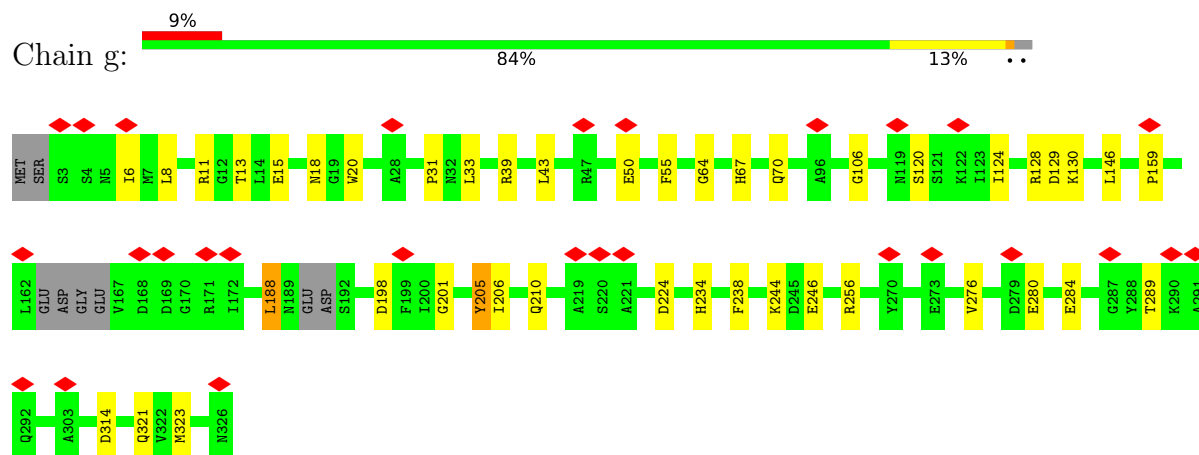
- Molecule 28: eS24



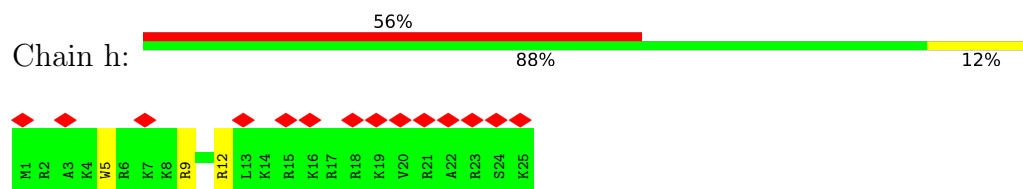
- Molecule 29: eS25



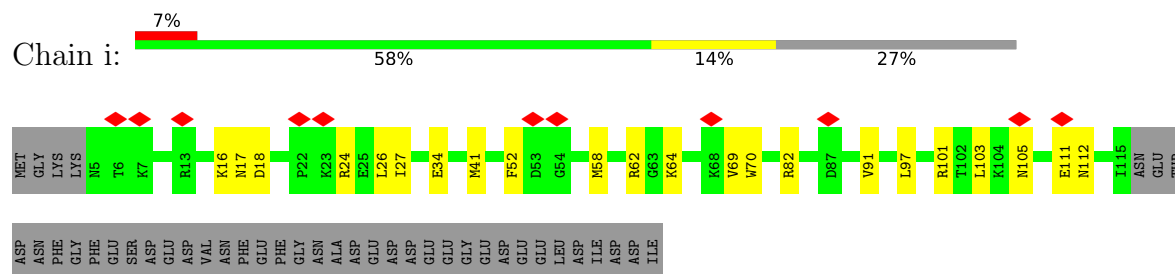
- Molecule 36: RACK1



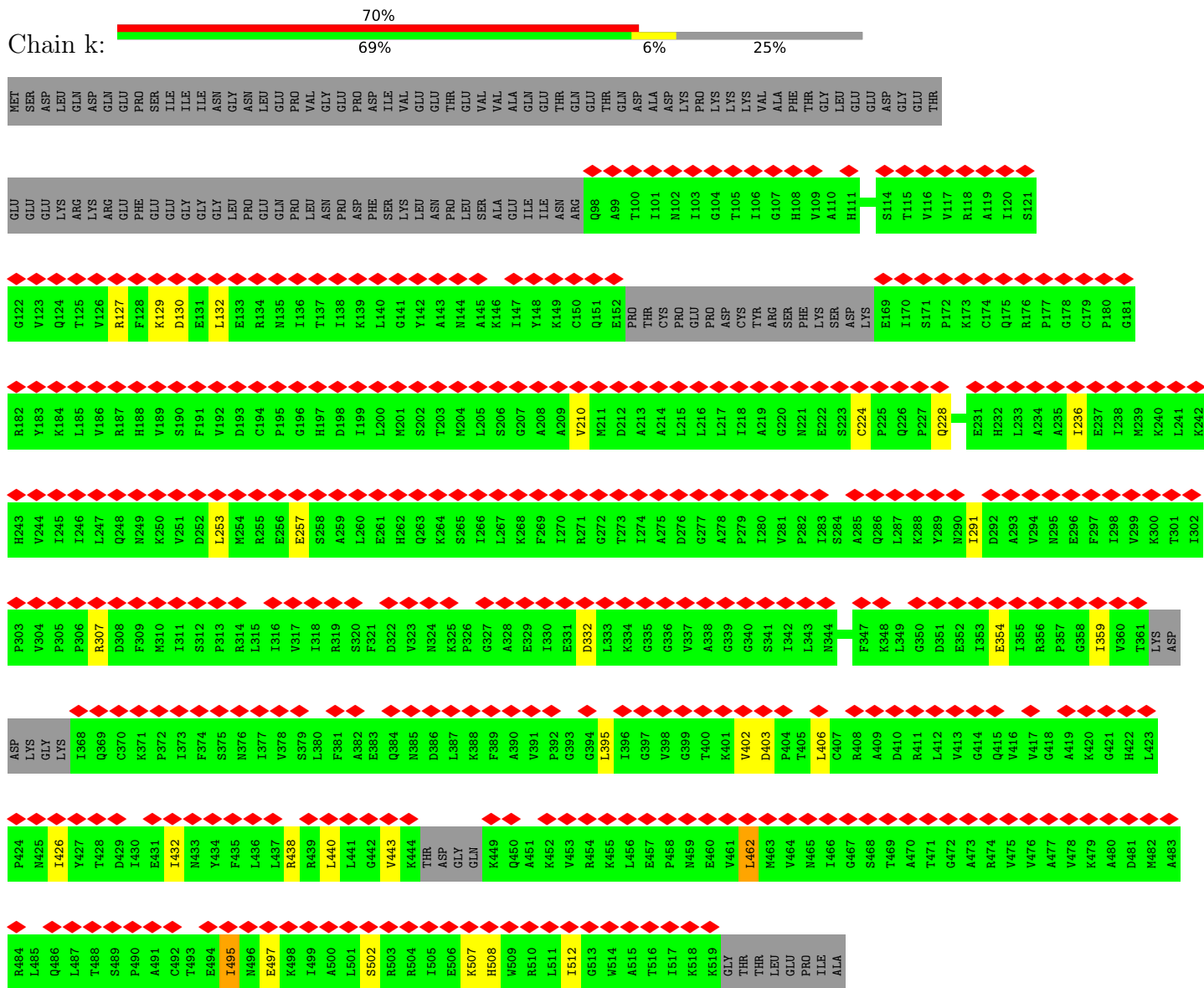
- Molecule 37: eL41



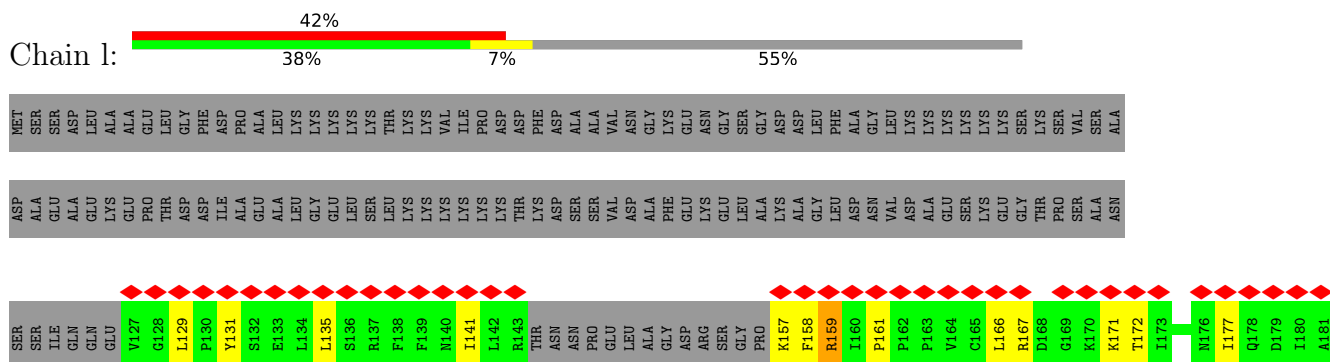
- Molecule 38: eIF1A

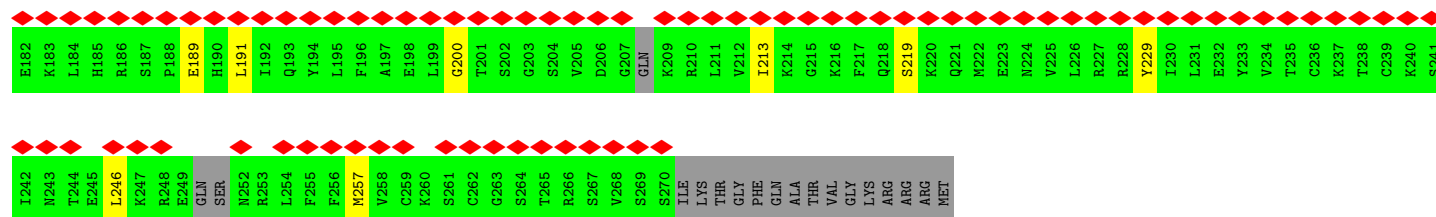


Chain k:

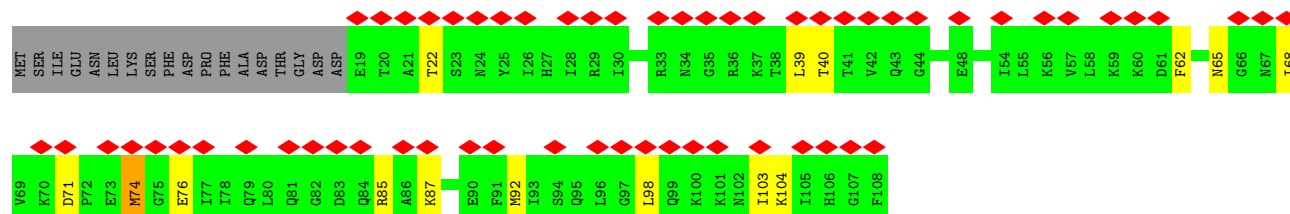


Chain 1:

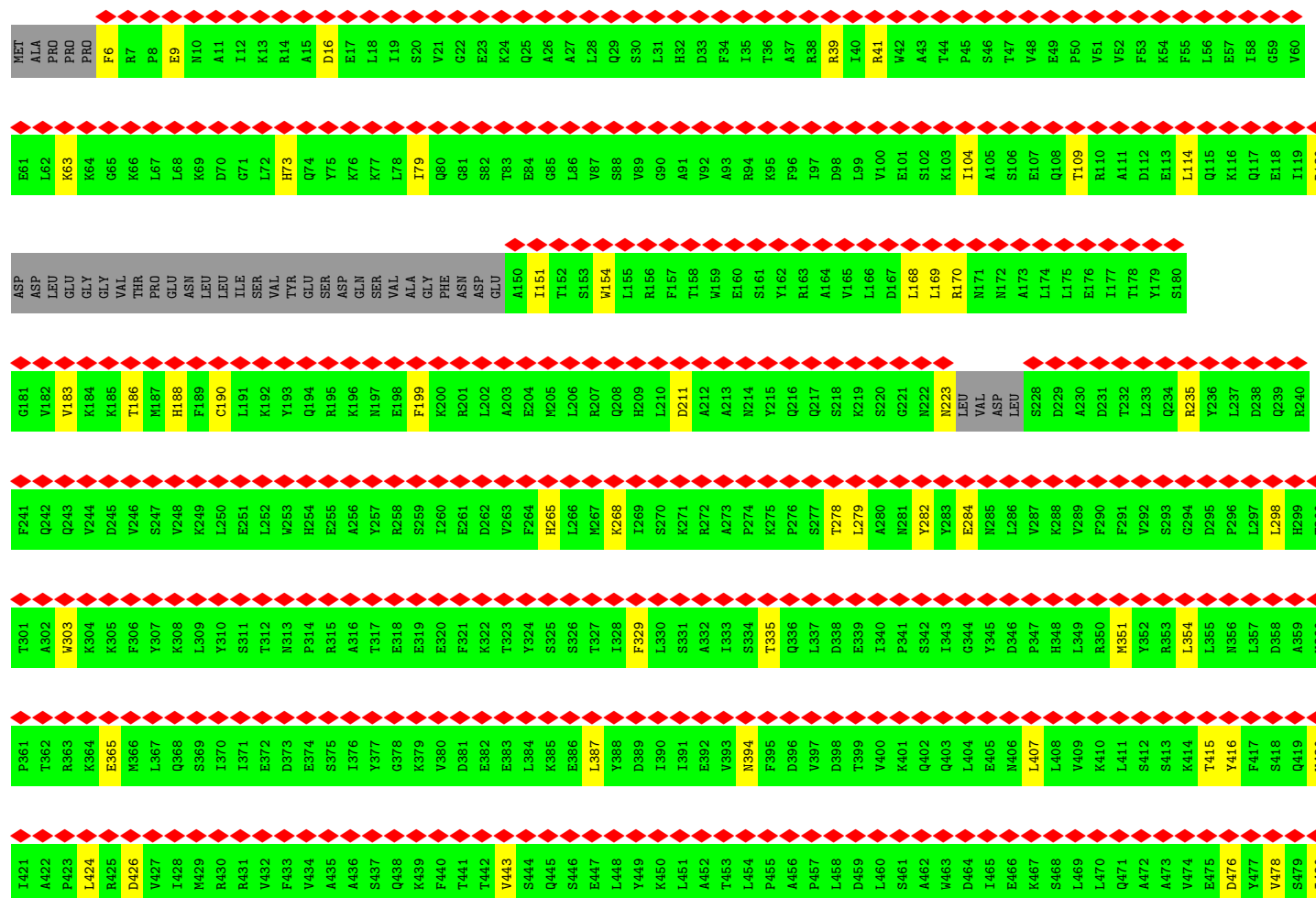
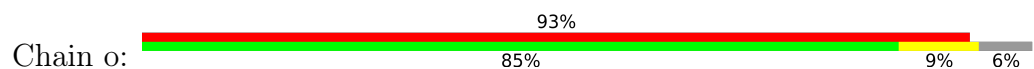




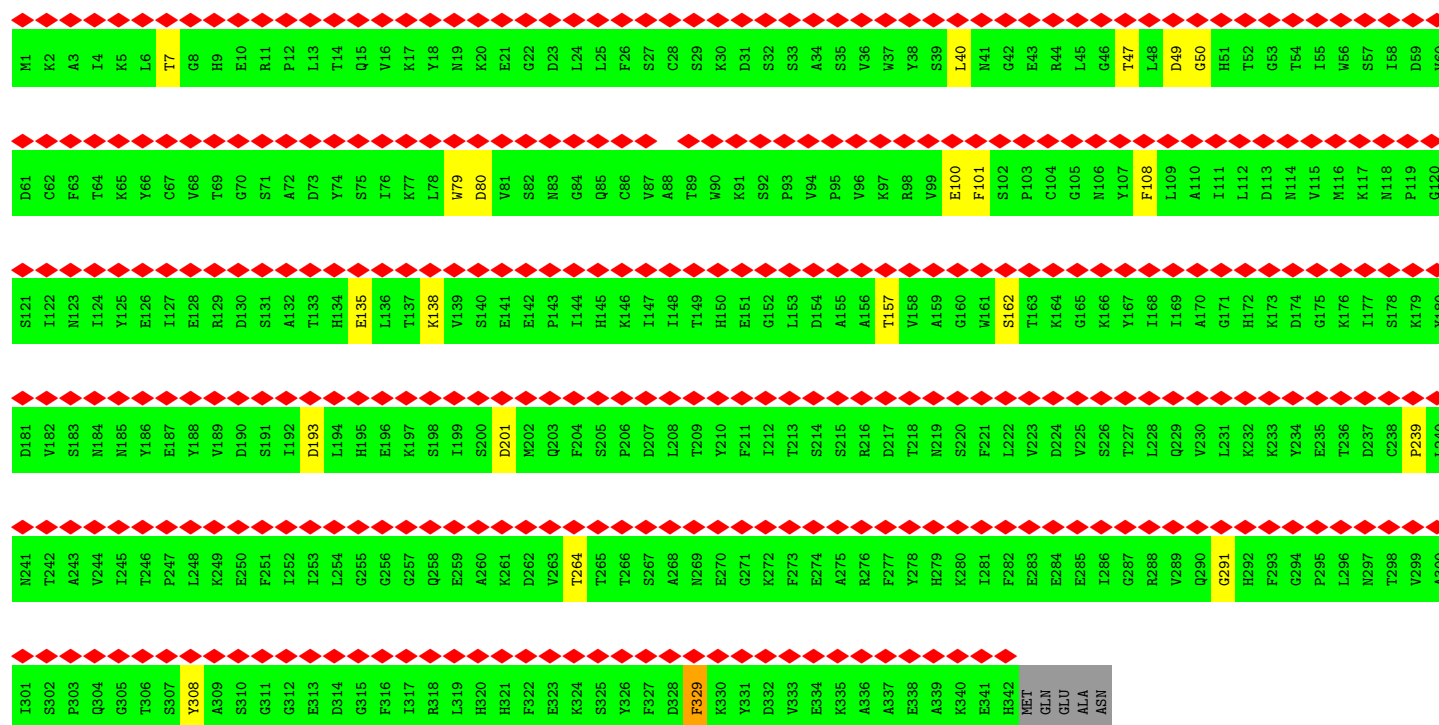
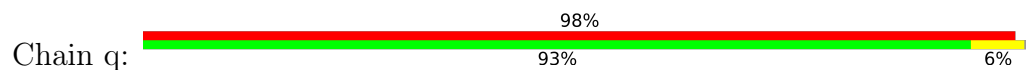
• Molecule 42: eIF1



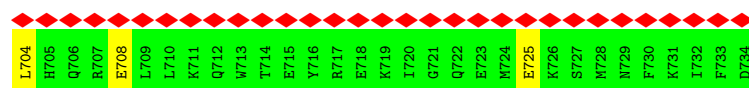
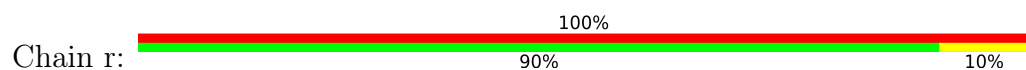
• Molecule 43: eIF3a



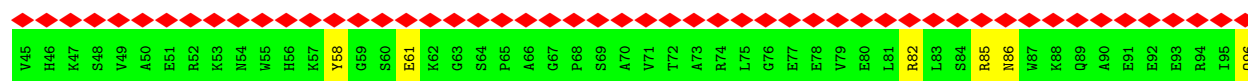
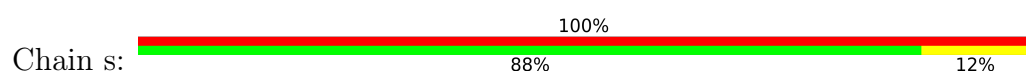
- Molecule 45: eIF3i



- Molecule 46: eIF3b



- Molecule 47: eIF3g



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21401	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, MG

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	0.38	1/1797 (0.1%)	0.69	0/2799
2	2	0.27	0/42269	0.69	7/65862 (0.0%)
3	3	0.30	0/317	0.69	0/489
4	A	0.42	0/1666	0.78	2/2279 (0.1%)
5	B	0.40	0/1793	0.72	2/2414 (0.1%)
6	C	0.39	0/1659	0.69	0/2252
7	D	0.42	0/1769	0.72	1/2378 (0.0%)
8	E	0.38	0/2122	0.67	0/2861
9	F	0.41	0/1628	0.75	0/2198
10	G	0.41	0/1835	0.72	1/2451 (0.0%)
11	H	0.42	0/1507	0.71	0/2028
12	I	0.41	0/1515	0.73	2/2029 (0.1%)
13	J	0.40	0/1495	0.75	1/2001 (0.0%)
14	K	0.48	0/831	0.77	1/1123 (0.1%)
15	L	0.41	0/1276	0.63	0/1718
16	M	0.46	0/891	0.80	1/1201 (0.1%)
17	N	0.41	0/1210	0.77	0/1628
18	O	0.38	0/953	0.68	0/1279
19	P	0.42	0/946	0.71	1/1273 (0.1%)
20	Q	0.43	0/1125	0.71	0/1510
21	R	0.43	0/969	0.77	1/1299 (0.1%)
22	S	0.43	0/1212	0.78	0/1629
23	T	0.40	0/1129	0.72	0/1520
24	U	0.40	0/857	0.73	0/1158
25	V	0.36	0/696	0.66	0/938
26	W	0.39	0/1039	0.74	1/1399 (0.1%)
27	X	0.40	0/1137	0.75	2/1516 (0.1%)
28	Y	0.40	0/1075	0.69	0/1433
29	Z	0.44	0/567	0.69	0/762
30	a	0.36	0/791	0.67	0/1059
31	b	0.38	0/619	0.65	0/837
32	c	0.38	0/489	0.71	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.41	0/457	0.62	0/607
34	e	0.40	0/440	0.73	0/586
35	f	0.49	0/559	0.73	1/747 (0.1%)
36	g	0.41	0/2521	0.64	1/3431 (0.0%)
37	h	0.36	0/234	0.75	0/300
38	i	0.39	0/894	0.70	0/1188
39	j	0.47	0/2034	0.77	2/2737 (0.1%)
40	k	0.47	0/3079	0.70	1/4157 (0.0%)
41	l	0.47	0/1051	0.76	1/1402 (0.1%)
42	m	0.41	0/724	0.75	1/968 (0.1%)
43	o	0.49	0/3796	0.80	0/5128
44	p	0.49	0/4602	0.76	2/6226 (0.0%)
45	q	0.50	0/2757	0.67	0/3733
46	r	0.49	0/282	0.74	0/373
47	s	0.47	0/426	0.64	0/571
All	All	0.38	1/103040 (0.0%)	0.71	32/148132 (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
9	F	0	1
27	X	0	1
28	Y	0	1
41	l	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.88	1.49	1.61

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	685	A	C2'-C3'-O3'	8.09	127.30	109.50
12	I	29	LEU	CA-CB-CG	7.26	132.00	115.30
39	j	166	LEU	CA-CB-CG	6.66	130.62	115.30
41	l	191	LEU	CA-CB-CG	6.50	130.25	115.30
26	W	26	LEU	CA-CB-CG	6.10	129.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1157	C	C4'-C3'-O3'	5.95	124.91	113.00
19	P	56	LEU	CA-CB-CG	5.90	128.87	115.30
44	p	550	LEU	CA-CB-CG	5.81	128.67	115.30
2	2	1491	A	C2'-C3'-O3'	5.74	122.88	113.70
12	I	190	LEU	CA-CB-CG	5.71	128.44	115.30
5	B	181	LEU	CA-CB-CG	5.70	128.40	115.30
27	X	9	LEU	CA-CB-CG	5.70	128.40	115.30
7	D	110	LEU	CA-CB-CG	5.67	128.35	115.30
13	J	49	LEU	CA-CB-CG	5.64	128.28	115.30
2	2	279	U	C2'-C3'-O3'	5.63	122.71	113.70
42	m	76	GLU	N-CA-C	-5.63	95.81	111.00
44	p	376	LEU	CA-CB-CG	5.61	128.21	115.30
39	j	126	LEU	CA-CB-CG	5.60	128.19	115.30
2	2	700	C	C2'-C3'-O3'	5.55	122.59	113.70
5	B	184	LEU	CA-CB-CG	5.54	128.04	115.30
2	2	704	C	N1-C1'-C2'	5.48	121.12	114.00
10	G	76	LEU	CA-CB-CG	5.42	127.76	115.30
35	f	100	LEU	CA-CB-CG	5.33	127.56	115.30
4	A	59	LEU	CA-CB-CG	5.24	127.36	115.30
2	2	1430	U	C2'-C3'-O3'	5.23	122.07	113.70
21	R	53	TYR	CB-CA-C	5.15	120.69	110.40
36	g	188	LEU	CA-CB-CG	5.15	127.14	115.30
4	A	201	LEU	CA-CB-CG	5.13	127.10	115.30
27	X	93	LEU	CA-CB-CG	5.06	126.94	115.30
14	K	15	LEU	CA-CB-CG	5.05	126.92	115.30
16	M	21	LEU	CA-CB-CG	5.03	126.87	115.30
40	k	462	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	191	THR	Peptide
27	X	63	GLN	Peptide
28	Y	29	HIS	Peptide
41	l	158	PHE	Peptide

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	
4	A	206/254 (81%)	170 (82%)	27 (13%)	9 (4%)	2	24
5	B	218/255 (86%)	185 (85%)	25 (12%)	8 (4%)	3	27
6	C	215/259 (83%)	186 (86%)	22 (10%)	7 (3%)	4	29
7	D	221/237 (93%)	196 (89%)	16 (7%)	9 (4%)	3	25
8	E	258/261 (99%)	225 (87%)	28 (11%)	5 (2%)	8	40
9	F	204/227 (90%)	169 (83%)	28 (14%)	7 (3%)	3	29
10	G	224/236 (95%)	197 (88%)	23 (10%)	4 (2%)	8	41
11	H	182/190 (96%)	157 (86%)	15 (8%)	10 (6%)	2	21
12	I	184/201 (92%)	160 (87%)	15 (8%)	9 (5%)	2	22
13	J	180/188 (96%)	154 (86%)	19 (11%)	7 (4%)	3	26
14	K	94/106 (89%)	81 (86%)	7 (7%)	6 (6%)	1	18
15	L	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	23
16	M	113/134 (84%)	85 (75%)	21 (19%)	7 (6%)	1	18
17	N	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	22	62
18	O	125/137 (91%)	102 (82%)	16 (13%)	7 (6%)	2	20
19	P	115/142 (81%)	96 (84%)	13 (11%)	6 (5%)	2	21
20	Q	139/143 (97%)	108 (78%)	20 (14%)	11 (8%)	1	14
21	R	116/136 (85%)	101 (87%)	13 (11%)	2 (2%)	9	43
22	S	143/146 (98%)	111 (78%)	21 (15%)	11 (8%)	1	14
23	T	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
24	U	104/117 (89%)	84 (81%)	16 (15%)	4 (4%)	3	26
25	V	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	23
26	W	127/130 (98%)	112 (88%)	10 (8%)	5 (4%)	3	26
27	X	142/145 (98%)	117 (82%)	14 (10%)	11 (8%)	1	14
28	Y	132/135 (98%)	118 (89%)	7 (5%)	7 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	68/108 (63%)	50 (74%)	17 (25%)	1 (2%)	10	46
30	a	96/119 (81%)	81 (84%)	11 (12%)	4 (4%)	3	24
31	b	79/82 (96%)	61 (77%)	15 (19%)	3 (4%)	3	26
32	c	60/67 (90%)	51 (85%)	6 (10%)	3 (5%)	2	22
33	d	51/56 (91%)	33 (65%)	15 (29%)	3 (6%)	1	19
34	e	52/63 (82%)	45 (86%)	6 (12%)	1 (2%)	8	40
35	f	67/150 (45%)	48 (72%)	9 (13%)	10 (15%)	0	4
36	g	312/326 (96%)	257 (82%)	45 (14%)	10 (3%)	4	30
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	92 (84%)	14 (13%)	3 (3%)	5	32
39	j	243/304 (80%)	205 (84%)	32 (13%)	6 (2%)	5	34
40	k	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	10	46
41	l	120/285 (42%)	100 (83%)	16 (13%)	4 (3%)	4	29
42	m	88/108 (82%)	76 (86%)	10 (11%)	2 (2%)	6	36
43	o	451/588 (77%)	417 (92%)	31 (7%)	3 (1%)	22	62
44	p	554/652 (85%)	497 (90%)	45 (8%)	12 (2%)	6	37
45	q	340/347 (98%)	302 (89%)	33 (10%)	5 (2%)	10	46
46	r	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
47	s	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
All	All	7149/8360 (86%)	6131 (86%)	778 (11%)	240 (3%)	6	29

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	95	ALA
4	A	166	GLY
6	C	141	VAL
6	C	235	TRP
7	D	216	PRO
7	D	220	PRO
8	E	245	LYS
10	G	69	LEU
11	H	14	THR
11	H	31	SER
11	H	64	VAL

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Mol	Chain	Res	Type
11	H	74	GLN
12	I	22	ARG
12	I	147	ARG
15	L	105	LYS
20	Q	97	VAL
21	R	85	VAL
22	S	19	ASN
22	S	27	ASN
22	S	28	VAL
22	S	82	PRO
22	S	91	ASP
24	U	96	PRO
26	W	83	ILE
27	X	12	ALA
27	X	64	PRO
27	X	90	ASP
27	X	92	CYS
28	Y	30	PRO
34	e	47	VAL
35	f	94	LYS
39	j	48	LEU
40	k	129	LYS
43	o	63	LYS
44	p	460	PRO
44	p	558	CYS
4	A	21	ARG
5	B	148	ASN
5	B	214	LYS
5	B	221	PRO
5	B	224	ASP
6	C	253	THR
7	D	221	SER
9	F	66	ILE
10	G	122	GLU
11	H	10	SER
11	H	136	VAL
11	H	163	ASP
12	I	40	THR
12	I	52	ASN
12	I	153	ILE
13	J	136	VAL
14	K	22	VAL

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Mol	Chain	Res	Type
14	K	54	PHE
14	K	64	TYR
15	L	7	VAL
16	M	82	VAL
16	M	84	ASP
16	M	110	SER
17	N	3	ARG
18	O	124	ASP
20	Q	39	VAL
20	Q	40	GLN
20	Q	122	ARG
22	S	7	GLU
22	S	83	ALA
22	S	145	ARG
25	V	12	TYR
25	V	45	ALA
26	W	78	ARG
27	X	115	GLY
28	Y	4	ALA
30	a	13	LYS
30	a	59	TYR
33	d	23	ILE
35	f	100	LEU
35	f	102	VAL
36	g	130	LYS
39	j	57	ARG
40	k	495	ILE
40	k	507	LYS
41	l	200	GLY
45	q	329	PHE
4	A	39	LYS
4	A	109	ASN
5	B	54	LEU
5	B	190	PRO
5	B	207	LEU
6	C	187	PRO
7	D	163	PRO
8	E	205	PHE
9	F	37	GLN
9	F	59	SER
9	F	190	LYS
12	I	120	SER

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Mol	Chain	Res	Type
13	J	20	GLU
13	J	134	ILE
13	J	150	LEU
14	K	23	ALA
15	L	4	GLU
15	L	30	LYS
15	L	55	ASP
16	M	98	ASP
18	O	18	ARG
18	O	40	ALA
18	O	51	ASP
18	O	114	ARG
19	P	89	MET
19	P	108	ARG
19	P	109	PRO
20	Q	14	LYS
20	Q	27	GLY
20	Q	115	THR
20	Q	116	LEU
21	R	5	ARG
22	S	8	GLN
25	V	9	VAL
26	W	29	PRO
26	W	58	SER
27	X	3	LYS
27	X	41	SER
27	X	54	LEU
27	X	97	ASP
28	Y	36	SER
31	b	21	LEU
35	f	111	GLU
35	f	122	PRO
35	f	140	GLY
35	f	143	HIS
36	g	106	GLY
36	g	120	SER
36	g	201	GLY
36	g	205	TYR
38	i	17	ASN
38	i	64	LYS
39	j	49	SER
39	j	64	ARG

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Mol	Chain	Res	Type
39	j	138	PHE
40	k	127	ARG
40	k	497	GLU
41	l	159	ARG
42	m	85	ARG
44	p	492	LYS
44	p	536	ASP
44	p	639	GLY
45	q	291	GLY
6	C	44	THR
6	C	65	SER
6	C	155	GLN
7	D	143	ARG
8	E	77	ARG
8	E	150	PRO
8	E	195	ILE
9	F	65	GLN
9	F	67	SER
11	H	13	PRO
11	H	110	GLN
12	I	148	ALA
13	J	120	LYS
13	J	171	ARG
14	K	25	LYS
16	M	81	LYS
18	O	42	VAL
19	P	90	ILE
24	U	89	ARG
25	V	10	GLU
26	W	72	CYS
29	Z	38	HIS
32	c	35	ASP
32	c	49	ARG
33	d	34	TYR
35	f	110	ASP
36	g	31	PRO
36	g	50	GLU
41	l	129	LEU
41	l	219	SER
42	m	74	MET
43	o	394	ASN
44	p	337	ASP

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Mol	Chain	Res	Type
44	p	650	LYS
44	p	774	THR
45	q	162	SER
4	A	103	THR
4	A	158	VAL
4	A	195	TRP
4	A	202	TYR
5	B	4	GLY
7	D	196	THR
11	H	98	ILE
12	I	149	ALA
13	J	147	MET
16	M	77	VAL
18	O	91	SER
19	P	100	LYS
20	Q	74	HIS
22	S	14	ILE
22	S	90	LYS
28	Y	31	ASN
28	Y	64	TYR
30	a	36	ILE
31	b	62	VAL
35	f	90	LYS
35	f	98	VAL
36	g	15	GLU
38	i	16	LYS
39	j	226	PRO
43	o	335	THR
44	p	351	ILE
44	p	645	ILE
44	p	704	PRO
7	D	63	GLY
7	D	219	GLU
9	F	100	MET
10	G	152	ASP
10	G	224	ALA
12	I	59	ARG
15	L	3	THR
16	M	122	GLN
28	Y	67	GLY
20	Q	33	GLY
24	U	118	ILE

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Mol	Chain	Res	Type
30	a	64	LEU
19	P	48	GLY
24	U	117	ILE
27	X	63	GLN
27	X	96	VAL
45	q	50	GLY
45	q	239	PRO
15	L	54	ILE
31	b	10	PRO
32	c	24	GLY
33	d	29	GLY
36	g	159	PRO
7	D	217	VAL
14	K	82	LEU
20	Q	73	GLY
36	g	64	GLY
40	k	210	VAL
44	p	336	ILE
28	Y	5	ILE

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	
4	A	174/211 (82%)	147 (84%)	27 (16%)	2	15
5	B	198/228 (87%)	174 (88%)	24 (12%)	5	22
6	C	176/203 (87%)	153 (87%)	23 (13%)	4	20
7	D	185/196 (94%)	152 (82%)	33 (18%)	2	11
8	E	223/224 (100%)	186 (83%)	37 (17%)	2	13
9	F	174/194 (90%)	140 (80%)	34 (20%)	1	9
10	G	192/200 (96%)	174 (91%)	18 (9%)	8	30
11	H	164/170 (96%)	138 (84%)	26 (16%)	2	15
12	I	147/159 (92%)	133 (90%)	14 (10%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J	153/158 (97%)	135 (88%)	18 (12%)	5	22
14	K	88/96 (92%)	70 (80%)	18 (20%)	1	7
15	L	136/137 (99%)	128 (94%)	8 (6%)	19	46
16	M	93/109 (85%)	82 (88%)	11 (12%)	5	22
17	N	127/128 (99%)	108 (85%)	19 (15%)	3	16
18	O	96/104 (92%)	88 (92%)	8 (8%)	11	36
19	P	100/119 (84%)	83 (83%)	17 (17%)	2	13
20	Q	117/119 (98%)	99 (85%)	18 (15%)	2	15
21	R	109/124 (88%)	91 (84%)	18 (16%)	2	14
22	S	128/129 (99%)	105 (82%)	23 (18%)	1	11
23	T	117/118 (99%)	97 (83%)	20 (17%)	2	12
24	U	96/107 (90%)	83 (86%)	13 (14%)	4	19
25	V	73/73 (100%)	66 (90%)	7 (10%)	8	29
26	W	110/111 (99%)	102 (93%)	8 (7%)	14	40
27	X	119/120 (99%)	102 (86%)	17 (14%)	3	17
28	Y	108/109 (99%)	102 (94%)	6 (6%)	21	48
29	Z	60/88 (68%)	55 (92%)	5 (8%)	11	36
30	a	83/100 (83%)	71 (86%)	12 (14%)	3	17
31	b	71/72 (99%)	67 (94%)	4 (6%)	21	48
32	c	54/59 (92%)	48 (89%)	6 (11%)	6	24
33	d	46/48 (96%)	39 (85%)	7 (15%)	3	16
34	e	47/55 (86%)	39 (83%)	8 (17%)	2	13
35	f	57/133 (43%)	48 (84%)	9 (16%)	2	15
36	g	265/272 (97%)	231 (87%)	34 (13%)	4	20
37	h	23/23 (100%)	20 (87%)	3 (13%)	4	20
38	i	93/130 (72%)	74 (80%)	19 (20%)	1	7
39	j	224/274 (82%)	185 (83%)	39 (17%)	2	12
40	k	332/449 (74%)	306 (92%)	26 (8%)	12	38
41	l	119/246 (48%)	103 (87%)	16 (13%)	4	19
42	m	77/96 (80%)	64 (83%)	13 (17%)	2	13
43	o	411/444 (93%)	364 (89%)	47 (11%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	p	507/536 (95%)	469 (92%)	38 (8%)	13	39
45	q	297/301 (99%)	280 (94%)	17 (6%)	20	47
46	r	30/30 (100%)	27 (90%)	3 (10%)	7	28
47	s	43/43 (100%)	37 (86%)	6 (14%)	3	18
All	All	6242/7045 (89%)	5465 (88%)	777 (12%)	8	21

All (777) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	ARG
4	A	34	GLU
4	A	41	ARG
4	A	43	ASP
4	A	58	VAL
4	A	59	LEU
4	A	69	ASN
4	A	71	GLU
4	A	79	ARG
4	A	80	THR
4	A	84	ARG
4	A	93	THR
4	A	96	THR
4	A	108	THR
4	A	112	THR
4	A	113	ARG
4	A	119	ARG
4	A	120	LEU
4	A	122	ILE
4	A	143	VAL
4	A	165	ARG
4	A	167	LYS
4	A	170	ILE
4	A	192	THR
4	A	193	GLN
4	A	198	MET
4	A	205	ARG
5	B	22	ASP
5	B	28	GLU
5	B	47	LEU
5	B	64	ARG
5	B	68	VAL

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Mol	Chain	Res	Type
5	B	70	LEU
5	B	78	ASP
5	B	82	ARG
5	B	84	VAL
5	B	104	ASP
5	B	111	ARG
5	B	118	GLN
5	B	119	THR
5	B	125	VAL
5	B	127	VAL
5	B	140	ILE
5	B	170	GLU
5	B	181	LEU
5	B	189	ILE
5	B	196	GLU
5	B	205	PHE
5	B	208	GLN
5	B	219	LYS
5	B	228	LEU
6	C	58	ILE
6	C	71	PHE
6	C	72	GLN
6	C	78	LEU
6	C	83	ASP
6	C	86	MET
6	C	91	VAL
6	C	93	LYS
6	C	99	GLN
6	C	109	VAL
6	C	113	ASN
6	C	125	GLU
6	C	131	ARG
6	C	145	ARG
6	C	146	ARG
6	C	166	LYS
6	C	199	GLU
6	C	223	ILE
6	C	234	LEU
6	C	235	TRP
6	C	236	GLU
6	C	240	LEU
6	C	246	ASP

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Mol	Chain	Res	Type
7	D	4	ILE
7	D	5	ILE
7	D	6	SER
7	D	16	VAL
7	D	20	GLU
7	D	31	GLU
7	D	57	ASP
7	D	68	GLU
7	D	69	LEU
7	D	70	THR
7	D	75	LYS
7	D	76	ARG
7	D	93	ASP
7	D	94	ARG
7	D	103	GLU
7	D	109	LEU
7	D	113	LEU
7	D	116	ARG
7	D	122	VAL
7	D	128	GLU
7	D	132	LYS
7	D	146	ARG
7	D	148	LYS
7	D	158	ILE
7	D	168	ILE
7	D	173	ARG
7	D	176	LEU
7	D	200	LYS
7	D	204	ASP
7	D	209	ILE
7	D	212	LYS
7	D	213	GLU
7	D	214	GLU
8	E	7	LYS
8	E	9	LEU
8	E	18	TRP
8	E	21	ASP
8	E	22	LYS
8	E	23	LEU
8	E	38	LEU
8	E	44	LEU
8	E	51	ARG

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Mol	Chain	Res	Type
8	E	60	GLU
8	E	65	LEU
8	E	68	ARG
8	E	75	LYS
8	E	77	ARG
8	E	79	ASP
8	E	102	VAL
8	E	104	ASP
8	E	108	ARG
8	E	113	ARG
8	E	117	GLU
8	E	125	LYS
8	E	133	LYS
8	E	147	ILE
8	E	168	THR
8	E	180	LEU
8	E	181	VAL
8	E	189	LEU
8	E	198	ARG
8	E	201	HIS
8	E	206	ASP
8	E	208	VAL
8	E	220	THR
8	E	221	ARG
8	E	225	VAL
8	E	233	ARG
8	E	248	ILE
8	E	259	HIS
9	F	31	ILE
9	F	34	GLU
9	F	37	GLN
9	F	42	ILE
9	F	50	PHE
9	F	54	GLU
9	F	62	ASP
9	F	70	ILE
9	F	72	VAL
9	F	83	ARG
9	F	86	LYS
9	F	88	GLN
9	F	91	ILE
9	F	98	SER

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Mol	Chain	Res	Type
9	F	104	ARG
9	F	108	LYS
9	F	111	LYS
9	F	132	LEU
9	F	163	ASP
9	F	164	VAL
9	F	168	ARG
9	F	174	ILE
9	F	177	LEU
9	F	178	THR
9	F	186	PHE
9	F	187	ARG
9	F	189	ILE
9	F	194	GLU
9	F	199	GLU
9	F	209	THR
9	F	216	LYS
9	F	221	ARG
9	F	224	LYS
9	F	226	ASN
10	G	15	CYS
10	G	21	GLU
10	G	26	VAL
10	G	39	GLU
10	G	52	ILE
10	G	76	LEU
10	G	95	LYS
10	G	121	ILE
10	G	127	ASP
10	G	151	ASP
10	G	164	LYS
10	G	169	TYR
10	G	170	THR
10	G	176	GLN
10	G	180	THR
10	G	195	ILE
10	G	215	ARG
10	G	220	LYS
11	H	5	GLN
11	H	7	LYS
11	H	11	GLN
11	H	15	GLU

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Mol	Chain	Res	Type
11	H	19	GLN
11	H	27	LEU
11	H	33	GLU
11	H	37	ASP
11	H	38	LEU
11	H	48	GLU
11	H	72	LYS
11	H	74	GLN
11	H	80	GLU
11	H	86	GLN
11	H	91	ILE
11	H	104	ARG
11	H	111	LYS
11	H	112	ARG
11	H	116	ARG
11	H	122	HIS
11	H	124	LYS
11	H	129	LEU
11	H	139	ARG
11	H	162	ILE
11	H	180	GLN
11	H	184	GLU
12	I	20	GLN
12	I	24	LYS
12	I	26	LYS
12	I	29	LEU
12	I	47	ARG
12	I	53	GLN
12	I	72	VAL
12	I	96	LEU
12	I	104	ILE
12	I	119	GLN
12	I	153	ILE
12	I	190	LEU
12	I	196	ARG
12	I	201	LYS
13	J	8	TYR
13	J	10	LYS
13	J	20	GLU
13	J	25	ASP
13	J	28	LEU
13	J	33	GLU

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Mol	Chain	Res	Type
13	J	37	LYS
13	J	40	ARG
13	J	49	LEU
13	J	63	ASP
13	J	64	GLU
13	J	69	ARG
13	J	83	ILE
13	J	100	LYS
13	J	107	ARG
13	J	127	VAL
13	J	131	GLN
13	J	161	THR
14	K	2	LEU
14	K	9	LYS
14	K	13	GLN
14	K	15	LEU
14	K	20	VAL
14	K	21	LEU
14	K	29	GLN
14	K	34	GLU
14	K	44	LYS
14	K	47	GLN
14	K	55	VAL
14	K	57	THR
14	K	64	TYR
14	K	71	GLU
14	K	75	TYR
14	K	76	LEU
14	K	85	HIS
14	K	91	TYR
15	L	5	LEU
15	L	10	GLU
15	L	36	LYS
15	L	55	ASP
15	L	80	MET
15	L	84	ILE
15	L	118	GLN
15	L	124	THR
16	M	22	LYS
16	M	26	ARG
16	M	52	LEU
16	M	61	GLU

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Mol	Chain	Res	Type
16	M	67	LEU
16	M	91	TRP
16	M	97	ILE
16	M	100	ASP
16	M	117	TRP
16	M	123	GLU
16	M	125	GLU
17	N	3	ARG
17	N	16	ILE
17	N	20	ARG
17	N	27	LYS
17	N	53	LEU
17	N	64	LYS
17	N	70	LYS
17	N	83	GLU
17	N	84	ILE
17	N	86	GLU
17	N	88	LEU
17	N	96	VAL
17	N	99	ARG
17	N	100	LYS
17	N	107	LYS
17	N	112	LYS
17	N	121	ARG
17	N	125	LEU
17	N	141	TYR
18	O	29	HIS
18	O	49	LYS
18	O	65	GLN
18	O	92	LYS
18	O	102	LEU
18	O	110	LEU
18	O	114	ARG
18	O	121	VAL
19	P	13	LYS
19	P	21	ASP
19	P	25	LEU
19	P	56	LEU
19	P	57	MET
19	P	71	GLU
19	P	72	LYS
19	P	76	VAL

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Mol	Chain	Res	Type
19	P	79	HIS
19	P	82	ASN
19	P	85	ILE
19	P	101	VAL
19	P	106	GLU
19	P	108	ARG
19	P	111	MET
19	P	122	THR
19	P	123	TYR
20	Q	13	LYS
20	Q	28	LEU
20	Q	37	THR
20	Q	38	LEU
20	Q	45	ARG
20	Q	46	PHE
20	Q	47	LYS
20	Q	68	LYS
20	Q	74	HIS
20	Q	82	ARG
20	Q	83	GLN
20	Q	89	LEU
20	Q	100	GLN
20	Q	105	LEU
20	Q	132	ARG
20	Q	137	ARG
20	Q	139	GLN
20	Q	143	ARG
21	R	3	ARG
21	R	5	ARG
21	R	6	THR
21	R	9	VAL
21	R	10	LYS
21	R	28	PHE
21	R	33	ARG
21	R	37	GLU
21	R	45	ARG
21	R	47	ARG
21	R	48	ASN
21	R	63	LYS
21	R	82	ASP
21	R	83	GLN
21	R	100	LEU

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Mol	Chain	Res	Type
21	R	102	VAL
21	R	103	ASP
21	R	117	LEU
22	S	6	GLN
22	S	20	THR
22	S	25	ASN
22	S	35	ILE
22	S	52	VAL
22	S	54	LEU
22	S	57	ARG
22	S	73	MET
22	S	78	HIS
22	S	84	TRP
22	S	86	LEU
22	S	91	ASP
22	S	97	ASP
22	S	99	HIS
22	S	105	LEU
22	S	111	ASP
22	S	114	GLU
22	S	115	ARG
22	S	120	ARG
22	S	122	HIS
22	S	126	ARG
22	S	136	GLN
22	S	144	ARG
23	T	8	ASP
23	T	16	ASN
23	T	25	GLN
23	T	37	VAL
23	T	45	LEU
23	T	64	HIS
23	T	65	ILE
23	T	85	ASN
23	T	86	ARG
23	T	91	HIS
23	T	95	ASP
23	T	103	LYS
23	T	106	GLN
23	T	107	SER
23	T	124	ILE
23	T	126	ASP

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Mol	Chain	Res	Type
23	T	131	ASP
23	T	132	LEU
23	T	142	ASP
23	T	144	GLU
24	U	34	LEU
24	U	35	GLU
24	U	37	VAL
24	U	41	ILE
24	U	57	ARG
24	U	67	THR
24	U	72	ASN
24	U	80	ASP
24	U	83	GLU
24	U	98	HIS
24	U	109	GLU
24	U	117	ILE
24	U	118	ILE
25	V	1	MET
25	V	7	GLN
25	V	8	LEU
25	V	12	TYR
25	V	44	ARG
25	V	76	ASP
25	V	80	LYS
26	W	7	LEU
26	W	24	GLN
26	W	25	VAL
26	W	26	LEU
26	W	31	SER
26	W	47	ILE
26	W	80	ASN
26	W	111	MET
27	X	14	LYS
27	X	17	VAL
27	X	19	ARG
27	X	30	LYS
27	X	54	LEU
27	X	55	GLU
27	X	79	ASN
27	X	83	VAL
27	X	84	THR
27	X	94	ASN

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Mol	Chain	Res	Type
27	X	97	ASP
27	X	98	GLU
27	X	107	PHE
27	X	117	ILE
27	X	127	VAL
27	X	133	LEU
27	X	144	ARG
28	Y	8	ARG
28	Y	13	ILE
28	Y	35	VAL
28	Y	84	LYS
28	Y	99	LYS
28	Y	121	THR
29	Z	38	HIS
29	Z	44	GLN
29	Z	70	LYS
29	Z	71	LEU
29	Z	84	GLU
30	a	12	LYS
30	a	15	ARG
30	a	19	LYS
30	a	28	ARG
30	a	30	VAL
30	a	34	LYS
30	a	38	ARG
30	a	46	GLU
30	a	53	LEU
30	a	64	LEU
30	a	69	ASN
30	a	75	ILE
31	b	3	LEU
31	b	20	LYS
31	b	57	GLU
31	b	67	THR
32	c	9	LEU
32	c	31	GLU
32	c	43	ASN
32	c	49	ARG
32	c	54	LEU
32	c	65	ARG
33	d	4	GLU
33	d	20	GLN

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Mol	Chain	Res	Type
33	d	21	CYS
33	d	22	ARG
33	d	30	LEU
33	d	34	TYR
33	d	38	ILE
34	e	17	GLN
34	e	22	GLU
34	e	24	GLN
34	e	33	ARG
34	e	38	LEU
34	e	39	LEU
34	e	49	LEU
34	e	54	ARG
35	f	85	TYR
35	f	91	ILE
35	f	92	ARG
35	f	100	LEU
35	f	108	VAL
35	f	109	ASP
35	f	119	LYS
35	f	129	PHE
35	f	138	TYR
36	g	6	ILE
36	g	8	LEU
36	g	11	ARG
36	g	13	THR
36	g	18	ASN
36	g	20	TRP
36	g	33	LEU
36	g	39	ARG
36	g	43	LEU
36	g	55	PHE
36	g	67	HIS
36	g	70	GLN
36	g	124	ILE
36	g	128	ARG
36	g	129	ASP
36	g	146	LEU
36	g	188	LEU
36	g	198	ASP
36	g	205	TYR
36	g	206	ILE

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Mol	Chain	Res	Type
36	g	210	GLN
36	g	224	ASP
36	g	234	HIS
36	g	238	PHE
36	g	244	LYS
36	g	246	GLU
36	g	256	ARG
36	g	276	VAL
36	g	280	GLU
36	g	284	GLU
36	g	289	THR
36	g	314	ASP
36	g	321	GLN
36	g	323	MET
37	h	5	TRP
37	h	9	ARG
37	h	12	ARG
38	i	18	ASP
38	i	24	ARG
38	i	26	LEU
38	i	27	ILE
38	i	34	GLU
38	i	41	MET
38	i	52	PHE
38	i	58	MET
38	i	62	ARG
38	i	69	VAL
38	i	70	TRP
38	i	82	ARG
38	i	91	VAL
38	i	97	LEU
38	i	101	ARG
38	i	103	LEU
38	i	105	ASN
38	i	111	GLU
38	i	112	ASN
39	j	6	CYS
39	j	7	ARG
39	j	11	ASN
39	j	15	GLU
39	j	17	ASP
39	j	18	ASP

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Mol	Chain	Res	Type
39	j	19	ILE
39	j	23	ASN
39	j	33	TYR
39	j	39	TYR
39	j	42	ILE
39	j	45	MET
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	79	GLU
39	j	87	LYS
39	j	90	VAL
39	j	96	ILE
39	j	97	LYS
39	j	114	TYR
39	j	119	PHE
39	j	129	THR
39	j	143	GLU
39	j	159	GLU
39	j	163	LYS
39	j	164	ASP
39	j	166	LEU
39	j	169	LEU
39	j	185	ARG
39	j	195	TYR
39	j	203	ASP
39	j	230	LEU
39	j	235	LEU
39	j	236	ASP
39	j	244	LEU
39	j	251	ILE
39	j	261	VAL
39	j	264	ILE
40	k	130	ASP
40	k	132	LEU
40	k	224	CYS
40	k	228	GLN
40	k	236	ILE
40	k	253	LEU
40	k	257	GLU
40	k	291	ILE
40	k	307	ARG

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Mol	Chain	Res	Type
40	k	332	ASP
40	k	354	GLU
40	k	359	ILE
40	k	395	LEU
40	k	402	VAL
40	k	403	ASP
40	k	406	LEU
40	k	426	ILE
40	k	432	ILE
40	k	438	ARG
40	k	440	LEU
40	k	443	VAL
40	k	462	LEU
40	k	495	ILE
40	k	502	SER
40	k	508	HIS
40	k	512	ILE
41	l	131	TYR
41	l	135	LEU
41	l	141	ILE
41	l	157	LYS
41	l	159	ARG
41	l	161	PRO
41	l	166	LEU
41	l	167	ARG
41	l	171	LYS
41	l	172	THR
41	l	177	ILE
41	l	189	GLU
41	l	213	ILE
41	l	229	TYR
41	l	246	LEU
41	l	257	MET
42	m	22	THR
42	m	39	LEU
42	m	40	THR
42	m	62	PHE
42	m	65	ASN
42	m	68	ILE
42	m	71	ASP
42	m	74	MET
42	m	87	LYS

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Mol	Chain	Res	Type
42	m	92	MET
42	m	98	LEU
42	m	103	ILE
42	m	104	LYS
43	o	6	PHE
43	o	9	GLU
43	o	16	ASP
43	o	39	ARG
43	o	41	ARG
43	o	73	HIS
43	o	79	ILE
43	o	104	ILE
43	o	109	THR
43	o	114	LEU
43	o	120	ASP
43	o	151	ILE
43	o	154	TRP
43	o	168	LEU
43	o	169	LEU
43	o	170	ARG
43	o	183	VAL
43	o	186	THR
43	o	188	HIS
43	o	190	CYS
43	o	199	PHE
43	o	211	ASP
43	o	223	ASN
43	o	235	ARG
43	o	265	HIS
43	o	268	LYS
43	o	278	THR
43	o	279	LEU
43	o	282	TYR
43	o	284	GLU
43	o	298	LEU
43	o	303	TRP
43	o	329	PHE
43	o	351	MET
43	o	354	LEU
43	o	365	GLU
43	o	387	LEU
43	o	407	LEU

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Mol	Chain	Res	Type
43	o	415	THR
43	o	416	TYR
43	o	420	TYR
43	o	424	LEU
43	o	426	ASP
43	o	443	VAL
43	o	476	ASP
43	o	478	VAL
43	o	480	ILE
44	p	195	TYR
44	p	251	GLN
44	p	253	ASP
44	p	257	ARG
44	p	275	LEU
44	p	297	LEU
44	p	315	ILE
44	p	317	GLN
44	p	335	THR
44	p	336	ILE
44	p	354	GLU
44	p	374	GLU
44	p	388	ASP
44	p	404	ILE
44	p	409	LEU
44	p	413	LEU
44	p	416	GLU
44	p	438	ASP
44	p	462	GLN
44	p	467	PHE
44	p	480	ASP
44	p	540	GLN
44	p	559	LEU
44	p	561	GLU
44	p	608	TYR
44	p	611	HIS
44	p	616	LEU
44	p	644	ARG
44	p	659	TYR
44	p	663	SER
44	p	671	LEU
44	p	681	SER
44	p	707	GLU

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Mol	Chain	Res	Type
44	p	722	LEU
44	p	733	TYR
44	p	744	LEU
44	p	750	ASN
44	p	793	LYS
45	q	7	THR
45	q	40	LEU
45	q	47	THR
45	q	49	ASP
45	q	79	TRP
45	q	80	ASP
45	q	100	GLU
45	q	101	PHE
45	q	108	PHE
45	q	135	GLU
45	q	138	LYS
45	q	157	THR
45	q	193	ASP
45	q	201	ASP
45	q	264	THR
45	q	308	TYR
45	q	329	PHE
46	r	704	LEU
46	r	708	GLU
46	r	725	GLU
47	s	58	TYR
47	s	61	GLU
47	s	82	ARG
47	s	85	ARG
47	s	86	ASN
47	s	96	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	30	GLN
4	A	33	GLN
4	A	46	ASN
4	A	109	ASN
4	A	131	GLN
4	A	140	ASN
5	B	101	HIS

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Mol	Chain	Res	Type
5	B	148	ASN
5	B	183	GLN
6	C	64	HIS
6	C	72	GLN
6	C	76	GLN
6	C	87	ASN
6	C	92	GLN
6	C	99	GLN
6	C	194	GLN
6	C	225	ASN
6	C	233	ASN
8	E	69	HIS
8	E	188	ASN
9	F	37	GLN
9	F	65	GLN
9	F	81	ASN
9	F	105	ASN
9	F	172	GLN
9	F	188	ASN
10	G	4	ASN
10	G	10	ASN
10	G	13	GLN
11	H	19	GLN
11	H	110	GLN
12	I	53	GLN
15	L	8	GLN
15	L	118	GLN
17	N	36	GLN
17	N	49	GLN
17	N	58	HIS
17	N	105	ASN
18	O	80	HIS
20	Q	83	GLN
21	R	48	ASN
22	S	13	HIS
22	S	21	ASN
22	S	25	ASN
22	S	75	ASN
22	S	99	HIS
23	T	43	ASN
24	U	72	ASN
25	V	33	GLN

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Mol	Chain	Res	Type
25	V	70	ASN
26	W	24	GLN
27	X	22	ASN
27	X	48	HIS
27	X	79	ASN
31	b	51	GLN
33	d	10	HIS
33	d	41	GLN
36	g	161	ASN
38	i	37	GLN
38	i	44	ASN
38	i	60	HIS
38	i	85	GLN
40	k	98	GLN
40	k	248	GLN
40	k	415	GLN
40	k	508	HIS
41	l	176	ASN
41	l	190	HIS
41	l	243	ASN
42	m	67	ASN
42	m	79	GLN
43	o	32	HIS
43	o	194	GLN
43	o	209	HIS
43	o	216	GLN
43	o	242	GLN
43	o	254	HIS
43	o	299	HIS
43	o	348	HIS
43	o	403	GLN
44	p	582	GLN
44	p	683	GLN
45	q	9	HIS
45	q	195	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	32 (43%)	7 (9%)
2	2	1778/1781 (99%)	879 (49%)	146 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	13/25 (52%)	11 (84%)	1 (7%)
All	All	1865/1881 (99%)	922 (49%)	154 (8%)

All (922) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	G
1	1	10	G
1	1	14	A
1	1	15	G
1	1	16	U
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A
1	1	22	G
1	1	23	C
1	1	25	C
1	1	28	A
1	1	34	C
1	1	40	C
1	1	41	C
1	1	44	A
1	1	45	U
1	1	46	G
1	1	48	C
1	1	49	C
1	1	52	G
1	1	56	C
1	1	59	A
1	1	60	A
1	1	61	C
1	1	63	G
1	1	69	C
1	1	71	C
1	1	75	C
1	1	76	A
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U

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Mol	Chain	Res	Type
2	2	9	U
2	2	11	A
2	2	14	C
2	2	16	G
2	2	17	C
2	2	19	A
2	2	20	G
2	2	24	U
2	2	25	C
2	2	26	A
2	2	27	U
2	2	29	U
2	2	30	G
2	2	31	C
2	2	34	G
2	2	35	U
2	2	36	C
2	2	37	U
2	2	39	A
2	2	40	A
2	2	42	G
2	2	43	A
2	2	44	U
2	2	45	U
2	2	47	A
2	2	51	A
2	2	54	C
2	2	56	U
2	2	57	G
2	2	59	C
2	2	60	U
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U

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Mol	Chain	Res	Type
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	81	G
2	2	87	C
2	2	92	A
2	2	95	G
2	2	104	A
2	2	111	U
2	2	114	C
2	2	115	G
2	2	123	G
2	2	124	A
2	2	125	U
2	2	127	G
2	2	128	U
2	2	129	U
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	141	U
2	2	144	A
2	2	146	A
2	2	147	U
2	2	148	C
2	2	149	U
2	2	150	G
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	161	A
2	2	167	A
2	2	169	U
2	2	172	A

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Mol	Chain	Res	Type
2	2	173	U
2	2	176	U
2	2	177	U
2	2	178	A
2	2	183	C
2	2	185	C
2	2	186	G
2	2	187	A
2	2	190	C
2	2	191	U
2	2	192	U
2	2	193	U
2	2	194	G
2	2	195	G
2	2	198	G
2	2	199	A
2	2	203	G
2	2	209	A
2	2	214	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	226	U
2	2	227	G
2	2	228	U
2	2	230	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	237	U
2	2	239	C
2	2	240	U
2	2	245	G
2	2	248	U
2	2	249	C
2	2	254	U
2	2	256	A
2	2	259	U
2	2	264	A
2	2	265	A
2	2	266	U

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Mol	Chain	Res	Type
2	2	268	G
2	2	270	A
2	2	274	C
2	2	275	C
2	2	276	U
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	286	G
2	2	288	U
2	2	289	G
2	2	294	A
2	2	298	A
2	2	301	U
2	2	307	C
2	2	308	C
2	2	311	A
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	319	U
2	2	320	C
2	2	321	G
2	2	322	A
2	2	332	A
2	2	336	G
2	2	337	C
2	2	345	G
2	2	349	U
2	2	350	C
2	2	351	A
2	2	358	A
2	2	359	A
2	2	360	C
2	2	368	A
2	2	371	G
2	2	372	G
2	2	377	A
2	2	380	C

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Mol	Chain	Res	Type
2	2	382	G
2	2	384	A
2	2	388	G
2	2	389	G
2	2	390	A
2	2	395	G
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	403	G
2	2	404	C
2	2	406	A
2	2	409	A
2	2	411	A
2	2	412	U
2	2	413	C
2	2	415	A
2	2	416	A
2	2	417	G
2	2	418	G
2	2	420	A
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	426	C
2	2	433	G
2	2	438	U
2	2	439	U
2	2	440	A
2	2	443	C
2	2	447	C
2	2	448	C
2	2	452	U
2	2	454	C
2	2	455	A
2	2	456	G
2	2	457	G
2	2	458	G
2	2	459	A

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Mol	Chain	Res	Type
2	2	461	G
2	2	467	A
2	2	468	C
2	2	473	A
2	2	475	U
2	2	479	G
2	2	480	A
2	2	482	A
2	2	483	C
2	2	487	G
2	2	488	C
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	497	G
2	2	499	C
2	2	500	U
2	2	501	U
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	511	A
2	2	512	U
2	2	513	G
2	2	515	G
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	521	U
2	2	522	G
2	2	523	U
2	2	525	A
2	2	527	U
2	2	530	C
2	2	531	U
2	2	533	A

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Mol	Chain	Res	Type
2	2	534	A
2	2	535	C
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	544	A
2	2	545	C
2	2	547	G
2	2	550	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	559	U
2	2	560	G
2	2	564	C
2	2	565	C
2	2	566	A
2	2	567	G
2	2	568	C
2	2	569	A
2	2	570	G
2	2	571	C
2	2	573	G
2	2	574	C
2	2	576	G
2	2	577	U
2	2	578	A
2	2	579	A
2	2	580	U
2	2	581	U
2	2	584	A
2	2	586	C
2	2	589	C
2	2	590	A
2	2	593	A
2	2	594	G

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Mol	Chain	Res	Type
2	2	597	U
2	2	599	U
2	2	600	A
2	2	601	U
2	2	605	A
2	2	610	U
2	2	612	G
2	2	613	C
2	2	614	A
2	2	615	G
2	2	616	U
2	2	617	U
2	2	618	A
2	2	619	A
2	2	621	A
2	2	622	A
2	2	624	C
2	2	634	A
2	2	638	U
2	2	641	G
2	2	647	G
2	2	649	U
2	2	651	U
2	2	652	C
2	2	653	C
2	2	654	G
2	2	655	G
2	2	657	C
2	2	677	G
2	2	678	U
2	2	680	U
2	2	681	U
2	2	684	A
2	2	685	A
2	2	686	C
2	2	687	C
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U

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Mol	Chain	Res	Type
2	2	700	C
2	2	701	U
2	2	702	G
2	2	703	G
2	2	704	C
2	2	705	U
2	2	706	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	713	A
2	2	714	C
2	2	715	U
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	723	G
2	2	725	U
2	2	727	C
2	2	729	G
2	2	731	C
2	2	732	G
2	2	733	A
2	2	734	A
2	2	735	C
2	2	736	C
2	2	738	G
2	2	741	C
2	2	742	U
2	2	743	U
2	2	744	U
2	2	745	U
2	2	753	A
2	2	755	A
2	2	762	A
2	2	763	G
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C

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Mol	Chain	Res	Type
2	2	771	A
2	2	774	A
2	2	775	G
2	2	778	G
2	2	779	A
2	2	780	A
2	2	781	A
2	2	783	C
2	2	784	U
2	2	785	C
2	2	788	A
2	2	790	A
2	2	793	U
2	2	794	U
2	2	796	G
2	2	803	A
2	2	805	A
2	2	806	A
2	2	809	G
2	2	811	A
2	2	812	U
2	2	813	A
2	2	814	G
2	2	817	C
2	2	819	U
2	2	820	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	832	U
2	2	834	U
2	2	836	G
2	2	837	G
2	2	839	U
2	2	840	U
2	2	841	C
2	2	845	G
2	2	847	C

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Mol	Chain	Res	Type
2	2	851	C
2	2	855	A
2	2	856	U
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	864	A
2	2	872	U
2	2	875	G
2	2	883	A
2	2	885	U
2	2	886	A
2	2	895	U
2	2	896	C
2	2	897	A
2	2	898	G
2	2	904	A
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	919	U
2	2	920	U
2	2	925	A
2	2	927	U
2	2	930	C
2	2	931	U
2	2	932	A
2	2	934	U
2	2	936	C
2	2	938	A
2	2	939	A
2	2	941	G
2	2	944	U
2	2	946	U
2	2	947	G

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Mol	Chain	Res	Type
2	2	950	A
2	2	956	G
2	2	957	U
2	2	958	U
2	2	959	U
2	2	962	A
2	2	965	A
2	2	970	A
2	2	978	A
2	2	981	U
2	2	982	A
2	2	983	G
2	2	987	A
2	2	991	A
2	2	992	A
2	2	993	G
2	2	994	A
2	2	995	U
2	2	996	G
2	2	998	U
2	2	999	C
2	2	1000	A
2	2	1003	U
2	2	1004	A
2	2	1007	G
2	2	1008	U
2	2	1009	C
2	2	1012	A
2	2	1013	G
2	2	1015	C
2	2	1018	A
2	2	1020	C
2	2	1022	A
2	2	1023	U
2	2	1024	A
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A

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Mol	Chain	Res	Type
2	2	1039	G
2	2	1041	G
2	2	1042	A
2	2	1043	U
2	2	1046	G
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1060	U
2	2	1062	U
2	2	1064	A
2	2	1065	C
2	2	1066	C
2	2	1069	C
2	2	1070	U
2	2	1075	A
2	2	1076	C
2	2	1077	C
2	2	1079	U
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1086	A
2	2	1089	C
2	2	1090	A
2	2	1091	A
2	2	1092	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1098	U
2	2	1099	G

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Mol	Chain	Res	Type
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1107	G
2	2	1108	G
2	2	1110	G
2	2	1111	G
2	2	1112	A
2	2	1113	G
2	2	1114	U
2	2	1117	G
2	2	1118	G
2	2	1123	A
2	2	1125	G
2	2	1133	C
2	2	1135	U
2	2	1136	A
2	2	1137	A
2	2	1138	A
2	2	1145	G
2	2	1149	G
2	2	1150	A
2	2	1154	G
2	2	1155	C
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1163	G
2	2	1164	G
2	2	1166	G
2	2	1168	G
2	2	1169	G
2	2	1172	C
2	2	1174	U
2	2	1175	G
2	2	1176	C
2	2	1184	U
2	2	1185	U
2	2	1186	U
2	2	1188	A
2	2	1189	C

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Mol	Chain	Res	Type
2	2	1190	U
2	2	1191	C
2	2	1192	A
2	2	1193	A
2	2	1195	A
2	2	1196	C
2	2	1197	G
2	2	1198	G
2	2	1199	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1206	C
2	2	1207	A
2	2	1211	G
2	2	1213	U
2	2	1216	A
2	2	1217	G
2	2	1218	A
2	2	1224	U
2	2	1225	A
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1237	A
2	2	1240	G
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1247	C
2	2	1250	U
2	2	1254	G
2	2	1255	A
2	2	1256	U
2	2	1258	U
2	2	1259	U
2	2	1260	G
2	2	1268	U
2	2	1272	G
2	2	1273	C
2	2	1275	U
2	2	1282	U

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Mol	Chain	Res	Type
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1286	A
2	2	1287	G
2	2	1292	U
2	2	1294	G
2	2	1295	A
2	2	1296	G
2	2	1298	G
2	2	1300	U
2	2	1303	G
2	2	1305	C
2	2	1306	U
2	2	1309	U
2	2	1311	A
2	2	1312	A
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1317	G
2	2	1320	A
2	2	1321	A
2	2	1324	A
2	2	1332	C
2	2	1336	A
2	2	1337	C
2	2	1338	C
2	2	1339	U
2	2	1340	A
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1346	U
2	2	1347	A
2	2	1348	G
2	2	1352	U
2	2	1353	G
2	2	1357	G
2	2	1358	C
2	2	1359	A

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Mol	Chain	Res	Type
2	2	1361	U
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1366	G
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1374	C
2	2	1376	U
2	2	1377	C
2	2	1380	A
2	2	1381	G
2	2	1383	G
2	2	1386	A
2	2	1387	C
2	2	1388	U
2	2	1389	A
2	2	1390	U
2	2	1393	G
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1408	A
2	2	1409	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1416	G
2	2	1417	G
2	2	1418	C
2	2	1419	A
2	2	1420	A
2	2	1423	A
2	2	1425	A
2	2	1426	G
2	2	1428	U
2	2	1429	C
2	2	1430	U
2	2	1431	G

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Mol	Chain	Res	Type
2	2	1433	G
2	2	1434	A
2	2	1435	U
2	2	1442	A
2	2	1444	A
2	2	1448	U
2	2	1449	C
2	2	1450	U
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1458	A
2	2	1459	C
2	2	1461	C
2	2	1465	C
2	2	1466	U
2	2	1467	A
2	2	1469	A
2	2	1470	C
2	2	1471	U
2	2	1476	G
2	2	1478	G
2	2	1479	C
2	2	1480	C
2	2	1481	A
2	2	1482	G
2	2	1484	G
2	2	1487	U
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1496	G
2	2	1498	C
2	2	1499	C
2	2	1501	A
2	2	1504	G
2	2	1512	U
2	2	1513	A
2	2	1514	A

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Mol	Chain	Res	Type
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1528	C
2	2	1529	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1537	G
2	2	1538	G
2	2	1540	G
2	2	1544	G
2	2	1554	A
2	2	1555	U
2	2	1557	A
2	2	1558	U
2	2	1559	U
2	2	1566	C
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1574	A
2	2	1575	A
2	2	1578	C
2	2	1579	C
2	2	1580	U
2	2	1581	A
2	2	1582	G
2	2	1583	U
2	2	1584	A
2	2	1588	G
2	2	1590	A
2	2	1593	U
2	2	1594	C
2	2	1597	C
2	2	1598	A
2	2	1599	G

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Mol	Chain	Res	Type
2	2	1604	C
2	2	1608	G
2	2	1611	U
2	2	1612	A
2	2	1613	C
2	2	1614	G
2	2	1616	C
2	2	1631	A
2	2	1632	C
2	2	1633	A
2	2	1634	C
2	2	1635	C
2	2	1636	G
2	2	1637	C
2	2	1638	C
2	2	1648	U
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1667	U
2	2	1678	G
2	2	1679	A
2	2	1682	U
2	2	1685	U
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1699	A
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1705	A
2	2	1706	U
2	2	1707	C

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Mol	Chain	Res	Type
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1719	A
2	2	1725	G
2	2	1728	A
2	2	1730	A
2	2	1742	A
2	2	1743	G
2	2	1748	A
2	2	1750	U
2	2	1753	A
2	2	1754	A
2	2	1758	G
2	2	1763	A
2	2	1764	A
2	2	1765	G
2	2	1766	G
2	2	1767	U
2	2	1768	U
2	2	1778	G
2	2	1779	A
2	2	1781	C
2	2	1782	C
2	2	1786	G
2	2	1787	G
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1794	C
2	2	1795	A
2	2	1796	U
2	2	1797	U
2	2	1798	A
3	3	4	U
3	3	5	C
3	3	6	U
3	3	7	C
3	3	8	U
3	3	9	C
3	3	10	U

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Mol	Chain	Res	Type
3	3	11	C
3	3	12	U
3	3	13	A
3	3	16	C

All (154) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	7	G
1	1	43	G
1	1	44	A
1	1	47	U
1	1	48	C
1	1	59	A
1	1	74	C
2	2	42	G
2	2	46	A
2	2	66	U
2	2	68	A
2	2	72	A
2	2	73	U
2	2	74	U
2	2	103	A
2	2	115	G
2	2	126	A
2	2	129	U
2	2	130	C
2	2	131	C
2	2	133	U
2	2	134	U
2	2	140	A
2	2	157	U
2	2	177	U
2	2	186	G
2	2	190	C
2	2	193	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	248	U
2	2	258	U
2	2	265	A

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Mol	Chain	Res	Type
2	2	277	U
2	2	278	G
2	2	279	U
2	2	294	A
2	2	312	U
2	2	320	C
2	2	321	G
2	2	344	U
2	2	349	U
2	2	368	A
2	2	388	G
2	2	389	G
2	2	403	G
2	2	451	A
2	2	473	A
2	2	497	G
2	2	517	A
2	2	538	G
2	2	540	A
2	2	542	C
2	2	554	A
2	2	564	C
2	2	570	G
2	2	588	C
2	2	589	C
2	2	593	A
2	2	600	A
2	2	617	U
2	2	620	A
2	2	654	G
2	2	685	A
2	2	693	U
2	2	695	U
2	2	700	C
2	2	704	C
2	2	721	U
2	2	736	C
2	2	781	A
2	2	793	U
2	2	810	A
2	2	811	A
2	2	826	C

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Mol	Chain	Res	Type
2	2	828	A
2	2	854	A
2	2	855	A
2	2	860	U
2	2	896	C
2	2	907	U
2	2	938	A
2	2	946	U
2	2	956	G
2	2	986	G
2	2	995	U
2	2	998	U
2	2	1010	G
2	2	1030	U
2	2	1038	A
2	2	1056	U
2	2	1080	A
2	2	1089	C
2	2	1092	A
2	2	1095	C
2	2	1096	U
2	2	1099	G
2	2	1107	G
2	2	1110	G
2	2	1117	G
2	2	1136	A
2	2	1157	C
2	2	1188	A
2	2	1192	A
2	2	1194	C
2	2	1195	A
2	2	1196	C
2	2	1198	G
2	2	1202	A
2	2	1206	C
2	2	1225	A
2	2	1226	A
2	2	1283	C
2	2	1314	U
2	2	1315	G
2	2	1320	A
2	2	1343	A

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Mol	Chain	Res	Type
2	2	1345	A
2	2	1360	C
2	2	1363	G
2	2	1375	U
2	2	1389	A
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1416	G
2	2	1419	A
2	2	1423	A
2	2	1425	A
2	2	1430	U
2	2	1445	C
2	2	1455	C
2	2	1457	C
2	2	1465	C
2	2	1479	C
2	2	1481	A
2	2	1482	G
2	2	1489	C
2	2	1491	A
2	2	1533	U
2	2	1534	G
2	2	1571	A
2	2	1579	C
2	2	1580	U
2	2	1604	C
2	2	1613	C
2	2	1655	U
2	2	1678	G
2	2	1763	A
2	2	1765	G
2	2	1766	G
2	2	1792	A
3	3	10	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	GCP	k	603	48	27,34,34	1.96	8 (29%)	34,54,54	1.98	8 (23%)
50	MET	k	601	-	6,7,8	0.43	0	2,7,9	0.19	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
51	GCP	k	603	48	-	2/15/38/38	0/3/3/3
50	MET	k	601	-	-	1/5/6/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.43	1.61	1.50
51	k	603	GCP	C5-C6	4.82	1.49	1.41
51	k	603	GCP	PB-O3A	3.15	1.61	1.58
51	k	603	GCP	PG-O2G	2.86	1.61	1.54
51	k	603	GCP	C5-C4	2.82	1.48	1.40
51	k	603	GCP	PG-O3G	-2.78	1.48	1.54
51	k	603	GCP	PB-O2B	2.09	1.61	1.56
51	k	603	GCP	O4'-C1'	2.04	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.46	121.60	115.36
51	k	603	GCP	C2-N1-C6	4.11	122.46	115.93
51	k	603	GCP	C5-C6-N1	-3.86	118.16	123.43
51	k	603	GCP	C4-C5-C6	-3.77	117.20	120.80
51	k	603	GCP	N3-C2-N1	-3.63	122.38	127.22
51	k	603	GCP	PB-O3A-PA	-3.45	121.61	132.56
51	k	603	GCP	C3'-C2'-C1'	2.82	105.23	100.98
51	k	603	GCP	C4-C5-N7	-2.79	106.49	109.40

There are no chirality outliers.

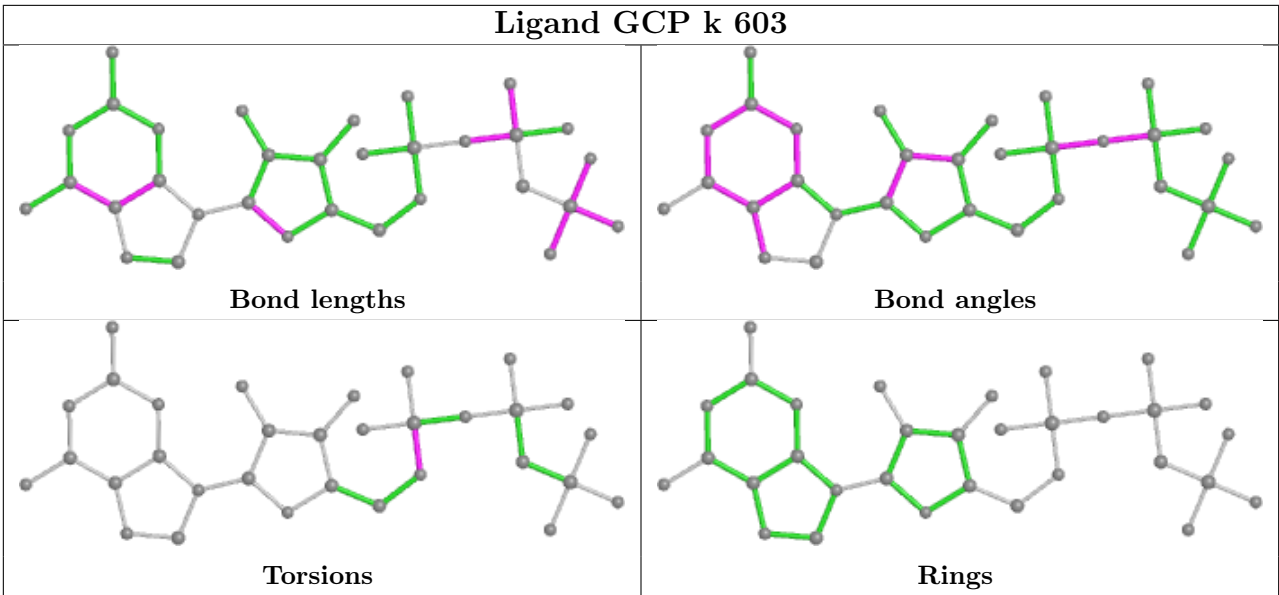
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	k	603	GCP	C5'-O5'-PA-O3A
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	C5'-O5'-PA-O1A

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	o	7
44	p	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	495:PRO	C	753:UNK	N	221.30
1	p	218:UNK	C	251:GLN	N	63.04
1	p	32:UNK	C	116:UNK	N	42.95
1	p	185:UNK	C	193:ARG	N	15.92
1	o	818:UNK	C	828:UNK	N	14.63
1	p	158:UNK	C	170:UNK	N	13.31
1	o	846:UNK	C	850:UNK	N	8.27
1	o	769:UNK	C	772:UNK	N	6.84
1	p	135:UNK	C	139:UNK	N	5.98
1	o	802:UNK	C	806:UNK	N	4.31
1	o	834:UNK	C	837:UNK	N	4.08
1	o	785:UNK	C	788:UNK	N	3.70

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	206:SER	C	211:UNK	N	3.67
1	p	148:UNK	C	150:UNK	N	3.24

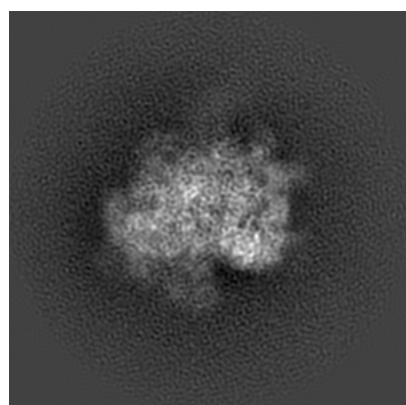
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3048. These allow visual inspection of the internal detail of the map and identification of artifacts.

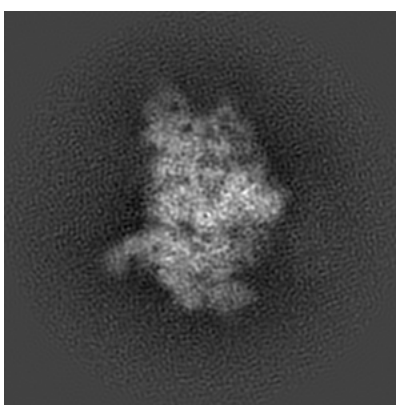
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

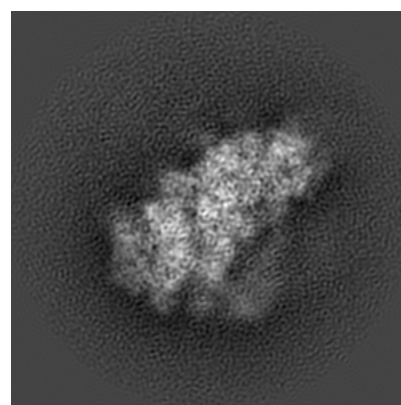
6.1.1 Primary map



X



Y

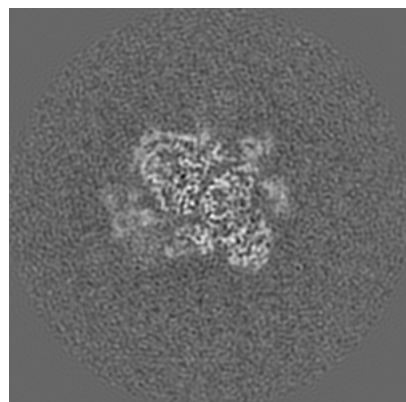


Z

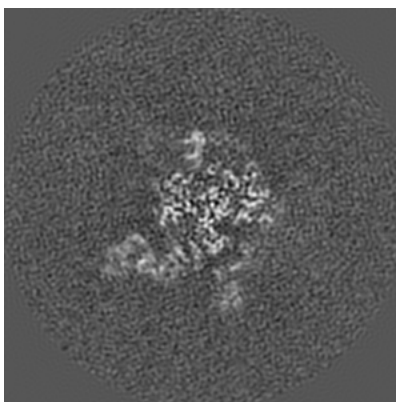
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

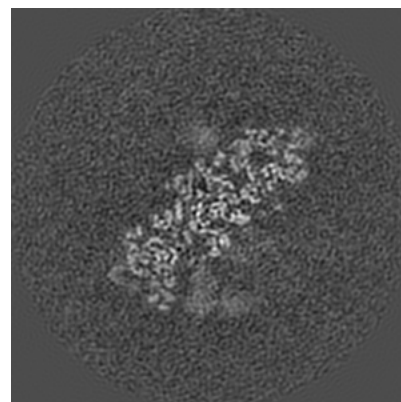
6.2.1 Primary map



X Index: 150



Y Index: 150

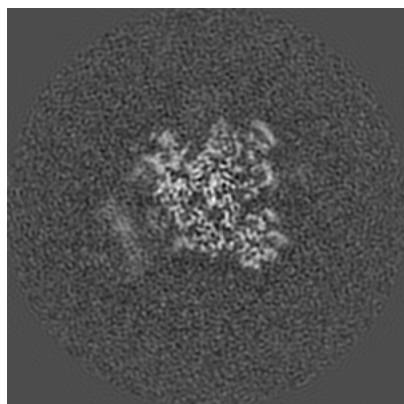


Z Index: 150

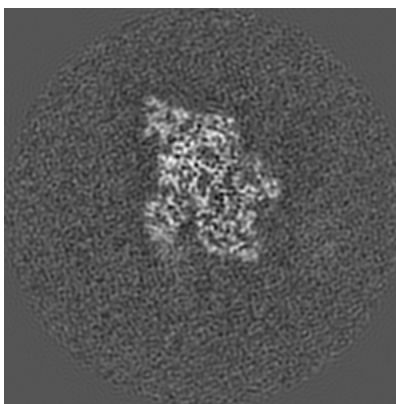
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

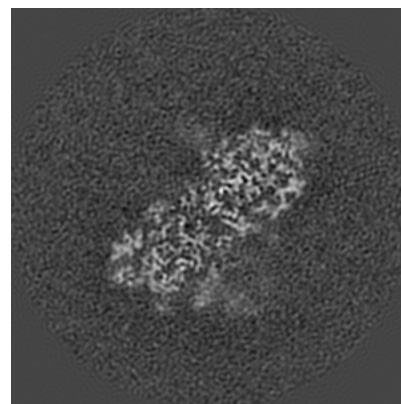
6.3.1 Primary map



X Index: 161



Y Index: 171



Z Index: 143

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

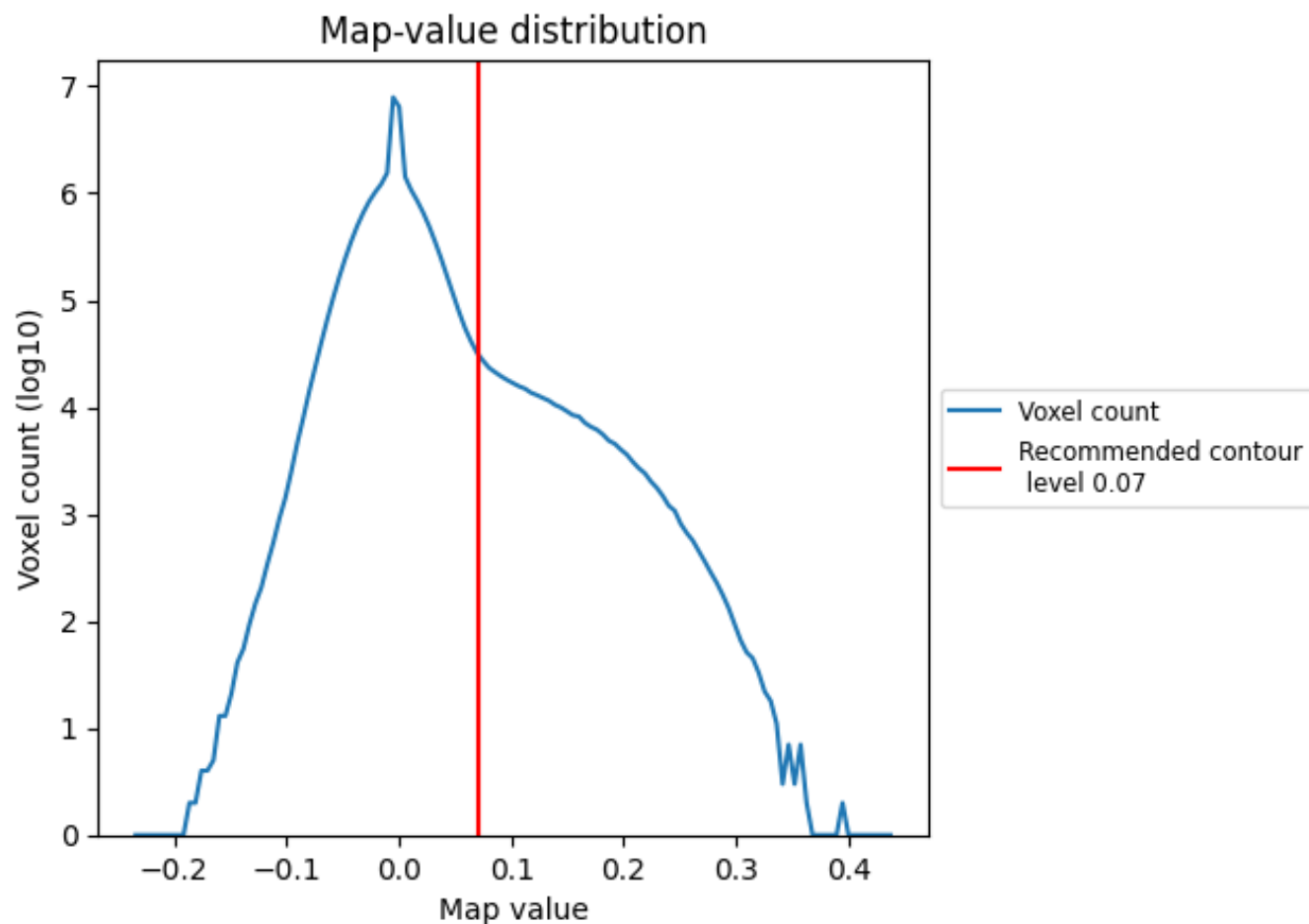
6.5 Mask visualisation

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

7 Map analysis [i](#)

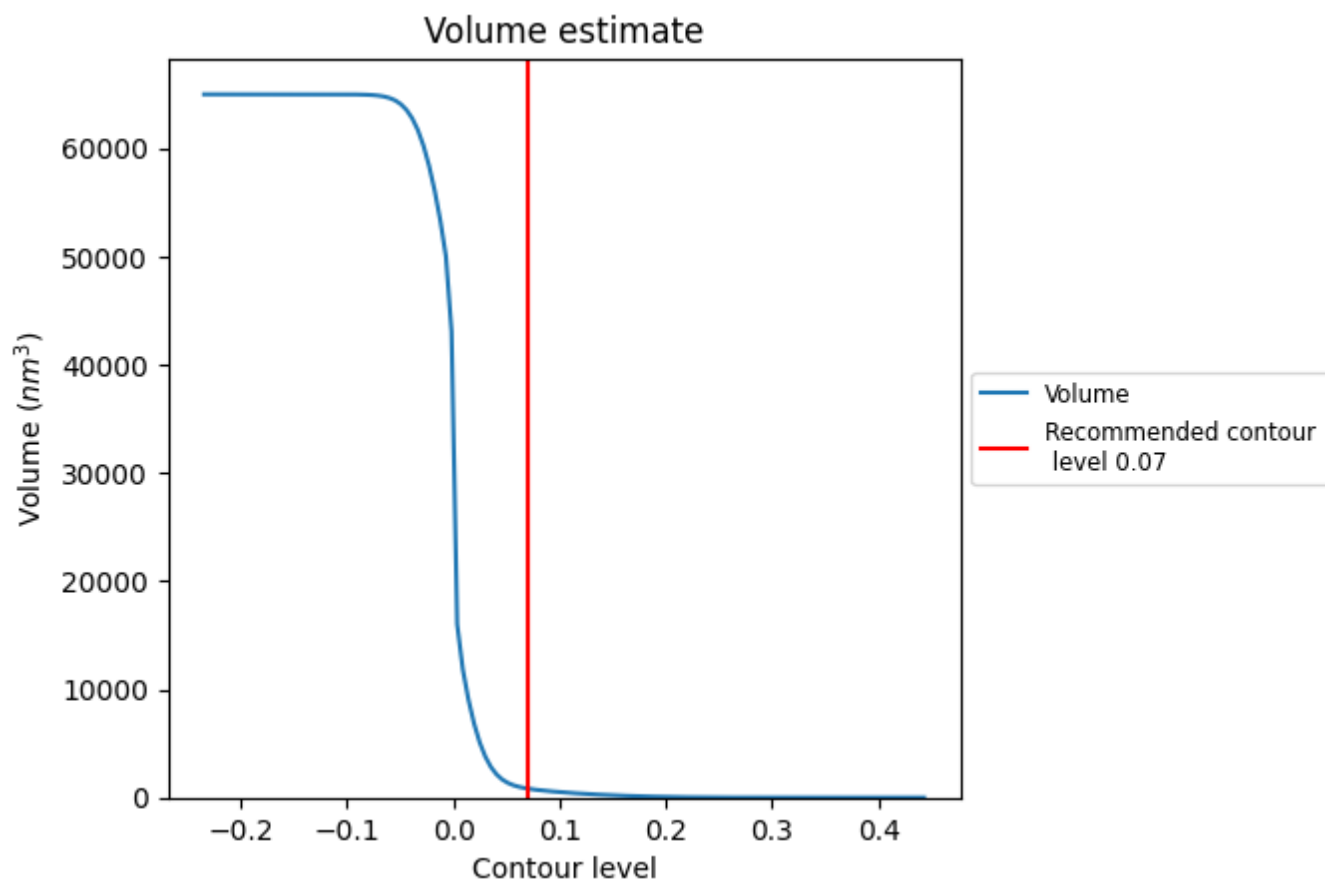
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

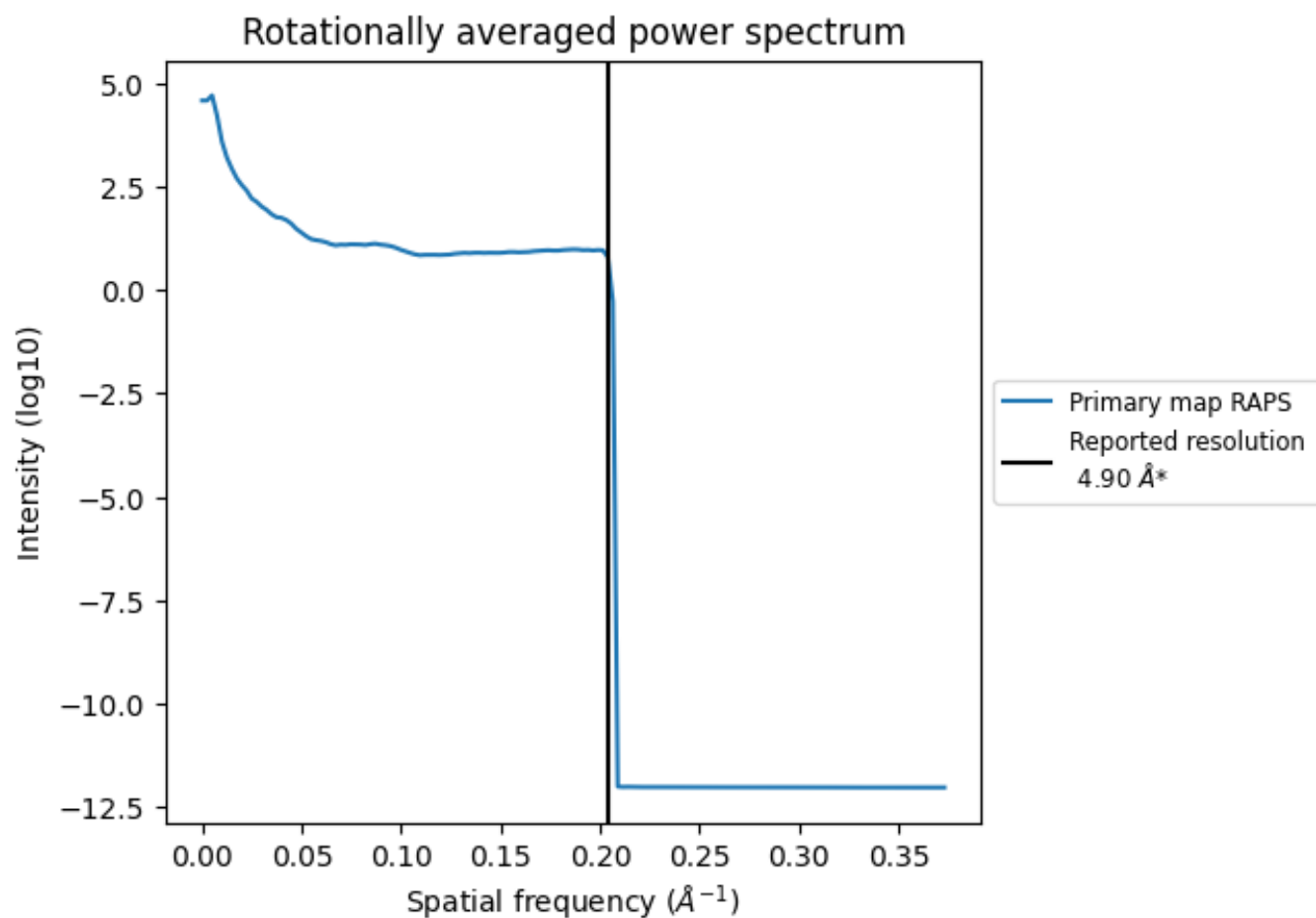
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; this corresponds to an approximate mass of 750 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 ⓘ

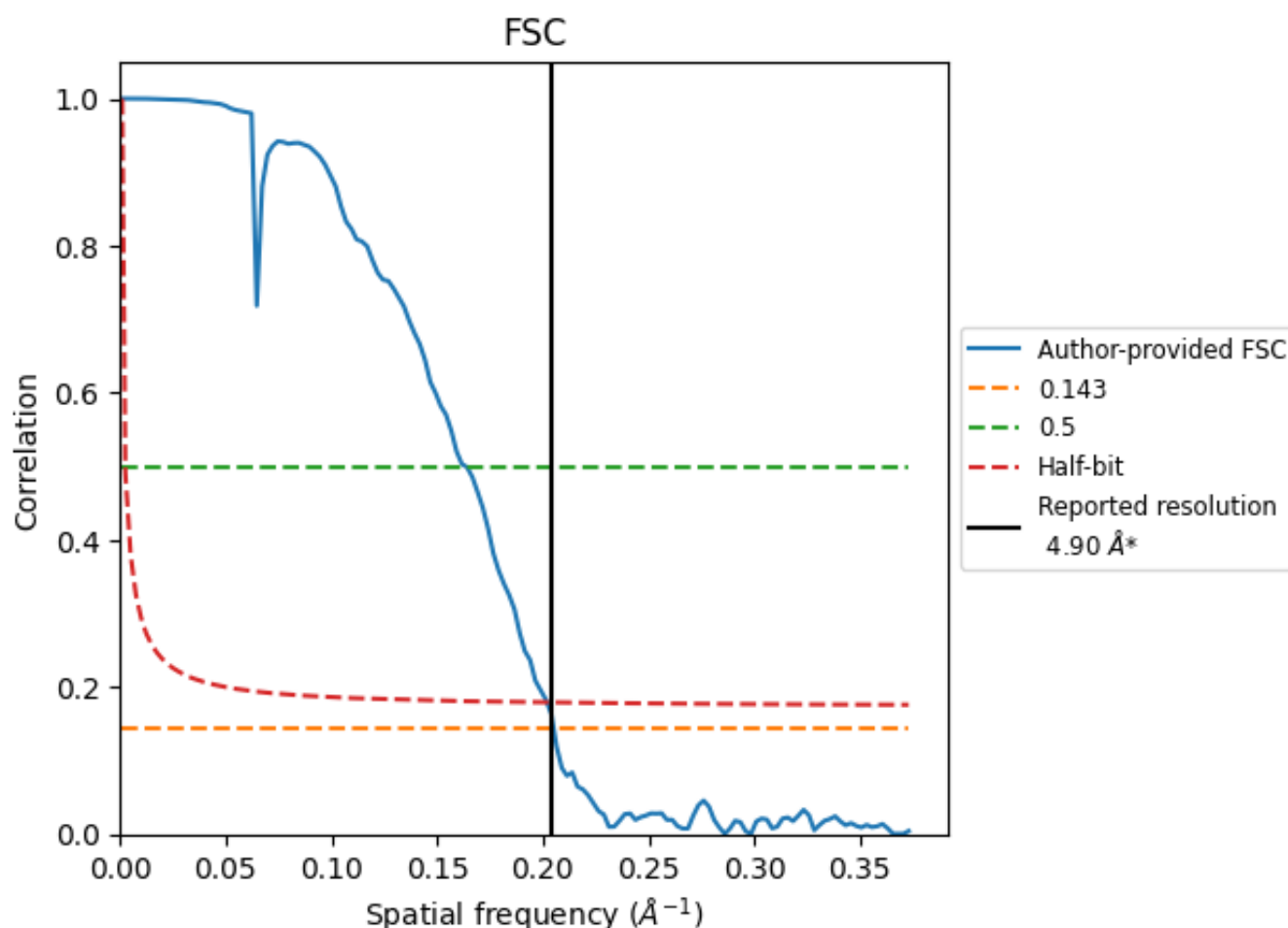


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

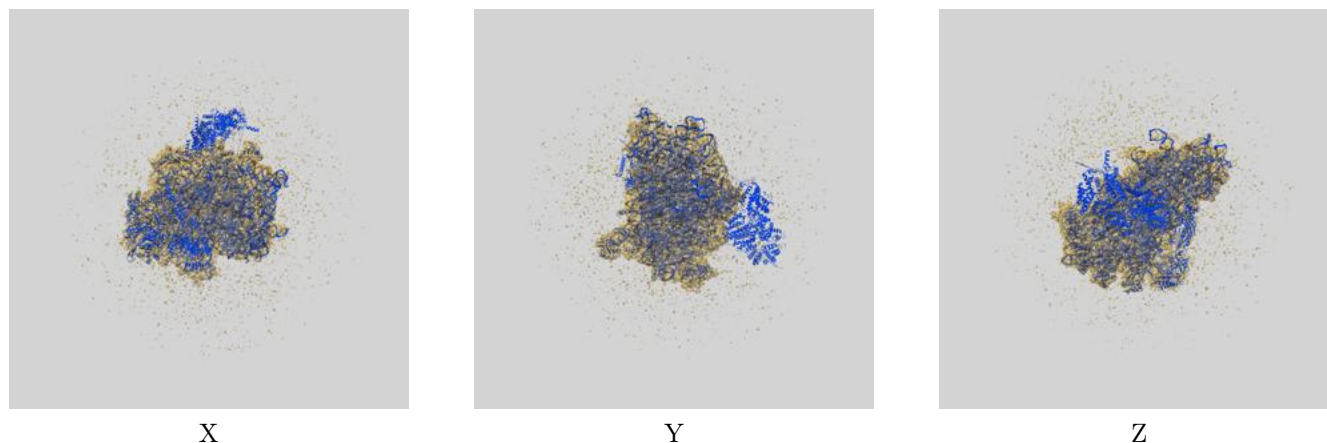
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.88	6.12	4.95
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

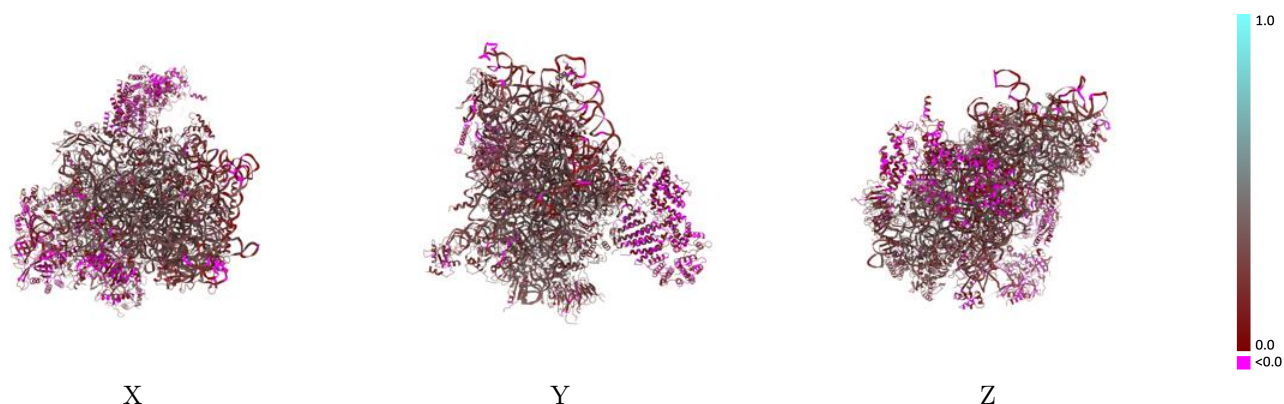
This section contains information regarding the fit between EMDB map EMD-3048 and PDB model 3JAP. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



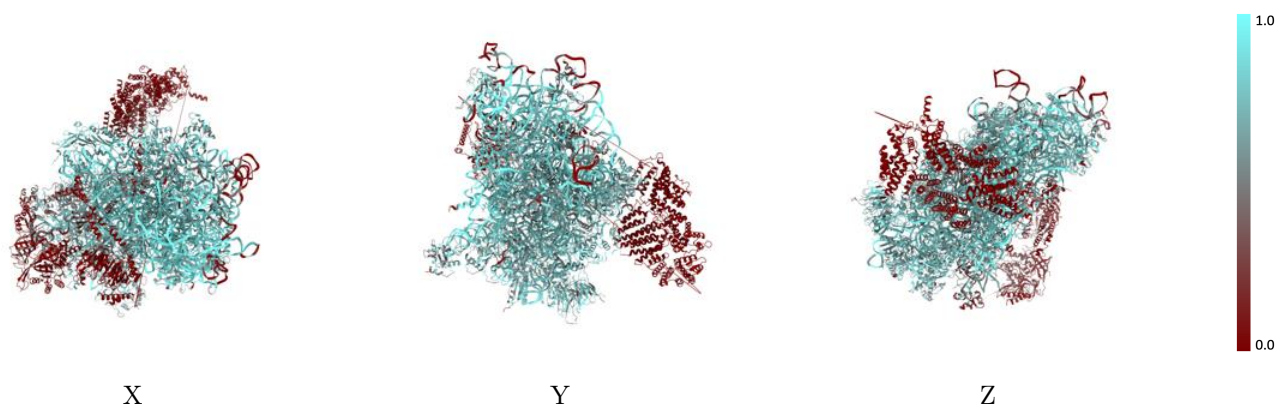
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



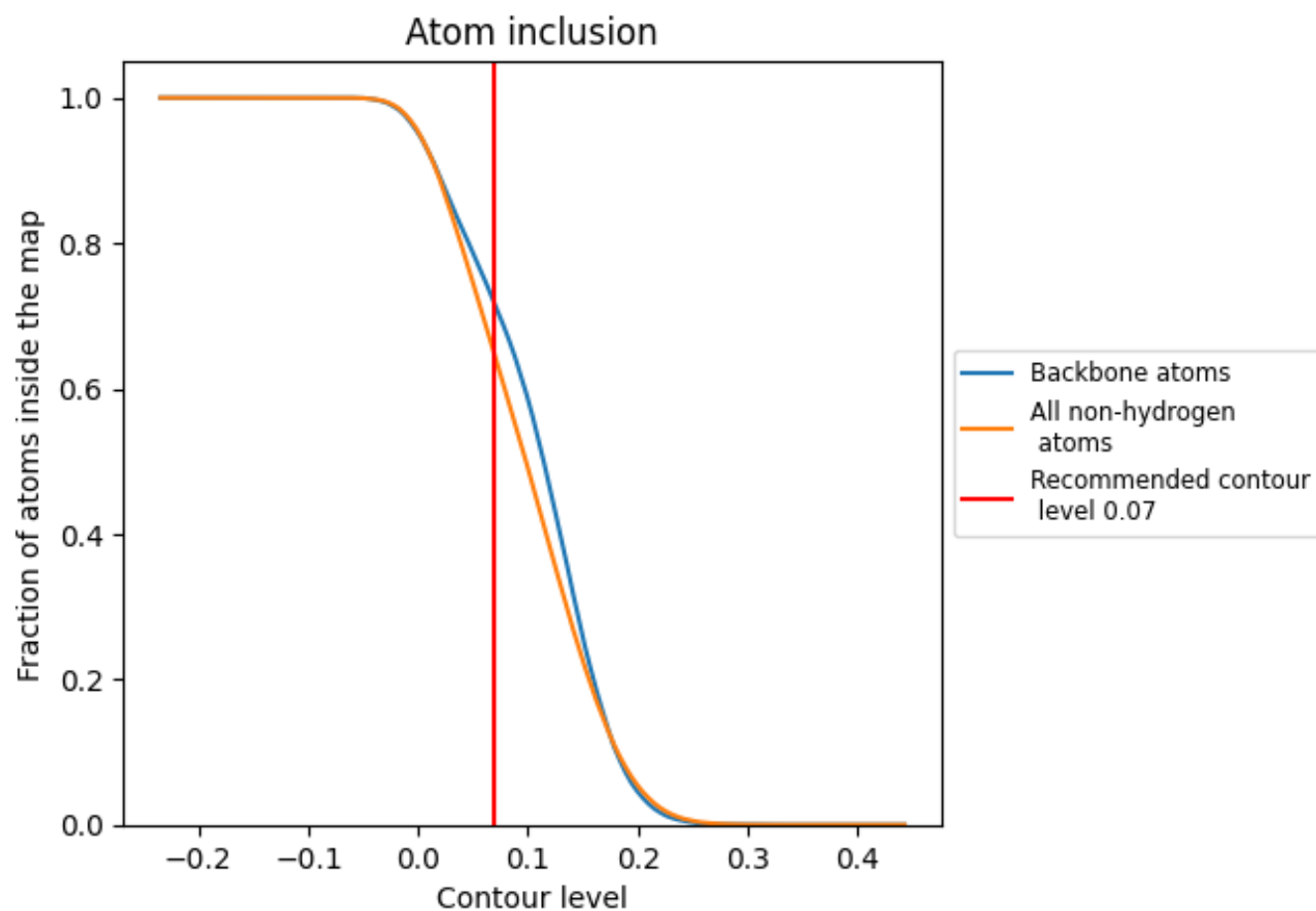
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6445	 0.2440
1	 0.5980	 0.1680
2	 0.8675	 0.2900
3	 0.5505	 0.2110
A	 0.7511	 0.2890
B	 0.7503	 0.2810
C	 0.7189	 0.3090
D	 0.6808	 0.2810
E	 0.7303	 0.2980
F	 0.6794	 0.2580
G	 0.7146	 0.2460
H	 0.6706	 0.2540
I	 0.7155	 0.2620
J	 0.7288	 0.2960
K	 0.7123	 0.2710
L	 0.6856	 0.2970
M	 0.5650	 0.2000
N	 0.7277	 0.2870
O	 0.7508	 0.2800
P	 0.7201	 0.2620
Q	 0.7093	 0.2650
R	 0.7166	 0.2850
S	 0.6782	 0.2640
T	 0.7287	 0.2560
U	 0.6470	 0.2680
V	 0.7316	 0.3010
W	 0.7130	 0.2930
X	 0.7189	 0.3190
Y	 0.7646	 0.2910
Z	 0.6188	 0.2420
a	 0.7426	 0.3170
b	 0.7176	 0.2800
c	 0.6938	 0.2950
d	 0.7588	 0.3010
e	 0.7160	 0.3180



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Chain	Atom inclusion	Q-score
f	 0.6555	 0.2270
g	 0.7093	 0.2410
h	 0.3726	 0.2170
i	 0.6404	 0.2810
j	 0.3060	 0.1650
k	 0.1174	 0.1100
l	 0.1039	 0.1240
m	 0.2756	 0.2020
o	 0.0131	 0.0720
p	 0.0307	 0.0920
q	 0.0264	 0.0530
r	 0.0185	 0.0550
s	 0.0025	 0.0760