



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:39 pm GMT

PDB ID : 5NGM
EMDB ID : EMD-3640
Title : 2.9S structure of the 70S ribosome composing the S. aureus 100S complex
Authors : Matzov, D.; Aibara, S.; Zimmerman, E.; Bashan, A.; Amunts, A.; Yonath, A.
Deposited on : 2017-03-18
Resolution : 2.90 Å (reported)

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:

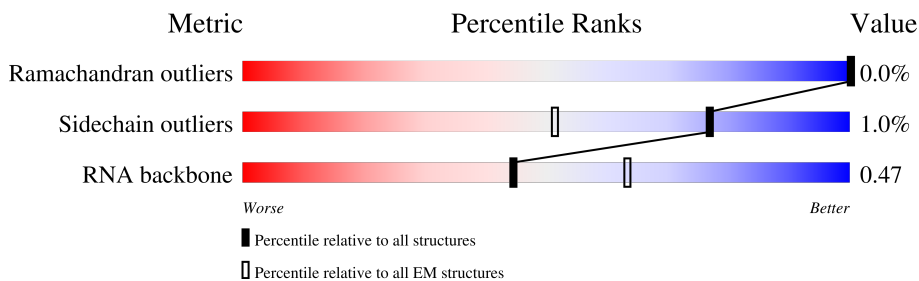
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.90 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	Aa	1555	
2	Ab	255	
3	Ac	217	
4	Ad	200	
5	Ae	166	
6	Af	98	
7	Ag	156	
8	Ah	132	

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Mol	Chain	Length	Quality of chain
9	Ai	132	92% 93% • •
10	Aj	102	88% 94% • 5%
11	Ak	129	39% 88% 12%
12	Al	137	10% 96% • •
13	Am	121	79% 85% • 14%
14	An	61	82% 95% • •
15	Ao	89	10% 98% • •
16	Ap	91	21% 96% • •
17	Aq	87	7% 92% 8%
18	Ar	80	14% 66% • 32%
19	As	92	77% 86% • 13%
20	At	83	27% 96% • •
21	Au	58	90% 90% 10%
22	Av	190	65% 82% • 15%
23	AA	2923	8% 70% 27% • •
24	AB	115	• 82% 17% •
25	AC	277	98% • •
26	AD	220	• 97% • •
27	AE	207	99%
28	AF	179	27% 97% • •
29	AG	178	• 97% • •
30	AH	145	• 99% •
31	AI	122	97% •
32	AJ	146	97% •
33	AK	144	• 94% • 5%

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Mol	Chain	Length	Quality of chain
34	AL	122	98%
35	AM	119	97%
36	AN	116	97%
37	AO	118	97%
38	AP	102	98%
39	AQ	117	95%
40	AR	91	96%
41	AS	105	97%
42	AT	217	43% 57%
43	AU	94	83% 13%
44	AV	62	92% 6%
45	AW	73	92% 8%
46	AX	59	98%
47	AY	84	70% 30%
48	AZ	57	84% 16%
49	A1	49	96%
50	A2	45	96%
51	A3	66	97%
52	A4	37	97%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 140965 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Aa	1539	32969	14719	6017	10694	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ab	226	1819	1159	317	335	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ac	202	1501	945	284	271	1	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Ad	198	1497	952	275	268	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Ae	156	1145	723	211	209	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Af	95	778	493	138	145	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ag	152	1161	722	218	217	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Ah	131	1026	650	183	189	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Ai	127	922	576	179	166	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Aj	97	752	475	140	136	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Ak	114	810	498	151	159	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Al	135	1037	646	211	178	2	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Am	104	727	453	139	135	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	60	Total	C	N	O	S	0	0
			487	307	98	77	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	88	Total	C	N	O	S	0	0
			723	448	150	124	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	89	Total	C	N	O	S	0	0
			694	436	128	129	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Aq	80	Total	C	N	O	0	0
			621	392	112	117		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			445	284	86	73	2		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	80	Total	C	N	O	S	0	0
			636	410	113	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	81	Total	C	N	O	S	0	0
			591	358	117	115	1		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Au	52	Total	C	N	O	0	0
			400	249	79	72		

- Molecule 22 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	162	Total	C	N	O	S	0	0
			1333	835	242	254	2		

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AA	2905	Total	C	N	O	P	0	0
			62277	27803	11387	20182	2905		

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AB	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AC	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AD	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AE	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AF	175	1325	837	227	255	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AG	175	1263	790	239	231	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AH	145	1143	714	208	218	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AI	122	918	572	174	168	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AJ	146	1086	674	214	197	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	AK	137	1071	689	203	175	4	0	0

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AL	120	932	576	182	173	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AM	119	891	557	174	159	1	0	0

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AN	114	889	563	175	151		0	0

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AO	116	942	593	189	156	4	0	0

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AP	102	790	503	142	144	1	0	0

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	AQ	112	854	534	164	153	3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	AR	89	715	453	127	131	4	0	0

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AS	103	770	486	142	141	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	AT	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	AU	82	Total	C	N	O	0	0
			622	385	122	115		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	AV	58	Total	C	N	O	0	0
			445	277	96	72		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	AW	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	AX	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AY	59	Total	C	N	O	S	0	0
			370	225	68	76	1		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AZ	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

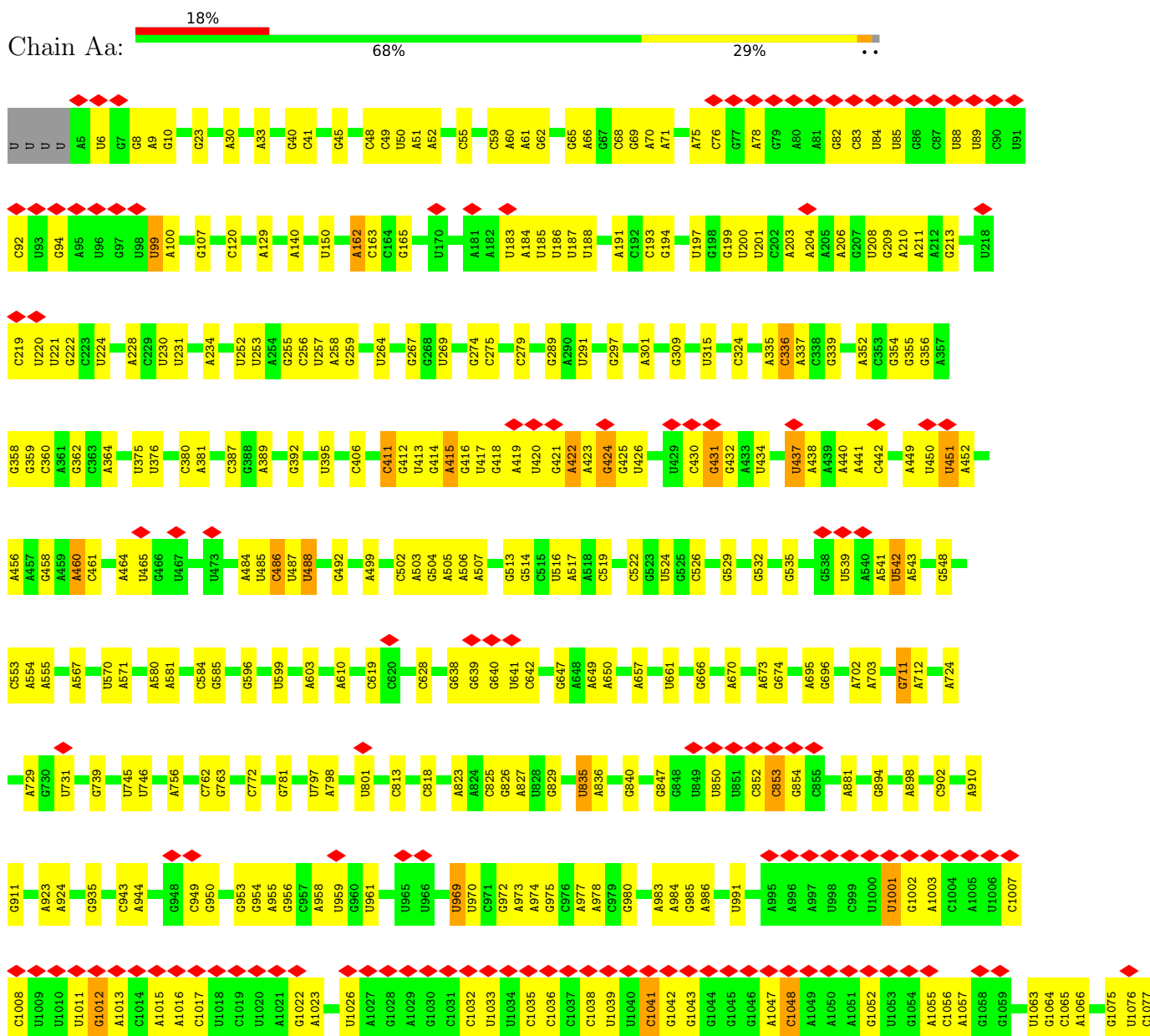
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

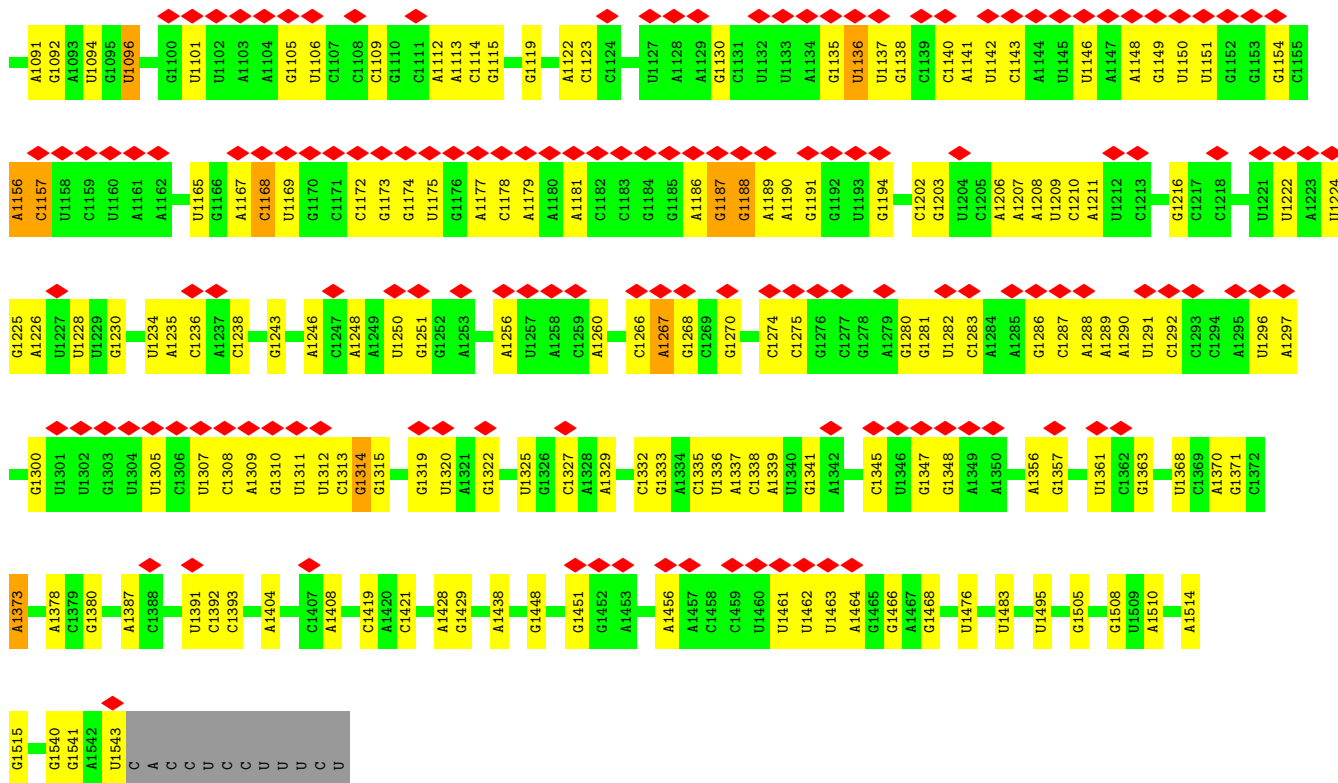
Mol	Chain	Residues	Atoms		AltConf
53	AA	199	Total	Mg	0
			199	199	
53	AB	2	Total	Mg	0
			2	2	
53	AC	2	Total	Mg	0
			2	2	
53	AU	1	Total	Mg	0
			1	1	
53	AZ	1	Total	Mg	0
			1	1	

3 Residue-property plots

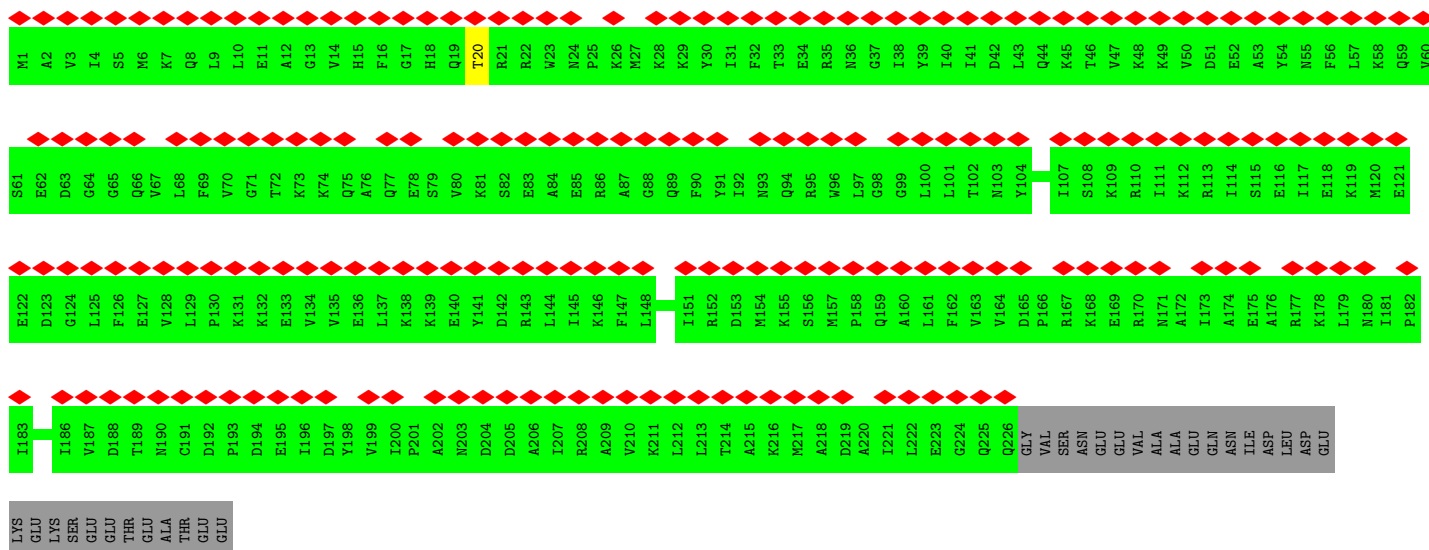
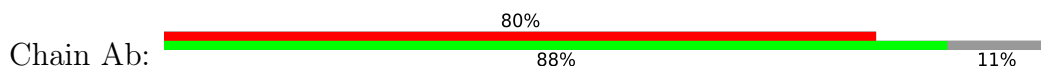
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

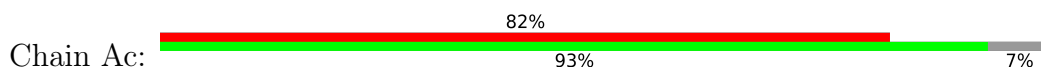


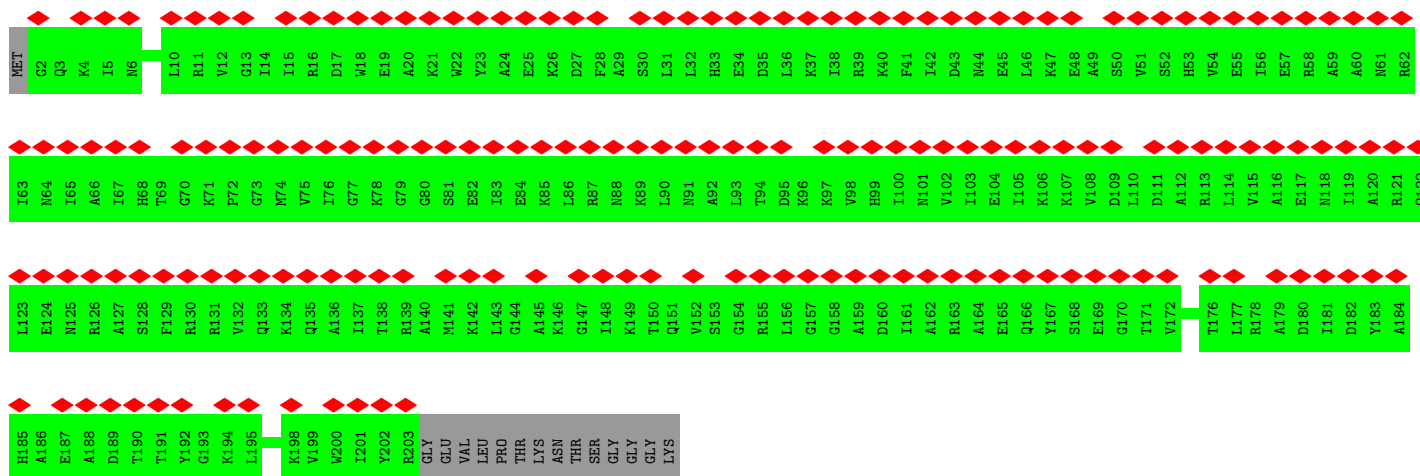


• Molecule 2: 30S ribosomal protein S2

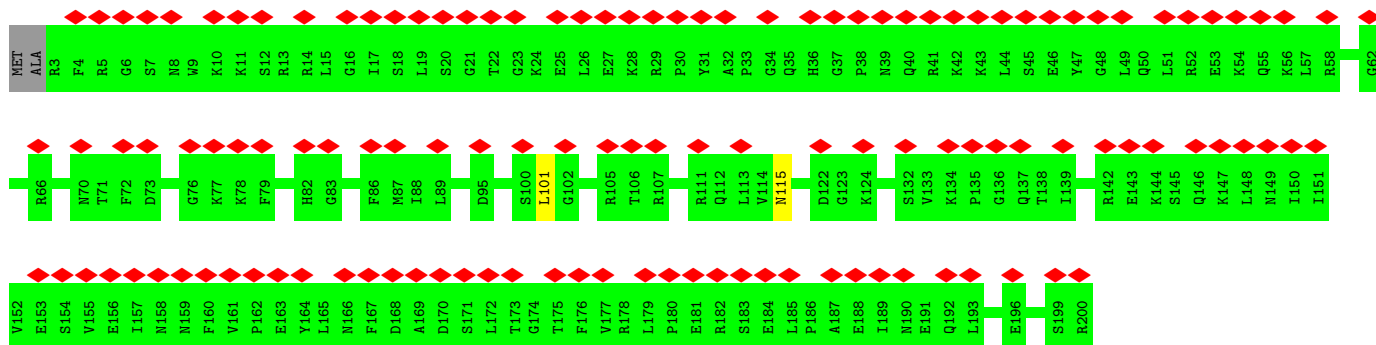


• Molecule 3: 30S ribosomal protein S3

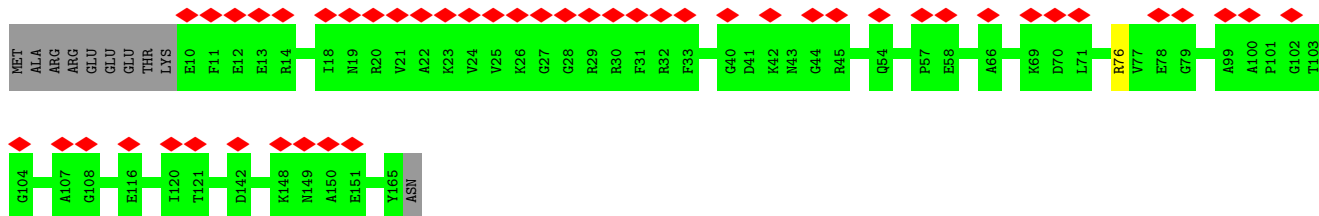




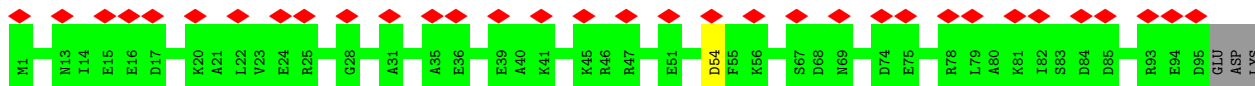
• Molecule 4: 30S ribosomal protein S4



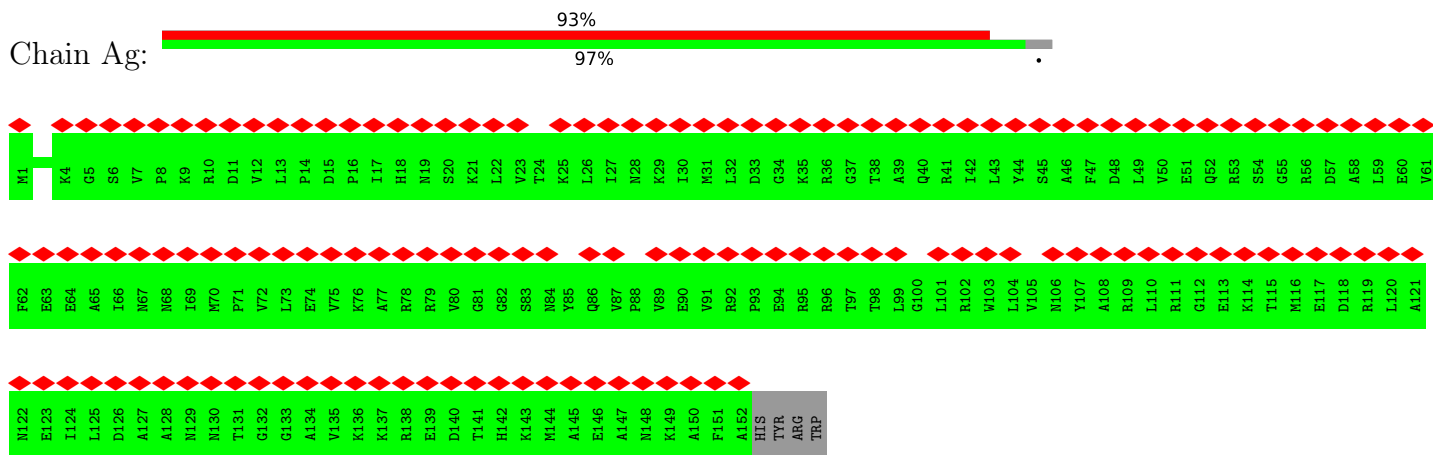
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



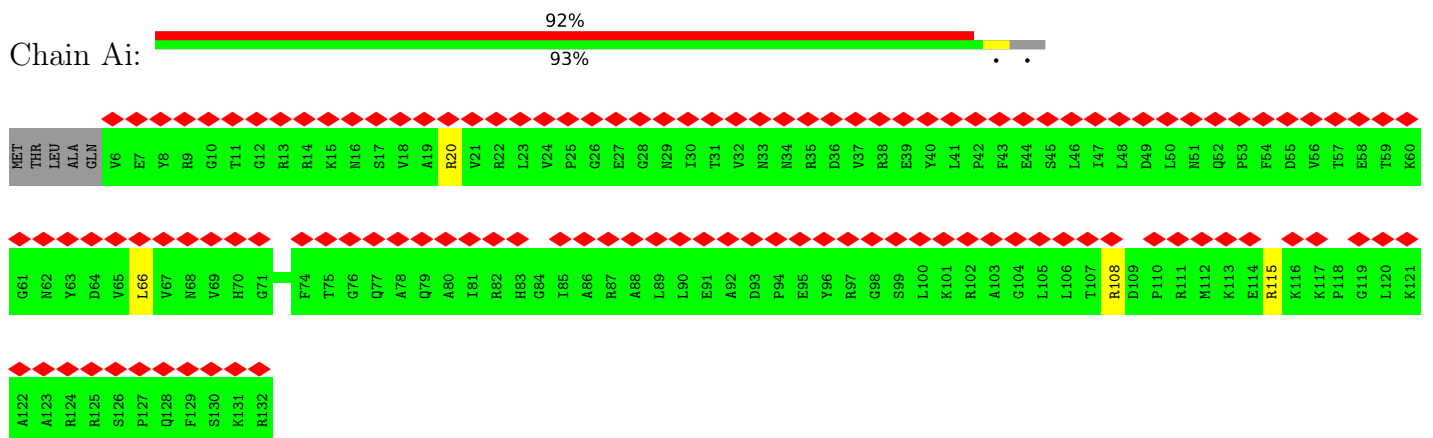
• Molecule 7: 30S ribosomal protein S7



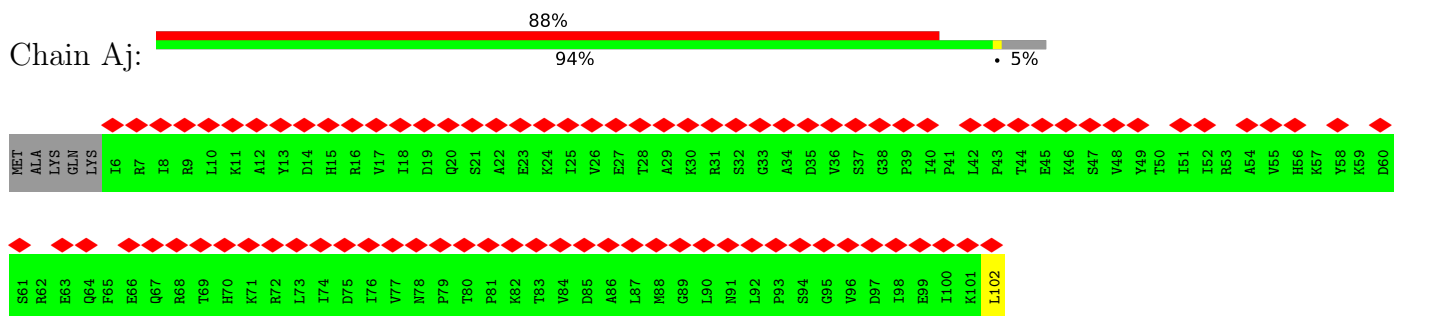
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

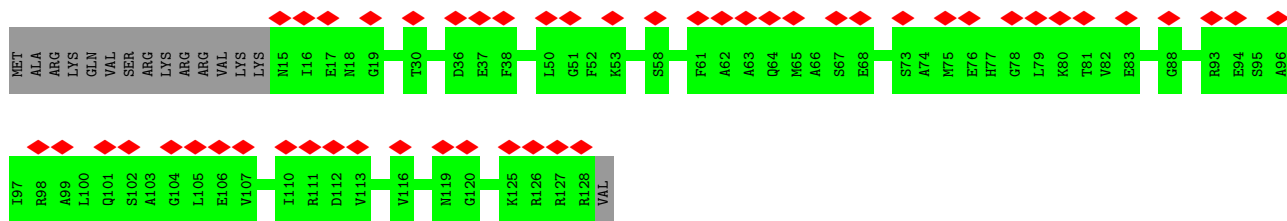


• Molecule 10: 30S ribosomal protein S10

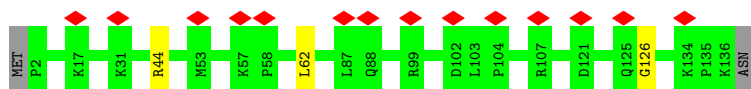


• Molecule 11: 30S ribosomal protein S11

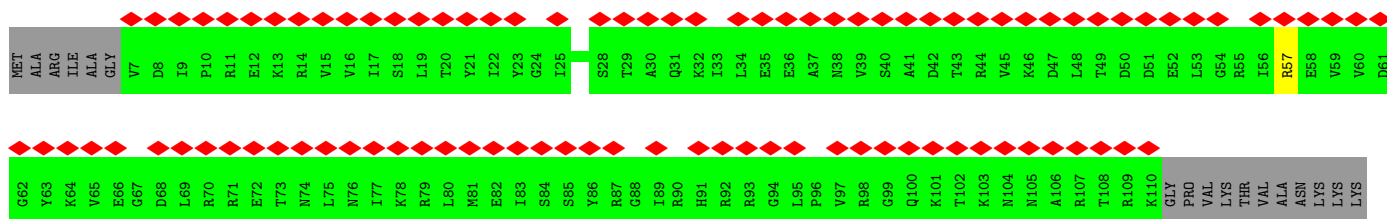
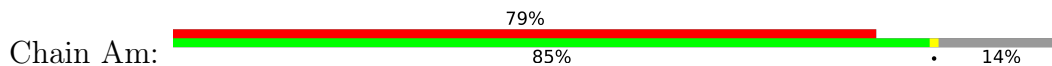




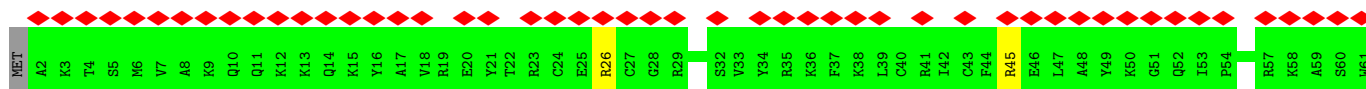
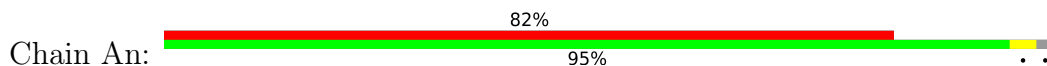
- Molecule 12: 30S ribosomal protein S12



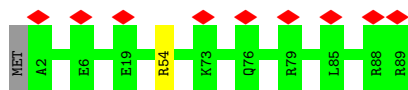
- Molecule 13: 30S ribosomal protein S13



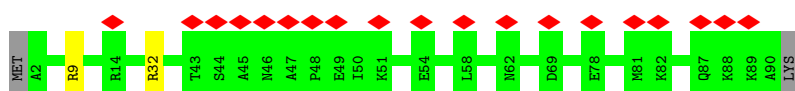
- Molecule 14: 30S ribosomal protein S14 type Z



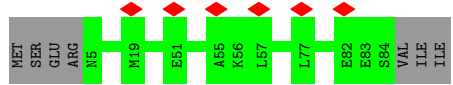
- Molecule 15: 30S ribosomal protein S15



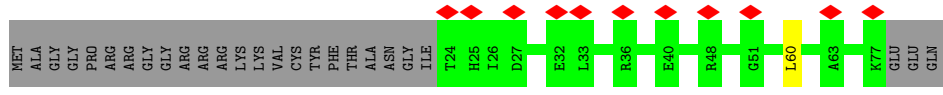
- Molecule 16: 30S ribosomal protein S16



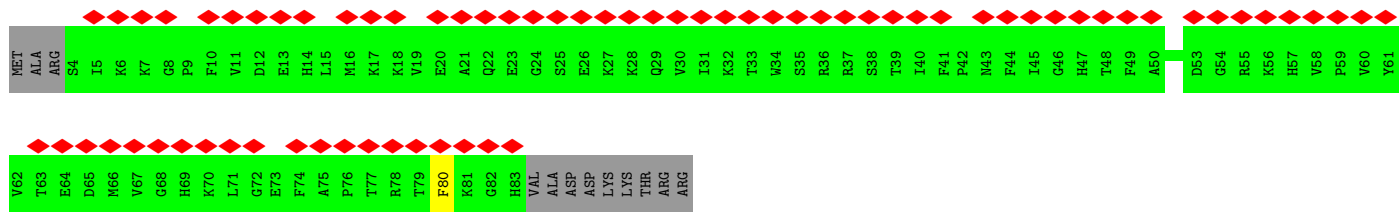
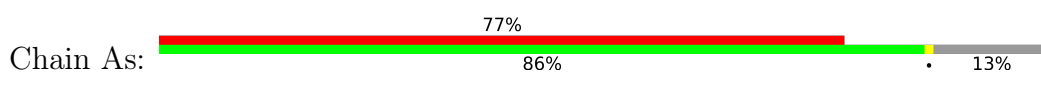
- Molecule 17: 30S ribosomal protein S17



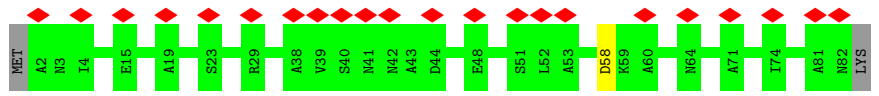
• Molecule 18: 30S ribosomal protein S18



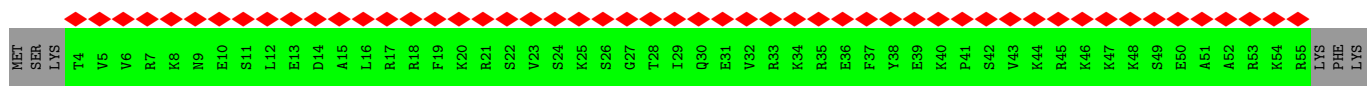
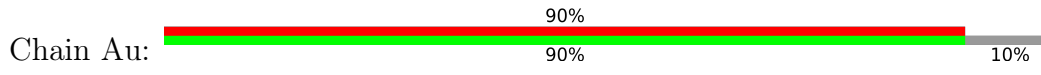
• Molecule 19: 30S ribosomal protein S19



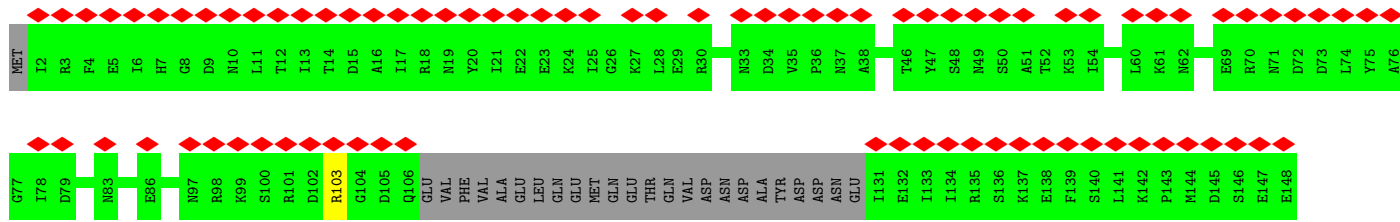
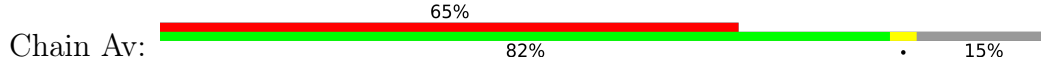
• Molecule 20: 30S ribosomal protein S20

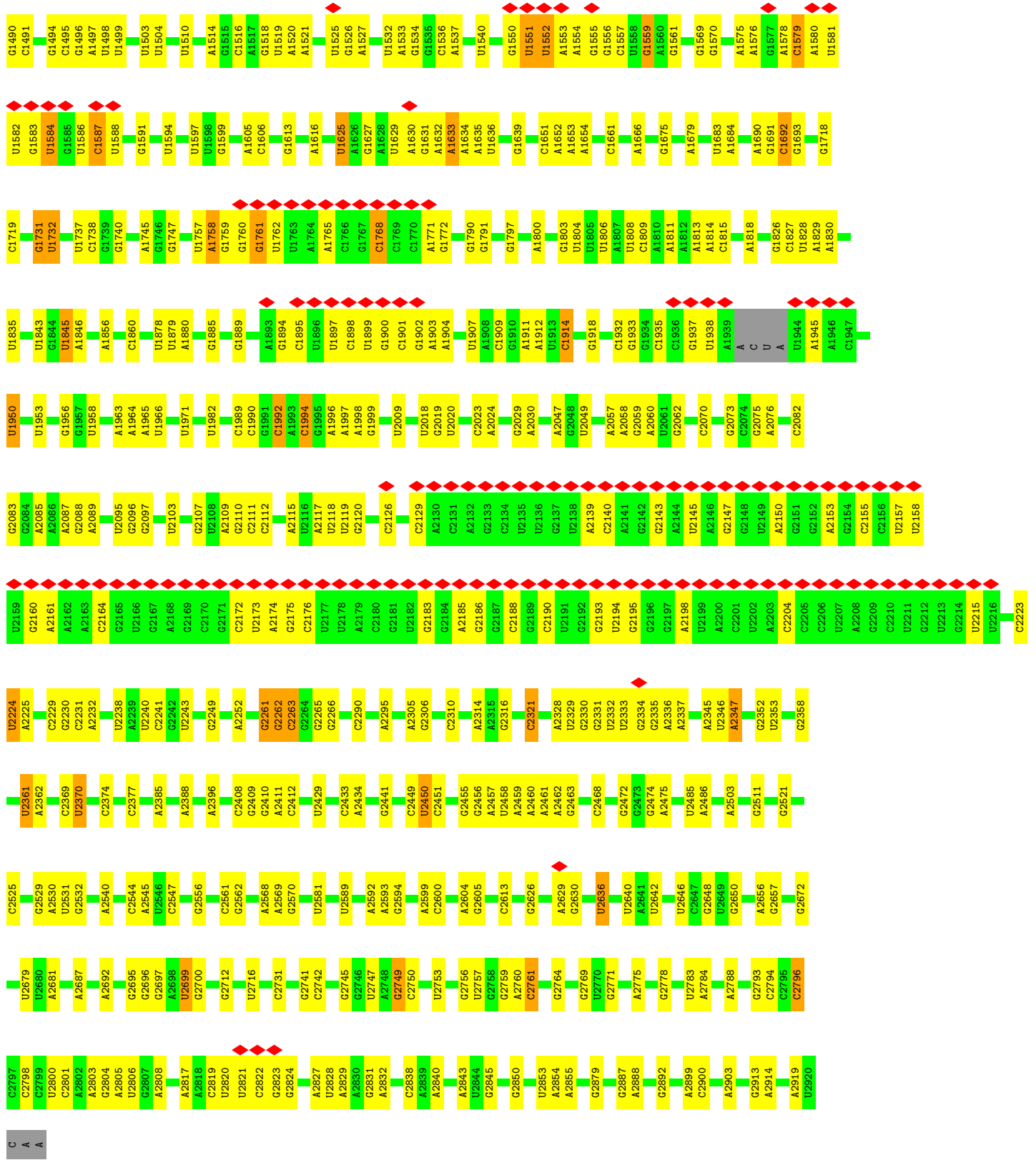


• Molecule 21: 30S ribosomal protein S21

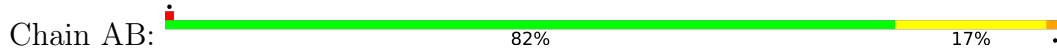


• Molecule 22: Ribosome hibernation promoting factor





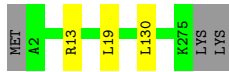
• Molecule 24: 5S Ribosomal RNA





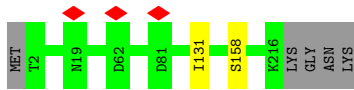
- Molecule 25: 50S ribosomal protein L2

Chain AC: 98%



- Molecule 26: 50S ribosomal protein L3

Chain AD: 97%



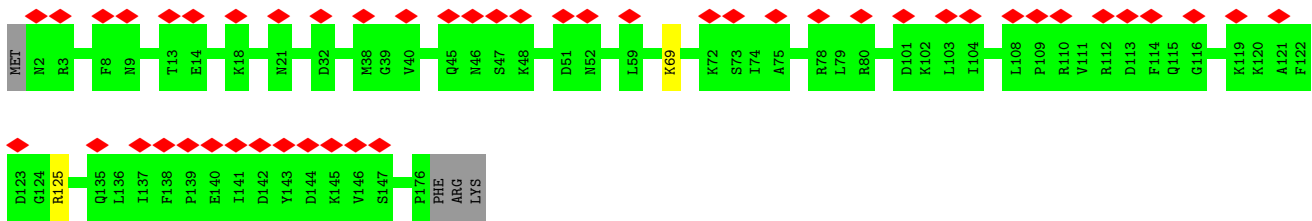
- Molecule 27: 50S ribosomal protein L4

Chain AE: 99%



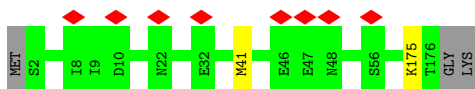
- Molecule 28: 50S ribosomal protein L5

Chain AF: 27% 97%



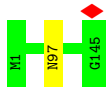
- Molecule 29: 50S ribosomal protein L6

Chain AG: 97%



- Molecule 30: 50S ribosomal protein L13

Chain AH: 99%



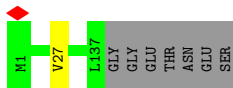
- Molecule 31: 50S ribosomal protein L14



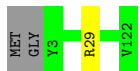
- Molecule 32: 50S ribosomal protein L15



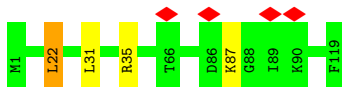
- Molecule 33: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L17



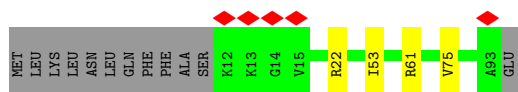
- Molecule 35: 50S ribosomal protein L18



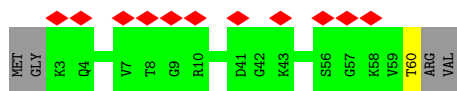
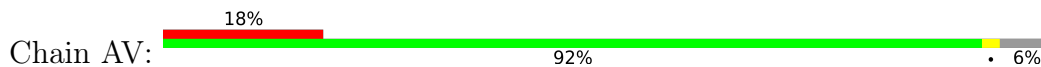
- Molecule 36: 50S ribosomal protein L19



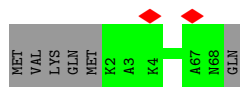
- Molecule 37: 50S ribosomal protein L20



• Molecule 44: 50S ribosomal protein L28



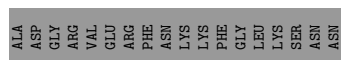
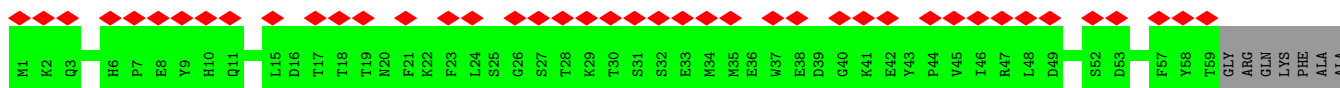
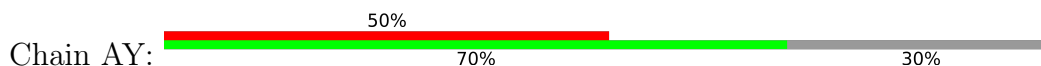
• Molecule 45: 50S ribosomal protein L29



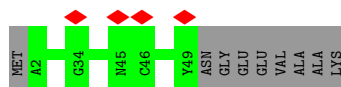
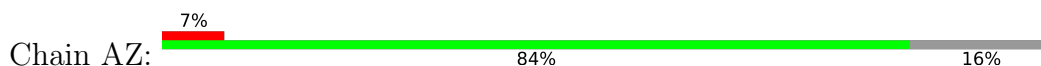
• Molecule 46: 50S ribosomal protein L30



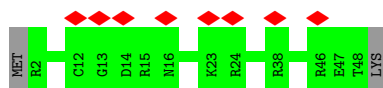
• Molecule 47: 50S ribosomal protein L31 type B



• Molecule 48: 50S ribosomal protein L32

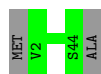


• Molecule 49: 50S ribosomal protein L33



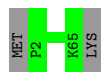
- Molecule 50: 50S ribosomal protein L34

Chain A2:  96%



- Molecule 51: 50S ribosomal protein L35

Chain A3:  97%



- Molecule 52: 50S ribosomal protein L36

Chain A4:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.056	Depositor
Minimum map value	-0.644	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	Aa	0.38	0/36913	0.95	102/57564 (0.2%)
2	Ab	0.26	0/1846	0.54	1/2477 (0.0%)
3	Ac	0.27	0/1523	0.59	0/2062
4	Ad	0.28	0/1526	0.62	1/2063 (0.0%)
5	Ae	0.28	0/1159	0.59	0/1566
6	Af	0.30	0/789	0.60	1/1060 (0.1%)
7	Ag	0.26	0/1176	0.54	0/1588
8	Ah	0.31	0/1038	0.63	0/1395
9	Ai	0.27	0/937	0.67	1/1269 (0.1%)
10	Aj	0.27	0/764	0.56	0/1034
11	Ak	0.29	0/824	0.59	0/1119
12	Al	0.30	0/1054	0.63	1/1415 (0.1%)
13	Am	0.26	0/732	0.56	0/991
14	An	0.32	0/497	0.63	0/662
15	Ao	0.26	0/732	0.53	0/979
16	Ap	0.33	0/705	0.57	0/952
17	Aq	0.31	0/629	0.58	0/849
18	Ar	0.28	0/452	0.65	1/604 (0.2%)
19	As	0.31	0/654	0.58	0/879
20	At	0.23	0/591	0.50	0/793
21	Au	0.27	0/403	0.51	0/535
22	Av	0.49	0/1350	0.81	2/1812 (0.1%)
23	AA	0.74	3/69738 (0.0%)	1.02	202/108747 (0.2%)
24	AB	0.61	0/2732	1.16	20/4253 (0.5%)
25	AC	0.48	0/2129	0.67	3/2858 (0.1%)
26	AD	0.49	0/1651	0.66	0/2215
27	AE	0.47	0/1595	0.66	0/2154
28	AF	0.31	0/1339	0.63	0/1805
29	AG	0.35	0/1281	0.58	0/1736
30	AH	0.48	0/1165	0.65	0/1570
31	AI	0.47	0/925	0.73	3/1242 (0.2%)
32	AJ	0.45	0/1100	0.71	2/1467 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AK	0.46	0/1095	0.61	0/1472
34	AL	0.43	0/936	0.71	0/1253
35	AM	0.43	0/900	0.68	2/1205 (0.2%)
36	AN	0.43	0/901	0.65	1/1209 (0.1%)
37	AO	0.52	0/954	0.64	0/1264
38	AP	0.47	0/800	0.67	0/1070
39	AQ	0.45	0/862	0.70	0/1161
40	AR	0.43	0/723	0.63	0/966
41	AS	0.39	0/779	0.67	0/1043
42	AT	0.37	0/730	0.66	1/981 (0.1%)
43	AU	0.54	0/628	0.68	1/833 (0.1%)
44	AV	0.38	0/451	0.66	0/603
45	AW	0.39	0/542	0.69	0/722
46	AX	0.40	0/451	0.61	0/606
47	AY	0.25	0/378	0.53	0/521
48	AZ	0.43	0/366	0.65	0/489
49	A1	0.34	0/395	0.60	0/530
50	A2	0.48	0/371	0.67	0/484
51	A3	0.40	0/526	0.61	0/690
52	A4	0.52	0/298	0.63	0/392
All	All	0.58	3/153035 (0.0%)	0.92	345/229209 (0.2%)

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
5	Ae	0	1
9	Ai	0	1
12	Al	0	1
19	As	0	1
20	At	0	1
26	AD	0	1
38	AP	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	1584	U	C1'-N1	5.36	1.56	1.48
23	AA	1065	A	N9-C4	-5.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	1186	A	N9-C4	-5.08	1.34	1.37

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	87	C	N1-C2-O2	12.65	126.49	118.90
24	AB	87	C	C2-N1-C1'	12.12	132.13	118.80
23	AA	576	U	C2-N1-C1'	11.98	132.08	117.70
1	Aa	745	U	OP1-P-O3'	-11.40	80.13	105.20
23	AA	2150	A	N7-C8-N9	10.80	119.20	113.80
24	AB	111	C	N1-C2-O2	10.61	125.27	118.90
23	AA	576	U	N1-C2-O2	10.61	130.22	122.80
24	AB	87	C	N3-C2-O2	-10.51	114.55	121.90
23	AA	1179	C	N1-C2-O2	10.45	125.17	118.90
23	AA	576	U	N3-C2-O2	-10.00	115.20	122.20
23	AA	2150	A	C5-N7-C8	9.88	108.84	103.90
23	AA	1994	C	N1-C2-O2	9.73	124.74	118.90
23	AA	1994	C	C2-N1-C1'	9.61	129.37	118.80
23	AA	1932	C	N1-C2-O2	9.48	124.59	118.90
23	AA	1932	C	C2-N1-C1'	9.36	129.10	118.80
24	AB	87	C	C6-N1-C1'	-9.05	109.94	120.80
23	AA	1179	C	N3-C2-O2	-8.75	115.77	121.90
23	AA	1179	C	C2-N1-C1'	8.72	128.39	118.80
24	AB	111	C	N3-C2-O2	-8.69	115.82	121.90
23	AA	593	U	C2-N1-C1'	8.62	128.04	117.70
24	AB	111	C	C2-N1-C1'	8.59	128.24	118.80
24	AB	108	U	N3-C2-O2	-8.42	116.31	122.20
23	AA	439	U	C2-N1-C1'	8.36	127.73	117.70
23	AA	1894	G	C4-N9-C1'	8.34	137.35	126.50
23	AA	576	U	C6-N1-C1'	-8.33	109.54	121.20
9	Ai	66	LEU	CA-CB-CG	8.30	134.39	115.30
23	AA	1378	U	N3-C2-O2	-8.23	116.44	122.20
23	AA	1804	U	C2-N1-C1'	8.16	127.50	117.70
1	Aa	55	C	N1-C2-O2	8.13	123.78	118.90
1	Aa	99	U	C2-N1-C1'	8.07	127.39	117.70
24	AB	108	U	C2-N1-C1'	8.04	127.34	117.70
1	Aa	599	U	C2-N1-C1'	8.03	127.33	117.70
23	AA	1378	U	N1-C2-O2	8.02	128.41	122.80
24	AB	100	U	C2-N1-C1'	8.02	127.32	117.70
23	AA	759	U	N1-C2-O2	8.01	128.41	122.80
1	Aa	55	C	C2-N1-C1'	7.99	127.59	118.80
23	AA	1994	C	N3-C2-O2	-7.99	116.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	759	U	C2-N1-C1'	7.98	127.28	117.70
1	Aa	1187	G	C4-N9-C1'	7.94	136.82	126.50
23	AA	439	U	N3-C2-O2	-7.83	116.72	122.20
23	AA	439	U	N1-C2-O2	7.82	128.27	122.80
23	AA	1227	U	N3-C2-O2	-7.82	116.73	122.20
1	Aa	745	U	OP2-P-O3'	-7.80	88.05	105.20
23	AA	2370	U	N3-C2-O2	-7.73	116.79	122.20
23	AA	882	C	C2-N1-C1'	7.70	127.27	118.80
23	AA	1378	U	C2-N1-C1'	7.65	126.88	117.70
24	AB	108	U	N1-C2-O2	7.59	128.11	122.80
23	AA	1932	C	N3-C2-O2	-7.58	116.60	121.90
31	AI	20	LEU	CA-CB-CG	7.56	132.69	115.30
23	AA	1894	G	C8-N9-C1'	-7.53	117.21	127.00
1	Aa	1136	U	C2-N1-C1'	7.45	126.64	117.70
35	AM	31	LEU	CA-CB-CG	7.44	132.40	115.30
23	AA	1599	G	N3-C2-N2	-7.37	114.74	119.90
1	Aa	415	A	P-O3'-C3'	7.32	128.49	119.70
23	AA	1692	C	C2-N1-C1'	7.25	126.78	118.80
23	AA	1579	C	N1-C2-O2	7.22	123.23	118.90
1	Aa	835	U	C2-N1-C1'	7.14	126.27	117.70
1	Aa	902	C	C2-N1-C1'	7.13	126.64	118.80
23	AA	1994	C	C6-N1-C1'	-7.13	112.25	120.80
23	AA	2223	C	N1-C2-O2	7.11	123.17	118.90
1	Aa	746	U	OP1-P-OP2	7.09	130.24	119.60
23	AA	1597	U	N3-C2-O2	-7.08	117.25	122.20
1	Aa	99	U	N1-C2-O2	7.07	127.75	122.80
1	Aa	99	U	N3-C2-O2	-7.07	117.25	122.20
23	AA	1932	C	C6-N1-C1'	-7.05	112.34	120.80
1	Aa	460	A	P-O3'-C3'	6.97	128.06	119.70
23	AA	2261	G	P-O3'-C3'	-6.97	111.34	119.70
23	AA	759	U	N3-C2-O2	-6.96	117.32	122.20
1	Aa	1187	G	N3-C4-N9	6.95	130.17	126.00
23	AA	1914	C	N1-C2-O2	6.93	123.06	118.90
23	AA	2819	C	N1-C2-O2	6.90	123.04	118.90
23	AA	575	G	C4-N9-C1'	6.88	135.44	126.50
23	AA	1894	G	N3-C4-N9	6.87	130.12	126.00
1	Aa	431	G	C4-N9-C1'	6.85	135.41	126.50
1	Aa	424	G	C4-N9-C1'	6.85	135.41	126.50
23	AA	1160	C	N1-C2-O2	6.85	123.01	118.90
23	AA	1214	C	N1-C2-O2	6.85	123.01	118.90
23	AA	2361	U	C2-N1-C1'	6.82	125.88	117.70
22	Av	176	ARG	NE-CZ-NH1	6.81	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	853	C	P-O3'-C3'	6.76	127.81	119.70
1	Aa	55	C	N3-C2-O2	-6.72	117.19	121.90
1	Aa	1187	G	N3-C4-C5	-6.67	125.26	128.60
1	Aa	431	G	N3-C4-N9	6.65	129.99	126.00
23	AA	1227	U	N1-C2-O2	6.64	127.45	122.80
1	Aa	424	G	N3-C4-C5	-6.60	125.30	128.60
1	Aa	711	G	P-O3'-C3'	6.60	127.62	119.70
1	Aa	451	U	P-O3'-C3'	6.57	127.58	119.70
1	Aa	1041	C	P-O3'-C3'	6.57	127.58	119.70
1	Aa	65	G	P-O3'-C3'	6.57	127.58	119.70
1	Aa	1187	G	C8-N9-C1'	-6.53	118.52	127.00
4	Ad	101	LEU	CA-CB-CG	6.51	130.27	115.30
1	Aa	1075	G	P-O3'-C3'	6.50	127.50	119.70
23	AA	1597	U	N1-C2-O2	6.50	127.35	122.80
1	Aa	1136	U	N3-C2-O2	-6.49	117.66	122.20
1	Aa	336	C	C2-N1-C1'	6.49	125.93	118.80
23	AA	2049	U	C2-N1-C1'	6.48	125.48	117.70
1	Aa	835	U	N3-C2-O2	-6.44	117.69	122.20
1	Aa	315	U	C2-N1-C1'	6.44	125.42	117.70
23	AA	268	A	P-O3'-C3'	6.43	127.41	119.70
23	AA	1213	C	N1-C2-O2	6.42	122.75	118.90
23	AA	2223	C	N3-C2-O2	-6.42	117.41	121.90
23	AA	1731	G	P-O3'-C3'	6.41	127.39	119.70
23	AA	2699	U	N1-C2-O2	6.41	127.28	122.80
23	AA	2450	U	P-O3'-C3'	6.40	127.38	119.70
23	AA	1651	C	N1-C2-O2	6.38	122.73	118.90
23	AA	1992	C	C2-N1-C1'	6.36	125.80	118.80
24	AB	111	C	C6-N1-C1'	-6.36	113.17	120.80
1	Aa	1136	U	N1-C2-O2	6.36	127.25	122.80
23	AA	1552	U	N3-C2-O2	-6.34	117.76	122.20
23	AA	74	U	N1-C2-O2	6.34	127.24	122.80
1	Aa	902	C	N3-C2-O2	-6.33	117.47	121.90
23	AA	1804	U	C6-N1-C1'	-6.33	112.33	121.20
23	AA	1804	U	N3-C2-O2	-6.33	117.77	122.20
1	Aa	431	G	N3-C4-C5	-6.33	125.44	128.60
23	AA	975	U	N1-C2-O2	6.31	127.22	122.80
23	AA	2262	G	O5'-P-OP1	-6.30	100.03	105.70
23	AA	2747	U	C2-N1-C1'	6.30	125.26	117.70
23	AA	1692	C	N1-C2-O2	6.29	122.68	118.90
1	Aa	424	G	N3-C4-N9	6.29	129.78	126.00
23	AA	575	G	N3-C4-N9	6.29	129.78	126.00
1	Aa	762	C	C2-N1-C1'	6.26	125.69	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	862	C	N1-C2-O2	6.26	122.66	118.90
23	AA	988	C	N1-C2-O2	6.26	122.66	118.90
1	Aa	902	C	N1-C2-O2	6.26	122.65	118.90
1	Aa	797	U	C2-N1-C1'	6.24	125.19	117.70
24	AB	94	C	N1-C2-O2	6.22	122.63	118.90
23	AA	1804	U	N1-C2-O2	6.21	127.15	122.80
1	Aa	599	U	N1-C2-O2	6.20	127.14	122.80
23	AA	184	C	C2-N1-C1'	6.19	125.61	118.80
23	AA	1953	U	C2-N1-C1'	6.18	125.12	117.70
23	AA	1227	U	C2-N1-C1'	6.18	125.11	117.70
23	AA	1579	C	N3-C2-O2	-6.17	117.58	121.90
1	Aa	1168	C	N1-C2-O2	6.17	122.60	118.90
23	AA	1914	C	N3-C2-O2	-6.17	117.58	121.90
1	Aa	835	U	N1-C2-O2	6.17	127.12	122.80
18	Ar	60	LEU	CA-CB-CG	6.16	129.48	115.30
1	Aa	387	C	C2-N1-C1'	6.16	125.57	118.80
1	Aa	460	A	C2-N3-C4	6.14	113.67	110.60
1	Aa	1001	U	P-O3'-C3'	6.14	127.07	119.70
23	AA	2845	G	N3-C2-N2	-6.14	115.60	119.90
1	Aa	502	C	C2-N1-C1'	6.13	125.54	118.80
23	AA	882	C	C6-N1-C1'	-6.13	113.45	120.80
1	Aa	524	U	C2-N1-C1'	6.12	125.04	117.70
23	AA	593	U	C6-N1-C1'	-6.09	112.67	121.20
1	Aa	762	C	N1-C2-O2	6.09	122.55	118.90
23	AA	2845	G	N3-C4-N9	-6.08	122.36	126.00
23	AA	575	G	C8-N9-C1'	-6.07	119.11	127.00
23	AA	2112	C	N1-C2-O2	6.04	122.53	118.90
36	AN	15	LEU	CA-CB-CG	6.04	129.18	115.30
1	Aa	1140	C	N1-C2-O2	6.02	122.51	118.90
1	Aa	162	A	C2-N3-C4	6.02	113.61	110.60
1	Aa	1314	G	P-O3'-C3'	6.01	126.92	119.70
1	Aa	969	U	P-O3'-C3'	6.01	126.92	119.70
1	Aa	1096	U	C2-N1-C1'	5.99	124.88	117.70
23	AA	2347	A	C2-N3-C4	5.97	113.58	110.60
1	Aa	1096	U	N1-C2-O2	5.97	126.98	122.80
23	AA	882	C	N3-C2-O2	-5.97	117.72	121.90
23	AA	463	C	N1-C2-O2	5.96	122.48	118.90
23	AA	987	U	P-O3'-C3'	5.96	126.86	119.70
23	AA	882	C	N1-C2-O2	5.96	122.48	118.90
23	AA	576	U	P-O3'-C3'	5.95	126.84	119.70
23	AA	2223	C	C2-N1-C1'	5.95	125.34	118.80
23	AA	1179	C	C6-N1-C1'	-5.95	113.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1267	A	P-O3'-C3'	5.95	126.84	119.70
1	Aa	1325	U	C2-N1-C1'	5.93	124.82	117.70
23	AA	439	U	C6-N1-C1'	-5.93	112.89	121.20
24	AB	87	C	C6-N1-C2	-5.93	117.93	120.30
23	AA	1731	G	OP1-P-O3'	5.93	118.25	105.20
23	AA	577	A	P-O3'-C3'	5.93	126.81	119.70
23	AA	1179	C	C6-N1-C2	-5.92	117.93	120.30
1	Aa	431	G	C8-N9-C1'	-5.91	119.32	127.00
24	AB	100	U	C6-N1-C1'	-5.90	112.93	121.20
31	AI	89	ASP	CB-CG-OD1	5.90	123.61	118.30
23	AA	2049	U	N1-C2-O2	5.89	126.93	122.80
1	Aa	315	U	N1-C2-O2	5.89	126.92	122.80
23	AA	1768	C	N1-C2-O2	5.88	122.43	118.90
1	Aa	415	A	OP1-P-O3'	5.87	118.12	105.20
23	AA	402	C	N1-C2-O2	5.87	122.42	118.90
1	Aa	415	A	C2-N3-C4	5.86	113.53	110.60
43	AU	53	ILE	C-N-CA	5.86	136.34	121.70
1	Aa	387	C	N1-C2-O2	5.84	122.41	118.90
1	Aa	599	U	N3-C2-O2	-5.84	118.11	122.20
1	Aa	315	U	N3-C2-O2	-5.84	118.11	122.20
23	AA	897	A	C5-C6-N6	-5.84	119.03	123.70
23	AA	2370	U	N1-C2-O2	5.84	126.89	122.80
23	AA	688	A	P-O3'-C3'	5.82	126.68	119.70
1	Aa	336	C	N1-C2-O2	5.80	122.38	118.90
23	AA	2796	C	N1-C2-O2	5.80	122.38	118.90
23	AA	828	A	C4-N9-C1'	5.79	136.72	126.30
23	AA	74	U	N3-C2-O2	-5.79	118.15	122.20
1	Aa	437	U	P-O3'-C3'	5.78	126.64	119.70
23	AA	268	A	O4'-C1'-N9	5.78	112.83	108.20
23	AA	2369	C	N1-C2-O2	5.77	122.36	118.90
1	Aa	1156	A	P-O3'-C3'	5.77	126.62	119.70
23	AA	755	C	N1-C2-O2	5.77	122.36	118.90
23	AA	2742	C	N1-C2-O2	5.76	122.35	118.90
23	AA	1287	U	N1-C2-O2	5.72	126.81	122.80
23	AA	1588	U	O4'-C1'-N1	5.72	112.78	108.20
23	AA	1213	C	N3-C2-O2	-5.70	117.91	121.90
23	AA	759	U	C6-N1-C1'	-5.69	113.24	121.20
23	AA	2749	G	P-O3'-C3'	5.67	126.51	119.70
23	AA	943	C	N1-C2-O2	5.67	122.30	118.90
23	AA	1552	U	N1-C2-O2	5.66	126.76	122.80
23	AA	2361	U	N1-C2-O2	5.66	126.76	122.80
23	AA	1287	U	C2-N1-C1'	5.66	124.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1370	A	P-O3'-C3'	5.65	126.48	119.70
23	AA	1287	U	N3-C2-O2	-5.65	118.24	122.20
1	Aa	486	C	N1-C2-O2	5.65	122.29	118.90
1	Aa	65	G	C4-N9-C1'	5.65	133.84	126.50
23	AA	975	U	N3-C2-O2	-5.63	118.26	122.20
23	AA	1803	G	C4-N9-C1'	5.63	133.82	126.50
23	AA	2370	U	C2-N1-C1'	5.62	124.45	117.70
23	AA	1214	C	N3-C2-O2	-5.61	117.97	121.90
1	Aa	599	U	C6-N1-C1'	-5.61	113.35	121.20
23	AA	593	U	C5-C6-N1	5.60	125.50	122.70
23	AA	1228	A	N7-C8-N9	5.60	116.60	113.80
23	AA	872	U	N1-C2-O2	5.60	126.72	122.80
23	AA	577	A	C2-N3-C4	5.59	113.40	110.60
23	AA	862	C	N3-C2-O2	-5.59	117.99	121.90
1	Aa	1136	U	P-O3'-C3'	5.59	126.40	119.70
23	AA	1845	U	P-O3'-C3'	5.59	126.40	119.70
23	AA	754	U	N1-C2-O2	5.58	126.71	122.80
1	Aa	424	G	C8-N9-C1'	-5.58	119.75	127.00
22	Av	153	MET	CG-SD-CE	-5.56	91.30	100.20
23	AA	1579	C	C6-N1-C2	-5.56	118.08	120.30
23	AA	2761	C	N1-C2-O2	5.56	122.23	118.90
24	AB	69	C	N1-C2-O2	5.56	122.23	118.90
23	AA	1633	A	C2-N3-C4	5.55	113.37	110.60
23	AA	1343	U	C2-N1-C1'	5.54	124.35	117.70
35	AM	22	LEU	CA-CB-CG	5.54	128.05	115.30
23	AA	1692	C	C6-N1-C1'	-5.54	114.16	120.80
1	Aa	553	C	O4'-C1'-N1	5.53	112.63	108.20
1	Aa	1048	C	N1-C2-O2	5.53	122.22	118.90
1	Aa	1122	A	P-O3'-C3'	5.52	126.32	119.70
23	AA	1451	U	N1-C2-O2	5.51	126.66	122.80
23	AA	862	C	C6-N1-C2	-5.51	118.10	120.30
23	AA	256	C	N1-C2-O2	5.50	122.20	118.90
23	AA	1992	C	N1-C2-O2	5.50	122.20	118.90
23	AA	1894	G	C6-C5-N7	-5.49	127.11	130.40
1	Aa	55	C	C6-N1-C1'	-5.49	114.22	120.80
23	AA	2699	U	N3-C2-O2	-5.48	118.36	122.20
1	Aa	387	C	N3-C2-O2	-5.48	118.07	121.90
23	AA	2408	C	N1-C2-O2	5.48	122.19	118.90
23	AA	398	C	N1-C2-O2	5.47	122.18	118.90
23	AA	1049	C	N1-C2-O2	5.45	122.17	118.90
23	AA	1815	C	N1-C2-O2	5.44	122.17	118.90
23	AA	1514	A	N1-C6-N6	5.44	121.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	975	U	C2-N1-C1'	5.43	124.22	117.70
23	AA	1216	U	C2-N1-C1'	5.43	124.21	117.70
23	AA	872	U	N3-C2-O2	-5.41	118.41	122.20
1	Aa	1168	C	C2-N1-C1'	5.41	124.75	118.80
23	AA	2747	U	N3-C2-O2	-5.41	118.42	122.20
24	AB	115	C	N1-C2-O2	5.41	122.14	118.90
1	Aa	486	C	N3-C2-O2	-5.39	118.12	121.90
23	AA	327	G	O4'-C1'-N9	5.39	112.51	108.20
1	Aa	1157	C	N1-C2-O2	5.38	122.13	118.90
23	AA	2321	C	N1-C2-O2	5.38	122.13	118.90
24	AB	94	C	N3-C2-O2	-5.35	118.15	121.90
23	AA	1692	C	N3-C2-O2	-5.34	118.16	121.90
24	AB	100	U	N1-C2-O2	5.34	126.54	122.80
23	AA	2249	G	O4'-C1'-N9	5.34	112.47	108.20
23	AA	2112	C	N3-C2-O2	-5.34	118.16	121.90
25	AC	130	LEU	CA-CB-CG	5.34	127.57	115.30
23	AA	2361	U	N3-C2-O2	-5.33	118.47	122.20
23	AA	1732	U	O5'-P-OP2	-5.33	100.90	105.70
31	AI	64	ARG	CA-CB-CG	5.33	125.13	113.40
1	Aa	411	C	C6-N1-C2	-5.32	118.17	120.30
25	AC	19	LEU	CA-CB-CG	5.32	127.53	115.30
23	AA	2636	U	C2-N1-C1'	5.32	124.08	117.70
23	AA	988	C	N3-C2-O2	-5.31	118.19	121.90
1	Aa	422	A	C2-N3-C4	5.30	113.25	110.60
23	AA	2049	U	N3-C2-O2	-5.30	118.49	122.20
23	AA	340	C	N1-C2-O2	5.30	122.08	118.90
1	Aa	1012	G	C4-N9-C1'	5.29	133.38	126.50
23	AA	575	G	N3-C4-C5	-5.29	125.95	128.60
23	AA	1101	A	C2-N3-C4	5.29	113.25	110.60
23	AA	1758	A	C2-N3-C4	5.28	113.24	110.60
23	AA	2796	C	N3-C2-O2	-5.28	118.20	121.90
1	Aa	55	C	C6-N1-C2	-5.28	118.19	120.30
23	AA	1894	G	N3-C4-C5	-5.28	125.96	128.60
23	AA	2731	C	N1-C2-O2	5.28	122.07	118.90
23	AA	460	C	N1-C2-O2	5.27	122.06	118.90
23	AA	971	U	N1-C2-O2	5.27	126.49	122.80
23	AA	1551	U	O5'-P-OP1	-5.27	100.95	105.70
23	AA	1557	C	N1-C2-O2	5.26	122.06	118.90
23	AA	714	G	C4-N9-C1'	5.26	133.34	126.50
23	AA	394	U	N1-C2-O2	5.23	126.46	122.80
23	AA	2263	C	N1-C2-O2	5.22	122.03	118.90
23	AA	1950	U	N1-C2-O2	5.22	126.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	1451	U	N3-C2-O2	-5.21	118.56	122.20
12	Al	62	LEU	CA-CB-CG	5.20	127.27	115.30
25	AC	13	ARG	CA-CB-CG	5.20	124.84	113.40
23	AA	1101	A	C4-N9-C1'	5.20	135.65	126.30
23	AA	1228	A	O4'-C1'-N9	5.19	112.35	108.20
1	Aa	1063	U	C2-N1-C1'	5.18	123.92	117.70
1	Aa	1188	G	C4-N9-C1'	5.18	133.24	126.50
23	AA	1101	A	N7-C8-N9	5.18	116.39	113.80
23	AA	1214	C	C2-N1-C1'	5.18	124.50	118.80
1	Aa	1096	U	N3-C2-O2	-5.18	118.58	122.20
1	Aa	797	U	N1-C2-O2	5.17	126.42	122.80
32	AJ	6	LEU	CA-CB-CG	5.17	127.19	115.30
32	AJ	61	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	Aa	502	C	N1-C2-O2	5.15	121.99	118.90
23	AA	2263	C	C6-N1-C2	-5.15	118.24	120.30
1	Aa	324	C	C6-N1-C2	-5.14	118.24	120.30
1	Aa	1186	A	C2-N3-C4	5.14	113.17	110.60
6	Af	54	ASP	CB-CG-OD1	5.14	122.92	118.30
1	Aa	99	U	C5-C6-N1	5.14	125.27	122.70
23	AA	1160	C	N3-C2-O2	-5.13	118.31	121.90
23	AA	57	C	N1-C2-O2	5.13	121.98	118.90
23	AA	1587	C	N1-C2-O2	5.13	121.98	118.90
23	AA	1651	C	N3-C2-O2	-5.13	118.31	121.90
23	AA	1953	U	N3-C2-O2	-5.13	118.61	122.20
23	AA	556	U	N1-C2-O2	5.13	126.39	122.80
23	AA	1385	G	P-O3'-C3'	5.13	125.85	119.70
23	AA	1625	U	N3-C2-O2	-5.12	118.62	122.20
23	AA	576	U	C5-C6-N1	5.11	125.25	122.70
1	Aa	542	U	C2-N1-C1'	5.11	123.83	117.70
23	AA	1758	A	C4-N9-C1'	5.10	135.48	126.30
24	AB	108	U	C6-N1-C1'	-5.10	114.06	121.20
23	AA	1803	G	C8-N9-C1'	-5.10	120.38	127.00
23	AA	754	U	N3-C2-O2	-5.09	118.63	122.20
1	Aa	1114	C	C6-N1-C2	-5.08	118.27	120.30
23	AA	1761	G	N3-C4-C5	5.08	131.14	128.60
1	Aa	488	U	C2-N1-C1'	5.08	123.80	117.70
1	Aa	797	U	N3-C2-O2	-5.08	118.65	122.20
1	Aa	460	A	N3-C4-N9	5.07	131.46	127.40
23	AA	1216	U	N1-C2-O2	5.07	126.35	122.80
42	AT	82	LEU	C-N-CA	5.07	134.38	121.70
23	AA	1380	G	C4-N9-C1'	5.07	133.09	126.50
23	AA	256	C	N3-C2-O2	-5.06	118.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	2819	C	C2-N1-C1'	5.06	124.36	118.80
23	AA	530	C	N1-C2-O2	5.05	121.93	118.90
23	AA	1552	U	C6-N1-C2	-5.04	117.98	121.00
1	Aa	99	U	P-O3'-C3'	5.04	125.74	119.70
23	AA	2369	C	N3-C2-O2	-5.03	118.38	121.90
23	AA	1559	G	N3-C2-N2	-5.03	116.38	119.90
23	AA	1992	C	N3-C2-O2	-5.03	118.38	121.90
2	Ab	20	THR	C-N-CA	5.02	134.26	121.70
1	Aa	1373	A	C2-N3-C4	5.02	113.11	110.60
23	AA	2095	U	N1-C2-O2	5.02	126.31	122.80
23	AA	2224	U	N3-C2-O2	-5.01	118.69	122.20
1	Aa	599	U	O4'-C1'-N1	5.01	112.20	108.20
23	AA	2742	C	N3-C2-O2	-5.00	118.40	121.90
1	Aa	65	G	OP2-P-O3'	5.00	116.21	105.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	AD	158	SER	Peptide
38	AP	50	ALA	Peptide
5	Ae	76	ARG	Peptide
9	Ai	108	ARG	Peptide
12	Al	126	GLY	Peptide
19	As	80	PHE	Peptide
20	At	58	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	224/255 (88%)	213 (95%)	11 (5%)	0	100	100
3	Ac	200/217 (92%)	177 (88%)	23 (12%)	0	100	100
4	Ad	196/200 (98%)	170 (87%)	26 (13%)	0	100	100
5	Ae	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
6	Af	93/98 (95%)	85 (91%)	8 (9%)	0	100	100
7	Ag	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
8	Ah	129/132 (98%)	121 (94%)	8 (6%)	0	100	100
9	Ai	125/132 (95%)	112 (90%)	13 (10%)	0	100	100
10	Aj	95/102 (93%)	88 (93%)	7 (7%)	0	100	100
11	Ak	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
12	Al	133/137 (97%)	118 (89%)	15 (11%)	0	100	100
13	Am	100/121 (83%)	90 (90%)	10 (10%)	0	100	100
14	An	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	Ao	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	Ap	87/91 (96%)	78 (90%)	9 (10%)	0	100	100
17	Aq	78/87 (90%)	72 (92%)	6 (8%)	0	100	100
18	Ar	52/80 (65%)	51 (98%)	1 (2%)	0	100	100
19	As	78/92 (85%)	69 (88%)	9 (12%)	0	100	100
20	At	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
21	Au	50/58 (86%)	48 (96%)	2 (4%)	0	100	100
22	Av	158/190 (83%)	149 (94%)	9 (6%)	0	100	100
25	AC	272/277 (98%)	257 (94%)	15 (6%)	0	100	100
26	AD	213/220 (97%)	194 (91%)	19 (9%)	0	100	100
27	AE	204/207 (99%)	192 (94%)	12 (6%)	0	100	100
28	AF	173/179 (97%)	142 (82%)	31 (18%)	0	100	100
29	AG	173/178 (97%)	155 (90%)	18 (10%)	0	100	100
30	AH	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
31	AI	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
32	AJ	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
33	AK	135/144 (94%)	127 (94%)	8 (6%)	0	100	100
34	AL	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
35	AM	117/119 (98%)	103 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AN	112/116 (97%)	99 (88%)	13 (12%)	0	100	100
37	AO	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
38	AP	100/102 (98%)	93 (93%)	6 (6%)	1 (1%)	15	45
39	AQ	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
40	AR	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
41	AS	101/105 (96%)	89 (88%)	12 (12%)	0	100	100
42	AT	92/217 (42%)	87 (95%)	5 (5%)	0	100	100
43	AU	80/94 (85%)	72 (90%)	8 (10%)	0	100	100
44	AV	56/62 (90%)	53 (95%)	3 (5%)	0	100	100
45	AW	65/73 (89%)	58 (89%)	7 (11%)	0	100	100
46	AX	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	AY	57/84 (68%)	45 (79%)	12 (21%)	0	100	100
48	AZ	46/57 (81%)	40 (87%)	6 (13%)	0	100	100
49	A1	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
50	A2	41/45 (91%)	39 (95%)	2 (5%)	0	100	100
51	A3	62/66 (94%)	57 (92%)	5 (8%)	0	100	100
52	A4	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5508/6027 (91%)	5052 (92%)	455 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	AP	51	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ab	196/221 (89%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ac	138/175 (79%)	138 (100%)	0	100	100
4	Ad	147/175 (84%)	146 (99%)	1 (1%)	84	95
5	Ae	118/131 (90%)	118 (100%)	0	100	100
6	Af	80/86 (93%)	80 (100%)	0	100	100
7	Ag	118/132 (89%)	118 (100%)	0	100	100
8	Ah	111/113 (98%)	109 (98%)	2 (2%)	59	85
9	Ai	86/109 (79%)	84 (98%)	2 (2%)	50	80
10	Aj	81/91 (89%)	80 (99%)	1 (1%)	71	91
11	Ak	82/104 (79%)	82 (100%)	0	100	100
12	Al	111/119 (93%)	110 (99%)	1 (1%)	78	93
13	Am	62/104 (60%)	61 (98%)	1 (2%)	62	86
14	An	48/53 (91%)	46 (96%)	2 (4%)	30	63
15	Ao	77/81 (95%)	76 (99%)	1 (1%)	69	90
16	Ap	73/77 (95%)	71 (97%)	2 (3%)	44	77
17	Aq	65/82 (79%)	65 (100%)	0	100	100
18	Ar	48/68 (71%)	48 (100%)	0	100	100
19	As	67/80 (84%)	67 (100%)	0	100	100
20	At	61/69 (88%)	61 (100%)	0	100	100
21	Au	40/54 (74%)	40 (100%)	0	100	100
22	Av	147/173 (85%)	143 (97%)	4 (3%)	44	77
25	AC	221/224 (99%)	221 (100%)	0	100	100
26	AD	173/177 (98%)	172 (99%)	1 (1%)	86	96
27	AE	168/169 (99%)	167 (99%)	1 (1%)	86	96
28	AF	141/158 (89%)	139 (99%)	2 (1%)	67	89
29	AG	124/155 (80%)	122 (98%)	2 (2%)	62	86
30	AH	122/123 (99%)	121 (99%)	1 (1%)	81	94
31	AI	100/100 (100%)	99 (99%)	1 (1%)	76	92
32	AJ	109/112 (97%)	107 (98%)	2 (2%)	59	85
33	AK	108/119 (91%)	107 (99%)	1 (1%)	78	93
34	AL	96/102 (94%)	95 (99%)	1 (1%)	76	92
35	AM	86/95 (90%)	83 (96%)	3 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	AN	93/102 (91%)	92 (99%)	1 (1%)	73	92
37	AO	96/98 (98%)	95 (99%)	1 (1%)	76	92
38	AP	84/86 (98%)	84 (100%)	0	100	100
39	AQ	89/94 (95%)	88 (99%)	1 (1%)	73	92
40	AR	78/82 (95%)	76 (97%)	2 (3%)	46	77
41	AS	81/90 (90%)	80 (99%)	1 (1%)	71	91
42	AT	78/190 (41%)	78 (100%)	0	100	100
43	AU	63/75 (84%)	60 (95%)	3 (5%)	25	58
44	AV	44/52 (85%)	43 (98%)	1 (2%)	50	80
45	AW	58/66 (88%)	58 (100%)	0	100	100
46	AX	52/53 (98%)	52 (100%)	0	100	100
47	AY	23/75 (31%)	23 (100%)	0	100	100
48	AZ	35/50 (70%)	35 (100%)	0	100	100
49	A1	44/47 (94%)	44 (100%)	0	100	100
50	A2	39/40 (98%)	39 (100%)	0	100	100
51	A3	55/57 (96%)	55 (100%)	0	100	100
52	A4	35/35 (100%)	34 (97%)	1 (3%)	42	76
All	All	4451/5123 (87%)	4408 (99%)	43 (1%)	77	92

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Ad	115	ASN
8	Ah	56	LYS
8	Ah	105	LEU
9	Ai	20	ARG
9	Ai	115	ARG
10	Aj	102	LEU
12	Al	44	ARG
13	Am	57	ARG
14	An	26	ARG
14	An	45	ARG
15	Ao	54	ARG
16	Ap	9	ARG
16	Ap	32	ARG
22	Av	103	ARG

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Mol	Chain	Res	Type
22	Av	151	LEU
22	Av	164	THR
22	Av	179	ASP
26	AD	131	ILE
27	AE	193	VAL
28	AF	69	LYS
28	AF	125	ARG
29	AG	41	MET
29	AG	175	LYS
30	AH	97	ASN
31	AI	122	LEU
32	AJ	30	THR
32	AJ	114	ASN
33	AK	27	VAL
34	AL	29	ARG
35	AM	22	LEU
35	AM	35	ARG
35	AM	87	LYS
36	AN	11	THR
37	AO	4	VAL
39	AQ	98	LYS
40	AR	47	ASN
40	AR	56	MET
41	AS	8	ASN
43	AU	22	ARG
43	AU	61	ARG
43	AU	75	VAL
44	AV	60	THR
52	A4	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	190	ASN
3	Ac	64	ASN
4	Ad	112	GLN
4	Ad	115	ASN
4	Ad	146	GLN
5	Ae	83	HIS
6	Af	70	ASN
7	Ag	67	ASN
9	Ai	33	ASN

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Mol	Chain	Res	Type
9	Ai	77	GLN
11	Ak	22	HIS
11	Ak	40	ASN
11	Ak	101	GLN
12	Al	42	GLN
12	Al	85	HIS
14	An	52	GLN
17	Aq	33	HIS
18	Ar	57	GLN
19	As	22	GLN
20	At	21	ASN
22	Av	82	ASN
22	Av	152	GLN
25	AC	86	ASN
25	AC	133	GLN
25	AC	230	HIS
26	AD	128	GLN
26	AD	148	HIS
26	AD	167	GLN
26	AD	200	ASN
27	AE	75	GLN
28	AF	127	ASN
29	AG	77	GLN
30	AH	48	HIS
30	AH	97	ASN
31	AI	4	GLN
32	AJ	4	HIS
32	AJ	114	ASN
35	AM	43	GLN
36	AN	4	HIS
36	AN	79	HIS
37	AO	37	GLN
37	AO	91	ASN
38	AP	81	ASN
39	AQ	77	ASN
40	AR	47	ASN
41	AS	8	ASN
41	AS	39	ASN
41	AS	44	HIS
43	AU	20	ASN
44	AV	16	ASN
48	AZ	19	HIS

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Mol	Chain	Res	Type
48	AZ	40	HIS
49	A1	26	ASN
49	A1	45	HIS
50	A2	17	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1537/1555 (98%)	461 (29%)	0
23	AA	2895/2923 (99%)	794 (27%)	28 (0%)
24	AB	113/115 (98%)	16 (14%)	0
All	All	4545/4593 (98%)	1271 (27%)	28 (0%)

All (1271) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	6	U
1	Aa	8	G
1	Aa	9	A
1	Aa	10	G
1	Aa	23	G
1	Aa	30	A
1	Aa	33	A
1	Aa	40	G
1	Aa	41	C
1	Aa	45	G
1	Aa	48	C
1	Aa	49	C
1	Aa	50	U
1	Aa	51	A
1	Aa	52	A
1	Aa	59	C
1	Aa	60	A
1	Aa	61	A
1	Aa	62	G
1	Aa	66	A
1	Aa	68	C
1	Aa	69	G
1	Aa	70	A
1	Aa	71	A
1	Aa	75	A

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Mol	Chain	Res	Type
1	Aa	76	C
1	Aa	78	A
1	Aa	82	G
1	Aa	83	C
1	Aa	84	U
1	Aa	85	U
1	Aa	88	U
1	Aa	89	U
1	Aa	92	C
1	Aa	94	G
1	Aa	99	U
1	Aa	100	A
1	Aa	107	G
1	Aa	120	C
1	Aa	129	A
1	Aa	140	A
1	Aa	150	U
1	Aa	162	A
1	Aa	163	C
1	Aa	165	G
1	Aa	183	U
1	Aa	184	A
1	Aa	185	U
1	Aa	186	U
1	Aa	187	U
1	Aa	188	U
1	Aa	191	A
1	Aa	193	C
1	Aa	194	G
1	Aa	197	U
1	Aa	199	G
1	Aa	200	U
1	Aa	201	U
1	Aa	203	A
1	Aa	204	A
1	Aa	206	A
1	Aa	208	U
1	Aa	209	G
1	Aa	210	A
1	Aa	211	A
1	Aa	213	G
1	Aa	219	C

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Mol	Chain	Res	Type
1	Aa	220	U
1	Aa	221	U
1	Aa	222	G
1	Aa	224	U
1	Aa	228	A
1	Aa	230	U
1	Aa	231	U
1	Aa	234	A
1	Aa	252	U
1	Aa	253	U
1	Aa	255	G
1	Aa	256	C
1	Aa	257	U
1	Aa	258	A
1	Aa	259	G
1	Aa	264	U
1	Aa	267	G
1	Aa	269	U
1	Aa	274	G
1	Aa	275	C
1	Aa	279	C
1	Aa	289	G
1	Aa	291	U
1	Aa	297	G
1	Aa	301	A
1	Aa	309	G
1	Aa	335	A
1	Aa	336	C
1	Aa	337	A
1	Aa	339	G
1	Aa	352	A
1	Aa	354	G
1	Aa	355	G
1	Aa	356	G
1	Aa	358	G
1	Aa	359	G
1	Aa	360	C
1	Aa	362	G
1	Aa	364	A
1	Aa	375	U
1	Aa	376	U
1	Aa	380	C

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Mol	Chain	Res	Type
1	Aa	381	A
1	Aa	389	A
1	Aa	392	G
1	Aa	395	U
1	Aa	406	C
1	Aa	411	C
1	Aa	412	G
1	Aa	413	U
1	Aa	414	G
1	Aa	415	A
1	Aa	416	G
1	Aa	417	U
1	Aa	418	G
1	Aa	419	A
1	Aa	420	U
1	Aa	421	G
1	Aa	422	A
1	Aa	423	A
1	Aa	424	G
1	Aa	425	G
1	Aa	426	U
1	Aa	430	C
1	Aa	431	G
1	Aa	432	G
1	Aa	434	U
1	Aa	437	U
1	Aa	438	A
1	Aa	440	A
1	Aa	441	A
1	Aa	442	C
1	Aa	449	A
1	Aa	450	U
1	Aa	451	U
1	Aa	452	A
1	Aa	456	A
1	Aa	458	G
1	Aa	460	A
1	Aa	461	C
1	Aa	464	A
1	Aa	465	U
1	Aa	484	A
1	Aa	485	U

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Mol	Chain	Res	Type
1	Aa	486	C
1	Aa	487	U
1	Aa	488	U
1	Aa	492	G
1	Aa	499	A
1	Aa	503	A
1	Aa	504	G
1	Aa	505	A
1	Aa	506	A
1	Aa	507	A
1	Aa	513	G
1	Aa	514	G
1	Aa	516	U
1	Aa	517	A
1	Aa	519	C
1	Aa	522	C
1	Aa	526	C
1	Aa	529	G
1	Aa	532	G
1	Aa	535	G
1	Aa	539	U
1	Aa	541	A
1	Aa	542	U
1	Aa	543	A
1	Aa	548	G
1	Aa	554	A
1	Aa	555	A
1	Aa	567	A
1	Aa	570	U
1	Aa	571	A
1	Aa	580	A
1	Aa	581	A
1	Aa	584	C
1	Aa	585	G
1	Aa	596	G
1	Aa	603	A
1	Aa	610	A
1	Aa	619	C
1	Aa	628	C
1	Aa	638	G
1	Aa	639	G
1	Aa	640	G

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Mol	Chain	Res	Type
1	Aa	641	U
1	Aa	642	C
1	Aa	647	G
1	Aa	649	A
1	Aa	650	A
1	Aa	657	A
1	Aa	661	U
1	Aa	666	G
1	Aa	670	A
1	Aa	673	A
1	Aa	674	G
1	Aa	695	A
1	Aa	696	G
1	Aa	702	A
1	Aa	703	A
1	Aa	711	G
1	Aa	712	A
1	Aa	724	A
1	Aa	729	A
1	Aa	731	U
1	Aa	739	G
1	Aa	756	A
1	Aa	763	G
1	Aa	772	C
1	Aa	781	G
1	Aa	798	A
1	Aa	801	U
1	Aa	813	C
1	Aa	818	C
1	Aa	823	A
1	Aa	825	C
1	Aa	826	G
1	Aa	827	A
1	Aa	829	G
1	Aa	835	U
1	Aa	836	A
1	Aa	840	G
1	Aa	847	G
1	Aa	850	U
1	Aa	852	C
1	Aa	853	C
1	Aa	854	G

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Mol	Chain	Res	Type
1	Aa	881	A
1	Aa	894	G
1	Aa	898	A
1	Aa	910	A
1	Aa	911	G
1	Aa	923	A
1	Aa	924	A
1	Aa	935	G
1	Aa	943	C
1	Aa	944	A
1	Aa	949	C
1	Aa	950	G
1	Aa	953	G
1	Aa	954	G
1	Aa	955	A
1	Aa	956	G
1	Aa	958	A
1	Aa	959	U
1	Aa	961	U
1	Aa	969	U
1	Aa	970	U
1	Aa	972	G
1	Aa	973	A
1	Aa	974	A
1	Aa	975	G
1	Aa	977	A
1	Aa	978	A
1	Aa	980	G
1	Aa	983	A
1	Aa	984	A
1	Aa	985	G
1	Aa	986	A
1	Aa	991	U
1	Aa	1001	U
1	Aa	1002	G
1	Aa	1003	A
1	Aa	1007	C
1	Aa	1008	C
1	Aa	1011	U
1	Aa	1012	G
1	Aa	1013	A
1	Aa	1015	A

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Mol	Chain	Res	Type
1	Aa	1016	A
1	Aa	1017	C
1	Aa	1022	G
1	Aa	1023	A
1	Aa	1026	U
1	Aa	1032	C
1	Aa	1033	U
1	Aa	1035	C
1	Aa	1036	C
1	Aa	1038	C
1	Aa	1039	U
1	Aa	1041	C
1	Aa	1042	G
1	Aa	1043	G
1	Aa	1047	A
1	Aa	1048	C
1	Aa	1052	G
1	Aa	1055	A
1	Aa	1056	C
1	Aa	1057	A
1	Aa	1064	G
1	Aa	1065	C
1	Aa	1066	A
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1091	A
1	Aa	1092	G
1	Aa	1094	U
1	Aa	1096	U
1	Aa	1101	U
1	Aa	1105	G
1	Aa	1106	U
1	Aa	1109	C
1	Aa	1112	A
1	Aa	1113	A
1	Aa	1115	G
1	Aa	1119	G
1	Aa	1123	C
1	Aa	1130	G
1	Aa	1135	G
1	Aa	1136	U
1	Aa	1137	U

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Mol	Chain	Res	Type
1	Aa	1138	G
1	Aa	1141	A
1	Aa	1142	U
1	Aa	1143	C
1	Aa	1146	U
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1150	U
1	Aa	1151	U
1	Aa	1154	G
1	Aa	1156	A
1	Aa	1157	C
1	Aa	1165	U
1	Aa	1167	A
1	Aa	1168	C
1	Aa	1169	U
1	Aa	1172	C
1	Aa	1173	G
1	Aa	1174	G
1	Aa	1175	U
1	Aa	1177	A
1	Aa	1178	C
1	Aa	1179	A
1	Aa	1181	A
1	Aa	1187	G
1	Aa	1188	G
1	Aa	1189	A
1	Aa	1190	A
1	Aa	1191	G
1	Aa	1194	G
1	Aa	1202	C
1	Aa	1203	G
1	Aa	1206	A
1	Aa	1207	A
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1210	C
1	Aa	1211	A
1	Aa	1216	G
1	Aa	1222	U
1	Aa	1224	U
1	Aa	1225	G

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Mol	Chain	Res	Type
1	Aa	1226	A
1	Aa	1228	U
1	Aa	1230	G
1	Aa	1234	U
1	Aa	1235	A
1	Aa	1236	C
1	Aa	1238	C
1	Aa	1243	G
1	Aa	1246	A
1	Aa	1248	A
1	Aa	1250	U
1	Aa	1251	G
1	Aa	1256	A
1	Aa	1260	A
1	Aa	1266	C
1	Aa	1267	A
1	Aa	1268	G
1	Aa	1270	G
1	Aa	1274	C
1	Aa	1275	C
1	Aa	1280	G
1	Aa	1281	G
1	Aa	1282	U
1	Aa	1283	C
1	Aa	1286	G
1	Aa	1287	C
1	Aa	1288	A
1	Aa	1289	A
1	Aa	1290	A
1	Aa	1291	U
1	Aa	1292	C
1	Aa	1296	U
1	Aa	1297	A
1	Aa	1300	G
1	Aa	1305	U
1	Aa	1307	U
1	Aa	1308	C
1	Aa	1309	A
1	Aa	1310	G
1	Aa	1311	U
1	Aa	1312	U
1	Aa	1313	C

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Mol	Chain	Res	Type
1	Aa	1314	G
1	Aa	1315	G
1	Aa	1319	G
1	Aa	1320	U
1	Aa	1322	G
1	Aa	1327	C
1	Aa	1329	A
1	Aa	1332	C
1	Aa	1333	G
1	Aa	1335	C
1	Aa	1336	U
1	Aa	1337	A
1	Aa	1338	C
1	Aa	1339	A
1	Aa	1341	G
1	Aa	1345	C
1	Aa	1347	G
1	Aa	1348	G
1	Aa	1356	A
1	Aa	1357	G
1	Aa	1361	U
1	Aa	1363	G
1	Aa	1368	U
1	Aa	1371	G
1	Aa	1373	A
1	Aa	1378	A
1	Aa	1380	G
1	Aa	1387	A
1	Aa	1391	U
1	Aa	1392	C
1	Aa	1393	C
1	Aa	1404	A
1	Aa	1408	A
1	Aa	1419	C
1	Aa	1421	C
1	Aa	1428	A
1	Aa	1429	G
1	Aa	1438	A
1	Aa	1448	G
1	Aa	1451	G
1	Aa	1456	A
1	Aa	1461	U

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Mol	Chain	Res	Type
1	Aa	1462	U
1	Aa	1463	U
1	Aa	1464	A
1	Aa	1466	G
1	Aa	1468	G
1	Aa	1476	U
1	Aa	1483	U
1	Aa	1495	U
1	Aa	1505	G
1	Aa	1508	G
1	Aa	1510	A
1	Aa	1514	A
1	Aa	1515	G
1	Aa	1540	G
1	Aa	1541	G
1	Aa	1543	U
23	AA	11	U
23	AA	15	G
23	AA	27	G
23	AA	28	A
23	AA	34	U
23	AA	36	G
23	AA	43	A
23	AA	51	G
23	AA	52	A
23	AA	53	A
23	AA	55	G
23	AA	63	U
23	AA	70	G
23	AA	71	A
23	AA	74	U
23	AA	75	G
23	AA	83	G
23	AA	84	A
23	AA	90	A
23	AA	92	G
23	AA	93	U
23	AA	96	G
23	AA	101	G
23	AA	102	A
23	AA	104	C
23	AA	117	A

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Mol	Chain	Res	Type
23	AA	119	U
23	AA	124	A
23	AA	141	U
23	AA	148	U
23	AA	149	U
23	AA	152	C
23	AA	156	A
23	AA	157	U
23	AA	158	G
23	AA	161	A
23	AA	164	A
23	AA	167	U
23	AA	168	A
23	AA	170	C
23	AA	172	U
23	AA	173	A
23	AA	177	G
23	AA	178	A
23	AA	180	G
23	AA	184	C
23	AA	185	A
23	AA	199	A
23	AA	202	A
23	AA	213	C
23	AA	215	G
23	AA	216	A
23	AA	218	G
23	AA	219	A
23	AA	224	A
23	AA	225	A
23	AA	233	U
23	AA	246	U
23	AA	251	G
23	AA	255	G
23	AA	268	A
23	AA	269	G
23	AA	270	C
23	AA	279	A
23	AA	280	C
23	AA	285	U
23	AA	286	U
23	AA	287	G

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Mol	Chain	Res	Type
23	AA	292	U
23	AA	293	U
23	AA	298	U
23	AA	299	U
23	AA	300	G
23	AA	301	U
23	AA	302	A
23	AA	307	A
23	AA	309	U
23	AA	310	C
23	AA	311	U
23	AA	312	A
23	AA	316	G
23	AA	320	U
23	AA	321	U
23	AA	327	G
23	AA	328	G
23	AA	333	C
23	AA	335	U
23	AA	345	C
23	AA	353	A
23	AA	365	A
23	AA	366	G
23	AA	373	A
23	AA	388	A
23	AA	389	A
23	AA	392	U
23	AA	394	U
23	AA	397	U
23	AA	402	C
23	AA	404	U
23	AA	406	A
23	AA	410	G
23	AA	411	A
23	AA	417	A
23	AA	432	G
23	AA	435	A
23	AA	444	C
23	AA	447	A
23	AA	449	U
23	AA	451	U
23	AA	452	G

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Mol	Chain	Res	Type
23	AA	458	A
23	AA	460	C
23	AA	481	C
23	AA	482	U
23	AA	486	G
23	AA	490	C
23	AA	492	G
23	AA	493	A
23	AA	501	C
23	AA	502	C
23	AA	503	A
23	AA	504	G
23	AA	506	A
23	AA	512	A
23	AA	513	G
23	AA	518	A
23	AA	523	A
23	AA	527	G
23	AA	535	G
23	AA	538	G
23	AA	539	G
23	AA	550	A
23	AA	553	A
23	AA	554	C
23	AA	557	G
23	AA	558	A
23	AA	559	A
23	AA	563	G
23	AA	566	U
23	AA	572	C
23	AA	574	A
23	AA	576	U
23	AA	577	A
23	AA	578	G
23	AA	580	C
23	AA	591	A
23	AA	592	A
23	AA	594	G
23	AA	606	G
23	AA	611	U
23	AA	616	G
23	AA	617	A

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Mol	Chain	Res	Type
23	AA	618	A
23	AA	639	U
23	AA	644	C
23	AA	645	A
23	AA	646	A
23	AA	647	G
23	AA	659	A
23	AA	672	A
23	AA	679	G
23	AA	682	A
23	AA	689	A
23	AA	690	U
23	AA	698	U
23	AA	699	U
23	AA	702	U
23	AA	713	A
23	AA	715	A
23	AA	720	A
23	AA	722	A
23	AA	730	A
23	AA	731	U
23	AA	735	C
23	AA	750	A
23	AA	754	U
23	AA	755	C
23	AA	759	U
23	AA	760	A
23	AA	761	A
23	AA	762	C
23	AA	763	A
23	AA	765	U
23	AA	766	G
23	AA	768	A
23	AA	771	G
23	AA	775	A
23	AA	792	U
23	AA	793	G
23	AA	797	A
23	AA	802	G
23	AA	809	A
23	AA	810	A
23	AA	816	G

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Mol	Chain	Res	Type
23	AA	820	G
23	AA	822	G
23	AA	827	A
23	AA	829	U
23	AA	830	U
23	AA	834	A
23	AA	835	U
23	AA	836	C
23	AA	837	G
23	AA	840	C
23	AA	841	C
23	AA	842	U
23	AA	850	G
23	AA	856	U
23	AA	857	C
23	AA	868	A
23	AA	870	C
23	AA	872	U
23	AA	891	A
23	AA	892	U
23	AA	904	G
23	AA	911	A
23	AA	914	G
23	AA	918	G
23	AA	920	A
23	AA	926	G
23	AA	928	C
23	AA	940	U
23	AA	943	C
23	AA	949	C
23	AA	952	A
23	AA	955	A
23	AA	957	C
23	AA	960	C
23	AA	964	U
23	AA	968	A
23	AA	969	A
23	AA	970	U
23	AA	971	U
23	AA	972	A
23	AA	973	A
23	AA	975	U

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Mol	Chain	Res	Type
23	AA	977	A
23	AA	985	A
23	AA	986	G
23	AA	988	C
23	AA	989	A
23	AA	990	G
23	AA	992	A
23	AA	997	G
23	AA	1003	A
23	AA	1005	G
23	AA	1012	G
23	AA	1018	A
23	AA	1019	A
23	AA	1024	A
23	AA	1025	A
23	AA	1027	A
23	AA	1034	A
23	AA	1040	A
23	AA	1043	U
23	AA	1047	G
23	AA	1049	C
23	AA	1056	U
23	AA	1057	A
23	AA	1066	G
23	AA	1067	U
23	AA	1069	G
23	AA	1070	A
23	AA	1076	A
23	AA	1077	U
23	AA	1078	G
23	AA	1086	G
23	AA	1087	C
23	AA	1088	C
23	AA	1089	C
23	AA	1091	G
23	AA	1092	A
23	AA	1093	C
23	AA	1094	A
23	AA	1095	A
23	AA	1100	G
23	AA	1102	U
23	AA	1105	U

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Mol	Chain	Res	Type
23	AA	1106	G
23	AA	1109	U
23	AA	1111	A
23	AA	1113	A
23	AA	1114	A
23	AA	1115	G
23	AA	1116	C
23	AA	1117	A
23	AA	1118	G
23	AA	1119	C
23	AA	1120	C
23	AA	1122	U
23	AA	1126	U
23	AA	1127	U
23	AA	1128	A
23	AA	1132	A
23	AA	1133	G
23	AA	1137	G
23	AA	1138	U
23	AA	1139	A
23	AA	1140	A
23	AA	1143	G
23	AA	1145	U
23	AA	1148	C
23	AA	1150	A
23	AA	1151	G
23	AA	1155	A
23	AA	1156	G
23	AA	1158	G
23	AA	1160	C
23	AA	1161	A
23	AA	1162	C
23	AA	1163	U
23	AA	1174	U
23	AA	1176	U
23	AA	1178	C
23	AA	1179	C
23	AA	1186	A
23	AA	1200	A
23	AA	1201	G
23	AA	1208	A
23	AA	1214	C

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Mol	Chain	Res	Type
23	AA	1215	U
23	AA	1216	U
23	AA	1217	U
23	AA	1218	G
23	AA	1225	G
23	AA	1245	G
23	AA	1250	G
23	AA	1258	A
23	AA	1265	G
23	AA	1267	A
23	AA	1274	G
23	AA	1275	A
23	AA	1276	G
23	AA	1284	A
23	AA	1285	A
23	AA	1286	G
23	AA	1290	G
23	AA	1291	A
23	AA	1294	G
23	AA	1298	G
23	AA	1300	G
23	AA	1304	G
23	AA	1309	G
23	AA	1310	A
23	AA	1320	G
23	AA	1326	C
23	AA	1337	A
23	AA	1338	U
23	AA	1339	U
23	AA	1340	G
23	AA	1342	C
23	AA	1344	A
23	AA	1348	U
23	AA	1349	U
23	AA	1351	C
23	AA	1354	G
23	AA	1358	A
23	AA	1367	C
23	AA	1370	C
23	AA	1386	U
23	AA	1387	C
23	AA	1389	U

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Mol	Chain	Res	Type
23	AA	1392	G
23	AA	1394	U
23	AA	1402	A
23	AA	1405	G
23	AA	1415	A
23	AA	1416	U
23	AA	1417	G
23	AA	1420	U
23	AA	1422	A
23	AA	1423	C
23	AA	1432	A
23	AA	1440	A
23	AA	1443	A
23	AA	1445	C
23	AA	1447	A
23	AA	1450	A
23	AA	1451	U
23	AA	1453	G
23	AA	1454	U
23	AA	1455	U
23	AA	1457	U
23	AA	1459	A
23	AA	1463	A
23	AA	1464	U
23	AA	1471	A
23	AA	1472	C
23	AA	1481	A
23	AA	1489	A
23	AA	1490	G
23	AA	1491	C
23	AA	1494	G
23	AA	1495	C
23	AA	1496	G
23	AA	1497	A
23	AA	1498	U
23	AA	1499	U
23	AA	1503	U
23	AA	1504	U
23	AA	1510	U
23	AA	1516	C
23	AA	1518	G
23	AA	1519	U

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Mol	Chain	Res	Type
23	AA	1520	A
23	AA	1521	A
23	AA	1525	U
23	AA	1526	G
23	AA	1527	A
23	AA	1532	U
23	AA	1533	A
23	AA	1534	G
23	AA	1536	C
23	AA	1537	A
23	AA	1540	U
23	AA	1550	G
23	AA	1551	U
23	AA	1552	U
23	AA	1553	A
23	AA	1554	A
23	AA	1555	G
23	AA	1556	G
23	AA	1559	G
23	AA	1561	G
23	AA	1569	G
23	AA	1570	G
23	AA	1575	A
23	AA	1576	A
23	AA	1578	A
23	AA	1579	C
23	AA	1580	A
23	AA	1581	U
23	AA	1582	U
23	AA	1583	G
23	AA	1584	U
23	AA	1586	U
23	AA	1587	C
23	AA	1591	G
23	AA	1594	U
23	AA	1605	A
23	AA	1606	C
23	AA	1613	G
23	AA	1616	A
23	AA	1625	U
23	AA	1627	G
23	AA	1629	U

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Mol	Chain	Res	Type
23	AA	1630	A
23	AA	1631	G
23	AA	1632	A
23	AA	1633	A
23	AA	1634	A
23	AA	1635	A
23	AA	1636	U
23	AA	1639	G
23	AA	1652	A
23	AA	1653	A
23	AA	1654	A
23	AA	1661	C
23	AA	1666	A
23	AA	1675	G
23	AA	1679	A
23	AA	1683	U
23	AA	1684	A
23	AA	1690	A
23	AA	1691	G
23	AA	1692	C
23	AA	1693	G
23	AA	1718	G
23	AA	1719	C
23	AA	1732	U
23	AA	1737	U
23	AA	1738	C
23	AA	1740	G
23	AA	1745	A
23	AA	1747	G
23	AA	1757	U
23	AA	1758	A
23	AA	1759	G
23	AA	1760	G
23	AA	1761	G
23	AA	1762	U
23	AA	1765	A
23	AA	1768	C
23	AA	1771	A
23	AA	1772	G
23	AA	1790	G
23	AA	1791	G
23	AA	1797	G

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Mol	Chain	Res	Type
23	AA	1800	A
23	AA	1806	U
23	AA	1808	U
23	AA	1809	C
23	AA	1811	A
23	AA	1813	A
23	AA	1814	A
23	AA	1818	A
23	AA	1826	G
23	AA	1827	C
23	AA	1828	U
23	AA	1829	A
23	AA	1830	A
23	AA	1835	U
23	AA	1843	U
23	AA	1846	A
23	AA	1856	A
23	AA	1860	C
23	AA	1878	U
23	AA	1879	U
23	AA	1880	A
23	AA	1885	G
23	AA	1889	G
23	AA	1895	C
23	AA	1897	U
23	AA	1898	C
23	AA	1899	U
23	AA	1900	G
23	AA	1901	C
23	AA	1902	G
23	AA	1903	A
23	AA	1904	A
23	AA	1907	U
23	AA	1909	C
23	AA	1911	A
23	AA	1912	A
23	AA	1914	C
23	AA	1918	G
23	AA	1933	G
23	AA	1935	C
23	AA	1937	G
23	AA	1938	U

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Mol	Chain	Res	Type
23	AA	1945	A
23	AA	1950	U
23	AA	1956	G
23	AA	1958	U
23	AA	1963	A
23	AA	1964	A
23	AA	1965	A
23	AA	1966	U
23	AA	1971	U
23	AA	1982	U
23	AA	1989	C
23	AA	1990	C
23	AA	1992	C
23	AA	1994	C
23	AA	1996	A
23	AA	1997	A
23	AA	1998	A
23	AA	1999	G
23	AA	2009	U
23	AA	2018	U
23	AA	2019	G
23	AA	2020	U
23	AA	2023	C
23	AA	2024	A
23	AA	2029	G
23	AA	2030	A
23	AA	2047	A
23	AA	2057	A
23	AA	2058	A
23	AA	2059	G
23	AA	2060	A
23	AA	2062	G
23	AA	2070	C
23	AA	2073	G
23	AA	2075	G
23	AA	2076	A
23	AA	2082	C
23	AA	2083	G
23	AA	2085	A
23	AA	2087	A
23	AA	2088	G
23	AA	2089	A

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Mol	Chain	Res	Type
23	AA	2096	G
23	AA	2097	G
23	AA	2103	U
23	AA	2107	G
23	AA	2109	A
23	AA	2110	G
23	AA	2111	C
23	AA	2115	A
23	AA	2117	A
23	AA	2118	U
23	AA	2119	U
23	AA	2120	G
23	AA	2126	C
23	AA	2129	C
23	AA	2139	A
23	AA	2140	C
23	AA	2143	G
23	AA	2145	U
23	AA	2147	G
23	AA	2153	A
23	AA	2155	C
23	AA	2157	U
23	AA	2158	U
23	AA	2160	G
23	AA	2161	A
23	AA	2164	C
23	AA	2172	C
23	AA	2173	U
23	AA	2174	A
23	AA	2175	G
23	AA	2176	C
23	AA	2183	G
23	AA	2185	A
23	AA	2186	G
23	AA	2188	C
23	AA	2190	C
23	AA	2193	G
23	AA	2194	U
23	AA	2195	G
23	AA	2198	A
23	AA	2204	C
23	AA	2215	U

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Mol	Chain	Res	Type
23	AA	2224	U
23	AA	2225	A
23	AA	2229	C
23	AA	2230	G
23	AA	2231	C
23	AA	2232	A
23	AA	2238	U
23	AA	2240	U
23	AA	2241	C
23	AA	2243	U
23	AA	2252	A
23	AA	2261	G
23	AA	2262	G
23	AA	2263	C
23	AA	2265	G
23	AA	2266	G
23	AA	2290	C
23	AA	2295	A
23	AA	2305	A
23	AA	2306	G
23	AA	2310	C
23	AA	2314	A
23	AA	2316	G
23	AA	2321	C
23	AA	2328	A
23	AA	2329	U
23	AA	2330	G
23	AA	2331	G
23	AA	2332	U
23	AA	2333	U
23	AA	2334	G
23	AA	2335	G
23	AA	2336	A
23	AA	2337	A
23	AA	2345	A
23	AA	2346	U
23	AA	2347	A
23	AA	2352	G
23	AA	2353	U
23	AA	2358	G
23	AA	2361	U
23	AA	2362	A

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Mol	Chain	Res	Type
23	AA	2370	U
23	AA	2374	C
23	AA	2377	C
23	AA	2385	A
23	AA	2388	A
23	AA	2396	A
23	AA	2409	G
23	AA	2410	G
23	AA	2411	A
23	AA	2412	C
23	AA	2429	U
23	AA	2433	C
23	AA	2434	A
23	AA	2441	G
23	AA	2449	C
23	AA	2450	U
23	AA	2451	C
23	AA	2455	G
23	AA	2456	G
23	AA	2457	A
23	AA	2458	U
23	AA	2459	A
23	AA	2460	A
23	AA	2461	A
23	AA	2462	A
23	AA	2463	G
23	AA	2468	C
23	AA	2472	G
23	AA	2474	G
23	AA	2475	A
23	AA	2485	U
23	AA	2486	A
23	AA	2503	A
23	AA	2511	G
23	AA	2521	G
23	AA	2525	C
23	AA	2529	G
23	AA	2530	A
23	AA	2531	U
23	AA	2532	G
23	AA	2540	A
23	AA	2544	C

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Mol	Chain	Res	Type
23	AA	2545	A
23	AA	2547	C
23	AA	2556	G
23	AA	2561	C
23	AA	2562	G
23	AA	2568	A
23	AA	2569	A
23	AA	2570	G
23	AA	2581	U
23	AA	2589	U
23	AA	2592	A
23	AA	2593	A
23	AA	2594	G
23	AA	2599	A
23	AA	2600	C
23	AA	2604	A
23	AA	2605	G
23	AA	2613	C
23	AA	2626	G
23	AA	2629	A
23	AA	2630	G
23	AA	2636	U
23	AA	2640	U
23	AA	2642	U
23	AA	2646	U
23	AA	2648	G
23	AA	2650	G
23	AA	2656	A
23	AA	2657	G
23	AA	2672	G
23	AA	2679	U
23	AA	2681	A
23	AA	2687	A
23	AA	2692	A
23	AA	2695	G
23	AA	2696	G
23	AA	2697	G
23	AA	2699	U
23	AA	2700	G
23	AA	2712	G
23	AA	2716	U
23	AA	2741	G

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Mol	Chain	Res	Type
23	AA	2745	G
23	AA	2750	C
23	AA	2753	U
23	AA	2756	G
23	AA	2757	U
23	AA	2759	G
23	AA	2760	A
23	AA	2761	C
23	AA	2764	G
23	AA	2769	G
23	AA	2771	G
23	AA	2775	A
23	AA	2778	G
23	AA	2784	A
23	AA	2788	A
23	AA	2793	G
23	AA	2794	C
23	AA	2796	C
23	AA	2798	C
23	AA	2800	U
23	AA	2801	C
23	AA	2803	A
23	AA	2804	G
23	AA	2805	A
23	AA	2806	U
23	AA	2808	A
23	AA	2817	A
23	AA	2820	U
23	AA	2821	U
23	AA	2822	C
23	AA	2823	G
23	AA	2824	G
23	AA	2827	A
23	AA	2828	U
23	AA	2829	A
23	AA	2831	G
23	AA	2832	A
23	AA	2838	C
23	AA	2840	A
23	AA	2843	A
23	AA	2850	G
23	AA	2853	U

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Mol	Chain	Res	Type
23	AA	2854	A
23	AA	2855	A
23	AA	2879	G
23	AA	2887	G
23	AA	2888	A
23	AA	2892	G
23	AA	2899	A
23	AA	2900	C
23	AA	2903	A
23	AA	2913	G
23	AA	2914	A
23	AA	2919	A
24	AB	10	U
24	AB	22	G
24	AB	23	U
24	AB	24	C
24	AB	33	U
24	AB	39	G
24	AB	40	C
24	AB	43	A
24	AB	51	A
24	AB	55	A
24	AB	64	A
24	AB	87	C
24	AB	88	G
24	AB	106	G
24	AB	111	C
24	AB	113	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	AA	99	U
23	AA	160	G
23	AA	267	G
23	AA	268	A
23	AA	291	G
23	AA	451	U
23	AA	487	U
23	AA	513	G
23	AA	576	U
23	AA	577	A

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Mol	Chain	Res	Type
23	AA	688	A
23	AA	697	U
23	AA	711	G
23	AA	840	C
23	AA	987	U
23	AA	1024	A
23	AA	1075	G
23	AA	1190	A
23	AA	1267	A
23	AA	1372	C
23	AA	1385	G
23	AA	1731	G
23	AA	1845	U
23	AA	2117	A
23	AA	2450	U
23	AA	2568	A
23	AA	2749	G
23	AA	2783	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 205 ligands modelled in this entry, 205 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	AA	6
1	Aa	1
24	AB	1
13	Am	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	2207:U	O3'	2208:A	P	9.06
1	AA	2132:A	O3'	2133:G	P	8.44
1	AA	1096:C	O3'	1097:U	P	6.77
1	Aa	465:U	O3'	466:G	P	3.97
1	AA	1153:C	O3'	1154:G	P	3.61
1	AA	1448:U	O3'	1449:A	P	3.51
1	AB	114:G	O3'	115:C	P	3.40
1	AA	2217:G	O3'	2218:G	P	3.39
1	Am	93:ARG	C	94:GLY	N	3.26

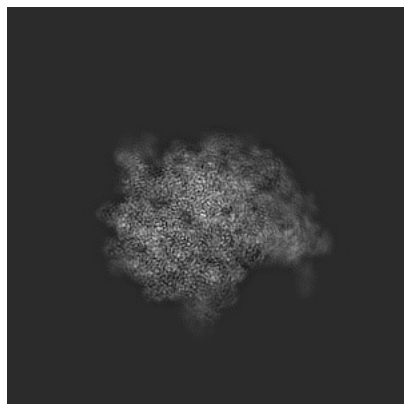
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3640. These allow visual inspection of the internal detail of the map and identification of artifacts.

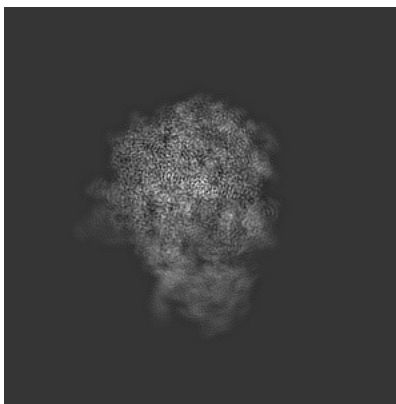
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

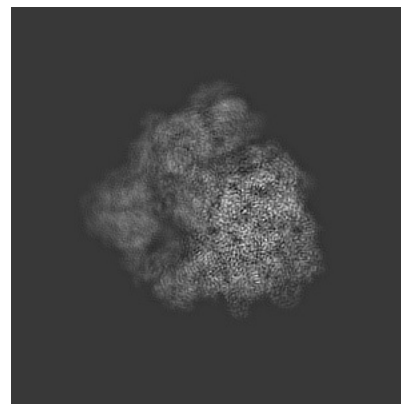
6.1.1 Primary map



X

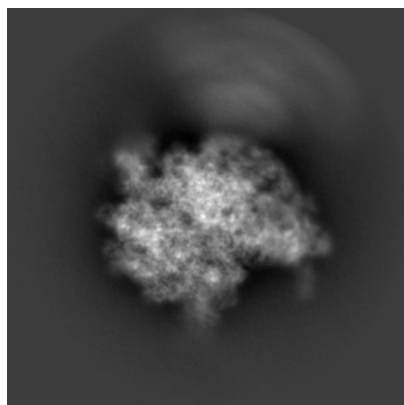


Y

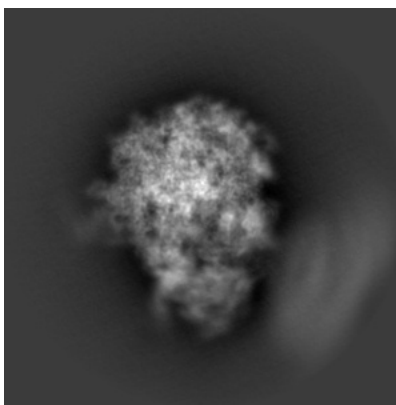


Z

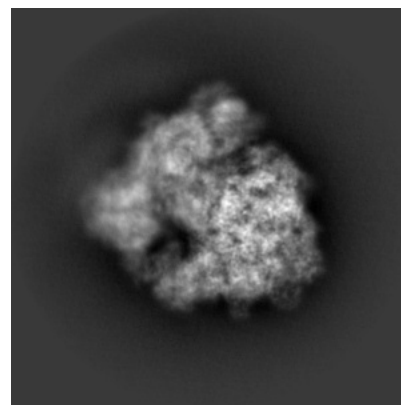
6.1.2 Raw map



X



Y

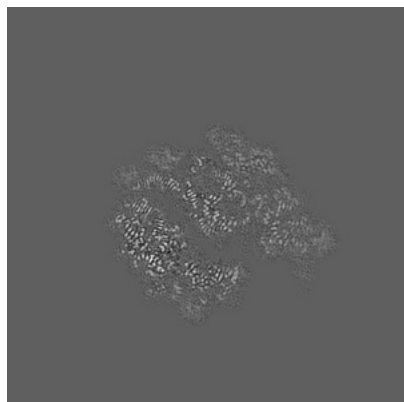


Z

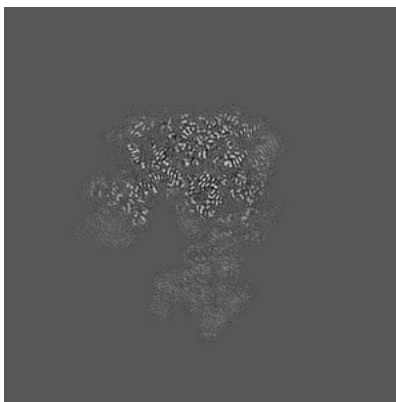
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

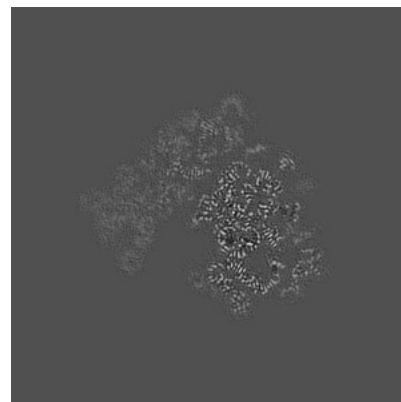
6.2.1 Primary map



X Index: 200

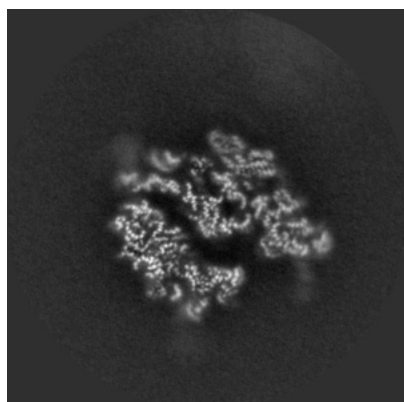


Y Index: 200

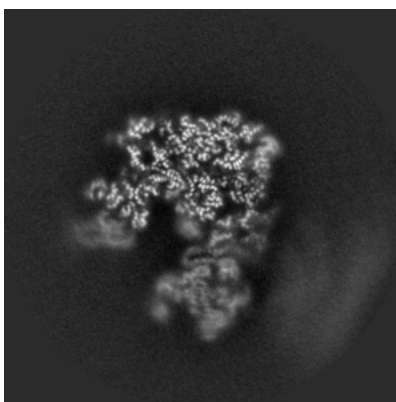


Z Index: 200

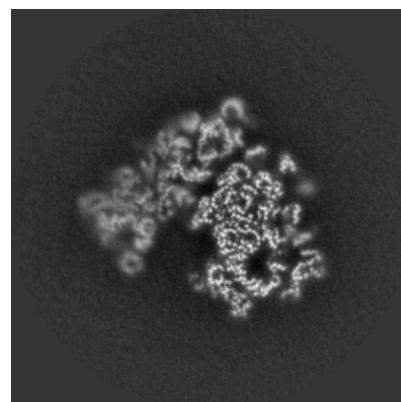
6.2.2 Raw map



X Index: 200



Y Index: 200

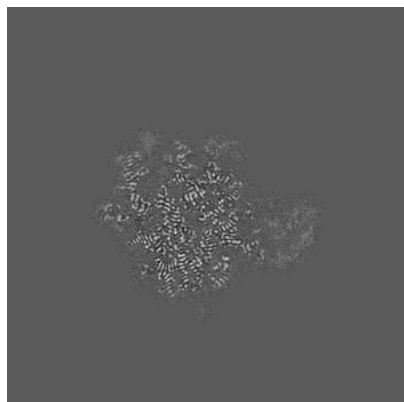


Z Index: 200

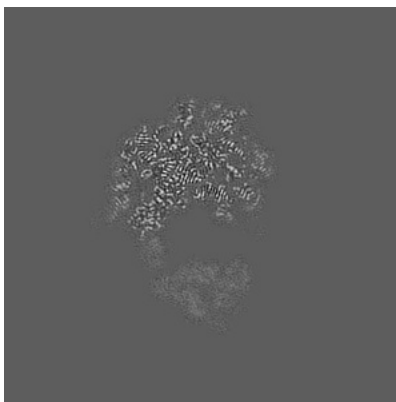
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

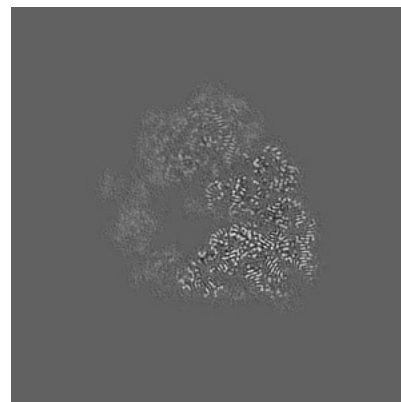
6.3.1 Primary map



X Index: 232

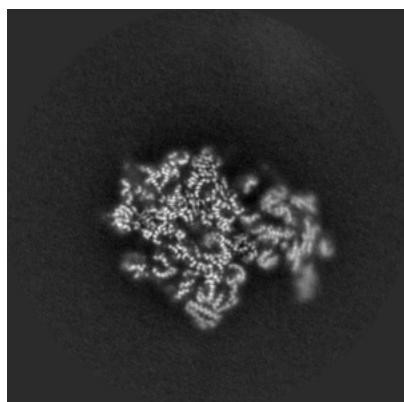


Y Index: 169

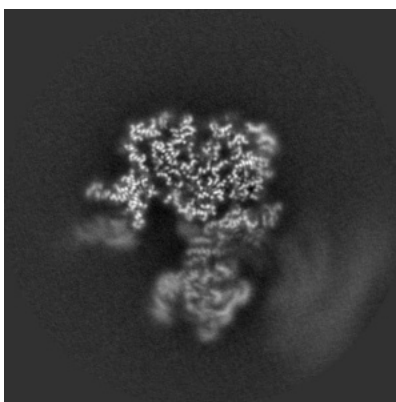


Z Index: 177

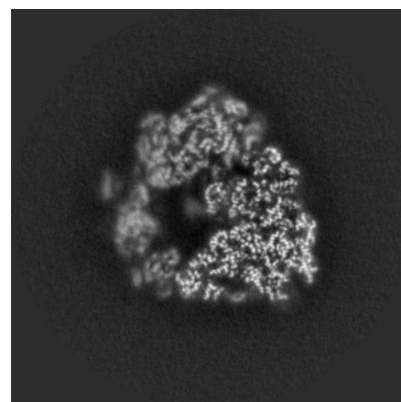
6.3.2 Raw map



X Index: 215



Y Index: 206

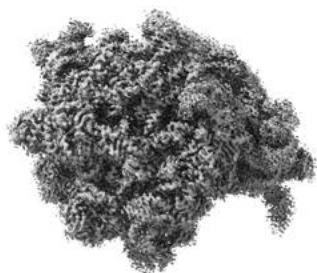


Z Index: 176

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

6.4 Orthogonal surface views [i](#)

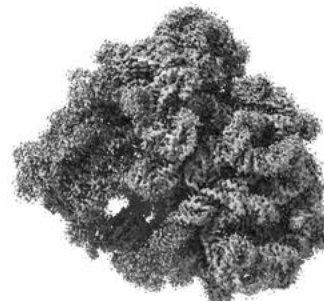
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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

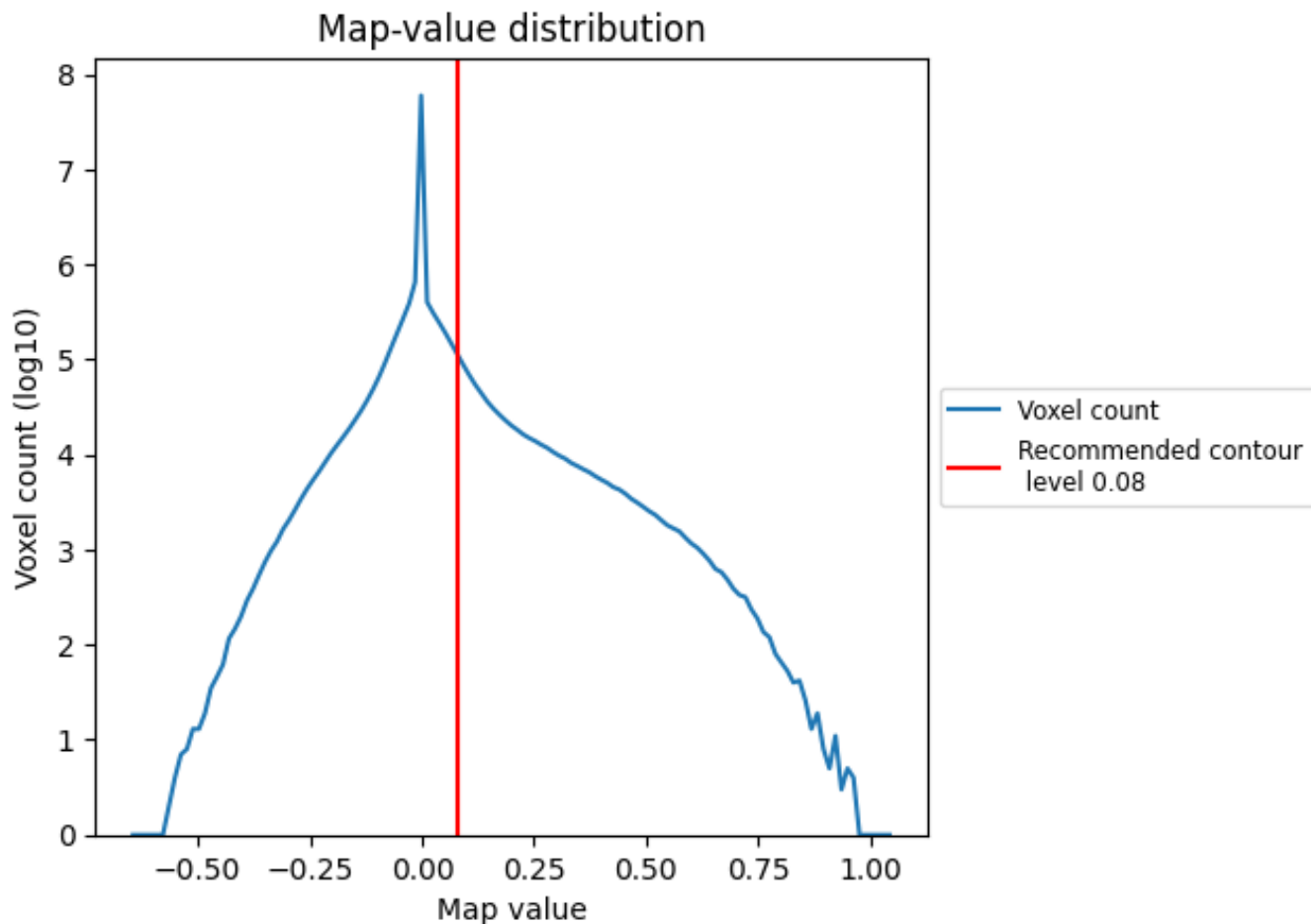
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

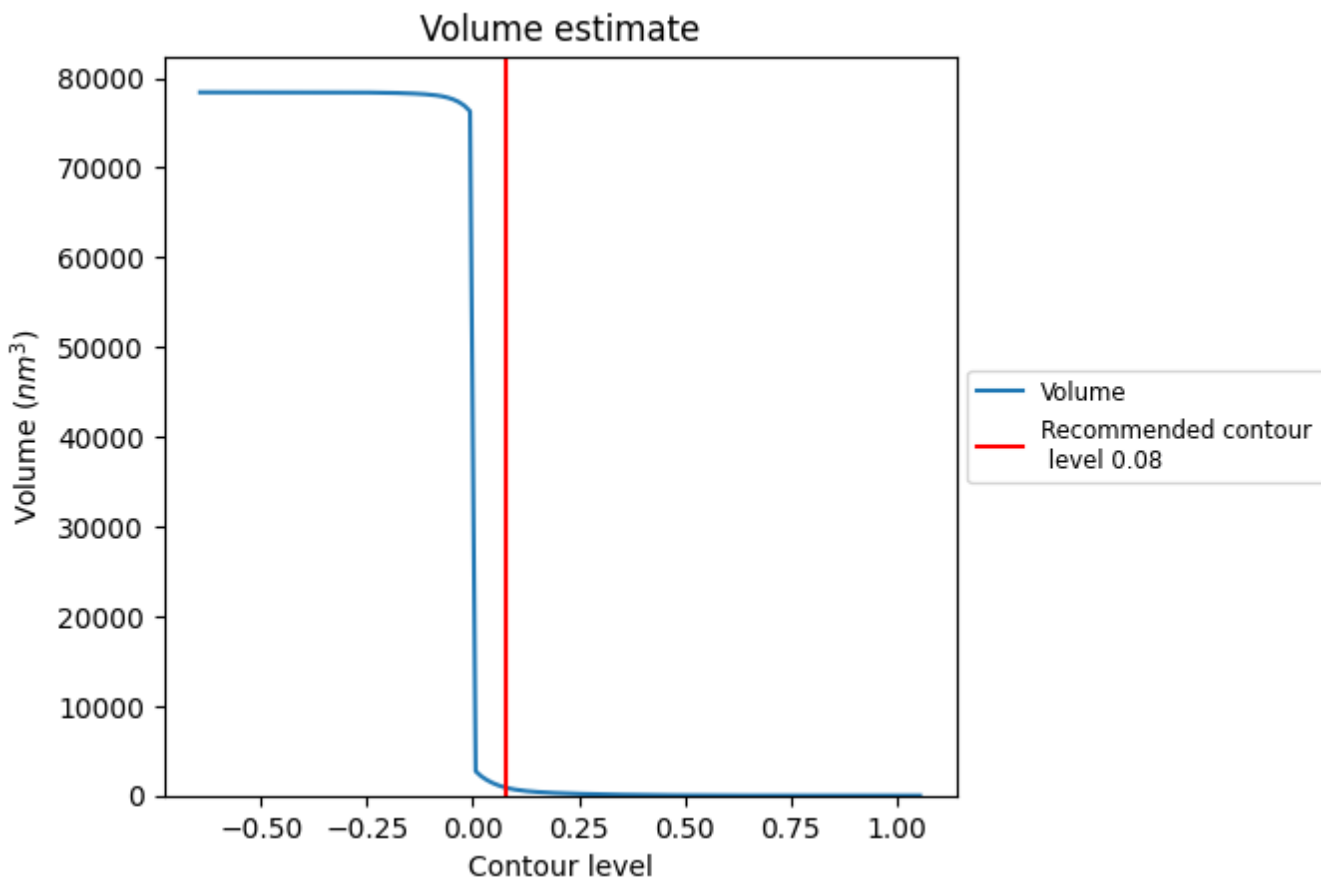
This section contains the results of statistical analysis of the map.

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.

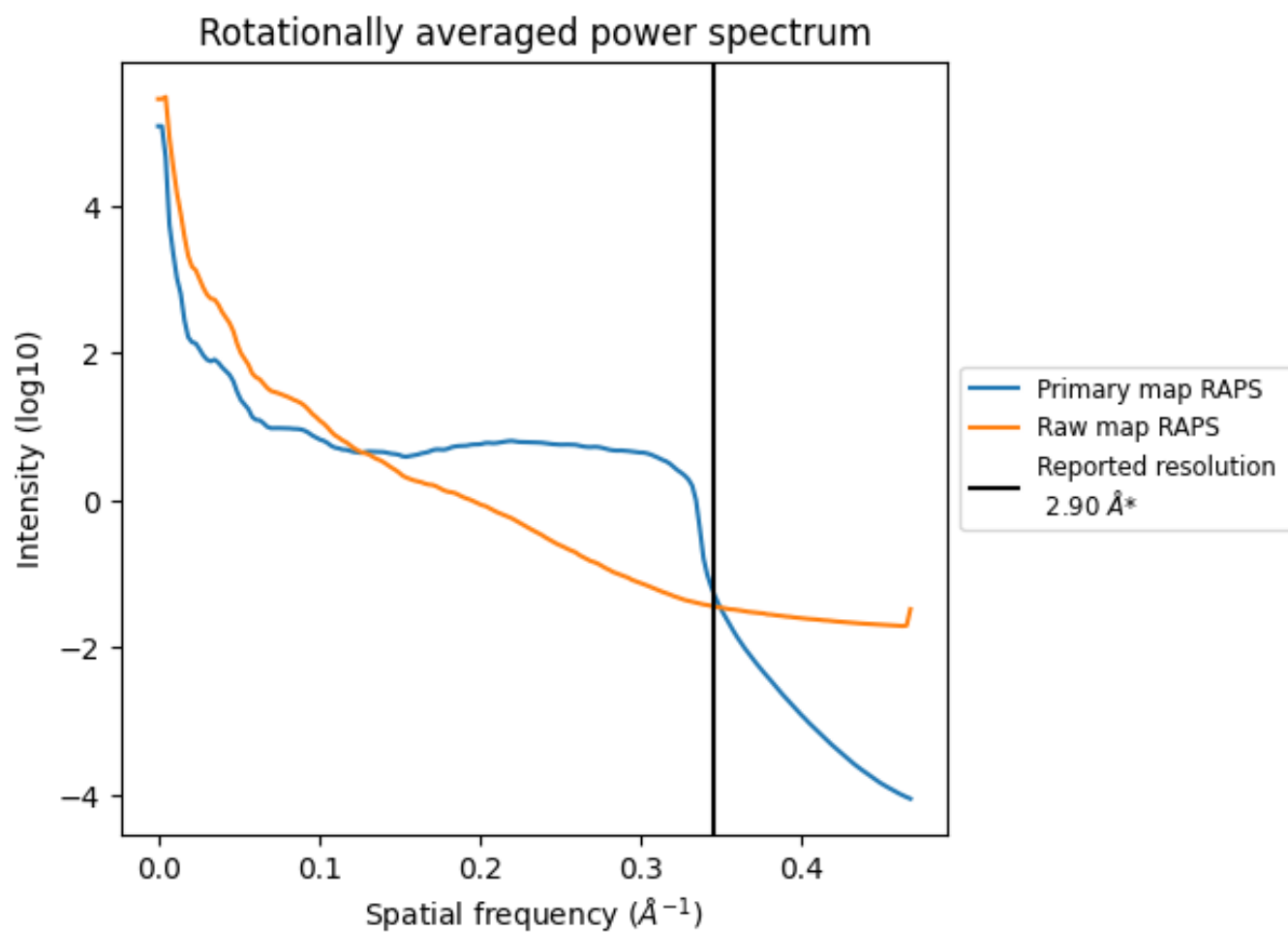
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 863 nm³; this corresponds to an approximate mass of 780 kDa.

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

7.3 Rotationally averaged power spectrum i

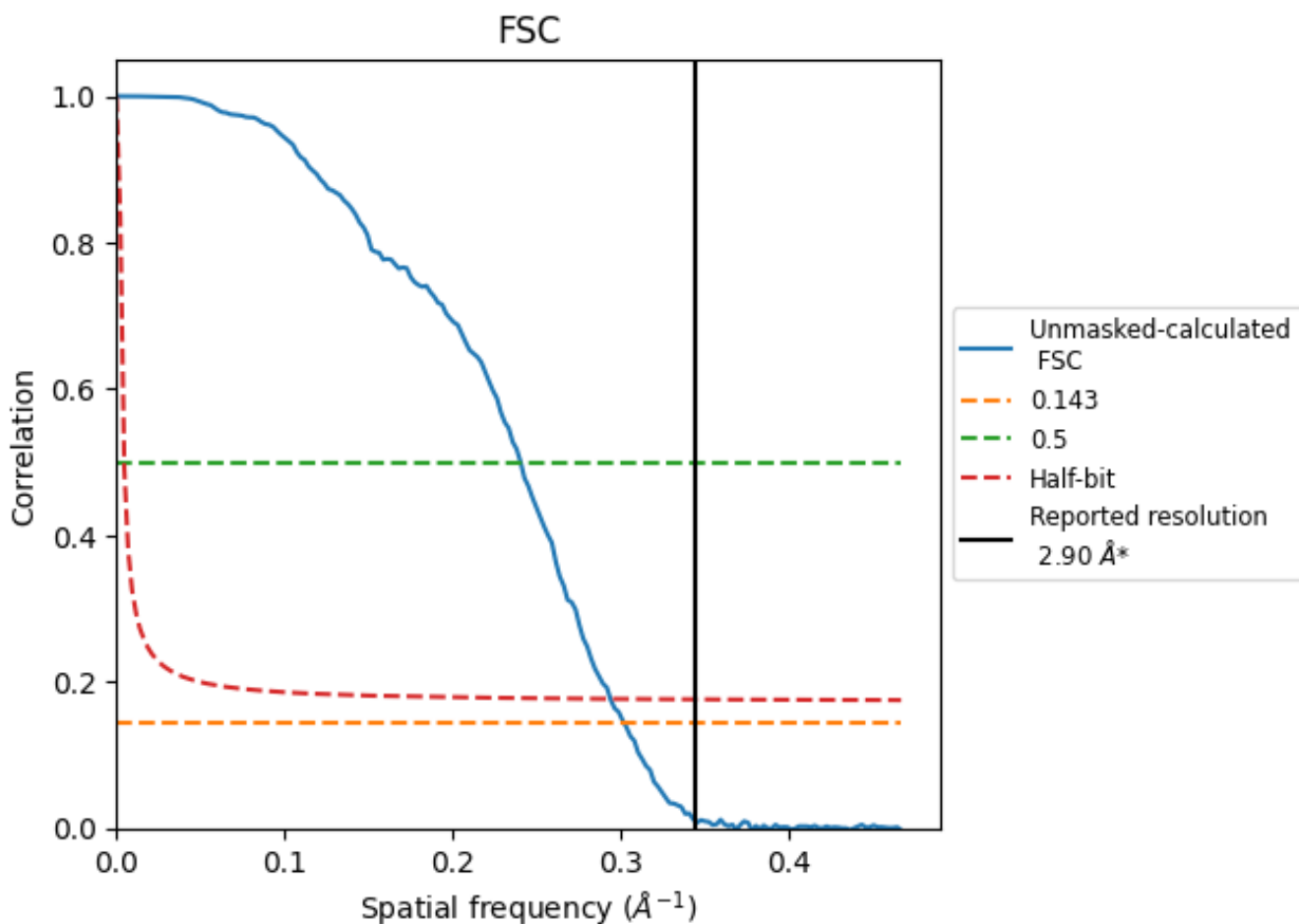


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

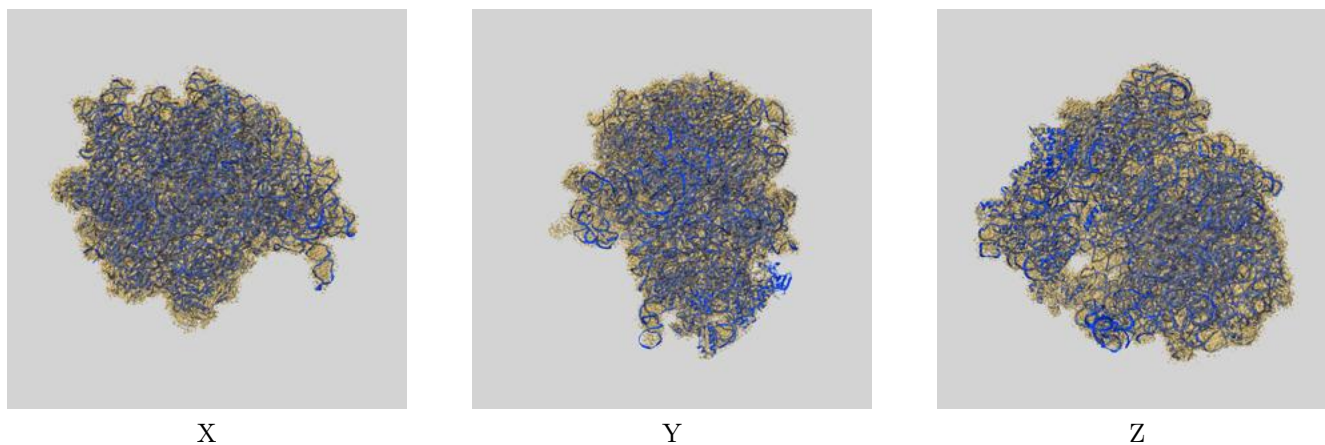
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	4.16	3.40

*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 3.31 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3640 and PDB model 5NGM. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



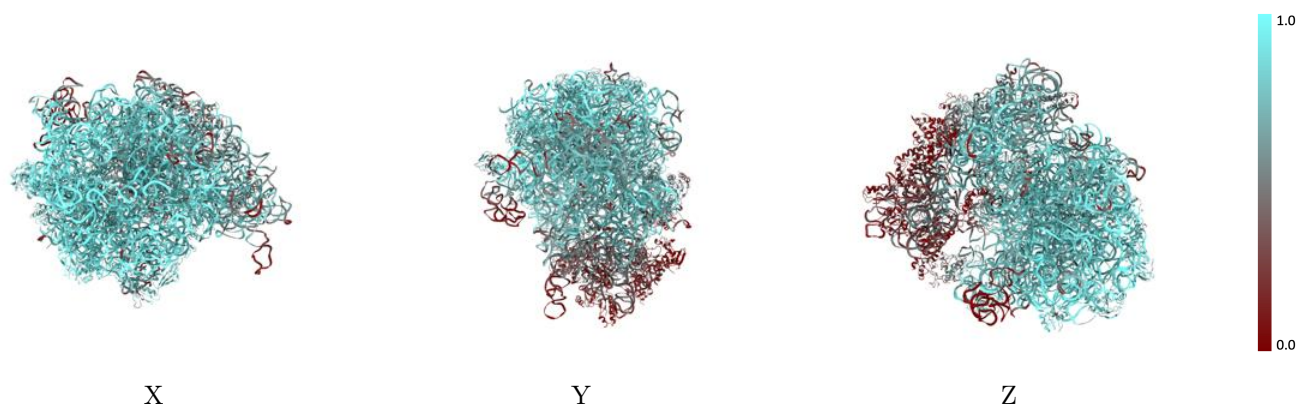
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



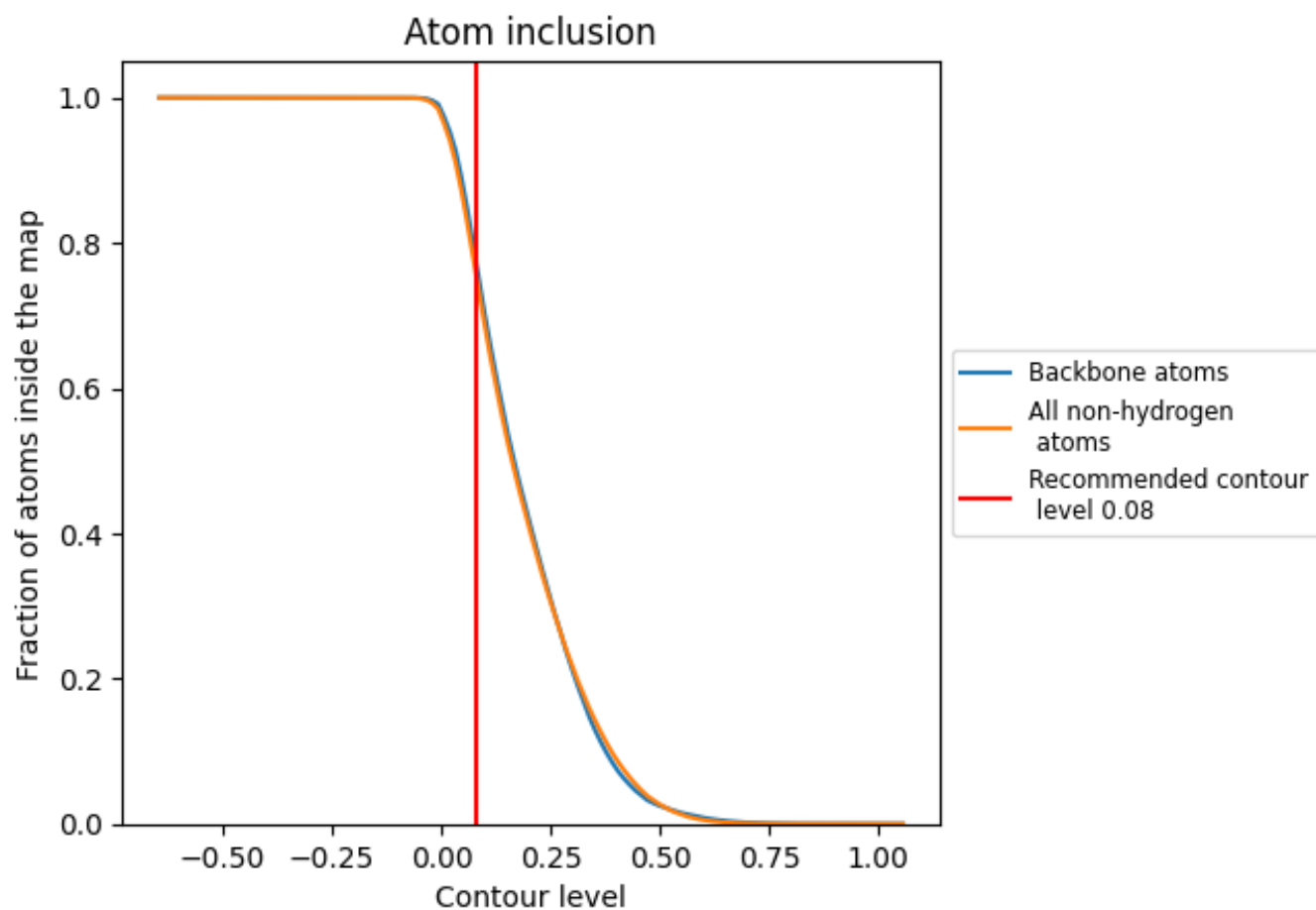
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 75% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.4520
A1	 0.6560	 0.4890
A2	 0.9249	 0.5950
A3	 0.8825	 0.5910
A4	 0.8754	 0.5680
AA	 0.8805	 0.5260
AB	 0.9375	 0.5580
AC	 0.9059	 0.5860
AD	 0.8971	 0.5680
AE	 0.8683	 0.5610
AF	 0.5464	 0.3310
AG	 0.7838	 0.4900
AH	 0.8899	 0.5780
AI	 0.8659	 0.5410
AJ	 0.8843	 0.5680
AK	 0.9017	 0.5920
AL	 0.8954	 0.5720
AM	 0.8078	 0.5050
AN	 0.8533	 0.5500
AO	 0.9186	 0.5980
AP	 0.8856	 0.5640
AQ	 0.8822	 0.5640
AR	 0.8383	 0.5420
AS	 0.7693	 0.4990
AT	 0.7475	 0.5170
AU	 0.8609	 0.5730
AV	 0.7389	 0.5070
AW	 0.7924	 0.5130
AX	 0.8912	 0.5870
AY	 0.3125	 0.2160
AZ	 0.8506	 0.5440
Aa	 0.6727	 0.3630
Ab	 0.1620	 0.1860
Ac	 0.2096	 0.1390
Ad	 0.3692	 0.2370



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Chain	Atom inclusion	Q-score
Ae	 0.4933	 0.3440
Af	 0.4987	 0.3060
Ag	 0.1405	 0.0880
Ah	 0.6670	 0.4180
Ai	 0.1449	 0.1050
Aj	 0.1760	 0.1230
Ak	 0.4580	 0.2860
Al	 0.6706	 0.4360
Am	 0.1697	 0.0950
An	 0.2511	 0.1810
Ao	 0.6566	 0.3970
Ap	 0.5879	 0.3650
Aq	 0.6287	 0.3820
Ar	 0.6215	 0.4040
As	 0.2010	 0.1570
At	 0.5540	 0.3390
Au	 0.0672	 0.1930
Av	 0.2052	 0.1700