



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 08:14 PM EDT

PDB ID : 6P5N
EMDB ID : EMD-20258
Title : Structure of a mammalian 80S ribosome in complex with a single translocated Israeli Acute Paralysis Virus IRES and eRF1
Authors : Acosta-Reyes, F.J.; Neupane, R.; Frank, J.; Fernandez, I.S.
Deposited on : 2019-05-30
Resolution : 3.20 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:

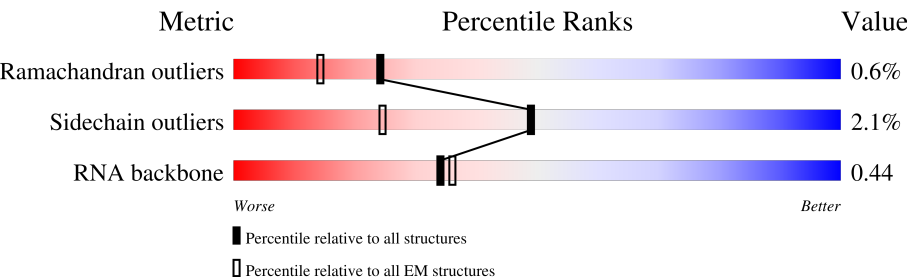
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





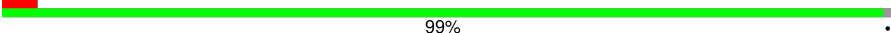
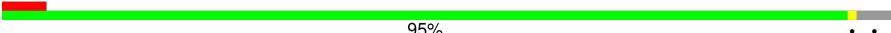
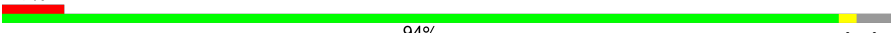















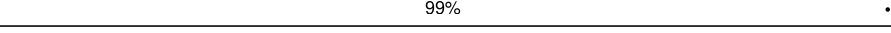
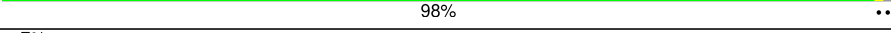


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	5	3594	
2	7	119	
3	8	156	
4	AA	257	
5	AB	402	
6	AC	392	
7	AD	297	
8	AE	291	

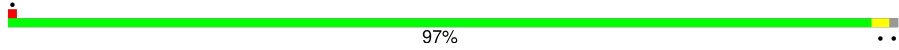

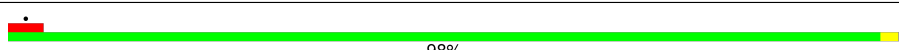
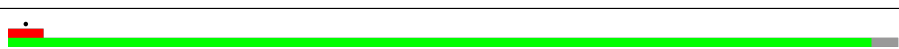
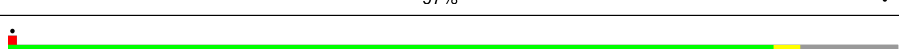
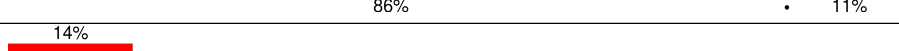
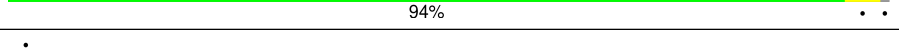
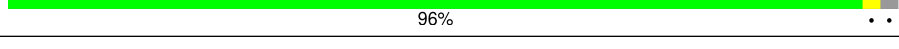
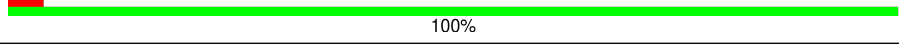
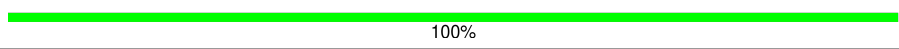
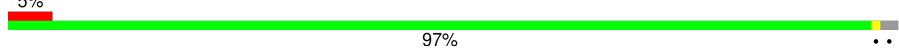

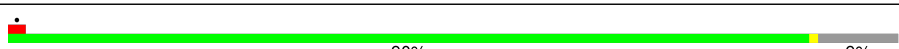


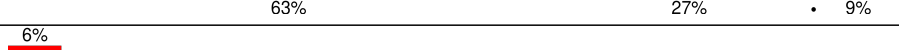




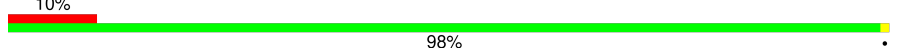


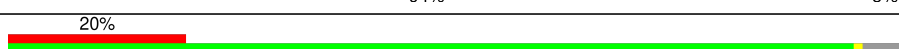
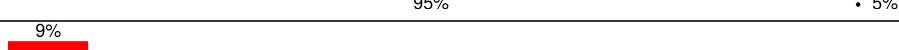
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Mol	Chain	Length	Quality of chain
9	AF	249	
10	AG	242	
11	AH	192	
12	AI	214	
13	AJ	178	
14	AL	211	
15	AM	198	
16	AN	204	
17	AO	203	
18	AP	184	
19	AQ	188	
20	AR	196	
21	AS	176	
22	AT	160	
23	AU	128	
24	AV	140	
25	AW	157	
26	AX	156	
27	AY	145	
28	AZ	136	
29	Aa	148	
30	Ab	226	
31	Ac	115	
32	Ad	125	
33	Ae	135	

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Mol	Chain	Length	Quality of chain
34	Af	110	
35	Ag	126	
36	Ah	123	
37	Ai	105	
38	Aj	97	
39	Ak	70	
40	Al	51	
41	Am	52	
42	An	25	
43	Ao	106	
44	Ap	92	
45	Ar	137	
46	AK	217	
47	2	1869	
48	B	295	
49	C	264	
50	D	255	
51	E	281	
52	F	263	
53	G	204	
54	H	249	
55	I	194	
56	J	207	
57	K	194	
58	L	149	

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Mol	Chain	Length	Quality of chain
59	M	158	
60	N	132	
61	O	151	
62	P	151	
63	Q	145	
64	R	172	
65	S	135	
66	T	152	
67	U	145	
68	V	119	
69	W	83	
70	X	130	
71	Y	143	
72	Z	134	
73	a	125	
74	b	115	
75	c	84	
76	d	69	
77	e	56	
78	f	133	
79	g	156	
80	h	317	
81	Aq	437	
82	1	251	

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 219295 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3594	Total	C	N	O	P	0	0
			77074	34325	14116	25039	3594		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	248	Total	C	N	O	S	0	0
			1895	1186	389	314	6		

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 7 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 8 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 9 is a protein called L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	225	Total	C	N	O	S	0	0
			1819	1161	351	303	4		

- Molecule 11 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 13 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 14 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	201	Total	C	N	O	S	0	0
			1627	1020	341	262	4		

- Molecule 15 is a protein called L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 16 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AO	199	Total	C	N	O	S	0	0
			1631	1052	319	255	5		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	187	Total	C	N	O	S	0	0
			1526	964	306	252	4		

- Molecule 20 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	180	Total	C	N	O	S	0	0
			1503	931	324	238	10		

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	176	Total	C	N	O	S	0	0
			1457	928	283	235	11		

- Molecule 22 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	99	Total	C	N	O	S	0	0
			818	520	146	150	2		

- Molecule 24 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 25 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 26 is a protein called eL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 27 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 30 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Af	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 35 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ag	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called eL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ah	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 37 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ai	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 38 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Aj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ak	69	Total	C	N	O	S	0	0
			569	366	101	99	3		

- Molecule 40 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Al	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Am	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	An	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ao	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ar	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 46 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AK	212	Total	C	N	O	S	0	0
			1705	1091	306	300	8		

- Molecule 47 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 48 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B	217	Total	C	N	O	S	0	0
			1706	1085	295	317	9		

- Molecule 49 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 50 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	D	221	Total	C	N	O	S	0	0
			1712	1107	296	299	10		

- Molecule 51 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 52 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	F	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

- Molecule 53 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	G	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 54 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 55 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 56 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 57 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 58 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 59 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	M	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 60 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 61 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 62 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 63 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Q	119	Total	C	N	O	S	0	0
			990	630	186	167	7		

- Molecule 64 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 65 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 66 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 67 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 68 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 69 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	W	83	Total	C	N	O	S	0	0
			630	387	118	120	5		

- Molecule 70 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	X	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 71 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Y	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 72 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 73 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 74 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	b	98	Total	C	N	O	S	0	0
			778	485	158	129	6		

- Molecule 75 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	c	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 76 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 77 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	e	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 78 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	f	56	Total	C	N	O	S	0	0
			447	276	98	72	1		

- Molecule 79 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 80 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 81 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Aq	416	Total	C	N	O	S	0	0
			3278	2085	559	623	11		

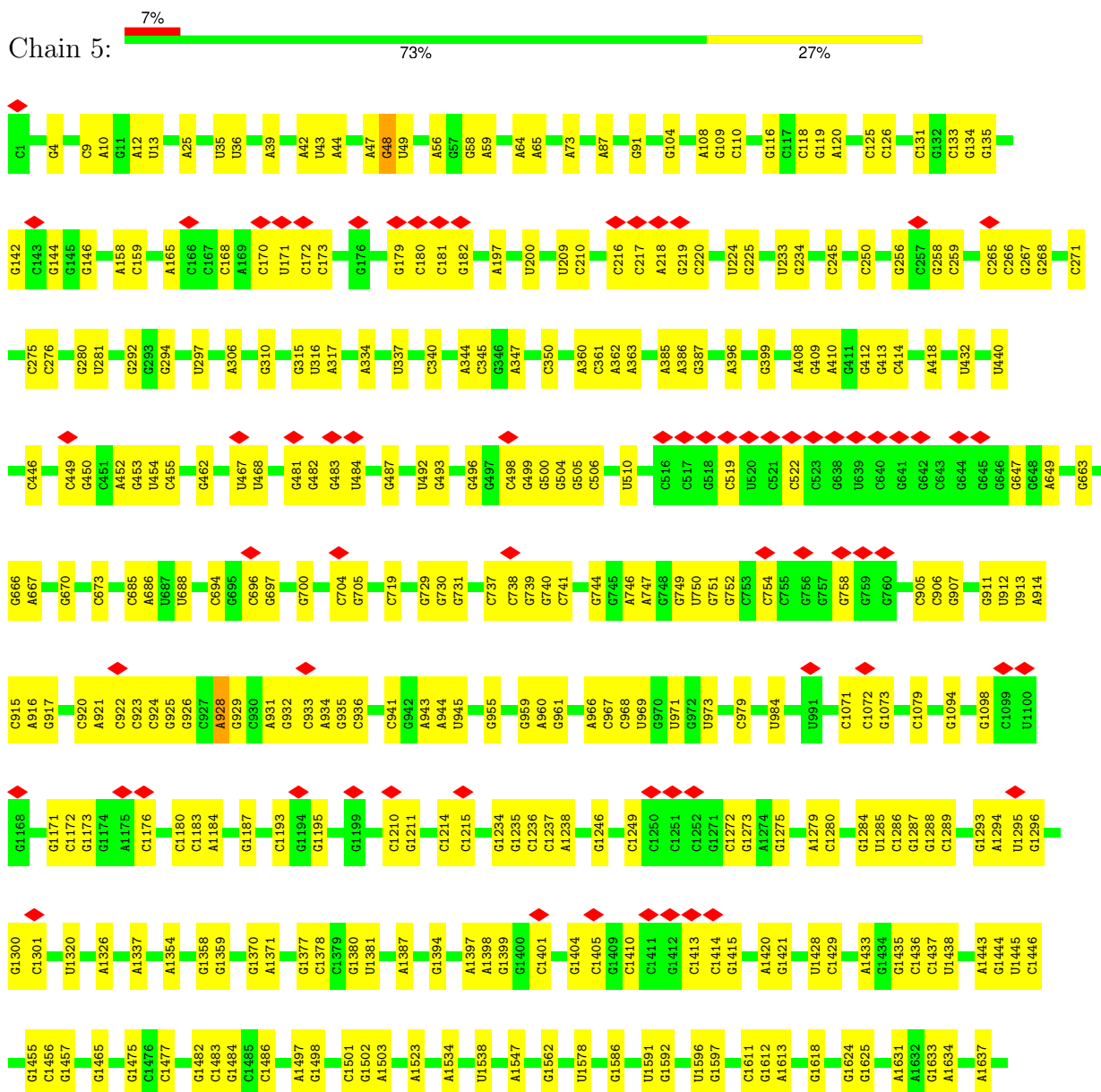
- Molecule 82 is a RNA chain called IAPV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	207	Total	C	N	O	P	0	0
			4407	1970	781	1449	207		

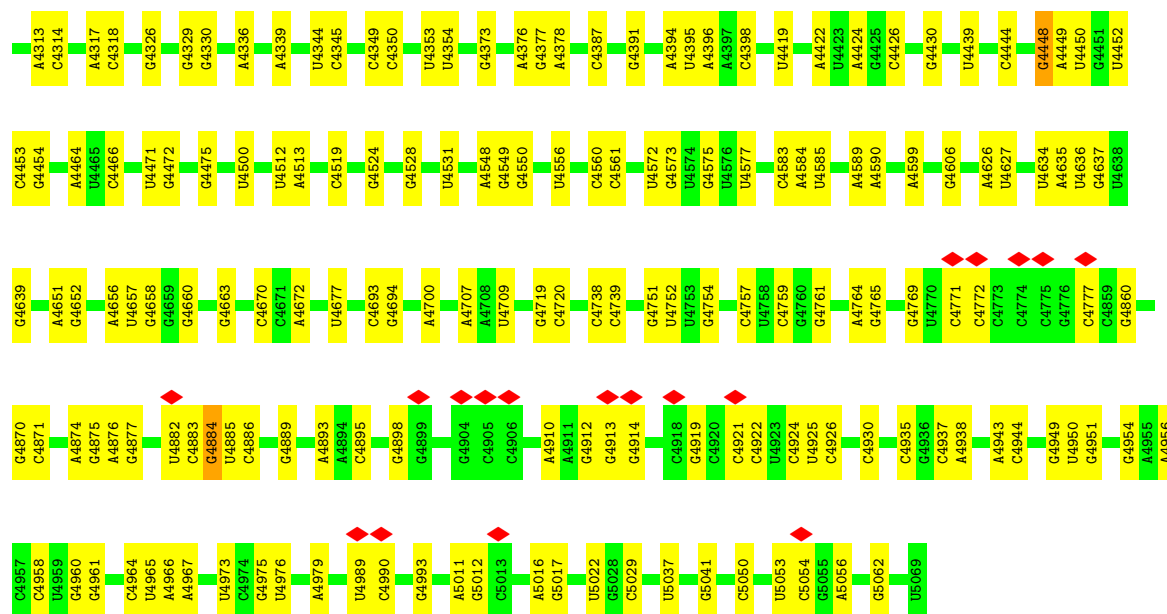
3 Residue-property plots

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: 28S rRNA

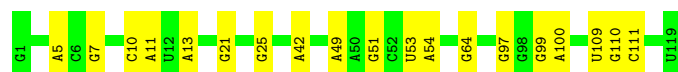






• Molecule 2: 5S rRNA

Chain 7: 84% 16%



• Molecule 3: 5.8S rRNA

Chain 8: 74% 22%



• Molecule 4: uL2

Chain AA: 94%



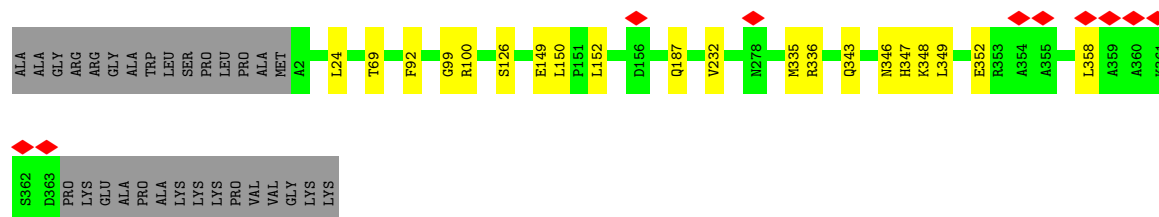
• Molecule 5: uL3

Chain AB: 96%

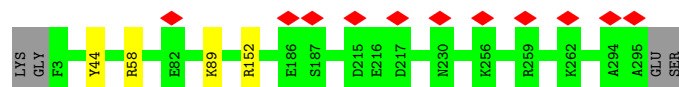


• Molecule 6: uL4

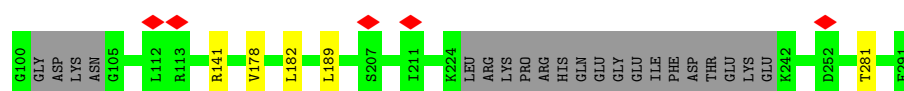
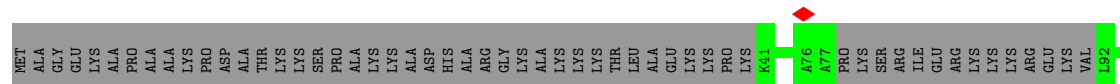
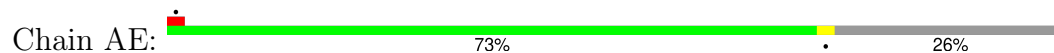
Chain AC: 87% 5% 8%



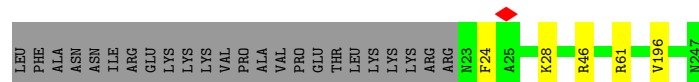
• Molecule 7: uL18



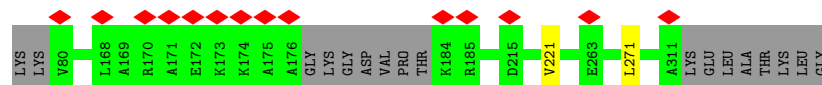
• Molecule 8: eL6



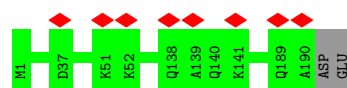
• Molecule 9: L30



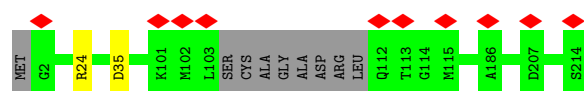
• Molecule 10: eL8



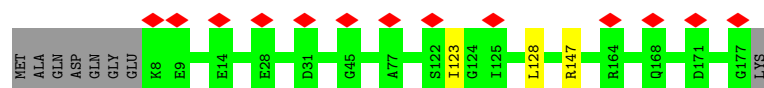
• Molecule 11: uL6



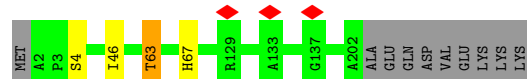
• Molecule 12: uL16



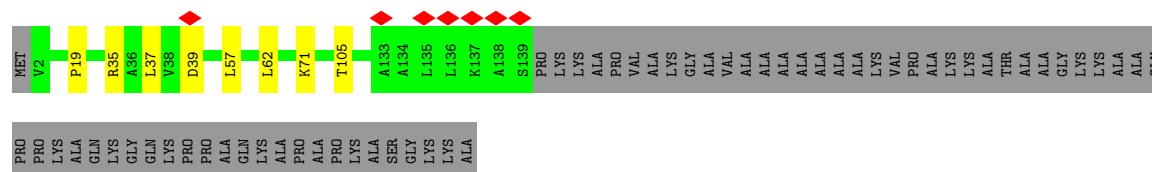
- Molecule 13: uL11



- Molecule 14: eL13



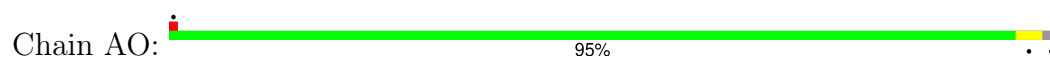
- Molecule 15: L14e



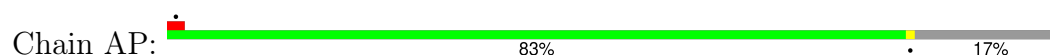
- Molecule 16: eL15

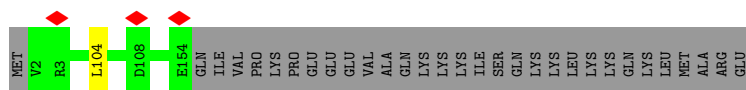


- Molecule 17: uL13



- Molecule 18: uL22

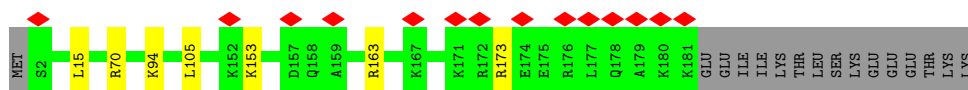
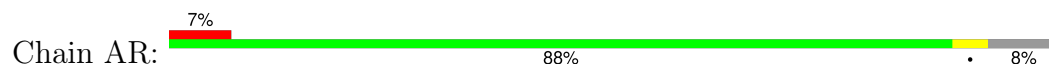




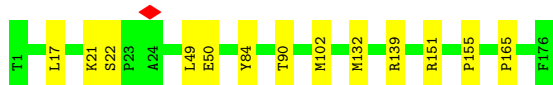
- Molecule 19: eL18



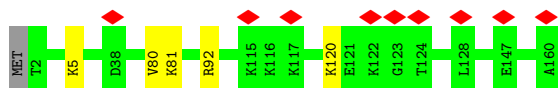
- Molecule 20: eL19



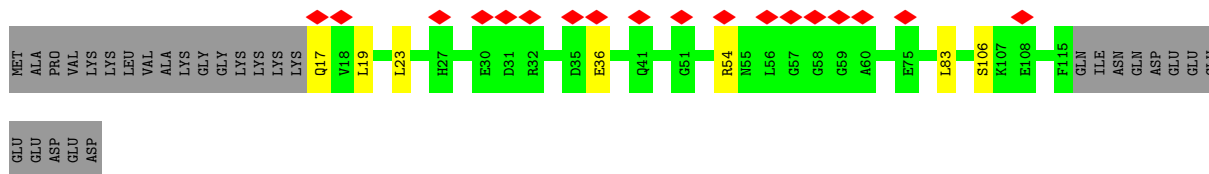
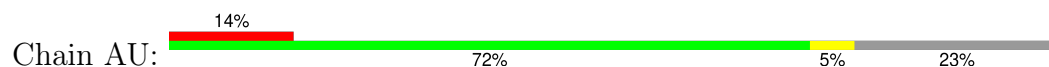
- Molecule 21: eL20



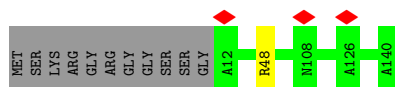
- Molecule 22: eL21

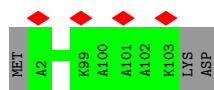


- Molecule 23: eL22

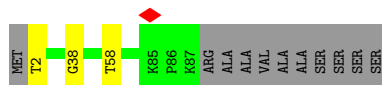
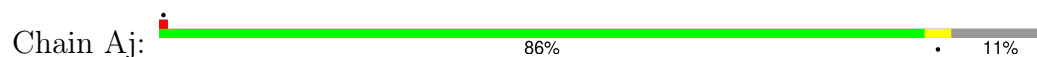


- Molecule 24: uL14

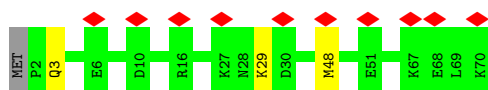




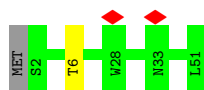
- Molecule 38: eL37



- Molecule 39: eL38



- Molecule 40: eL39



- Molecule 41: eL40

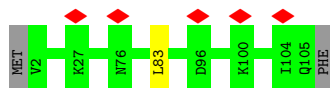


- Molecule 42: eL41



There are no outlier residues recorded for this chain.

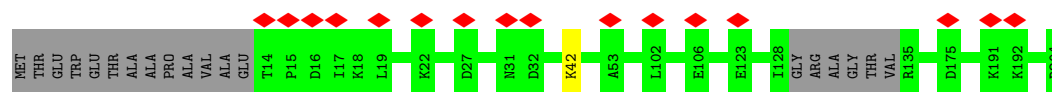
- Molecule 43: eL42



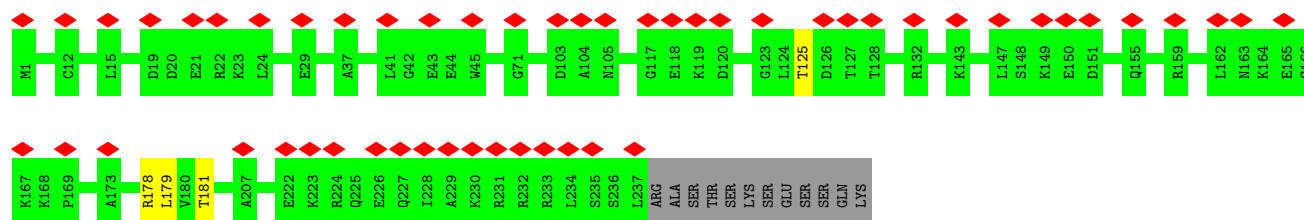
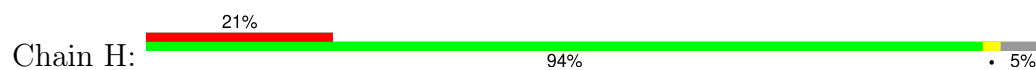
- Molecule 44: eL43



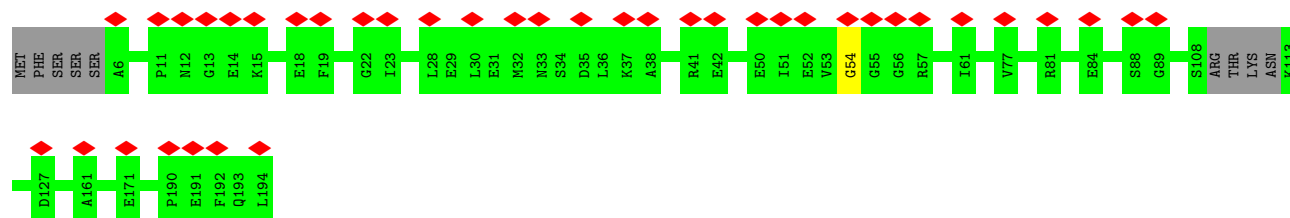
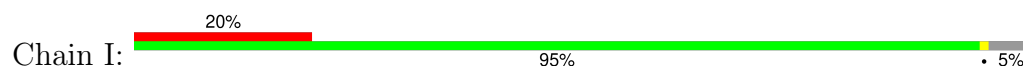




• Molecule 54: eS6



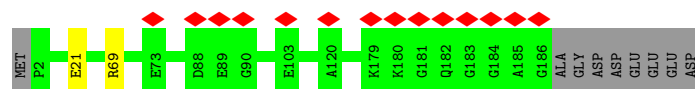
• Molecule 55: eS7



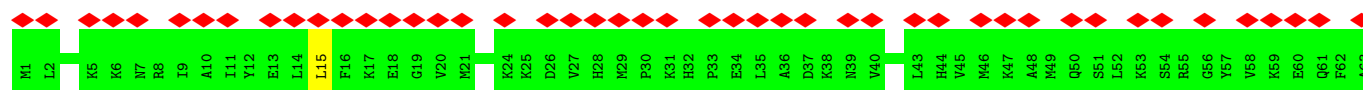
• Molecule 56: eS8

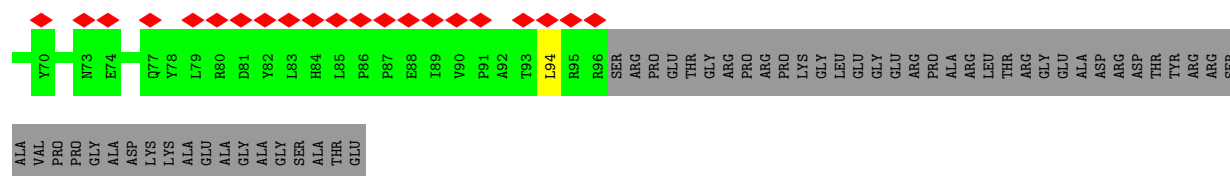


• Molecule 57: uS4

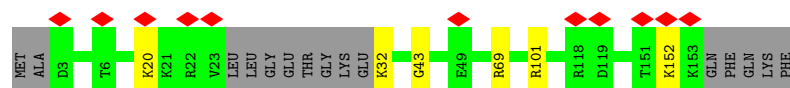
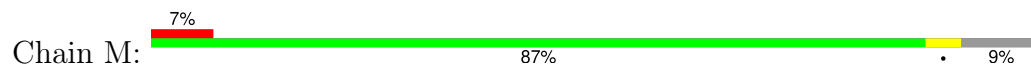


• Molecule 58: eS10

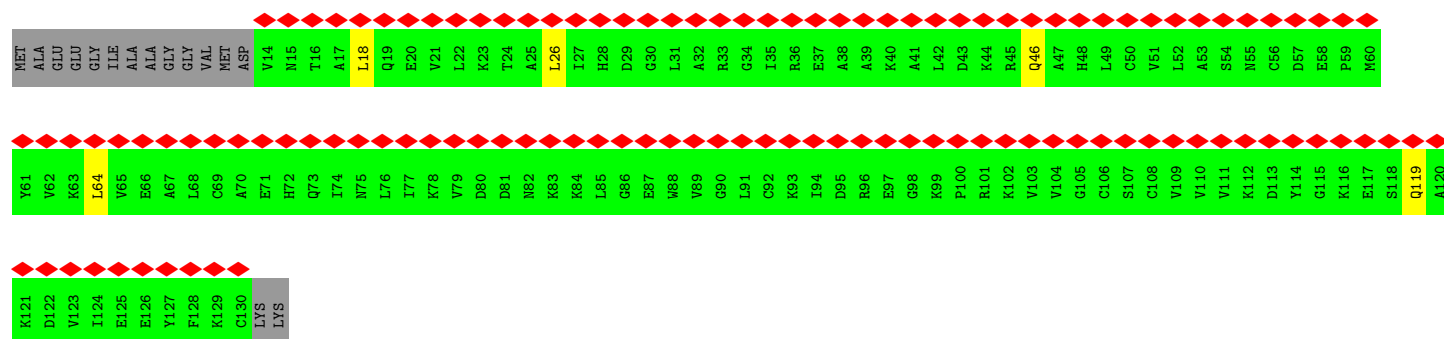
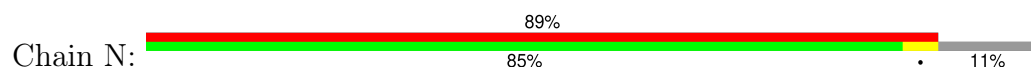




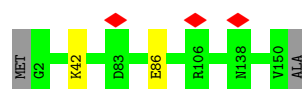
• Molecule 59: uS17



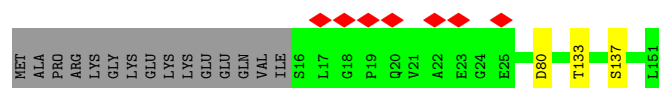
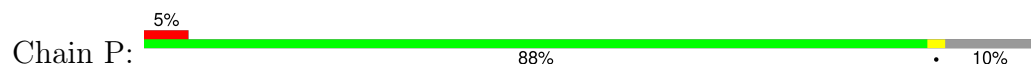
• Molecule 60: eS12



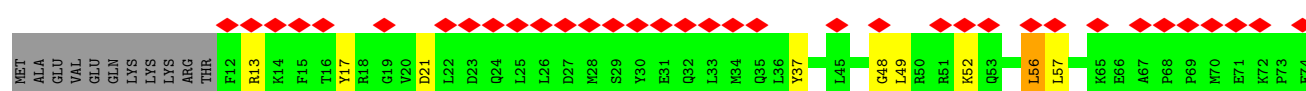
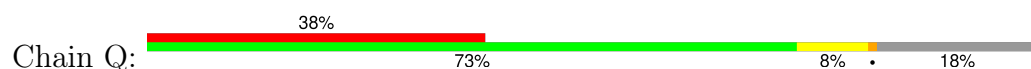
• Molecule 61: uS15

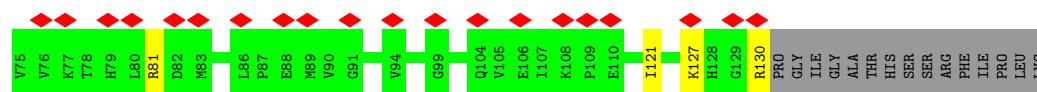


• Molecule 62: uS11

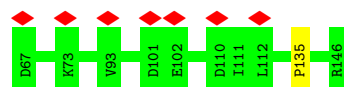
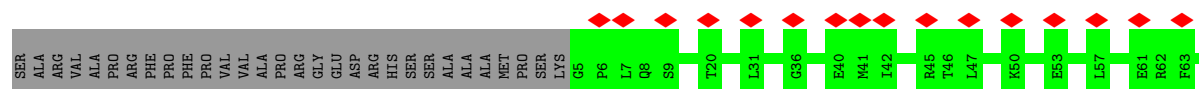
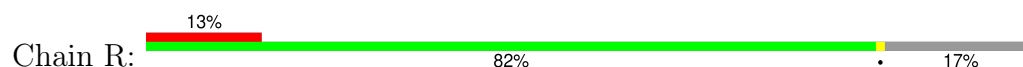


• Molecule 63: uS19

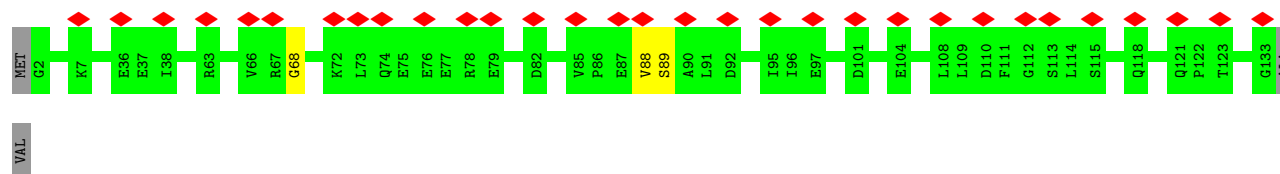




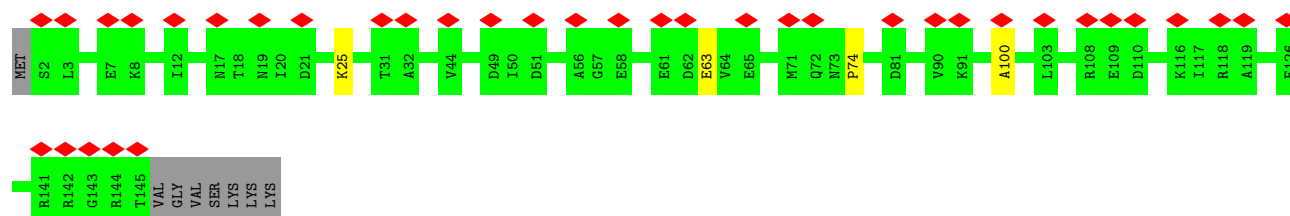
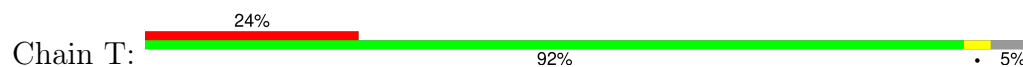
• Molecule 64: uS9



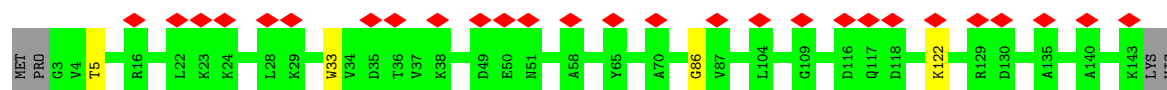
• Molecule 65: eS17



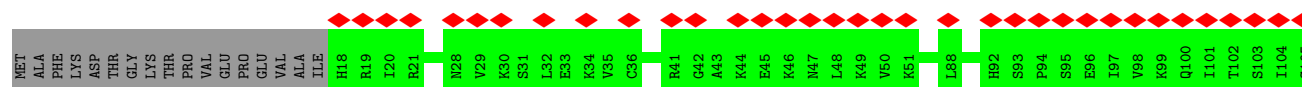
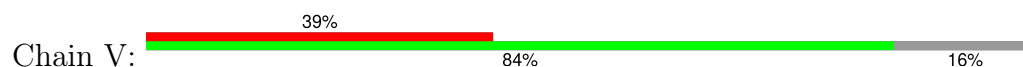
• Molecule 66: uS13

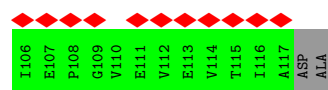


• Molecule 67: eS19

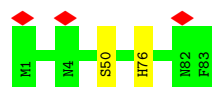


• Molecule 68: uS10





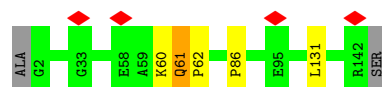
• Molecule 69: eS21



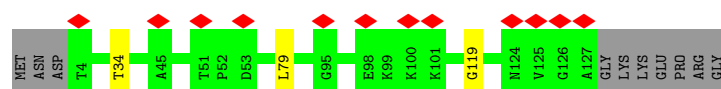
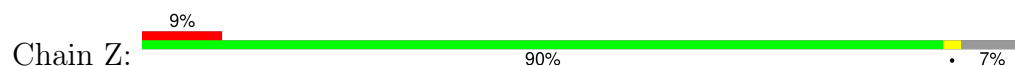
• Molecule 70: uS8



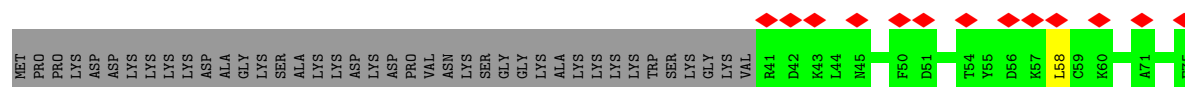
• Molecule 71: uS12



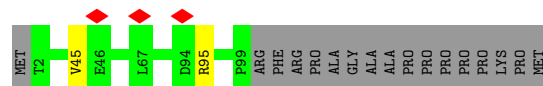
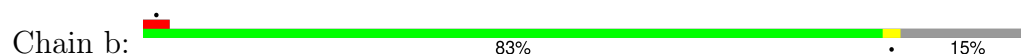
• Molecule 72: eS24



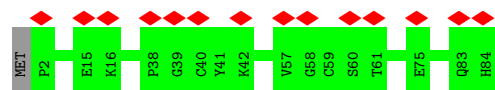
• Molecule 73: eS25



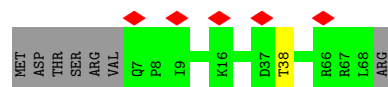
• Molecule 74: eS26



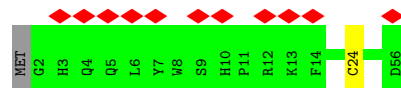
- Molecule 75: eS27



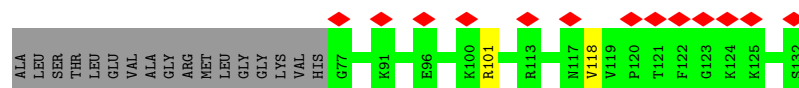
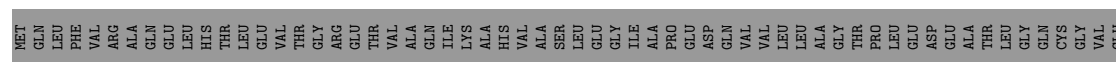
- Molecule 76: eS28



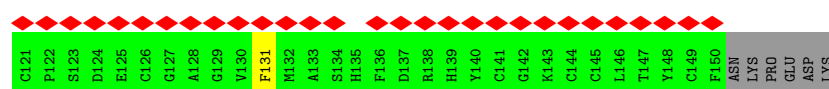
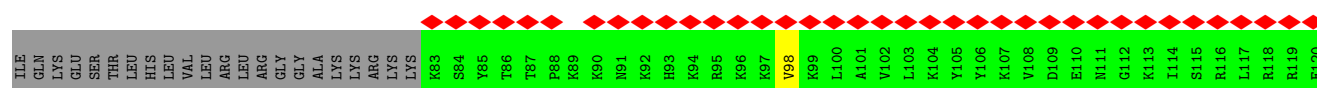
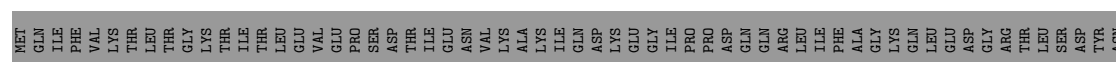
- Molecule 77: eS29



- Molecule 78: eS30

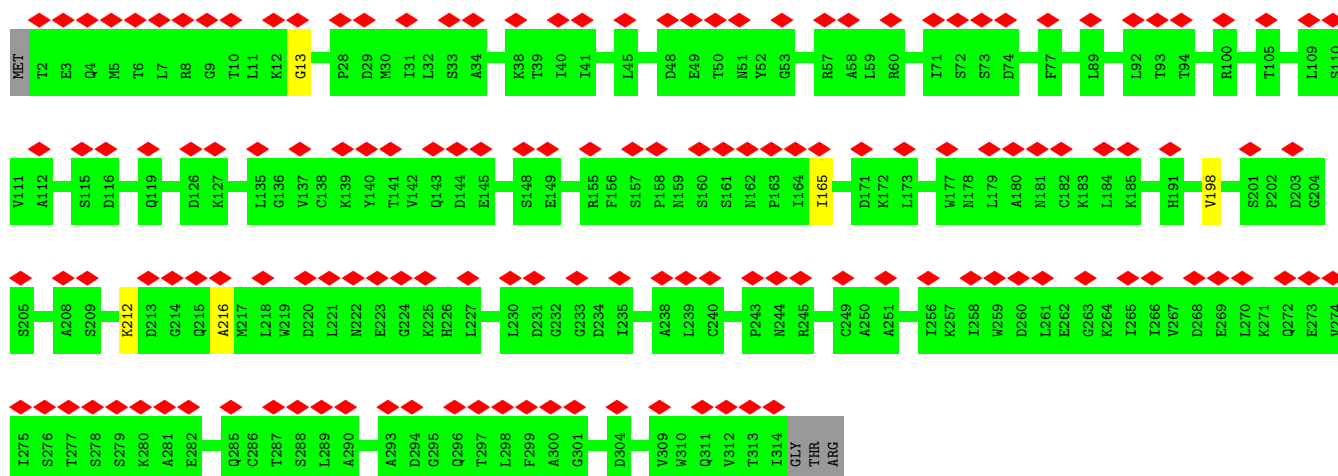


- Molecule 79: eS31



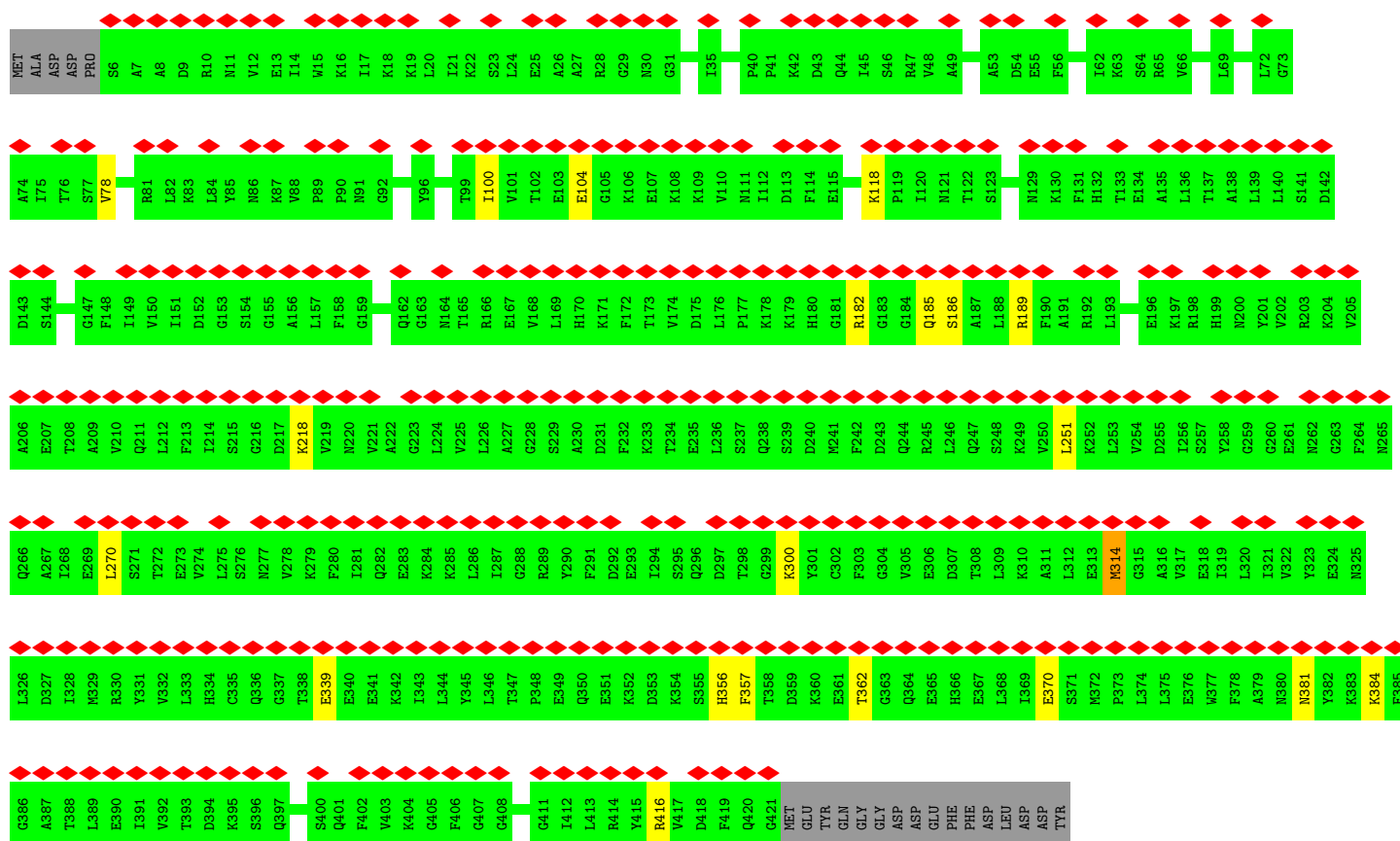
- Molecule 80: RACK1





- Molecule 81: Eukaryotic peptide chain release factor subunit 1

Chain Aq:



- Molecule 82: IAPV-IRES

Chain 1:

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.90	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4900	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	441.168, 441.168, 441.168	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0605, 1.0605, 1.0605	Depositor

5 Model quality

5.1 Standard geometry

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	5	0.24	0/86214	0.68	7/134455 (0.0%)
2	7	0.22	0/2836	0.66	0/4421
3	8	0.25	0/3581	0.68	0/5577
4	AA	0.68	0/1933	0.84	0/2592
5	AB	0.66	0/3240	0.80	0/4339
6	AC	0.65	0/2937	0.79	0/3946
7	AD	0.67	0/2437	0.79	0/3264
8	AE	0.68	0/1762	0.83	0/2362
9	AF	0.66	0/1911	0.79	0/2549
10	AG	0.67	0/1850	0.82	0/2491
11	AH	0.70	0/1535	0.81	0/2063
12	AI	0.66	0/1702	0.82	0/2272
13	AJ	0.68	0/1385	0.80	0/1852
14	AL	0.66	0/1658	0.85	0/2219
15	AM	0.67	0/1158	0.79	0/1547
16	AN	0.64	0/1746	0.84	0/2338
17	AO	0.67	0/1663	0.81	0/2223
18	AP	0.65	0/1268	0.80	0/1700
19	AQ	0.65	0/1557	0.82	0/2086
20	AR	0.66	0/1519	0.82	0/2006
21	AS	0.65	0/1498	0.79	0/2012
22	AT	0.65	0/1326	0.81	0/1770
23	AU	0.67	0/832	0.76	0/1116
24	AV	0.71	0/983	0.81	0/1319
25	AW	0.65	0/541	0.82	0/720
26	AX	0.65	0/984	0.78	0/1323
27	AY	0.66	0/1132	0.82	0/1504
28	AZ	0.66	0/1130	0.83	0/1507
29	Aa	0.65	0/1191	0.82	0/1590
30	Ab	0.68	0/861	0.83	0/1138
31	Ac	0.70	0/771	0.76	0/1034
32	Ad	0.66	0/903	0.82	0/1216
33	Ae	0.66	0/1071	0.80	0/1429
34	Af	0.66	0/895	0.82	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	Ag	0.68	0/916	0.86	0/1220
36	Ah	0.67	0/1021	0.82	0/1348
37	Ai	0.68	0/841	0.82	0/1112
38	Aj	0.65	0/720	0.86	0/952
39	Ak	0.67	0/575	0.81	0/759
40	Al	0.63	0/459	0.78	0/608
41	Am	0.66	0/435	0.79	0/575
42	An	0.61	0/240	0.87	0/305
43	Ao	0.65	0/864	0.82	0/1140
44	Ap	0.69	0/718	0.84	0/953
45	Ar	0.68	0/1010	0.84	0/1354
46	AK	0.70	0/1733	0.85	0/2324
47	2	0.24	0/40509	0.70	14/63128 (0.0%)
48	B	0.68	0/1744	0.76	0/2371
49	C	0.67	0/1756	0.79	0/2350
50	D	0.68	0/1748	0.77	0/2362
51	E	0.70	0/1796	0.82	0/2417
52	F	0.67	0/2115	0.80	0/2843
53	G	0.69	0/1492	0.78	0/2005
54	H	0.68	0/1946	0.84	0/2590
55	I	0.68	0/1510	0.79	0/2022
56	J	0.67	0/1715	0.80	0/2287
57	K	0.68	0/1550	0.83	0/2069
58	L	0.66	0/834	0.77	0/1125
59	M	0.66	0/1195	0.82	0/1597
60	N	0.72	0/918	0.82	0/1233
61	O	0.67	0/1226	0.79	0/1649
62	P	0.69	0/1029	0.84	0/1380
63	Q	0.68	0/1009	0.81	0/1346
64	R	0.68	0/1146	0.82	0/1534
65	S	0.69	0/1082	0.80	0/1452
66	T	0.69	0/1208	0.82	0/1618
67	U	0.70	0/1115	0.81	0/1493
68	V	0.69	0/805	0.82	0/1081
69	W	0.70	0/638	0.79	0/855
70	X	0.67	0/1051	0.80	0/1406
71	Y	0.69	0/1116	0.81	0/1490
72	Z	0.67	0/1028	0.82	0/1366
73	a	0.70	0/604	0.84	0/810
74	b	0.67	0/791	0.82	0/1062
75	c	0.68	0/665	0.81	0/891
76	d	0.68	0/490	0.82	0/656
77	e	0.67	0/470	0.83	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
78	f	0.71	0/451	0.85	0/592
79	g	0.69	0/567	0.88	0/753
80	h	0.69	0/2493	0.80	0/3394
81	Aq	0.71	0/3331	0.81	1/4479 (0.0%)
82	l	0.23	0/4927	0.72	1/7675 (0.0%)
All	All	0.47	0/235612	0.74	23/345832 (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
5	AB	0	3
14	AL	0	1
30	Ab	0	1
34	Af	0	1
36	Ah	0	1
46	AK	0	4
49	C	0	1
53	G	0	1
60	N	0	1
63	Q	0	1
65	S	0	1
66	T	0	1
70	X	0	1
71	Y	0	1
79	g	0	1
All	All	0	20

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1858	G	C2'-C3'-O3'	8.65	128.52	109.50
1	5	928	A	C2'-C3'-O3'	5.98	123.27	113.70
1	5	48	G	C2'-C3'-O3'	5.86	123.07	113.70
82	1	6506	U	C2'-C3'-O3'	5.85	123.05	113.70
47	2	885	U	C2'-C3'-O3'	5.83	123.02	113.70
1	5	4180	G	C2'-C3'-O3'	5.79	122.97	113.70
47	2	874	G	C2'-C3'-O3'	5.79	122.96	113.70
47	2	24	C	C2'-C3'-O3'	5.79	122.96	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2046	G	C2'-C3'-O3'	5.77	122.94	113.70
47	2	1685	U	C2'-C3'-O3'	5.62	122.70	113.70
47	2	917	U	C2'-C3'-O3'	5.48	122.47	113.70
47	2	884	C	C4'-C3'-O3'	-5.47	97.91	109.40
1	5	4884	G	C2'-C3'-O3'	5.33	122.23	113.70
47	2	110	U	C2'-C3'-O3'	5.32	122.21	113.70
47	2	1664	A	C4'-C3'-O3'	5.31	123.62	113.00
1	5	4448	G	C2'-C3'-O3'	5.17	121.97	113.70
81	Aq	314	MET	CA-C-N	5.17	126.53	116.20
47	2	461	U	C2'-C3'-O3'	5.13	121.90	113.70
1	5	3888	G	C4'-C3'-O3'	5.06	123.12	113.00
47	2	1535	U	N1-C1'-C2'	5.06	120.57	114.00
47	2	293	C	N1-C1'-C2'	5.04	120.55	114.00
47	2	55	U	N1-C1'-C2'	5.01	120.51	114.00
47	2	501	C	N1-C1'-C2'	5.00	120.50	114.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AB	241	PRO	Peptide
5	AB	257	TRP	Peptide
5	AB	258	HIS	Peptide
46	AK	136	SER	Peptide
46	AK	139	THR	Peptide
46	AK	150	GLU	Peptide
46	AK	17	VAL	Peptide
14	AL	46	ILE	Peptide
30	Ab	101	HIS	Peptide
34	Af	106	TYR	Peptide
36	Ah	86	LYS	Peptide
49	C	189	ILE	Peptide
53	G	42	LYS	Peptide
60	N	26	LEU	Peptide
63	Q	56	LEU	Peptide
65	S	89	SER	Peptide
66	T	25	LYS	Peptide
70	X	27	ILE	Peptide
71	Y	61	GLN	Peptide
79	g	131	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	AA	246/257 (96%)	222 (90%)	24 (10%)	0	100	100
5	AB	392/402 (98%)	372 (95%)	18 (5%)	2 (0%)	25	60
6	AC	360/392 (92%)	329 (91%)	28 (8%)	3 (1%)	16	51
7	AD	291/297 (98%)	272 (94%)	18 (6%)	1 (0%)	37	69
8	AE	208/291 (72%)	187 (90%)	20 (10%)	1 (0%)	25	60
9	AF	223/249 (90%)	210 (94%)	11 (5%)	2 (1%)	14	49
10	AG	221/242 (91%)	208 (94%)	13 (6%)	0	100	100
11	AH	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
12	AI	201/214 (94%)	181 (90%)	20 (10%)	0	100	100
13	AJ	168/178 (94%)	160 (95%)	7 (4%)	1 (1%)	22	57
14	AL	199/211 (94%)	191 (96%)	7 (4%)	1 (0%)	25	60
15	AM	136/198 (69%)	122 (90%)	13 (10%)	1 (1%)	19	54
16	AN	201/204 (98%)	194 (96%)	6 (3%)	1 (0%)	25	60
17	AO	197/203 (97%)	191 (97%)	5 (2%)	1 (0%)	25	60
18	AP	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
19	AQ	185/188 (98%)	170 (92%)	14 (8%)	1 (0%)	25	60
20	AR	178/196 (91%)	171 (96%)	6 (3%)	1 (1%)	22	57
21	AS	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	12	44
22	AT	157/160 (98%)	145 (92%)	9 (6%)	3 (2%)	6	34
23	AU	97/128 (76%)	90 (93%)	7 (7%)	0	100	100
24	AV	127/140 (91%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	AW	61/157 (39%)	57 (93%)	4 (7%)	0	100	100
26	AX	116/156 (74%)	111 (96%)	5 (4%)	0	100	100
27	AY	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
28	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
29	Aa	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
30	Ab	100/226 (44%)	92 (92%)	6 (6%)	2 (2%)	6	32
31	Ac	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	Ad	105/125 (84%)	96 (91%)	7 (7%)	2 (2%)	6	34
33	Ae	126/135 (93%)	118 (94%)	8 (6%)	0	100	100
34	Af	107/110 (97%)	95 (89%)	11 (10%)	1 (1%)	14	49
35	Ag	112/126 (89%)	108 (96%)	4 (4%)	0	100	100
36	Ah	120/123 (98%)	119 (99%)	0	1 (1%)	16	51
37	Ai	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
38	Aj	84/97 (87%)	77 (92%)	6 (7%)	1 (1%)	11	43
39	Ak	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
40	Al	48/51 (94%)	43 (90%)	5 (10%)	0	100	100
41	Am	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
42	An	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	Ao	102/106 (96%)	95 (93%)	7 (7%)	0	100	100
44	Ap	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Ar	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	51
46	AK	210/217 (97%)	149 (71%)	53 (25%)	8 (4%)	2	18
48	B	215/295 (73%)	194 (90%)	21 (10%)	0	100	100
49	C	211/264 (80%)	192 (91%)	19 (9%)	0	100	100
50	D	219/255 (86%)	208 (95%)	11 (5%)	0	100	100
51	E	226/281 (80%)	204 (90%)	22 (10%)	0	100	100
52	F	260/263 (99%)	237 (91%)	23 (9%)	0	100	100
53	G	181/204 (89%)	167 (92%)	14 (8%)	0	100	100
54	H	235/249 (94%)	213 (91%)	20 (8%)	2 (1%)	14	49
55	I	181/194 (93%)	167 (92%)	13 (7%)	1 (1%)	22	57
56	J	204/207 (99%)	184 (90%)	18 (9%)	2 (1%)	13	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	K	183/194 (94%)	169 (92%)	14 (8%)	0	100	100
58	L	94/149 (63%)	83 (88%)	11 (12%)	0	100	100
59	M	139/158 (88%)	126 (91%)	12 (9%)	1 (1%)	19	54
60	N	115/132 (87%)	91 (79%)	24 (21%)	0	100	100
61	O	147/151 (97%)	138 (94%)	9 (6%)	0	100	100
62	P	134/151 (89%)	117 (87%)	16 (12%)	1 (1%)	19	54
63	Q	117/145 (81%)	100 (86%)	12 (10%)	5 (4%)	2	16
64	R	140/172 (81%)	128 (91%)	11 (8%)	1 (1%)	19	54
65	S	130/135 (96%)	112 (86%)	16 (12%)	2 (2%)	8	38
66	T	142/152 (93%)	124 (87%)	16 (11%)	2 (1%)	9	40
67	U	139/145 (96%)	127 (91%)	11 (8%)	1 (1%)	19	54
68	V	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
69	W	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
70	X	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	Y	139/143 (97%)	127 (91%)	8 (6%)	4 (3%)	3	24
72	Z	122/134 (91%)	112 (92%)	9 (7%)	1 (1%)	16	51
73	a	73/125 (58%)	69 (94%)	4 (6%)	0	100	100
74	b	96/115 (84%)	86 (90%)	10 (10%)	0	100	100
75	c	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
76	d	60/69 (87%)	55 (92%)	5 (8%)	0	100	100
77	e	53/56 (95%)	47 (89%)	6 (11%)	0	100	100
78	f	54/133 (41%)	47 (87%)	7 (13%)	0	100	100
79	g	66/156 (42%)	56 (85%)	10 (15%)	0	100	100
80	h	311/317 (98%)	263 (85%)	46 (15%)	2 (1%)	22	57
81	Aq	414/437 (95%)	359 (87%)	50 (12%)	5 (1%)	11	43
All	All	11735/13353 (88%)	10732 (92%)	936 (8%)	67 (1%)	24	57

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	Ar	68	SER
46	AK	152	LYS
56	J	206	LYS

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Mol	Chain	Res	Type
6	AC	126	SER
13	AJ	147	ARG
19	AQ	178	ARG
20	AR	153	LYS
22	AT	5	LYS
46	AK	19	HIS
46	AK	140	HIS
54	H	178	ARG
54	H	179	LEU
63	Q	48	GLY
63	Q	57	LEU
65	S	68	GLY
81	Aq	104	GLU
81	Aq	357	PHE
6	AC	187	GLN
7	AD	44	TYR
8	AE	189	LEU
9	AF	196	VAL
32	Ad	58	GLY
46	AK	127	GLY
56	J	123	ARG
62	P	137	SER
63	Q	52	LYS
67	U	86	GLY
71	Y	61	GLN
80	h	13	GLY
9	AF	24	PHE
17	AO	16	LEU
21	AS	155	PRO
22	AT	80	VAL
38	Aj	38	GLY
46	AK	84	HIS
46	AK	115	SER
46	AK	173	LYS
63	Q	49	LEU
65	S	88	VAL
71	Y	86	PRO
80	h	216	ALA
6	AC	99	GLY
22	AT	81	LYS
30	Ab	25	ARG
32	Ad	56	GLU

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Mol	Chain	Res	Type
36	Ah	40	ALA
63	Q	56	LEU
71	Y	60	LYS
81	Aq	314	MET
81	Aq	370	GLU
14	AL	63	THR
34	Af	107	PRO
66	T	100	ALA
71	Y	62	PRO
21	AS	165	PRO
30	Ab	102	PRO
55	I	54	GLY
59	M	43	GLY
66	T	74	PRO
72	Z	119	GLY
5	AB	37	PRO
16	AN	84	PRO
5	AB	18	PRO
15	AM	19	PRO
46	AK	213	PRO
64	R	135	PRO
81	Aq	118	LYS

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	AA	189/199 (95%)	182 (96%)	7 (4%)	29	62
5	AB	342/347 (99%)	339 (99%)	3 (1%)	75	89
6	AC	302/323 (94%)	285 (94%)	17 (6%)	17	50
7	AD	247/250 (99%)	244 (99%)	3 (1%)	67	85
8	AE	190/251 (76%)	186 (98%)	4 (2%)	48	74
9	AF	196/218 (90%)	193 (98%)	3 (2%)	60	81
10	AG	194/208 (93%)	192 (99%)	2 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AH	169/171 (99%)	169 (100%)	0	100	100
12	AI	175/181 (97%)	173 (99%)	2 (1%)	70	86
13	AJ	143/149 (96%)	141 (99%)	2 (1%)	62	82
14	AL	167/176 (95%)	164 (98%)	3 (2%)	54	77
15	AM	117/151 (78%)	110 (94%)	7 (6%)	16	48
16	AN	171/172 (99%)	167 (98%)	4 (2%)	45	72
17	AO	171/173 (99%)	165 (96%)	6 (4%)	31	63
18	AP	134/163 (82%)	133 (99%)	1 (1%)	81	92
19	AQ	166/167 (99%)	156 (94%)	10 (6%)	16	48
20	AR	159/175 (91%)	153 (96%)	6 (4%)	28	60
21	AS	155/155 (100%)	144 (93%)	11 (7%)	12	42
22	AT	139/140 (99%)	137 (99%)	2 (1%)	62	82
23	AU	91/116 (78%)	84 (92%)	7 (8%)	10	39
24	AV	100/107 (94%)	99 (99%)	1 (1%)	73	87
25	AW	55/126 (44%)	55 (100%)	0	100	100
26	AX	106/134 (79%)	105 (99%)	1 (1%)	75	89
27	AY	124/135 (92%)	119 (96%)	5 (4%)	27	59
28	AZ	117/118 (99%)	117 (100%)	0	100	100
29	Aa	119/120 (99%)	117 (98%)	2 (2%)	56	78
30	Ab	84/172 (49%)	83 (99%)	1 (1%)	67	85
31	Ac	84/98 (86%)	83 (99%)	1 (1%)	67	85
32	Ad	98/110 (89%)	98 (100%)	0	100	100
33	Ae	114/121 (94%)	112 (98%)	2 (2%)	54	77
34	Af	88/89 (99%)	88 (100%)	0	100	100
35	Ag	98/106 (92%)	95 (97%)	3 (3%)	35	66
36	Ah	109/110 (99%)	109 (100%)	0	100	100
37	Ai	86/89 (97%)	86 (100%)	0	100	100
38	Aj	73/80 (91%)	71 (97%)	2 (3%)	40	69
39	Ak	64/65 (98%)	61 (95%)	3 (5%)	22	55
40	Al	47/48 (98%)	46 (98%)	1 (2%)	48	74
41	Am	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	An	24/24 (100%)	24 (100%)	0	100	100
43	Ao	92/94 (98%)	91 (99%)	1 (1%)	70	86
44	Ap	74/75 (99%)	72 (97%)	2 (3%)	40	69
45	Ar	108/121 (89%)	108 (100%)	0	100	100
46	AK	190/196 (97%)	177 (93%)	13 (7%)	13	43
48	B	180/245 (74%)	179 (99%)	1 (1%)	84	92
49	C	194/231 (84%)	193 (100%)	1 (0%)	86	93
50	D	186/205 (91%)	184 (99%)	2 (1%)	70	86
51	E	190/232 (82%)	188 (99%)	2 (1%)	70	86
52	F	223/225 (99%)	220 (99%)	3 (1%)	65	83
53	G	158/170 (93%)	158 (100%)	0	100	100
54	H	207/218 (95%)	205 (99%)	2 (1%)	73	87
55	I	165/174 (95%)	165 (100%)	0	100	100
56	J	178/179 (99%)	175 (98%)	3 (2%)	56	78
57	K	161/168 (96%)	159 (99%)	2 (1%)	67	85
58	L	87/125 (70%)	85 (98%)	2 (2%)	45	72
59	M	130/142 (92%)	125 (96%)	5 (4%)	28	60
60	N	99/108 (92%)	95 (96%)	4 (4%)	27	59
61	O	130/131 (99%)	128 (98%)	2 (2%)	60	81
62	P	106/119 (89%)	104 (98%)	2 (2%)	52	76
63	Q	108/130 (83%)	100 (93%)	8 (7%)	11	40
64	R	117/140 (84%)	117 (100%)	0	100	100
65	S	119/121 (98%)	119 (100%)	0	100	100
66	T	125/132 (95%)	124 (99%)	1 (1%)	79	90
67	U	111/116 (96%)	108 (97%)	3 (3%)	40	69
68	V	92/107 (86%)	92 (100%)	0	100	100
69	W	68/68 (100%)	66 (97%)	2 (3%)	37	67
70	X	112/113 (99%)	112 (100%)	0	100	100
71	Y	113/114 (99%)	112 (99%)	1 (1%)	75	89
72	Z	107/115 (93%)	105 (98%)	2 (2%)	52	76
73	a	66/103 (64%)	64 (97%)	2 (3%)	36	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	b	86/99 (87%)	84 (98%)	2 (2%)	45	72
75	c	75/76 (99%)	75 (100%)	0	100	100
76	d	55/62 (89%)	54 (98%)	1 (2%)	54	77
77	e	48/49 (98%)	47 (98%)	1 (2%)	48	74
78	f	46/106 (43%)	44 (96%)	2 (4%)	25	57
79	g	61/140 (44%)	60 (98%)	1 (2%)	58	79
80	h	272/275 (99%)	269 (99%)	3 (1%)	70	86
81	Aq	358/376 (95%)	342 (96%)	16 (4%)	23	56
All	All	10252/11385 (90%)	10038 (98%)	214 (2%)	49	74

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AA	77	ILE
4	AA	80	GLU
4	AA	96	LEU
4	AA	97	ASN
4	AA	156	LYS
4	AA	165	VAL
4	AA	181	LYS
5	AB	157	CYS
5	AB	231	VAL
5	AB	261	ARG
6	AC	24	LEU
6	AC	69	THR
6	AC	92	PHE
6	AC	100	ARG
6	AC	149	GLU
6	AC	150	LEU
6	AC	152	LEU
6	AC	232	VAL
6	AC	335	MET
6	AC	336	ARG
6	AC	343	GLN
6	AC	346	ASN
6	AC	347	HIS
6	AC	348	LYS
6	AC	349	LEU
6	AC	352	GLU

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Mol	Chain	Res	Type
6	AC	358	LEU
7	AD	58	ARG
7	AD	89	LYS
7	AD	152	ARG
8	AE	141	ARG
8	AE	178	VAL
8	AE	182	LEU
8	AE	281	THR
9	AF	28	LYS
9	AF	46	ARG
9	AF	61	ARG
10	AG	221	VAL
10	AG	271	LEU
12	AI	24	ARG
12	AI	35	ASP
13	AJ	123	ILE
13	AJ	128	LEU
14	AL	4	SER
14	AL	63	THR
14	AL	67	HIS
15	AM	35	ARG
15	AM	37	LEU
15	AM	39	ASP
15	AM	57	LEU
15	AM	62	LEU
15	AM	71	LYS
15	AM	105	THR
16	AN	50	ARG
16	AN	87	HIS
16	AN	125	SER
16	AN	151	ILE
17	AO	43	ILE
17	AO	108	ILE
17	AO	113	ASP
17	AO	145	VAL
17	AO	174	ILE
17	AO	194	GLU
18	AP	104	LEU
19	AQ	14	TRP
19	AQ	23	MET
19	AQ	38	HIS
19	AQ	57	LYS

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Mol	Chain	Res	Type
19	AQ	66	VAL
19	AQ	74	ASP
19	AQ	110	HIS
19	AQ	120	ILE
19	AQ	122	THR
19	AQ	150	GLN
20	AR	15	LEU
20	AR	70	ARG
20	AR	94	LYS
20	AR	105	LEU
20	AR	163	ARG
20	AR	173	ARG
21	AS	17	LEU
21	AS	21	LYS
21	AS	22	SER
21	AS	49	LEU
21	AS	50	GLU
21	AS	84	TYR
21	AS	90	THR
21	AS	102	MET
21	AS	132	MET
21	AS	139	ARG
21	AS	151	ARG
22	AT	92	ARG
22	AT	120	LYS
23	AU	17	GLN
23	AU	19	LEU
23	AU	23	LEU
23	AU	36	GLU
23	AU	54	ARG
23	AU	83	LEU
23	AU	106	SER
24	AV	48	ARG
26	AX	95	THR
27	AY	2	LYS
27	AY	14	ASN
27	AY	17	ARG
27	AY	74	TYR
27	AY	97	VAL
29	Aa	82	VAL
29	Aa	124	VAL
30	Ab	101	HIS

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Mol	Chain	Res	Type
31	Ac	81	LEU
33	Ae	26	ASP
33	Ae	78	LEU
35	Ag	38	VAL
35	Ag	73	HIS
35	Ag	105	LYS
38	Aj	2	THR
38	Aj	58	THR
39	Ak	3	GLN
39	Ak	29	LYS
39	Ak	48	MET
40	Al	6	THR
43	Ao	83	LEU
44	Ap	16	THR
44	Ap	17	ARG
46	AK	7	ARG
46	AK	10	LEU
46	AK	39	LYS
46	AK	63	PHE
46	AK	67	VAL
46	AK	95	LYS
46	AK	105	LYS
46	AK	111	LEU
46	AK	128	LEU
46	AK	163	LEU
46	AK	169	VAL
46	AK	179	LEU
46	AK	216	LEU
48	B	128	GLN
49	C	98	THR
50	D	248	TYR
50	D	274	MET
51	E	76	ARG
51	E	90	LYS
52	F	23	LEU
52	F	156	MET
52	F	262	SER
54	H	125	THR
54	H	181	THR
56	J	130	THR
56	J	143	LYS
56	J	205	ARG

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Mol	Chain	Res	Type
57	K	21	GLU
57	K	69	ARG
58	L	15	LEU
58	L	94	LEU
59	M	20	LYS
59	M	32	LYS
59	M	69	ARG
59	M	101	ARG
59	M	152	LYS
60	N	18	LEU
60	N	46	GLN
60	N	64	LEU
60	N	119	GLN
61	O	42	LYS
61	O	86	GLU
62	P	80	ASP
62	P	133	THR
63	Q	13	ARG
63	Q	17	TYR
63	Q	21	ASP
63	Q	37	TYR
63	Q	81	ARG
63	Q	121	ILE
63	Q	127	LYS
63	Q	130	ARG
66	T	63	GLU
67	U	5	THR
67	U	33	TRP
67	U	122	LYS
69	W	50	SER
69	W	76	HIS
71	Y	131	LEU
72	Z	34	THR
72	Z	79	LEU
73	a	58	LEU
73	a	110	THR
74	b	45	VAL
74	b	95	ARG
76	d	38	THR
77	e	24	CYS
78	f	101	ARG
78	f	118	VAL

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Mol	Chain	Res	Type
79	g	98	VAL
80	h	165	ILE
80	h	198	VAL
80	h	212	LYS
81	Aq	78	VAL
81	Aq	100	ILE
81	Aq	182	ARG
81	Aq	185	GLN
81	Aq	186	SER
81	Aq	189	ARG
81	Aq	218	LYS
81	Aq	251	LEU
81	Aq	270	LEU
81	Aq	300	LYS
81	Aq	339	GLU
81	Aq	356	HIS
81	Aq	362	THR
81	Aq	381	ASN
81	Aq	384	LYS
81	Aq	416	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	140	ASN
4	AA	217	GLN
5	AB	203	GLN
5	AB	271	GLN
6	AC	38	ASN
6	AC	50	GLN
6	AC	119	GLN
6	AC	286	ASN
6	AC	346	ASN
6	AC	347	HIS
7	AD	138	GLN
7	AD	202	GLN
8	AE	253	GLN
9	AF	118	ASN
10	AG	91	ASN
10	AG	96	GLN
12	AI	202	ASN
13	AJ	104	ASN

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Mol	Chain	Res	Type
14	AL	159	ASN
14	AL	188	ASN
15	AM	33	GLN
15	AM	56	GLN
16	AN	99	GLN
16	AN	145	ASN
17	AO	42	ASN
18	AP	28	ASN
18	AP	75	GLN
18	AP	80	GLN
18	AP	120	ASN
19	AQ	8	ASN
19	AQ	150	GLN
19	AQ	188	ASN
21	AS	77	ASN
21	AS	146	HIS
22	AT	49	GLN
22	AT	127	GLN
22	AT	131	GLN
23	AU	41	GLN
24	AV	27	ASN
26	AX	93	ASN
26	AX	111	GLN
26	AX	125	ASN
26	AX	151	ASN
27	AY	14	ASN
28	AZ	76	ASN
28	AZ	79	HIS
29	Aa	67	GLN
30	Ab	50	ASN
32	Ad	100	ASN
33	Ae	52	GLN
33	Ae	92	ASN
34	Af	56	ASN
35	Ag	100	GLN
36	Ah	20	GLN
41	Am	61	GLN
46	AK	197	ASN
46	AK	199	GLN
48	B	128	GLN
48	B	141	ASN
48	B	180	GLN

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Mol	Chain	Res	Type
50	D	235	ASN
51	E	101	GLN
53	G	65	GLN
53	G	83	ASN
53	G	107	ASN
53	G	118	ASN
53	G	137	GLN
53	G	165	ASN
54	H	65	GLN
54	H	177	GLN
55	I	114	GLN
55	I	165	ASN
56	J	168	GLN
57	K	140	GLN
59	M	19	ASN
59	M	100	ASN
60	N	73	GLN
60	N	75	ASN
62	P	20	GLN
64	R	80	GLN
64	R	86	GLN
65	S	26	ASN
66	T	17	ASN
67	U	85	ASN
69	W	35	ASN
70	X	16	ASN
70	X	90	GLN
70	X	113	HIS
77	e	5	GLN
80	h	4	GLN
80	h	133	ASN
81	Aq	401	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3569/3594 (99%)	943 (26%)	77 (2%)
2	7	118/119 (99%)	18 (15%)	1 (0%)
3	8	149/156 (95%)	34 (22%)	1 (0%)
47	2	1685/1869 (90%)	504 (29%)	50 (2%)
82	1	206/251 (82%)	115 (55%)	14 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5727/5989 (95%)	1614 (28%)	143 (2%)

All (1614) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	4	G
1	5	9	C
1	5	10	A
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	36	U
1	5	39	A
1	5	42	A
1	5	43	U
1	5	44	A
1	5	48	G
1	5	49	U
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	73	A
1	5	87	A
1	5	91	G
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	116	G
1	5	118	C
1	5	119	G
1	5	120	A
1	5	126	C
1	5	131	C
1	5	133	C
1	5	134	G
1	5	135	G
1	5	142	G
1	5	144	G

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Mol	Chain	Res	Type
1	5	146	G
1	5	158	A
1	5	159	C
1	5	165	A
1	5	168	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	179	G
1	5	180	C
1	5	181	C
1	5	182	G
1	5	197	A
1	5	200	U
1	5	209	U
1	5	210	C
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	225	G
1	5	233	U
1	5	234	G
1	5	245	C
1	5	250	C
1	5	256	G
1	5	258	G
1	5	259	C
1	5	265	C
1	5	266	C
1	5	267	G
1	5	268	G
1	5	271	C
1	5	276	C
1	5	280	G
1	5	281	U
1	5	292	G
1	5	294	G
1	5	297	U
1	5	306	A

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Mol	Chain	Res	Type
1	5	310	G
1	5	315	G
1	5	316	U
1	5	317	A
1	5	334	A
1	5	337	U
1	5	340	C
1	5	344	A
1	5	345	C
1	5	347	A
1	5	350	C
1	5	360	A
1	5	361	C
1	5	362	A
1	5	363	A
1	5	386	A
1	5	387	G
1	5	396	A
1	5	399	G
1	5	408	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C
1	5	418	A
1	5	432	U
1	5	440	U
1	5	446	C
1	5	449	C
1	5	450	G
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	462	G
1	5	467	U
1	5	468	U
1	5	481	G
1	5	482	G
1	5	483	G
1	5	484	U

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Mol	Chain	Res	Type
1	5	487	G
1	5	492	U
1	5	493	G
1	5	496	G
1	5	498	C
1	5	499	G
1	5	500	G
1	5	505	G
1	5	506	C
1	5	510	U
1	5	519	C
1	5	522	C
1	5	647	G
1	5	649	A
1	5	663	G
1	5	666	G
1	5	667	A
1	5	670	G
1	5	673	C
1	5	685	C
1	5	686	A
1	5	688	U
1	5	694	C
1	5	696	C
1	5	697	G
1	5	700	G
1	5	704	C
1	5	705	G
1	5	719	C
1	5	729	G
1	5	730	G
1	5	731	G
1	5	737	C
1	5	738	C
1	5	739	G
1	5	740	G
1	5	741	C
1	5	744	G
1	5	746	A
1	5	747	A
1	5	749	G
1	5	750	U

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Mol	Chain	Res	Type
1	5	751	G
1	5	752	G
1	5	754	C
1	5	758	G
1	5	905	C
1	5	906	C
1	5	907	G
1	5	911	G
1	5	912	U
1	5	913	U
1	5	914	A
1	5	915	C
1	5	916	A
1	5	917	G
1	5	920	C
1	5	921	A
1	5	922	C
1	5	923	C
1	5	924	C
1	5	925	G
1	5	926	G
1	5	928	A
1	5	929	G
1	5	931	A
1	5	932	G
1	5	933	C
1	5	934	A
1	5	935	G
1	5	936	C
1	5	941	C
1	5	943	A
1	5	944	A
1	5	945	U
1	5	959	G
1	5	960	A
1	5	961	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	U
1	5	971	U
1	5	973	U

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Mol	Chain	Res	Type
1	5	979	C
1	5	984	U
1	5	1071	C
1	5	1072	C
1	5	1073	G
1	5	1079	C
1	5	1094	G
1	5	1098	G
1	5	1171	G
1	5	1172	C
1	5	1173	G
1	5	1176	C
1	5	1180	C
1	5	1184	A
1	5	1187	G
1	5	1193	C
1	5	1195	G
1	5	1210	C
1	5	1211	G
1	5	1214	C
1	5	1215	C
1	5	1234	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1246	G
1	5	1249	C
1	5	1272	C
1	5	1273	G
1	5	1275	G
1	5	1279	A
1	5	1280	C
1	5	1284	G
1	5	1285	U
1	5	1286	C
1	5	1287	G
1	5	1288	G
1	5	1289	C
1	5	1293	G
1	5	1294	A
1	5	1295	U

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Mol	Chain	Res	Type
1	5	1296	G
1	5	1301	C
1	5	1320	U
1	5	1326	A
1	5	1337	A
1	5	1354	A
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1371	A
1	5	1377	G
1	5	1378	C
1	5	1380	G
1	5	1381	U
1	5	1387	A
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1399	G
1	5	1401	C
1	5	1404	G
1	5	1405	C
1	5	1410	C
1	5	1413	C
1	5	1414	C
1	5	1415	G
1	5	1420	A
1	5	1421	G
1	5	1428	U
1	5	1429	C
1	5	1433	A
1	5	1435	G
1	5	1436	C
1	5	1437	C
1	5	1438	U
1	5	1443	A
1	5	1444	G
1	5	1445	U
1	5	1446	C
1	5	1456	C
1	5	1457	G
1	5	1465	G

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Mol	Chain	Res	Type
1	5	1475	G
1	5	1477	C
1	5	1482	G
1	5	1483	C
1	5	1484	G
1	5	1486	C
1	5	1497	A
1	5	1498	G
1	5	1501	C
1	5	1502	G
1	5	1503	A
1	5	1523	A
1	5	1534	A
1	5	1538	U
1	5	1547	A
1	5	1562	G
1	5	1578	U
1	5	1586	G
1	5	1591	U
1	5	1592	G
1	5	1596	U
1	5	1597	G
1	5	1611	C
1	5	1612	G
1	5	1613	A
1	5	1618	G
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1637	A
1	5	1640	C
1	5	1651	G
1	5	1654	G
1	5	1658	G
1	5	1660	U
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1679	A
1	5	1721	G

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Mol	Chain	Res	Type
1	5	1731	C
1	5	1734	G
1	5	1742	A
1	5	1743	A
1	5	1750	G
1	5	1754	U
1	5	1756	U
1	5	1757	U
1	5	1758	G
1	5	1760	G
1	5	1763	C
1	5	1764	G
1	5	1769	G
1	5	1770	A
1	5	1771	U
1	5	1772	C
1	5	1773	U
1	5	1775	A
1	5	1787	A
1	5	1797	G
1	5	1804	A
1	5	1805	A
1	5	1809	C
1	5	1815	G
1	5	1820	U
1	5	1821	G
1	5	1828	C
1	5	1830	G
1	5	1833	G
1	5	1834	U
1	5	1836	G
1	5	1837	A
1	5	1842	G
1	5	1855	G
1	5	1865	G
1	5	1869	G
1	5	1881	C
1	5	1882	U
1	5	1886	G
1	5	1889	U
1	5	1897	A
1	5	1899	G

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Mol	Chain	Res	Type
1	5	1910	G
1	5	1915	C
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1931	C
1	5	1939	A
1	5	1940	G
1	5	1941	A
1	5	1947	U
1	5	1952	G
1	5	1957	U
1	5	1958	A
1	5	1959	U
1	5	1960	A
1	5	1961	G
1	5	1962	A
1	5	1963	C
1	5	1964	A
1	5	1966	C
1	5	1967	A
1	5	1972	G
1	5	1974	U
1	5	1975	G
1	5	1976	G
1	5	1977	C
1	5	1978	C
1	5	1979	A
1	5	1980	U
1	5	1981	G
1	5	1982	G
1	5	1983	A
1	5	1984	A
1	5	1985	G
1	5	1987	C
1	5	1988	G
1	5	1989	G
1	5	1990	A
1	5	1991	A
1	5	1992	U
1	5	1993	C

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Mol	Chain	Res	Type
1	5	1995	G
1	5	1996	C
1	5	1997	U
1	5	1998	A
1	5	1999	A
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2008	U
1	5	2009	A
1	5	2010	A
1	5	2011	C
1	5	2012	A
1	5	2013	A
1	5	2014	C
1	5	2018	C
1	5	2020	U
1	5	2021	G
1	5	2022	C
1	5	2024	G
1	5	2025	A
1	5	2026	A
1	5	2042	A
1	5	2044	U
1	5	2046	G
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2058	G
1	5	2069	A
1	5	2070	U
1	5	2084	U
1	5	2088	A
1	5	2089	G
1	5	2090	U
1	5	2093	G
1	5	2094	C
1	5	2097	A
1	5	2098	G
1	5	2100	G

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Mol	Chain	Res	Type
1	5	2102	G
1	5	2104	A
1	5	2107	A
1	5	2108	G
1	5	2110	G
1	5	2259	G
1	5	2260	C
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2275	G
1	5	2277	C
1	5	2280	G
1	5	2289	C
1	5	2294	G
1	5	2300	A
1	5	2301	G
1	5	2313	A
1	5	2314	G
1	5	2325	C
1	5	2332	A
1	5	2333	G
1	5	2348	G
1	5	2350	U
1	5	2351	C
1	5	2364	G
1	5	2366	A
1	5	2374	A
1	5	2387	G
1	5	2395	A
1	5	2396	A
1	5	2398	U
1	5	2400	G
1	5	2409	U
1	5	2417	A
1	5	2422	C
1	5	2428	A
1	5	2433	G
1	5	2437	C
1	5	2441	C
1	5	2444	U

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Mol	Chain	Res	Type
1	5	2447	U
1	5	2450	G
1	5	2471	G
1	5	2475	G
1	5	2477	A
1	5	2478	C
1	5	2481	G
1	5	2483	G
1	5	2486	G
1	5	2487	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2493	G
1	5	2495	U
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2511	A
1	5	2513	A
1	5	2514	G
1	5	2529	A
1	5	2530	U
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2552	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2558	C
1	5	2562	G
1	5	2564	G
1	5	2565	A
1	5	2569	G
1	5	2570	U
1	5	2575	U
1	5	2586	G

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Mol	Chain	Res	Type
1	5	2587	A
1	5	2589	C
1	5	2601	A
1	5	2618	G
1	5	2623	A
1	5	2627	C
1	5	2628	U
1	5	2639	U
1	5	2649	G
1	5	2653	C
1	5	2655	C
1	5	2656	U
1	5	2659	A
1	5	2661	U
1	5	2662	G
1	5	2663	G
1	5	2669	C
1	5	2670	C
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2701	U
1	5	2704	C
1	5	2708	U
1	5	2709	C
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2714	G
1	5	2716	C
1	5	2719	C
1	5	2723	U
1	5	2724	G
1	5	2732	G
1	5	2735	G
1	5	2740	U
1	5	2743	A
1	5	2744	A
1	5	2750	G
1	5	2761	U
1	5	2763	U

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Mol	Chain	Res	Type
1	5	2764	A
1	5	2769	U
1	5	2770	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2796	G
1	5	2798	A
1	5	2815	A
1	5	2826	U
1	5	2827	G
1	5	2829	U
1	5	2842	G
1	5	2844	A
1	5	2848	G
1	5	2850	A
1	5	2855	G
1	5	2856	C
1	5	2862	G
1	5	2874	U
1	5	2875	C
1	5	2898	G
1	5	3604	A
1	5	3617	G
1	5	3618	C
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3644	U
1	5	3646	A
1	5	3648	A
1	5	3653	A
1	5	3662	A
1	5	3663	A
1	5	3670	C
1	5	3673	C
1	5	3679	U
1	5	3696	C
1	5	3705	G
1	5	3710	G
1	5	3711	A

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Mol	Chain	Res	Type
1	5	3712	A
1	5	3713	U
1	5	3714	G
1	5	3729	U
1	5	3734	U
1	5	3740	G
1	5	3748	A
1	5	3753	G
1	5	3759	A
1	5	3760	A
1	5	3761	C
1	5	3763	A
1	5	3764	U
1	5	3765	G
1	5	3766	A
1	5	3767	C
1	5	3774	A
1	5	3775	A
1	5	3776	G
1	5	3777	G
1	5	3778	U
1	5	3784	A
1	5	3786	U
1	5	3795	A
1	5	3809	G
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3839	G
1	5	3840	U
1	5	3862	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3880	G
1	5	3887	C
1	5	3889	G
1	5	3897	G
1	5	3901	A

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Mol	Chain	Res	Type
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3916	G
1	5	3917	A
1	5	3923	A
1	5	3938	G
1	5	3939	G
1	5	3944	G
1	5	3945	A
1	5	3947	A
1	5	3948	C
1	5	3950	U
1	5	3951	G
1	5	3954	A
1	5	3956	G
1	5	3958	G
1	5	3960	A
1	5	3962	A
1	5	3964	U
1	5	3965	A
1	5	3966	A
1	5	3967	G
1	5	3970	G
1	5	3972	A
1	5	3975	C
1	5	3977	C
1	5	4036	G
1	5	4039	G
1	5	4044	U
1	5	4046	A
1	5	4047	A
1	5	4048	A
1	5	4049	U
1	5	4050	A
1	5	4051	C
1	5	4052	C
1	5	4053	A
1	5	4054	C
1	5	4055	U

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Mol	Chain	Res	Type
1	5	4062	A
1	5	4063	U
1	5	4064	C
1	5	4065	G
1	5	4070	U
1	5	4071	U
1	5	4072	C
1	5	4074	C
1	5	4076	G
1	5	4077	A
1	5	4085	A
1	5	4086	G
1	5	4094	G
1	5	4095	G
1	5	4099	G
1	5	4101	C
1	5	4108	G
1	5	4118	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4122	G
1	5	4124	G
1	5	4127	A
1	5	4131	G
1	5	4135	G
1	5	4136	G
1	5	4138	C
1	5	4147	G
1	5	4148	C
1	5	4149	C
1	5	4152	G
1	5	4156	G
1	5	4157	A
1	5	4159	C
1	5	4162	C
1	5	4163	U
1	5	4170	A
1	5	4171	C
1	5	4172	A
1	5	4179	G
1	5	4181	U

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Mol	Chain	Res	Type
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4204	C
1	5	4206	C
1	5	4229	U
1	5	4232	U
1	5	4233	A
1	5	4237	C
1	5	4249	G
1	5	4251	A
1	5	4252	C
1	5	4254	G
1	5	4257	A
1	5	4266	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4280	A
1	5	4281	A
1	5	4291	G
1	5	4297	G
1	5	4305	G
1	5	4306	U
1	5	4307	A
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4336	A
1	5	4339	A
1	5	4344	U
1	5	4345	C
1	5	4349	C
1	5	4350	C
1	5	4353	U
1	5	4354	U
1	5	4373	G

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Mol	Chain	Res	Type
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4387	C
1	5	4391	G
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4398	C
1	5	4419	U
1	5	4422	A
1	5	4424	A
1	5	4426	C
1	5	4430	G
1	5	4439	U
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4450	U
1	5	4452	U
1	5	4453	C
1	5	4454	G
1	5	4464	A
1	5	4466	C
1	5	4471	U
1	5	4472	G
1	5	4475	G
1	5	4500	U
1	5	4512	U
1	5	4513	A
1	5	4519	C
1	5	4524	G
1	5	4528	G
1	5	4531	U
1	5	4548	A
1	5	4549	G
1	5	4550	G
1	5	4556	U
1	5	4560	C
1	5	4561	C
1	5	4573	G
1	5	4575	G

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Mol	Chain	Res	Type
1	5	4577	U
1	5	4583	C
1	5	4584	A
1	5	4585	U
1	5	4589	A
1	5	4590	A
1	5	4599	A
1	5	4606	G
1	5	4627	U
1	5	4634	U
1	5	4635	A
1	5	4636	U
1	5	4637	G
1	5	4639	G
1	5	4651	A
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4658	G
1	5	4660	G
1	5	4663	G
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4693	C
1	5	4694	G
1	5	4700	A
1	5	4707	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4738	C
1	5	4739	C
1	5	4751	G
1	5	4752	U
1	5	4754	G
1	5	4757	C
1	5	4759	C
1	5	4761	G
1	5	4764	A
1	5	4765	G
1	5	4769	G

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Mol	Chain	Res	Type
1	5	4771	C
1	5	4772	C
1	5	4777	C
1	5	4860	G
1	5	4870	G
1	5	4871	C
1	5	4874	A
1	5	4875	G
1	5	4876	A
1	5	4877	G
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4886	C
1	5	4889	G
1	5	4893	A
1	5	4895	C
1	5	4898	G
1	5	4910	A
1	5	4912	G
1	5	4913	G
1	5	4914	G
1	5	4919	G
1	5	4921	C
1	5	4922	C
1	5	4924	C
1	5	4925	U
1	5	4926	C
1	5	4930	C
1	5	4935	C
1	5	4937	C
1	5	4938	A
1	5	4943	A
1	5	4944	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4954	G
1	5	4956	A
1	5	4958	C
1	5	4960	G
1	5	4961	G

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Mol	Chain	Res	Type
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4967	A
1	5	4973	U
1	5	4975	G
1	5	4976	U
1	5	4979	A
1	5	4989	U
1	5	4990	C
1	5	4993	G
1	5	5011	A
1	5	5012	G
1	5	5016	A
1	5	5017	G
1	5	5022	U
1	5	5029	C
1	5	5037	U
1	5	5041	G
1	5	5050	C
1	5	5053	U
1	5	5054	C
1	5	5056	A
1	5	5062	G
2	7	5	A
2	7	7	G
2	7	10	C
2	7	11	A
2	7	13	A
2	7	21	G
2	7	25	G
2	7	42	A
2	7	49	A
2	7	51	G
2	7	53	U
2	7	54	A
2	7	64	G
2	7	97	G
2	7	99	G
2	7	100	A
2	7	110	G
2	7	111	C

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Mol	Chain	Res	Type
3	8	2	G
3	8	3	A
3	8	23	C
3	8	32	C
3	8	34	U
3	8	35	C
3	8	59	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	95	A
3	8	96	C
3	8	105	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	112	G
3	8	113	C
3	8	114	G
3	8	117	C
3	8	121	G
3	8	122	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	128	C
3	8	137	A
3	8	143	G
3	8	147	G
3	8	150	C
3	8	151	G
3	8	156	U
47	2	3	C
47	2	4	C
47	2	5	U
47	2	17	C
47	2	25	A
47	2	33	G
47	2	42	A
47	2	46	A

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Mol	Chain	Res	Type
47	2	56	G
47	2	59	U
47	2	62	G
47	2	64	A
47	2	65	C
47	2	66	G
47	2	67	C
47	2	68	A
47	2	69	C
47	2	72	C
47	2	73	C
47	2	74	G
47	2	76	U
47	2	77	A
47	2	79	A
47	2	81	U
47	2	84	A
47	2	88	G
47	2	91	A
47	2	92	A
47	2	99	A
47	2	100	U
47	2	103	A
47	2	111	A
47	2	113	G
47	2	115	U
47	2	123	G
47	2	125	C
47	2	126	G
47	2	128	U
47	2	129	C
47	2	142	C
47	2	143	U
47	2	145	G
47	2	146	G
47	2	147	A
47	2	155	G
47	2	158	A
47	2	160	U
47	2	162	C
47	2	163	U
47	2	164	A

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Mol	Chain	Res	Type
47	2	170	A
47	2	172	U
47	2	173	A
47	2	175	A
47	2	182	C
47	2	183	G
47	2	184	G
47	2	187	G
47	2	189	U
47	2	190	G
47	2	191	A
47	2	192	C
47	2	196	C
47	2	200	G
47	2	201	C
47	2	203	G
47	2	210	U
47	2	212	C
47	2	213	G
47	2	214	U
47	2	215	G
47	2	216	C
47	2	217	A
47	2	218	U
47	2	219	U
47	2	221	A
47	2	224	A
47	2	292	A
47	2	294	U
47	2	297	A
47	2	304	C
47	2	305	U
47	2	308	G
47	2	309	G
47	2	310	C
47	2	312	G
47	2	317	C
47	2	319	C
47	2	320	G
47	2	321	C
47	2	322	C
47	2	323	C

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Mol	Chain	Res	Type
47	2	335	G
47	2	336	A
47	2	347	G
47	2	360	A
47	2	361	U
47	2	362	C
47	2	364	A
47	2	368	U
47	2	370	G
47	2	373	G
47	2	381	C
47	2	382	C
47	2	385	G
47	2	386	C
47	2	389	A
47	2	391	C
47	2	400	C
47	2	407	G
47	2	409	C
47	2	418	A
47	2	420	G
47	2	429	C
47	2	441	C
47	2	447	A
47	2	448	A
47	2	450	C
47	2	462	C
47	2	464	A
47	2	465	A
47	2	466	G
47	2	467	G
47	2	468	A
47	2	472	C
47	2	473	A
47	2	474	G
47	2	482	G
47	2	487	U
47	2	488	U
47	2	489	A
47	2	492	C
47	2	493	A
47	2	494	C

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Mol	Chain	Res	Type
47	2	496	C
47	2	497	C
47	2	498	C
47	2	500	A
47	2	501	C
47	2	507	G
47	2	517	C
47	2	525	A
47	2	526	A
47	2	528	A
47	2	530	U
47	2	531	A
47	2	532	C
47	2	533	A
47	2	537	C
47	2	541	U
47	2	542	U
47	2	543	C
47	2	544	G
47	2	547	G
47	2	548	C
47	2	549	C
47	2	550	C
47	2	551	U
47	2	553	U
47	2	554	A
47	2	556	U
47	2	559	G
47	2	561	A
47	2	562	U
47	2	564	A
47	2	568	C
47	2	575	A
47	2	576	A
47	2	577	U
47	2	579	C
47	2	587	A
47	2	588	G
47	2	590	A
47	2	591	U
47	2	592	C
47	2	594	A

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Mol	Chain	Res	Type
47	2	600	G
47	2	604	A
47	2	606	G
47	2	607	U
47	2	608	C
47	2	609	U
47	2	614	C
47	2	615	C
47	2	617	G
47	2	627	U
47	2	629	A
47	2	643	A
47	2	644	G
47	2	655	A
47	2	657	U
47	2	659	G
47	2	660	C
47	2	664	A
47	2	668	A
47	2	669	A
47	2	671	A
47	2	672	A
47	2	673	G
47	2	674	C
47	2	684	G
47	2	687	C
47	2	692	G
47	2	694	G
47	2	697	G
47	2	731	G
47	2	732	U
47	2	733	C
47	2	735	C
47	2	744	G
47	2	750	C
47	2	751	G
47	2	752	G
47	2	753	C
47	2	754	G
47	2	755	C
47	2	789	G
47	2	790	C

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Mol	Chain	Res	Type
47	2	792	C
47	2	794	A
47	2	795	A
47	2	796	G
47	2	797	C
47	2	798	G
47	2	799	U
47	2	811	A
47	2	812	A
47	2	818	A
47	2	821	G
47	2	822	U
47	2	825	A
47	2	827	A
47	2	829	C
47	2	834	C
47	2	845	G
47	2	847	A
47	2	849	A
47	2	850	C
47	2	862	A
47	2	869	A
47	2	870	A
47	2	871	U
47	2	873	G
47	2	874	G
47	2	875	A
47	2	877	C
47	2	878	G
47	2	879	C
47	2	883	U
47	2	884	C
47	2	885	U
47	2	886	A
47	2	887	U
47	2	890	U
47	2	891	G
47	2	893	U
47	2	894	G
47	2	898	U
47	2	901	G
47	2	908	A

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Mol	Chain	Res	Type
47	2	909	G
47	2	910	G
47	2	913	A
47	2	914	U
47	2	918	U
47	2	920	A
47	2	921	G
47	2	930	C
47	2	933	G
47	2	943	U
47	2	955	A
47	2	956	G
47	2	963	A
47	2	970	G
47	2	976	G
47	2	977	C
47	2	978	G
47	2	990	A
47	2	992	A
47	2	999	G
47	2	1002	U
47	2	1017	U
47	2	1023	A
47	2	1044	G
47	2	1045	U
47	2	1046	U
47	2	1058	A
47	2	1059	G
47	2	1060	A
47	2	1070	A
47	2	1078	C
47	2	1083	A
47	2	1085	C
47	2	1100	A
47	2	1110	G
47	2	1115	U
47	2	1116	C
47	2	1117	C
47	2	1118	C
47	2	1121	G
47	2	1126	G
47	2	1133	A

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Mol	Chain	Res	Type
47	2	1138	C
47	2	1139	C
47	2	1144	A
47	2	1148	A
47	2	1149	A
47	2	1150	A
47	2	1153	C
47	2	1154	U
47	2	1175	G
47	2	1194	A
47	2	1195	A
47	2	1200	A
47	2	1204	A
47	2	1207	G
47	2	1215	C
47	2	1242	U
47	2	1243	U
47	2	1251	A
47	2	1253	A
47	2	1256	G
47	2	1257	G
47	2	1258	A
47	2	1259	A
47	2	1260	A
47	2	1261	C
47	2	1263	U
47	2	1265	A
47	2	1274	G
47	2	1275	G
47	2	1277	C
47	2	1278	A
47	2	1283	C
47	2	1284	A
47	2	1285	G
47	2	1286	G
47	2	1288	U
47	2	1291	A
47	2	1292	C
47	2	1293	A
47	2	1294	G
47	2	1298	G
47	2	1299	A

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Mol	Chain	Res	Type
47	2	1300	U
47	2	1301	A
47	2	1302	G
47	2	1303	C
47	2	1307	U
47	2	1308	U
47	2	1309	C
47	2	1312	G
47	2	1313	A
47	2	1316	C
47	2	1318	G
47	2	1320	G
47	2	1321	G
47	2	1330	G
47	2	1342	U
47	2	1348	G
47	2	1354	G
47	2	1371	U
47	2	1372	U
47	2	1375	G
47	2	1378	A
47	2	1379	A
47	2	1380	C
47	2	1395	C
47	2	1396	A
47	2	1397	U
47	2	1399	C
47	2	1400	U
47	2	1401	A
47	2	1402	A
47	2	1403	C
47	2	1404	U
47	2	1409	A
47	2	1411	G
47	2	1415	C
47	2	1428	G
47	2	1429	G
47	2	1442	U
47	2	1447	G
47	2	1450	G
47	2	1452	A
47	2	1453	C

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Mol	Chain	Res	Type
47	2	1454	A
47	2	1455	A
47	2	1462	U
47	2	1463	U
47	2	1464	C
47	2	1473	G
47	2	1475	G
47	2	1476	A
47	2	1478	U
47	2	1479	G
47	2	1480	A
47	2	1489	A
47	2	1490	G
47	2	1491	G
47	2	1494	U
47	2	1495	G
47	2	1498	A
47	2	1499	U
47	2	1506	A
47	2	1507	G
47	2	1509	U
47	2	1514	G
47	2	1518	C
47	2	1519	U
47	2	1520	G
47	2	1521	C
47	2	1522	A
47	2	1523	C
47	2	1533	A
47	2	1548	G
47	2	1551	U
47	2	1552	G
47	2	1553	C
47	2	1554	C
47	2	1555	U
47	2	1556	A
47	2	1557	C
47	2	1558	C
47	2	1560	U
47	2	1570	G
47	2	1574	C
47	2	1580	A

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Mol	Chain	Res	Type
47	2	1584	G
47	2	1585	U
47	2	1588	A
47	2	1595	U
47	2	1599	U
47	2	1601	A
47	2	1604	G
47	2	1612	G
47	2	1618	C
47	2	1621	U
47	2	1623	A
47	2	1625	U
47	2	1637	A
47	2	1638	G
47	2	1639	G
47	2	1641	A
47	2	1647	A
47	2	1648	G
47	2	1654	G
47	2	1661	A
47	2	1662	U
47	2	1664	A
47	2	1665	G
47	2	1680	G
47	2	1683	C
47	2	1684	C
47	2	1685	U
47	2	1686	G
47	2	1697	A
47	2	1698	C
47	2	1699	A
47	2	1700	C
47	2	1711	U
47	2	1721	U
47	2	1722	G
47	2	1726	G
47	2	1744	G
47	2	1745	A
47	2	1746	U
47	2	1749	G
47	2	1756	C
47	2	1757	G

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Mol	Chain	Res	Type
47	2	1760	G
47	2	1761	U
47	2	1777	G
47	2	1778	C
47	2	1782	G
47	2	1783	C
47	2	1784	G
47	2	1785	C
47	2	1800	A
47	2	1817	G
47	2	1819	A
47	2	1823	A
47	2	1824	A
47	2	1825	A
47	2	1826	G
47	2	1829	G
47	2	1831	A
47	2	1835	A
47	2	1837	G
47	2	1838	U
47	2	1841	C
47	2	1842	C
47	2	1845	A
47	2	1849	G
47	2	1851	A
47	2	1852	C
47	2	1858	G
47	2	1859	A
47	2	1861	G
47	2	1862	G
47	2	1863	A
47	2	1864	U
47	2	1865	C
47	2	1869	A
82	1	6420	A
82	1	6424	U
82	1	6425	A
82	1	6426	U
82	1	6427	G
82	1	6428	G
82	1	6429	U
82	1	6430	U

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Mol	Chain	Res	Type
82	1	6431	A
82	1	6432	C
82	1	6433	C
82	1	6434	C
82	1	6435	A
82	1	6438	A
82	1	6445	G
82	1	6449	U
82	1	6450	U
82	1	6451	U
82	1	6455	A
82	1	6457	A
82	1	6470	A
82	1	6472	G
82	1	6473	C
82	1	6474	U
82	1	6475	U
82	1	6482	A
82	1	6483	U
82	1	6484	G
82	1	6485	G
82	1	6486	U
82	1	6487	C
82	1	6488	G
82	1	6492	U
82	1	6493	G
82	1	6494	C
82	1	6499	U
82	1	6501	U
82	1	6502	A
82	1	6505	G
82	1	6506	U
82	1	6507	G
82	1	6509	G
82	1	6510	G
82	1	6511	A
82	1	6512	G
82	1	6513	C
82	1	6514	C
82	1	6515	U
82	1	6516	C
82	1	6517	G

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Mol	Chain	Res	Type
82	1	6518	G
82	1	6521	G
82	1	6522	C
82	1	6523	A
82	1	6526	C
82	1	6527	C
82	1	6528	C
82	1	6532	A
82	1	6533	A
82	1	6534	A
82	1	6535	U
82	1	6536	C
82	1	6538	U
82	1	6540	U
82	1	6541	A
82	1	6542	U
82	1	6544	G
82	1	6545	G
82	1	6548	A
82	1	6549	G
82	1	6550	G
82	1	6551	A
82	1	6552	A
82	1	6554	A
82	1	6555	G
82	1	6556	C
82	1	6557	U
82	1	6558	G
82	1	6562	U
82	1	6567	A
82	1	6568	G
82	1	6571	A
82	1	6572	C
82	1	6575	C
82	1	6577	G
82	1	6581	U
82	1	6585	G
82	1	6586	U
82	1	6587	A
82	1	6588	A
82	1	6589	C
82	1	6590	A

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Mol	Chain	Res	Type
82	1	6591	C
82	1	6597	G
82	1	6598	C
82	1	6599	G
82	1	6601	U
82	1	6602	C
82	1	6603	C
82	1	6604	G
82	1	6605	A
82	1	6606	A
82	1	6607	A
82	1	6608	U
82	1	6609	A
82	1	6610	C
82	1	6611	C
82	1	6612	A
82	1	6613	U
82	1	6616	C
82	1	6617	U
82	1	6618	U
82	1	6620	A
82	1	6621	U
82	1	6622	A

All (143) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	47	A
1	5	48	G
1	5	125	C
1	5	170	C
1	5	209	U
1	5	217	C
1	5	275	C
1	5	385	A
1	5	408	A
1	5	449	C
1	5	504	G
1	5	920	C
1	5	922	C
1	5	923	C
1	5	925	G

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Mol	Chain	Res	Type
1	5	928	A
1	5	935	G
1	5	936	C
1	5	955	G
1	5	1183	C
1	5	1236	C
1	5	1237	C
1	5	1287	G
1	5	1300	G
1	5	1370	G
1	5	1445	U
1	5	1455	G
1	5	1633	G
1	5	1654	G
1	5	1676	C
1	5	1733	G
1	5	1740	C
1	5	1881	C
1	5	1960	A
1	5	1974	U
1	5	2046	G
1	5	2259	G
1	5	2313	A
1	5	2370	A
1	5	2428	A
1	5	2490	U
1	5	2502	A
1	5	2529	A
1	5	2554	U
1	5	2587	A
1	5	2661	U
1	5	2782	U
1	5	2848	G
1	5	3603	G
1	5	3710	G
1	5	3758	U
1	5	3759	A
1	5	3765	G
1	5	3774	A
1	5	3784	A
1	5	3785	A
1	5	3876	A

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Mol	Chain	Res	Type
1	5	3888	G
1	5	3904	G
1	5	3938	G
1	5	4054	C
1	5	4076	G
1	5	4119	C
1	5	4170	A
1	5	4180	G
1	5	4221	C
1	5	4232	U
1	5	4448	G
1	5	4560	C
1	5	4572	U
1	5	4583	C
1	5	4626	A
1	5	4719	G
1	5	4882	U
1	5	4884	G
1	5	4925	U
1	5	5016	A
2	7	109	U
3	8	94	G
47	2	24	C
47	2	73	C
47	2	80	G
47	2	98	C
47	2	110	U
47	2	172	U
47	2	293	C
47	2	316	G
47	2	407	G
47	2	449	A
47	2	461	U
47	2	465	A
47	2	493	A
47	2	500	A
47	2	532	C
47	2	553	U
47	2	561	A
47	2	587	A
47	2	659	G
47	2	752	G

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Mol	Chain	Res	Type
47	2	874	G
47	2	885	U
47	2	886	A
47	2	908	A
47	2	917	U
47	2	1165	G
47	2	1258	A
47	2	1260	A
47	2	1262	C
47	2	1277	C
47	2	1298	G
47	2	1300	U
47	2	1312	G
47	2	1452	A
47	2	1462	U
47	2	1474	A
47	2	1488	C
47	2	1490	G
47	2	1497	G
47	2	1519	U
47	2	1554	C
47	2	1556	A
47	2	1637	A
47	2	1664	A
47	2	1685	U
47	2	1743	G
47	2	1744	G
47	2	1824	A
47	2	1858	G
47	2	1862	G
82	1	6432	C
82	1	6450	U
82	1	6456	U
82	1	6472	G
82	1	6493	G
82	1	6506	U
82	1	6514	C
82	1	6538	U
82	1	6551	A
82	1	6589	C
82	1	6604	G
82	1	6607	A

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Mol	Chain	Res	Type
82	1	6608	U
82	1	6617	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
1	5	26

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.75
1	5	1252:C	O3'	1271:G	P	37.28
1	5	1405:C	O3'	1409:G	P	20.58
1	5	1219:G	O3'	1233:G	P	19.67
1	5	1696:C	O3'	1720:C	P	18.85
1	5	4138:C	O3'	4146:G	P	18.54
1	5	991:U	O3'	1064:G	P	17.85
1	5	4101:C	O3'	4107:G	P	17.31
1	5	3977:C	O3'	4034:G	P	16.55
1	5	523:C	O3'	638:G	P	16.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	5022:U	O3'	5028:G	P	15.62
1	5	760:G	O3'	903:C	P	14.99
1	5	1364:U	O3'	1368:A	P	14.85
1	5	4777:C	O3'	4859:C	P	14.39
1	5	2901:G	O3'	3597:G	P	12.73
1	5	4729:A	O3'	4735:G	P	9.82
1	5	1180:C	O3'	1183:C	P	9.58
1	5	182:G	O3'	189:G	P	8.45
1	5	4740:G	O3'	4743:G	P	8.00
1	5	512:U	O3'	515:C	P	7.78
1	5	500:G	O3'	504:G	P	7.67
1	5	1438:U	O3'	1440:U	P	4.58
1	5	1411:C	O3'	1412:G	P	4.41
1	5	1100:U	O3'	1168:G	P	4.02
1	5	1239:C	O3'	1244:G	P	3.64
1	5	4899:G	O3'	4902:C	P	3.30

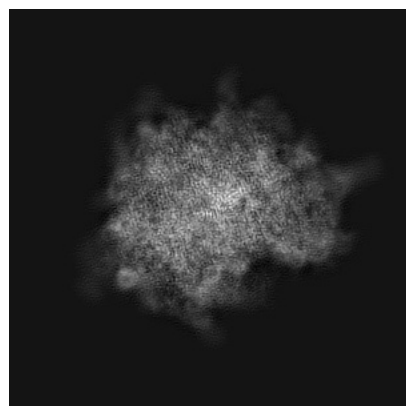
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20258. These allow visual inspection of the internal detail of the map and identification of artifacts.

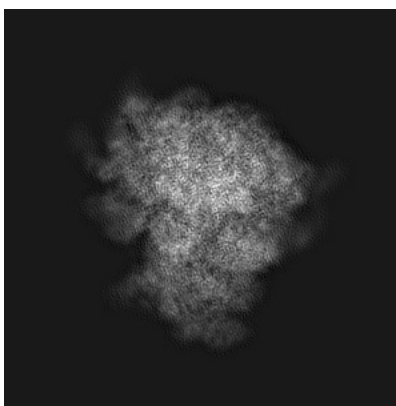
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

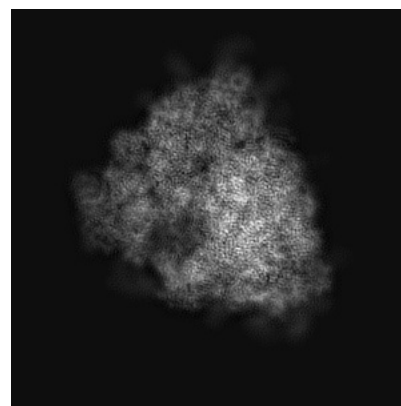
6.1.1 Primary map



X

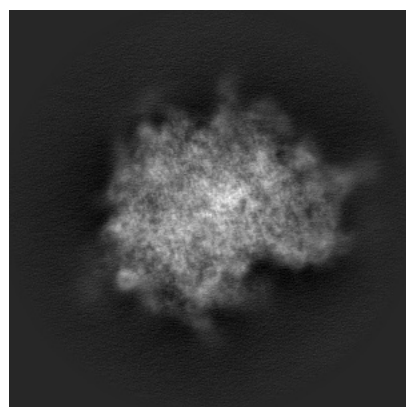


Y

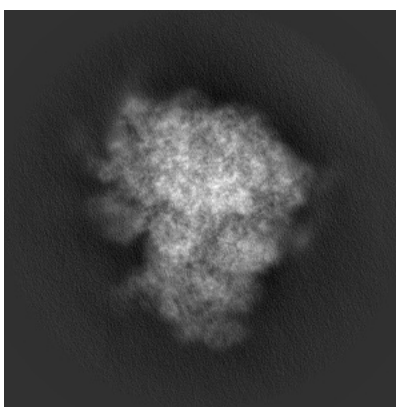


Z

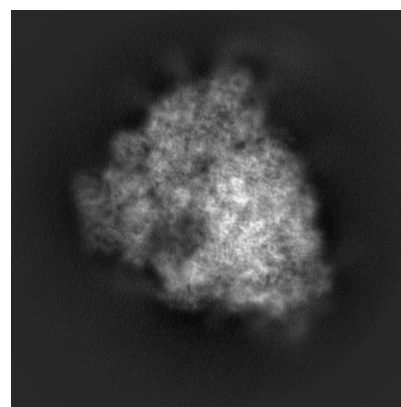
6.1.2 Raw map



X



Y

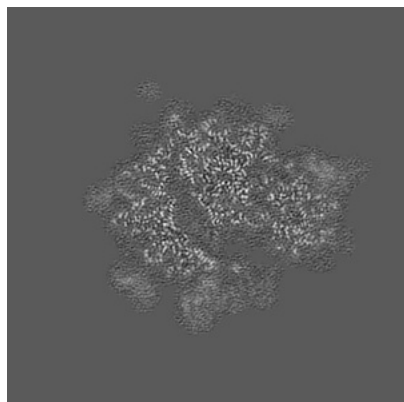


Z

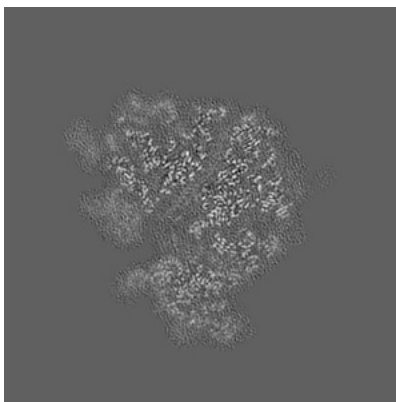
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

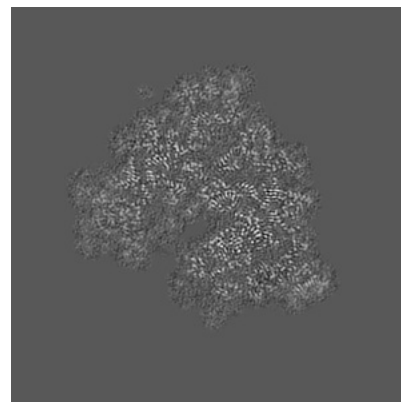
6.2.1 Primary map



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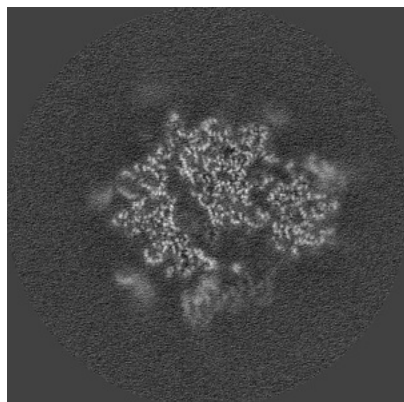


Y Index: 208

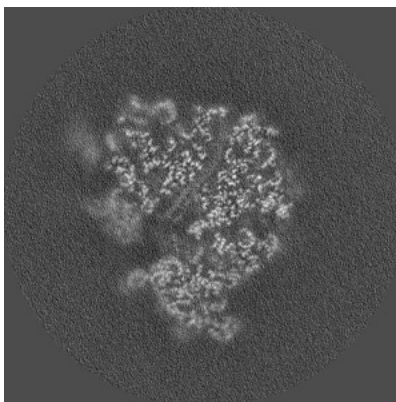


Z Index: 208

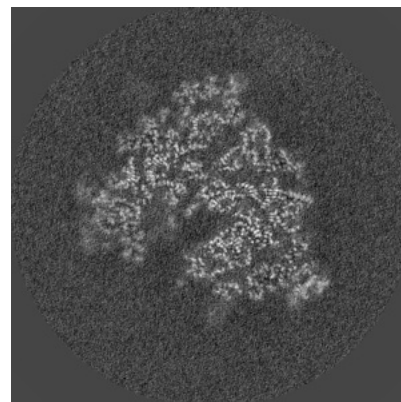
6.2.2 Raw map



X Index: 208



Y Index: 208

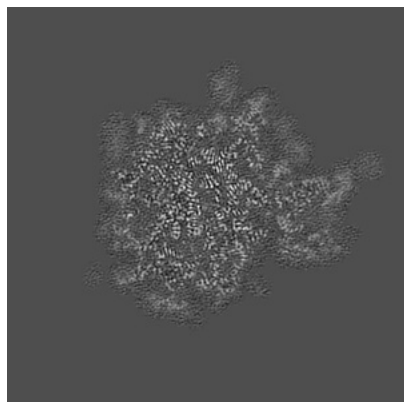


Z Index: 208

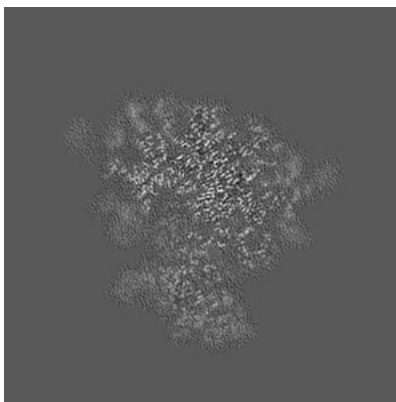
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

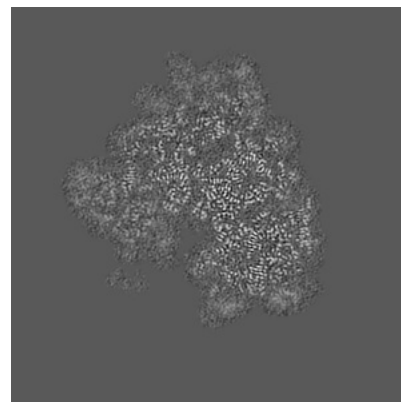
6.3.1 Primary map



X Index: 239

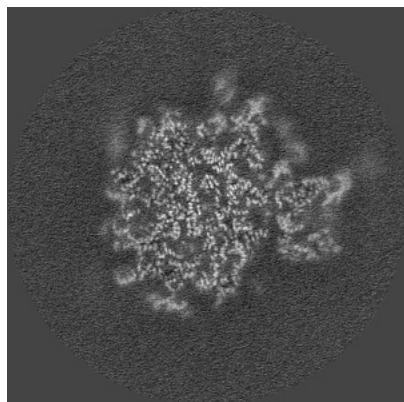


Y Index: 217

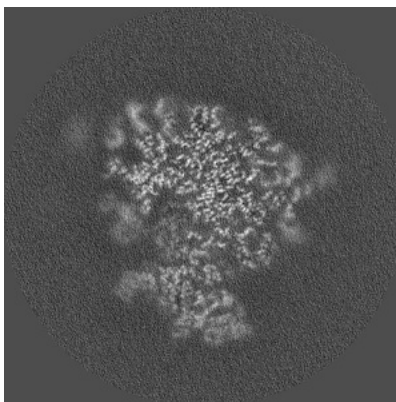


Z Index: 225

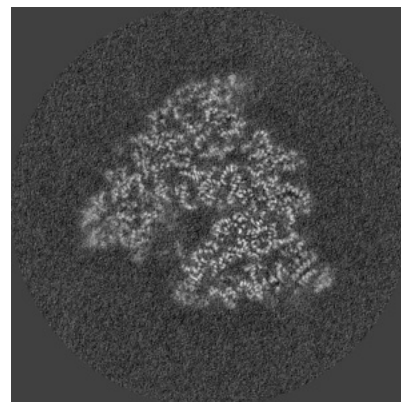
6.3.2 Raw map



X Index: 239



Y Index: 217

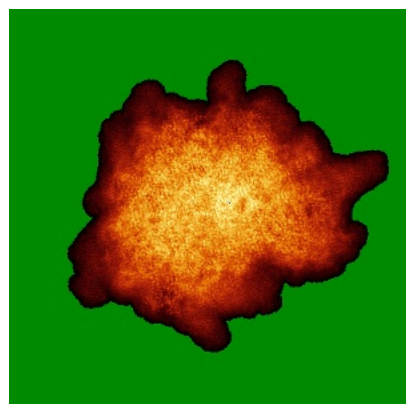


Z Index: 199

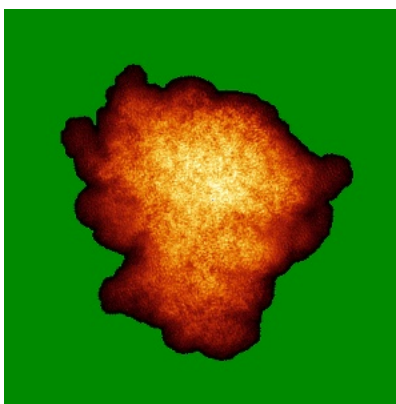
The images above show the largest variance slices of the map in three orthogonal directions.

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

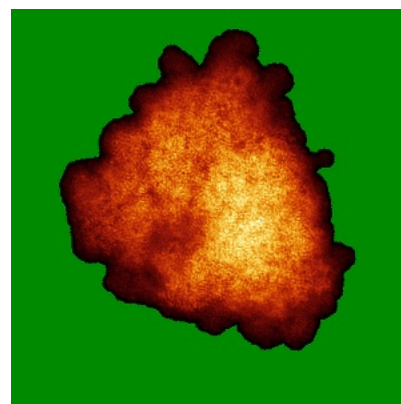
6.4.1 Primary map



X

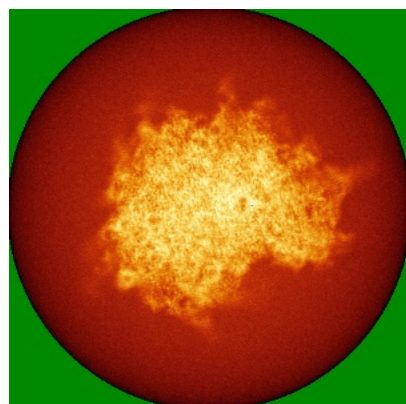


Y

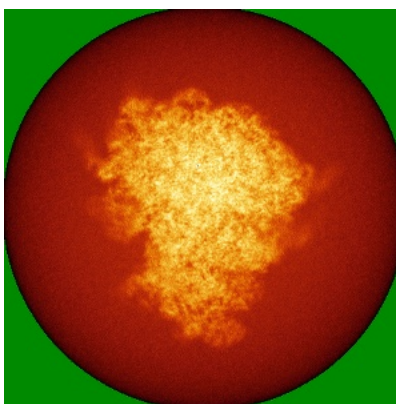


Z

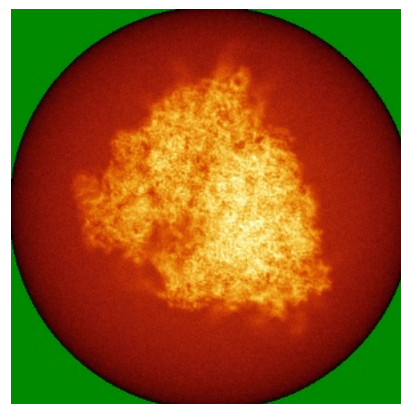
6.4.2 Raw map



X



Y

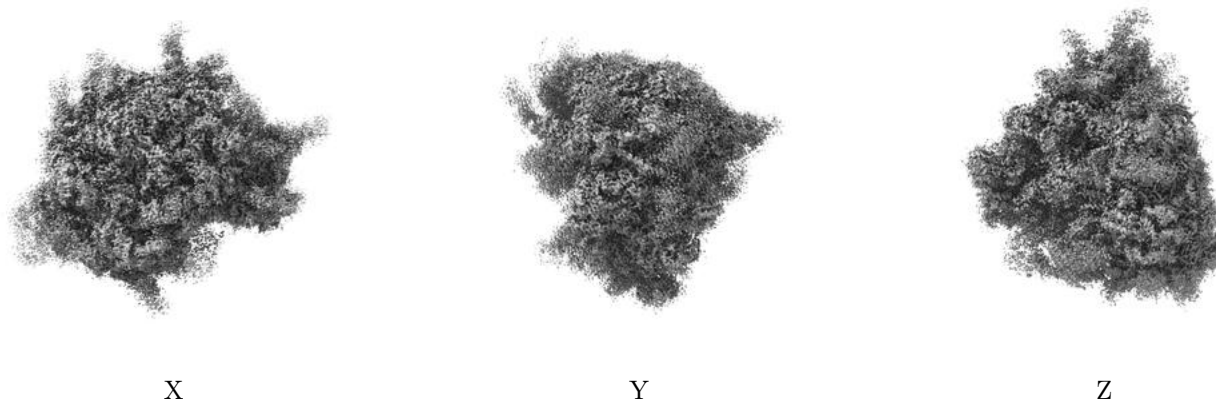


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

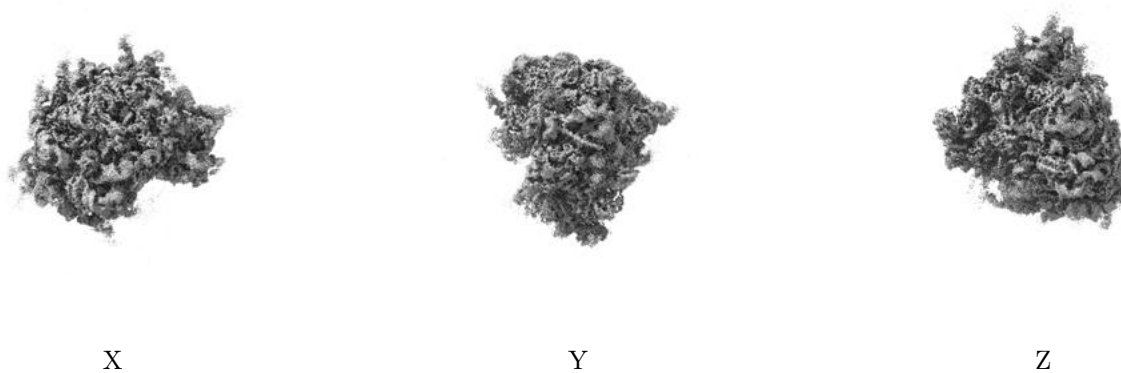
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

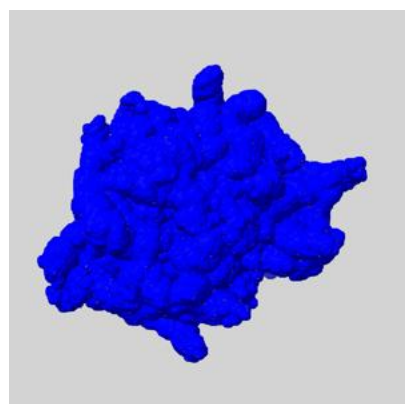
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

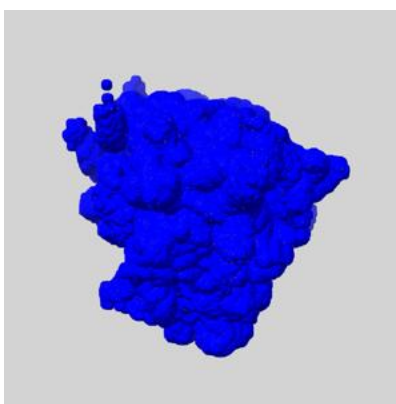
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

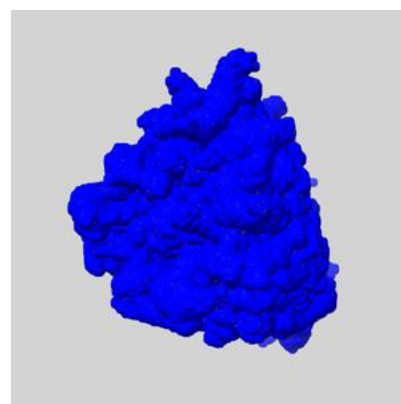
6.6.1 emd_20258_msk_1.map [i](#)



X



Y

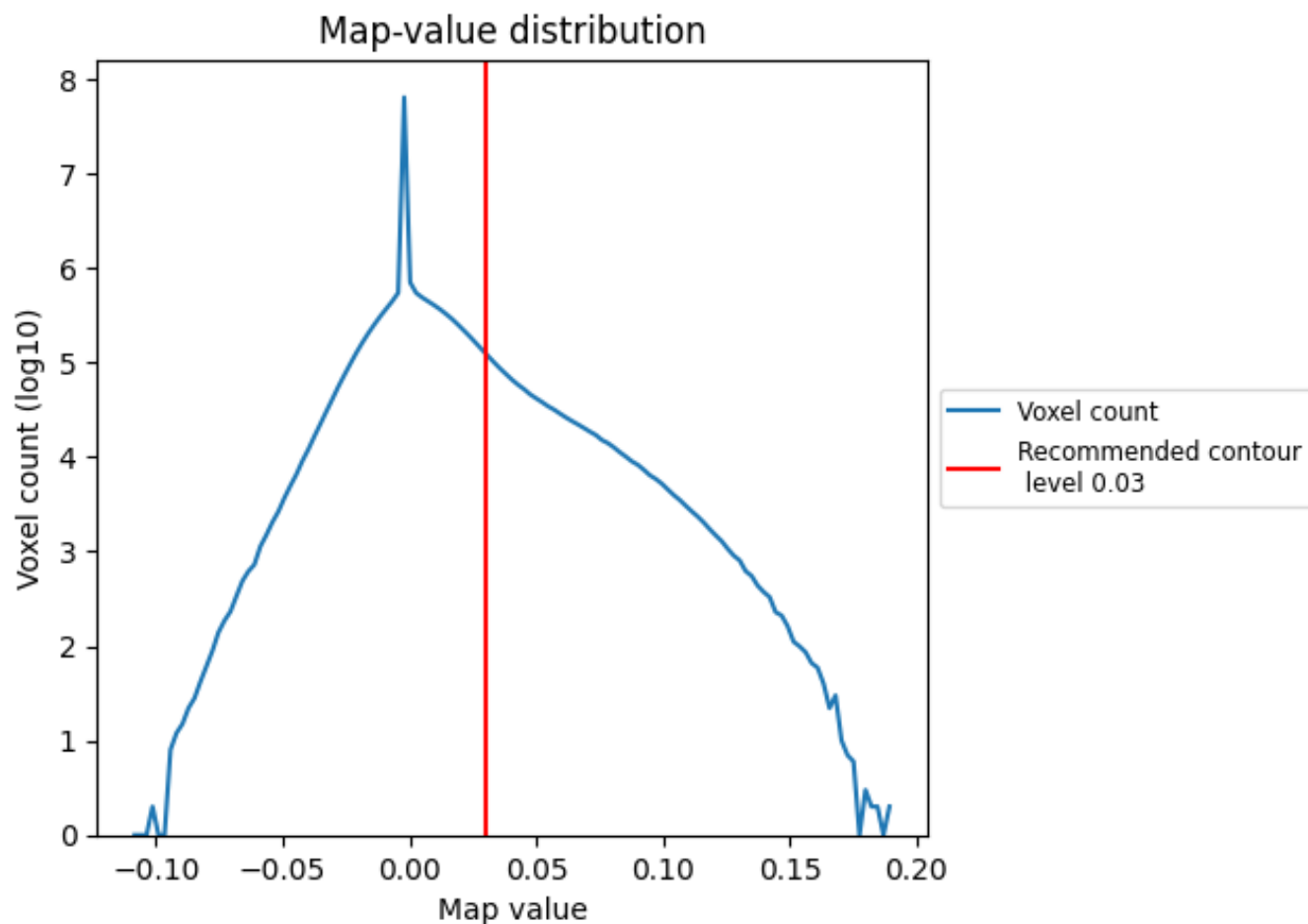


Z

7 Map analysis [i](#)

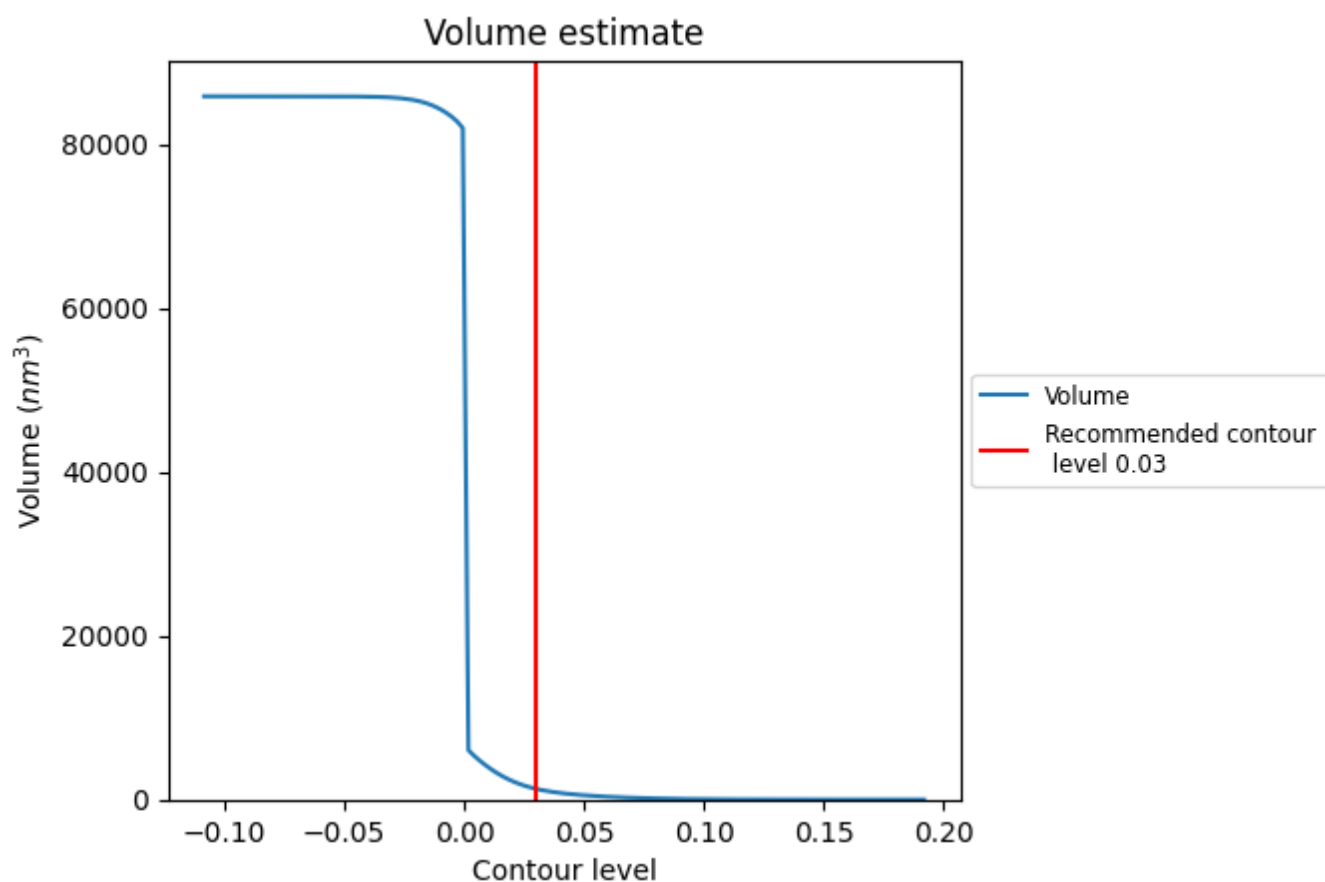
This section contains the results of statistical analysis of the map.

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.

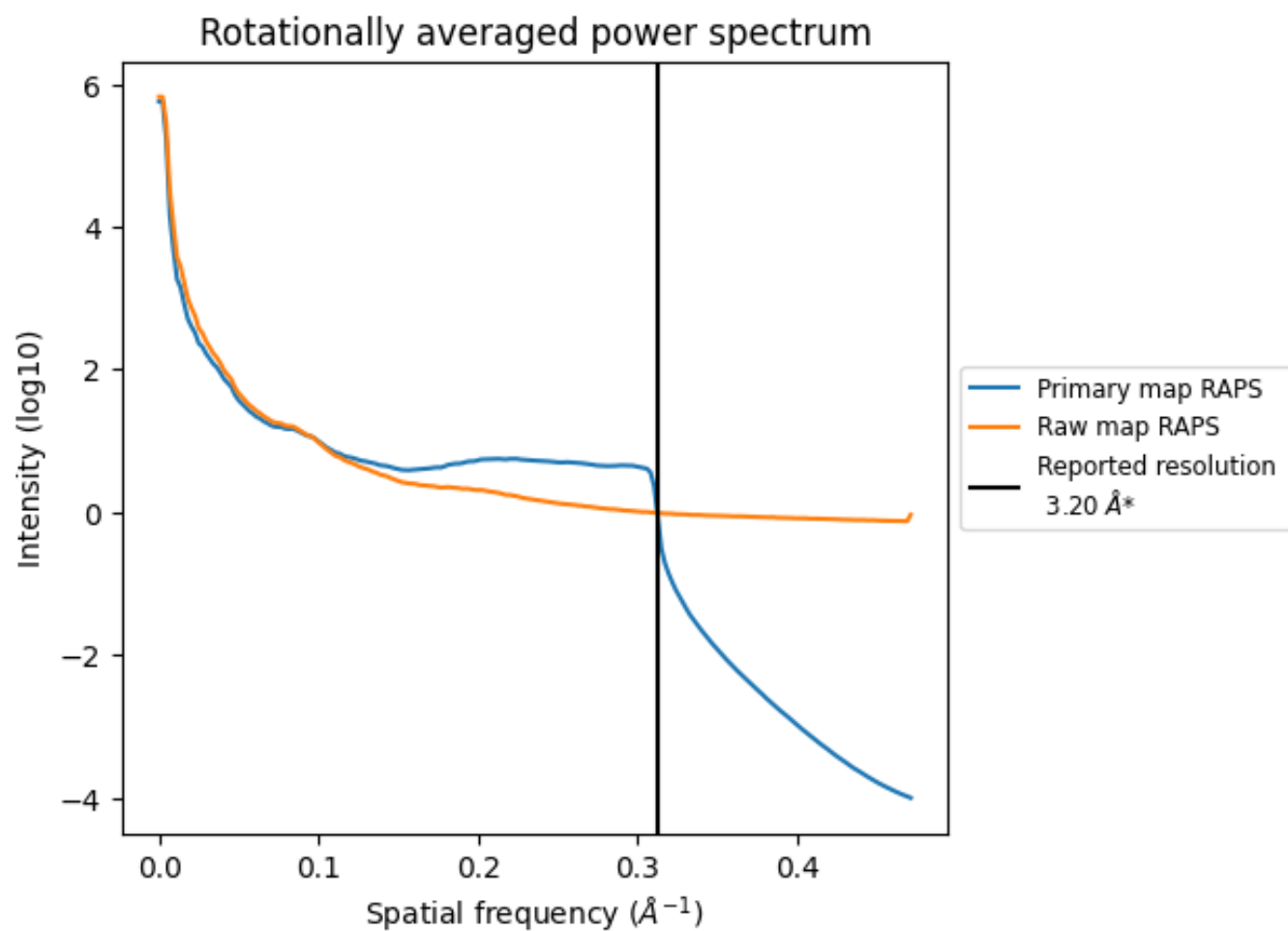
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309 nm³; this corresponds to an approximate mass of 1182 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 ⓘ

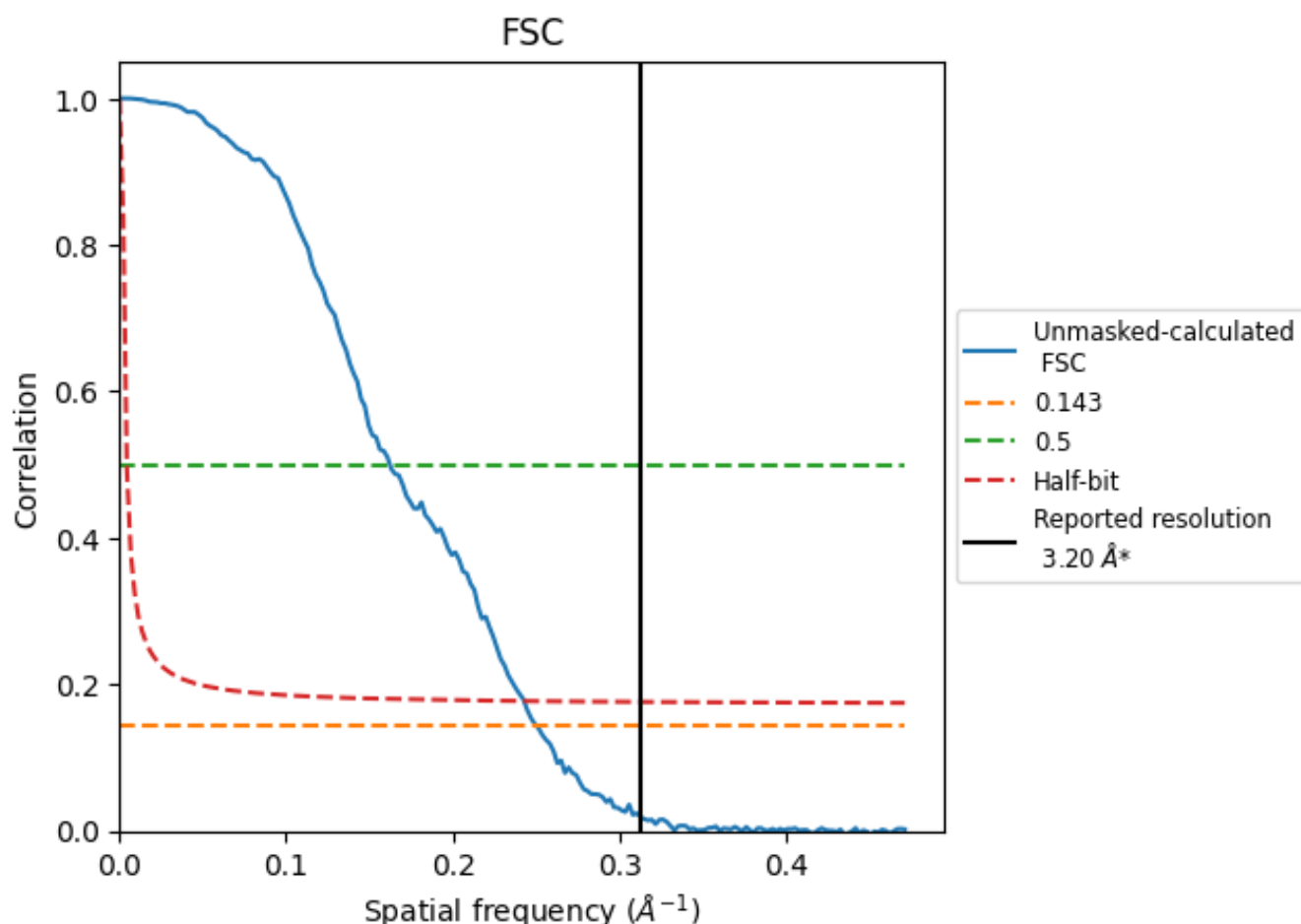


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

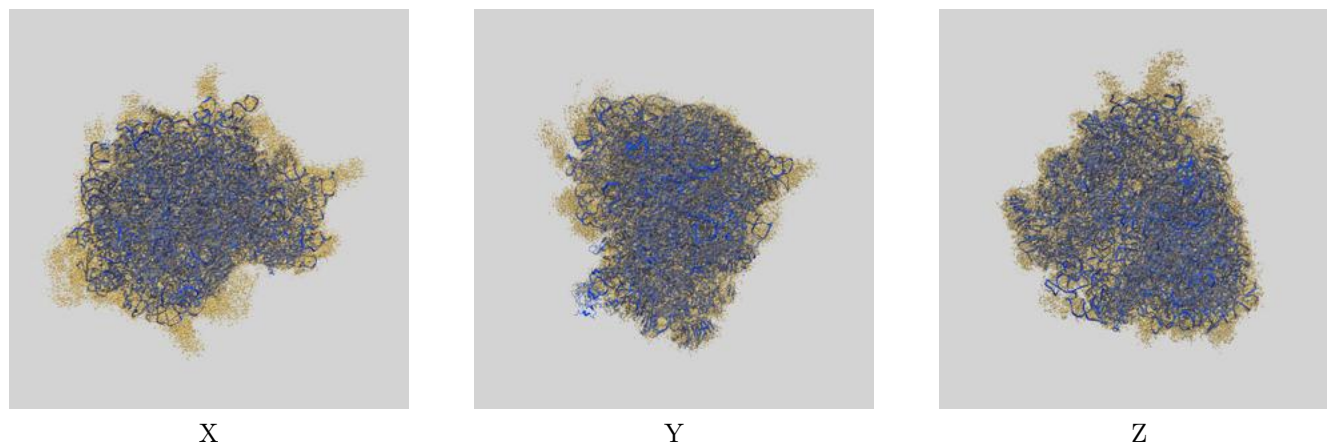
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	6.16	4.12

*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 3.99 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

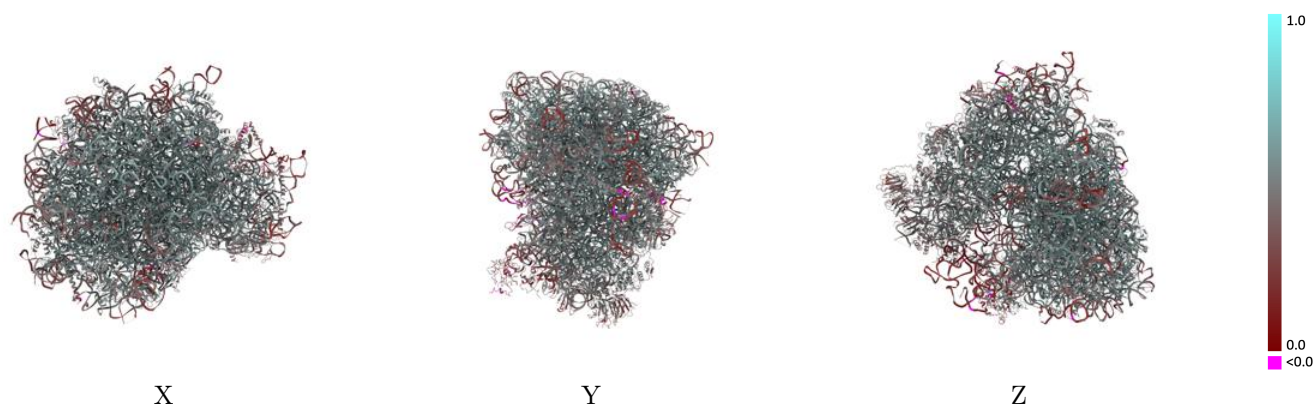
This section contains information regarding the fit between EMDB map EMD-20258 and PDB model 6P5N. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



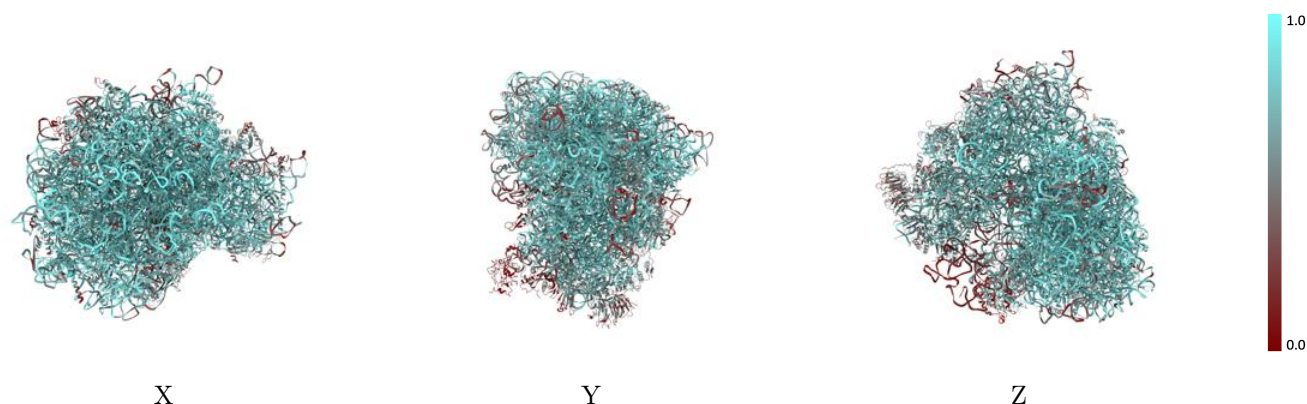
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



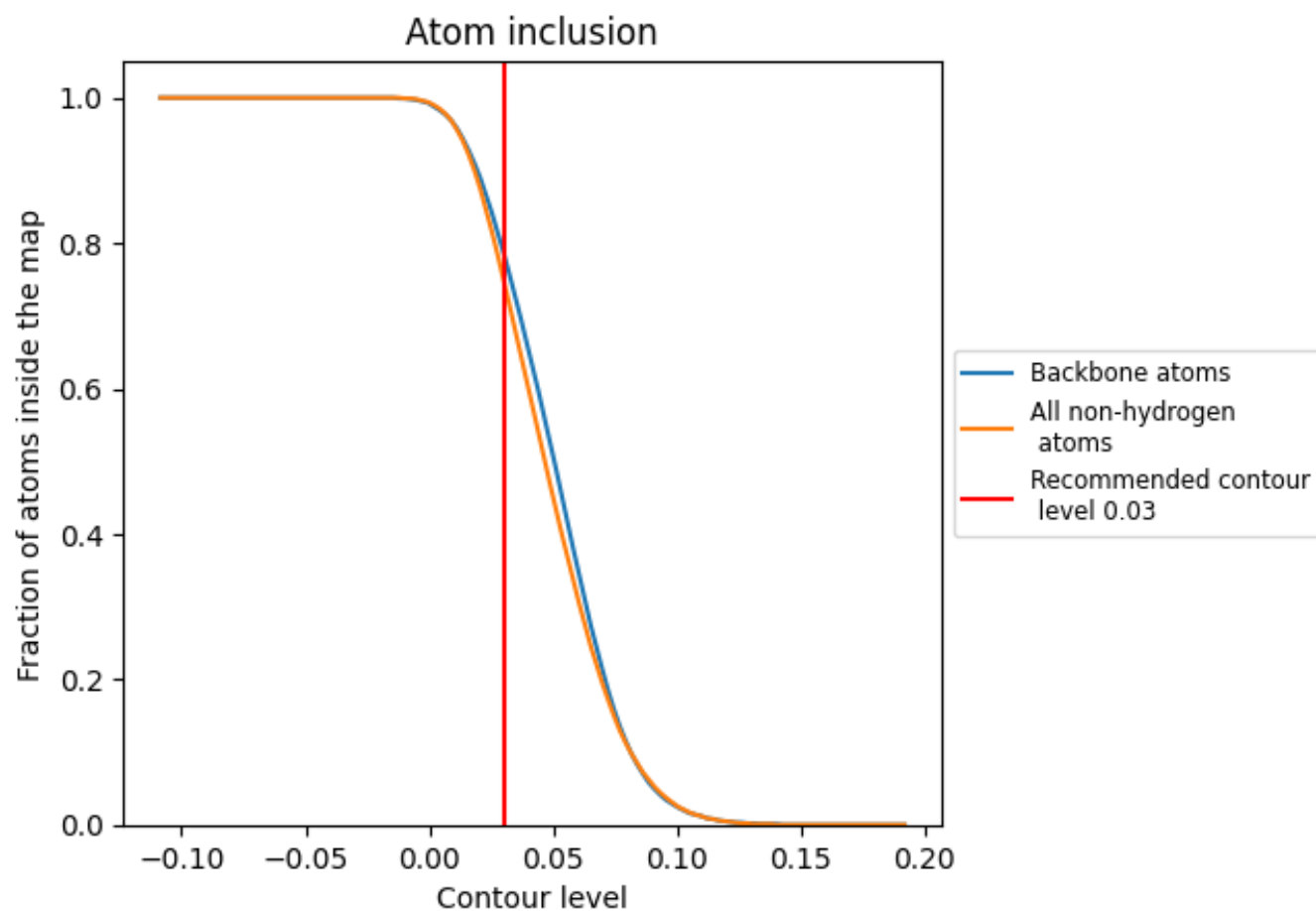
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.4850
1	 0.2500	 0.2150
2	 0.8020	 0.4770
5	 0.8370	 0.4960
7	 0.9270	 0.5430
8	 0.8660	 0.5170
AA	 0.8280	 0.5530
AB	 0.8060	 0.5410
AC	 0.7950	 0.5350
AD	 0.7600	 0.5180
AE	 0.7440	 0.5010
AF	 0.8030	 0.5440
AG	 0.7180	 0.5010
AH	 0.7190	 0.5150
AI	 0.7530	 0.5300
AJ	 0.7010	 0.4970
AK	 0.1630	 0.2730
AL	 0.7700	 0.5280
AM	 0.7580	 0.5210
AN	 0.8590	 0.5640
AO	 0.7950	 0.5310
AP	 0.8040	 0.5460
AQ	 0.7950	 0.5490
AR	 0.7290	 0.4860
AS	 0.8020	 0.5340
AT	 0.7610	 0.5360
AU	 0.6580	 0.4710
AV	 0.7830	 0.5410
AW	 0.7840	 0.5430
AX	 0.7480	 0.5300
AY	 0.7680	 0.5330
AZ	 0.7640	 0.5230
Aa	 0.8380	 0.5550
Ab	 0.6810	 0.4740
Ac	 0.7900	 0.5340















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Chain	Atom inclusion	Q-score
Ad	 0.7360	 0.5270
Ae	 0.7950	 0.5480
Af	 0.8210	 0.5500
Ag	 0.7710	 0.5320
Ah	 0.7340	 0.5040
Ai	 0.7240	 0.5050
Aj	 0.8500	 0.5560
Ak	 0.6460	 0.4770
Al	 0.7890	 0.5420
Am	 0.7590	 0.5380
An	 0.7890	 0.5430
Ao	 0.7830	 0.5460
Ap	 0.7640	 0.5340
Aq	 0.2120	 0.3460
Ar	 0.7940	 0.5400
B	 0.6870	 0.4970
C	 0.6960	 0.5030
D	 0.7290	 0.5150
E	 0.4890	 0.4330
F	 0.7010	 0.5030
G	 0.6380	 0.4810
H	 0.5800	 0.4290
I	 0.5890	 0.4480
J	 0.7190	 0.5110
K	 0.6970	 0.4950
L	 0.3140	 0.3490
M	 0.7260	 0.5250
N	 0.0270	 0.2410
O	 0.7570	 0.5240
P	 0.7220	 0.5180
Q	 0.4420	 0.3940
R	 0.6160	 0.4630
S	 0.5710	 0.4440
T	 0.5390	 0.4260
U	 0.5600	 0.4150
V	 0.4630	 0.4270
W	 0.6900	 0.4890
X	 0.7720	 0.5240
Y	 0.7300	 0.5240
Z	 0.6630	 0.4740
a	 0.5160	 0.4170
b	 0.7460	 0.5230

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Chain	Atom inclusion	Q-score
c	 0.6530	 0.4970
d	 0.6470	 0.5090
e	 0.6120	 0.4390
f	 0.5650	 0.4630
g	 0.0820	 0.2690
h	 0.4220	 0.3740