



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 10:51 AM UTC

PDB ID : 9H3G / pdb_00009h3g
EMDB ID : EMD-51820
Title : Structure of the Arabidopsis thaliana 80S ribosome in complex with P- and E-site tRNAs and mRNA
Authors : Faille, A.; Warren, A.J.
Deposited on : 2024-10-16
Resolution : 1.82 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

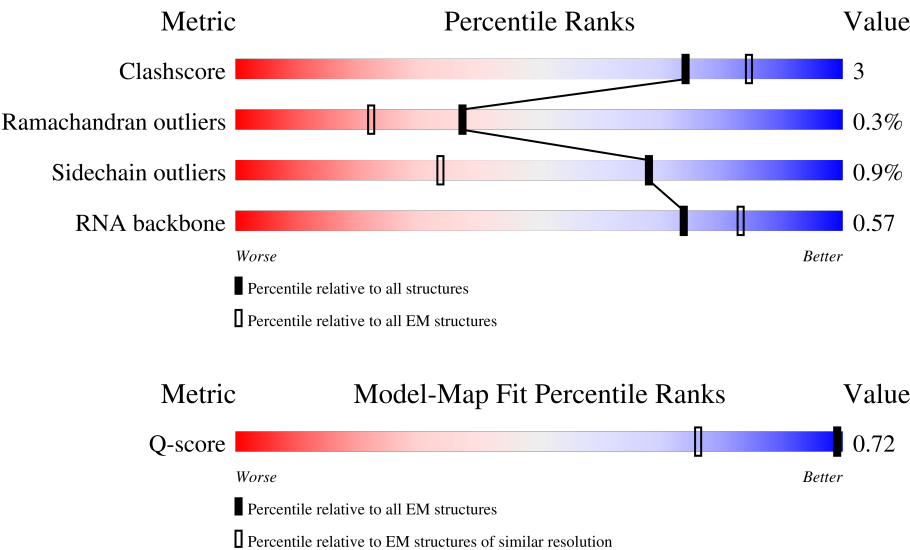
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.82 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	882 (1.33 - 2.32)

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	3	164	<div><div>6%</div><div>71%</div><div>25%</div><div>...</div></div>
2	A	3385	<div><div>6%</div><div>67%</div><div>22%</div><div>7%</div></div>
3	W2	76	<div><div>30%</div><div>74%</div><div>22%</div><div>...</div></div>



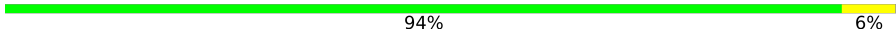

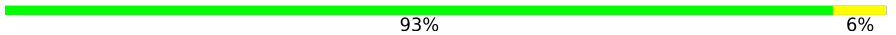




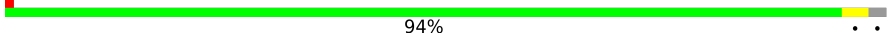















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Mol	Chain	Length	Quality of chain
3	i2	76	
4	C3	121	
5	BC	25	
6	BM	176	
7	BO	146	
8	AR	83	
9	AU	119	
10	Ma	131	
11	Ia	194	
12	AE	130	
13	AX	112	
14	AP	135	
15	Ja	262	
16	Ea	204	
17	AL	217	
18	Va	142	
19	Ka	133	
20	AW	112	
21	BD	105	
22	BS	389	
23	AM	164	
24	AC	284	
25	BI	140	
26	AH	134	
27	BT	406	

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Mol	Chain	Length	Quality of chain
28	AV	133	
29	AD	207	
30	AJ	187	
31	BQ	258	
32	BH	206	
33	Da	151	
34	BK	301	
35	AT	112	
36	Pa	62	
37	BP	123	
38	BN	154	
39	BG	256	
40	Fa	120	
41	Ha	146	
42	BU	182	
43	BR	247	
44	Xa	160	
45	BV	262	
46	BJ	221	
47	AO	164	
48	BW	82	
49	AK	214	
50	Na	86	
51	AB	197	
52	BF	233	

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Mol	Chain	Length	Quality of chain
53	AA	250	
54	AG	206	
55	Ga	128	
56	BA	51	
57	AF	146	
58	Wa	152	
59	Ta	249	
60	AZ	69	
61	BE	92	
62	Za	298	
63	AQ	143	
64	Oa	64	
65	Ua	150	
66	Ya	150	
67	BB	141	
68	AN	124	
69	Ra	190	
70	BL	143	
71	La	108	
72	Aa	222	
73	AY	95	
74	Ca	56	
75	h1	1805	
76	B1	12	
77	Ba	122	

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Mol	Chain	Length	Quality of chain
78	AI	177	<div><div></div><div>14%</div><div>46%</div><div>6%</div><div>48%</div></div>
79	L3	23	<div><div></div><div>83%</div><div>96%</div><div></div><div></div></div>

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 209234 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 Ribosomal RNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	162	Total	C	N	O	P	0	0
			3453	1544	617	1130	162		

- Molecule 2 is a RNA chain called Ribosomal RNA 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3149	Total	C	N	O	P	1	0
			67525	30162	12266	21947	3150		

- Molecule 3 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i2	76	Total	C	N	O	P	0	0
			1630	726	298	530	76		
3	W2	76	Total	C	N	O	P	0	0
			1629	726	298	529	76		

- Molecule 4 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	119	Total	C	N	O	P	0	0
			2536	1132	454	831	119		

- Molecule 5 is a protein called Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BM	155	Total	C	N	O	S	0	0
			1246	774	247	221	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BO	125	Total	C	N	O	S	0	0
			1030	637	211	179	3		

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AR	51	Total	C	N	O	S	0	0
			425	258	100	66	1		

- Molecule 9 is a protein called Large ribosomal subunit protein eL31y.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AU	109	Total	C	N	O	S	0	0
			888	558	168	160	2		

- Molecule 10 is a protein called Small ribosomal subunit protein eS26y.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ma	98	Total	C	N	O	S	0	0
			789	485	166	132	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ia	190	Total	C	N	O	S	0	0
			1512	961	270	275	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8z/uS8w.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	129	Total	C	N	O	S	0	0
			1033	660	188	180	5		

- Molecule 13 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AX	97	Total	C	N	O	S	0	0
			786	492	166	126	2		

- Molecule 14 is a protein called Large ribosomal subunit protein eL27x.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AP	134	Total	C	N	O	S	0	0
			1092	706	200	183	3		

- Molecule 15 is a protein called Small ribosomal subunit protein eS4x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ja	258	Total	C	N	O	S	0	0
			2074	1325	386	357	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ea	203	Total	C	N	O	S	1	0
			1713	1070	361	279	3		

- Molecule 17 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AL	175	Total	C	N	O	S	0	0
			1485	960	273	244	8		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12y.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Va	139	Total	C	N	O	S	0	0
			1082	689	207	183	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS24y.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ka	120	Total	C	N	O	S	0	0
			986	627	191	165	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL33y.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AW	111	Total	C	N	O	S	0	0
			901	568	174	155	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BD	97	Total	C	N	O	S	0	0
			792	497	158	132	5		

- Molecule 22 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	386	Total	C	N	O	S	0	0
			3111	1981	581	532	17		

- Molecule 23 is a protein called Large ribosomal subunit protein eL21z/eL21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	163	Total	C	N	O	S	0	0
			1307	827	254	222	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS5y/uS5u/uS5v.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AC	215	Total	C	N	O	S	0	0
			1672	1075	300	290	7		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BI	131	Total	C	N	O	S	0	0
			986	624	183	171	8		

- Molecule 26 is a protein called Large ribosomal subunit protein eL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AH	128	Total	C	N	O	S	0	0
			1042	665	194	179	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	393	Total	C	N	O	S	0	0
			3056	1934	573	535	14		

- Molecule 28 is a protein called Large ribosomal subunit protein eL32z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AV	126	Total	C	N	O	S	0	0
			1028	649	204	171	4		

- Molecule 29 is a protein called Small ribosomal subunit protein uS7y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	184	Total	C	N	O	S	0	0
			1454	912	275	261	6		

- Molecule 30 is a protein called Large ribosomal subunit protein eL18x.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AJ	186	Total	C	N	O	S	0	0
			1468	932	283	249	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BQ	245	Total	C	N	O	S	1	0
			1881	1179	379	316	7		

- Molecule 32 is a protein called Large ribosomal subunit protein uL13y.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	205	Total	C	N	O	S	0	0
			1636	1038	314	273	11		

- Molecule 33 is a protein called Small ribosomal subunit protein uS15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Da	149	Total	C	N	O	S	0	0
			1190	759	223	206	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BK	281	Total	C	N	O	S	0	0
			2277	1441	418	414	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AT	94	Total	C	N	O	S	0	0
			720	457	127	131	5		

- Molecule 36 is a protein called Small ribosomal subunit protein eS30z/eS30y/eS30x.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Pa	49	Total	C	N	O	0	0
			389	236	92	61		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	120	Total	C	N	O	S	0	0
			975	617	191	166	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	117	Total	C	N	O	S	0	0
			955	615	170	168	2		

- Molecule 39 is a protein called Large ribosomal subunit protein eL8y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	234	Total	C	N	O	S	0	0
			1874	1207	339	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Fa	111	Total	C	N	O	S	0	0
			896	560	187	148	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ha	145	Total	C	N	O	S	0	0
			1156	744	225	184	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	169	Total	C	N	O	S	0	0
			1366	863	254	242	7		

- Molecule 43 is a protein called Ribosomal protein L30/L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	232	Total	C	N	O	S	0	0
			1898	1221	348	325	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Xa	146	Total	C	N	O	S	0	0
			1163	742	224	192	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS1y.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BV	212	Total	C	N	O	S	0	0
			1718	1087	313	310	8		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BJ	207	Total	C	N	O	S	0	0
			1653	1047	327	268	11		

- Molecule 47 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AO	62	Total	C	N	O	S	0	0
			528	343	100	81	4		

- Molecule 48 is a protein called Small ribosomal subunit protein eS21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	73	Total	C	N	O	S	0	0
			568	355	104	107	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AK	178	Total	C	N	O	S	0	0
			1480	920	308	241	11		

- Molecule 50 is a protein called Small ribosomal subunit protein eS27y.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	83	Total	C	N	O	S	0	0
			647	405	118	117	7		

- Molecule 51 is a protein called Small ribosomal subunit protein uS4y.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AB	180	Total	C	N	O	S	0	0
			1514	953	303	254	4		

- Molecule 52 is a protein called Large ribosomal subunit protein eL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1491	966	273	250	2		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	208	Total	C	N	O	S	0	0
			1625	1031	296	290	8		

- Molecule 54 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	203	Total	C	N	O	S	0	0
			1648	1041	326	277	4		

- Molecule 55 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ga	52	Total	C	N	O	S	0	0
			433	271	89	66	7		

- Molecule 56 is a protein called Large ribosomal subunit protein eL39z/eL39x.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BA	50	Total	C	N	O	S	0	0
			444	282	97	63	2		

- Molecule 57 is a protein called Small ribosomal subunit protein uS9z.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	138	Total	C	N	O	S	0	0
			1113	708	213	187	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS13z/uS13y/uS13x.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Wa	139	Total	C	N	O	S	0	0
			1136	709	224	198	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ta	225	Total	C	N	O	S	0	0
			1795	1123	354	310	8		

- Molecule 60 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AZ	68	Total	C	N	O	S	0	0
			562	359	103	98	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL43y.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BE	90	Total	C	N	O	S	0	0
			702	441	135	120	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Za	198	Total	C	N	O	S	0	0
			1575	1000	283	279	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL28z.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AQ	136	Total	C	N	O	S	0	0
			1056	667	197	190	2		

- Molecule 64 is a protein called Small ribosomal subunit protein eS28x.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Oa	59	Total	C	N	O	S	0	0
			471	289	96	84	2		

- Molecule 65 is a protein called Small ribosomal subunit protein uS11y.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ua	127	Total	C	N	O	S	0	0
			962	591	189	177	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS19y.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ya	129	Total	C	N	O	S	0	0
			1024	657	190	172	5		

- Molecule 67 is a protein called Small ribosomal subunit protein eS17w.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BB	119	Total	C	N	O	S	0	0
			955	597	175	178	5		

- Molecule 68 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	99	Total	C	N	O	S	0	0
			808	517	143	146	2		

- Molecule 69 is a protein called Small ribosomal subunit protein eS7x.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ra	184	Total	C	N	O	S	0	0
			1506	955	275	270	6		

- Molecule 70 is a protein called Small ribosomal subunit protein eS19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BL	136	Total	C	N	O	S	0	0
			1064	673	202	186	3		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25w.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	La	71	Total	C	N	O	S	0	0
			562	354	105	99	4		

- Molecule 72 is a protein called Small ribosomal subunit protein eS8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aa	185	Total	C	N	O	S	0	0
			1494	928	296	266	4		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AY	87	Total	C	N	O	S	0	0
			705	429	157	113	6		

- Molecule 74 is a protein called Small ribosomal subunit protein uS14z/uS14y/uS14x.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ca	55	Total	C	N	O	S	0	0
			440	273	91	71	5		

- Molecule 75 is a RNA chain called Ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h1	1612	Total	C	N	O	P	0	0
			34449	15422	6154	11261	1612		

- Molecule 76 is a RNA chain called Messenger RNA (poly-U).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	B1	12	Total	C	N	O	P	0	0
			240	108	24	96	12		

- Molecule 77 is a protein called Small ribosomal subunit protein uS10y.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ba	101	Total	C	N	O	S	0	0
			799	505	149	142	3		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10z.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AI	92	Total	C	N	O	S	0	0
			779	514	127	133	5		

- Molecule 79 is a protein called Nascent polypeptide (poly-A).

Mol	Chain	Residues	Atoms				AltConf	Trace
79	L3	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	3	5	Total	Mg	0
			5	5	
80	A	197	Total	Mg	0
			197	197	
80	i2	1	Total	Mg	0
			1	1	
80	C3	4	Total	Mg	0
			4	4	
80	BM	1	Total	Mg	0
			1	1	
80	BS	4	Total	Mg	0
			4	4	
80	AM	1	Total	Mg	0
			1	1	
80	AC	1	Total	Mg	0
			1	1	
80	BI	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	BR	1	Total 1	Mg 1	0
80	AG	1	Total 1	Mg 1	0
80	Wa	1	Total 1	Mg 1	0
80	Ta	1	Total 1	Mg 1	0
80	AY	2	Total 2	Mg 2	0
80	h1	78	Total 78	Mg 78	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

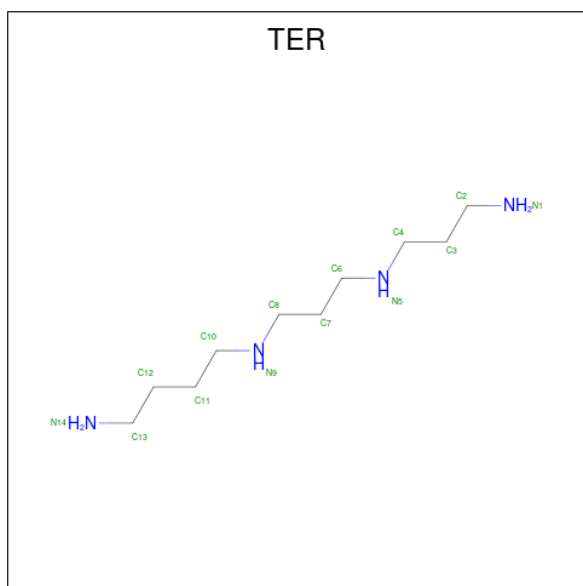
Mol	Chain	Residues	Atoms		AltConf
81	3	4	Total 4	K 4	0
81	A	127	Total 127	K 127	0
81	C3	1	Total 1	K 1	0
81	BM	1	Total 1	K 1	0
81	AR	1	Total 1	K 1	0
81	Ea	1	Total 1	K 1	0
81	Va	1	Total 1	K 1	0
81	BD	1	Total 1	K 1	0
81	BS	2	Total 2	K 2	0
81	AV	1	Total 1	K 1	0
81	AD	1	Total 1	K 1	0
81	AJ	1	Total 1	K 1	0
81	BQ	2	Total 2	K 2	0

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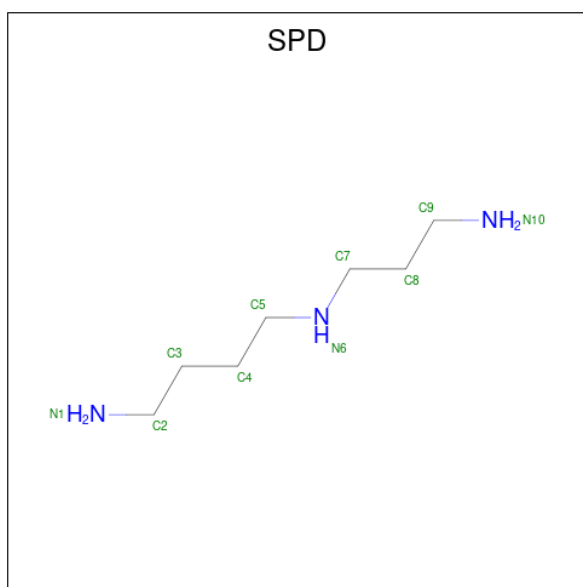
Mol	Chain	Residues	Atoms		AltConf
81	Fa	1	Total	K	0
			1	1	
81	BJ	1	Total	K	0
			1	1	
81	Wa	1	Total	K	0
			1	1	
81	Ua	1	Total	K	0
			1	1	
81	Ca	1	Total	K	0
			1	1	
81	h1	40	Total	K	0
			40	40	

- Molecule 82 is N-(3-AMINO-PROPYL)-N-(5-AMINOPROPYL)-1,4-DIAMINOBUTANE (CCD ID: TER) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



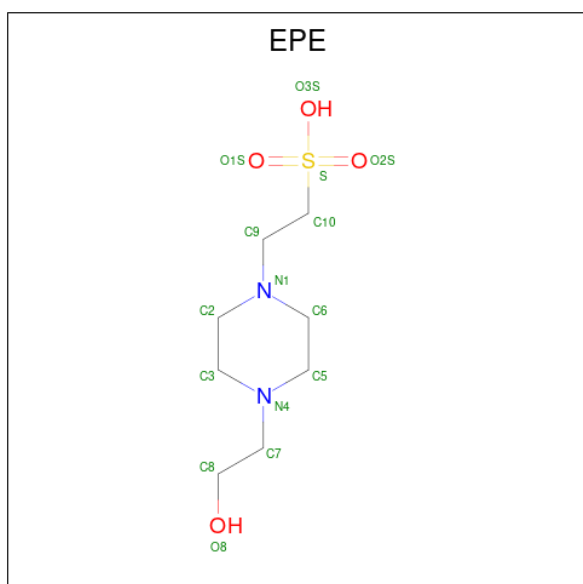
Mol	Chain	Residues	Atoms			AltConf
82	A	1	Total	C	N	0
			14	10	4	

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	

- Molecule 84 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					AltConf
84	A	1	Total	C	N	O	S	0
			15	8	2	4	1	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Ma	1	Total	Zn	0
			1	1	
85	BD	1	Total	Zn	0
			1	1	
85	Ga	1	Total	Zn	0
			1	1	
85	BE	1	Total	Zn	0
			1	1	
85	AY	1	Total	Zn	0
			1	1	
85	Ca	1	Total	Zn	0
			1	1	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	3	341	Total	O	0
			341	341	
86	A	7528	Total	O	0
			7528	7528	
86	i2	7	Total	O	0
			7	7	
86	C3	178	Total	O	0
			178	178	
86	BC	10	Total	O	0
			10	10	
86	BM	66	Total	O	0
			66	66	
86	BO	31	Total	O	0
			31	31	
86	AR	38	Total	O	0
			38	38	
86	AU	28	Total	O	0
			28	28	
86	Ma	26	Total	O	0
			26	26	
86	Ia	24	Total	O	0
			24	24	

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Mol	Chain	Residues	Atoms		AltConf
86	AE	22	Total 22	O 22	0
86	AX	28	Total 28	O 28	0
86	AP	16	Total 16	O 16	0
86	Ja	16	Total 16	O 16	0
86	Ea	133	Total 133	O 133	0
86	AL	65	Total 65	O 65	0
86	Va	30	Total 30	O 30	0
86	Ka	2	Total 2	O 2	0
86	AW	58	Total 58	O 58	0
86	BD	65	Total 65	O 65	0
86	BS	170	Total 170	O 170	0
86	AM	79	Total 79	O 79	0
86	AC	23	Total 23	O 23	0
86	BI	41	Total 41	O 41	0
86	AH	24	Total 24	O 24	0
86	BT	138	Total 138	O 138	0
86	AV	69	Total 69	O 69	0
86	AD	8	Total 8	O 8	0
86	AJ	117	Total 117	O 117	0
86	BQ	131	Total 131	O 131	0
86	BH	90	Total 90	O 90	0

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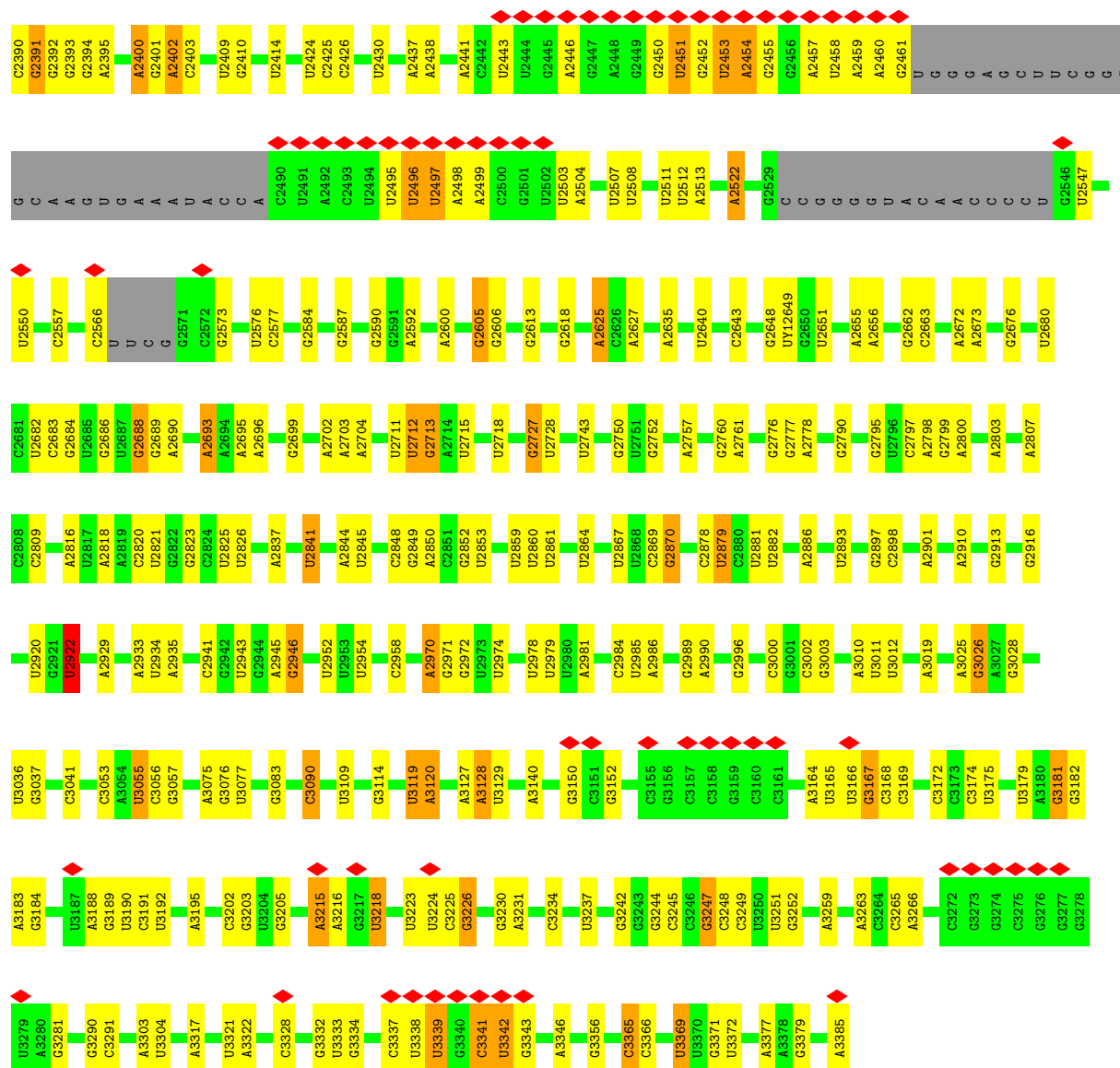
Mol	Chain	Residues	Atoms		AltConf
86	Da	23	Total 23	O 23	0
86	BK	70	Total 70	O 70	0
86	AT	16	Total 16	O 16	0
86	Pa	3	Total 3	O 3	0
86	BP	22	Total 22	O 22	0
86	BN	34	Total 34	O 34	0
86	BG	40	Total 40	O 40	0
86	Fa	51	Total 51	O 51	0
86	Ha	87	Total 87	O 87	0
86	BU	11	Total 11	O 11	0
86	BR	77	Total 77	O 77	0
86	Xa	17	Total 17	O 17	0
86	BV	16	Total 16	O 16	0
86	BJ	36	Total 36	O 36	0
86	AO	22	Total 22	O 22	0
86	BW	1	Total 1	O 1	0
86	AK	46	Total 46	O 46	0
86	Na	3	Total 3	O 3	0
86	AB	7	Total 7	O 7	0
86	BF	17	Total 17	O 17	0
86	AA	3	Total 3	O 3	0

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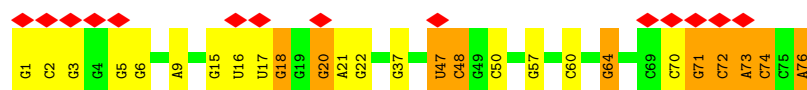
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Mol	Chain	Residues	Atoms		AltConf
86	AG	91	Total 91	O 91	0
86	Ga	18	Total 18	O 18	0
86	BA	22	Total 22	O 22	0
86	AF	9	Total 9	O 9	0
86	Wa	1	Total 1	O 1	0
86	Ta	7	Total 7	O 7	0
86	AZ	4	Total 4	O 4	0
86	BE	34	Total 34	O 34	0
86	Za	3	Total 3	O 3	0
86	AQ	3	Total 3	O 3	0
86	Oa	2	Total 2	O 2	0
86	Ua	29	Total 29	O 29	0
86	Ya	1	Total 1	O 1	0
86	BL	3	Total 3	O 3	0
86	Aa	6	Total 6	O 6	0
86	AY	71	Total 71	O 71	0
86	h1	1709	Total 1709	O 1709	0
86	B1	22	Total 22	O 22	0
86	W2	22	Total 22	O 22	0
86	Ba	4	Total 4	O 4	0
86	L3	1	Total 1	O 1	0

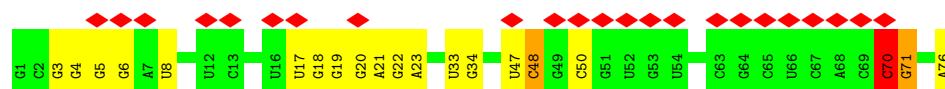
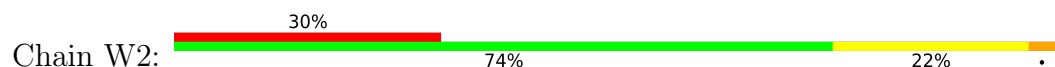
A2953	A2254	G2095	G1816	G1661	G1545	G1413	G1215	U1091	U985	A845	G700
A2255	G2256	U2101	U1817	G1662	A1557	G1419	U1218	U1092	C986	C848	A701
G2257	G2258	G2110	G1818	A1676	U1564	U1420	G1219	G1097	G987	G702	U703
A2259	U2260	U2111	C1819	A1677	U1565	G1421	U1220	C1104	A989	A856	C709
G2261	G2262	C2117	C1820	G1678	U1566	G1422	G1222	G1105	C990	A857	G710
G2263	U2264	A2118	U1821	U1681	A1567	G1428	G1223	G1106	C991	C858	G711
G2267	G2271	G2121	U1822	U1682	A1568	G1429	U1229	A1107	C992	C870	U711
G2272	U2273	G2122	C1823	A1683	U1569	G1443	U1230	U1001	C993	A712	A712
G2276	G2277	A2130	C1824	U1686	U1572	G1446	A1231	G1111	U880	A719	A719
G2278	U2279	G2131	C1845	U1687	U1573	C1446	A1232	A1112	C882	C726	C726
G2280	A2157	U2134	G1848	U1688	U1574	U1447	G1233	C1119	U883	U727	U727
G2304	G2188	U2139	G1853	G1692	A1575	U1451	G1236	A1120	U888	G728	G728
G2305	A2181	U2142	A1860	A1697	A1576	U1454	G1237	G1124	A892	A730	A730
G2306	U2182	G2143	A1868	C1706	G1580	U1455	A	G1125	A893	U731	U731
G2307	G2183	G2144	G1880	G1714	A1581	A1459	G	G1126	U884	G732	G732
G2308	U2184	U2145	A1881	U1718	A1582	A1460	A	U1131	U901	U742	U742
G2309	G2185	U2146	U1882	G1719	A1583	A1461	C	U1132	A905	C743	C743
A2310	U2186	U2147	U1883	G1720	A1584	A1462	C	U1133	C906	C744	C744
A2311	G2187	U2148	U1884	G1721	A1585	A1463	G	U1134	G909	G745	G745
A2312	U2188	U2149	U1885	G1722	A1586	A1464	G	U1135	G910	C746	C746
G2313	A2189	U2150	U1886	G1723	A1587	A1465	A	U1136	G911	G747	G747
G2314	G2189	U2151	U1887	A1724	A1588	A1466	C	U1137	G912	U750	U750
U2316	U2190	U2152	U1888	G1725	A1589	A1467	C	U1138	G913	G751	G751
A2319	U2191	U2153	U1889	G1726	A1590	A1468	C	U1139	G914	C758	C758
A2324	G2192	U2154	U1890	U1727	A1591	A1469	C	U1140	A923	U774	U774
U2332	U2193	U2155	U1891	G1728	A1592	A1470	C	U1141	A924	C775	C775
G2333	A2205	U2156	U1892	U1729	A1593	A1471	C	U1142	G925	U776	U776
U2334	G2206	U2157	U1893	U1730	A1594	A1472	C	U1143	A926	U785	U785
U2345	U2207	U2158	U1894	U1731	A1595	A1473	C	U1144	A927	U786	U786
G2362	G2208	U2159	U1895	G1732	A1596	A1474	C	U1145	A928	C787	C787
C2363	U2209	U2160	U1896	U1733	A1597	A1475	C	U1146	A929	G788	G788
A2370	A2212	U2161	U1897	U1734	A1598	A1476	C	U1147	A930	A789	A789
C2372	G2218	U2162	U1898	U1735	A1599	A1477	C	U1148	A931	G790	G790
G2373	U2224	U2163	U1899	U1736	A1600	A1478	C	U1149	A932	G794	G794
G2374	G2225	U2164	U1900	U1737	A1601	A1479	C	U1150	A933	A795	A795
C2381	A2226	U2165	U1901	U1738	A1602	A1480	C	U1151	A934	G814	G814
G2389	G2227	U2166	U1902	U1739	A1603	A1481	C	U1152	A935	G821	G821
	U2252	U2167	U1903	U1740	A1604	A1482	C	U1153	A936	A826	A826
		U2168	U1904	U1741	A1605	A1483	C	U1154	A937	C827	C827
		U2169	U1905	U1742	A1606	A1484	C	U1155	A938	U828	U828
		U2170	U1906	U1743	A1607	A1485	C	U1156	A939	A829	A829
		U2171	U1907	U1744	A1608	A1486	C	U1157	A940	U830	U830
		U2172	U1908	U1745	A1609	A1487	C	U1158	A941	U831	U831
		U2173	U1909	U1746	A1610	A1488	C	U1159	A942	A832	A832
		U2174	U1910	U1747	A1611	A1489	C	U1160	A943	G833	G833
		U2175	U1911	U1748	A1612	A1490	C	U1161	A944	U834	U834
		U2176	U1912	U1749	A1613	A1491	C	U1162	A945	A835	A835
		U2177	U1913	U1750	A1614	A1492	C	U1163	A946	U836	U836
		U2178	U1914	U1751	A1615	A1493	C	U1164	A947	A837	A837
		U2179	U1915	U1752	A1616	A1494	C	U1165	A948	U838	U838
		U2180	U1916	U1753	A1617	A1495	C	U1166	A949	A839	A839
		U2181	U1917	U1754	A1618	A1496	C	U1167	A950	U840	U840
		U2182	U1918	U1755	A1619	A1497	C	U1168	A951	A841	A841
		U2183	U1919	U1756	A1620	A1498	C	U1169	A952	U842	U842
		U2184	U1920	U1757	A1621	A1499	C	U1170	A953	A843	A843
		U2185	U1921	U1758	A1622	A1500	C	U1171	A954	U844	U844
		U2186	U1922	U1759	A1623	A1501	C	U1172	A955	A845	A845
		U2187	U1923	U1760	A1624	A1502	C	U1173	A956	U846	U846
		U2188	U1924	U1761	A1625	A1503	C	U1174	A957	A847	A847
		U2189	U1925	U1762	A1626	A1504	C	U1175	A958	U848	U848
		U2190	U1926	U1763	A1627	A1505	C	U1176	A959	A849	A849
		U2191	U1927	U1764	A1628	A1506	C	U1177	A960	U850	U850
		U2192	U1928	U1765	A1629	A1507	C	U1178	A961	A851	A851
		U2193	U1929	U1766	A1630	A1508	C	U1179	A962	U852	U852
		U2194	U1930	U1767	A1631	A1509	C	U1180	A963	A853	A853
		U2195	U1931	U1768	A1632	A1510	C	U1181	A964	U854	U854
		U2196	U1932	U1769	A1633	A1511	C	U1182	A965	A855	A855
		U2197	U1933	U1770	A1634	A1512	C	U1183	A966	U856	U856
		U2198	U1934	U1771	A1635	A1513	C	U1184	A967	A857	A857
		U2199	U1935	U1772	A1636	A1514	C	U1185	A968	U858	U858
		U2200	U1936	U1773	A1637	A1515	C	U1186	A969	A859	A859
		U2201	U1937	U1774	A1638	A1516	C	U1187	A970	U860	U860
		U2202	U1938	U1775	A1639	A1517	C	U1188	A971	A861	A861
		U2203	U1939	U1776	A1640	A1518	C	U1189	A972	U862	U862
		U2204	U1940	U1777	A1641	A1519	C	U1190	A973	A863	A863
		U2205	U1941	U1778	A1642	A1520	C	U1191	A974	U864	U864
		U2206	U1942	U1779	A1643	A1521	C	U1192	A975	A865	A865
		U2207	U1943	U1780	A1644	A1522	C	U1193	A976	U866	U866
		U2208	U1944	U1781	A1645	A1523	C	U1194	A977	A867	A867
		U2209	U1945	U1782	A1646	A1524	C	U1195	A978	U868	U868
		U2210	U1946	U1783	A1647	A1525	C	U1196	A979	A869	A869
		U2211	U1947	U1784	A1648	A1526	C	U1197	A980	U870	U870
		U2212	U1948	U1785	A1649	A1527	C	U1198	A981	A871	A871
		U2213	U1949	U1786	A1650	A1528	C	U1199	A982	U872	U872
		U2214	U1950	U1787	A1651	A1529	C	U1200	A983	A873	A873
		U2215	U1951	U1788	A1652	A1530	C	U1201	A984	U874	U874
		U2216	U1952	U1789	A1653	A1531	C	U1202	A985	A875	A875
		U2217	U1953	U1790	A1654	A1532	C	U1203	A986	U876	U876
		U2218	U1954	U1791	A1655	A1533	C	U1204	A987	A877	A877
		U2219	U1955	U1792	A1656	A1534	C	U1205	A988	U878	U878
		U2220	U1956	U1793	A1657	A1535	C	U1206	A989	A879	A879
		U2221	U1957	U1794	A1658	A1536	C	U1207	A990	U880	U880
		U2222	U1958	U1795	A1659	A1537	C	U1208	A991	A881	A881
		U2223	U1959	U1796	A1660	A1538	C	U1209	A992	U882	U882
		U2224	U1960	U1797	A1661	A1539	C	U1210	A993	A883	A883
		U2225	U1961	U1798	A1662	A1540	C	U1211	A994	U884	U884
		U2226	U1962	U1799	A1663	A1541	C	U1212	A995	A885	A885
		U2227	U1963	U1800	A1664	A1542	C	U1213	A996	U886	U886
		U2228	U1964	U1801	A1665	A1543	C	U1214	A997	A887	A887
		U2229	U1965	U1802	A1666	A1544	C	U1215	A998	U888	U888
		U2230	U1966	U1803	A1667	A1545	C	U1216	A999	A889	A889
		U2231	U1967	U1804	A1668	A1546	C	U1217	A1000	U890	U890
		U2232	U1968	U1805	A1669	A1547	C	U1218	A1001	A891	A891
		U2233	U1969	U1806	A1670	A1548	C	U1219	A1002	U892	U892
		U2234	U1970	U1807	A1671	A1549	C	U1220	A1003	A893	A893
		U2235	U1971	U1808	A1672	A1550	C	U1221	A1004	U894	U894
		U2236	U1972	U1809	A1673	A1551	C	U1222	A1005	A895	A895
		U2237	U1973	U1810	A1674	A1552	C	U1223	A1006	U896	U896
		U2238	U1974	U1811	A1675	A1553	C	U1224	A1007	A897	A897
		U2239	U1975	U1812	A1676	A1554	C	U1225	A1008	U898	U898
		U2240	U1976	U1813	A1677	A1555	C	U1226	A1009	A899	A899
		U2241	U1977	U1814	A1678	A1556	C	U1227	A1010	U900	U900
		U2242	U1978	U1815	A1679	A1557	C	U1228	A1011	A901	A901
		U2243	U1979	U1816	A1680	A1558	C	U1229	A1012	U902	U902
		U2244	U1980	U1817	A1681	A1559	C	U1230	A1013	A903	A903
		U2245	U1981	U1818	A1682	A1560	C	U1231	A1014	U904	U904
		U2246	U1982	U1819	A1683	A1561	C	U1232	A1015	A905	A905
		U2247	U1983	U1820	A1684	A1562	C	U1233	A1016	U906	U906
		U2248	U1984	U1821							




• Molecule 3: Transfer RNA Phe

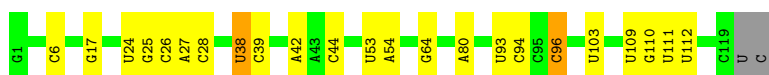


• Molecule 3: Transfer RNA Phe



• Molecule 4: Ribosomal RNA 5S

Chain C3:  79% 17% ..




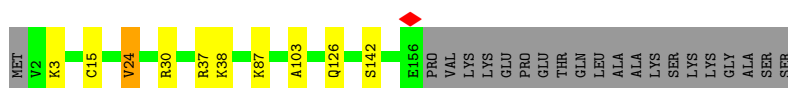
- Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v

Chain BC:  100%

There are no outlier residues recorded for this chain.

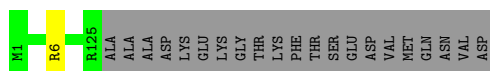
- Molecule 6: Large ribosomal subunit protein uL22z

Chain BM:  82% 5% • 12%



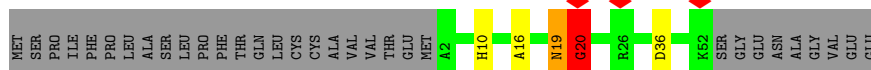
- Molecule 7: Large ribosomal subunit protein uL24z

Chain BO:  85% • 14%




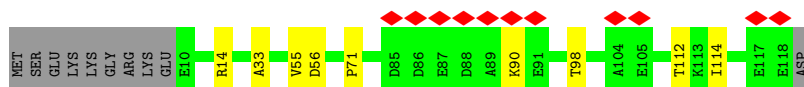
- Molecule 8: 60S ribosomal protein L29

Chain AR:  55% • • 39%



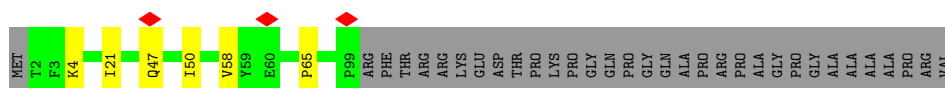
- Molecule 9: Large ribosomal subunit protein eL31y

Chain AU:  9% 84% 8% 8%




- Molecule 10: Small ribosomal subunit protein eS26y

Chain Ma:  70% 5% 25%



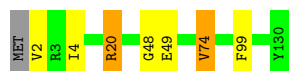
- Molecule 11: Large ribosomal subunit protein uL6z/uL6y

Chain Ia:  89% 9%




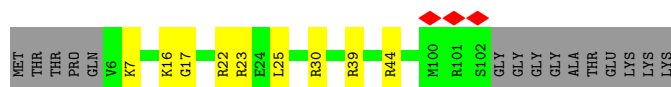
- Molecule 12: Small ribosomal subunit protein uS8z/uS8w

Chain AE:  94%



- Molecule 13: Large ribosomal subunit protein eL36y

Chain AX:  79% 8% 13%




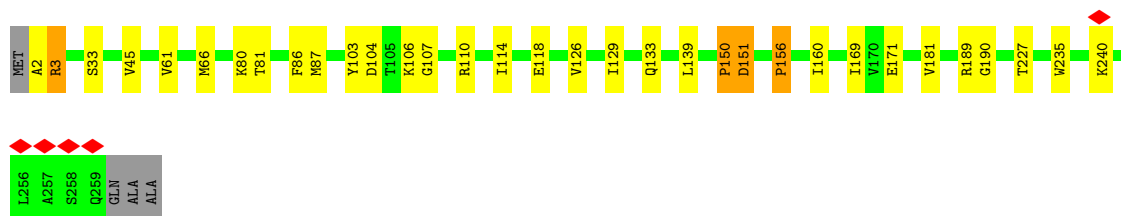
- Molecule 14: Large ribosomal subunit protein eL27x

Chain AP:  90% 9%



- Molecule 15: Small ribosomal subunit protein eS4x

Chain Ja:  86% 11%



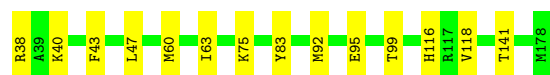
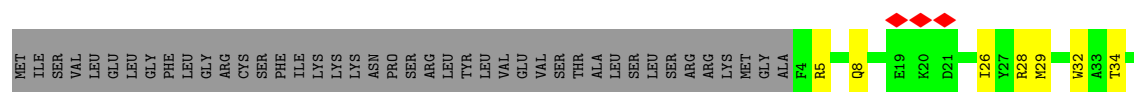
- Molecule 16: Large ribosomal subunit protein eL15z

Chain Ea:  93% 7%



- Molecule 17: Ribosomal protein L18ae/LX family protein

Chain AL:  71% 10% 19%



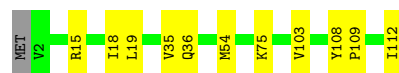
- Molecule 18: Small ribosomal subunit protein uS12y



- Molecule 19: Small ribosomal subunit protein eS24y



- Molecule 20: Large ribosomal subunit protein eL33y



- Molecule 21: Large ribosomal subunit protein eL42z/eL42y

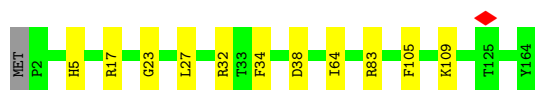


- Molecule 22: Large ribosomal subunit protein uL3z



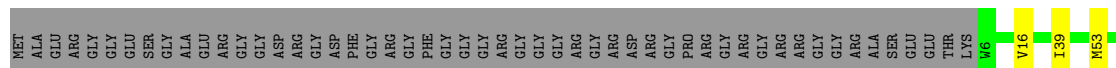
- Molecule 23: Large ribosomal subunit protein eL21z/eL21y





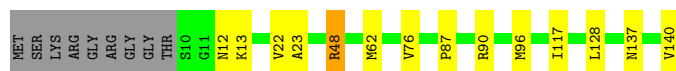
- Molecule 24: Small ribosomal subunit protein uS5y/uS5u/uS5v

Chain AC: 68% 7% 24%



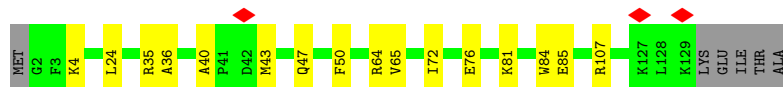
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI: 84% 9% 6%



- Molecule 26: Large ribosomal subunit protein eL14y

Chain AH: 84% 12% 4%



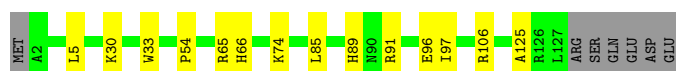
- Molecule 27: Large ribosomal subunit protein uL4z

Chain BT: 85% 12% 3%



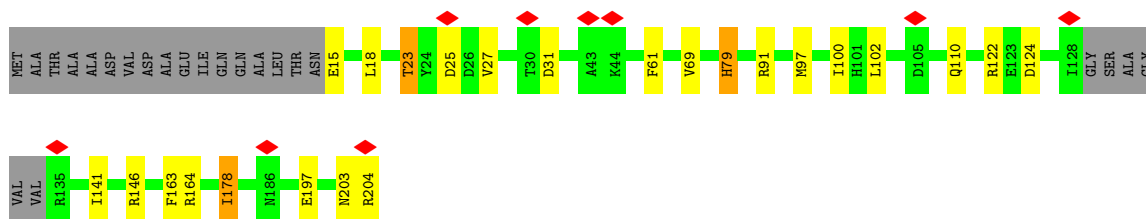
- Molecule 28: Large ribosomal subunit protein eL32z

Chain AV: 84% 11% 5%



- Molecule 29: Small ribosomal subunit protein uS7y

Chain AD: 77% 10% 11%



- Molecule 30: Large ribosomal subunit protein eL18x

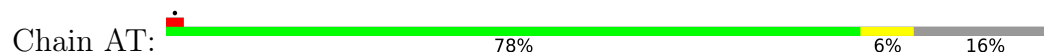
- Molecule 31: Large ribosomal subunit protein uL2z

- Molecule 32: Large ribosomal subunit protein uL13y

- Molecule 33: Small ribosomal subunit protein uS15y

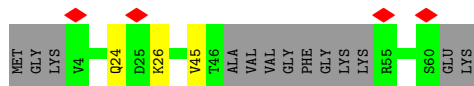
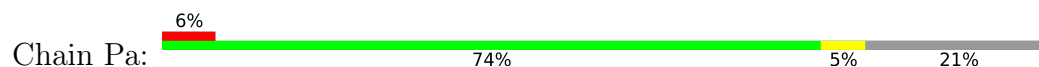
- Molecule 34: Large ribosomal subunit protein uL18z

- Molecule 35: Large ribosomal subunit protein eL30y

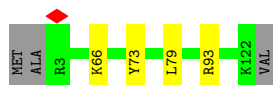




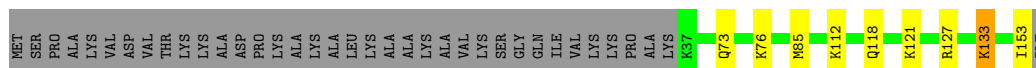
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x



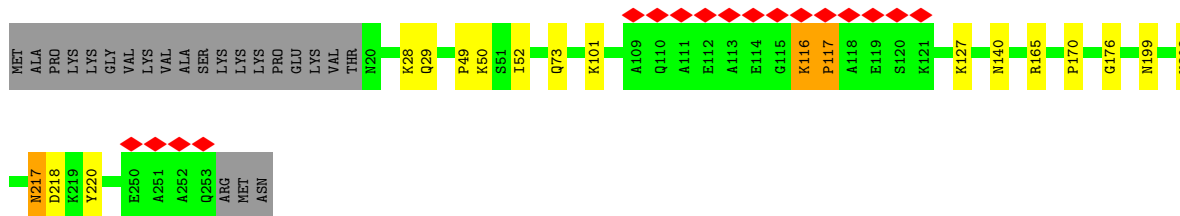
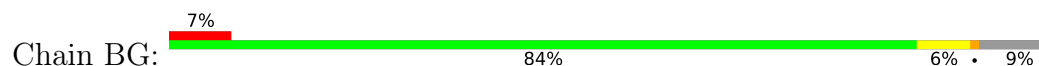
- Molecule 37: Large ribosomal subunit protein uL29x



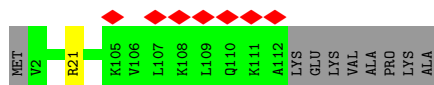
- Molecule 38: Large ribosomal subunit protein uL23y



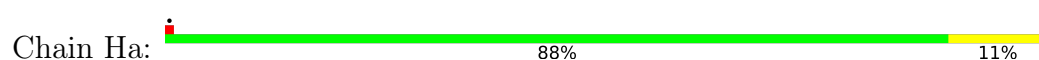
- Molecule 39: Large ribosomal subunit protein eL8y



- Molecule 40: Large ribosomal subunit protein eL34z

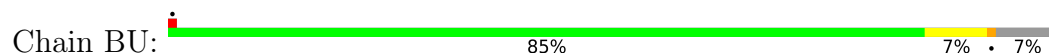


- Molecule 41: Large ribosomal subunit protein uL15x





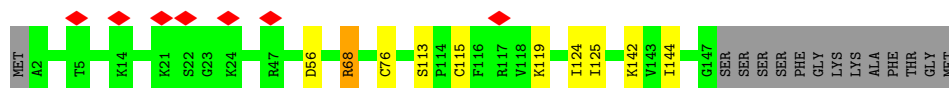
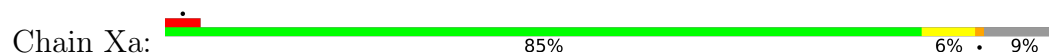
- Molecule 42: Large ribosomal subunit protein uL5z



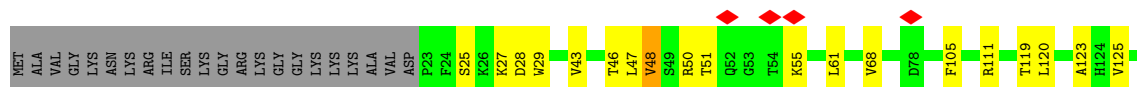
- Molecule 43: Ribosomal protein L30/L7 family protein



- Molecule 44: Small ribosomal subunit protein uS17z



- Molecule 45: Small ribosomal subunit protein eS1y

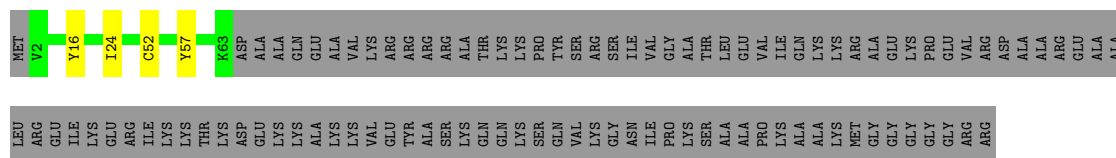


- Molecule 46: Large ribosomal subunit protein uL16y




- Molecule 47: Large ribosomal subunit protein eL24z

Chain AO:  35% 62%




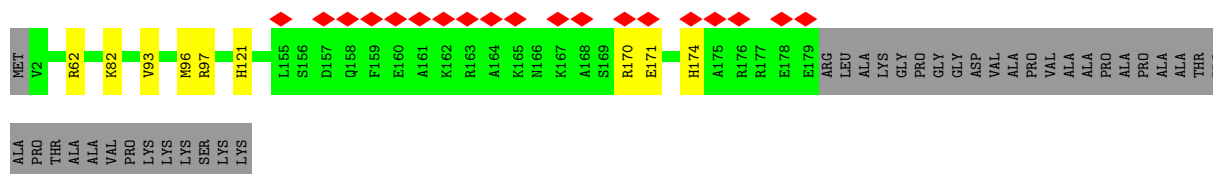
- Molecule 48: Small ribosomal subunit protein eS21y

Chain BW:  79% 9% 11%




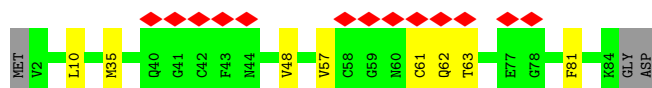
- Molecule 49: Large ribosomal subunit protein eL19x

Chain AK:  79% 17% 9%




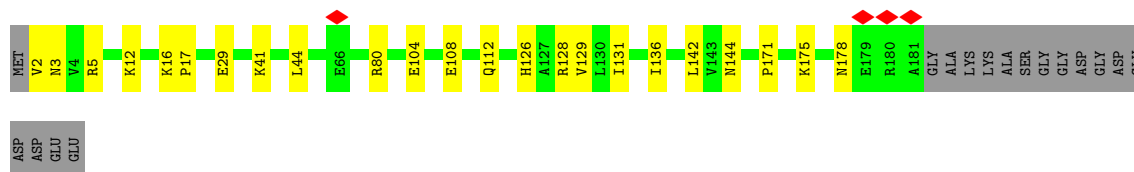
- Molecule 50: Small ribosomal subunit protein eS27y

Chain Na:  87% 9% 15%




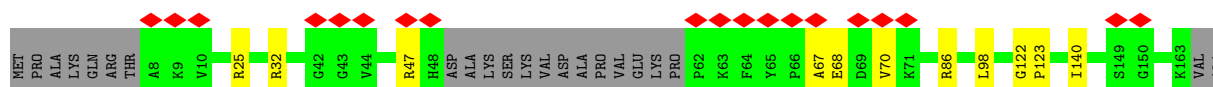
- Molecule 51: Small ribosomal subunit protein uS4y

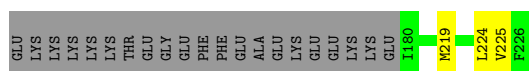
Chain AB:  80% 12% 9%



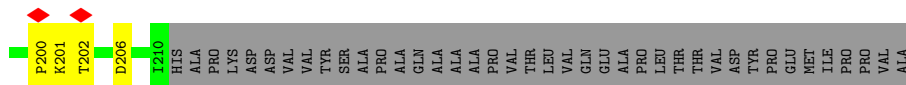
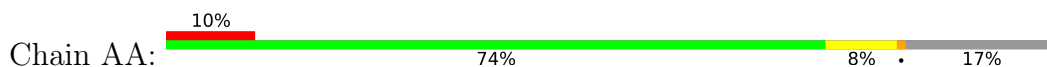
- Molecule 52: Large ribosomal subunit protein eL6y

Chain BF:  76% 6% 18% 8%

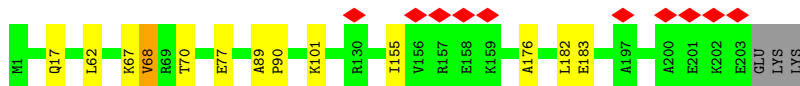




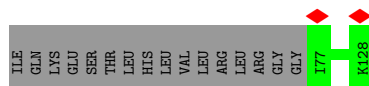
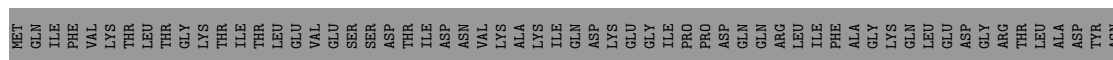
- Molecule 53: Small ribosomal subunit protein uS3z



- Molecule 54: Large ribosomal subunit protein eL13z



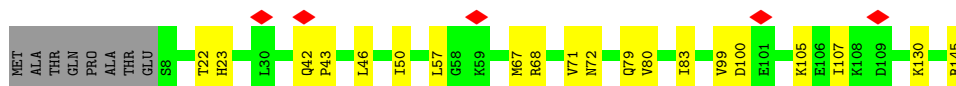
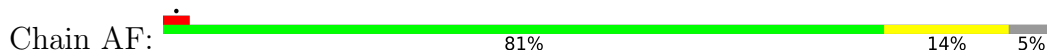
- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein



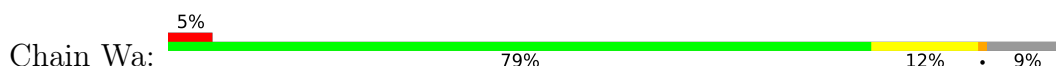
- Molecule 56: Large ribosomal subunit protein eL39z/eL39x



- Molecule 57: Small ribosomal subunit protein uS9z

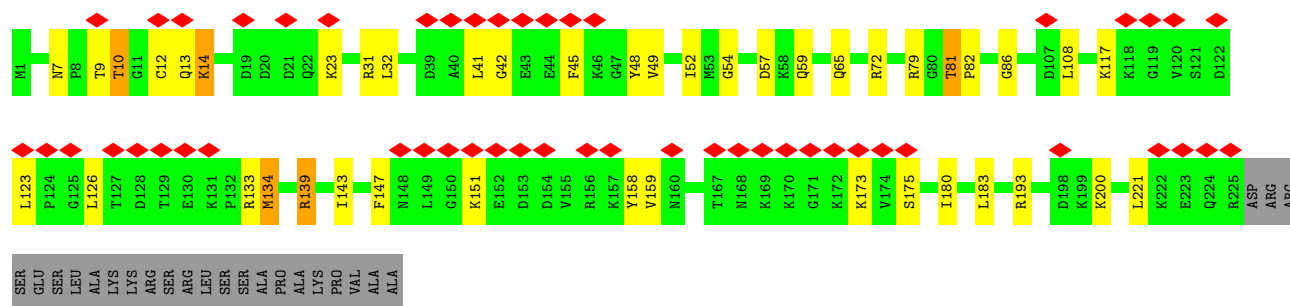
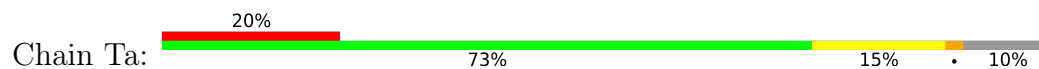


- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x

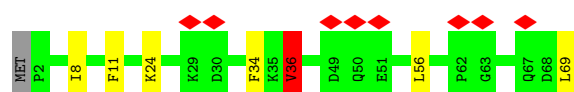
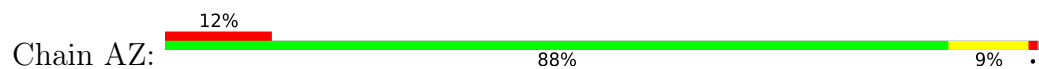




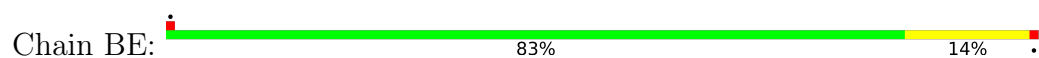
- Molecule 59: Small ribosomal subunit protein eS6y



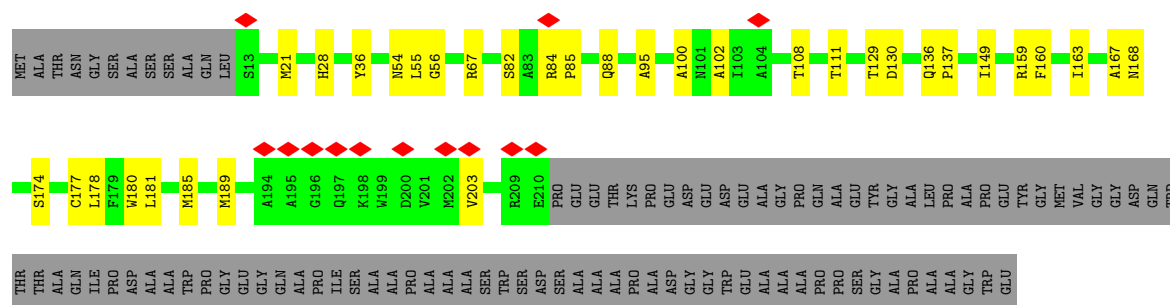
- Molecule 60: Large ribosomal subunit protein eL38z/eL38y



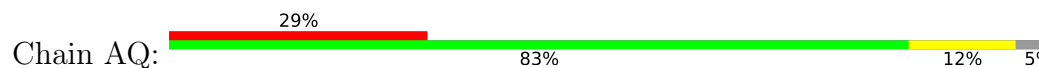
- Molecule 61: Large ribosomal subunit protein eL43y

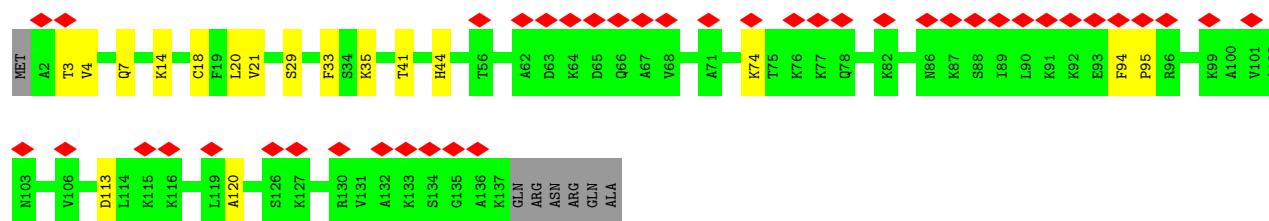


- Molecule 62: Small ribosomal subunit protein uS2z

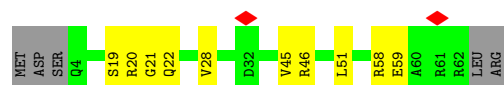
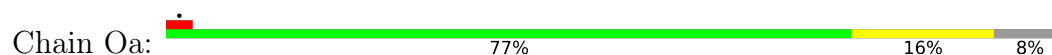


- Molecule 63: Large ribosomal subunit protein eL28z

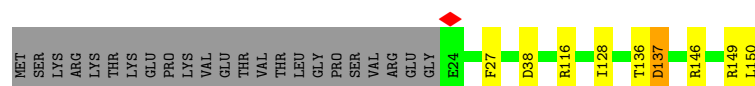
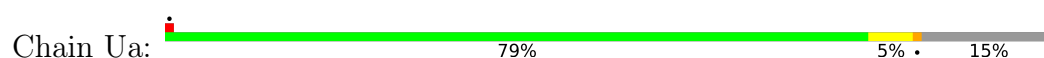




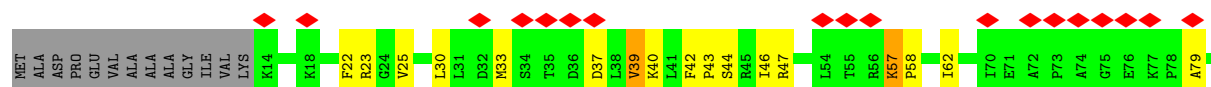
- Molecule 64: Small ribosomal subunit protein eS28x



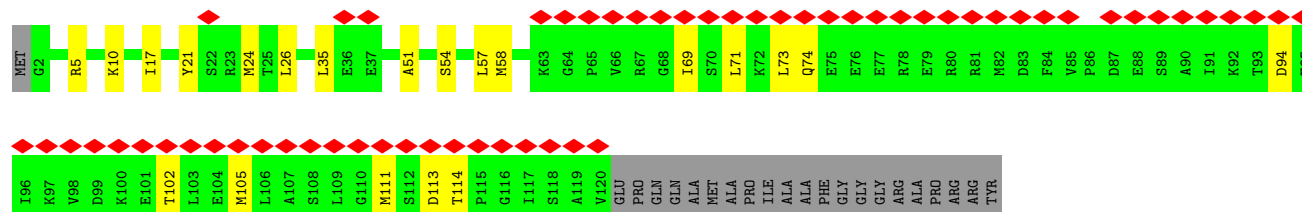
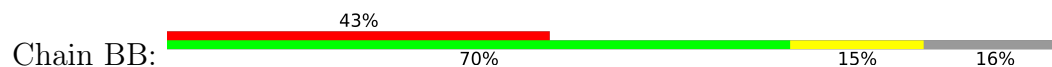
- Molecule 65: Small ribosomal subunit protein uS11y



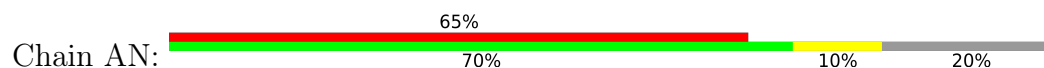
- Molecule 66: Small ribosomal subunit protein uS19y

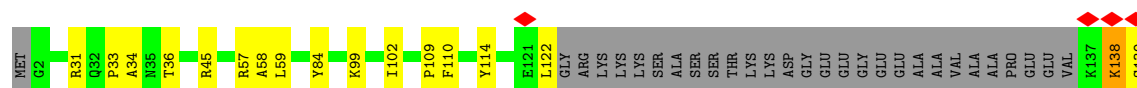


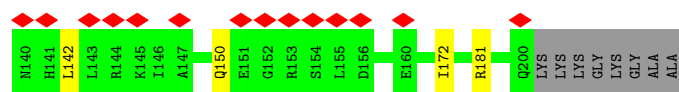
- Molecule 67: Small ribosomal subunit protein eS17w



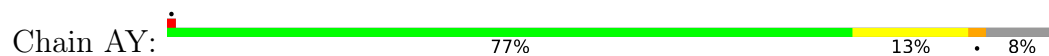
- Molecule 68: Large ribosomal subunit protein eL22z



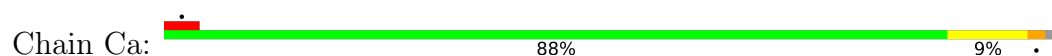




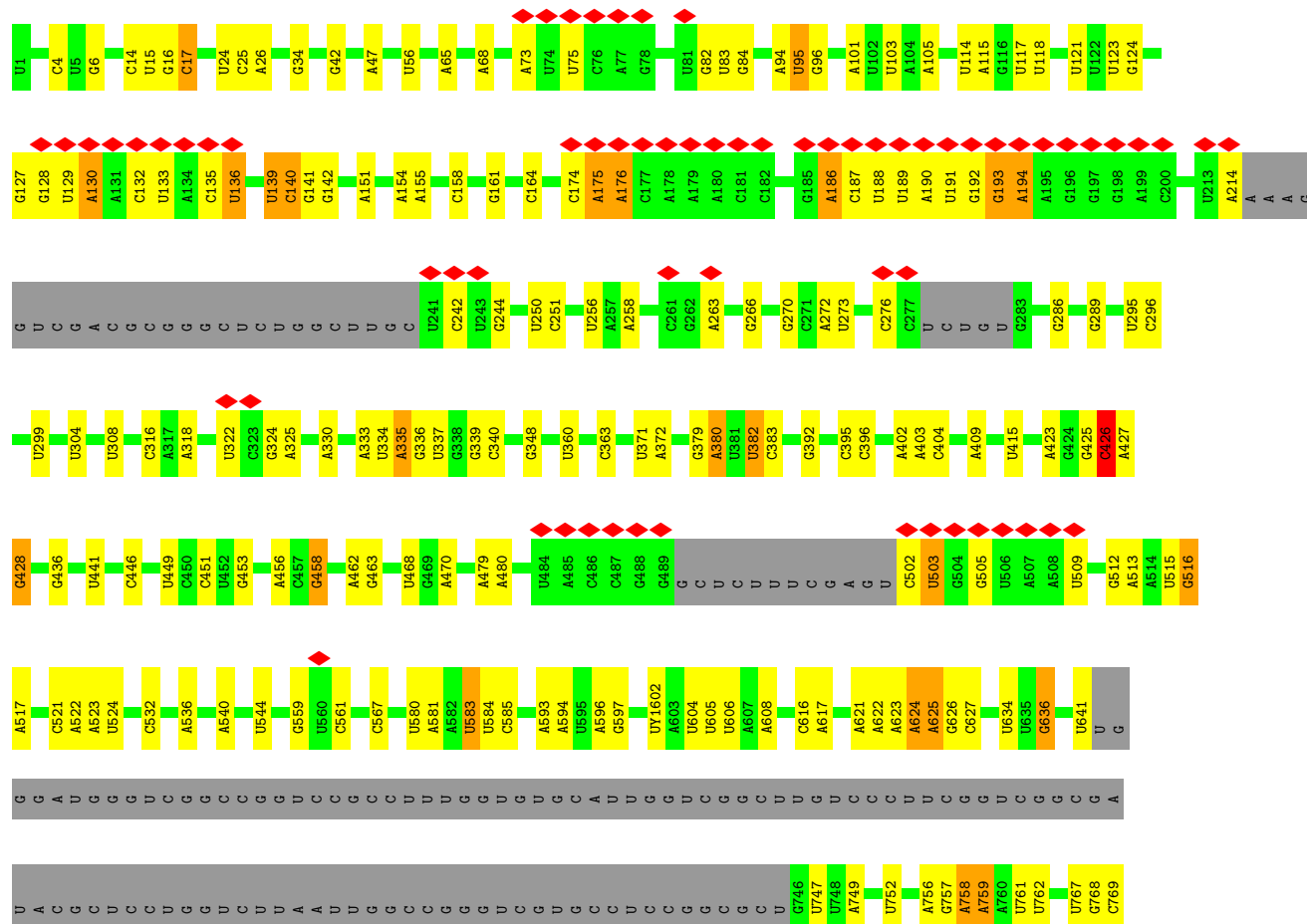
- Molecule 73: Large ribosomal subunit protein eL37z

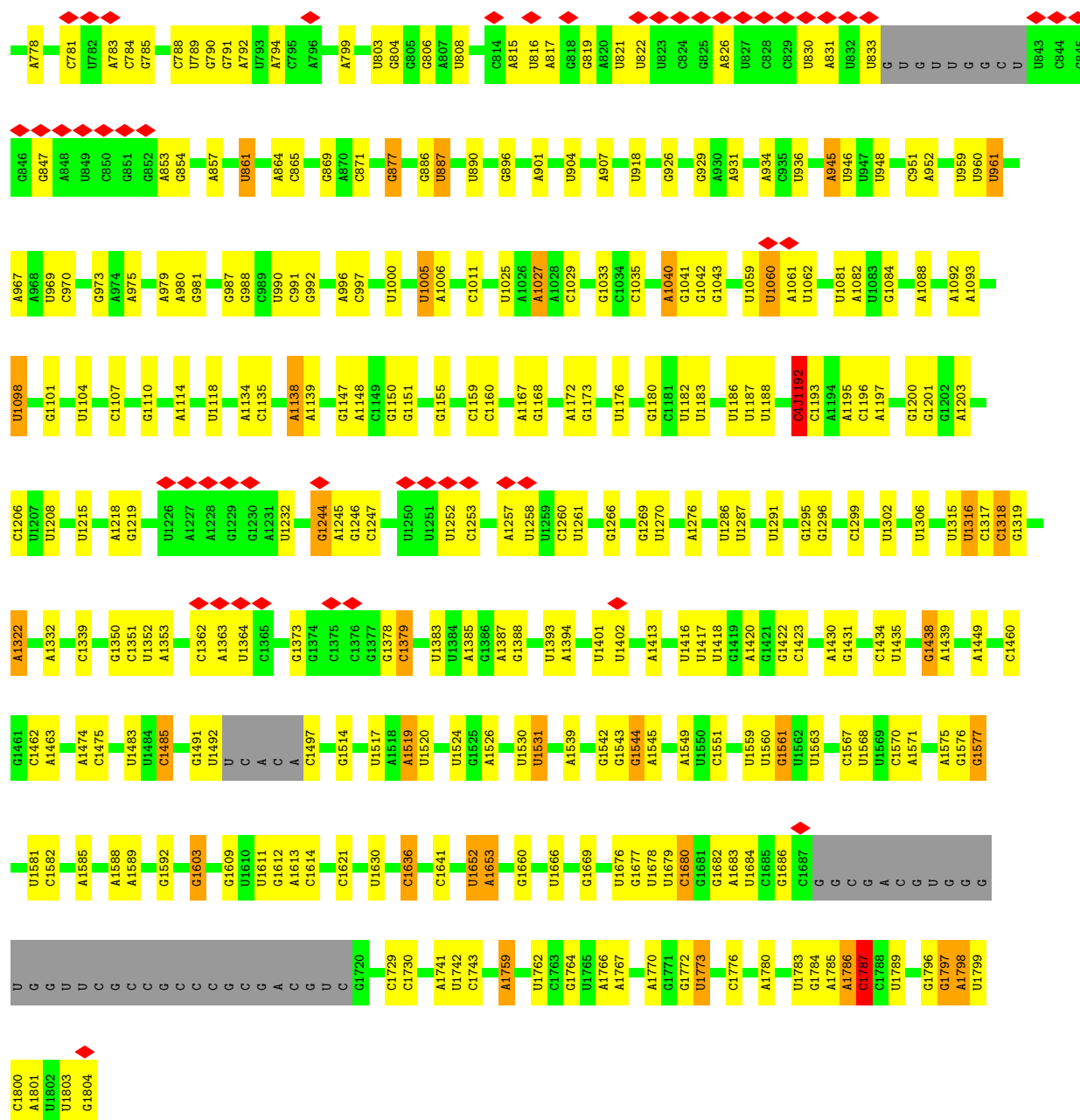


- Molecule 74: Small ribosomal subunit protein uS14z/uS14y/uS14x

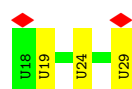
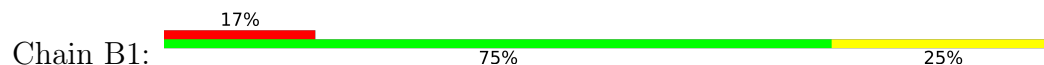


- Molecule 75: Ribosomal RNA 18S

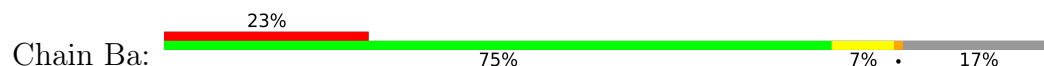


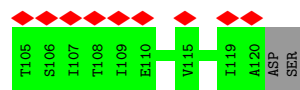


- Molecule 76: Messenger RNA (poly-U)

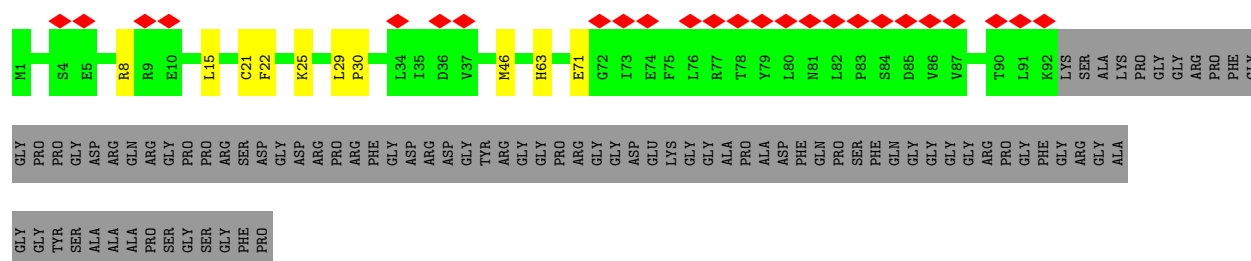


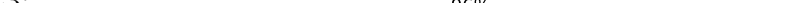
- Molecule 77: Small ribosomal subunit protein uS10y

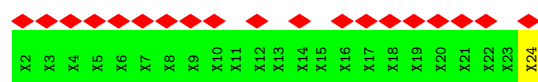




- Chain AI: 



- Chain L3:  83% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	243821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.827	Depositor
Minimum map value	-3.649	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.245	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	495.978, 495.978, 495.978	wwPDB
Map dimensions	686, 686, 686	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, SPD, 4AC, C4J, K, G7M, PSU, 5MC, 1MG, TER, UR3, OMC, EPE, 1MA, HIC, OMG, 6MZ, MA6, OMU, A2M, ZN, UY1, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3	0.47	0/3713	0.95	8/5784 (0.1%)
2	A	0.49	1/72590 (0.0%)	0.97	137/113222 (0.1%)
3	W2	0.53	0/1822	0.85	2/2840 (0.1%)
3	i2	0.52	0/1823	0.85	4/2840 (0.1%)
4	C3	0.46	0/2834	0.93	4/4415 (0.1%)
5	BC	0.53	0/238	0.95	0/302
6	BM	0.53	0/1269	0.89	0/1705
7	BO	0.51	0/1042	0.86	0/1390
8	AR	0.55	0/435	0.94	0/577
9	AU	0.49	0/900	0.85	0/1202
10	Ma	0.51	0/804	0.76	0/1081
11	Ia	0.47	0/1533	0.79	0/2050
12	AE	0.47	0/1051	0.83	0/1406
13	AX	0.50	0/793	0.93	0/1047
14	AP	0.47	0/1110	0.82	0/1477
15	Ja	0.46	0/2116	0.81	0/2841
16	Ea	0.53	0/1754	0.86	0/2349
17	AL	0.49	0/1523	0.85	1/2042 (0.0%)
18	Va	0.49	0/1100	0.83	0/1465
19	Ka	0.45	0/1001	0.81	0/1329
20	AW	0.51	0/921	0.81	0/1234
21	BD	0.51	0/806	0.85	0/1065
22	BS	0.50	0/3165	0.83	0/4238
23	AM	0.49	0/1335	0.86	0/1789
24	AC	0.49	0/1709	0.84	1/2310 (0.0%)
25	BI	0.52	0/1002	0.86	0/1347
26	AH	0.46	0/1054	0.81	0/1408
27	BT	0.51	0/3112	0.84	1/4187 (0.0%)
28	AV	0.51	0/1045	0.82	0/1399
29	AD	0.45	0/1473	0.87	1/1985 (0.1%)
30	AJ	0.53	0/1492	0.87	0/1995

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BQ	0.54	0/1928	0.86	1/2594 (0.0%)
32	BH	0.52	0/1664	0.85	1/2224 (0.0%)
33	Da	0.50	0/1214	0.86	0/1630
34	BK	0.47	0/2321	0.83	0/3119
35	AT	0.50	0/731	0.83	0/982
36	Pa	0.50	0/394	0.88	0/519
37	BP	0.49	0/984	0.83	0/1306
38	BN	0.49	0/972	0.83	0/1309
39	BG	0.48	0/1908	0.87	1/2561 (0.0%)
40	Fa	0.52	0/909	0.91	0/1214
41	Ha	0.55	0/1187	0.91	0/1584
42	BU	0.44	0/1388	0.81	0/1858
43	BR	0.48	0/1931	0.87	0/2584
44	Xa	0.48	0/1189	0.73	0/1590
45	BV	0.45	0/1746	0.81	0/2341
46	BJ	0.48	0/1691	0.82	0/2263
47	AO	0.48	0/541	0.76	0/718
48	BW	0.46	0/577	0.83	0/777
49	AK	0.50	0/1499	0.86	0/1975
50	Na	0.46	0/657	0.80	0/883
51	AB	0.44	0/1540	0.83	0/2061
52	BF	0.48	0/1521	0.83	0/2040
53	AA	0.45	0/1647	0.82	0/2212
54	AG	0.49	0/1680	0.87	0/2251
55	Ga	0.49	0/428	0.80	0/564
56	BA	0.56	0/456	0.81	0/603
57	AF	0.46	0/1133	0.82	0/1513
58	Wa	0.44	0/1152	0.84	0/1541
59	Ta	0.45	0/1819	0.87	0/2422
60	AZ	0.49	0/570	0.84	1/758 (0.1%)
61	BE	0.51	0/711	0.92	1/942 (0.1%)
62	Za	0.45	0/1609	0.83	0/2173
63	AQ	0.46	0/1070	0.85	0/1436
64	Oa	0.44	0/474	0.75	0/632
65	Ua	0.49	0/974	0.87	0/1305
66	Ya	0.48	0/1044	0.85	0/1398
67	BB	0.45	0/965	0.90	0/1287
68	AN	0.45	0/820	0.83	0/1097
69	Ra	0.44	0/1530	0.87	0/2052
70	BL	0.47	0/1086	0.90	1/1459 (0.1%)
71	La	0.45	0/568	0.85	0/762
72	Aa	0.45	0/1517	0.81	0/2027
73	AY	1.45	1/718 (0.1%)	1.04	1/954 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Ca	1.98	1/451 (0.2%)	0.94	3/601 (0.5%)
75	h1	0.50	0/36567	0.91	49/56975 (0.1%)
76	B1	0.52	0/263	0.87	0/404
77	Ba	0.45	0/809	0.82	0/1090
78	AI	0.44	0/801	0.82	0/1082
All	All	0.50	3/205919 (0.0%)	0.91	218/301993 (0.1%)

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
2	A	0	7
8	AR	0	2
14	AP	0	1
22	BS	0	1
23	AM	0	2
25	BI	0	1
27	BT	0	1
34	BK	0	1
37	BP	0	1
41	Ha	0	1
42	BU	0	1
44	Xa	0	1
46	BJ	0	1
49	AK	0	1
69	Ra	0	1
73	AY	0	2
All	All	0	25

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Ca	53	ILE	C-N	40.62	1.90	1.33
73	AY	76	THR	C-N	35.88	1.85	1.33
2	A	2279	A2M	O3'-P	5.24	1.61	1.56

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	AY	76	THR	O-C-N	-14.09	101.86	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	426	C	O3'-P-O5'	-11.10	87.36	104.00
2	A	3127	A	O3'-P-O5'	-10.99	87.51	104.00
75	h1	1422	G	O3'-P-O5'	-10.38	88.44	104.00
2	A	1111	G	O3'-P-O5'	-9.96	89.06	104.00

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	113	G	Sidechain
2	A	1413	G	Sidechain
2	A	403	G	Sidechain
2	A	653	C	Sidechain
2	A	92	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	3453	0	1754	17	0
2	A	67525	0	34103	294	0
3	W2	1629	0	823	6	0
3	i2	1630	0	823	16	0
4	C3	2536	0	1284	9	0
5	BC	237	0	289	0	0
6	BM	1246	0	1264	6	0
7	BO	1030	0	1110	1	0
8	AR	425	0	440	4	0
9	AU	888	0	933	5	0
10	Ma	789	0	810	5	0
11	Ia	1512	0	1598	10	0
12	AE	1033	0	1070	7	0
13	AX	786	0	888	6	0
14	AP	1092	0	1182	10	0
15	Ja	2074	0	2180	28	0
16	Ea	1713	0	1777	12	0
17	AL	1485	0	1547	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Va	1082	0	1153	3	0
19	Ka	986	0	1053	13	0
20	AW	901	0	926	10	0
21	BD	792	0	843	2	0
22	BS	3111	0	3221	33	0
23	AM	1307	0	1359	7	0
24	AC	1672	0	1748	15	0
25	BI	986	0	1048	13	0
26	AH	1042	0	1119	9	0
27	BT	3056	0	3214	37	0
28	AV	1028	0	1105	13	0
29	AD	1454	0	1512	15	0
30	AJ	1468	0	1577	8	0
31	BQ	1881	0	1931	11	0
32	BH	1636	0	1752	11	0
33	Da	1190	0	1273	6	0
34	BK	2277	0	2311	9	0
35	AT	720	0	754	6	0
36	Pa	389	0	419	2	0
37	BP	975	0	1100	2	0
38	BN	955	0	1037	5	0
39	BG	1874	0	2015	16	0
40	Fa	896	0	975	1	0
41	Ha	1156	0	1207	12	0
42	BU	1366	0	1407	11	0
43	BR	1898	0	2005	10	0
44	Xa	1163	0	1222	6	0
45	BV	1718	0	1774	26	0
46	BJ	1653	0	1707	15	0
47	AO	528	0	557	4	0
48	BW	568	0	566	5	0
49	AK	1480	0	1610	5	0
50	Na	647	0	663	4	0
51	AB	1514	0	1576	15	0
52	BF	1491	0	1596	12	0
53	AA	1625	0	1718	14	0
54	AG	1648	0	1755	15	0
55	Ga	433	0	475	0	0
56	BA	444	0	477	3	0
57	AF	1113	0	1169	11	0
58	Wa	1136	0	1177	10	0
59	Ta	1795	0	1920	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	AZ	562	0	606	7	0
61	BE	702	0	741	11	0
62	Za	1575	0	1578	25	0
63	AQ	1056	0	1128	13	0
64	Oa	471	0	497	9	0
65	Ua	962	0	994	21	0
66	Ya	1024	0	1090	21	0
67	BB	955	0	1012	12	0
68	AN	808	0	845	6	0
69	Ra	1506	0	1571	25	0
70	BL	1064	0	1097	6	0
71	La	562	0	599	9	0
72	Aa	1494	0	1538	17	0
73	AY	705	0	724	10	0
74	Ca	440	0	431	6	0
75	h1	34449	0	17384	167	0
76	B1	240	0	120	1	0
77	Ba	799	0	868	6	0
78	AI	779	0	790	8	0
79	L3	115	0	36	1	0
80	3	5	0	0	0	0
80	A	197	0	0	0	0
80	AC	1	0	0	0	0
80	AG	1	0	0	0	0
80	AM	1	0	0	0	0
80	AY	2	0	0	0	0
80	BI	1	0	0	0	0
80	BM	1	0	0	0	0
80	BR	1	0	0	0	0
80	BS	4	0	0	0	0
80	C3	4	0	0	0	0
80	Ta	1	0	0	0	0
80	Wa	1	0	0	0	0
80	h1	78	0	0	0	0
80	i2	1	0	0	0	0
81	3	4	0	0	0	0
81	A	127	0	0	1	0
81	AD	1	0	0	0	0
81	AJ	1	0	0	0	0
81	AR	1	0	0	0	0
81	AV	1	0	0	0	0
81	BD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BJ	1	0	0	0	0
81	BM	1	0	0	0	0
81	BQ	2	0	0	0	0
81	BS	2	0	0	0	0
81	C3	1	0	0	0	0
81	Ca	1	0	0	0	0
81	Ea	1	0	0	0	0
81	Fa	1	0	0	0	0
81	Ua	1	0	0	0	0
81	Va	1	0	0	0	0
81	Wa	1	0	0	0	0
81	h1	40	0	0	0	0
82	A	14	0	26	1	0
83	A	40	0	76	2	0
84	A	15	0	18	0	0
85	AY	1	0	0	0	0
85	BD	1	0	0	0	0
85	BE	1	0	0	0	0
85	Ca	1	0	0	0	0
85	Ga	1	0	0	0	0
85	Ma	1	0	0	0	0
86	3	341	0	0	1	0
86	A	7528	0	0	45	0
86	AA	3	0	0	0	0
86	AB	7	0	0	0	0
86	AC	23	0	0	2	0
86	AD	8	0	0	0	0
86	AE	22	0	0	1	0
86	AF	9	0	0	0	0
86	AG	91	0	0	3	0
86	AH	24	0	0	0	0
86	AJ	117	0	0	1	0
86	AK	46	0	0	1	0
86	AL	65	0	0	2	0
86	AM	79	0	0	4	0
86	AO	22	0	0	0	0
86	AP	16	0	0	1	0
86	AQ	3	0	0	0	0
86	AR	38	0	0	1	0
86	AT	16	0	0	2	0
86	AU	28	0	0	0	0
86	AV	69	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	AW	58	0	0	0	0
86	AX	28	0	0	1	0
86	AY	71	0	0	3	0
86	AZ	4	0	0	0	0
86	Aa	6	0	0	1	0
86	B1	22	0	0	0	0
86	BA	22	0	0	1	0
86	BC	10	0	0	0	0
86	BD	65	0	0	0	0
86	BE	34	0	0	0	0
86	BF	17	0	0	0	0
86	BG	40	0	0	3	0
86	BH	90	0	0	0	0
86	BI	41	0	0	0	0
86	BJ	36	0	0	2	0
86	BK	70	0	0	1	0
86	BL	3	0	0	0	0
86	BM	66	0	0	0	0
86	BN	34	0	0	0	0
86	BO	31	0	0	1	0
86	BP	22	0	0	0	0
86	BQ	131	0	0	3	0
86	BR	77	0	0	3	0
86	BS	170	0	0	9	0
86	BT	138	0	0	2	0
86	BU	11	0	0	0	0
86	BV	16	0	0	2	0
86	BW	1	0	0	0	0
86	Ba	4	0	0	1	0
86	C3	178	0	0	0	0
86	Da	23	0	0	0	0
86	Ea	133	0	0	3	0
86	Fa	51	0	0	0	0
86	Ga	18	0	0	0	0
86	Ha	87	0	0	4	0
86	Ia	24	0	0	0	0
86	Ja	16	0	0	1	0
86	Ka	2	0	0	0	0
86	L3	1	0	0	0	0
86	Ma	26	0	0	0	0
86	Na	3	0	0	0	0
86	Oa	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Pa	3	0	0	0	0
86	Ta	7	0	0	2	0
86	Ua	29	0	0	2	0
86	Va	30	0	0	1	0
86	W2	22	0	0	0	0
86	Wa	1	0	0	0	0
86	Xa	17	0	0	0	0
86	Ya	1	0	0	0	0
86	Za	3	0	0	0	0
86	h1	1709	0	0	6	0
86	i2	7	0	0	0	0
All	All	209234	0	145670	1072	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 1072 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AY:76:THR:C	73:AY:77:CYS:N	1.85	1.35
74:Ca:53:ILE:C	74:Ca:54:LYS:N	1.90	1.30
43:BR:201:LYS:NZ	86:BR:401:HOH:O	1.66	1.26
14:AP:43:VAL:HB	86:AP:215:HOH:O	1.38	1.23
22:BS:182:MET:SD	86:BS:662:HOH:O	2.02	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	BC	23/25 (92%)	23 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BM	153/176 (87%)	149 (97%)	4 (3%)	0	100	100
7	BO	123/146 (84%)	122 (99%)	1 (1%)	0	100	100
8	AR	49/83 (59%)	45 (92%)	3 (6%)	1 (2%)	6	1
9	AU	107/119 (90%)	105 (98%)	2 (2%)	0	100	100
10	Ma	96/131 (73%)	93 (97%)	3 (3%)	0	100	100
11	Ia	188/194 (97%)	185 (98%)	3 (2%)	0	100	100
12	AE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
13	AX	95/112 (85%)	94 (99%)	0	1 (1%)	11	4
14	AP	132/135 (98%)	127 (96%)	5 (4%)	0	100	100
15	Ja	256/262 (98%)	247 (96%)	6 (2%)	3 (1%)	10	3
16	Ea	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
17	AL	173/217 (80%)	170 (98%)	3 (2%)	0	100	100
18	Va	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
19	Ka	118/133 (89%)	111 (94%)	7 (6%)	0	100	100
20	AW	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
21	BD	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
22	BS	383/389 (98%)	377 (98%)	6 (2%)	0	100	100
23	AM	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
24	AC	213/284 (75%)	210 (99%)	3 (1%)	0	100	100
25	BI	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
26	AH	126/134 (94%)	125 (99%)	1 (1%)	0	100	100
27	BT	389/406 (96%)	380 (98%)	9 (2%)	0	100	100
28	AV	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
29	AD	180/207 (87%)	169 (94%)	10 (6%)	1 (1%)	21	11
30	AJ	184/187 (98%)	178 (97%)	6 (3%)	0	100	100
31	BQ	244/258 (95%)	235 (96%)	9 (4%)	0	100	100
32	BH	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
33	Da	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
34	BK	279/301 (93%)	273 (98%)	5 (2%)	1 (0%)	30	19
35	AT	92/112 (82%)	92 (100%)	0	0	100	100
36	Pa	45/62 (73%)	43 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BP	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
38	BN	115/154 (75%)	115 (100%)	0	0	100	100
39	BG	232/256 (91%)	224 (97%)	6 (3%)	2 (1%)	14	5
40	Fa	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
41	Ha	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	18	8
42	BU	167/182 (92%)	165 (99%)	2 (1%)	0	100	100
43	BR	230/247 (93%)	226 (98%)	4 (2%)	0	100	100
44	Xa	144/160 (90%)	138 (96%)	5 (4%)	1 (1%)	18	8
45	BV	210/262 (80%)	204 (97%)	6 (3%)	0	100	100
46	BJ	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
47	AO	60/164 (37%)	59 (98%)	1 (2%)	0	100	100
48	BW	71/82 (87%)	70 (99%)	0	1 (1%)	9	2
49	AK	176/214 (82%)	175 (99%)	1 (1%)	0	100	100
50	Na	81/86 (94%)	70 (86%)	11 (14%)	0	100	100
51	AB	178/197 (90%)	173 (97%)	5 (3%)	0	100	100
52	BF	184/233 (79%)	177 (96%)	7 (4%)	0	100	100
53	AA	206/250 (82%)	194 (94%)	10 (5%)	2 (1%)	12	4
54	AG	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
55	Ga	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
56	BA	48/51 (94%)	48 (100%)	0	0	100	100
57	AF	136/146 (93%)	127 (93%)	8 (6%)	1 (1%)	18	8
58	Wa	137/152 (90%)	133 (97%)	3 (2%)	1 (1%)	18	8
59	Ta	223/249 (90%)	203 (91%)	16 (7%)	4 (2%)	6	1
60	AZ	66/69 (96%)	61 (92%)	5 (8%)	0	100	100
61	BE	88/92 (96%)	83 (94%)	4 (4%)	1 (1%)	11	4
62	Za	196/298 (66%)	190 (97%)	6 (3%)	0	100	100
63	AQ	134/143 (94%)	123 (92%)	10 (8%)	1 (1%)	18	8
64	Oa	57/64 (89%)	57 (100%)	0	0	100	100
65	Ua	125/150 (83%)	120 (96%)	3 (2%)	2 (2%)	7	2
66	Ya	127/150 (85%)	118 (93%)	6 (5%)	3 (2%)	4	0
67	BB	117/141 (83%)	108 (92%)	7 (6%)	2 (2%)	7	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	AN	97/124 (78%)	90 (93%)	6 (6%)	1 (1%)	12	4
69	Ra	182/190 (96%)	163 (90%)	18 (10%)	1 (0%)	24	14
70	BL	134/143 (94%)	133 (99%)	1 (1%)	0	100	100
71	La	69/108 (64%)	67 (97%)	2 (3%)	0	100	100
72	Aa	181/222 (82%)	176 (97%)	5 (3%)	0	100	100
73	AY	85/95 (90%)	83 (98%)	1 (1%)	1 (1%)	10	3
74	Ca	53/56 (95%)	53 (100%)	0	0	100	100
77	Ba	99/122 (81%)	97 (98%)	2 (2%)	0	100	100
78	AI	90/177 (51%)	87 (97%)	3 (3%)	0	100	100
All	All	10403/11933 (87%)	10077 (97%)	294 (3%)	32 (0%)	37	26

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Ja	151	ASP
34	BK	261	LYS
39	BG	218	ASP
59	Ta	14	LYS
59	Ta	139	ARG

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	
5	BC	24/24 (100%)	24 (100%)	0	100	100
6	BM	131/148 (88%)	130 (99%)	1 (1%)	73	67
7	BO	116/133 (87%)	116 (100%)	0	100	100
8	AR	44/71 (62%)	44 (100%)	0	100	100
9	AU	96/105 (91%)	95 (99%)	1 (1%)	68	60
10	Ma	87/110 (79%)	87 (100%)	0	100	100
11	Ia	171/175 (98%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AE	111/112 (99%)	109 (98%)	2 (2%)	51	39
13	AX	84/94 (89%)	83 (99%)	1 (1%)	63	54
14	AP	116/117 (99%)	116 (100%)	0	100	100
15	Ja	225/227 (99%)	223 (99%)	2 (1%)	70	62
16	Ea	180/180 (100%)	179 (99%)	1 (1%)	78	74
17	AL	161/198 (81%)	159 (99%)	2 (1%)	63	54
18	Va	111/114 (97%)	110 (99%)	1 (1%)	70	62
19	Ka	104/114 (91%)	102 (98%)	2 (2%)	50	37
20	AW	97/98 (99%)	97 (100%)	0	100	100
21	BD	87/93 (94%)	87 (100%)	0	100	100
22	BS	326/329 (99%)	326 (100%)	0	100	100
23	AM	137/138 (99%)	137 (100%)	0	100	100
24	AC	183/225 (81%)	180 (98%)	3 (2%)	55	44
25	BI	104/110 (94%)	104 (100%)	0	100	100
26	AH	112/117 (96%)	112 (100%)	0	100	100
27	BT	323/331 (98%)	316 (98%)	7 (2%)	45	30
28	AV	114/121 (94%)	114 (100%)	0	100	100
29	AD	156/171 (91%)	152 (97%)	4 (3%)	40	23
30	AJ	157/158 (99%)	156 (99%)	1 (1%)	78	74
31	BQ	192/197 (98%)	191 (100%)	1 (0%)	81	77
32	BH	176/177 (99%)	176 (100%)	0	100	100
33	Da	132/133 (99%)	131 (99%)	1 (1%)	73	67
34	BK	238/254 (94%)	237 (100%)	1 (0%)	84	81
35	AT	81/97 (84%)	81 (100%)	0	100	100
36	Pa	40/49 (82%)	40 (100%)	0	100	100
37	BP	108/110 (98%)	108 (100%)	0	100	100
38	BN	108/136 (79%)	107 (99%)	1 (1%)	70	62
39	BG	200/219 (91%)	197 (98%)	3 (2%)	57	46
40	Fa	97/104 (93%)	97 (100%)	0	100	100
41	Ha	120/121 (99%)	119 (99%)	1 (1%)	73	67
42	BU	147/158 (93%)	145 (99%)	2 (1%)	59	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BR	199/212 (94%)	198 (100%)	1 (0%)	81	77
44	Xa	124/135 (92%)	123 (99%)	1 (1%)	73	67
45	BV	187/226 (83%)	184 (98%)	3 (2%)	55	44
46	BJ	170/179 (95%)	168 (99%)	2 (1%)	63	54
47	AO	58/137 (42%)	58 (100%)	0	100	100
48	BW	60/68 (88%)	59 (98%)	1 (2%)	53	41
49	AK	158/181 (87%)	156 (99%)	2 (1%)	61	50
50	Na	76/78 (97%)	74 (97%)	2 (3%)	40	23
51	AB	161/172 (94%)	161 (100%)	0	100	100
52	BF	157/194 (81%)	157 (100%)	0	100	100
53	AA	174/207 (84%)	172 (99%)	2 (1%)	65	56
54	AG	174/177 (98%)	172 (99%)	2 (1%)	65	56
55	Ga	47/114 (41%)	47 (100%)	0	100	100
56	BA	47/48 (98%)	47 (100%)	0	100	100
57	AF	117/123 (95%)	116 (99%)	1 (1%)	70	62
58	Wa	121/132 (92%)	117 (97%)	4 (3%)	33	15
59	Ta	193/213 (91%)	189 (98%)	4 (2%)	47	32
60	AZ	64/65 (98%)	63 (98%)	1 (2%)	55	44
61	BE	72/73 (99%)	71 (99%)	1 (1%)	59	49
62	Za	166/228 (73%)	166 (100%)	0	100	100
63	AQ	116/122 (95%)	116 (100%)	0	100	100
64	Oa	52/57 (91%)	50 (96%)	2 (4%)	29	11
65	Ua	100/121 (83%)	100 (100%)	0	100	100
66	Ya	110/126 (87%)	109 (99%)	1 (1%)	70	62
67	BB	108/122 (88%)	108 (100%)	0	100	100
68	AN	88/104 (85%)	88 (100%)	0	100	100
69	Ra	165/169 (98%)	161 (98%)	4 (2%)	43	27
70	BL	110/113 (97%)	108 (98%)	2 (2%)	51	39
71	La	61/92 (66%)	61 (100%)	0	100	100
72	Aa	158/183 (86%)	155 (98%)	3 (2%)	50	37
73	AY	73/78 (94%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	Ca	47/48 (98%)	47 (100%)	0	100	100
77	Ba	93/110 (84%)	90 (97%)	3 (3%)	34	16
78	AI	87/139 (63%)	87 (100%)	0	100	100
All	All	9089/10114 (90%)	9009 (99%)	80 (1%)	68	62

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	Wa	84	LEU
69	Ra	97	THR
59	Ta	10	THR
64	Oa	45	VAL
72	Aa	138	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
55	Ga	117	HIS
73	AY	83	GLN
59	Ta	65	GLN
66	Ya	109	GLN
78	AI	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	161/164 (98%)	20 (12%)	2 (1%)
2	A	3142/3385 (92%)	410 (13%)	51 (1%)
3	W2	75/76 (98%)	15 (20%)	1 (1%)
3	i2	75/76 (98%)	15 (20%)	0
4	C3	118/121 (97%)	6 (5%)	1 (0%)
75	h1	1604/1805 (88%)	238 (14%)	0
76	B1	11/12 (91%)	2 (18%)	0
All	All	5186/5639 (91%)	706 (13%)	55 (1%)

5 of 706 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	6	G

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Mol	Chain	Res	Type
1	3	38	U
1	3	39	C
1	3	63	A
1	3	66	C

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1606	A
2	A	2370	A
3	W2	70	C
2	A	3225	C
2	A	1643	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	2134	2	18,21,22	0.88	1 (5%)	21,30,33	0.80	0
75	A2M	h1	1754	75	22,25,26	0.20	0	30,36,39	0.62	0
75	OMC	h1	416	75	19,22,23	0.28	0	25,31,34	0.55	0
2	PSU	A	1015	81,2	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
2	OMU	A	2882	2	19,22,23	0.24	0	25,31,34	0.64	0
2	OMG	A	3290	2,80	23,26,27	0.35	0	32,38,41	0.74	2 (6%)
75	PSU	h1	761	75	18,21,22	0.94	1 (5%)	21,30,33	0.83	0
2	A2M	A	816	2	22,25,26	0.29	0	30,36,39	0.73	0
2	A2M	A	1458	2,80	22,25,26	0.29	0	30,36,39	0.61	0
75	OMG	h1	1272	81,75	23,26,27	0.31	0	32,38,41	0.46	0
2	UR3	A	2952	81,2	19,22,23	0.35	0	26,32,35	0.76	1 (3%)
2	OMC	A	2335	2	19,22,23	0.32	0	25,31,34	0.59	0
2	OMU	A	144	81,2	19,22,23	0.33	0	25,31,34	0.37	0
55	MLY	Ga	113	55	9,10,11	0.49	0	6,11,13	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	1182	75	18,21,22	0.99	1 (5%)	21,30,33	0.85	0
75	A2M	h1	1327	75	22,25,26	0.20	0	30,36,39	0.40	0
2	PSU	A	2853	2	18,21,22	0.89	1 (5%)	21,30,33	0.77	0
2	OMC	A	2363	2	19,22,23	0.31	0	25,31,34	0.56	0
75	A2M	h1	621	75,80	22,25,26	0.29	0	30,36,39	0.73	0
75	PSU	h1	1783	75	18,21,22	1.08	1 (5%)	21,30,33	0.88	2 (9%)
2	PSU	A	2264	2	18,21,22	0.91	1 (5%)	21,30,33	0.72	0
2	OMG	A	1459	2,80	23,26,27	0.47	0	32,38,41	0.66	0
2	PSU	A	1133	2	18,21,22	0.87	1 (5%)	21,30,33	1.01	2 (9%)
1	A2M	3	47	1	22,25,26	0.24	0	30,36,39	0.72	1 (3%)
75	PSU	h1	948	75	18,21,22	0.98	1 (5%)	21,30,33	0.71	0
75	G7M	h1	1577	3,75	23,26,27	0.78	1 (4%)	34,39,42	0.57	1 (2%)
2	A2M	A	2212	2,80	22,25,26	0.22	0	30,36,39	0.69	1 (3%)
2	PSU	A	975	81,2	18,21,22	0.92	1 (5%)	21,30,33	0.87	0
2	PSU	A	150	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.63	0
2	5MC	A	2869	81,2	19,22,23	0.85	1 (5%)	26,32,35	0.88	1 (3%)
75	4AC	h1	1281	75	21,24,25	0.37	0	28,34,37	0.63	0
1	PSU	3	78	1	18,21,22	1.03	1 (5%)	21,30,33	0.71	0
2	OMC	A	1848	2,80	19,22,23	0.29	0	25,31,34	0.50	0
75	A2M	h1	799	75	22,25,26	0.20	0	30,36,39	0.77	1 (3%)
2	PSU	A	2879	2	18,21,22	0.90	1 (5%)	21,30,33	0.79	0
2	PSU	A	2893	2	18,21,22	0.97	1 (5%)	21,30,33	0.84	0
75	PSU	h1	752	75	18,21,22	0.94	1 (5%)	21,30,33	0.72	0
75	PSU	h1	1104	75	18,21,22	0.88	1 (5%)	21,30,33	0.76	0
2	PSU	A	2256	2	18,21,22	0.94	1 (5%)	21,30,33	0.71	0
2	OMU	A	44	81,2	19,22,23	0.34	0	25,31,34	0.57	0
75	PSU	h1	121	75,80	18,21,22	0.85	1 (5%)	21,30,33	0.68	0
2	OMU	A	1066	2	19,22,23	0.30	0	25,31,34	0.74	0
2	1MG	A	1646	2	23,26,27	0.67	0	33,39,42	0.63	0
75	6MZ	h1	1767	81,75,80	22,25,26	0.35	0	29,36,39	0.72	0
2	PSU	A	969	2	18,21,22	0.88	1 (5%)	21,30,33	1.06	1 (4%)
2	OMC	A	2291	2	19,22,23	0.29	0	25,31,34	0.59	0
75	A2M	h1	778	75	22,25,26	0.19	0	30,36,39	0.42	0
2	PSU	A	2262	2	18,21,22	0.92	1 (5%)	21,30,33	0.80	0
75	PSU	h1	360	75	18,21,22	0.93	1 (5%)	21,30,33	0.79	0
2	OMC	A	2958	2,80	19,22,23	0.35	0	25,31,34	0.80	1 (4%)
2	PSU	A	277	2	18,21,22	1.03	1 (5%)	21,30,33	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	MA6	h1	1785	75	23,26,27	0.33	0	33,38,41	0.72	1 (3%)
75	PSU	h1	606	75	18,21,22	1.01	1 (5%)	21,30,33	0.74	0
2	A2M	A	1142	2	22,25,26	0.27	0	30,36,39	0.69	0
2	OMC	A	2947	2	19,22,23	0.32	0	25,31,34	0.51	0
2	PSU	A	3109	2	18,21,22	0.94	1 (5%)	21,30,33	0.97	0
2	A2M	A	945	2	22,25,26	0.32	0	30,36,39	0.88	1 (3%)
75	PSU	h1	1291	75	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
2	OMU	A	2920	81,2	19,22,23	0.27	0	25,31,34	0.47	0
75	PSU	h1	1630	75	18,21,22	0.96	1 (5%)	21,30,33	0.75	0
2	A2M	A	2324	2	22,25,26	0.20	0	30,36,39	0.75	2 (6%)
2	OMC	A	1845	2	19,22,23	0.34	0	25,31,34	0.42	0
2	OMU	A	2345	2	19,22,23	0.32	0	25,31,34	0.51	0
75	A2M	h1	466	75	22,25,26	0.18	0	30,36,39	0.53	0
1	OMG	3	79	1	23,26,27	0.33	0	32,38,41	0.46	0
75	PSU	h1	415	75	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
2	OMG	A	2650	2	23,26,27	0.35	0	32,38,41	0.52	0
2	OMU	A	2734	2,80	19,22,23	0.30	0	25,31,34	0.58	0
75	OMC	h1	38	75	19,22,23	0.29	0	25,31,34	0.62	0
2	PSU	A	228	2	18,21,22	0.96	1 (5%)	21,30,33	0.70	0
2	OMU	A	2408	81,2	19,22,23	0.30	0	25,31,34	0.35	0
75	PSU	h1	605	75	18,21,22	0.97	1 (5%)	21,30,33	0.79	0
2	OMG	A	2921	2	23,26,27	0.29	0	32,38,41	0.40	0
2	A2M	A	661	2	22,25,26	0.25	0	30,36,39	0.37	0
75	4AC	h1	1777	75	21,24,25	0.41	0	28,34,37	0.42	0
75	OMC	h1	471	75	19,22,23	0.29	0	25,31,34	0.55	0
2	OMG	A	2122	2	23,26,27	0.31	0	32,38,41	0.72	1 (3%)
2	PSU	A	2825	81,2	18,21,22	0.94	1 (5%)	21,30,33	0.71	0
1	OMG	3	155	2,1	23,26,27	0.34	0	32,38,41	0.36	0
75	PSU	h1	1188	75	18,21,22	0.89	1 (5%)	21,30,33	0.74	0
2	OMC	A	1478	2	19,22,23	0.32	0	25,31,34	0.41	0
2	PSU	A	2974	2	18,21,22	1.03	1 (5%)	21,30,33	1.00	2 (9%)
2	PSU	A	42	81,2	18,21,22	1.09	2 (11%)	21,30,33	1.06	3 (14%)
75	PSU	h1	337	81,75	18,21,22	0.93	1 (5%)	21,30,33	0.72	0
2	PSU	A	2430	2	18,21,22	0.84	1 (5%)	21,30,33	0.77	0
75	OMG	h1	390	81,75	23,26,27	0.33	0	32,38,41	0.54	0
75	A2M	h1	1575	75	22,25,26	0.24	0	30,36,39	0.64	1 (3%)
2	PSU	A	894	2	18,21,22	0.98	1 (5%)	21,30,33	0.94	0
75	PSU	h1	1000	75	18,21,22	0.94	1 (5%)	21,30,33	0.84	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	A	2716	2	19,22,23	0.26	0	25,31,34	0.54	0
2	PSU	A	2258	2	18,21,22	0.92	1 (5%)	21,30,33	0.71	0
2	OMG	A	2286	2	23,26,27	0.33	0	32,38,41	0.32	0
2	OMC	A	2835	2	19,22,23	0.30	0	25,31,34	0.59	0
75	A2M	h1	543	75	22,25,26	0.23	0	30,36,39	0.62	0
2	PSU	A	2954	2	18,21,22	1.03	1 (5%)	21,30,33	0.81	1 (4%)
75	PSU	h1	468	75	18,21,22	1.00	1 (5%)	21,30,33	0.76	0
75	OMU	h1	1270	75,80	19,22,23	0.23	0	25,31,34	0.59	0
2	PSU	A	685	2	18,21,22	1.07	1 (5%)	21,30,33	0.91	1 (4%)
75	PSU	h1	1215	75	18,21,22	0.94	1 (5%)	21,30,33	0.64	0
75	PSU	h1	1302	75	18,21,22	0.92	1 (5%)	21,30,33	0.77	0
2	PSU	A	2922	2	18,21,22	0.92	1 (5%)	21,30,33	0.79	0
75	PSU	h1	1306	75	18,21,22	0.94	1 (5%)	21,30,33	0.62	0
75	UY1	h1	602	75	19,22,23	1.01	1 (5%)	21,31,34	0.82	0
75	PSU	h1	583	75	18,21,22	0.99	1 (5%)	21,30,33	0.72	0
2	PSU	A	2316	2,80	18,21,22	0.91	1 (5%)	21,30,33	0.70	0
2	OMG	A	2407	81,2	23,26,27	0.38	0	32,38,41	0.40	0
2	PSU	A	1132	2	18,21,22	0.94	1 (5%)	21,30,33	1.04	1 (4%)
75	OMU	h1	123	75	19,22,23	0.23	0	25,31,34	0.84	0
75	OMU	h1	1261	75	19,22,23	0.23	0	25,31,34	0.51	0
2	A2M	A	826	81,2,80	22,25,26	0.31	0	30,36,39	0.76	1 (3%)
75	PSU	h1	1025	75	18,21,22	0.99	1 (5%)	21,30,33	0.92	1 (4%)
2	OMC	A	675	2	19,22,23	0.35	0	25,31,34	0.68	0
75	PSU	h1	1531	75	18,21,22	0.98	1 (5%)	21,30,33	0.64	0
75	PSU	h1	1118	75	18,21,22	0.94	1 (5%)	21,30,33	0.85	0
75	PSU	h1	103	81,75	18,21,22	0.92	1 (5%)	21,30,33	0.80	0
2	A2M	A	2124	2	22,25,26	0.18	0	30,36,39	0.50	0
75	PSU	h1	1208	75	18,21,22	0.98	1 (5%)	21,30,33	0.71	0
75	A2M	h1	438	75	22,25,26	0.19	0	30,36,39	0.32	0
75	PSU	h1	449	81,75	18,21,22	0.98	1 (5%)	21,30,33	0.77	0
75	PSU	h1	1563	75	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
2	PSU	A	2312	81,2	18,21,22	0.93	1 (5%)	21,30,33	0.83	0
75	OMU	h1	1445	75	19,22,23	0.23	0	25,31,34	0.50	0
22	HIC	BS	246	22	10,11,12	0.46	0	9,14,16	1.06	1 (11%)
2	OMU	A	3299	2	19,22,23	0.33	0	25,31,34	0.55	0
2	OMU	A	803	2	19,22,23	0.28	0	25,31,34	0.51	0
2	PSU	A	901	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.85	0
75	OMC	h1	1216	75	19,22,23	0.29	0	25,31,34	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	1681	2	18,21,22	1.03	1 (5%)	21,30,33	0.79	0
75	A2M	h1	422	75	22,25,26	0.17	0	30,36,39	0.63	0
2	OMG	A	2234	2	23,26,27	0.34	0	32,38,41	0.49	0
75	PSU	h1	1611	75	18,21,22	0.99	1 (5%)	21,30,33	0.87	0
2	A2M	A	2933	2	22,25,26	0.22	0	30,36,39	0.50	0
2	OMG	A	2389	2	23,26,27	0.34	0	32,38,41	0.32	0
2	OMG	A	814	2	23,26,27	0.30	0	32,38,41	0.61	1 (3%)
75	OMC	h1	1641	75,80	19,22,23	0.33	0	25,31,34	0.55	0
75	OMU	h1	580	75	19,22,23	0.21	0	25,31,34	0.48	0
2	OMG	A	1853	2	23,26,27	0.38	0	32,38,41	0.65	1 (3%)
2	A2M	A	2279	2	22,25,26	0.37	0	30,36,39	0.78	1 (3%)
2	OMG	A	2814	2	23,26,27	0.31	0	32,38,41	0.27	0
2	OMC	A	2878	2	19,22,23	0.35	0	25,31,34	0.70	0
75	OMU	h1	1263	75	19,22,23	0.24	0	25,31,34	0.40	0
2	PSU	A	2943	81,2,80	18,21,22	0.93	1 (5%)	21,30,33	0.99	1 (4%)
75	OMU	h1	1381	75,80	19,22,23	0.23	0	25,31,34	0.54	0
2	OMG	A	2618	3,2	23,26,27	0.30	0	32,38,41	0.37	0
2	OMC	A	1858	2	19,22,23	0.39	0	25,31,34	0.60	0
2	PSU	A	1062	81,2	18,21,22	0.92	1 (5%)	21,30,33	0.82	0
2	OMU	A	1890	2	19,22,23	0.30	0	25,31,34	0.94	2 (8%)
2	A2M	A	2254	2	22,25,26	0.23	0	30,36,39	0.54	0
2	1MA	A	657	2,80	21,25,26	0.52	0	30,37,40	0.75	0
75	OMG	h1	597	75	23,26,27	0.31	0	32,38,41	0.55	0
75	OMG	h1	244	75	23,26,27	0.35	0	32,38,41	0.40	0
75	PSU	h1	604	75	18,21,22	0.93	1 (5%)	21,30,33	0.89	0
2	OMC	A	1517	2,80	19,22,23	0.33	0	25,31,34	0.68	0
75	OMG	h1	1431	75,80	23,26,27	0.37	0	32,38,41	0.42	0
2	PSU	A	509	2	18,21,22	1.02	1 (5%)	21,30,33	0.90	1 (4%)
2	PSU	A	2209	2	18,21,22	0.93	1 (5%)	21,30,33	0.72	0
2	OMU	A	2111	2	19,22,23	0.21	0	25,31,34	0.50	0
2	OMU	A	676	2	19,22,23	0.37	0	25,31,34	0.74	0
2	OMG	A	917	81,2	23,26,27	0.30	0	32,38,41	0.48	0
2	PSU	A	2252	2	18,21,22	0.91	1 (5%)	21,30,33	0.84	1 (4%)
2	PSU	A	1480	2	18,21,22	1.01	1 (5%)	21,30,33	0.76	0
2	PSU	A	2743	2	18,21,22	0.96	2 (11%)	21,30,33	0.74	0
2	PSU	A	2864	2	18,21,22	0.96	1 (5%)	21,30,33	0.81	0
2	PSU	A	785	2	18,21,22	0.91	1 (5%)	21,30,33	0.87	0
2	A2M	A	2639	2	22,25,26	0.18	0	30,36,39	0.36	0
2	PSU	A	828	2	18,21,22	0.93	1 (5%)	21,30,33	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	2189	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.79	0
2	OMG	A	2393	2,80	23,26,27	0.36	0	32,38,41	0.68	1 (3%)
75	OMU	h1	1232	75	19,22,23	0.25	0	25,31,34	0.37	0
75	A2M	h1	162	75	22,25,26	0.21	0	30,36,39	0.63	0
2	OMU	A	2419	2	19,22,23	0.28	0	25,31,34	0.71	0
75	PSU	h1	808	75	18,21,22	0.96	1 (5%)	21,30,33	0.69	0
75	A2M	h1	28	75,80	22,25,26	0.20	0	30,36,39	0.59	0
2	PSU	A	34	2	18,21,22	1.04	1 (5%)	21,30,33	1.08	2 (9%)
2	PSU	A	1054	2	18,21,22	0.90	1 (5%)	21,30,33	0.83	0
75	PSU	h1	1483	75	18,21,22	0.91	1 (5%)	21,30,33	0.61	0
2	A2M	A	2319	2	22,25,26	0.27	0	30,36,39	0.67	1 (3%)
2	PSU	A	1001	2	18,21,22	1.01	1 (5%)	21,30,33	0.91	0
2	A2M	A	2945	2,80	22,25,26	0.24	0	30,36,39	0.66	1 (3%)
75	OMU	h1	613	75	19,22,23	0.28	0	25,31,34	0.45	0
75	PSU	h1	256	75	18,21,22	0.95	1 (5%)	21,30,33	0.72	0
75	C4J	h1	1192	75	25,29,30	1.05	2 (8%)	28,42,45	1.04	2 (7%)
2	A2M	A	2910	2	22,25,26	0.33	0	30,36,39	0.42	0
2	A2M	A	885	2	22,25,26	0.27	0	30,36,39	0.37	0
2	OMG	A	2790	2	23,26,27	0.31	0	32,38,41	0.37	0
75	PSU	h1	959	81,75	18,21,22	0.89	1 (5%)	21,30,33	0.75	0
75	PSU	h1	762	75	18,21,22	0.93	1 (5%)	21,30,33	0.67	0
2	PSU	A	2132	81,2	18,21,22	1.00	1 (5%)	21,30,33	0.92	0
2	A2M	A	1376	2,80	22,25,26	0.22	0	30,36,39	0.62	0
2	A2M	A	2359	2	22,25,26	0.25	0	30,36,39	0.44	0
75	PSU	h1	308	75	18,21,22	1.05	2 (11%)	21,30,33	0.96	1 (4%)
75	PSU	h1	1520	75	18,21,22	0.96	1 (5%)	21,30,33	0.63	0
2	PSU	A	2414	2,80	18,21,22	1.09	1 (5%)	21,30,33	0.89	1 (4%)
2	OMC	A	2681	2	19,22,23	0.27	0	25,31,34	0.59	0
2	OMG	A	2916	2	23,26,27	0.35	0	32,38,41	0.48	0
75	OMU	h1	1010	75	19,22,23	0.25	0	25,31,34	0.49	0
75	PSU	h1	95	75	18,21,22	1.04	1 (5%)	21,30,33	0.79	0
2	PSU	A	1131	2	18,21,22	0.97	1 (5%)	21,30,33	0.84	0
75	PSU	h1	634	75	18,21,22	1.02	1 (5%)	21,30,33	0.96	0
2	OMC	A	1446	2	19,22,23	0.36	0	25,31,34	0.68	1 (4%)
1	PSU	3	97	81,1	18,21,22	0.97	1 (5%)	21,30,33	0.77	0
2	PSU	A	311	81,2	18,21,22	1.18	2 (11%)	21,30,33	1.07	2 (9%)
2	PSU	A	1472	2	18,21,22	0.95	1 (5%)	21,30,33	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	A	2195	81,2	19,22,23	0.34	0	25,31,34	0.77	0
75	A2M	h1	975	75	22,25,26	0.19	0	30,36,39	0.47	0
2	PSU	A	965	2	18,21,22	1.12	2 (11%)	21,30,33	0.85	0
75	PSU	h1	304	75	18,21,22	0.93	1 (5%)	21,30,33	0.79	0
2	A2M	A	2218	2	22,25,26	0.18	0	30,36,39	0.62	1 (3%)
75	MA6	h1	1786	75	23,26,27	0.28	0	33,38,41	0.84	1 (3%)
2	OMG	A	2792	2	23,26,27	0.32	0	32,38,41	0.52	0
2	5MC	A	2276	2,80	19,22,23	0.68	1 (5%)	26,32,35	0.70	0
1	PSU	3	22	2,1	18,21,22	0.88	1 (5%)	21,30,33	0.72	0
2	OMU	A	48	2	19,22,23	0.37	0	25,31,34	0.60	0
2	UY1	A	2649	2	19,22,23	1.04	1 (5%)	21,31,34	1.01	2 (9%)
75	PSU	h1	1176	75	18,21,22	0.90	1 (5%)	21,30,33	0.90	0
75	A2M	h1	794	75	22,25,26	0.19	0	30,36,39	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2134	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1754	75	-	0/9/27/28	0/3/3/3
75	OMC	h1	416	75	-	0/9/27/28	0/2/2/2
2	PSU	A	1015	81,2	-	0/7/25/26	0/2/2/2
2	OMU	A	2882	2	-	0/9/27/28	0/2/2/2
2	OMG	A	3290	2,80	-	0/9/27/28	0/3/3/3
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2
2	A2M	A	816	2	-	0/9/27/28	0/3/3/3
2	A2M	A	1458	2,80	-	0/9/27/28	0/3/3/3
75	OMG	h1	1272	81,75	-	0/9/27/28	0/3/3/3
2	UR3	A	2952	81,2	-	0/7/25/26	0/2/2/2
2	OMC	A	2335	2	-	0/9/27/28	0/2/2/2
2	OMU	A	144	81,2	-	0/9/27/28	0/2/2/2
55	MLY	Ga	113	55	-	0/8/9/11	-
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	1327	75	-	0/9/27/28	0/3/3/3
2	PSU	A	2853	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2363	2	-	1/9/27/28	0/2/2/2
75	A2M	h1	621	75,80	-	2/9/27/28	0/3/3/3
75	PSU	h1	1783	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A	1459	2,80	-	0/9/27/28	0/3/3/3
2	PSU	A	1133	2	-	0/7/25/26	0/2/2/2
1	A2M	3	47	1	-	0/9/27/28	0/3/3/3
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
75	G7M	h1	1577	3,75	-	0/7/25/26	0/3/3/3
2	A2M	A	2212	2,80	-	0/9/27/28	0/3/3/3
2	PSU	A	975	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	150	81,2	-	0/7/25/26	0/2/2/2
2	5MC	A	2869	81,2	-	4/7/25/26	0/2/2/2
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
1	PSU	3	78	1	-	0/7/25/26	0/2/2/2
2	OMC	A	1848	2,80	-	0/9/27/28	0/2/2/2
75	A2M	h1	799	75	-	0/9/27/28	0/3/3/3
2	PSU	A	2879	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2893	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	752	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2256	2	-	0/7/25/26	0/2/2/2
2	OMU	A	44	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	121	75,80	-	0/7/25/26	0/2/2/2
2	OMU	A	1066	2	-	0/9/27/28	0/2/2/2
2	1MG	A	1646	2	-	0/7/25/26	0/3/3/3
75	6MZ	h1	1767	81,75,80	-	0/9/27/28	0/3/3/3
2	PSU	A	969	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2291	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	778	75	-	2/9/27/28	0/3/3/3
2	PSU	A	2262	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
2	OMC	A	2958	2,80	-	0/9/27/28	0/2/2/2
2	PSU	A	277	2	-	0/7/25/26	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
75	PSU	h1	606	75	-	0/7/25/26	0/2/2/2
2	A2M	A	1142	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2947	2	-	0/9/27/28	0/2/2/2
2	PSU	A	3109	2	-	0/7/25/26	0/2/2/2
2	A2M	A	945	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2920	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2324	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1845	2	-	0/9/27/28	0/2/2/2
2	OMU	A	2345	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
1	OMG	3	79	1	-	0/9/27/28	0/3/3/3
75	PSU	h1	415	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2650	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2734	2,80	-	0/9/27/28	0/2/2/2
75	OMC	h1	38	75	-	0/9/27/28	0/2/2/2
2	PSU	A	228	2	-	1/7/25/26	0/2/2/2
2	OMU	A	2408	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2921	2	-	0/9/27/28	0/3/3/3
2	A2M	A	661	2	-	1/9/27/28	0/3/3/3
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
75	OMC	h1	471	75	-	0/9/27/28	0/2/2/2
2	OMG	A	2122	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2825	81,2	-	0/7/25/26	0/2/2/2
1	OMG	3	155	2,1	-	0/9/27/28	0/3/3/3
75	PSU	h1	1188	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1478	2	-	0/9/27/28	0/2/2/2
2	PSU	A	2974	2	-	0/7/25/26	0/2/2/2
2	PSU	A	42	81,2	-	0/7/25/26	0/2/2/2
75	PSU	h1	337	81,75	-	0/7/25/26	0/2/2/2
2	PSU	A	2430	2	-	0/7/25/26	0/2/2/2
75	OMG	h1	390	81,75	-	0/9/27/28	0/3/3/3
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
2	PSU	A	894	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2716	2	-	0/9/27/28	0/2/2/2
2	PSU	A	2258	2	-	0/7/25/26	0/2/2/2
2	OMG	A	2286	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2835	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	543	75	-	1/9/27/28	0/3/3/3
2	PSU	A	2954	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	468	75	-	0/7/25/26	0/2/2/2
75	OMU	h1	1270	75,80	-	2/9/27/28	0/2/2/2
2	PSU	A	685	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2922	2	-	1/7/25/26	0/2/2/2
75	PSU	h1	1306	75	-	1/7/25/26	0/2/2/2
75	UY1	h1	602	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	583	75	-	6/7/25/26	0/2/2/2
2	PSU	A	2316	2,80	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A	2407	81,2	-	0/9/27/28	0/3/3/3
2	PSU	A	1132	2	-	0/7/25/26	0/2/2/2
75	OMU	h1	123	75	-	2/9/27/28	0/2/2/2
75	OMU	h1	1261	75	-	0/9/27/28	0/2/2/2
2	A2M	A	826	81,2,80	-	2/9/27/28	0/3/3/3
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2
2	OMC	A	675	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	103	81,75	-	0/7/25/26	0/2/2/2
2	A2M	A	2124	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1208	75	-	1/7/25/26	0/2/2/2
75	A2M	h1	438	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	449	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2312	81,2	-	1/7/25/26	0/2/2/2
75	OMU	h1	1445	75	-	0/9/27/28	0/2/2/2
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
2	OMU	A	3299	2	-	0/9/27/28	0/2/2/2
2	OMU	A	803	2	-	0/9/27/28	0/2/2/2
2	PSU	A	901	81,2	-	0/7/25/26	0/2/2/2
75	OMC	h1	1216	75	-	0/9/27/28	0/2/2/2
2	PSU	A	1681	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	422	75	-	0/9/27/28	0/3/3/3
2	OMG	A	2234	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1611	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2933	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2389	2	-	0/9/27/28	0/3/3/3
2	OMG	A	814	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	1641	75,80	-	0/9/27/28	0/2/2/2
75	OMU	h1	580	75	-	2/9/27/28	0/2/2/2
2	OMG	A	1853	2	-	0/9/27/28	0/3/3/3
2	A2M	A	2279	2	-	3/9/27/28	0/3/3/3
2	OMG	A	2814	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2878	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	1263	75	-	1/9/27/28	0/2/2/2
2	PSU	A	2943	81,2,80	-	0/7/25/26	0/2/2/2
75	OMU	h1	1381	75,80	-	0/9/27/28	0/2/2/2
2	OMG	A	2618	3,2	-	1/9/27/28	0/3/3/3
2	OMC	A	1858	2	-	0/9/27/28	0/2/2/2
2	PSU	A	1062	81,2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	A	1890	2	-	0/9/27/28	0/2/2/2
2	A2M	A	2254	2	-	0/9/27/28	0/3/3/3
2	1MA	A	657	2,80	-	0/7/25/26	0/3/3/3
75	OMG	h1	597	75	-	3/9/27/28	0/3/3/3
75	OMG	h1	244	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1517	2,80	-	2/9/27/28	0/2/2/2
75	OMG	h1	1431	75,80	-	1/9/27/28	0/3/3/3
2	PSU	A	509	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2209	2	-	0/7/25/26	0/2/2/2
2	OMU	A	2111	2	-	2/9/27/28	0/2/2/2
2	OMU	A	676	2	-	0/9/27/28	0/2/2/2
2	OMG	A	917	81,2	-	0/9/27/28	0/3/3/3
2	PSU	A	2252	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1480	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2743	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2864	2	-	0/7/25/26	0/2/2/2
2	PSU	A	785	2	-	2/7/25/26	0/2/2/2
2	A2M	A	2639	2	-	0/9/27/28	0/3/3/3
2	PSU	A	828	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2189	81,2	-	0/7/25/26	0/2/2/2
2	OMG	A	2393	2,80	-	0/9/27/28	0/3/3/3
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
75	A2M	h1	162	75	-	0/9/27/28	0/3/3/3
2	OMU	A	2419	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	808	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	28	75,80	-	0/9/27/28	0/3/3/3
2	PSU	A	34	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1054	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1483	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2319	2	-	0/9/27/28	0/3/3/3
2	PSU	A	1001	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2945	2,80	-	0/9/27/28	0/3/3/3
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
75	C4J	h1	1192	75	-	5/16/34/35	0/2/2/2
2	A2M	A	2910	2	-	5/9/27/28	0/3/3/3
2	A2M	A	885	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2790	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	959	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2132	81,2	-	0/7/25/26	0/2/2/2
2	A2M	A	1376	2,80	-	0/9/27/28	0/3/3/3
2	A2M	A	2359	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	308	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1520	75	-	2/7/25/26	0/2/2/2
2	PSU	A	2414	2,80	-	0/7/25/26	0/2/2/2
2	OMC	A	2681	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2916	2	-	0/9/27/28	0/3/3/3
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	95	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1131	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1446	2	-	0/9/27/28	0/2/2/2
1	PSU	3	97	81,1	-	0/7/25/26	0/2/2/2
2	PSU	A	311	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	1472	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2195	81,2	-	4/9/27/28	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
2	PSU	A	965	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2218	2	-	0/9/27/28	0/3/3/3
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
2	OMG	A	2792	2	-	1/9/27/28	0/3/3/3
2	5MC	A	2276	2,80	-	0/7/25/26	0/2/2/2
1	PSU	3	22	2,1	-	0/7/25/26	0/2/2/2
2	OMU	A	48	2	-	0/9/27/28	0/2/2/2
2	UY1	A	2649	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	311	PSU	C6-C5	4.14	1.39	1.35
2	A	2414	PSU	C6-C5	4.02	1.39	1.35
2	A	2954	PSU	C6-C5	4.01	1.39	1.35
75	h1	1783	PSU	C6-C5	3.96	1.39	1.35
1	3	78	PSU	C6-C5	3.93	1.39	1.35

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	945	A2M	O2'-C2'-C1'	-3.68	101.99	108.99
75	h1	1786	MA6	C2-N1-C6	3.10	119.40	111.83
75	h1	1785	MA6	C2-N1-C6	3.07	119.32	111.83
75	h1	799	A2M	O2'-C2'-C1'	2.74	114.19	108.99
2	A	2279	A2M	O4'-C1'-N9	2.68	113.24	108.09

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	785	PSU	C2'-C1'-C5-C4
2	A	2111	OMU	O4'-C4'-C5'-O5'
2	A	2195	OMC	C2'-C1'-N1-C6
2	A	2618	OMG	C1'-C2'-O2'-CM2
2	A	2910	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

35 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2882	OMU	1	0
2	A	2879	PSU	1	0
2	A	44	OMU	1	0
75	h1	1767	6MZ	1	0
2	A	969	PSU	1	0
2	A	1142	A2M	1	0
2	A	2920	OMU	1	0
2	A	2324	A2M	1	0
2	A	2345	OMU	1	0
2	A	661	A2M	1	0
1	3	155	OMG	3	0
2	A	2258	PSU	1	0
2	A	2922	PSU	1	0
75	h1	1261	OMU	1	0
2	A	826	A2M	1	0
2	A	675	OMC	1	0
75	h1	1531	PSU	1	0
2	A	2312	PSU	1	0
2	A	2234	OMG	1	0
2	A	2933	A2M	2	0
2	A	2389	OMG	1	0
75	h1	1641	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1853	OMG	1	0
2	A	2878	OMC	1	0
2	A	2618	OMG	1	0
2	A	2254	A2M	1	0
75	h1	244	OMG	1	0
2	A	2189	PSU	1	0
75	h1	1192	C4J	1	0
2	A	2790	OMG	1	0
2	A	1376	A2M	1	0
75	h1	95	PSU	1	0
2	A	1446	OMC	2	0
75	h1	975	A2M	1	0
75	h1	794	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 494 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
83	SPD	A	3403	-	9,9,9	0.29	0	8,8,8	0.55	0
84	EPE	A	3404	-	15,15,15	0.68	1 (6%)	19,20,20	0.63	0
83	SPD	A	3405	-	9,9,9	0.17	0	8,8,8	0.29	0
82	TER	A	3401	-	13,13,13	0.16	0	12,12,12	0.27	0
83	SPD	A	3402	-	9,9,9	0.18	0	8,8,8	0.15	0
83	SPD	A	3406	-	9,9,9	0.17	0	8,8,8	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	SPD	A	3403	-	-	5/7/7/7	-
84	EPE	A	3404	-	-	5/9/19/19	0/1/1/1
83	SPD	A	3405	-	-	1/7/7/7	-
82	TER	A	3401	-	-	1/11/11/11	-
83	SPD	A	3402	-	-	3/7/7/7	-
83	SPD	A	3406	-	-	2/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	A	3404	EPE	O3S-S	2.44	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	A	3406	SPD	C3-C4-C5-N6
83	A	3403	SPD	C3-C4-C5-N6
83	A	3405	SPD	C3-C4-C5-N6
83	A	3403	SPD	N6-C7-C8-C9
83	A	3402	SPD	C3-C4-C5-N6

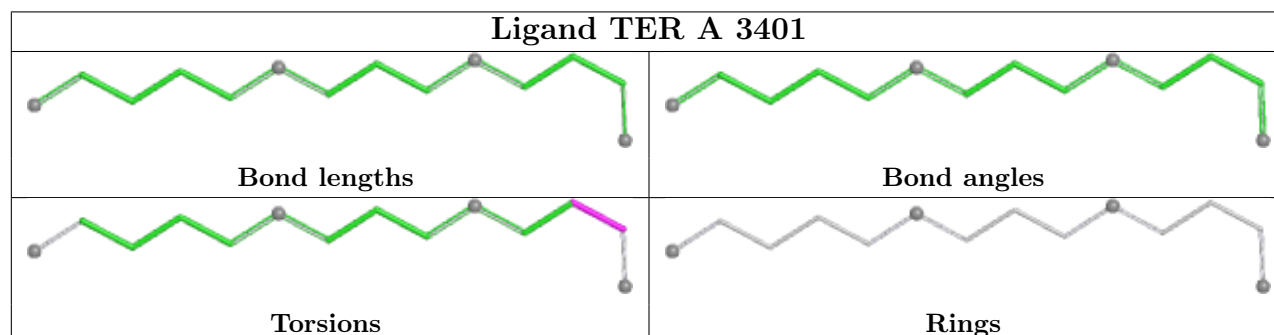
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	A	3403	SPD	1	0
83	A	3405	SPD	1	0
82	A	3401	TER	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
74	Ca	1
73	AY	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ca	53:ILE	C	54:LYS	N	1.90
1	AY	76:THR	C	77:CYS	N	1.85

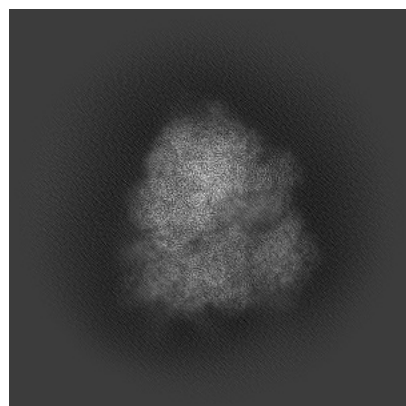
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51820. These allow visual inspection of the internal detail of the map and identification of artifacts.

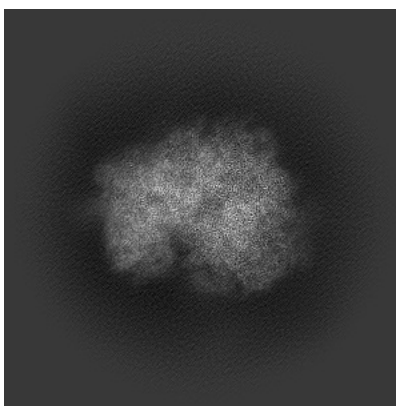
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

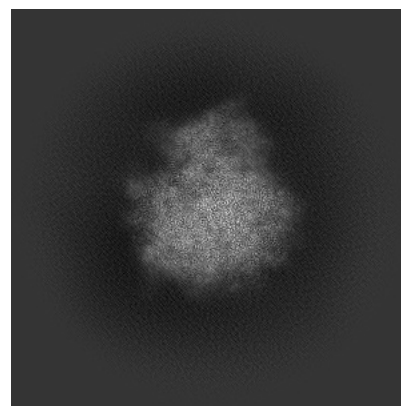
6.1.1 Primary map



X

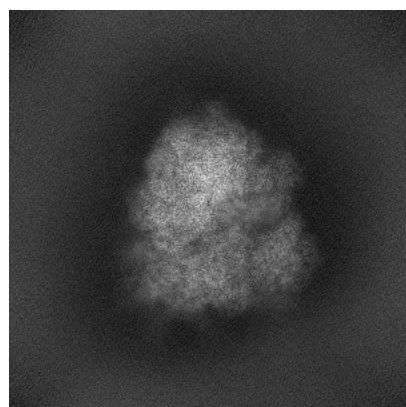


Y

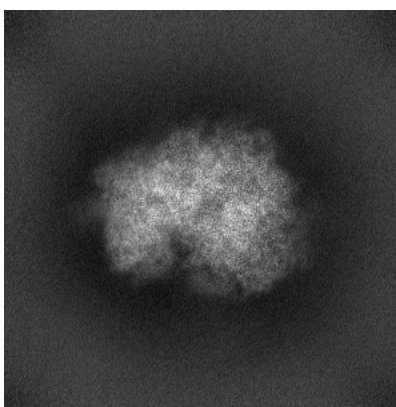


Z

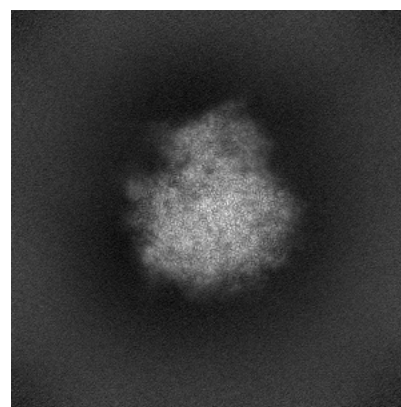
6.1.2 Raw map



X



Y

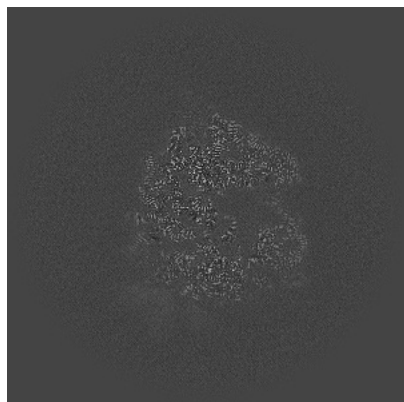


Z

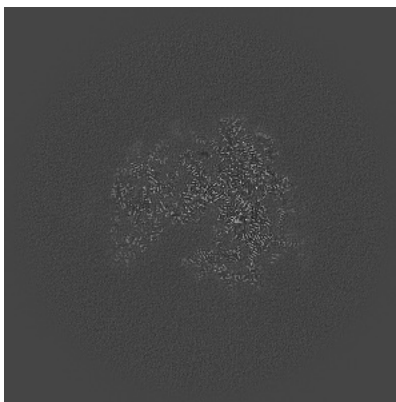
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

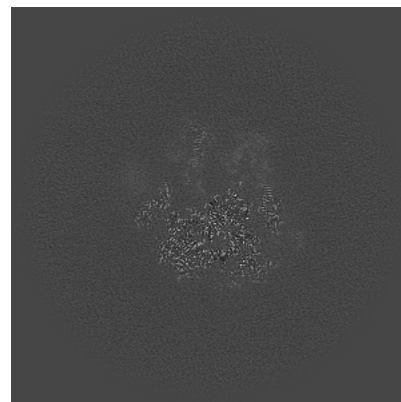
6.2.1 Primary map



X Index: 343

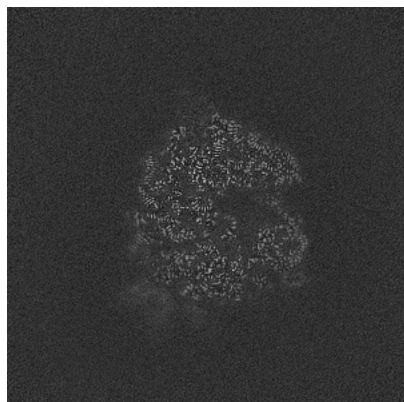


Y Index: 343

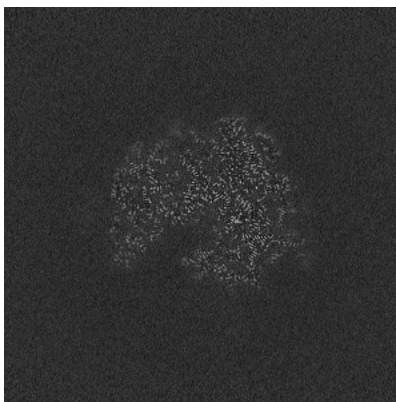


Z Index: 343

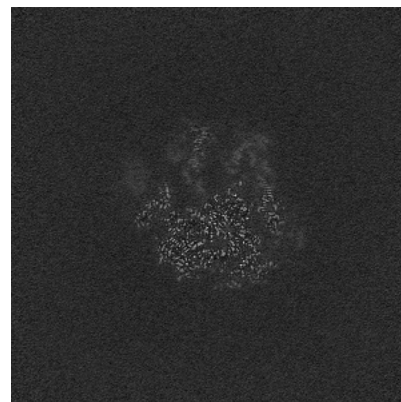
6.2.2 Raw map



X Index: 343



Y Index: 343

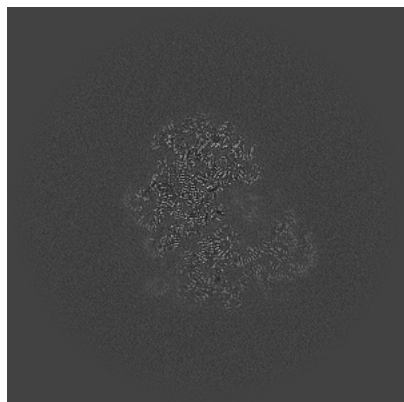


Z Index: 343

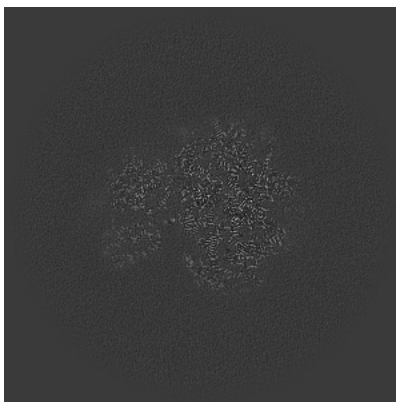
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

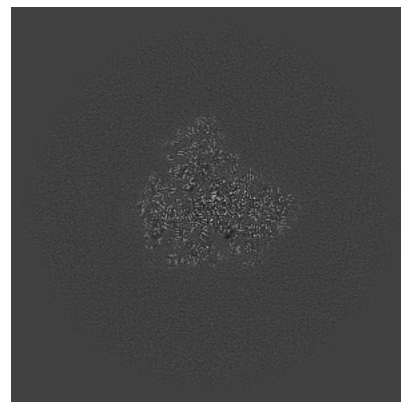
6.3.1 Primary map



X Index: 378

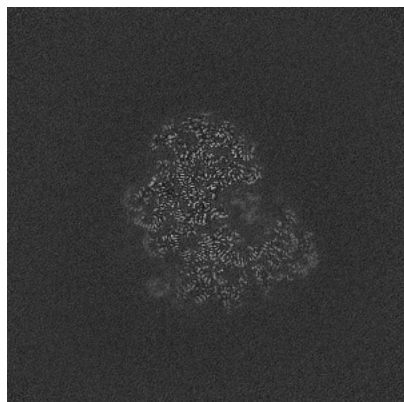


Y Index: 329

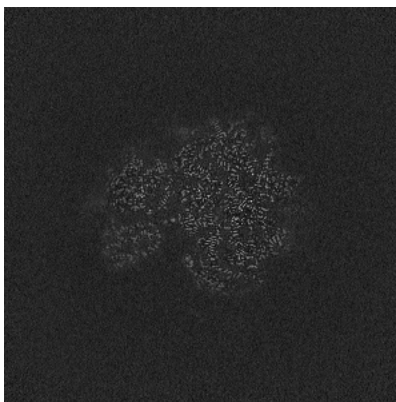


Z Index: 401

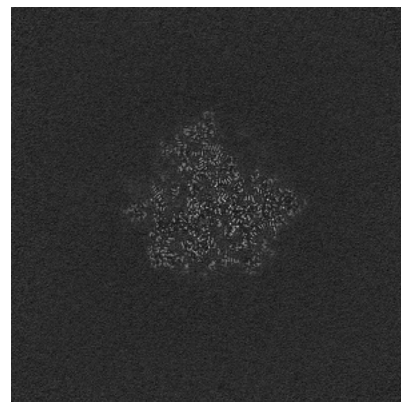
6.3.2 Raw map



X Index: 377



Y Index: 329

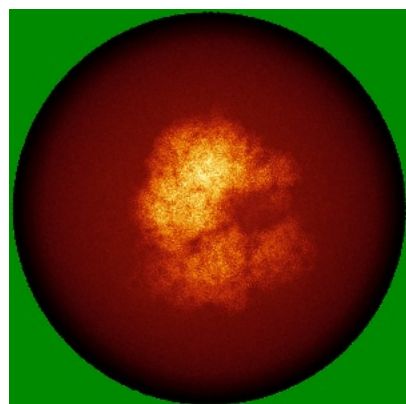


Z Index: 390

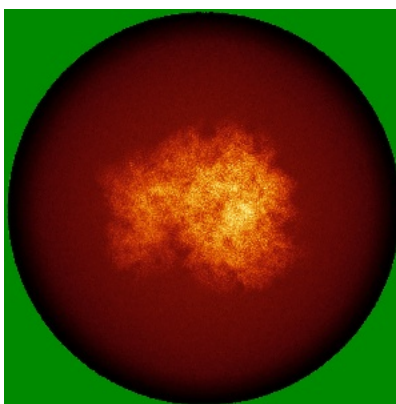
The images above show the largest variance slices of the map in three orthogonal directions.

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

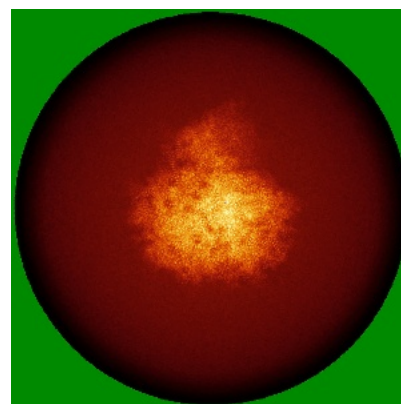
6.4.1 Primary map



X

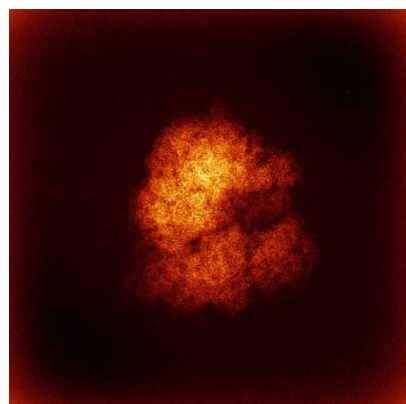


Y

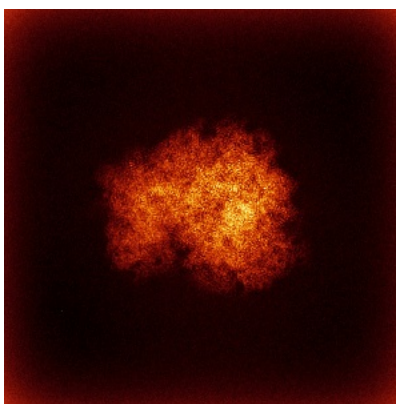


Z

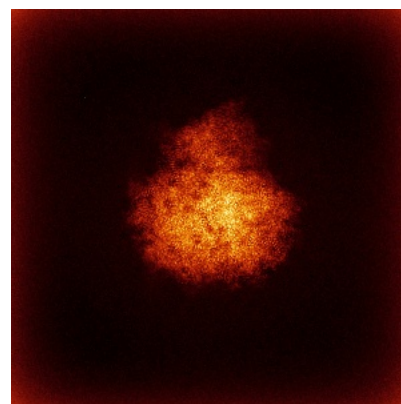
6.4.2 Raw map



X



Y

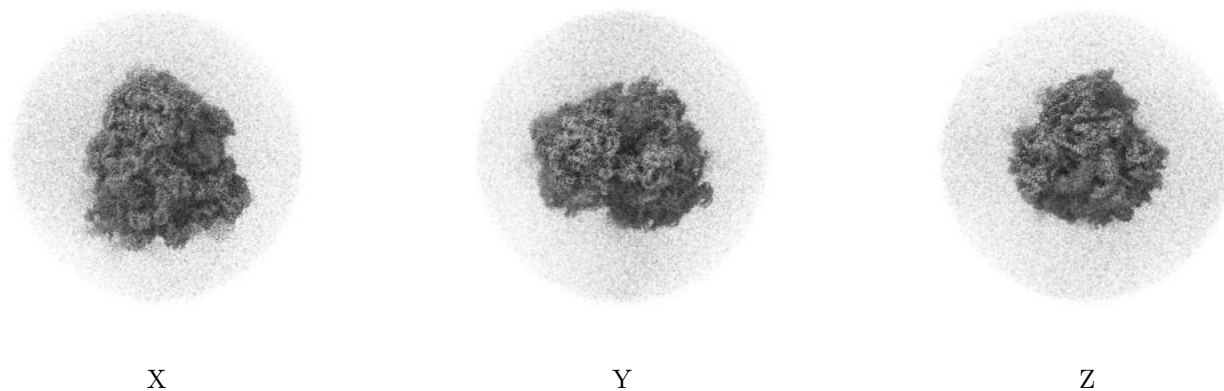


Z

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.

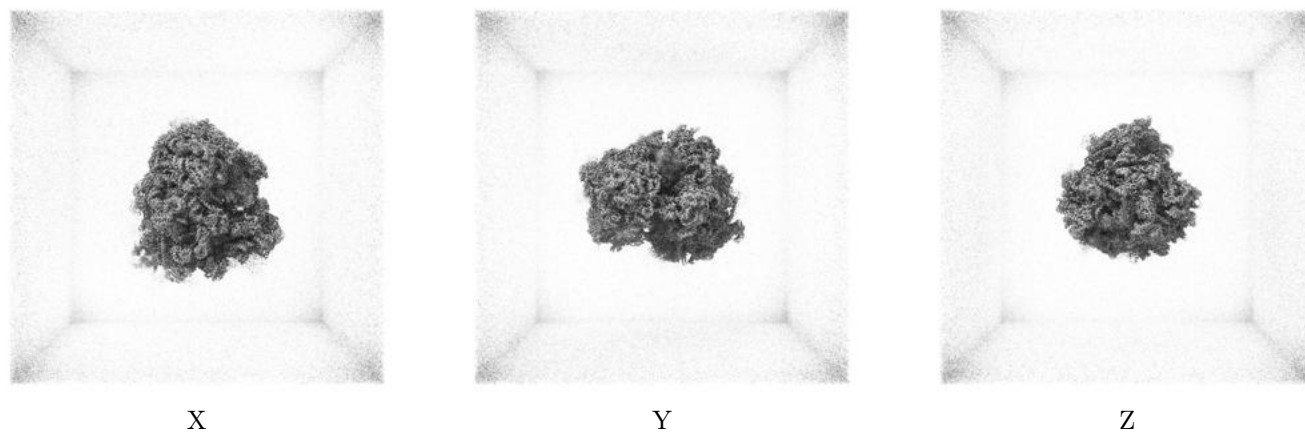
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

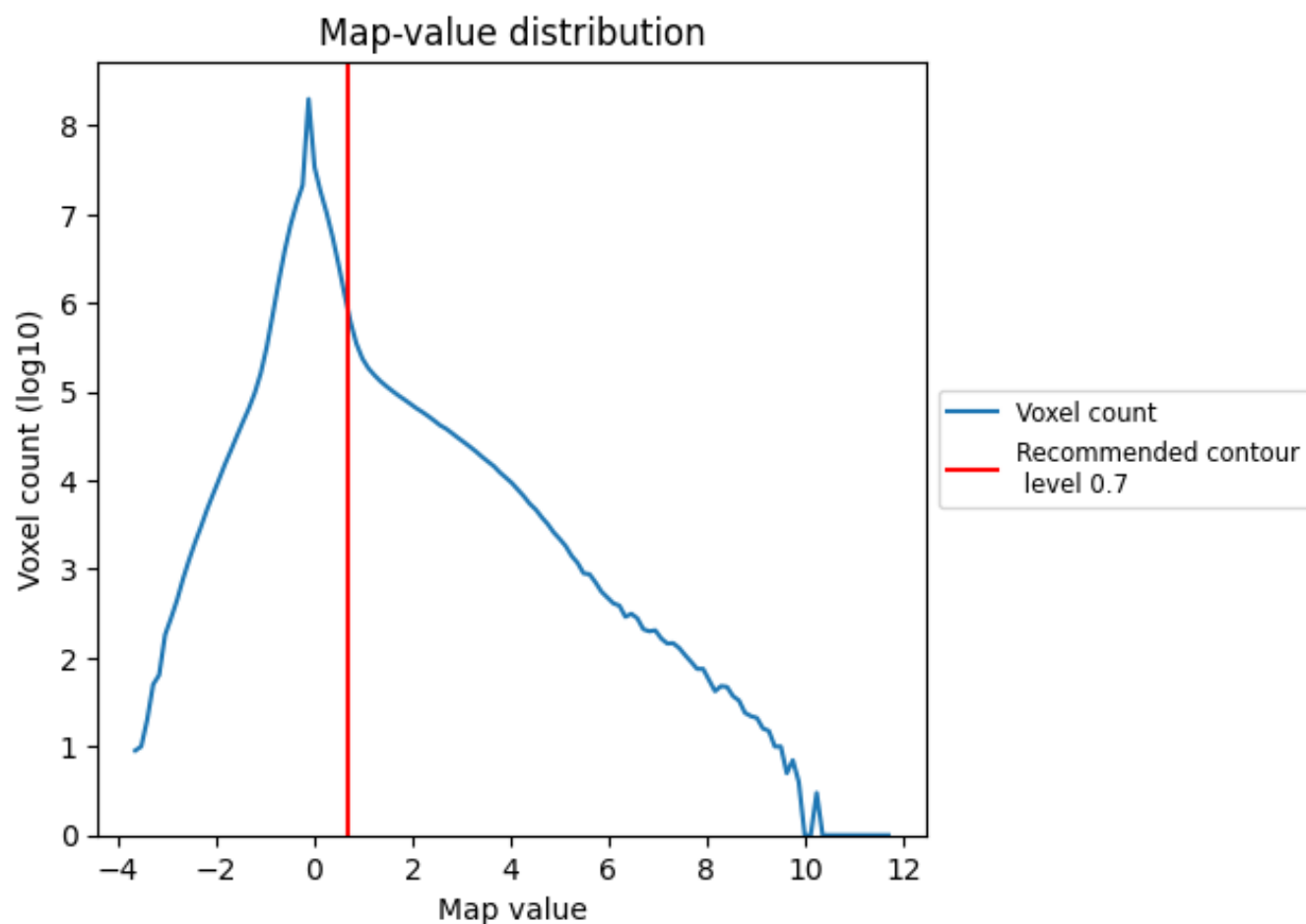
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

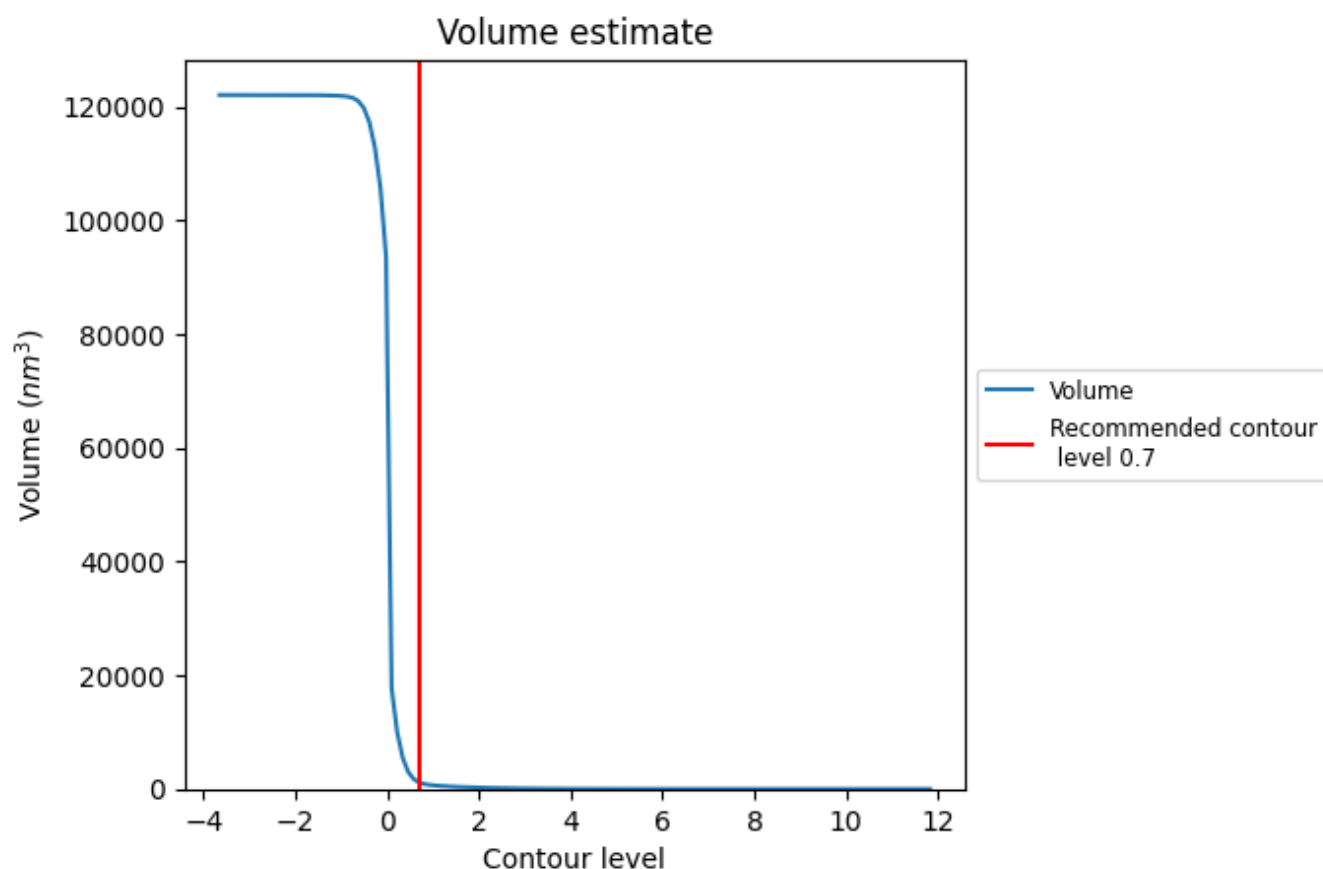
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

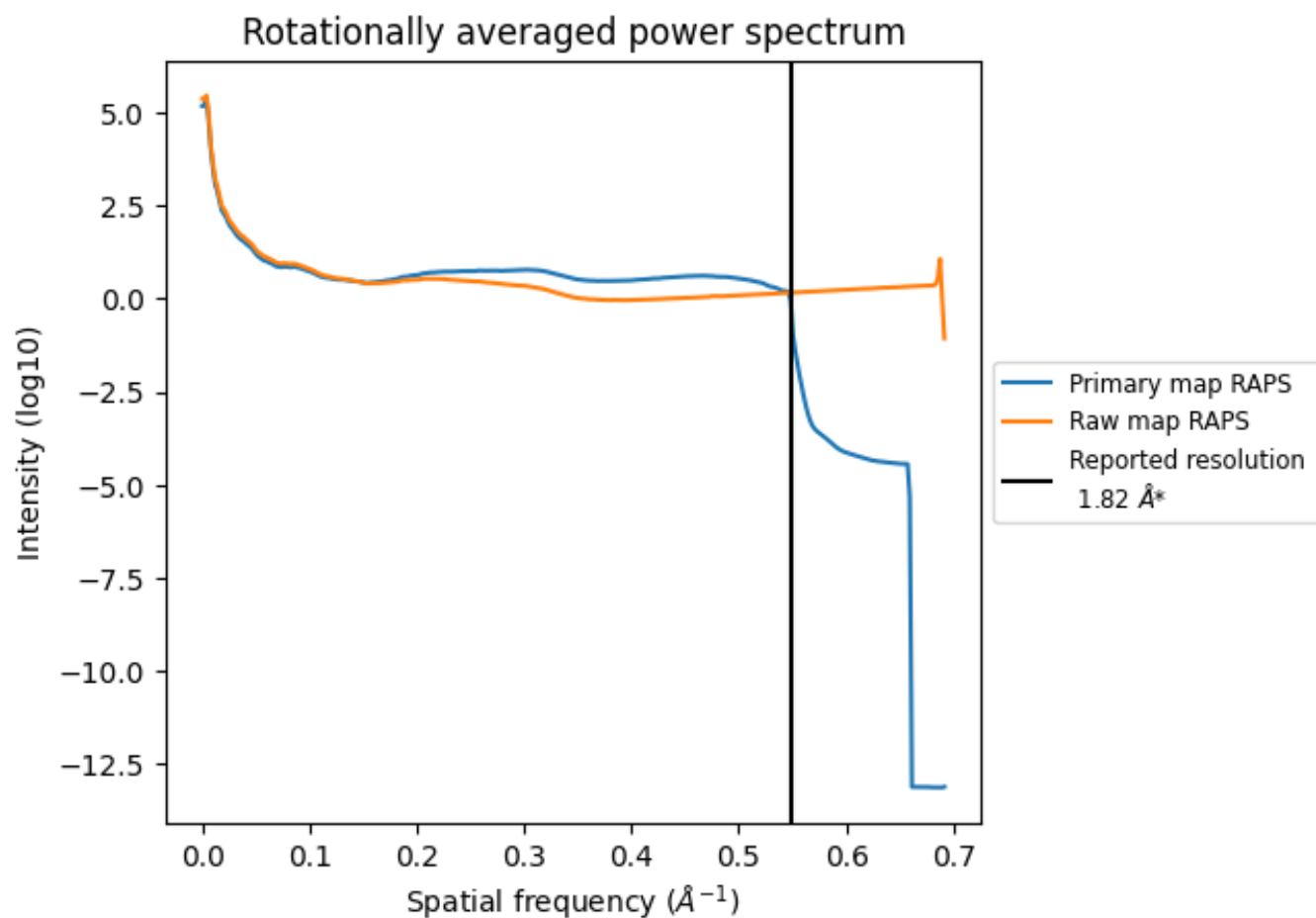
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1140 nm^3 ; this corresponds to an approximate mass of 1030 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 ⓘ

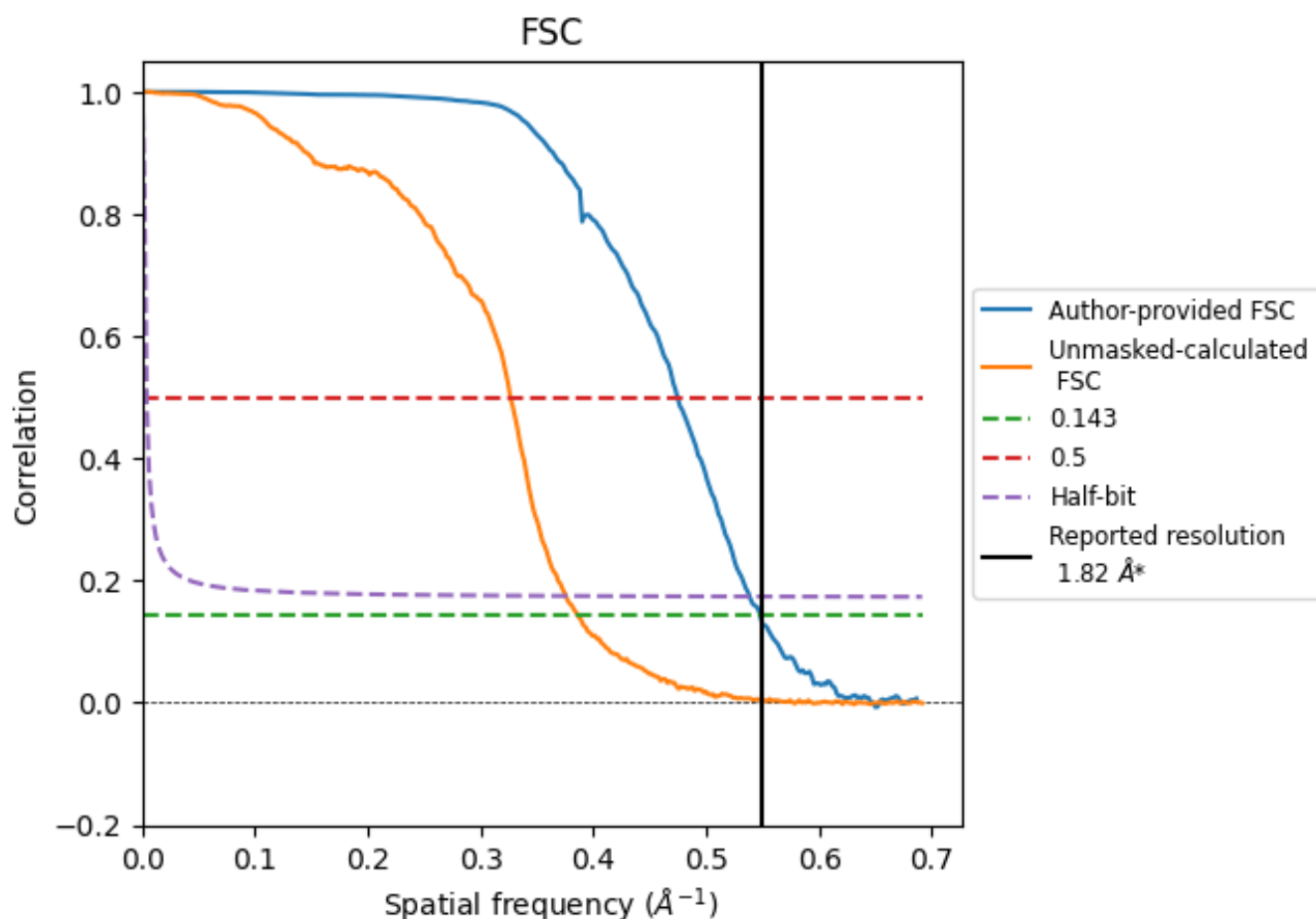


*Reported resolution corresponds to spatial frequency of 0.549 \AA^{-1}

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 0.549 Å⁻¹

8.2 Resolution estimates [i](#)

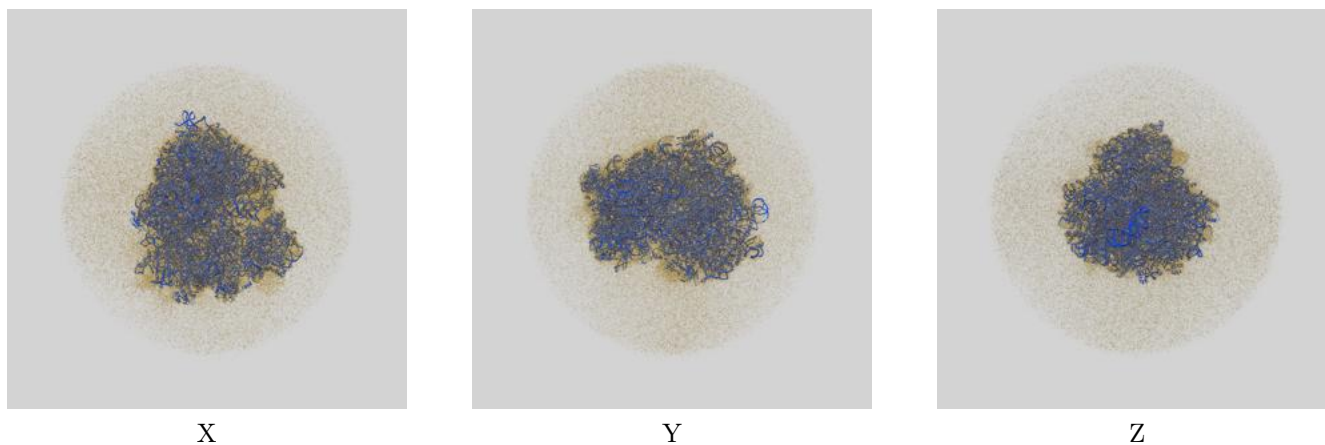
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.82	-	-
Author-provided FSC curve	1.82	2.11	1.86
Unmasked-calculated*	2.59	3.06	2.66

*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 2.59 differs from the reported value 1.82 by more than 10 %

9 Map-model fit [i](#)

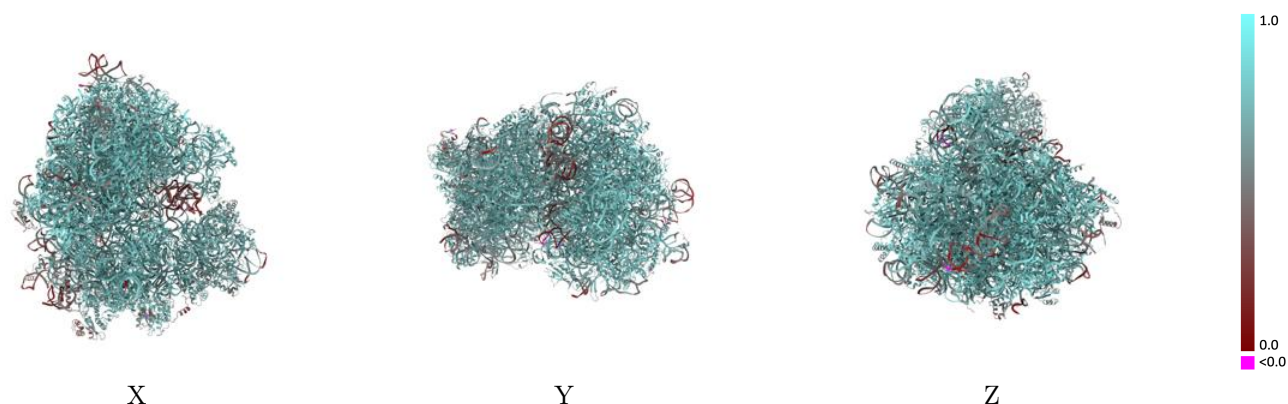
This section contains information regarding the fit between EMDB map EMD-51820 and PDB model 9H3G. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



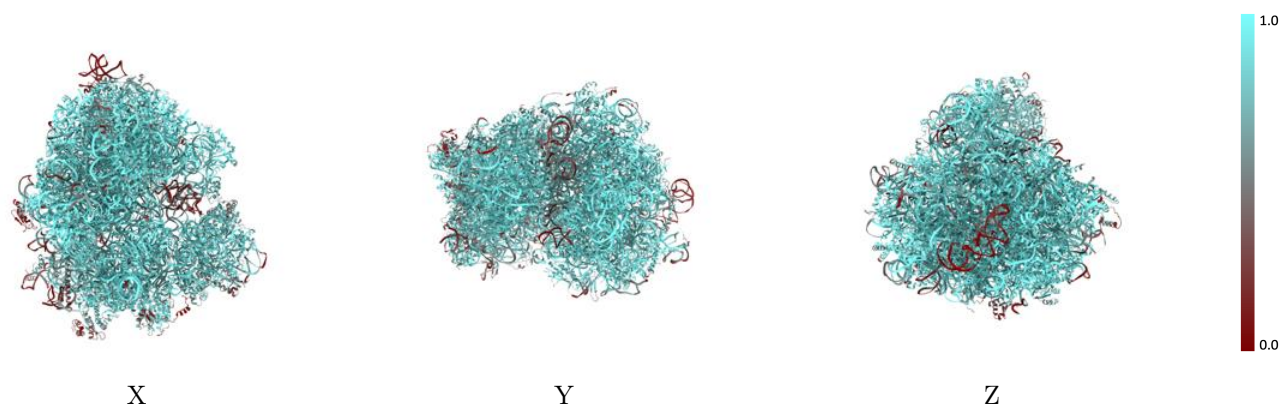
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



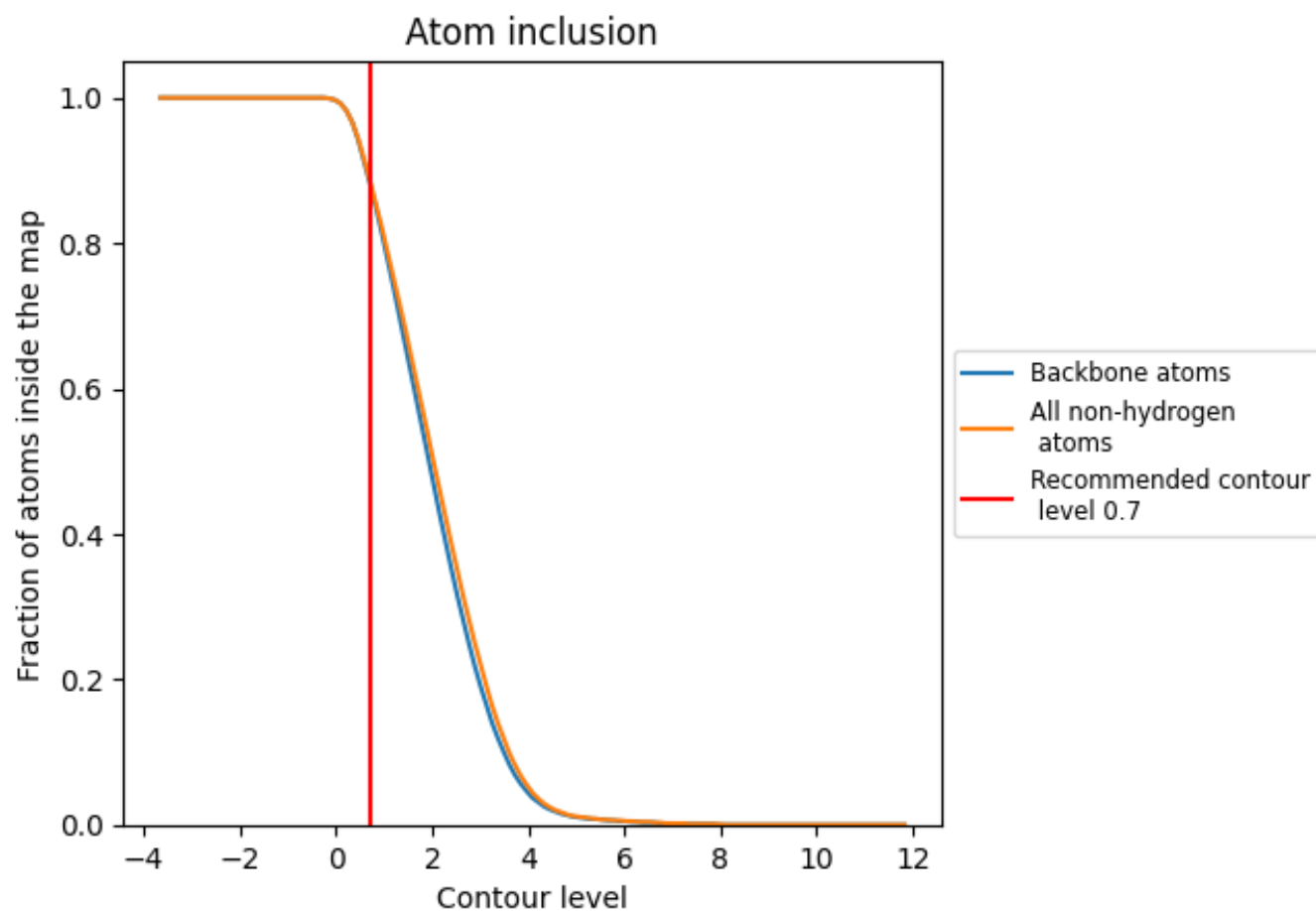
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.7200
3	 0.9100	 0.7230
A	 0.9170	 0.7350
AA	 0.7410	 0.6400
AB	 0.8740	 0.7060
AC	 0.9420	 0.7610
AD	 0.8520	 0.6890
AE	 0.9760	 0.7920
AF	 0.8350	 0.6660
AG	 0.9130	 0.7590
AH	 0.9090	 0.7490
AI	 0.6240	 0.5820
AJ	 0.9850	 0.8130
AK	 0.8480	 0.7130
AL	 0.9620	 0.7880
AM	 0.9270	 0.7670
AN	 0.2300	 0.4770
AO	 0.9550	 0.7840
AP	 0.9330	 0.7550
AQ	 0.5680	 0.6590
AR	 0.9440	 0.7790
AT	 0.9290	 0.7560
AU	 0.8690	 0.7380
AV	 0.9790	 0.8020
AW	 0.9800	 0.8100
AX	 0.9090	 0.7420
AY	 0.9780	 0.8130
AZ	 0.8010	 0.6760
Aa	 0.8040	 0.6580
B1	 0.8630	 0.6720
BA	 0.9810	 0.8050
BB	 0.4740	 0.5180
BC	 0.9360	 0.7690
BD	 0.9680	 0.8040
BE	 0.9600	 0.7920











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Chain	Atom inclusion	Q-score
BF	 0.8500	 0.7060
BG	 0.8440	 0.7110
BH	 0.9540	 0.7920
BI	 0.9690	 0.8030
BJ	 0.9340	 0.7430
BK	 0.9050	 0.7470
BL	 0.8550	 0.6810
BM	 0.9560	 0.7990
BN	 0.9390	 0.7720
BO	 0.9640	 0.7860
BP	 0.9220	 0.7600
BQ	 0.9920	 0.8220
BR	 0.9330	 0.7830
BS	 0.9760	 0.8090
BT	 0.9220	 0.7750
BU	 0.8750	 0.7100
BV	 0.8960	 0.7220
BW	 0.8940	 0.7310
Ba	 0.6330	 0.6200
C3	 0.9930	 0.7660
Ca	 0.9080	 0.7380
Da	 0.8820	 0.7170
Ea	 0.9990	 0.8250
Fa	 0.9230	 0.7750
Ga	 0.9350	 0.7650
Ha	 0.9630	 0.8020
Ia	 0.9080	 0.7440
Ja	 0.8830	 0.7050
Ka	 0.7680	 0.6510
L3	 0.2430	 0.3620
La	 0.6740	 0.6000
Ma	 0.9180	 0.7510
Na	 0.7570	 0.6460
Oa	 0.8150	 0.6750
Pa	 0.7960	 0.6730
Ra	 0.5480	 0.5470
Ta	 0.6390	 0.5790
Ua	 0.9510	 0.7480
Va	 0.9600	 0.7790
W2	 0.5810	 0.4500
Wa	 0.8190	 0.6780
Xa	 0.8900	 0.7120

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Chain	Atom inclusion	Q-score
Ya	 0.7050	 0.6230
Za	 0.8350	 0.6880
h1	 0.8930	 0.6910
i2	 0.6160	 0.4850