



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2026 – 07:54 pm BST

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:

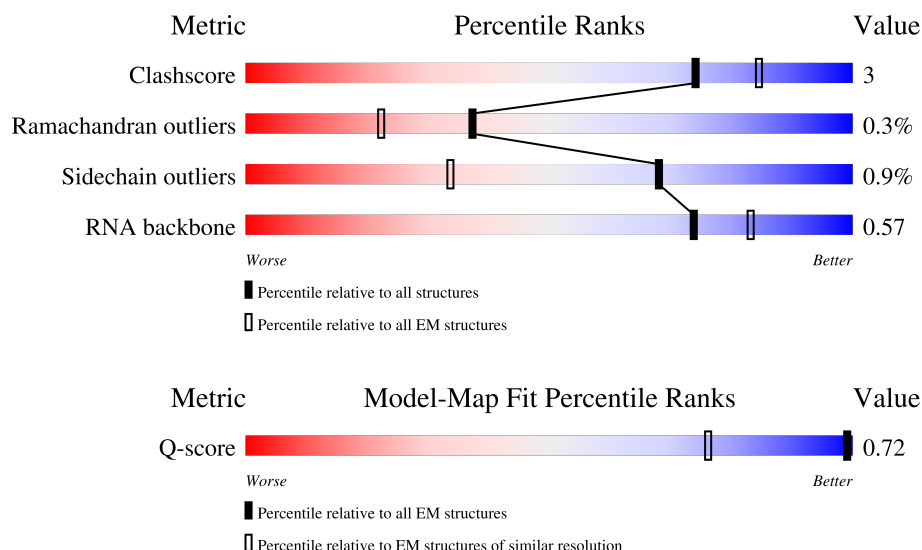
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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	 6% 71% 25% ...
2	A	3385	 6% 68% 21% 7%
3	W2	76	 30% 74% 22% ..

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

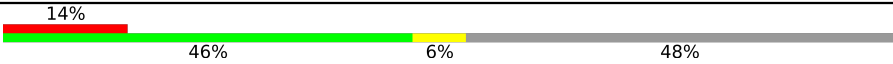
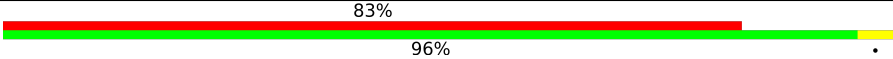
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	AI	177	
79	L3	23	

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	

Continued on next page...

Continued from previous page...

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).

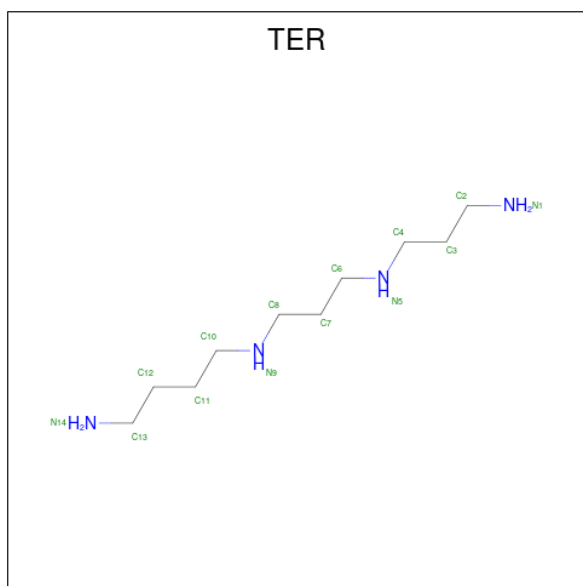
Mol	Chain	Residues	Atoms		AltConf
81	3	4	Total 4	K 4	0
81	A	127	Total 127	K 127	0
81	C3	1	Total 1	K 1	0
81	BM	1	Total 1	K 1	0
81	AR	1	Total 1	K 1	0
81	Ea	1	Total 1	K 1	0
81	Va	1	Total 1	K 1	0
81	BD	1	Total 1	K 1	0
81	BS	2	Total 2	K 2	0
81	AV	1	Total 1	K 1	0
81	AD	1	Total 1	K 1	0
81	AJ	1	Total 1	K 1	0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

Continued on next page...

Continued from previous page...

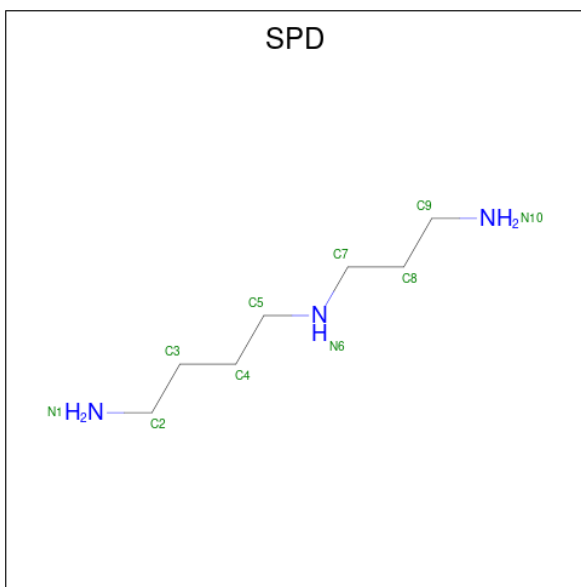
Mol	Chain	Residues	Atoms		AltConf
81	Fa	1	Total	K	0
			1	1	
81	BJ	1	Total	K	0
			1	1	
81	Wa	1	Total	K	0
			1	1	
81	Ua	1	Total	K	0
			1	1	
81	Ca	1	Total	K	0
			1	1	
81	h1	40	Total	K	0
			40	40	

- 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).



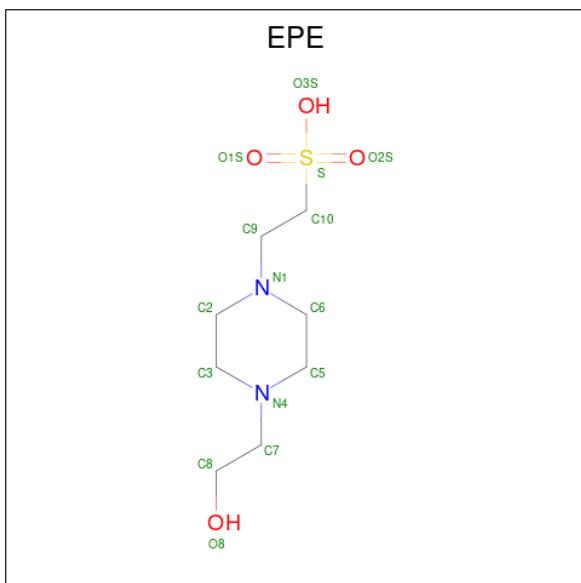
Mol	Chain	Residues	Atoms			AltConf
82	A	1	Total	C	N	0
			14	10	4	

- 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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

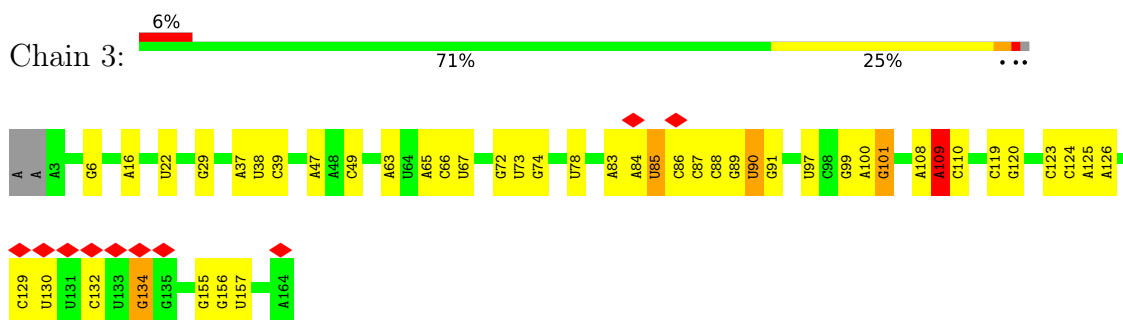
Continued from previous page...

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

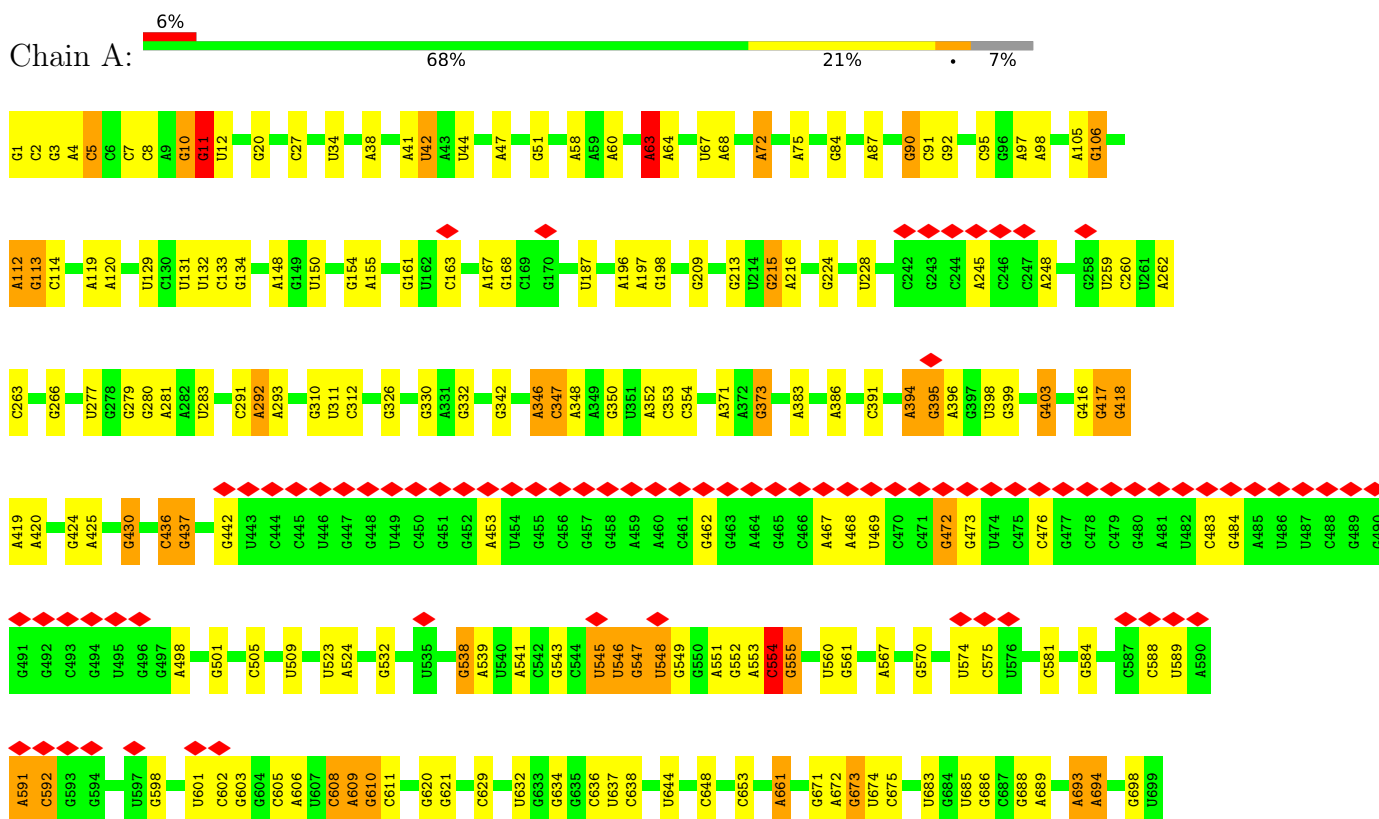
3 Residue-property plots

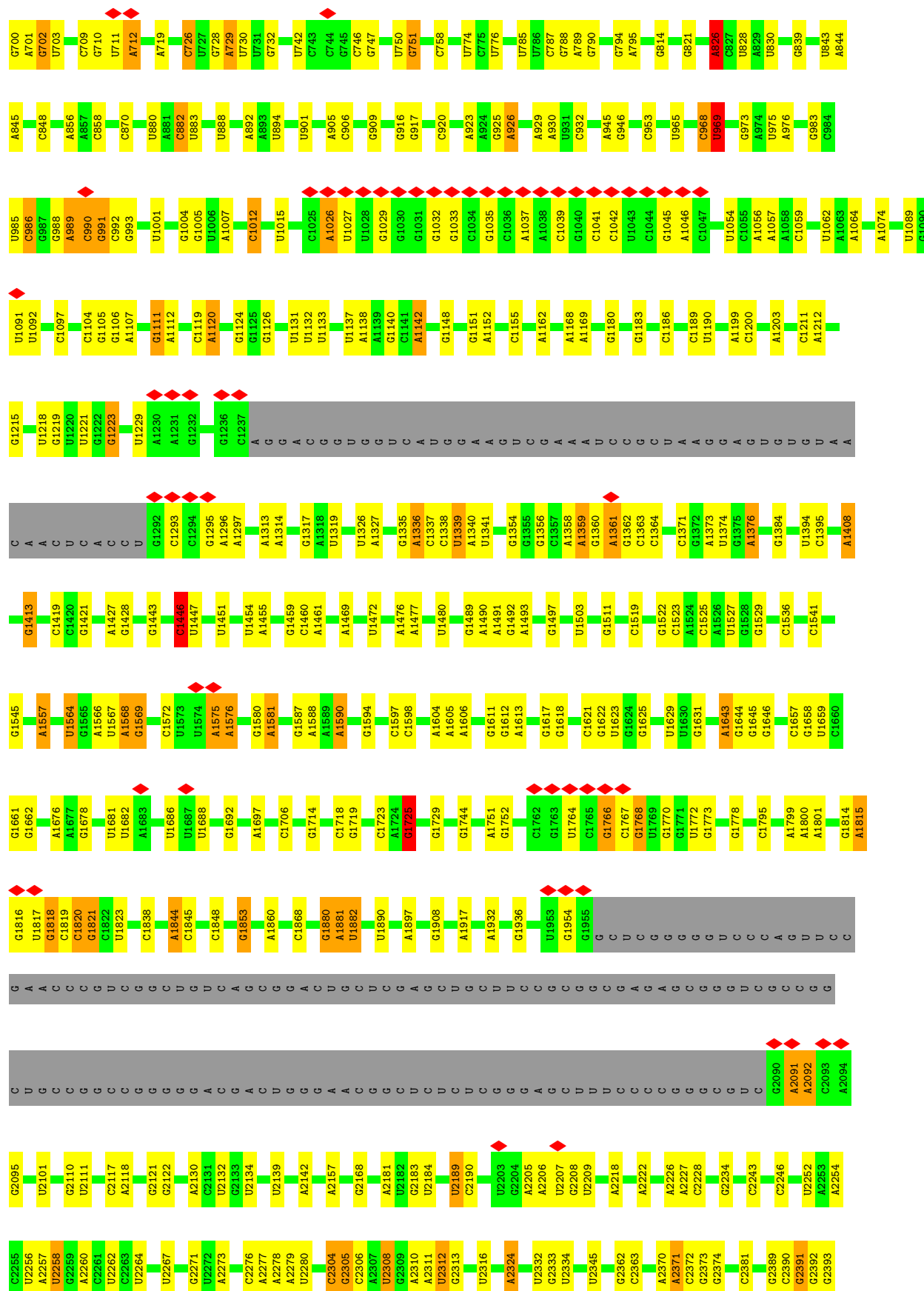
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

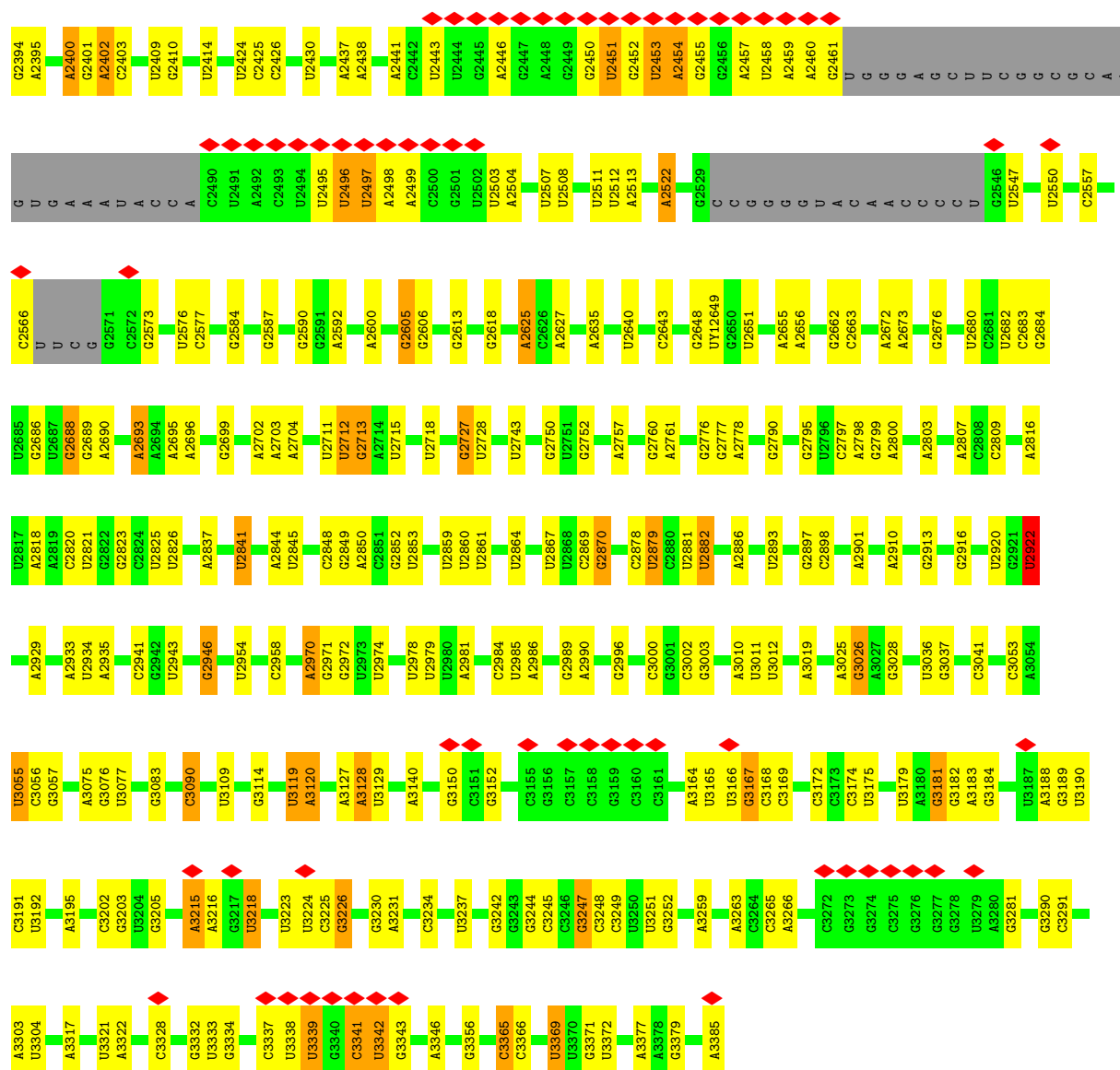
• Molecule 1: Ribosomal RNA 5.8S



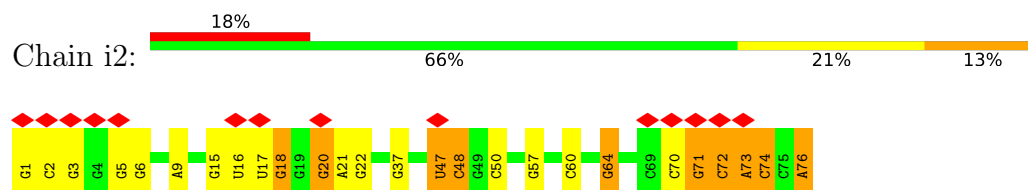
• Molecule 2: Ribosomal RNA 25S



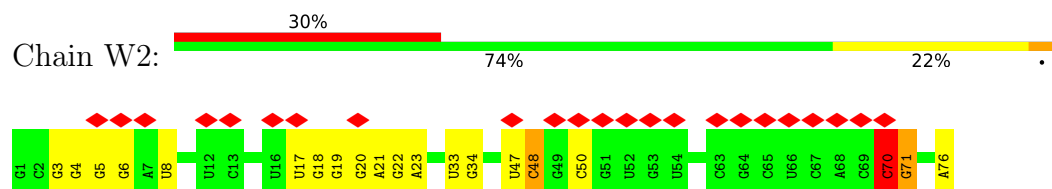




• Molecule 3: Transfer RNA Phe

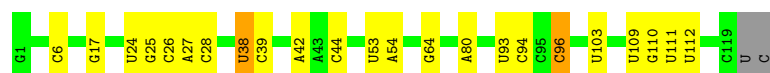


• Molecule 3: Transfer RNA Phe

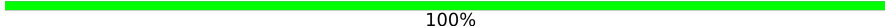


• Molecule 4: Ribosomal RNA 5S

Chain C3:  79% 17% ..



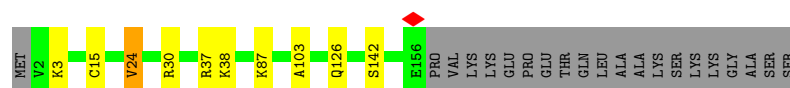
- Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v

Chain BC:  100%

There are no outlier residues recorded for this chain.

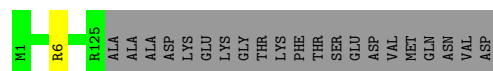
- Molecule 6: Large ribosomal subunit protein uL22z

Chain BM:  82% 5% • 12%



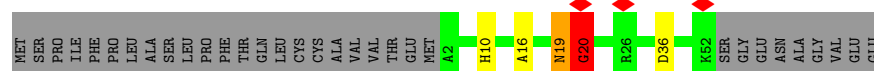
- Molecule 7: Large ribosomal subunit protein uL24z

Chain BO:  85% • 14%



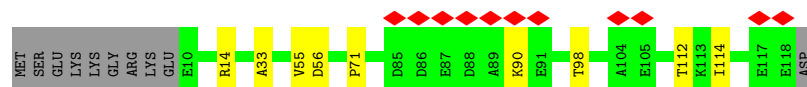
- Molecule 8: 60S ribosomal protein L29

Chain AR:  55% • • 39%



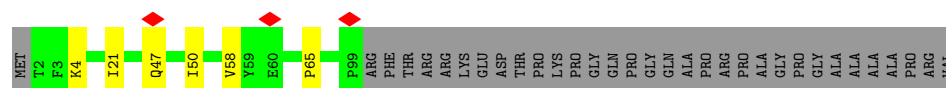
- Molecule 9: Large ribosomal subunit protein eL31y

Chain AU:  9% 84% 8% 8%



- Molecule 10: Small ribosomal subunit protein eS26y

Chain Ma:  70% 5% 25%

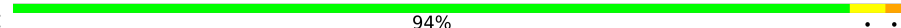


- Molecule 11: Large ribosomal subunit protein uL6z/uL6y

Chain Ia:  89% 9%



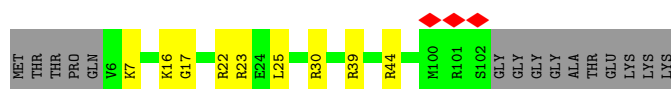
- Molecule 12: Small ribosomal subunit protein uS8z/uS8w

Chain AE:  94%



- Molecule 13: Large ribosomal subunit protein eL36y

Chain AX:  79% 8% 13%



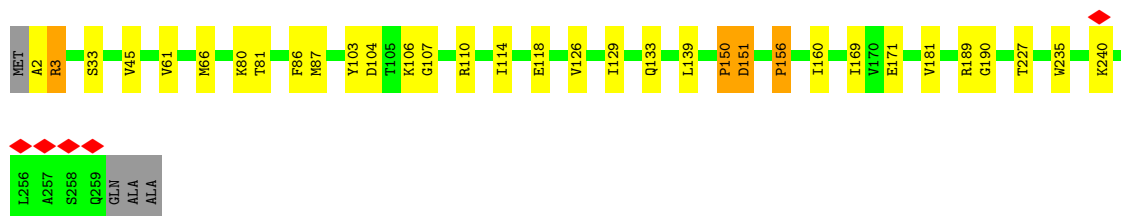
- Molecule 14: Large ribosomal subunit protein eL27x

Chain AP:  90% 9%

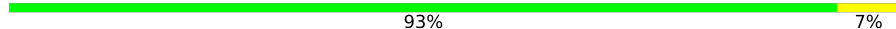


- Molecule 15: Small ribosomal subunit protein eS4x

Chain Ja:  86% 11%



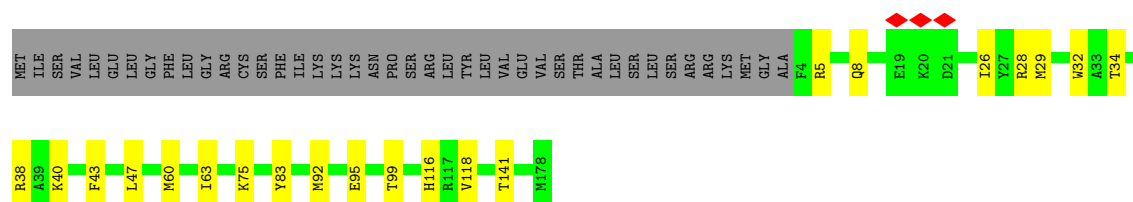
- Molecule 16: Large ribosomal subunit protein eL15z

Chain Ea:  93% 7%



- Molecule 17: Ribosomal protein L18ae/LX family protein

Chain AL:  71% 10% 19%



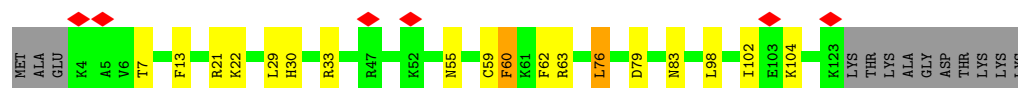
- Molecule 18: Small ribosomal subunit protein uS12y

Chain Va: 94%



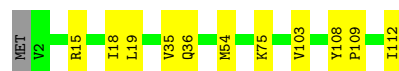
- Molecule 19: Small ribosomal subunit protein eS24y

Chain Ka: 5% 77% 12% 10%



- Molecule 20: Large ribosomal subunit protein eL33y

Chain AW: 89% 10%



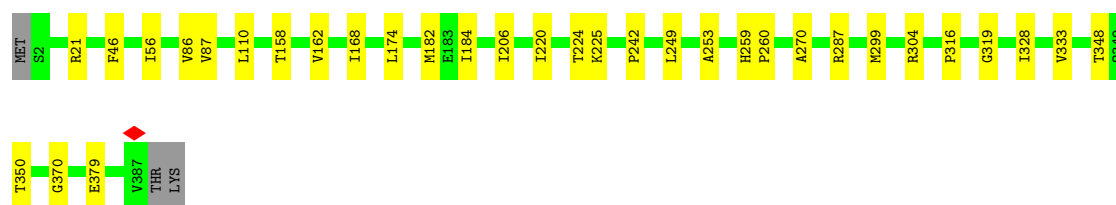
- Molecule 21: Large ribosomal subunit protein eL42z/eL42y

Chain BD: 89% 8%



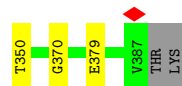
- Molecule 22: Large ribosomal subunit protein uL3z

Chain BS: 91% 8%



- Molecule 23: Large ribosomal subunit protein eL21z/eL21y

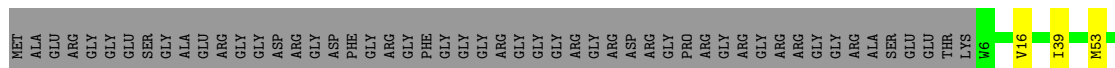
Chain AM: 93% 7%





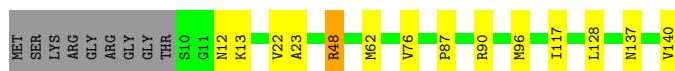
- Molecule 24: Small ribosomal subunit protein uS5y/uS5u/uS5v

Chain AC: 68% 7% 24%



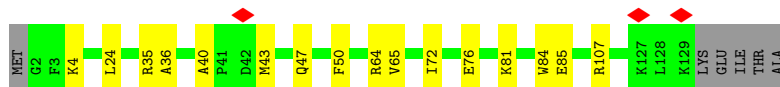
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI: 84% 9% 6%



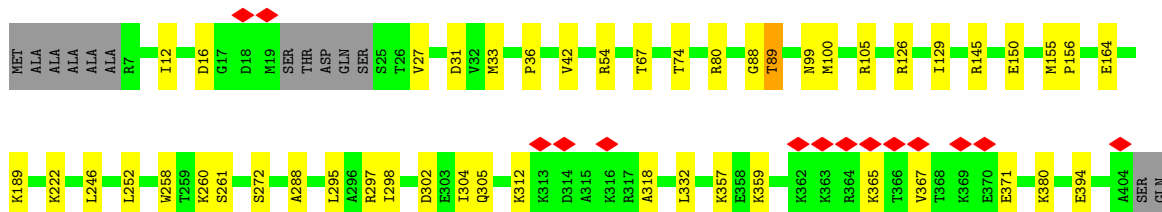
- Molecule 26: Large ribosomal subunit protein eL14y

Chain AH: 84% 12% 4%



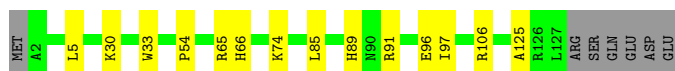
- Molecule 27: Large ribosomal subunit protein uL4z

Chain BT: 85% 12% 3%



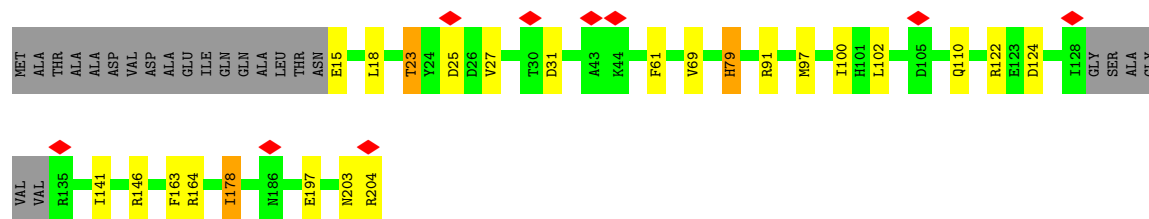
- Molecule 28: Large ribosomal subunit protein eL32z

Chain AV: 84% 11% 5%



- Molecule 29: Small ribosomal subunit protein uS7y

Chain AD: 77% 10% 11%



- Molecule 30: Large ribosomal subunit protein eL18x

Chain AJ: 94% 6%



- Molecule 31: Large ribosomal subunit protein uL2z

Chain BQ: 89% 6% 5%



- Molecule 32: Large ribosomal subunit protein uL13y

Chain BH: 93% 6%



- Molecule 33: Small ribosomal subunit protein uS15y

Chain Da: 91% 8%



- Molecule 34: Large ribosomal subunit protein uL18z

Chain BK: 88% 5% 7%

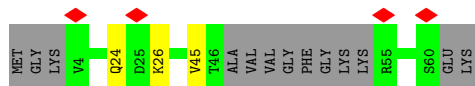
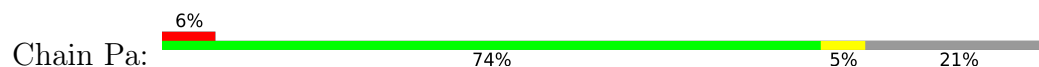


- Molecule 35: Large ribosomal subunit protein eL30y

Chain AT: 78% 6% 16%



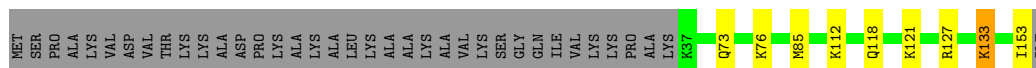
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x



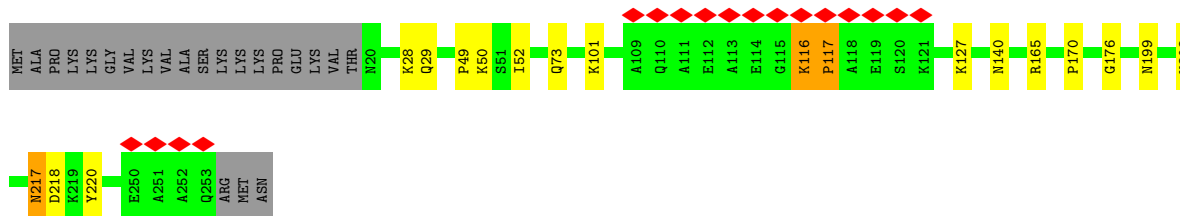
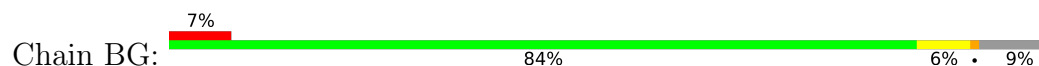
- Molecule 37: Large ribosomal subunit protein uL29x



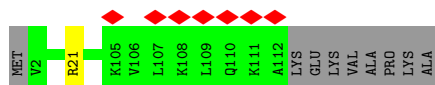
- Molecule 38: Large ribosomal subunit protein uL23y



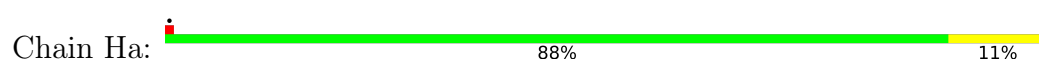
- Molecule 39: Large ribosomal subunit protein eL8y



- Molecule 40: Large ribosomal subunit protein eL34z

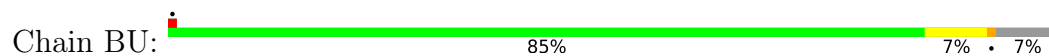


- Molecule 41: Large ribosomal subunit protein uL15x





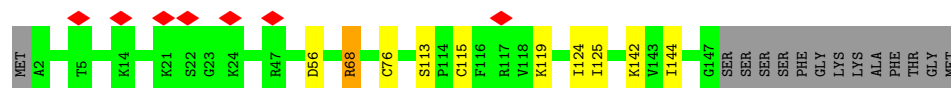
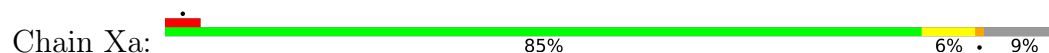
- Molecule 42: Large ribosomal subunit protein uL5z



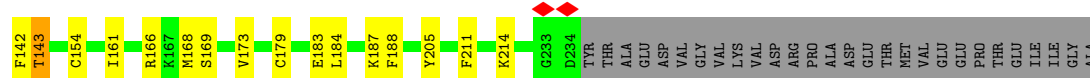
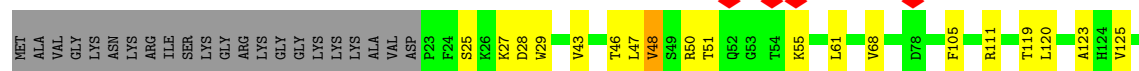
- Molecule 43: Ribosomal protein L30/L7 family protein



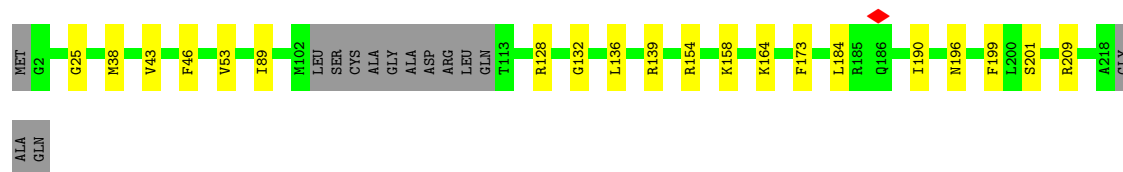
- Molecule 44: Small ribosomal subunit protein uS17z



- Molecule 45: Small ribosomal subunit protein eS1y

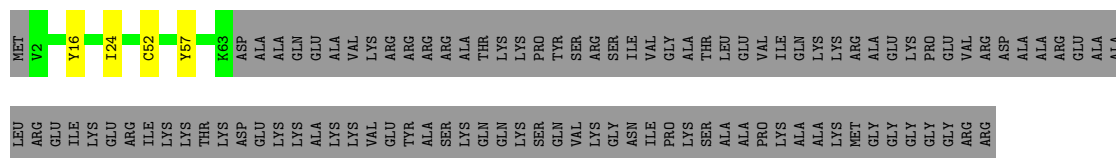


- Molecule 46: Large ribosomal subunit protein uL16y



- Molecule 47: Large ribosomal subunit protein eL24z

Chain AO:  35% 62%



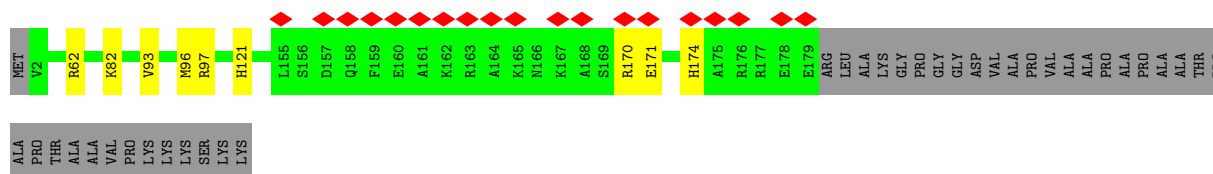
- Molecule 48: Small ribosomal subunit protein eS21y

Chain BW:  79% 9% 11%



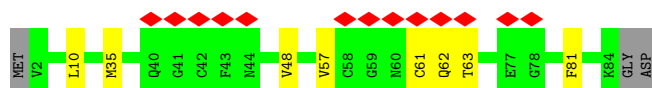
- Molecule 49: Large ribosomal subunit protein eL19x

Chain AK:  79% 17% 9%



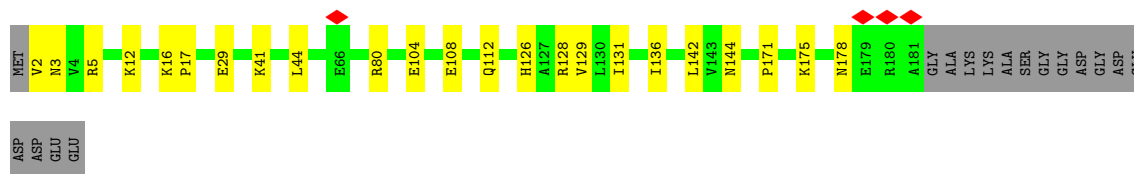
- Molecule 50: Small ribosomal subunit protein eS27y

Chain Na:  87% 9% 15%



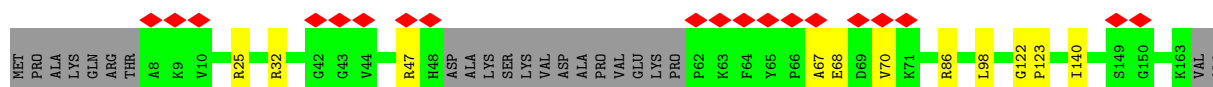
- Molecule 51: Small ribosomal subunit protein uS4y

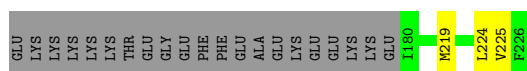
Chain AB:  80% 12% 9%



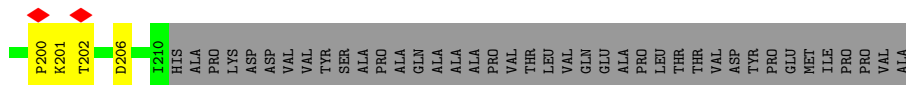
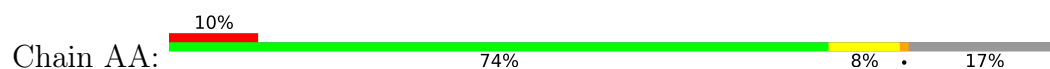
- Molecule 52: Large ribosomal subunit protein eL6y

Chain BF:  76% 6% 18% 8%

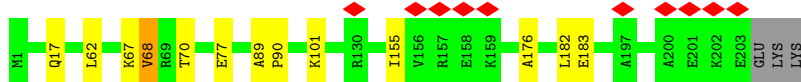




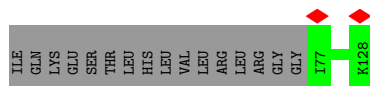
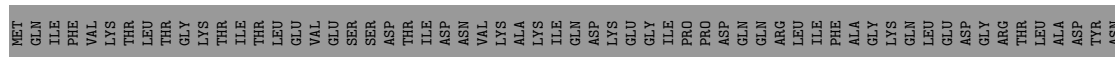
- Molecule 53: Small ribosomal subunit protein uS3z



- Molecule 54: Large ribosomal subunit protein eL13z



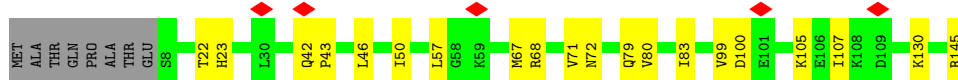
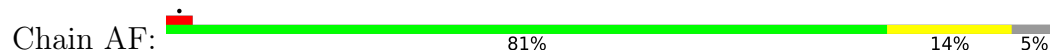
- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein



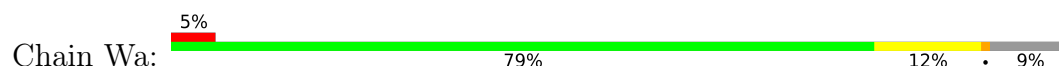
- Molecule 56: Large ribosomal subunit protein eL39z/eL39x

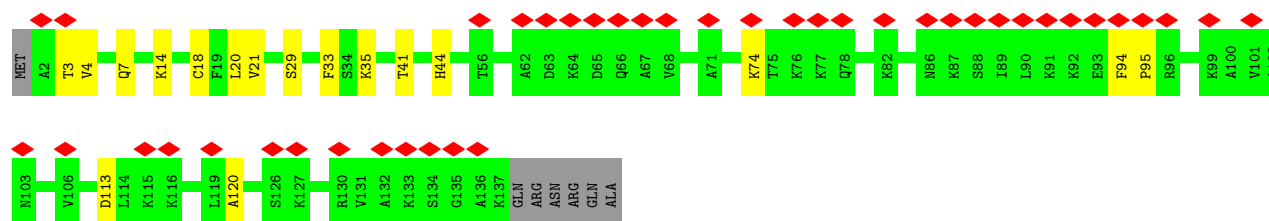


- Molecule 57: Small ribosomal subunit protein uS9z

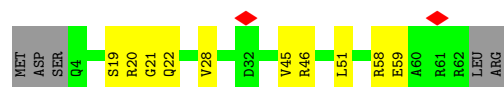
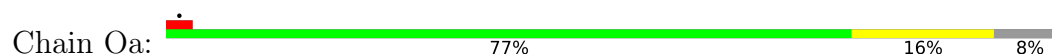


- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x

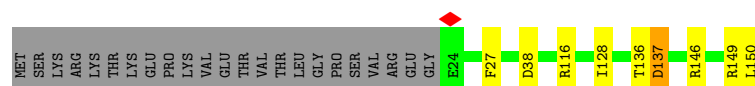
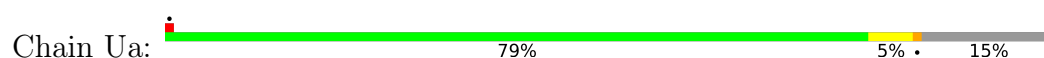




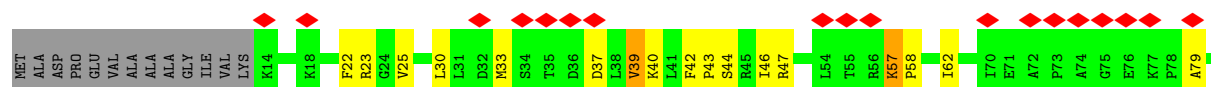
- Molecule 64: Small ribosomal subunit protein eS28x



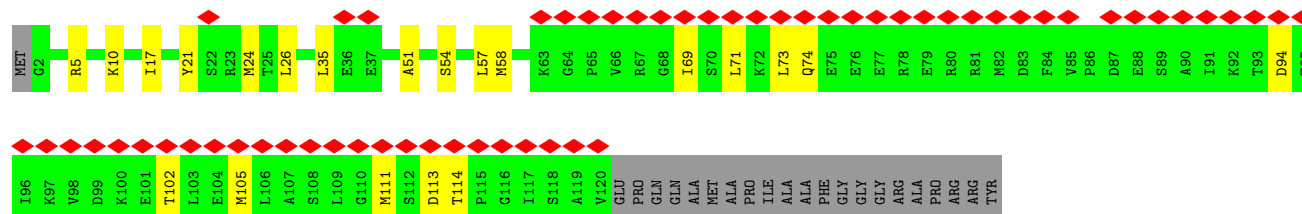
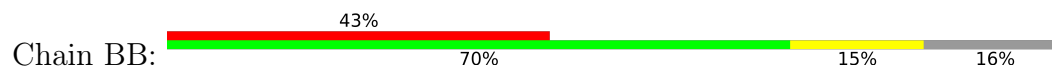
- Molecule 65: Small ribosomal subunit protein uS11y



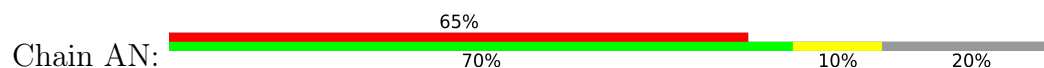
- Molecule 66: Small ribosomal subunit protein uS19y



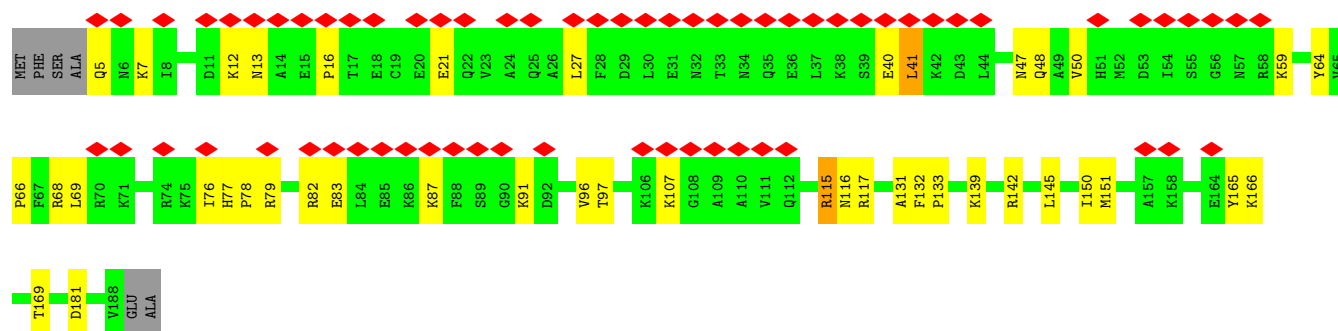
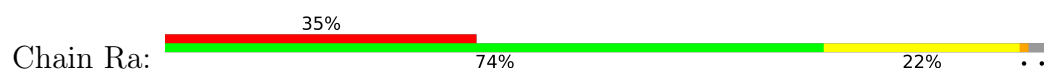
- Molecule 67: Small ribosomal subunit protein eS17w



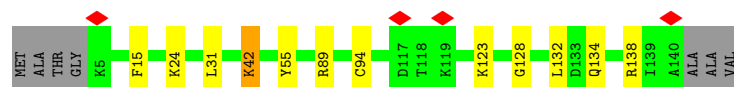
- Molecule 68: Large ribosomal subunit protein eL22z



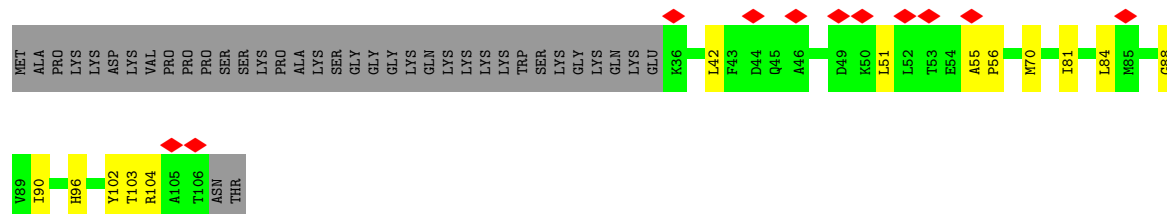
- Molecule 69: Small ribosomal subunit protein eS7x



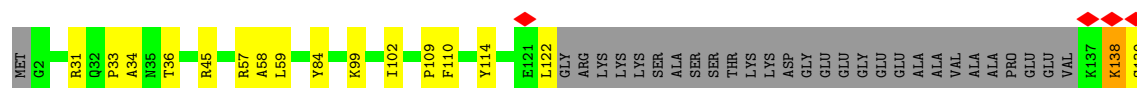
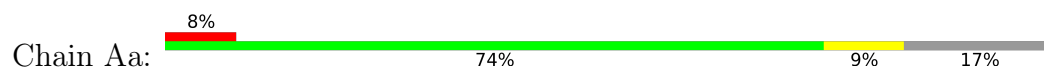
- Molecule 70: Small ribosomal subunit protein eS19x

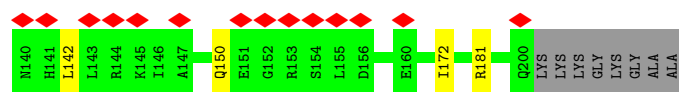


- Molecule 71: Small ribosomal subunit protein eS25w

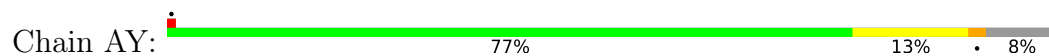


- Molecule 72: Small ribosomal subunit protein eS8z

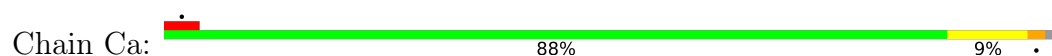




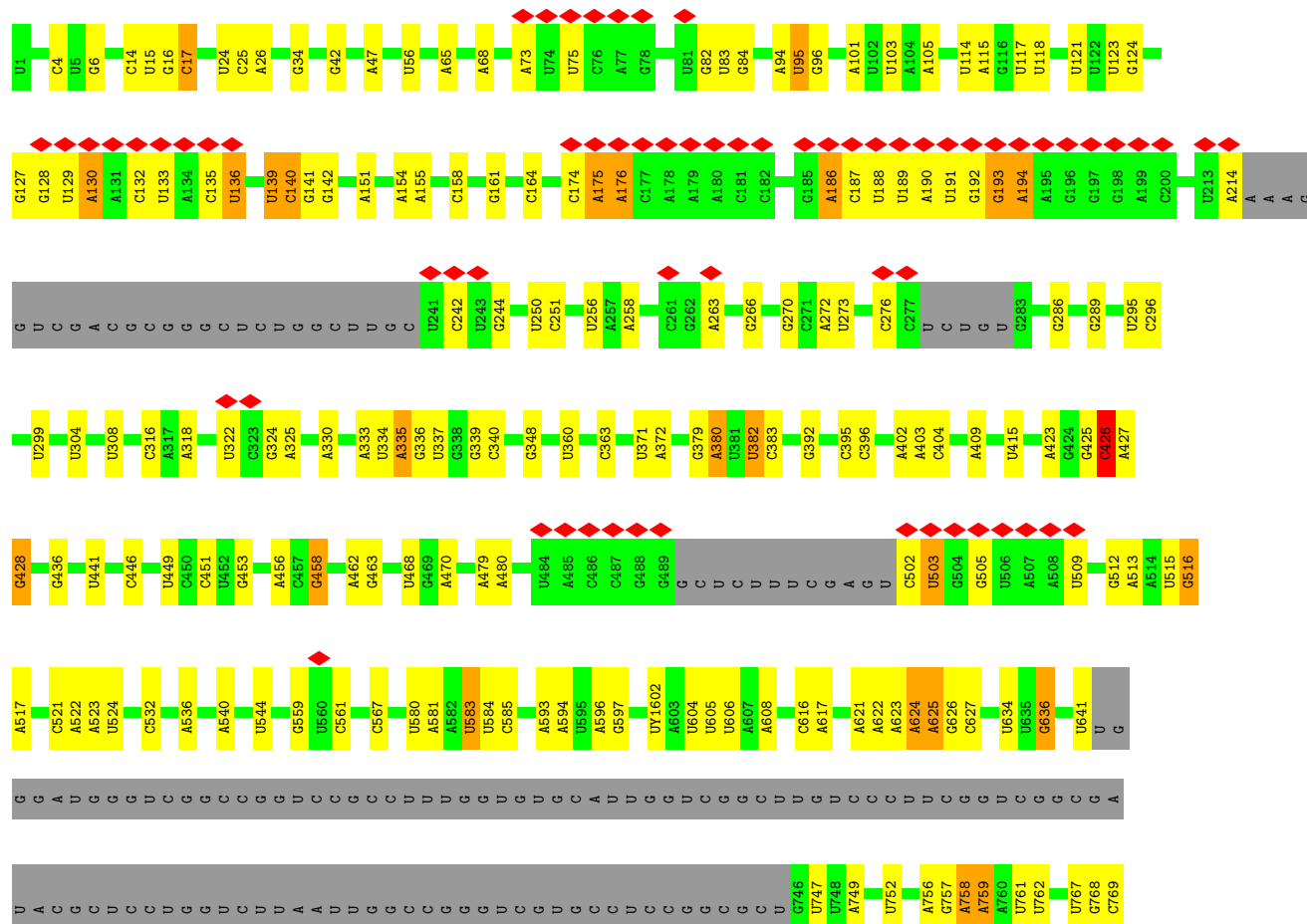
- Molecule 73: Large ribosomal subunit protein eL37z

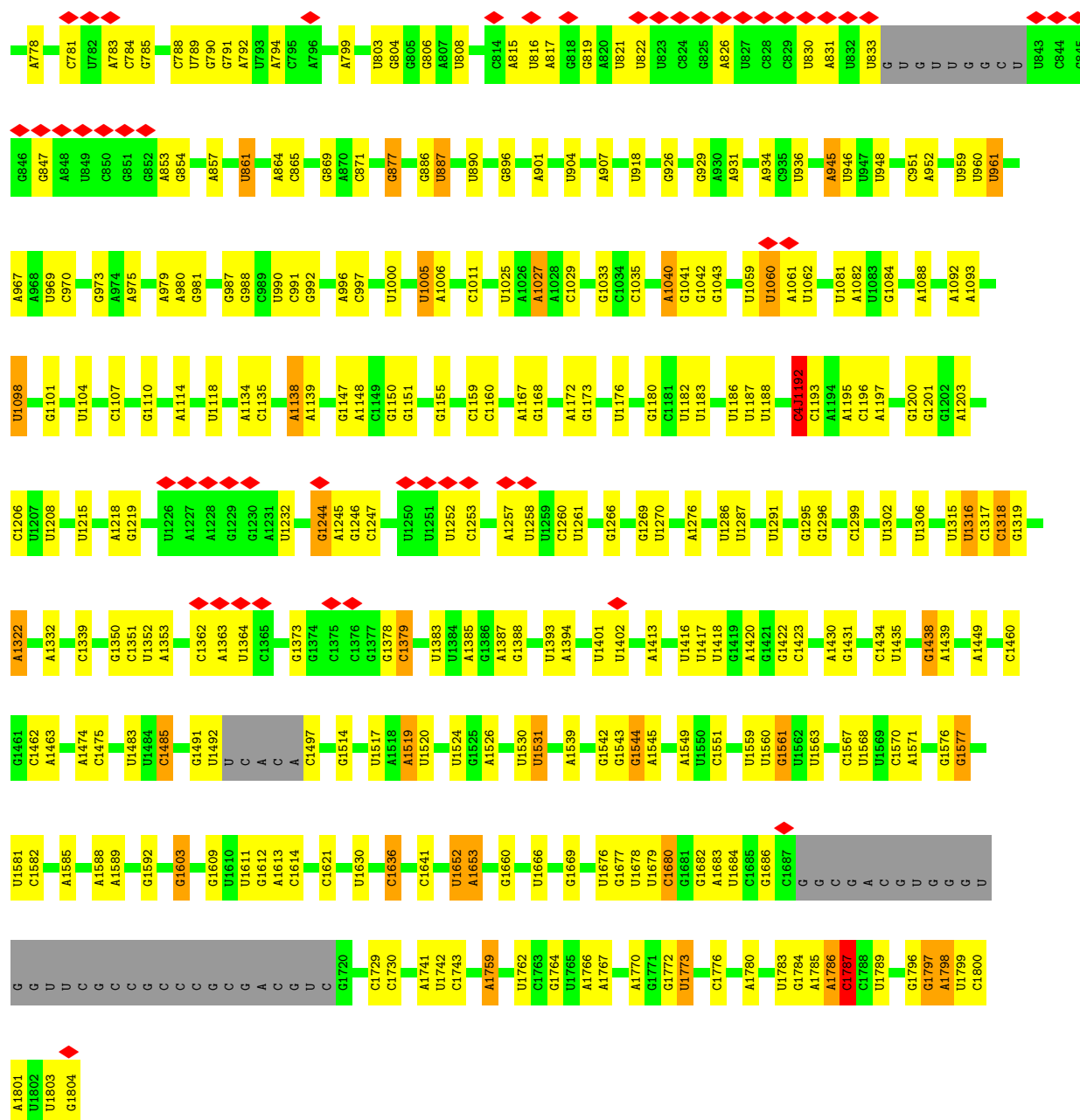


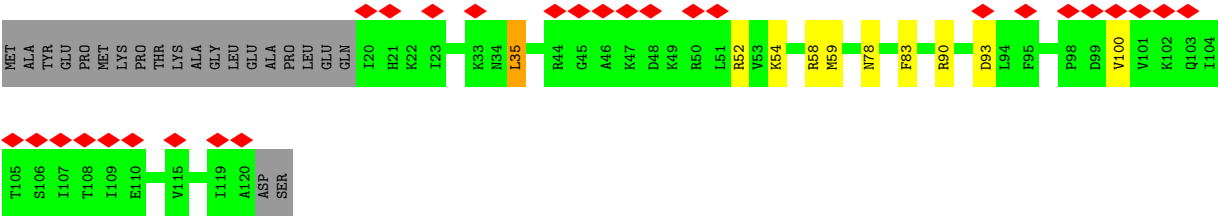
- Molecule 74: Small ribosomal subunit protein uS14z/uS14y/uS14x



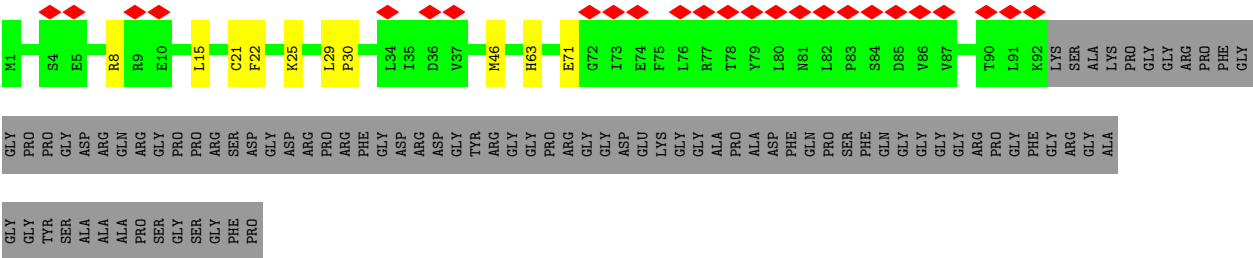
- Molecule 75: Ribosomal RNA 18S



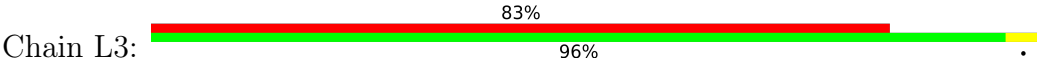




• Molecule 78: Small ribosomal subunit protein eS10z



• Molecule 79: Nascent polypeptide (poly-A)



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: G7M, K, OMU, MG, 5MC, ZN, MA6, OMC, EPE, MLY, A2M, SPD, TER, HIC, C4J, 1MA, 6MZ, UR3, PSU, 1MG, 4AC, UY1, OMG

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	$\# Z > 2$
75	PSU	h1	1000	75	18,21,22	0.89	1 (5%)	22,30,33	0.78	0
2	OMC	A	1848	2,80	19,22,23	0.30	0	26,31,34	0.49	0
2	OMU	A	3299	2	19,22,23	0.32	0	26,31,34	0.55	0
2	A2M	A	945	2	22,25,26	0.35	0	31,36,39	0.87	1 (3%)
75	PSU	h1	752	75	18,21,22	0.89	1 (5%)	22,30,33	0.68	0
75	PSU	h1	1025	75	18,21,22	0.94	1 (5%)	22,30,33	0.88	1 (4%)
75	PSU	h1	1531	75	18,21,22	0.93	1 (5%)	22,30,33	0.60	0
2	A2M	A	2324	2	22,25,26	0.22	0	31,36,39	0.71	2 (6%)
2	OMU	A	2920	2,81	19,22,23	0.29	0	26,31,34	0.47	0
75	OMG	h1	1431	80,75	23,26,27	0.36	0	33,38,41	0.41	0
75	OMU	h1	1263	75	19,22,23	0.22	0	26,31,34	0.39	0
75	PSU	h1	256	75	18,21,22	0.89	1 (5%)	22,30,33	0.68	0
2	1MG	A	1646	2	22,26,27	0.59	0	33,39,42	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	828	2	18,21,22	0.91	1 (5%)	22,30,33	0.90	0
2	A2M	A	2639	2	22,25,26	0.16	0	31,36,39	0.36	0
75	OMC	h1	416	75	19,22,23	0.26	0	26,31,34	0.53	0
2	A2M	A	2910	2	22,25,26	0.31	0	31,36,39	0.42	0
2	PSU	A	2430	2	18,21,22	0.80	1 (5%)	22,30,33	0.72	0
2	A2M	A	1376	2,80	22,25,26	0.20	0	31,36,39	0.61	0
2	OMC	A	2195	2,81	19,22,23	0.34	0	26,31,34	0.76	0
2	PSU	A	228	2	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
2	OMG	A	2393	2,80	23,26,27	0.39	0	33,38,41	0.66	1 (3%)
75	PSU	h1	121	80,75	18,21,22	0.80	1 (5%)	22,30,33	0.63	0
75	MA6	h1	1785	75	23,26,27	0.32	0	34,38,41	0.73	1 (2%)
75	UY1	h1	602	75	19,22,23	0.96	1 (5%)	22,31,34	0.75	0
75	PSU	h1	959	81,75	18,21,22	0.85	1 (5%)	22,30,33	0.71	0
75	PSU	h1	1118	75	18,21,22	0.89	1 (5%)	22,30,33	0.80	0
75	PSU	h1	1611	75	18,21,22	0.94	1 (5%)	22,30,33	0.82	0
2	OMG	A	1459	2,80	23,26,27	0.53	0	33,38,41	0.64	0
2	OMU	A	2345	2	19,22,23	0.33	0	26,31,34	0.51	0
55	MLY	Ga	113	55	9,10,11	0.49	0	6,11,13	0.38	0
75	PSU	h1	1104	75	18,21,22	0.83	1 (5%)	22,30,33	0.71	0
2	UR3	A	2952	2,81	19,22,23	0.34	0	26,32,35	0.66	0
2	PSU	A	965	2	18,21,22	1.07	2 (11%)	22,30,33	0.80	0
75	4AC	h1	1777	75	21,24,25	0.43	0	29,34,37	0.40	0
2	OMG	A	917	2,81	23,26,27	0.32	0	33,38,41	0.46	0
75	PSU	h1	1302	75	18,21,22	0.88	1 (5%)	22,30,33	0.72	0
2	PSU	A	2264	2	18,21,22	0.86	1 (5%)	22,30,33	0.68	0
2	PSU	A	2316	2,80	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
2	OMC	A	2335	2	19,22,23	0.32	0	26,31,34	0.59	0
2	OMG	A	2618	3,2	23,26,27	0.30	0	33,38,41	0.36	0
75	A2M	h1	1754	75	22,25,26	0.21	0	31,36,39	0.61	0
2	OMU	A	2111	2	19,22,23	0.22	0	26,31,34	0.49	0
75	A2M	h1	621	80,75	22,25,26	0.28	0	31,36,39	0.71	0
2	PSU	A	1133	2	18,21,22	0.82	1 (5%)	22,30,33	0.94	1 (4%)
2	OMU	A	44	2,81	19,22,23	0.33	0	26,31,34	0.56	0
2	OMU	A	2716	2	19,22,23	0.25	0	26,31,34	0.52	0
2	OMG	A	2389	2	23,26,27	0.34	0	33,38,41	0.35	0
75	PSU	h1	808	75	18,21,22	0.91	1 (5%)	22,30,33	0.64	0
2	PSU	A	2312	2,81	18,21,22	0.88	1 (5%)	22,30,33	0.79	0
2	PSU	A	2414	2,80	18,21,22	1.04	1 (5%)	22,30,33	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	OMG	h1	597	75	23,26,27	0.31	0	33,38,41	0.54	0
75	PSU	h1	634	75	18,21,22	0.98	1 (5%)	22,30,33	0.91	0
2	A2M	A	2254	2	22,25,26	0.21	0	31,36,39	0.54	0
1	PSU	3	22	1,2	18,21,22	0.84	1 (5%)	22,30,33	0.67	0
2	PSU	A	2825	2,81	18,21,22	0.90	1 (5%)	22,30,33	0.66	0
2	OMU	A	676	2	19,22,23	0.35	0	26,31,34	0.72	0
2	OMG	A	2650	2	23,26,27	0.34	0	33,38,41	0.52	0
2	A2M	A	2945	2,80	22,25,26	0.25	0	31,36,39	0.63	0
75	PSU	h1	360	75	18,21,22	0.88	1 (5%)	22,30,33	0.75	0
75	OMC	h1	1641	80,75	19,22,23	0.30	0	26,31,34	0.54	0
75	OMU	h1	1381	80,75	19,22,23	0.22	0	26,31,34	0.52	0
2	PSU	A	2189	2,81	18,21,22	0.92	1 (5%)	22,30,33	0.74	0
75	PSU	h1	1520	75	18,21,22	0.90	1 (5%)	22,30,33	0.58	0
75	PSU	h1	1563	75	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
2	PSU	A	2893	2	18,21,22	0.91	1 (5%)	22,30,33	0.79	0
2	1MA	A	657	2,80	21,25,26	0.51	0	31,37,40	0.73	0
2	OMG	A	2122	2	23,26,27	0.30	0	33,38,41	0.70	1 (3%)
75	A2M	h1	28	80,75	22,25,26	0.19	0	31,36,39	0.57	0
2	PSU	A	2134	2	18,21,22	0.84	1 (5%)	22,30,33	0.76	0
75	A2M	h1	466	75	22,25,26	0.19	0	31,36,39	0.52	0
2	OMG	A	2921	2	23,26,27	0.30	0	33,38,41	0.40	0
2	PSU	A	2258	2	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
75	PSU	h1	606	75	18,21,22	0.97	1 (5%)	22,30,33	0.70	0
75	G7M	h1	1577	3,75	23,26,27	0.75	1 (4%)	35,39,42	0.55	0
2	OMU	A	2734	2,80	19,22,23	0.29	0	26,31,34	0.57	0
75	PSU	h1	337	81,75	18,21,22	0.88	1 (5%)	22,30,33	0.68	0
2	PSU	A	1001	2	18,21,22	0.96	1 (5%)	22,30,33	0.85	0
2	OMC	A	1517	2,80	19,22,23	0.32	0	26,31,34	0.67	0
2	PSU	A	2943	81,2,80	18,21,22	0.90	1 (5%)	22,30,33	0.93	0
2	PSU	A	1132	2	18,21,22	0.90	1 (5%)	22,30,33	0.98	0
75	A2M	h1	1327	75	22,25,26	0.19	0	31,36,39	0.39	0
2	PSU	A	969	2	18,21,22	0.85	1 (5%)	22,30,33	1.02	1 (4%)
75	PSU	h1	415	75	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
75	PSU	h1	1630	75	18,21,22	0.91	1 (5%)	22,30,33	0.70	0
2	A2M	A	885	2	22,25,26	0.26	0	31,36,39	0.38	0
75	A2M	h1	543	75	22,25,26	0.21	0	31,36,39	0.61	0
2	PSU	A	2864	2	18,21,22	0.92	1 (5%)	22,30,33	0.76	0
2	OMC	A	2878	2	19,22,23	0.34	0	26,31,34	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	901	2,81	18,21,22	0.92	1 (5%)	22,30,33	0.79	0
2	OMG	A	2814	2	23,26,27	0.31	0	33,38,41	0.28	0
2	PSU	A	685	2	18,21,22	1.01	1 (5%)	22,30,33	0.85	1 (4%)
2	PSU	A	277	2	18,21,22	0.98	1 (5%)	22,30,33	0.76	0
2	PSU	A	2974	2	18,21,22	0.98	1 (5%)	22,30,33	0.94	1 (4%)
75	A2M	h1	1575	75	22,25,26	0.22	0	31,36,39	0.62	0
2	OMU	A	48	2	19,22,23	0.36	0	26,31,34	0.59	0
75	OMG	h1	390	81,75	23,26,27	0.32	0	33,38,41	0.53	0
75	OMG	h1	244	75	23,26,27	0.33	0	33,38,41	0.39	0
2	OMU	A	2419	2	19,22,23	0.28	0	26,31,34	0.68	0
75	PSU	h1	1483	75	18,21,22	0.86	1 (5%)	22,30,33	0.57	0
2	OMG	A	2790	2	23,26,27	0.31	0	33,38,41	0.37	0
2	A2M	A	2124	2	22,25,26	0.18	0	31,36,39	0.50	0
75	A2M	h1	438	75	22,25,26	0.17	0	31,36,39	0.32	0
2	PSU	A	785	2	18,21,22	0.87	1 (5%)	22,30,33	0.83	0
75	PSU	h1	304	75	18,21,22	0.89	1 (5%)	22,30,33	0.75	0
2	PSU	A	1054	2	18,21,22	0.86	1 (5%)	22,30,33	0.77	0
75	PSU	h1	1783	75	18,21,22	1.03	1 (5%)	22,30,33	0.82	0
2	PSU	A	2853	2	18,21,22	0.85	1 (5%)	22,30,33	0.73	0
75	PSU	h1	1306	75	18,21,22	0.89	1 (5%)	22,30,33	0.58	0
22	HIC	BS	246	22	10,11,12	0.46	0	8,14,16	0.85	0
2	A2M	A	2212	2,80	22,25,26	0.21	0	31,36,39	0.67	0
75	OMU	h1	1232	75	19,22,23	0.23	0	26,31,34	0.36	0
75	PSU	h1	449	81,75	18,21,22	0.92	1 (5%)	22,30,33	0.72	0
75	PSU	h1	948	75	18,21,22	0.93	1 (5%)	22,30,33	0.67	0
2	A2M	A	2359	2	22,25,26	0.25	0	31,36,39	0.44	0
2	A2M	A	1458	2,80	22,25,26	0.27	0	31,36,39	0.63	0
1	PSU	3	97	1,81	18,21,22	0.93	1 (5%)	22,30,33	0.72	0
2	OMG	A	2407	2,81	23,26,27	0.38	0	33,38,41	0.41	0
75	A2M	h1	162	75	22,25,26	0.18	0	31,36,39	0.61	0
75	OMU	h1	1010	75	19,22,23	0.23	0	26,31,34	0.49	0
2	OMU	A	2408	2,81	19,22,23	0.32	0	26,31,34	0.34	0
75	PSU	h1	103	81,75	18,21,22	0.87	1 (5%)	22,30,33	0.75	0
2	OMC	A	2363	2	19,22,23	0.31	0	26,31,34	0.56	0
2	PSU	A	1480	2	18,21,22	0.97	1 (5%)	22,30,33	0.71	0
75	PSU	h1	583	75	18,21,22	0.94	1 (5%)	22,30,33	0.69	0
75	6MZ	h1	1767	81,80,75	22,25,26	0.35	0	30,36,39	0.72	0
75	OMC	h1	38	75	19,22,23	0.28	0	26,31,34	0.61	0
75	A2M	h1	975	75	22,25,26	0.18	0	31,36,39	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	A	144	2,81	19,22,23	0.36	0	26,31,34	0.38	0
2	PSU	A	1062	2,81	18,21,22	0.87	1 (5%)	22,30,33	0.77	0
2	OMG	A	2286	2	23,26,27	0.33	0	33,38,41	0.32	0
75	A2M	h1	422	75	22,25,26	0.18	0	31,36,39	0.60	0
2	PSU	A	2879	2	18,21,22	0.86	1 (5%)	22,30,33	0.73	0
2	PSU	A	2922	2	18,21,22	0.88	1 (5%)	22,30,33	0.75	0
75	PSU	h1	1182	75	18,21,22	0.94	1 (5%)	22,30,33	0.80	0
2	UY1	A	2649	2	19,22,23	0.99	1 (5%)	22,31,34	0.94	2 (9%)
75	A2M	h1	794	75	22,25,26	0.18	0	31,36,39	0.41	0
2	OMG	A	2234	2	23,26,27	0.33	0	33,38,41	0.47	0
75	PSU	h1	1215	75	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
75	OMC	h1	1216	75	19,22,23	0.27	0	26,31,34	0.38	0
2	PSU	A	1472	2	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
75	PSU	h1	95	75	18,21,22	0.98	1 (5%)	22,30,33	0.76	0
75	PSU	h1	468	75	18,21,22	0.95	1 (5%)	22,30,33	0.71	0
75	OMU	h1	1270	80,75	19,22,23	0.26	0	26,31,34	0.58	0
2	OMC	A	2835	2	19,22,23	0.29	0	26,31,34	0.57	0
2	PSU	A	894	2	18,21,22	0.94	1 (5%)	22,30,33	0.88	0
2	PSU	A	2954	2	18,21,22	0.97	1 (5%)	22,30,33	0.77	1 (4%)
75	PSU	h1	1291	75	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
2	A2M	A	2218	2	22,25,26	0.18	0	31,36,39	0.59	1 (3%)
1	OMG	3	155	1,2	23,26,27	0.35	0	33,38,41	0.36	0
2	OMC	A	675	2	19,22,23	0.34	0	26,31,34	0.67	0
2	A2M	A	2319	2	22,25,26	0.26	0	31,36,39	0.64	0
2	OMG	A	2916	2	23,26,27	0.37	0	33,38,41	0.48	0
2	PSU	A	34	2	18,21,22	1.00	1 (5%)	22,30,33	1.01	2 (9%)
2	OMU	A	803	2	19,22,23	0.28	0	26,31,34	0.50	0
75	OMU	h1	1445	75	19,22,23	0.21	0	26,31,34	0.48	0
2	OMU	A	2882	2	19,22,23	0.23	0	26,31,34	0.63	1 (3%)
75	OMU	h1	580	75	19,22,23	0.21	0	26,31,34	0.48	0
2	OMC	A	2681	2	19,22,23	0.25	0	26,31,34	0.58	0
75	C4J	h1	1192	75	24,29,30	0.87	1 (4%)	29,42,45	1.03	0
2	A2M	A	2279	2	22,25,26	0.40	0	31,36,39	0.75	1 (3%)
75	A2M	h1	799	75	22,25,26	0.20	0	31,36,39	0.74	1 (3%)
2	PSU	A	1681	2	18,21,22	0.98	1 (5%)	22,30,33	0.74	0
2	A2M	A	2933	2	22,25,26	0.20	0	31,36,39	0.48	0
2	PSU	A	2252	2	18,21,22	0.87	1 (5%)	22,30,33	0.79	1 (4%)
75	OMG	h1	1272	81,75	23,26,27	0.30	0	33,38,41	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	150	2,81	18,21,22	0.92	1 (5%)	22,30,33	0.58	0
75	PSU	h1	1188	75	18,21,22	0.84	1 (5%)	22,30,33	0.70	0
1	OMG	3	79	1	23,26,27	0.32	0	33,38,41	0.45	0
2	A2M	A	661	2	22,25,26	0.27	0	31,36,39	0.38	0
2	PSU	A	975	2,81	18,21,22	0.88	1 (5%)	22,30,33	0.81	0
1	PSU	3	78	1	18,21,22	0.97	1 (5%)	22,30,33	0.66	0
2	PSU	A	311	2,81	18,21,22	1.11	2 (11%)	22,30,33	1.00	1 (4%)
2	OMC	A	1858	2	19,22,23	0.41	0	26,31,34	0.59	0
75	OMU	h1	123	75	19,22,23	0.23	0	26,31,34	0.81	0
75	PSU	h1	604	75	18,21,22	0.88	1 (5%)	22,30,33	0.84	0
2	OMC	A	2947	2	19,22,23	0.32	0	26,31,34	0.50	0
75	PSU	h1	762	75	18,21,22	0.88	1 (5%)	22,30,33	0.63	0
75	PSU	h1	1208	75	18,21,22	0.93	1 (5%)	22,30,33	0.67	0
1	A2M	3	47	1	22,25,26	0.24	0	31,36,39	0.68	1 (3%)
2	5MC	A	2869	2,81	18,22,23	0.40	0	26,32,35	0.86	1 (3%)
2	OMG	A	2792	2	23,26,27	0.32	0	33,38,41	0.51	0
2	PSU	A	1015	2,81	18,21,22	0.88	1 (5%)	22,30,33	0.66	0
75	PSU	h1	308	75	18,21,22	1.00	2 (11%)	22,30,33	0.91	1 (4%)
75	OMU	h1	1261	75	19,22,23	0.22	0	26,31,34	0.50	0
2	OMG	A	3290	2,80	23,26,27	0.34	0	33,38,41	0.73	2 (6%)
75	MA6	h1	1786	75	23,26,27	0.28	0	34,38,41	0.85	1 (2%)
2	PSU	A	1131	2	18,21,22	0.93	1 (5%)	22,30,33	0.79	0
2	OMC	A	1478	2	19,22,23	0.31	0	26,31,34	0.41	0
2	PSU	A	42	2,81	18,21,22	1.04	2 (11%)	22,30,33	0.99	2 (9%)
2	PSU	A	2262	2	18,21,22	0.88	1 (5%)	22,30,33	0.75	0
2	OMC	A	1845	2	19,22,23	0.33	0	26,31,34	0.42	0
2	OMU	A	1890	2	19,22,23	0.29	0	26,31,34	0.91	2 (7%)
2	OMC	A	2291	2	19,22,23	0.29	0	26,31,34	0.56	0
2	OMC	A	2958	2,80	19,22,23	0.34	0	26,31,34	0.77	2 (7%)
2	A2M	A	816	2	22,25,26	0.31	0	31,36,39	0.71	0
2	OMG	A	814	2	23,26,27	0.31	0	33,38,41	0.60	1 (3%)
75	OMU	h1	613	75	19,22,23	0.26	0	26,31,34	0.44	0
2	OMC	A	1446	2	19,22,23	0.36	0	26,31,34	0.69	1 (3%)
75	PSU	h1	1176	75	18,21,22	0.85	1 (5%)	22,30,33	0.85	0
2	PSU	A	509	2	18,21,22	0.98	1 (5%)	22,30,33	0.84	1 (4%)
2	OMU	A	1066	2	19,22,23	0.30	0	26,31,34	0.71	0
75	OMC	h1	471	75	19,22,23	0.27	0	26,31,34	0.53	0
75	A2M	h1	778	75	22,25,26	0.17	0	31,36,39	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	A	1142	2	22,25,26	0.26	0	31,36,39	0.67	1 (3%)
2	A2M	A	826	81,2,80	22,25,26	0.29	0	31,36,39	0.75	1 (3%)
2	PSU	A	2132	2,81	18,21,22	0.95	1 (5%)	22,30,33	0.86	0
2	PSU	A	2256	2	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
2	5MC	A	2276	2,80	18,22,23	0.34	0	26,32,35	0.70	1 (3%)
2	PSU	A	2743	2	18,21,22	0.91	2 (11%)	22,30,33	0.70	0
75	PSU	h1	605	75	18,21,22	0.92	1 (5%)	22,30,33	0.75	0
75	4AC	h1	1281	75	21,24,25	0.41	0	29,34,37	0.61	0
2	PSU	A	2209	2	18,21,22	0.88	1 (5%)	22,30,33	0.68	0
2	PSU	A	3109	2	18,21,22	0.90	1 (5%)	22,30,33	0.92	0
2	OMG	A	1853	2	23,26,27	0.38	0	33,38,41	0.64	1 (3%)
75	PSU	h1	761	75	18,21,22	0.89	1 (5%)	22,30,33	0.78	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
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1848	2,80	-	0/9/27/28	0/2/2/2
2	OMU	A	3299	2	-	0/9/27/28	0/2/2/2
2	A2M	A	945	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	752	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2324	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2920	2,81	-	0/9/27/28	0/2/2/2
75	OMG	h1	1431	80,75	-	1/9/27/28	0/3/3/3
75	OMU	h1	1263	75	-	1/9/27/28	0/2/2/2
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
2	1MG	A	1646	2	-	0/7/25/26	0/3/3/3
2	PSU	A	828	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2639	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	416	75	-	0/9/27/28	0/2/2/2
2	A2M	A	2910	2	-	5/9/27/28	0/3/3/3
2	PSU	A	2430	2	-	0/7/25/26	0/2/2/2
2	A2M	A	1376	2,80	-	0/9/27/28	0/3/3/3
2	OMC	A	2195	2,81	-	4/9/27/28	0/2/2/2
2	PSU	A	228	2	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A	2393	2,80	-	0/9/27/28	0/3/3/3
75	PSU	h1	121	80,75	-	0/7/25/26	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
75	UY1	h1	602	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	959	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1611	75	-	0/7/25/26	0/2/2/2
2	OMG	A	1459	2,80	-	0/9/27/28	0/3/3/3
2	OMU	A	2345	2	-	0/9/27/28	0/2/2/2
55	MLY	Ga	113	55	-	0/8/9/11	-
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
2	UR3	A	2952	2,81	-	0/7/25/26	0/2/2/2
2	PSU	A	965	2	-	0/7/25/26	0/2/2/2
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
2	OMG	A	917	2,81	-	0/9/27/28	0/3/3/3
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2316	2,80	-	0/7/25/26	0/2/2/2
2	OMC	A	2335	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2618	3,2	-	1/9/27/28	0/3/3/3
75	A2M	h1	1754	75	-	0/9/27/28	0/3/3/3
2	OMU	A	2111	2	-	2/9/27/28	0/2/2/2
75	A2M	h1	621	80,75	-	2/9/27/28	0/3/3/3
2	PSU	A	1133	2	-	0/7/25/26	0/2/2/2
2	OMU	A	44	2,81	-	0/9/27/28	0/2/2/2
2	OMU	A	2716	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2389	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	808	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2312	2,81	-	1/7/25/26	0/2/2/2
2	PSU	A	2414	2,80	-	0/7/25/26	0/2/2/2
75	OMG	h1	597	75	-	3/9/27/28	0/3/3/3
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2254	2	-	0/9/27/28	0/3/3/3
1	PSU	3	22	1,2	-	0/7/25/26	0/2/2/2
2	PSU	A	2825	2,81	-	0/7/25/26	0/2/2/2
2	OMU	A	676	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2650	2	-	0/9/27/28	0/3/3/3
2	A2M	A	2945	2,80	-	0/9/27/28	0/3/3/3
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
75	OMC	h1	1641	80,75	-	0/9/27/28	0/2/2/2
75	OMU	h1	1381	80,75	-	0/9/27/28	0/2/2/2
2	PSU	A	2189	2,81	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PSU	h1	1520	75	-	1/7/25/26	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2893	2	-	0/7/25/26	0/2/2/2
2	1MA	A	657	2,80	-	0/7/25/26	0/3/3/3
2	OMG	A	2122	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	28	80,75	-	0/9/27/28	0/3/3/3
2	PSU	A	2134	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
2	OMG	A	2921	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2258	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	606	75	-	0/7/25/26	0/2/2/2
75	G7M	h1	1577	3,75	-	0/7/25/26	0/3/3/3
2	OMU	A	2734	2,80	-	0/9/27/28	0/2/2/2
75	PSU	h1	337	81,75	-	0/7/25/26	0/2/2/2
2	PSU	A	1001	2	-	0/7/25/26	0/2/2/2
2	OMC	A	1517	2,80	-	2/9/27/28	0/2/2/2
2	PSU	A	2943	81,2,80	-	0/7/25/26	0/2/2/2
2	PSU	A	1132	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1327	75	-	0/9/27/28	0/3/3/3
2	PSU	A	969	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	415	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
2	A2M	A	885	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	543	75	-	1/9/27/28	0/3/3/3
2	PSU	A	2864	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2878	2	-	0/9/27/28	0/2/2/2
2	PSU	A	901	2,81	-	0/7/25/26	0/2/2/2
2	OMG	A	2814	2	-	0/9/27/28	0/3/3/3
2	PSU	A	685	2	-	0/7/25/26	0/2/2/2
2	PSU	A	277	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2974	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
2	OMU	A	48	2	-	0/9/27/28	0/2/2/2
75	OMG	h1	390	81,75	-	0/9/27/28	0/3/3/3
75	OMG	h1	244	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	1483	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2790	2	-	0/9/27/28	0/3/3/3
2	A2M	A	2124	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	438	75	-	0/9/27/28	0/3/3/3
2	PSU	A	785	2	-	1/7/25/26	0/2/2/2
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	1054	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1783	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2853	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1306	75	-	1/7/25/26	0/2/2/2
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
2	A2M	A	2212	2,80	-	0/9/27/28	0/3/3/3
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
75	PSU	h1	449	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2359	2	-	0/9/27/28	0/3/3/3
2	A2M	A	1458	2,80	-	0/9/27/28	0/3/3/3
1	PSU	3	97	1,81	-	0/7/25/26	0/2/2/2
2	OMG	A	2407	2,81	-	0/9/27/28	0/3/3/3
75	A2M	h1	162	75	-	0/9/27/28	0/3/3/3
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
2	OMU	A	2408	2,81	-	0/9/27/28	0/2/2/2
75	PSU	h1	103	81,75	-	0/7/25/26	0/2/2/2
2	OMC	A	2363	2	-	1/9/27/28	0/2/2/2
2	PSU	A	1480	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	583	75	-	5/7/25/26	0/2/2/2
75	6MZ	h1	1767	81,80,75	-	0/9/27/28	0/3/3/3
75	OMC	h1	38	75	-	0/9/27/28	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
2	OMU	A	144	2,81	-	1/9/27/28	0/2/2/2
2	PSU	A	1062	2,81	-	0/7/25/26	0/2/2/2
2	OMG	A	2286	2	-	0/9/27/28	0/3/3/3
75	A2M	h1	422	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	2922	2	-	1/7/25/26	0/2/2/2
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
2	UY1	A	2649	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3
2	OMG	A	2234	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2
75	OMC	h1	1216	75	-	0/9/27/28	0/2/2/2
2	PSU	A	1472	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	95	75	-	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	80,75	-	2/9/27/28	0/2/2/2
2	OMC	A	2835	2	-	0/9/27/28	0/2/2/2
2	PSU	A	894	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2954	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2218	2	-	0/9/27/28	0/3/3/3
1	OMG	3	155	1,2	-	0/9/27/28	0/3/3/3
2	OMC	A	675	2	-	0/9/27/28	0/2/2/2
2	A2M	A	2319	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2916	2	-	0/9/27/28	0/3/3/3
2	PSU	A	34	2	-	0/7/25/26	0/2/2/2
2	OMU	A	803	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	1445	75	-	0/9/27/28	0/2/2/2
2	OMU	A	2882	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	580	75	-	2/9/27/28	0/2/2/2
2	OMC	A	2681	2	-	0/9/27/28	0/2/2/2
75	C4J	h1	1192	75	-	4/16/34/35	0/2/2/2
2	A2M	A	2279	2	-	3/9/27/28	0/3/3/3
75	A2M	h1	799	75	-	0/9/27/28	0/3/3/3
2	PSU	A	1681	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2933	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2252	2	-	0/7/25/26	0/2/2/2
75	OMG	h1	1272	81,75	-	0/9/27/28	0/3/3/3
2	PSU	A	150	2,81	-	0/7/25/26	0/2/2/2
75	PSU	h1	1188	75	-	0/7/25/26	0/2/2/2
1	OMG	3	79	1	-	0/9/27/28	0/3/3/3
2	A2M	A	661	2	-	1/9/27/28	0/3/3/3
2	PSU	A	975	2,81	-	0/7/25/26	0/2/2/2
1	PSU	3	78	1	-	0/7/25/26	0/2/2/2
2	PSU	A	311	2,81	-	0/7/25/26	0/2/2/2
2	OMC	A	1858	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	123	75	-	2/9/27/28	0/2/2/2
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
2	OMC	A	2947	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1208	75	-	1/7/25/26	0/2/2/2
1	A2M	3	47	1	-	0/9/27/28	0/3/3/3
2	5MC	A	2869	2,81	-	4/7/25/26	0/2/2/2
2	OMG	A	2792	2	-	1/9/27/28	0/3/3/3
2	PSU	A	1015	2,81	-	0/7/25/26	0/2/2/2
75	PSU	h1	308	75	-	0/7/25/26	0/2/2/2
75	OMU	h1	1261	75	-	0/9/27/28	0/2/2/2
2	OMG	A	3290	2,80	-	0/9/27/28	0/3/3/3
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
2	PSU	A	1131	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	A	1478	2	-	0/9/27/28	0/2/2/2
2	PSU	A	42	2,81	-	0/7/25/26	0/2/2/2
2	PSU	A	2262	2	-	0/7/25/26	0/2/2/2
2	OMC	A	1845	2	-	0/9/27/28	0/2/2/2
2	OMU	A	1890	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2291	2	-	0/9/27/28	0/2/2/2
2	OMC	A	2958	2,80	-	0/9/27/28	0/2/2/2
2	A2M	A	816	2	-	0/9/27/28	0/3/3/3
2	OMG	A	814	2	-	0/9/27/28	0/3/3/3
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
2	OMC	A	1446	2	-	2/9/27/28	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
2	PSU	A	509	2	-	0/7/25/26	0/2/2/2
2	OMU	A	1066	2	-	0/9/27/28	0/2/2/2
75	OMC	h1	471	75	-	0/9/27/28	0/2/2/2
75	A2M	h1	778	75	-	2/9/27/28	0/3/3/3
2	A2M	A	1142	2	-	0/9/27/28	0/3/3/3
2	A2M	A	826	81,2,80	-	3/9/27/28	0/3/3/3
2	PSU	A	2132	2,81	-	0/7/25/26	0/2/2/2
2	PSU	A	2256	2	-	0/7/25/26	0/2/2/2
2	5MC	A	2276	2,80	-	0/7/25/26	0/2/2/2
2	PSU	A	2743	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
2	PSU	A	2209	2	-	0/7/25/26	0/2/2/2
2	PSU	A	3109	2	-	0/7/25/26	0/2/2/2
2	OMG	A	1853	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	311	PSU	C6-C5	3.91	1.39	1.35
2	A	2414	PSU	C6-C5	3.79	1.39	1.35
2	A	2954	PSU	C6-C5	3.79	1.39	1.35
75	h1	1783	PSU	C6-C5	3.74	1.39	1.35
1	3	78	PSU	C6-C5	3.71	1.39	1.35

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	945	A2M	O2'-C2'-C1'	-3.63	101.99	109.08
75	h1	1786	MA6	C2-N1-C6	3.24	119.40	111.75
75	h1	1785	MA6	C2-N1-C6	3.20	119.32	111.75
2	A	826	A2M	C3'-C2'-C1'	-2.67	97.87	102.89
2	A	2279	A2M	O4'-C1'-N9	2.63	113.24	108.06

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
75	h1	1531	PSU	1	0
2	A	2324	A2M	1	0
2	A	2920	OMU	1	0
2	A	1376	A2M	1	0
2	A	2345	OMU	1	0
2	A	2618	OMG	1	0
2	A	44	OMU	1	0
2	A	2389	OMG	1	0
2	A	2312	PSU	1	0
2	A	2254	A2M	1	0
75	h1	1641	OMC	1	0
2	A	2189	PSU	1	0
2	A	2258	PSU	1	0
2	A	969	PSU	1	0
2	A	2878	OMC	1	0
75	h1	244	OMG	1	0
2	A	2790	OMG	1	0
75	h1	1767	6MZ	1	0
75	h1	975	A2M	1	0
2	A	2879	PSU	1	0
2	A	2922	PSU	1	0
75	h1	794	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2234	OMG	1	0
75	h1	95	PSU	1	0
1	3	155	OMG	3	0
2	A	675	OMC	1	0
2	A	2882	OMU	1	0
75	h1	1192	C4J	1	0
2	A	2933	A2M	2	0
2	A	661	A2M	1	0
75	h1	1261	OMU	1	0
2	A	1446	OMC	2	0
2	A	1142	A2M	1	0
2	A	826	A2M	1	0
2	A	1853	OMG	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	3405	-	9,9,9	0.18	0	8,8,8	0.29	0
84	EPE	A	3404	-	15,15,15	0.68	1 (6%)	18,20,20	0.61	0
83	SPD	A	3403	-	9,9,9	0.30	0	8,8,8	0.54	0
82	TER	A	3401	-	13,13,13	0.15	0	12,12,12	0.28	0
83	SPD	A	3402	-	9,9,9	0.18	0	8,8,8	0.14	0
83	SPD	A	3406	-	9,9,9	0.17	0	8,8,8	0.22	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	3405	-	-	1/7/7/7	-
84	EPE	A	3404	-	-	5/9/19/19	0/1/1/1
83	SPD	A	3403	-	-	5/7/7/7	-
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	2.46	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
84	A	3404	EPE	S-C10-C9-N1
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	3406	SPD	C8-C7-N6-C5

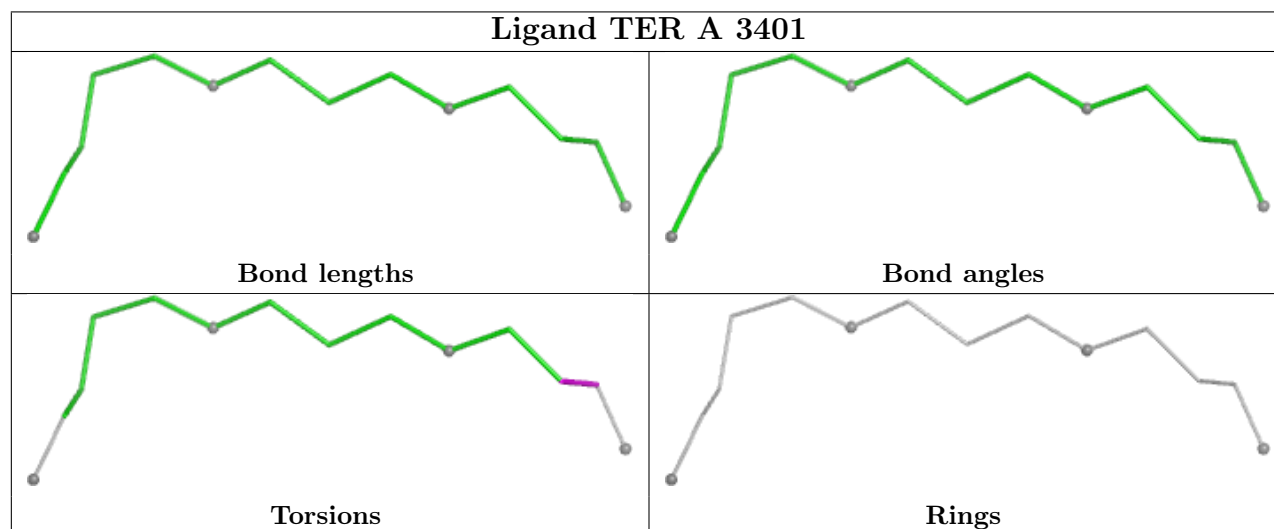
There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

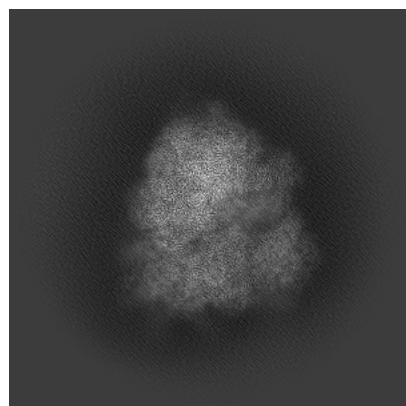
6 Map visualisation [i](#)

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.

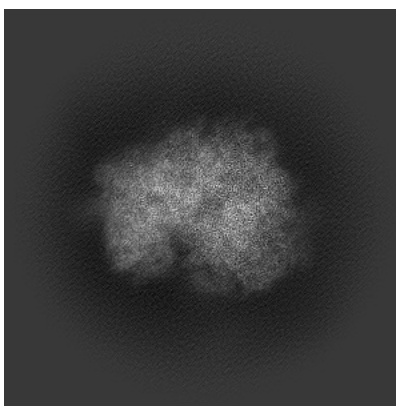
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

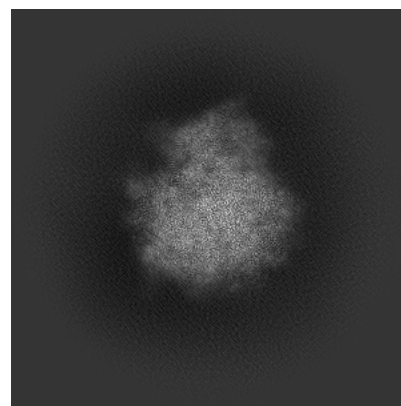
6.1.1 Primary map



X

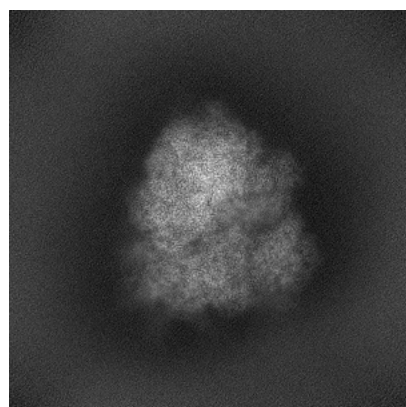


Y

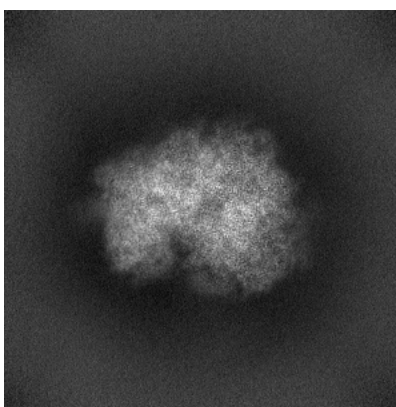


Z

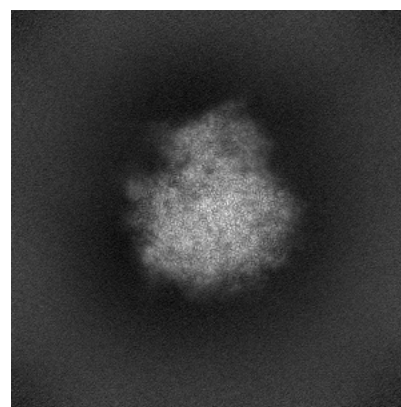
6.1.2 Raw map



X



Y

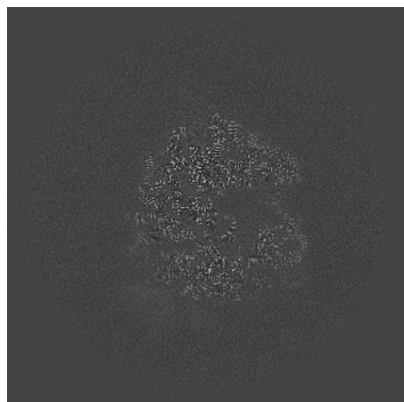


Z

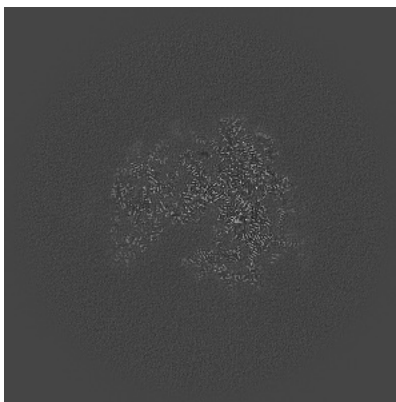
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

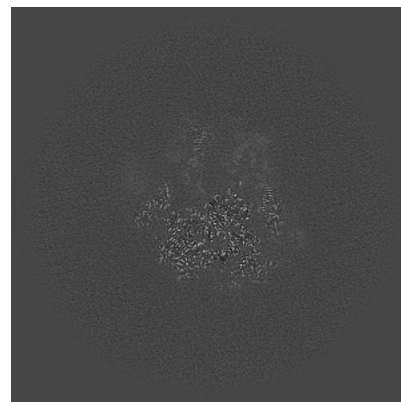
6.2.1 Primary map



X Index: 343

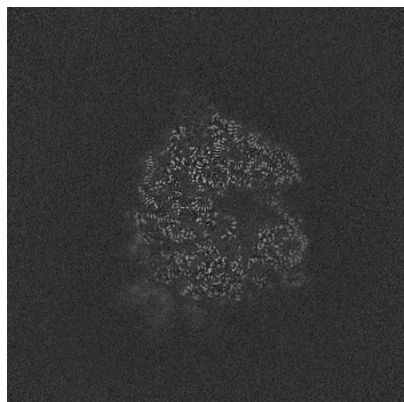


Y Index: 343

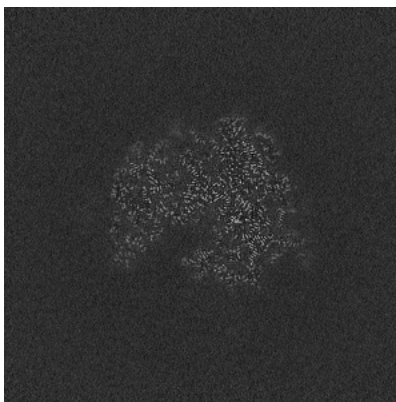


Z Index: 343

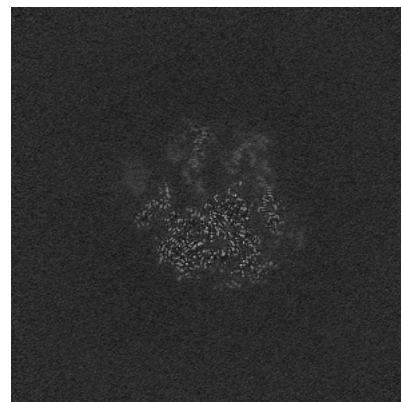
6.2.2 Raw map



X Index: 343



Y Index: 343

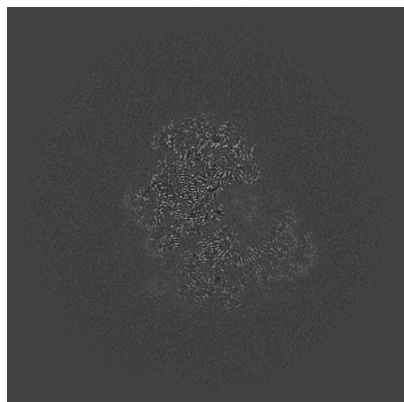


Z Index: 343

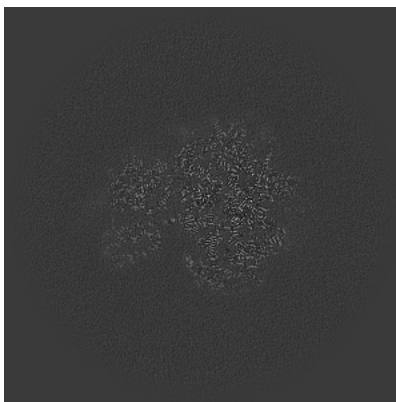
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

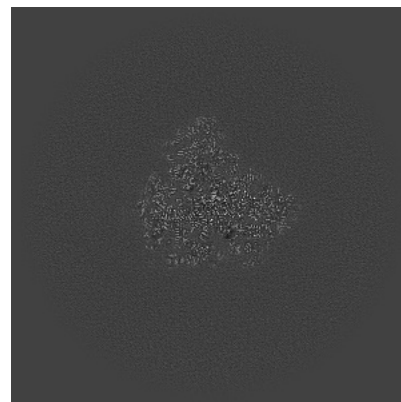
6.3.1 Primary map



X Index: 378

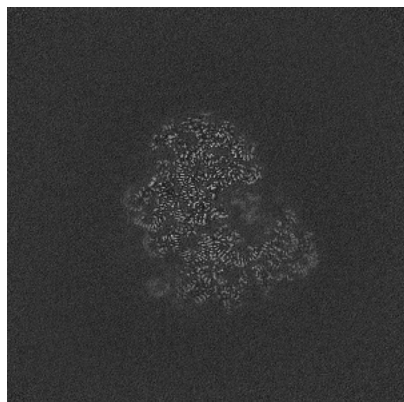


Y Index: 329

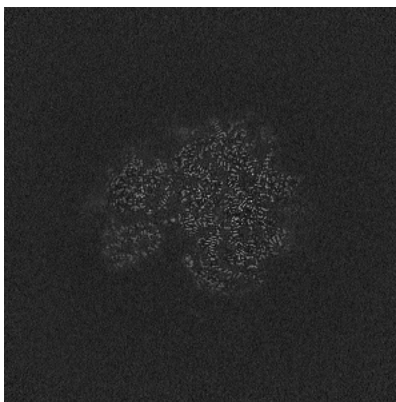


Z Index: 401

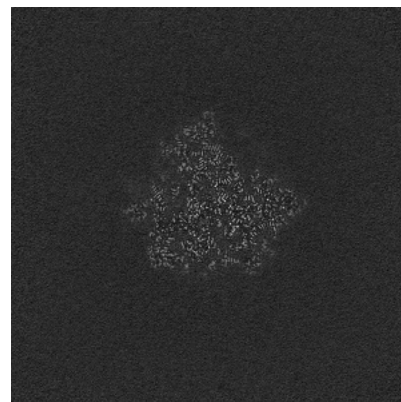
6.3.2 Raw map



X Index: 377



Y Index: 329

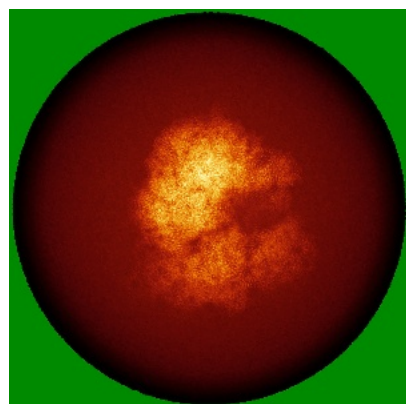


Z Index: 390

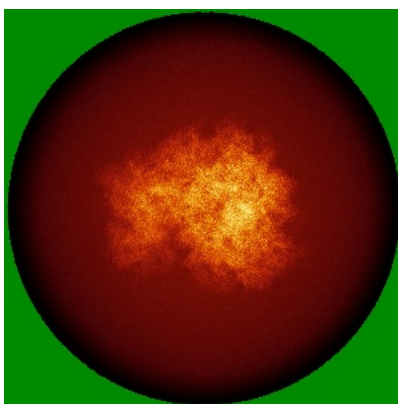
The images above show the largest variance slices of the map in three orthogonal directions.

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

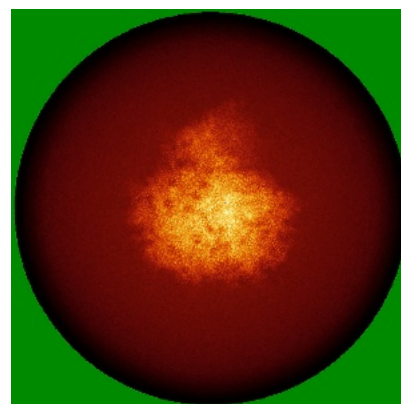
6.4.1 Primary map



X

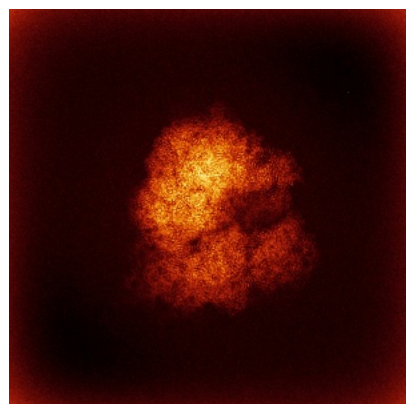


Y

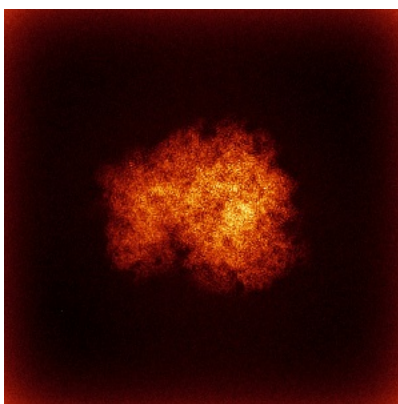


Z

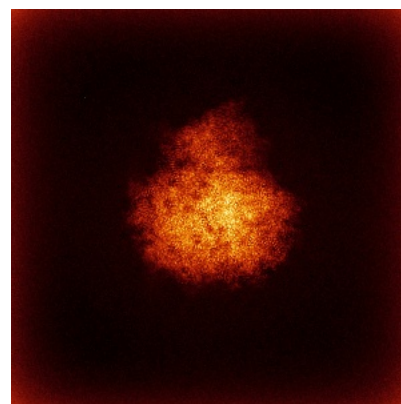
6.4.2 Raw map



X



Y

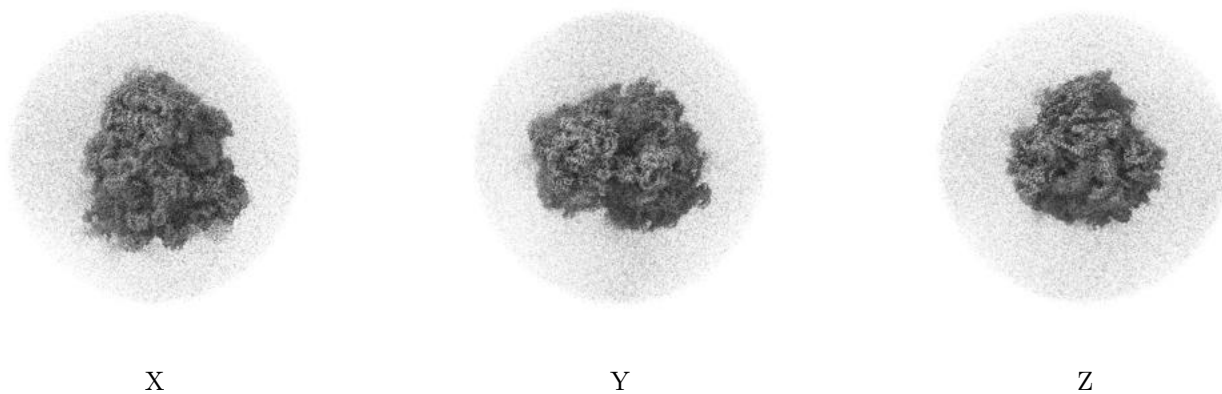


Z

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.

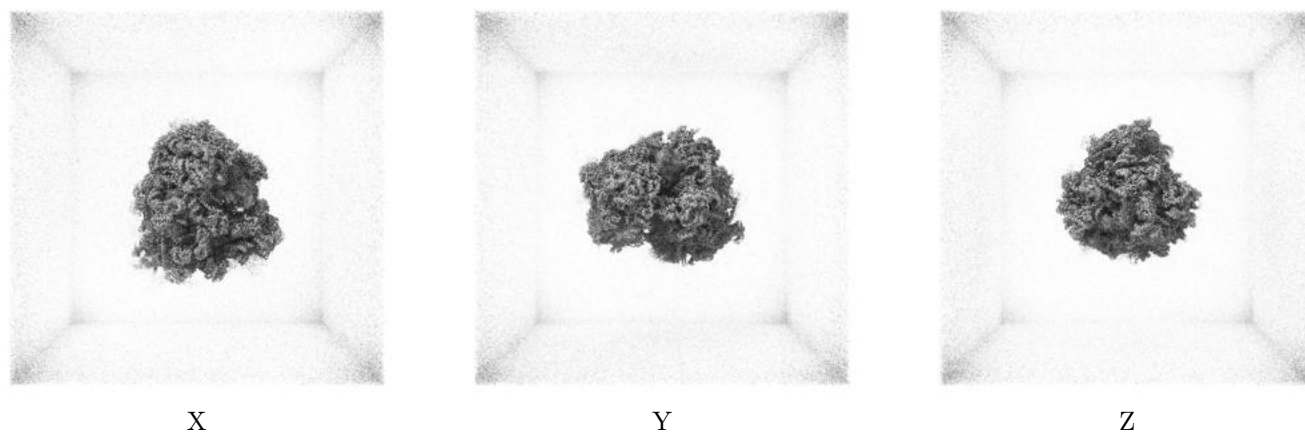
6.5 Orthogonal surface views [i](#)

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.

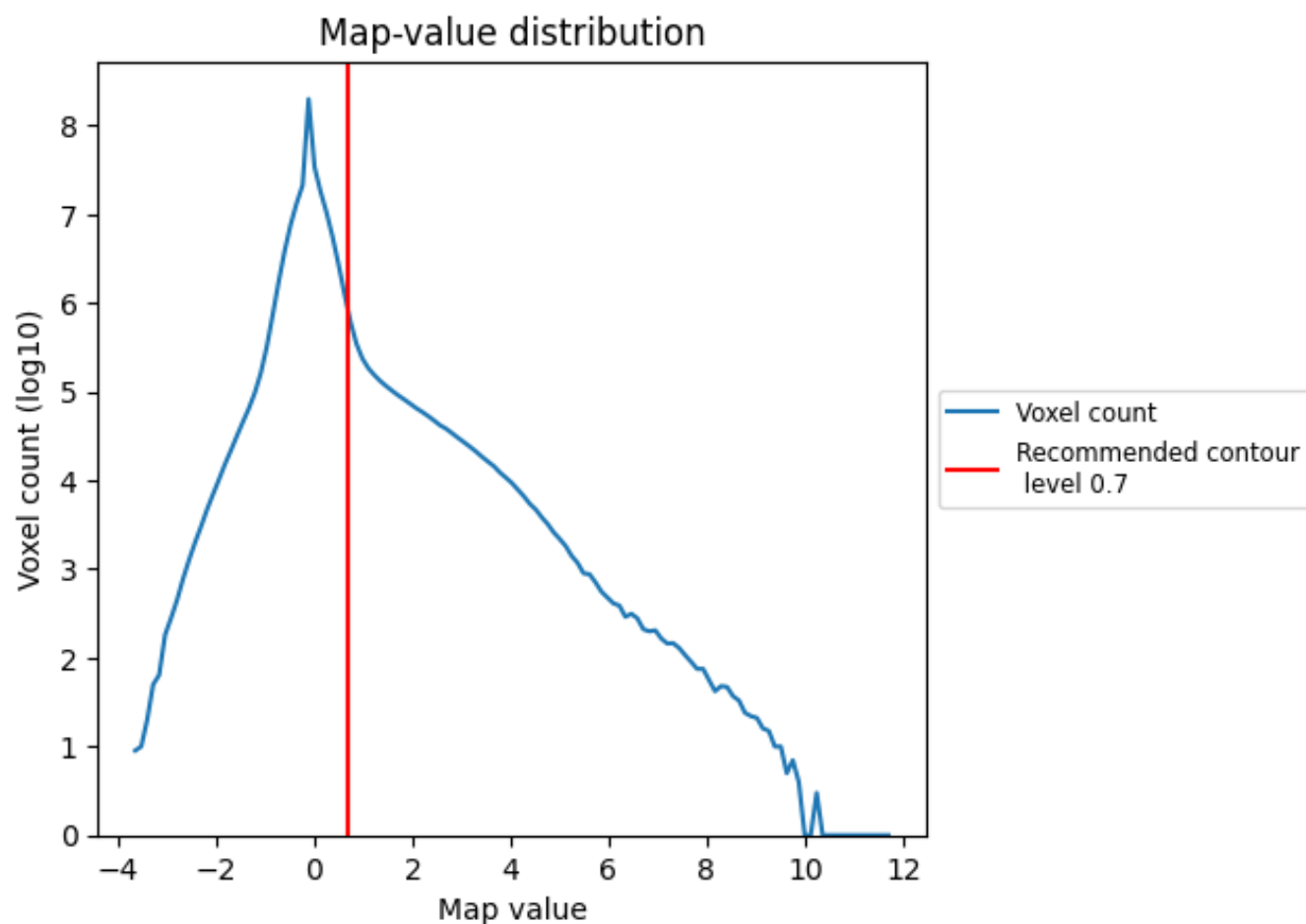
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

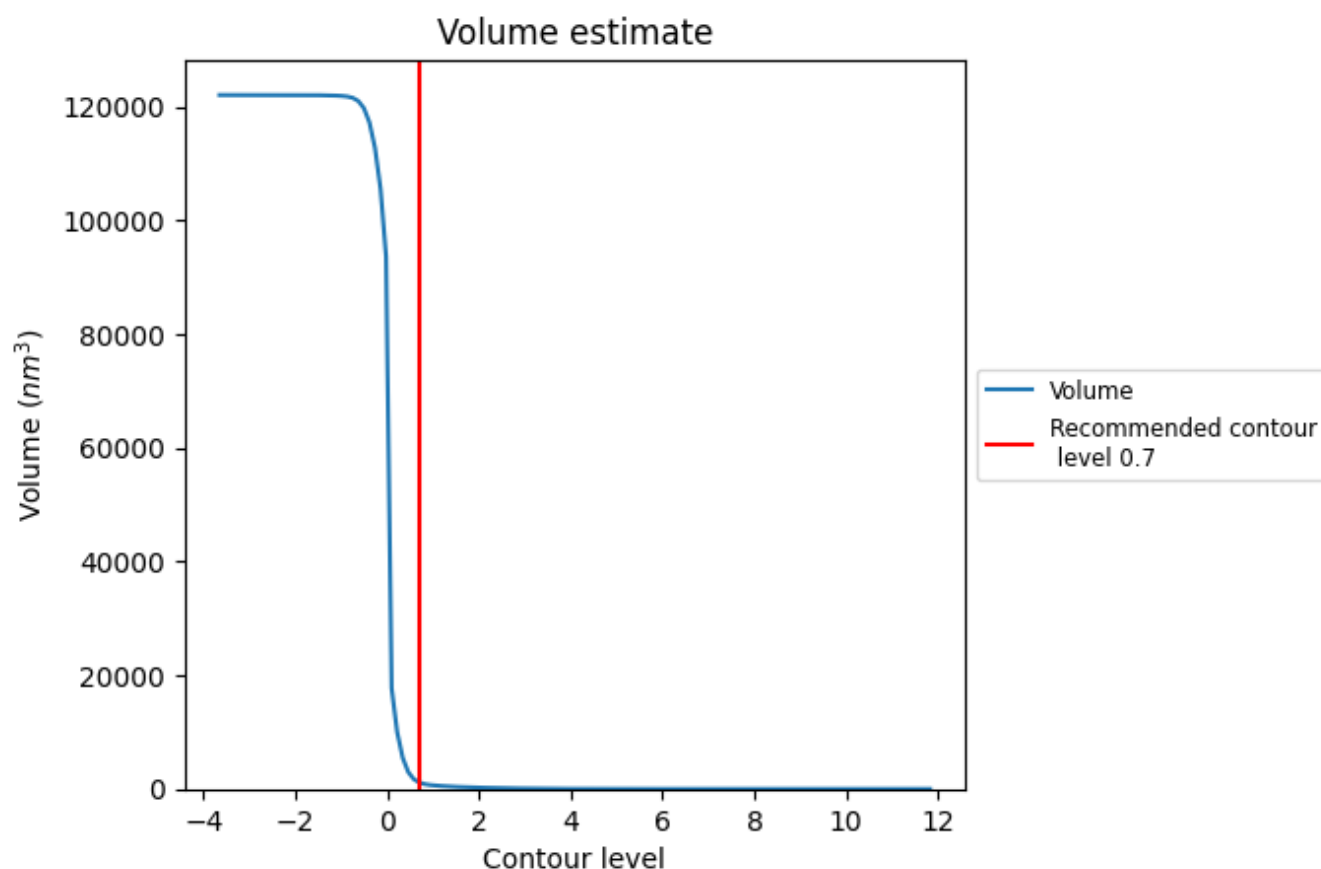
This section contains the results of statistical analysis of the map.

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.

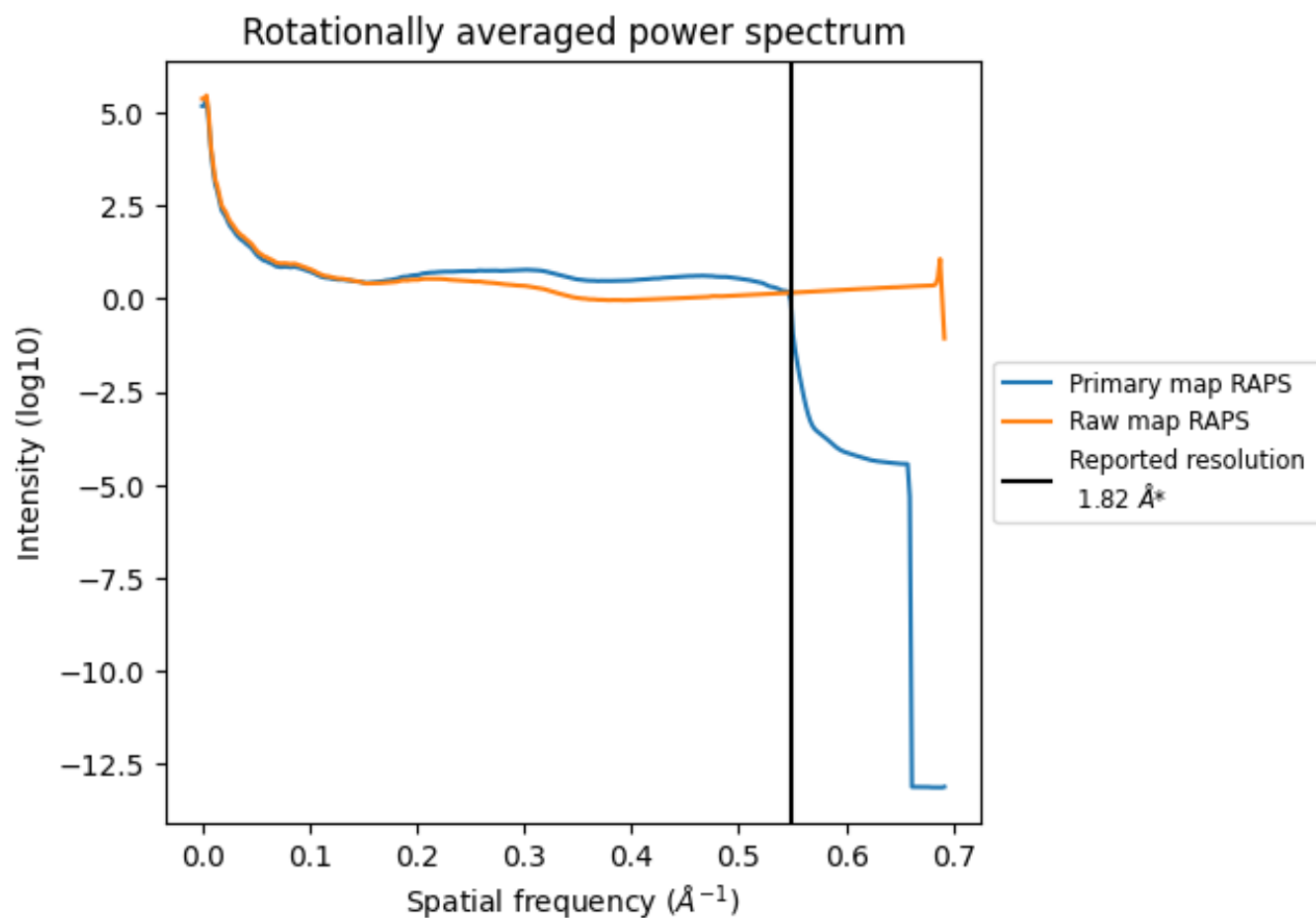
7.2 Volume estimate [i](#)



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 ⓘ

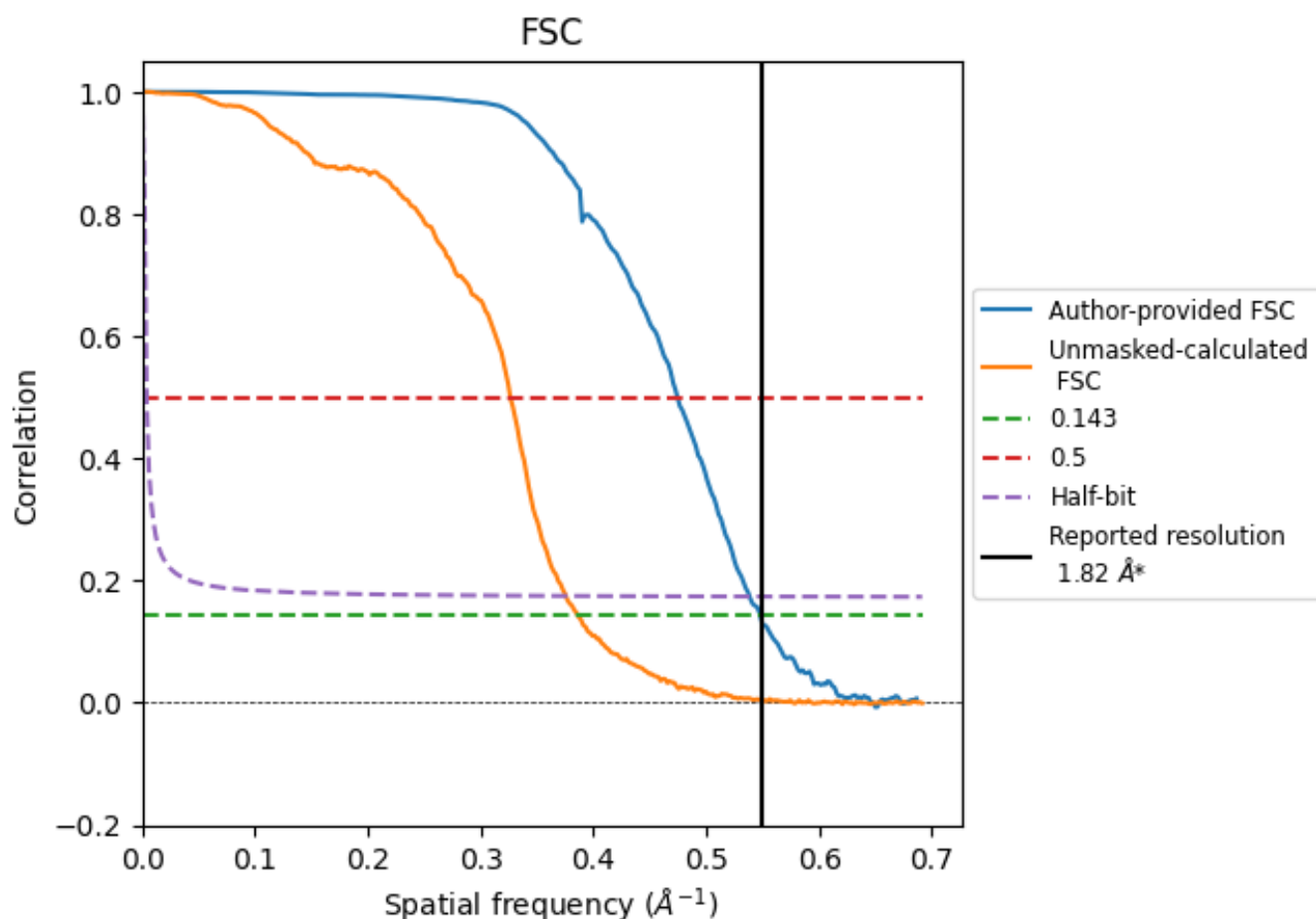


*Reported resolution corresponds to spatial frequency of 0.549 $\text{\AA}^{-1}$

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

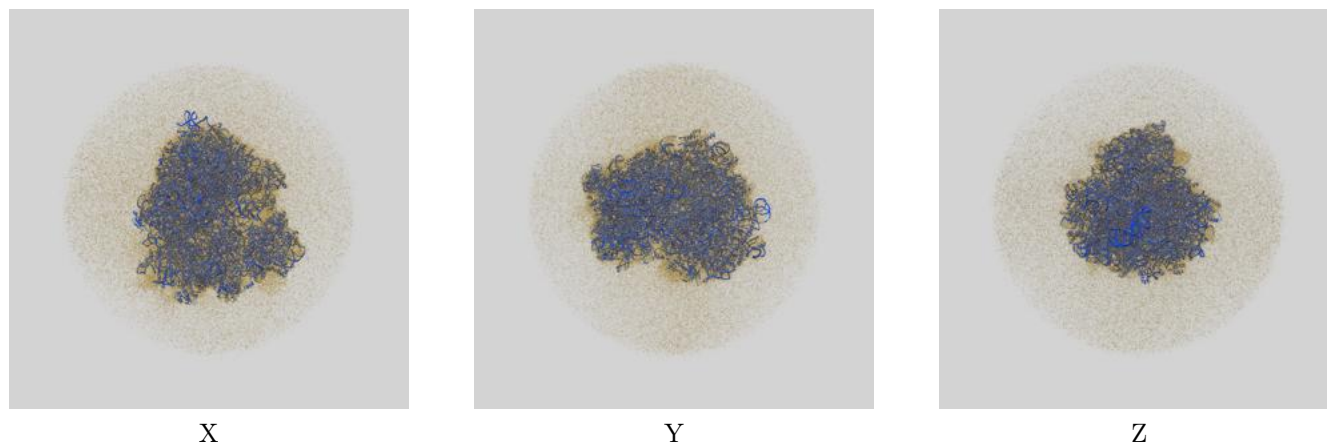
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.82	-	-
Author-provided FSC curve	1.82	2.11	1.86
Unmasked-calculated*	2.59	3.06	2.66

*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](#)

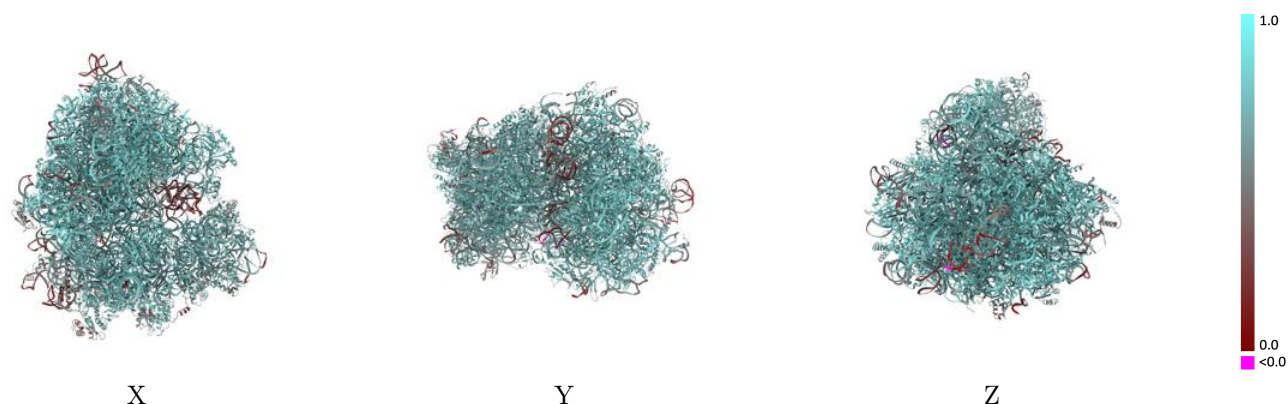
This section contains information regarding the fit between EMDB map EMD-51820 and PDB model 9H3G. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



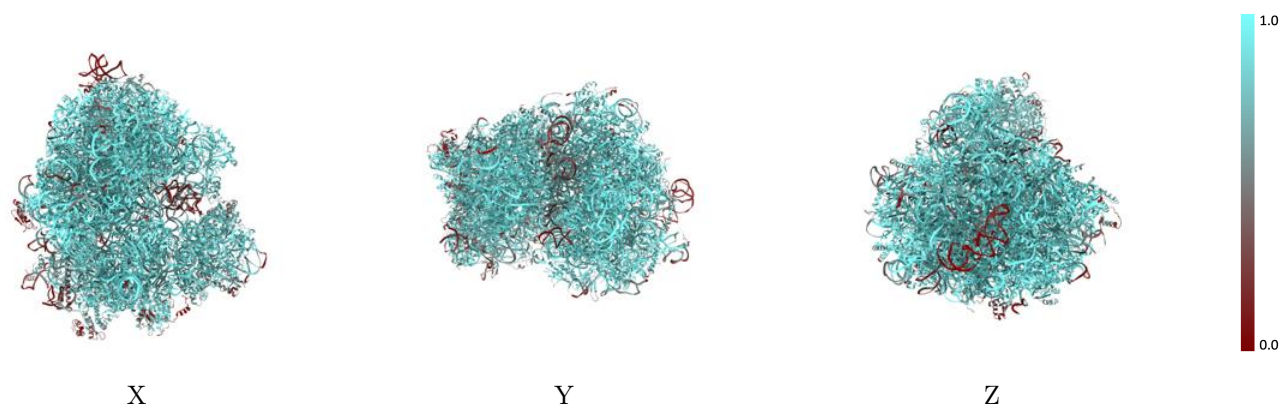
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



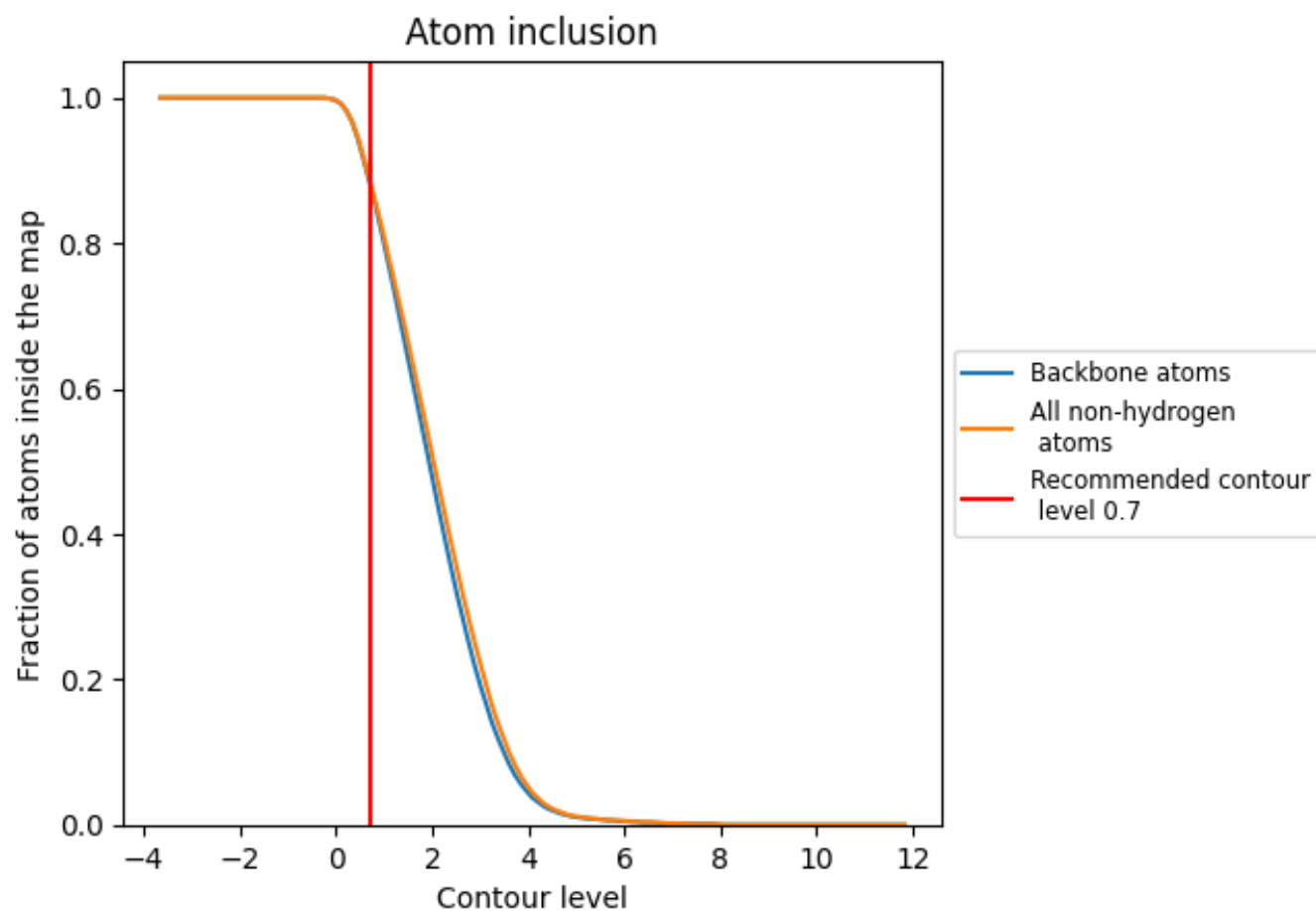
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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