



## wwPDB EM Validation Summary Report ⓘ

Apr 21, 2024 – 01:04 am BST

PDB ID : 8CEH  
EMDB ID : EMD-16609  
Title : Translocation intermediate 4 (TI-4) of 80S *S. cerevisiae* ribosome with ligands and eEF2 in the presence of sordarin  
Authors : Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2023-02-01  
Resolution : 2.05 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](mailto: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>.

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

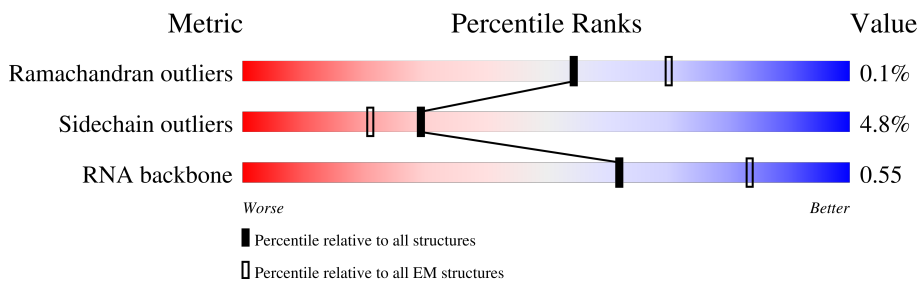
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.05 Å.

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




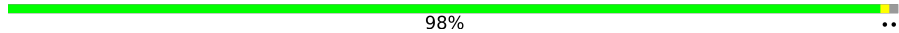

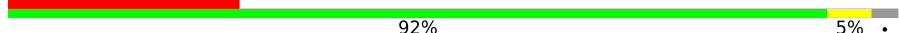












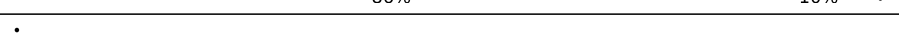
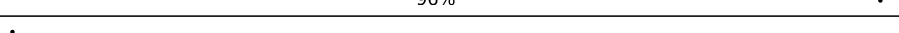
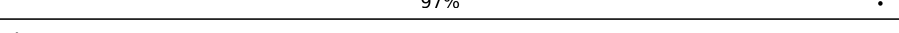

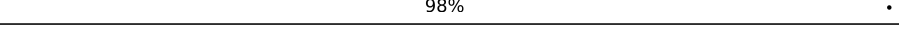
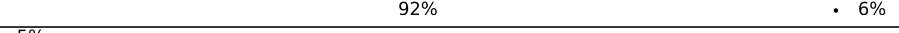
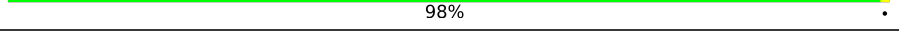


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	135	
2	1	108	
3	2	119	
4	3	82	
5	4	67	
6	5	56	
7	6	63	
8	7	319	


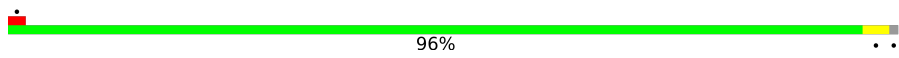
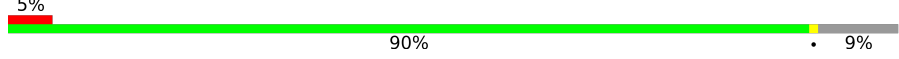
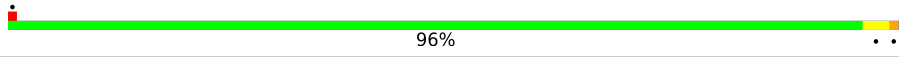
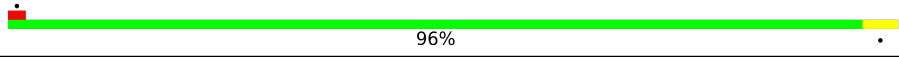
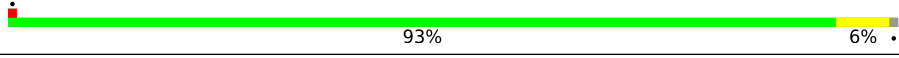
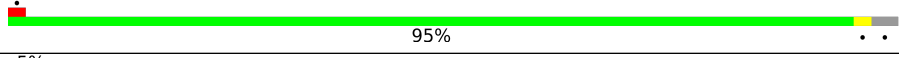
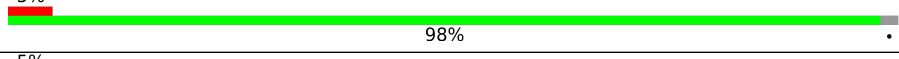
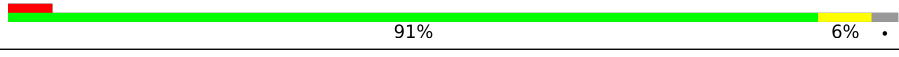
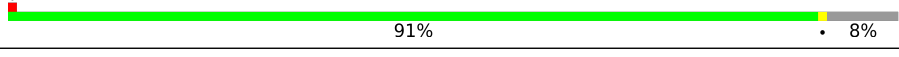
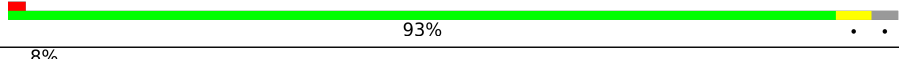
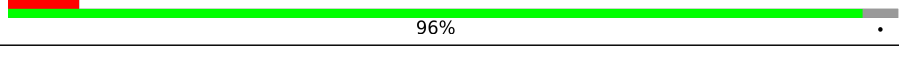
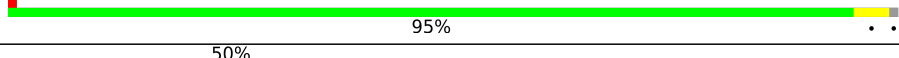

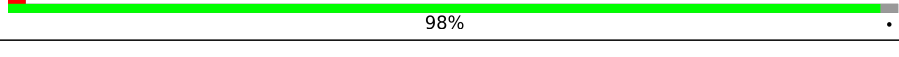
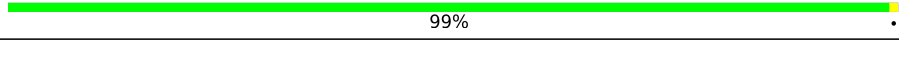
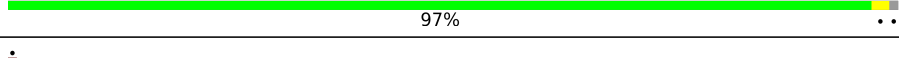
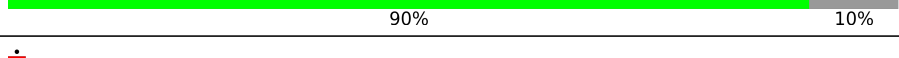
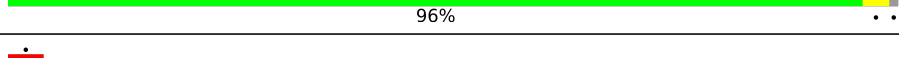
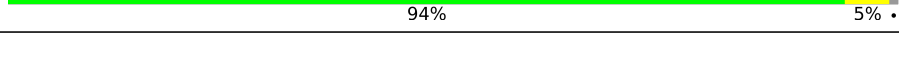
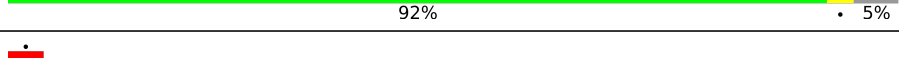
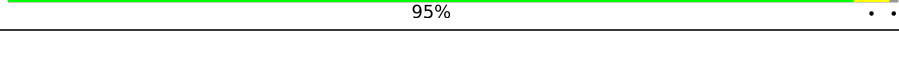
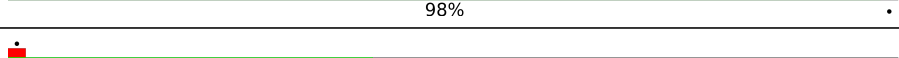
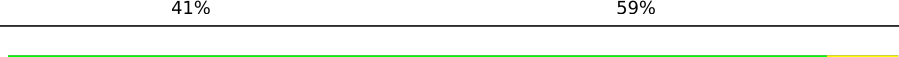
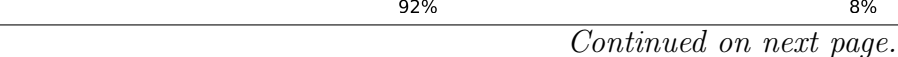
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Mol	Chain	Length	Quality of chain
9	8	152	
10	A	199	
11	AA	3396	
12	Aa	842	
13	B	184	
14	BB	121	
15	Bb	76	
16	C	186	
17	CC	158	
18	Cc	77	
19	D	189	
20	DD	312	
21	Dd	39	
22	E	172	
23	EE	254	
24	Ee	165	
25	F	160	
26	FF	387	
27	G	121	
28	GG	362	
29	H	137	
30	HH	297	
31	I	155	
32	II	176	
33	J	142	

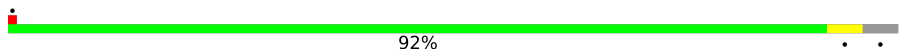
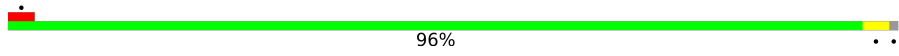

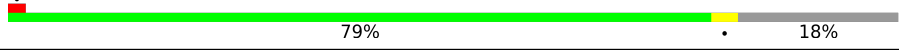
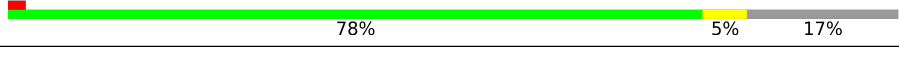


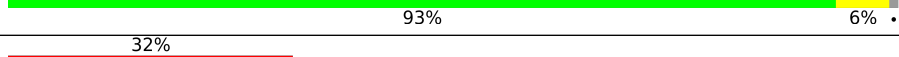
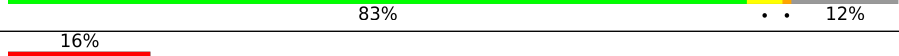
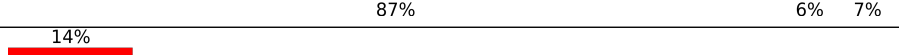
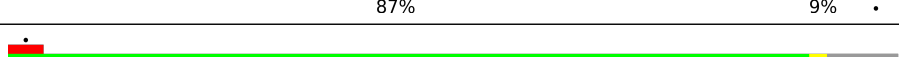
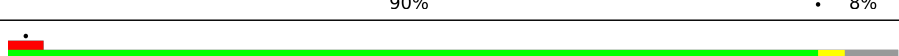
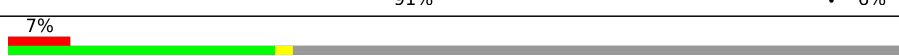
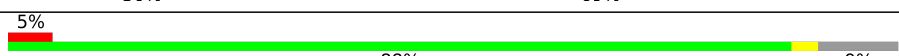
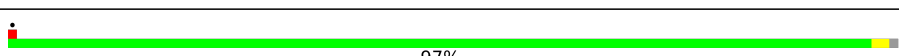
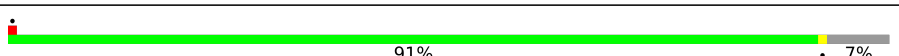



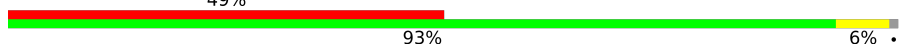
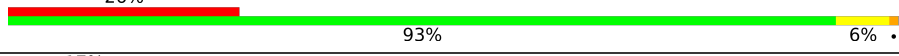
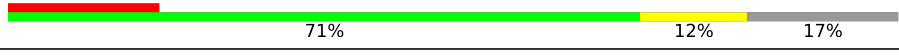
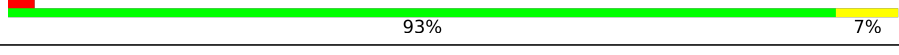
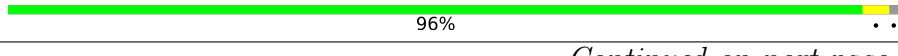

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Mol	Chain	Length	Quality of chain
34	JJ	244	 88% 9%
35	K	127	 96%
36	KK	256	 5% 90% 9%
37	L	136	 96%
38	LL	191	 96%
39	M	149	 93% 6%
40	MM	221	 95%
41	N	59	 5% 98%
42	NN	174	 5% 91% 6%
43	O	105	 91% 8%
44	OO	199	 93%
45	P	113	 8% 96%
46	PP	138	 95%
47	Pp	2	 50% 50%
48	Q	130	 98%
49	QQ	204	 99%
50	R	107	 97%
51	S	121	 90% 10%
52	T	120	 96%
53	U	100	 94% 5%
54	V	88	 92% 5%
55	W	78	 95%
56	X	51	 98%
57	Y	128	 41% 59%
58	Z	25	 92% 8%

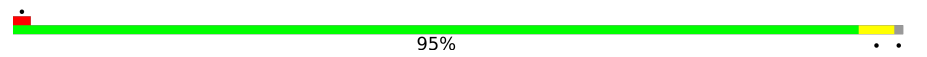
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Mol	Chain	Length	Quality of chain
59	a	106	 92%
60	b	92	 96%
61	c	1800	 70% 18% 11%
62	d	252	 79% 18%
63	e	255	 78% 5% 17%
64	f	254	 83% 15%
65	g	240	 12% 72% 5% 24%
66	h	261	 93% 6%
67	i	225	 32% 83% 12%
68	j	236	 16% 87% 6% 7%
69	k	190	 14% 87% 9%
70	l	200	 90% 8%
71	m	197	 91% 6%
72	n	105	 7% 30% 69%
73	o	156	 5% 88% 9%
74	p	151	 97%
75	q	137	 91% 7%
76	r	142	 25% 58% 6% 36%
77	s	143	 18% 85% 10%
78	t	136	 18% 80% 9% 11%
79	u	146	 49% 93% 6%
80	v	144	 26% 93% 6%
81	w	121	 17% 71% 12% 17%
82	x	87	 93% 7%
83	y	130	 96%

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Mol	Chain	Length	Quality of chain
84	z	145	

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 207126 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 protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1\_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	49	404	249	86	65	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	53	427	269	88	69	1	0	0

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	318	2436	1541	418	469	8	0	0

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	36	276	173	54	45	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	197	1555	1003	289	262	1	0	0

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AA	3197	68429	30589	12334	22309	3197	0	0

- Molecule 12 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Aa	816	6368	4051	1088	1198	31	0	0

- Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	B	154	1222	761	237	224	0	0

- Molecule 14 is a RNA chain called 5S ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	BB	121	2579	1152	461	845	121	0	0

- Molecule 15 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	Bb	76	1638	736	294	533	75	0	0

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	C	185	1441	908	290	241	2	0	0

- Molecule 17 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	CC	158	3353	1500	586	1109	158	0	0

- Molecule 18 is a RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	Cc	77	1644	732	298	537	77	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cc	18	C	U	conflict	GB 170517292

- Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	D	176	1423	875	308	240	0	0

- Molecule 20 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DD	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 21 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Dd	6	Total	C	N	O	P	0	0
			125	56	18	45	6		

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 23 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	EE	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 24 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 26 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 27 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	G	97	Total	C	N	O	0	0
			770	499	126	145		

- Molecule 28 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	GG	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 30 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HH	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 31 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 32 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	II	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 33 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 34 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	JJ	222	1784	1151	324	308	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	K	126	993	625	192	176		0	0

- Molecule 36 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	KK	233	1804	1151	323	327	3	0	0

- Molecule 37 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	L	135	1092	710	202	180		0	0

- Molecule 38 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LL	191	1518	963	274	277	4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	M	148	1173	749	231	190	3	0	0

- Molecule 40 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	MM	215	1743	1102	331	303	7	0	0

- Molecule 41 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	N	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NN	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 43 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	O	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 44 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	OO	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 45 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	P	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 46 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	PP	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 47 is a protein called Polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pp	2	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 48 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Q	127	1020	647	205	167	1	0	0

- Molecule 49 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	QQ	203	1720	1077	361	281	1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	R	106	850	540	165	144	1	0	0

- Molecule 51 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	S	109	861	533	175	149	4	0	0

- Molecule 52 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	T	119	969	615	186	167	1	0	0

- Molecule 53 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	U	99	771	481	156	132	2	0	0

- Molecule 54 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	V	84	665	405	145	110	5	0	0

- Molecule 55 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	W	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 56 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 57 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 58 is a protein called 60S ribosomal protein L41.

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

- Molecule 59 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	a	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 60 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	b	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 61 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	c	1608	Total	C	N	O	P	0	0
			34321	15360	6093	11260	1608		

- Molecule 62 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 63 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	f	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 65 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	g	183	Total	C	N	O	S	0	0
			1412	893	260	253	6		

- Molecule 66 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 67 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 68 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 69 is a protein called 40S ribosomal protein S7-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
69	k	184	1481	951	265	265	0	0

- Molecule 70 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	l	184	1457	906	291	258	2	0	0

- Molecule 71 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	m	185	1494	943	289	261	1	0	0

- Molecule 72 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	n	33	300	199	46	55	0	0

- Molecule 73 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	o	142	1146	735	217	191	3	0	0

- Molecule 74 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	p	150	1192	759	224	207	2	0	0

- Molecule 75 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	q	127	891	545	182	163	1	0	0

- Molecule 76 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	r	91	732	469	138	120	5	0	0

- Molecule 77 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	s	137	1080	692	199	189		0	0

- Molecule 78 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	t	121	961	599	182	178	2	0	0

- Molecule 79 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	u	145	1192	743	237	210	2	0	0

- Molecule 80 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	v	143	1112	694	208	208	2	0	0

- Molecule 81 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	w	100	800	509	144	146	1	0	0

- Molecule 82 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	x	87	684	420	125	137	2	0	0

- Molecule 83 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	y	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 84 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	z	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	2	1	Total	Zn	0
			1	1	
85	5	1	Total	Zn	0
			1	1	
85	8	1	Total	Zn	0
			1	1	
85	S	1	Total	Zn	0
			1	1	
85	V	1	Total	Zn	0
			1	1	
85	Y	1	Total	Zn	0
			1	1	
85	a	1	Total	Zn	0
			1	1	
85	b	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	AA	198	Total	Mg	0
			198	198	
86	Aa	1	Total	Mg	0
			1	1	
86	B	1	Total	Mg	0
			1	1	
86	BB	5	Total	Mg	0
			5	5	
86	Bb	1	Total	Mg	0
			1	1	

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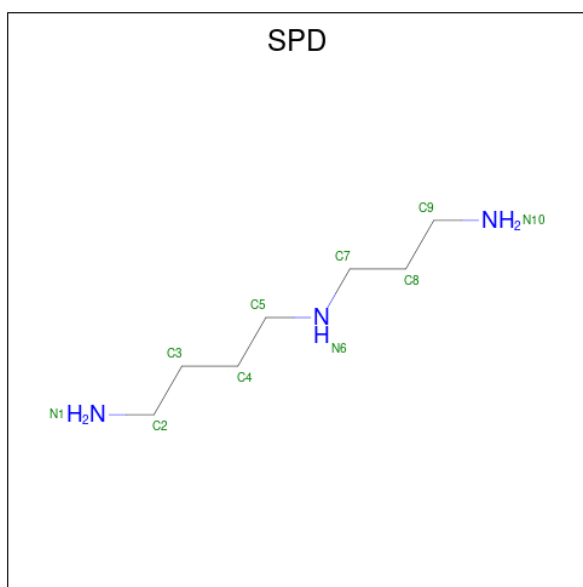
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Mol	Chain	Residues	Atoms		AltConf
86	CC	3	Total 3	Mg 3	0
86	Dd	1	Total 1	Mg 1	0
86	FF	1	Total 1	Mg 1	0
86	H	1	Total 1	Mg 1	0
86	QQ	1	Total 1	Mg 1	0
86	c	49	Total 49	Mg 49	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

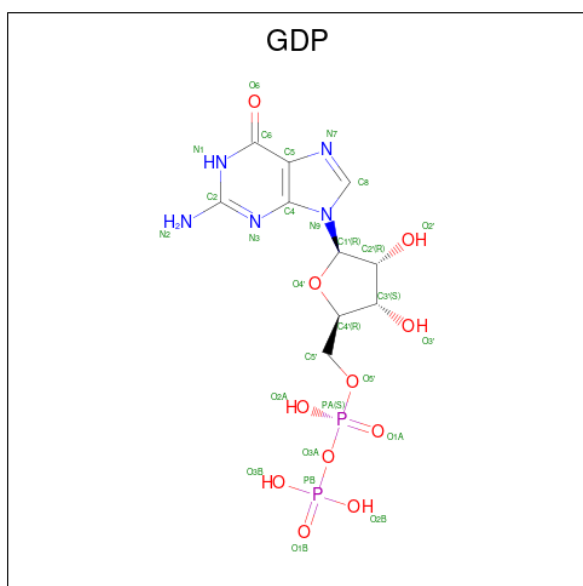
Mol	Chain	Residues	Atoms		AltConf
87	AA	14	Total 14	K 14	0
87	EE	1	Total 1	K 1	0
87	MM	1	Total 1	K 1	0
87	Q	1	Total 1	K 1	0
87	a	1	Total 1	K 1	0
87	c	2	Total 2	K 2	0
87	q	1	Total 1	K 1	0

- Molecule 88 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



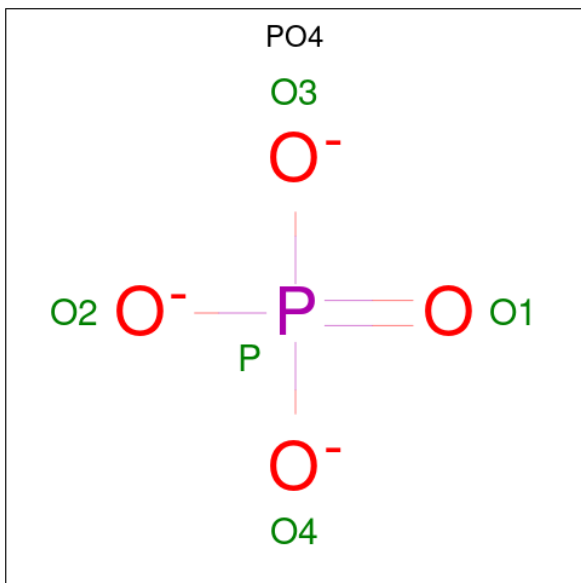
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
88	AA	1	10	7	3	0
88	AA	1	10	7	3	0
88	AA	1	10	7	3	0

- Molecule 89 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



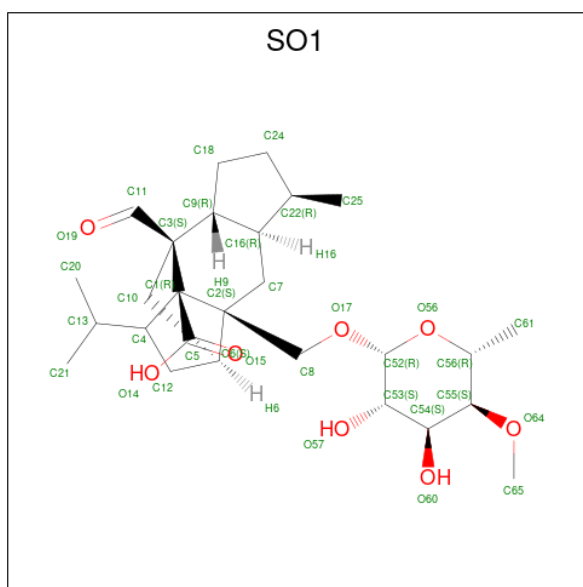
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
89	Aa	1	28	10	5	11	2	0

- Molecule 90 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms		AltConf	
			Total	O		P
90	Aa	1	5	4	1	0

- Molecule 91 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: C<sub>27</sub>H<sub>42</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
91	Aa	1	Total	C O	0
			35	27 8	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	2	1	Total	O	0
			1	1	
92	A	2	Total	O	0
			2	2	
92	AA	778	Total	O	0
			778	778	
92	B	3	Total	O	0
			3	3	
92	BB	13	Total	O	0
			13	13	
92	CC	13	Total	O	0
			13	13	
92	Cc	1	Total	O	0
			1	1	
92	D	1	Total	O	0
			1	1	
92	EE	6	Total	O	0
			6	6	
92	F	4	Total	O	0
			4	4	
92	FF	3	Total	O	0
			3	3	

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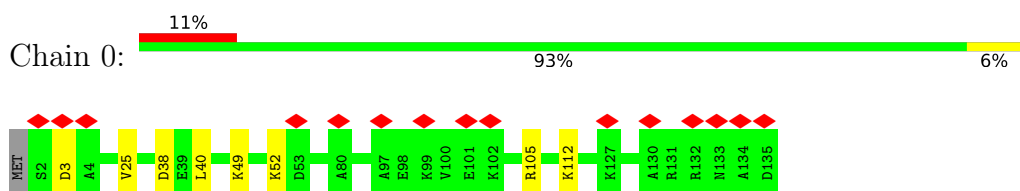
Mol	Chain	Residues	Atoms		AltConf
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92	H	3	Total 3	O 3	0
92	HH	1	Total 1	O 1	0
92	J	1	Total 1	O 1	0
92	JJ	1	Total 1	O 1	0
92	M	2	Total 2	O 2	0
92	MM	2	Total 2	O 2	0
92	N	1	Total 1	O 1	0
92	Q	4	Total 4	O 4	0
92	QQ	6	Total 6	O 6	0
92	V	2	Total 2	O 2	0
92	c	118	Total 118	O 118	0
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92	o	2	Total 2	O 2	0
92	p	2	Total 2	O 2	0



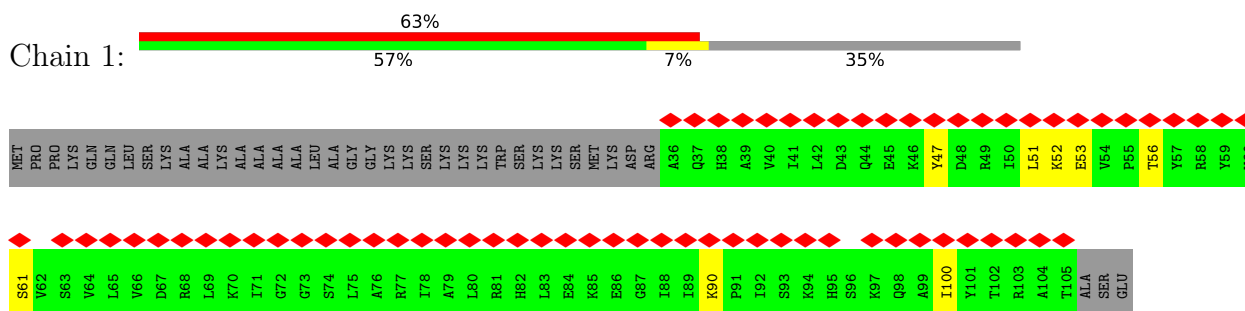
### 3 Residue-property plots [i](#)

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.

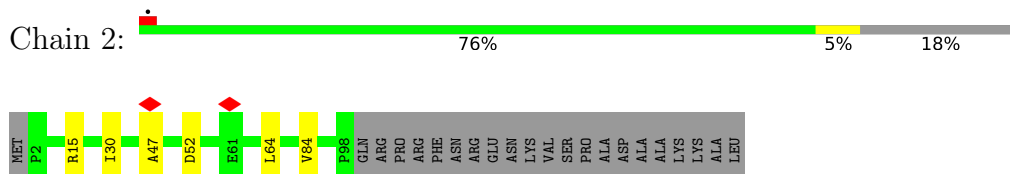
- Molecule 1: 40S ribosomal protein S24-A



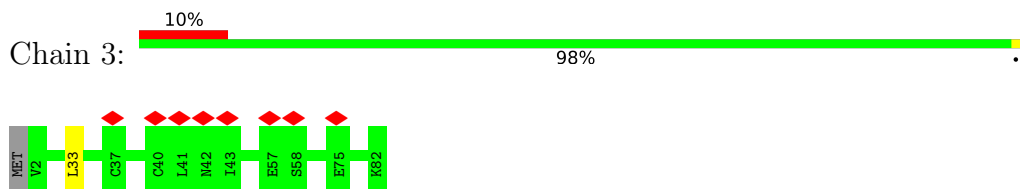
- Molecule 2: 40S ribosomal protein S25-A



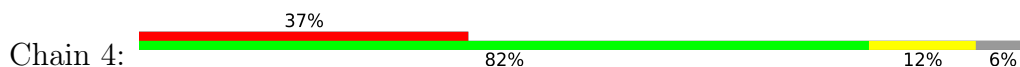
- Molecule 3: 40S ribosomal protein S26



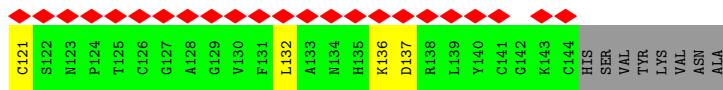
- Molecule 4: 40S ribosomal protein S27-A



- Molecule 5: 40S ribosomal protein S28-A



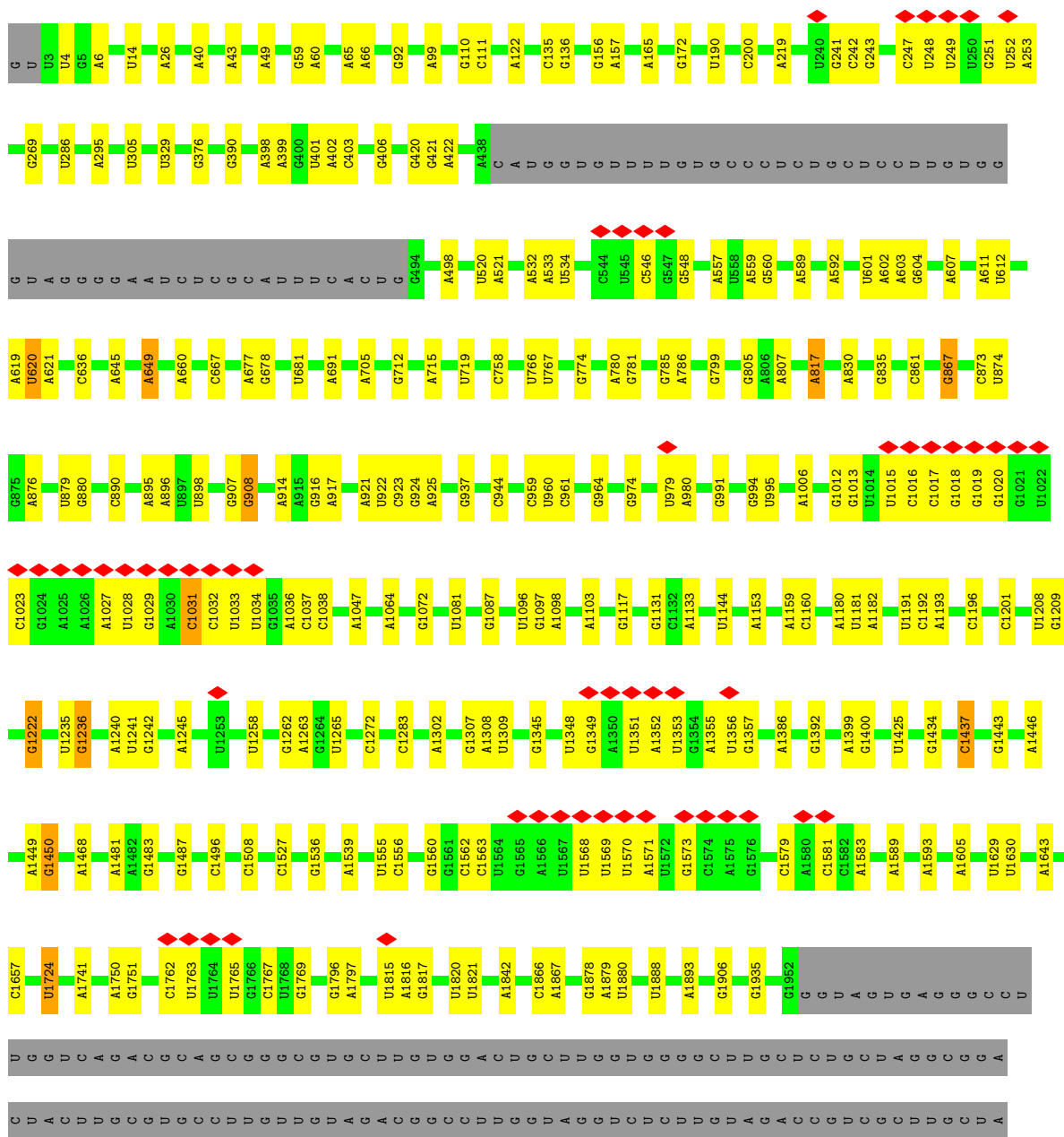
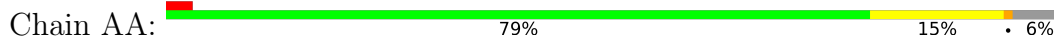


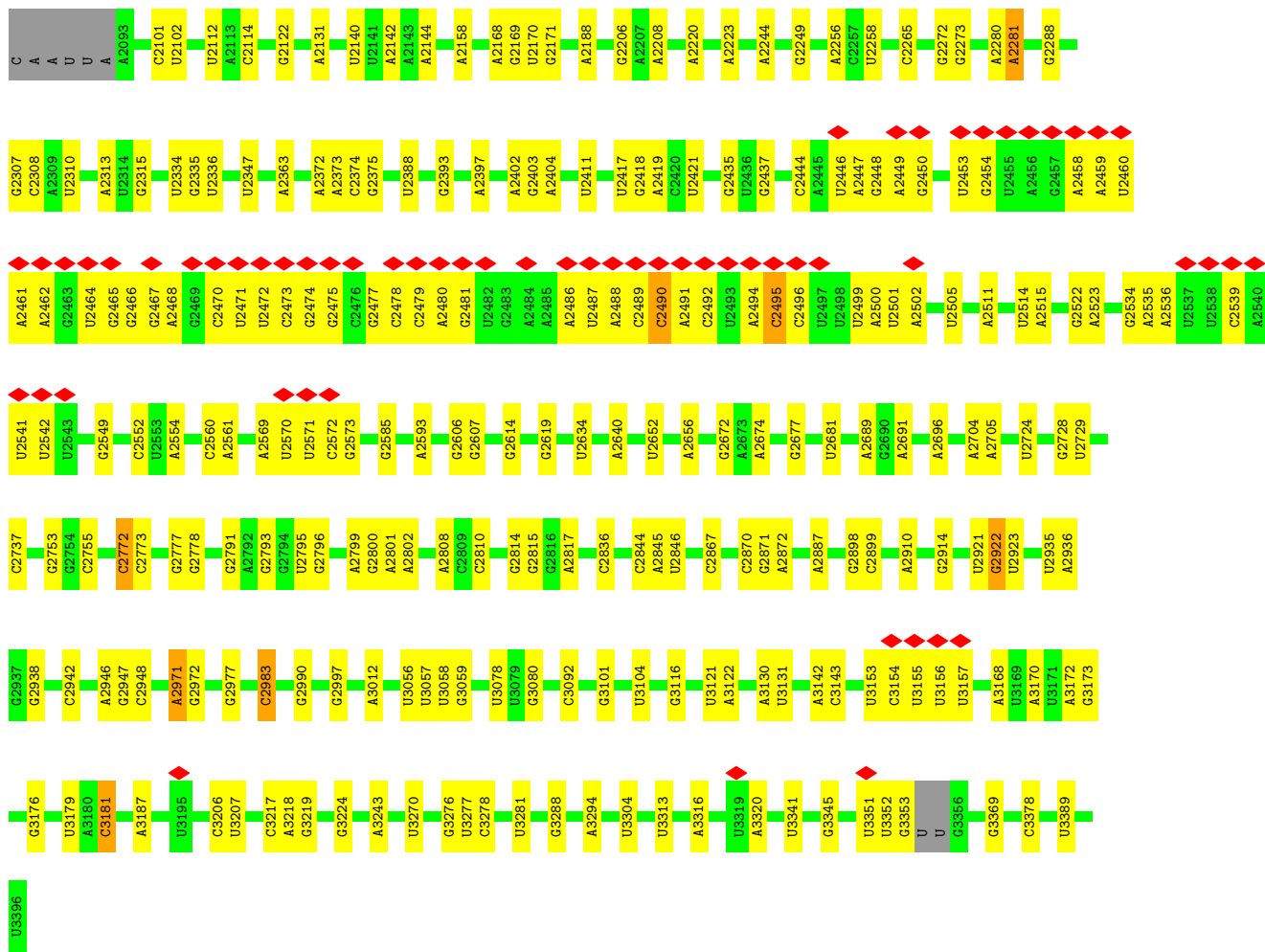


• Molecule 10: 60S ribosomal protein L16-A

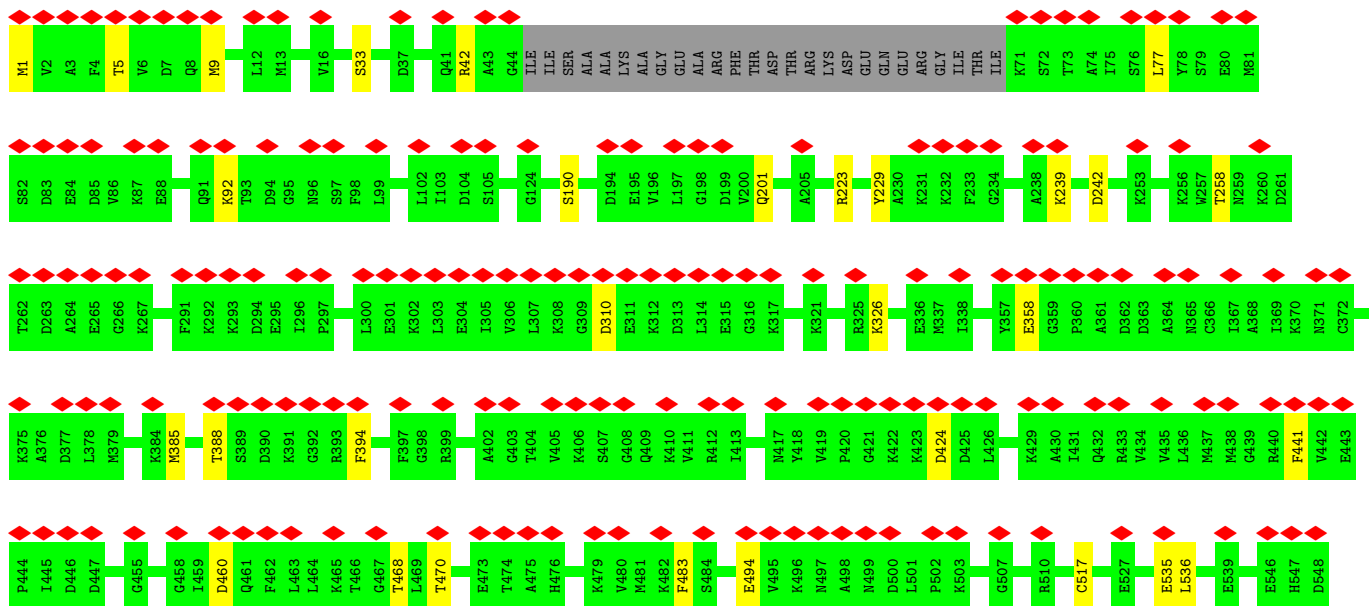
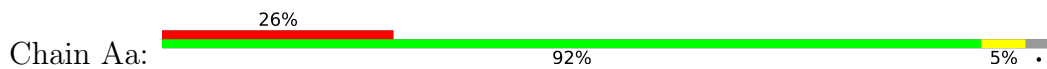


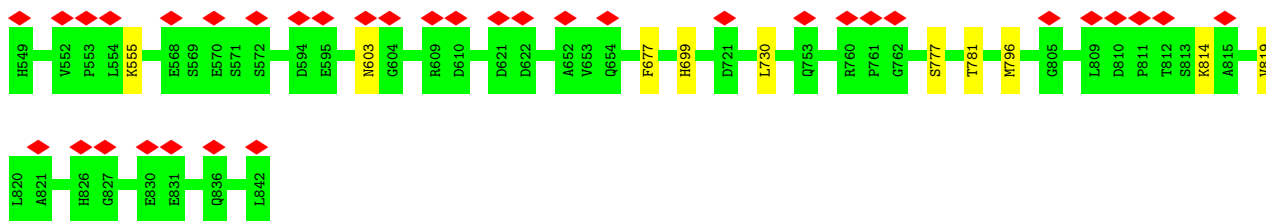
• Molecule 11: 25S ribosomal RNA



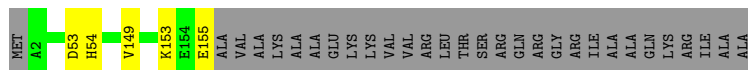
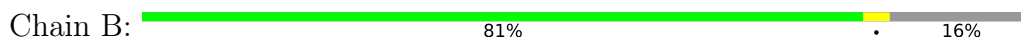


• Molecule 12: Elongation factor 2





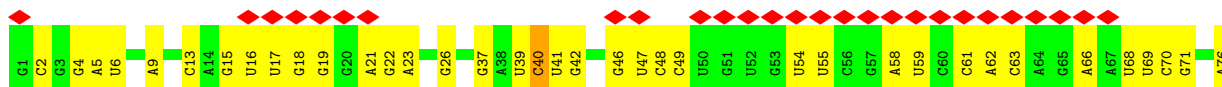
• Molecule 13: 60S ribosomal protein L17-A



• Molecule 14: 5S ribosomal RNA



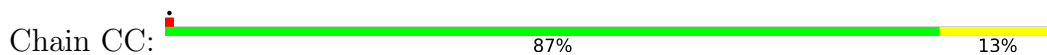
• Molecule 15: Transfer RNA Phe



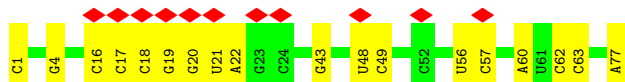
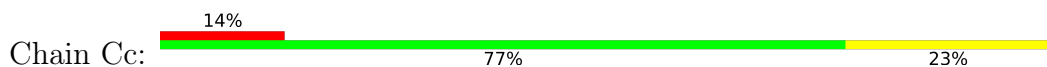
• Molecule 16: 60S ribosomal protein L18-A



• Molecule 17: 5.8S ribosomal RNA



• Molecule 18: Transfer RNA fMet







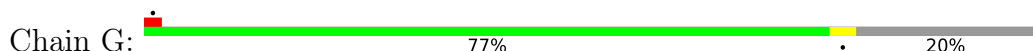
- Molecule 25: 60S ribosomal protein L21-A



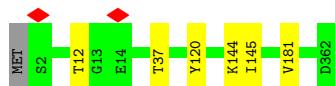
- Molecule 26: 60S ribosomal protein L3



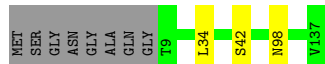
- Molecule 27: 60S ribosomal protein L22-A



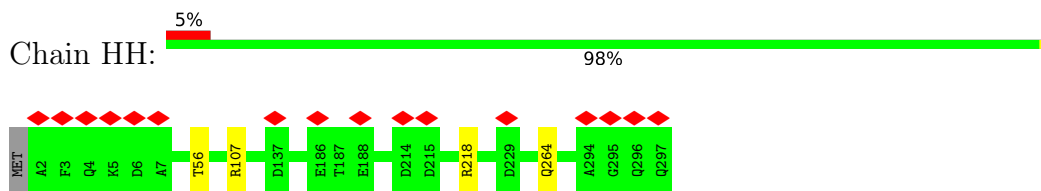
- Molecule 28: 60S ribosomal protein L4-A



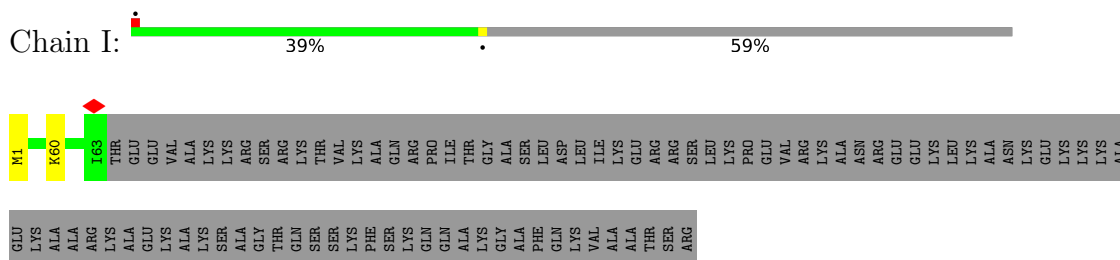
- Molecule 29: 60S ribosomal protein L23-A



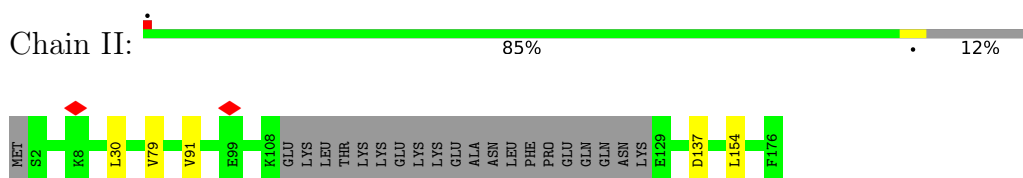
- Molecule 30: 60S ribosomal protein L5



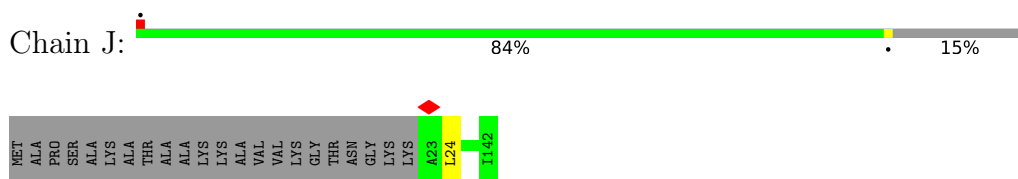
• Molecule 31: 60S ribosomal protein L24-A



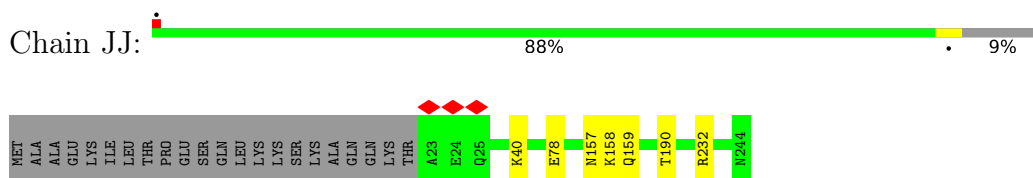
• Molecule 32: 60S ribosomal protein L6-A



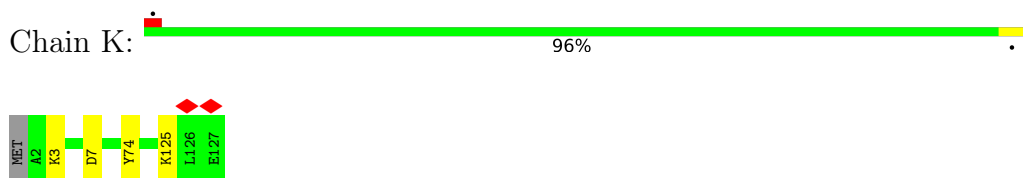
• Molecule 33: 60S ribosomal protein L25



• Molecule 34: 60S ribosomal protein L7-A



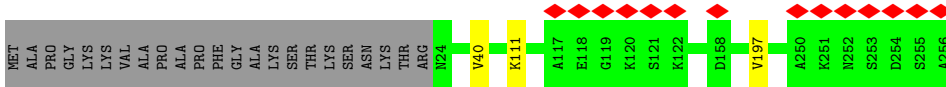
• Molecule 35: 60S ribosomal protein L26-A



• Molecule 36: 60S ribosomal protein L8-A



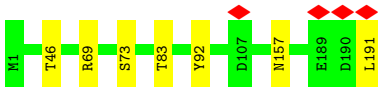




- Molecule 37: 60S ribosomal protein L27-A



- Molecule 38: RPL9A isoform 1



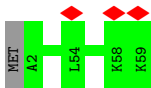
- Molecule 39: 60S ribosomal protein L28



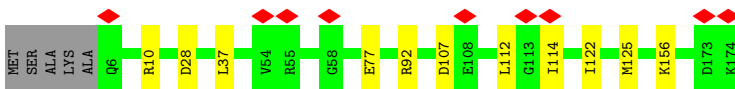
- Molecule 40: 60S ribosomal protein L10




- Molecule 41: 60S ribosomal protein L29

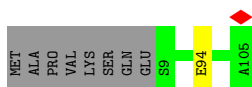


- Molecule 42: 60S ribosomal protein L11-A



- Molecule 43: 60S ribosomal protein L30

Chain O:  91% 8%



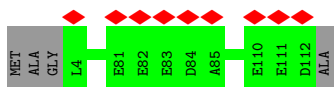
- Molecule 44: 60S ribosomal protein L13-A

Chain OO:  93%



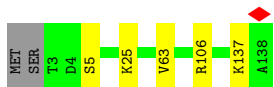
- Molecule 45: 60S ribosomal protein L31-A

Chain P:  8% 96%



- Molecule 46: 60S ribosomal protein L14-A

Chain PP:  95%



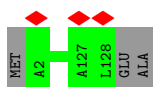
- Molecule 47: Polypeptide

Chain Pp:  50% 50%



- Molecule 48: 60S ribosomal protein L32

Chain Q:  98%



- Molecule 49: 60S ribosomal protein L15-A

Chain QQ:  99%




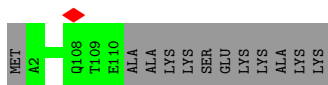
- Molecule 50: 60S ribosomal protein L33-A

Chain R:  97%



- Molecule 51: 60S ribosomal protein L34-A

Chain S:  90%



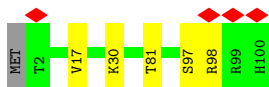
- Molecule 52: 60S ribosomal protein L35-A

Chain T:  96%



- Molecule 53: 60S ribosomal protein L36-A

Chain U:  94%



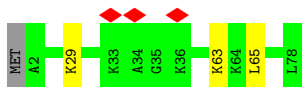
- Molecule 54: 60S ribosomal protein L37-A

Chain V:  92%



- Molecule 55: 60S ribosomal protein L38

Chain W:  95%



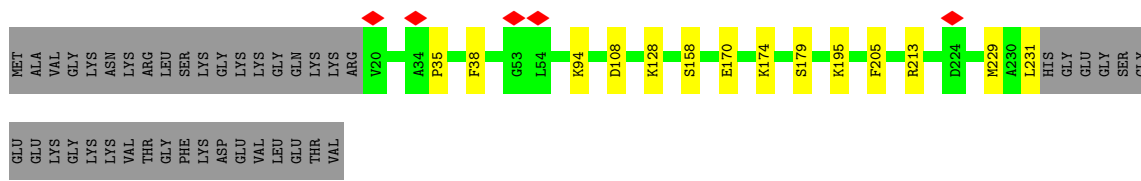
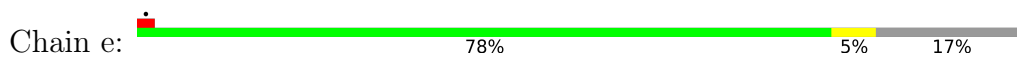
- Molecule 56: 60S ribosomal protein L39

Chain X:  98%

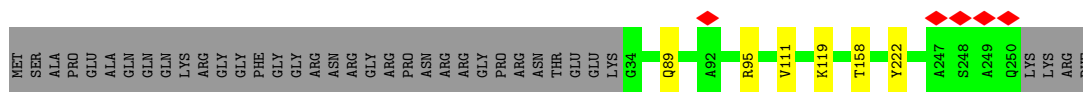
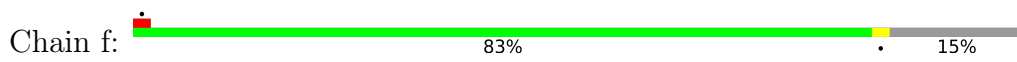




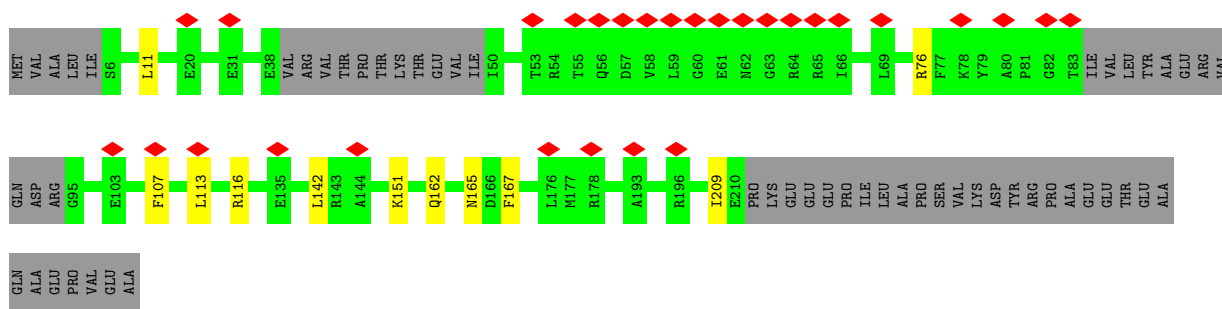
• Molecule 63: 40S ribosomal protein S1-A



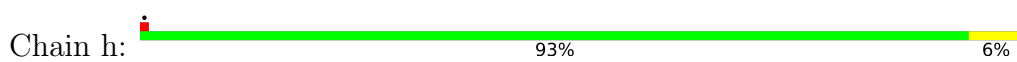
• Molecule 64: 40S ribosomal protein S2



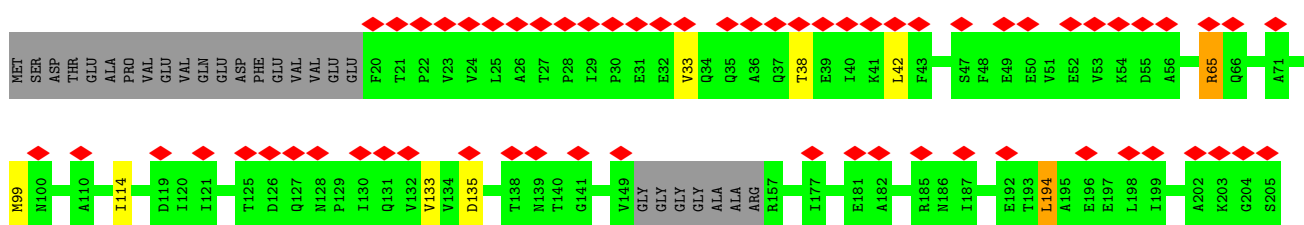
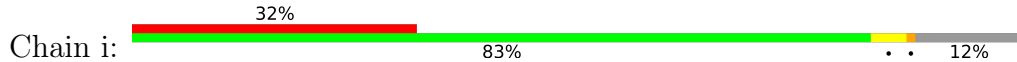
• Molecule 65: RPS3 isoform 1

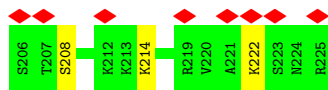


• Molecule 66: 40S ribosomal protein S4-A

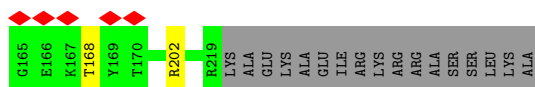
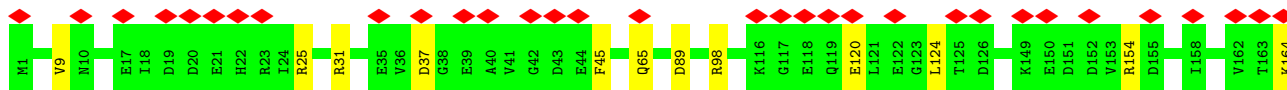
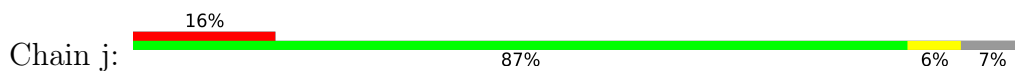


• Molecule 67: 40S ribosomal protein S5

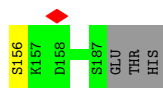
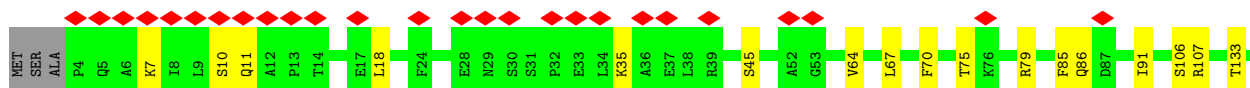
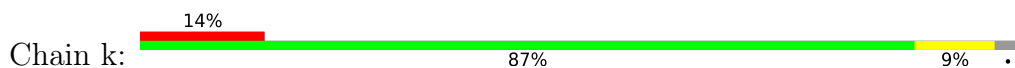




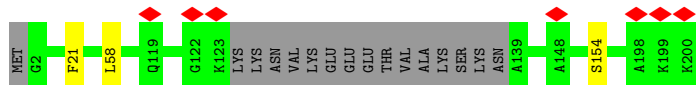
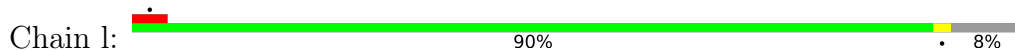
- Molecule 68: 40S ribosomal protein S6-A



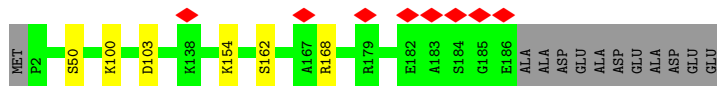
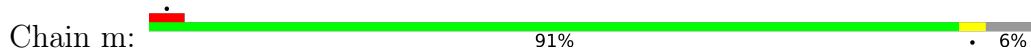
- Molecule 69: 40S ribosomal protein S7-A



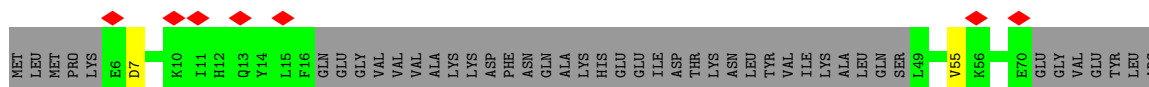
- Molecule 70: 40S ribosomal protein S8-B



- Molecule 71: 40S ribosomal protein S9-A

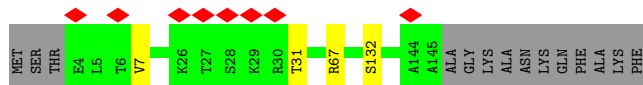
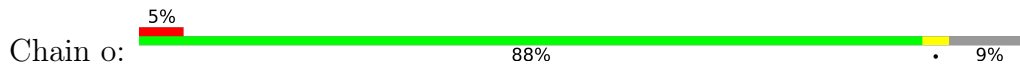


- Molecule 72: 40S ribosomal protein S10-A



GLU TYR LEU ASN LEU PRO PRG GUU HIS ILE VAL PRO GLY THR TYR ILE GLN GLU ARG ASN PRO THR GLN ARG ARG PRO GLN ARG ARG TYR

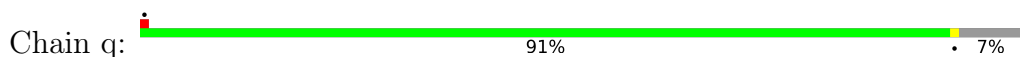
• Molecule 73: 40S ribosomal protein S11-A



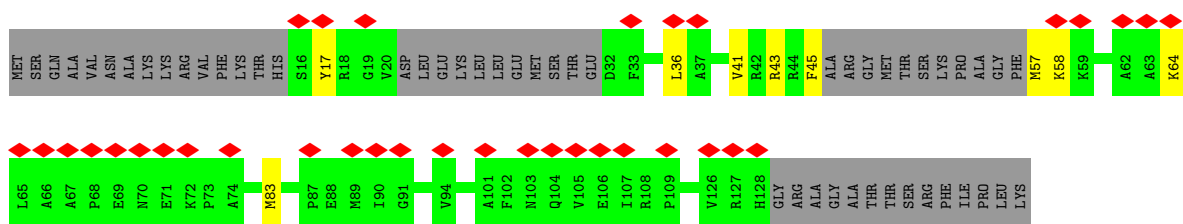
• Molecule 74: 40S ribosomal protein S13



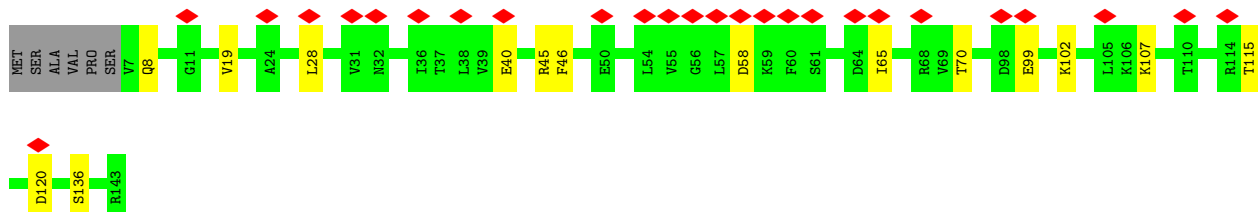
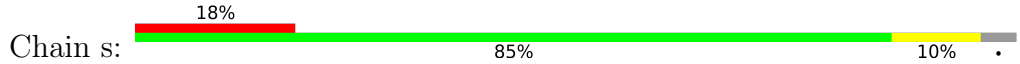
• Molecule 75: 40S ribosomal protein S14-A



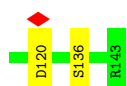
• Molecule 76: 40S ribosomal protein S15



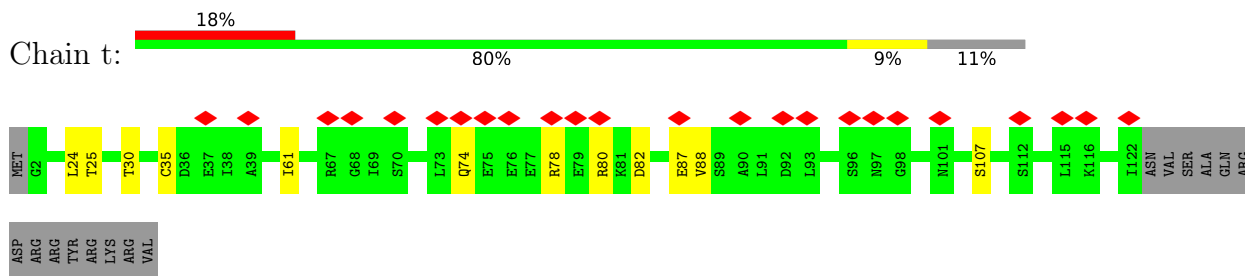
• Molecule 77: 40S ribosomal protein S16-A



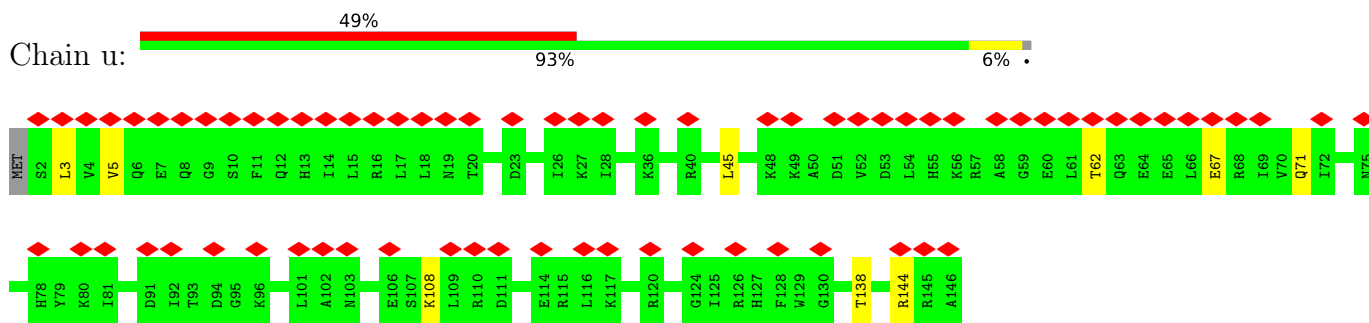
• Molecule 78: 40S ribosomal protein S17-A



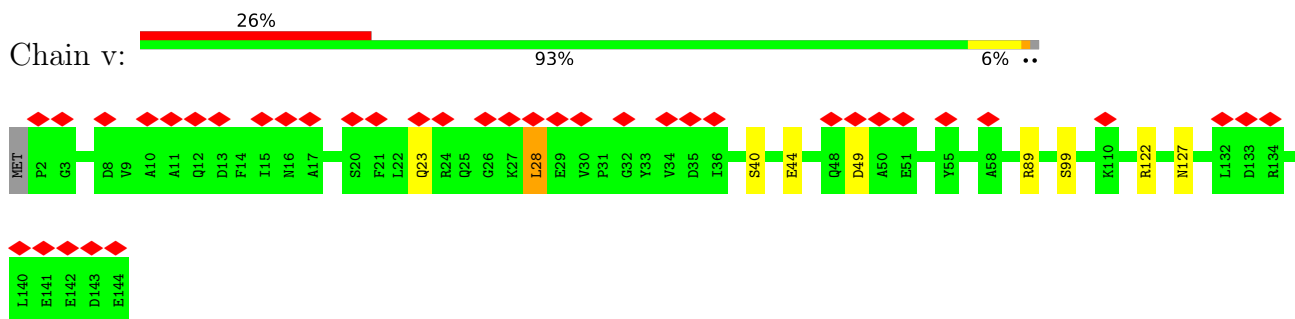




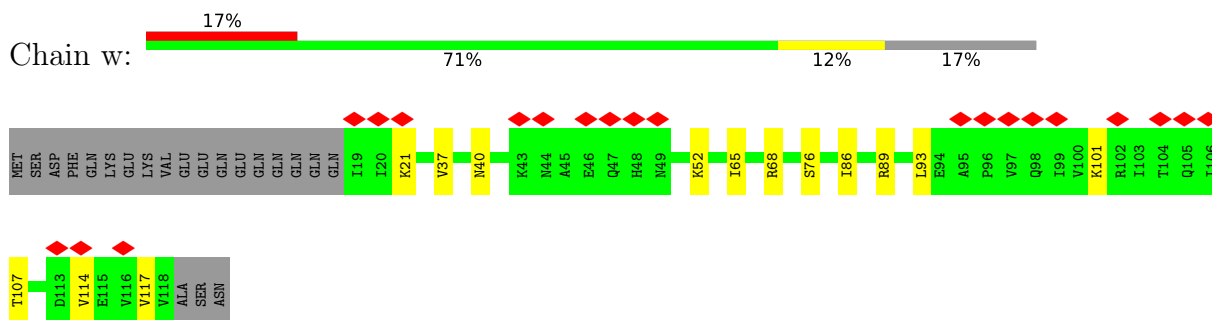
• Molecule 79: 40S ribosomal protein S18-A



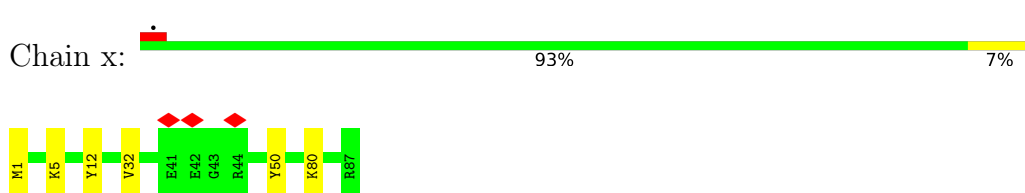
• Molecule 80: 40S ribosomal protein S19-A



• Molecule 81: 40S ribosomal protein S20



• Molecule 82: 40S ribosomal protein S21-A



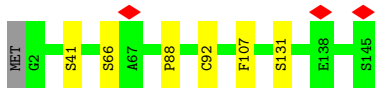
• Molecule 83: 40S ribosomal protein S22-A

Chain y:  96% ..



- Molecule 84: 40S ribosomal protein S23-A

Chain z:  95% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	270000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.697	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.161	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MA6, PO4, ZN, B8N, DDE, 1MA, 5MC, UR3, A2M, SO1, 4AC, SPD, K, YYG, OMG, G7M, OMU, GDP, OMC

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	0	0.28	0/1087	0.59	1/1449 (0.1%)
2	1	0.24	0/571	0.57	0/768
3	2	0.27	0/782	0.59	0/1047
4	3	0.27	0/620	0.56	0/838
5	4	0.27	0/499	0.63	0/670
6	5	0.27	0/412	0.61	0/544
7	6	0.26	0/433	0.65	0/575
8	7	0.26	0/2489	0.56	0/3389
9	8	0.23	0/279	0.52	0/369
10	A	0.29	0/1585	0.53	0/2128
11	AA	0.63	6/75545 (0.0%)	0.81	44/117782 (0.0%)
12	Aa	0.26	0/6470	0.53	0/8759
13	B	0.29	0/1245	0.53	0/1676
14	BB	0.34	0/2883	0.75	0/4491
15	Bb	0.26	0/1788	0.90	1/2786 (0.0%)
16	C	0.29	0/1465	0.56	0/1965
17	CC	0.39	0/3746	0.77	0/5832
18	Cc	0.34	1/1836 (0.1%)	0.78	0/2859
19	D	0.25	0/1440	0.56	0/1921
20	DD	0.26	0/1558	0.51	0/2107
21	Dd	0.24	0/138	0.76	0/212
22	E	0.29	0/1481	0.57	0/1990
23	EE	0.30	0/1948	0.57	0/2617
24	Ee	0.64	2/1210 (0.2%)	0.80	2/1627 (0.1%)
25	F	0.28	0/1300	0.52	0/1743
26	FF	0.29	0/3146	0.55	0/4228
27	G	0.28	0/786	0.52	0/1065
28	GG	0.27	0/2800	0.53	0/3790
29	H	0.29	0/978	0.56	0/1316
30	HH	0.28	0/2425	0.52	0/3271
31	I	0.29	0/533	0.52	0/707

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	II	0.28	0/1251	0.53	0/1682
33	J	0.29	0/974	0.52	0/1314
34	JJ	0.29	0/1821	0.53	1/2451 (0.0%)
35	K	0.27	0/1004	0.55	0/1341
36	KK	0.27	0/1836	0.48	0/2481
37	L	0.29	0/1118	0.49	0/1497
38	LL	0.28	0/1539	0.52	0/2073
39	M	0.28	0/1204	0.54	0/1612
40	MM	0.28	0/1779	0.55	0/2386
41	N	0.27	0/473	0.48	0/629
42	NN	0.27	0/1374	0.58	0/1842
43	O	0.28	0/750	0.46	0/1008
44	OO	0.27	0/1568	0.57	0/2106
45	P	0.27	0/897	0.56	0/1205
46	PP	0.27	0/1068	0.51	0/1438
47	Pp	0.35	0/19	0.71	0/23
48	Q	0.27	0/1041	0.51	0/1394
49	QQ	0.30	0/1757	0.58	0/2354
50	R	0.31	0/868	0.56	0/1168
51	S	0.28	0/871	0.57	0/1164
52	T	0.27	0/978	0.51	0/1301
53	U	0.26	0/778	0.59	0/1034
54	V	0.28	0/680	0.62	0/901
55	W	0.29	0/618	0.59	0/826
56	X	0.27	0/443	0.64	0/588
57	Y	0.26	0/423	0.54	0/562
58	Z	0.26	0/234	0.69	0/300
59	a	0.29	0/831	0.58	0/1097
60	b	0.27	0/701	0.57	0/934
61	c	0.31	0/37760	0.80	22/58811 (0.0%)
62	d	0.27	0/1623	0.52	0/2222
63	e	0.27	0/1714	0.55	0/2308
64	f	0.28	0/1665	0.55	0/2263
65	g	0.27	0/1429	0.58	0/1913
66	h	0.27	0/2097	0.55	0/2823
67	i	0.26	0/1591	0.60	1/2151 (0.0%)
68	j	0.25	0/1790	0.58	1/2393 (0.0%)
69	k	0.27	0/1506	0.60	1/2028 (0.0%)
70	l	0.27	0/1482	0.58	0/1980
71	m	0.26	0/1519	0.54	0/2035
72	n	0.26	0/309	0.48	0/416
73	o	0.28	0/1172	0.55	0/1580
74	p	0.27	0/1215	0.52	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	q	0.26	0/901	0.61	0/1217
76	r	0.26	0/747	0.59	0/1002
77	s	0.27	0/1099	0.54	0/1473
78	t	0.25	0/971	0.57	0/1303
79	u	0.24	0/1211	0.57	0/1628
80	v	0.26	0/1130	0.58	1/1517 (0.1%)
81	w	0.26	0/810	0.54	0/1095
82	x	0.28	0/693	0.55	0/935
83	y	0.29	0/1038	0.56	0/1395
84	z	0.26	0/1139	0.55	0/1518
All	All	0.44	9/218987 (0.0%)	0.72	75/320876 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	D	0	1
26	FF	0	1
34	JJ	0	2
37	L	0	2
54	V	0	1
59	a	0	1
63	e	0	2
67	i	0	1
69	k	0	3
77	s	0	1
84	z	0	1
All	All	0	16

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1236	G	N3-C4	73.32	1.86	1.35
11	AA	1236	G	C2-N3	65.52	1.85	1.32
11	AA	1236	G	C6-N1	53.02	1.76	1.39
11	AA	1236	G	N1-C2	47.08	1.75	1.37
11	AA	1236	G	C5-C4	45.13	1.70	1.38

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1236	G	C2-N3-C4	25.38	124.59	111.90
11	AA	1236	G	N3-C4-C5	-23.48	116.86	128.60
11	AA	1236	G	N3-C4-N9	21.57	138.94	126.00
24	Ee	16	ARG	CD-NE-CZ	21.19	153.26	123.60
11	AA	1236	G	N1-C2-N3	-21.09	111.24	123.90

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	D	130	ASN	Peptide
26	FF	349	LYS	Peptide
34	JJ	158	LYS	Peptide
34	JJ	232	ARG	Peptide
37	L	101	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	127 (96%)	5 (4%)	0	100	100
2	1	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
3	2	95/119 (80%)	88 (93%)	6 (6%)	1 (1%)	14	5
4	3	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
5	4	61/67 (91%)	61 (100%)	0	0	100	100
6	5	47/56 (84%)	47 (100%)	0	0	100	100
7	6	51/63 (81%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	316/319 (99%)	297 (94%)	19 (6%)	0	100	100
9	8	32/152 (21%)	20 (62%)	12 (38%)	0	100	100
10	A	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
12	Aa	811/842 (96%)	787 (97%)	24 (3%)	0	100	100
13	B	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
16	C	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
19	D	174/189 (92%)	170 (98%)	3 (2%)	1 (1%)	25	15
20	DD	195/312 (62%)	194 (100%)	1 (0%)	0	100	100
22	E	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
23	EE	250/254 (98%)	245 (98%)	5 (2%)	0	100	100
24	Ee	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
25	F	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
26	FF	384/387 (99%)	375 (98%)	9 (2%)	0	100	100
27	G	95/121 (78%)	94 (99%)	1 (1%)	0	100	100
28	GG	359/362 (99%)	344 (96%)	15 (4%)	0	100	100
29	H	127/137 (93%)	125 (98%)	2 (2%)	0	100	100
30	HH	294/297 (99%)	287 (98%)	7 (2%)	0	100	100
31	I	61/155 (39%)	61 (100%)	0	0	100	100
32	II	151/176 (86%)	146 (97%)	5 (3%)	0	100	100
33	J	118/142 (83%)	115 (98%)	3 (2%)	0	100	100
34	JJ	220/244 (90%)	212 (96%)	7 (3%)	1 (0%)	29	18
35	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
36	KK	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
37	L	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
38	LL	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
39	M	146/149 (98%)	139 (95%)	6 (4%)	1 (1%)	22	12
40	MM	213/221 (96%)	206 (97%)	7 (3%)	0	100	100
41	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
42	NN	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
43	O	95/105 (90%)	95 (100%)	0	0	100	100
44	OO	191/199 (96%)	176 (92%)	14 (7%)	1 (0%)	29	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	P	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
46	PP	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
48	Q	125/130 (96%)	125 (100%)	0	0	100	100
49	QQ	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
50	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
51	S	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
52	T	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
53	U	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
54	V	82/88 (93%)	77 (94%)	4 (5%)	1 (1%)	13	5
55	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
56	X	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
57	Y	50/128 (39%)	50 (100%)	0	0	100	100
58	Z	23/25 (92%)	23 (100%)	0	0	100	100
59	a	100/106 (94%)	95 (95%)	5 (5%)	0	100	100
60	b	89/92 (97%)	89 (100%)	0	0	100	100
62	d	204/252 (81%)	193 (95%)	11 (5%)	0	100	100
63	e	210/255 (82%)	199 (95%)	11 (5%)	0	100	100
64	f	215/254 (85%)	204 (95%)	11 (5%)	0	100	100
65	g	177/240 (74%)	168 (95%)	9 (5%)	0	100	100
66	h	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
67	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
68	j	217/236 (92%)	207 (95%)	10 (5%)	0	100	100
69	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
70	l	180/200 (90%)	169 (94%)	11 (6%)	0	100	100
71	m	183/197 (93%)	176 (96%)	7 (4%)	0	100	100
72	n	29/105 (28%)	25 (86%)	4 (14%)	0	100	100
73	o	140/156 (90%)	132 (94%)	8 (6%)	0	100	100
74	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
75	q	125/137 (91%)	115 (92%)	10 (8%)	0	100	100
76	r	85/142 (60%)	84 (99%)	1 (1%)	0	100	100
77	s	135/143 (94%)	127 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	t	119/136 (88%)	112 (94%)	7 (6%)	0	100	100
79	u	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
80	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
81	w	98/121 (81%)	98 (100%)	0	0	100	100
82	x	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
83	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
84	z	142/145 (98%)	129 (91%)	13 (9%)	0	100	100
All	All	11673/13056 (89%)	11237 (96%)	430 (4%)	6 (0%)	54	45

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	JJ	159	GLN
39	M	78	LEU
44	OO	63	VAL
54	V	65	ARG
3	2	47	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	112/113 (99%)	105 (94%)	7 (6%)	18	9
2	1	61/89 (68%)	53 (87%)	8 (13%)	4	1
3	2	83/101 (82%)	78 (94%)	5 (6%)	19	11
4	3	70/71 (99%)	69 (99%)	1 (1%)	67	65
5	4	56/60 (93%)	48 (86%)	8 (14%)	3	1
6	5	43/49 (88%)	39 (91%)	4 (9%)	9	3
7	6	46/54 (85%)	39 (85%)	7 (15%)	3	0
8	7	259/262 (99%)	237 (92%)	22 (8%)	10	4
9	8	30/135 (22%)	25 (83%)	5 (17%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	A	160/162 (99%)	158 (99%)	2 (1%)	69	67
12	Aa	694/714 (97%)	655 (94%)	39 (6%)	21	12
13	B	125/146 (86%)	120 (96%)	5 (4%)	31	24
16	C	150/151 (99%)	148 (99%)	2 (1%)	69	67
19	D	143/154 (93%)	139 (97%)	4 (3%)	43	37
20	DD	167/254 (66%)	157 (94%)	10 (6%)	19	11
22	E	156/156 (100%)	150 (96%)	6 (4%)	33	26
23	EE	193/196 (98%)	189 (98%)	4 (2%)	53	48
24	Ee	129/136 (95%)	114 (88%)	15 (12%)	5	1
25	F	136/137 (99%)	130 (96%)	6 (4%)	28	21
26	FF	320/323 (99%)	311 (97%)	9 (3%)	43	37
27	G	84/107 (78%)	80 (95%)	4 (5%)	25	18
28	GG	288/289 (100%)	282 (98%)	6 (2%)	53	48
29	H	101/105 (96%)	98 (97%)	3 (3%)	41	34
30	HH	244/245 (100%)	240 (98%)	4 (2%)	62	59
31	I	55/129 (43%)	53 (96%)	2 (4%)	35	28
32	II	133/153 (87%)	128 (96%)	5 (4%)	33	26
33	J	104/118 (88%)	103 (99%)	1 (1%)	76	75
34	JJ	186/205 (91%)	183 (98%)	3 (2%)	62	59
35	K	109/110 (99%)	105 (96%)	4 (4%)	34	27
36	KK	187/208 (90%)	184 (98%)	3 (2%)	62	59
37	L	115/116 (99%)	111 (96%)	4 (4%)	36	29
38	LL	171/171 (100%)	164 (96%)	7 (4%)	30	23
39	M	118/119 (99%)	110 (93%)	8 (7%)	16	8
40	MM	184/187 (98%)	179 (97%)	5 (3%)	44	38
41	N	46/47 (98%)	46 (100%)	0	100	100
42	NN	147/150 (98%)	136 (92%)	11 (8%)	13	6
43	O	81/88 (92%)	80 (99%)	1 (1%)	71	70
44	OO	154/159 (97%)	147 (96%)	7 (4%)	27	20
45	P	94/97 (97%)	94 (100%)	0	100	100
46	PP	107/109 (98%)	102 (95%)	5 (5%)	26	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Pp	2/2 (100%)	1 (50%)	1 (50%)	0	0
48	Q	109/111 (98%)	109 (100%)	0	100	100
49	QQ	175/176 (99%)	173 (99%)	2 (1%)	73	73
50	R	90/91 (99%)	88 (98%)	2 (2%)	52	46
51	S	94/103 (91%)	94 (100%)	0	100	100
52	T	104/105 (99%)	100 (96%)	4 (4%)	33	26
53	U	81/82 (99%)	76 (94%)	5 (6%)	18	10
54	V	69/71 (97%)	68 (99%)	1 (1%)	67	65
55	W	68/69 (99%)	65 (96%)	3 (4%)	28	21
56	X	45/46 (98%)	45 (100%)	0	100	100
57	Y	47/116 (40%)	47 (100%)	0	100	100
58	Z	23/23 (100%)	21 (91%)	2 (9%)	10	4
59	a	87/91 (96%)	84 (97%)	3 (3%)	37	30
60	b	71/72 (99%)	68 (96%)	3 (4%)	30	22
62	d	165/210 (79%)	157 (95%)	8 (5%)	25	18
63	e	189/224 (84%)	177 (94%)	12 (6%)	18	9
64	f	176/205 (86%)	170 (97%)	6 (3%)	37	30
65	g	145/195 (74%)	134 (92%)	11 (8%)	13	6
66	h	220/222 (99%)	204 (93%)	16 (7%)	14	6
67	i	172/191 (90%)	160 (93%)	12 (7%)	15	7
68	j	188/201 (94%)	175 (93%)	13 (7%)	15	8
69	k	165/170 (97%)	151 (92%)	14 (8%)	10	4
70	l	146/161 (91%)	143 (98%)	3 (2%)	53	48
71	m	158/166 (95%)	152 (96%)	6 (4%)	33	26
72	n	32/98 (33%)	30 (94%)	2 (6%)	18	9
73	o	127/137 (93%)	123 (97%)	4 (3%)	40	33
74	p	127/128 (99%)	124 (98%)	3 (2%)	49	42
75	q	81/105 (77%)	79 (98%)	2 (2%)	47	40
76	r	77/118 (65%)	68 (88%)	9 (12%)	5	1
77	s	114/119 (96%)	100 (88%)	14 (12%)	4	1
78	t	105/124 (85%)	93 (89%)	12 (11%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	u	128/129 (99%)	119 (93%)	9 (7%)	15	7
80	v	115/116 (99%)	106 (92%)	9 (8%)	12	5
81	w	94/114 (82%)	80 (85%)	14 (15%)	3	0
82	x	74/74 (100%)	68 (92%)	6 (8%)	11	5
83	y	110/111 (99%)	106 (96%)	4 (4%)	35	28
84	z	119/120 (99%)	114 (96%)	5 (4%)	30	22
All	All	9933/10971 (90%)	9461 (95%)	472 (5%)	29	18

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	NN	77	GLU
81	w	21	LYS
63	e	94	LYS
80	v	49	ASP
77	s	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
66	h	157	ASN
78	t	48	ASN
68	j	65	GLN
78	t	74	GLN
74	p	49	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	472 (14%)	24 (0%)
14	BB	120/121 (99%)	8 (6%)	1 (0%)
15	Bb	75/76 (98%)	36 (48%)	0
17	CC	157/158 (99%)	20 (12%)	0
18	Cc	76/77 (98%)	17 (22%)	0
21	Dd	5/39 (12%)	0	0
61	c	1593/1800 (88%)	320 (20%)	0
All	All	5219/5667 (92%)	873 (16%)	25 (0%)

5 of 873 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	4	U
11	AA	6	A
11	AA	14	U
11	AA	26	A
11	AA	40	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	2487	U
11	AA	2501	U
14	BB	72	A
11	AA	2500	A
11	AA	2535	A

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

68 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
11	A2M	AA	876	11	18,25,26	3.59	8 (44%)	18,36,39	3.35	4 (22%)
11	A2M	AA	2280	11	18,25,26	3.59	8 (44%)	18,36,39	3.36	3 (16%)
61	OMG	c	1126	61	18,26,27	1.19	2 (11%)	19,38,41	0.86	1 (5%)
11	A2M	AA	1449	11,86	18,25,26	3.60	8 (44%)	18,36,39	3.40	4 (22%)
11	OMG	AA	2793	11	18,26,27	1.18	2 (11%)	19,38,41	0.84	1 (5%)
11	OMC	AA	650	11	19,22,23	0.60	0	26,31,34	0.68	0
11	OMU	AA	2421	11	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
11	OMC	AA	2959	11,86	19,22,23	0.58	0	26,31,34	0.68	0
11	OMU	AA	2729	11	19,22,23	2.99	8 (42%)	26,31,34	1.63	5 (19%)
61	OMG	c	1572	61	18,26,27	1.13	2 (11%)	19,38,41	0.93	1 (5%)
61	OMC	c	414	61	19,22,23	0.54	0	26,31,34	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	A2M	AA	1133	11,86	18,25,26	3.60	7 (38%)	18,36,39	3.44	3 (16%)
11	UR3	AA	2634	11	19,22,23	2.83	7 (36%)	26,32,35	1.31	1 (3%)
11	OMG	AA	2922	11	18,26,27	1.20	2 (11%)	19,38,41	0.96	1 (5%)
11	A2M	AA	649	11	18,25,26	3.59	8 (44%)	18,36,39	3.35	3 (16%)
11	OMU	AA	2921	11,86	19,22,23	3.03	8 (42%)	26,31,34	1.71	5 (19%)
61	OMC	c	1639	86,61	19,22,23	0.56	0	26,31,34	0.55	0
11	OMG	AA	908	11	18,26,27	1.23	2 (11%)	19,38,41	0.89	1 (5%)
11	OMC	AA	1437	11,86	19,22,23	0.59	0	26,31,34	0.88	1 (3%)
11	5MC	AA	2870	11,87	18,22,23	0.69	0	26,32,35	0.64	0
61	A2M	c	796	61	18,25,26	3.61	8 (44%)	18,36,39	3.35	4 (22%)
11	OMC	AA	2948	11	19,22,23	0.57	0	26,31,34	0.73	1 (3%)
11	A2M	AA	2946	11,86	18,25,26	3.60	7 (38%)	18,36,39	3.30	3 (16%)
61	A2M	c	619	86,61	18,25,26	3.61	8 (44%)	18,36,39	3.39	3 (16%)
61	A2M	c	28	84,61	18,25,26	3.59	9 (50%)	18,36,39	3.41	5 (27%)
61	A2M	c	420	61	18,25,26	3.60	8 (44%)	18,36,39	3.37	4 (22%)
11	A2M	AA	2281	11	18,25,26	3.67	9 (50%)	18,36,39	3.36	4 (22%)
11	OMU	AA	898	11	19,22,23	2.99	8 (42%)	26,31,34	1.70	5 (19%)
11	OMG	AA	2288	11	18,26,27	1.18	2 (11%)	19,38,41	0.81	1 (5%)
11	A2M	AA	2256	11	18,25,26	3.60	8 (44%)	18,36,39	3.56	5 (27%)
61	OMU	c	1269	61	19,22,23	3.09	8 (42%)	26,31,34	1.71	5 (19%)
11	A2M	AA	807	11	18,25,26	3.61	8 (44%)	18,36,39	3.36	4 (22%)
11	OMG	AA	805	11	18,26,27	1.18	2 (11%)	19,38,41	0.86	1 (5%)
15	YYG	Bb	37	15	31,42,43	2.21	8 (25%)	33,62,65	1.81	10 (30%)
11	A2M	AA	2220	11	18,25,26	3.59	8 (44%)	18,36,39	3.37	3 (16%)
11	OMU	AA	2417	11	19,22,23	2.99	8 (42%)	26,31,34	1.70	5 (19%)
61	OMG	c	1428	61	18,26,27	1.13	2 (11%)	19,38,41	0.83	1 (5%)
61	MA6	c	1782	61	18,26,27	1.03	2 (11%)	19,38,41	3.47	2 (10%)
61	OMG	c	1271	61	18,26,27	1.11	2 (11%)	19,38,41	0.86	1 (5%)
12	DDE	Aa	699	12	14,20,21	1.01	1 (7%)	14,28,30	1.17	1 (7%)
61	OMC	c	1007	61	19,22,23	0.56	0	26,31,34	0.65	0
11	OMU	AA	1888	11	19,22,23	3.02	8 (42%)	26,31,34	1.82	6 (23%)
61	A2M	c	436	61	18,25,26	3.61	8 (44%)	18,36,39	3.39	3 (16%)
11	OMC	AA	663	11	19,22,23	0.58	0	26,31,34	0.75	0
11	A2M	AA	817	11,86	18,25,26	3.58	7 (38%)	18,36,39	3.53	3 (16%)
61	A2M	c	541	61	18,25,26	3.58	8 (44%)	18,36,39	3.32	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	OMG	AA	2619	11,15	18,26,27	1.18	2 (11%)	19,38,41	0.86	1 (5%)
11	OMG	AA	2815	11	18,26,27	1.16	2 (11%)	19,38,41	0.81	1 (5%)
11	1MA	AA	645	11,86	16,25,26	0.95	2 (12%)	18,37,40	1.08	2 (11%)
11	OMC	AA	2197	11,87	19,22,23	0.55	0	26,31,34	0.58	0
11	OMC	AA	2337	11	19,22,23	0.56	0	26,31,34	0.62	0
61	4AC	c	1280	61	21,24,25	3.56	10 (47%)	29,34,37	1.63	5 (17%)
11	OMU	AA	2724	11	19,22,23	2.99	8 (42%)	26,31,34	1.69	5 (19%)
11	OMG	AA	2791	11	18,26,27	1.15	2 (11%)	19,38,41	0.83	1 (5%)
11	OMG	AA	867	11,87	18,26,27	1.19	2 (11%)	19,38,41	0.90	1 (5%)
61	4AC	c	1773	61	21,24,25	3.39	10 (47%)	29,34,37	1.51	6 (20%)
61	OMU	c	578	61	19,22,23	3.09	8 (42%)	26,31,34	1.68	5 (19%)
61	A2M	c	100	86,61	18,25,26	3.61	8 (44%)	18,36,39	3.34	4 (22%)
61	MA6	c	1781	61	18,26,27	1.05	2 (11%)	19,38,41	3.37	2 (10%)
11	A2M	AA	2640	11	18,25,26	3.59	8 (44%)	18,36,39	3.32	4 (22%)
61	B8N	c	1191	61	24,29,30	3.05	6 (25%)	29,42,45	1.76	6 (20%)
61	OMG	c	562	7,61	18,26,27	1.12	2 (11%)	19,38,41	0.86	1 (5%)
11	1MA	AA	2142	11,86	16,25,26	0.98	2 (12%)	18,37,40	1.13	2 (11%)
61	G7M	c	1575	18,61	20,26,27	2.40	7 (35%)	17,39,42	1.15	1 (5%)
61	A2M	c	974	61	18,25,26	3.60	7 (38%)	18,36,39	3.35	3 (16%)
11	5MC	AA	2278	11,86	18,22,23	0.59	0	26,32,35	0.62	0
11	OMU	AA	2347	11	19,22,23	3.04	8 (42%)	26,31,34	1.73	5 (19%)
11	OMG	AA	1450	11	18,26,27	1.13	2 (11%)	19,38,41	0.80	1 (5%)

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
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2280	11	-	0/5/27/28	0/3/3/3
61	OMG	c	1126	61	-	0/5/27/28	0/3/3/3
11	A2M	AA	1449	11,86	-	0/5/27/28	0/3/3/3
11	OMG	AA	2793	11	-	2/5/27/28	0/3/3/3
11	OMC	AA	650	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2959	11,86	-	0/9/27/28	0/2/2/2
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	OMG	c	1572	61	-	3/5/27/28	0/3/3/3
61	OMC	c	414	61	-	1/9/27/28	0/2/2/2
11	A2M	AA	1133	11,86	-	0/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
11	OMG	AA	2922	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2921	11,86	-	0/9/27/28	0/2/2/2
61	OMC	c	1639	86,61	-	0/9/27/28	0/2/2/2
11	OMG	AA	908	11	-	1/5/27/28	0/3/3/3
11	OMC	AA	1437	11,86	-	2/9/27/28	0/2/2/2
11	5MC	AA	2870	11,87	-	4/7/25/26	0/2/2/2
61	A2M	c	796	61	-	0/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2946	11,86	-	0/5/27/28	0/3/3/3
61	A2M	c	619	86,61	-	3/5/27/28	0/3/3/3
61	A2M	c	28	84,61	-	2/5/27/28	0/3/3/3
61	A2M	c	420	61	-	2/5/27/28	0/3/3/3
11	A2M	AA	2281	11	-	3/5/27/28	0/3/3/3
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2256	11	-	2/5/27/28	0/3/3/3
61	OMU	c	1269	61	-	4/9/27/28	0/2/2/2
11	A2M	AA	807	11	-	1/5/27/28	0/3/3/3
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
15	YYG	Bb	37	15	-	14/20/42/43	0/3/4/4
11	A2M	AA	2220	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
61	OMG	c	1428	61	-	1/5/27/28	0/3/3/3
61	MA6	c	1782	61	-	1/7/29/30	0/3/3/3
61	OMG	c	1271	61	-	1/5/27/28	0/3/3/3
12	DDE	Aa	699	12	-	2/20/21/23	0/1/1/1
61	OMC	c	1007	61	-	0/9/27/28	0/2/2/2
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
61	A2M	c	436	61	-	0/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	817	11,86	-	2/5/27/28	0/3/3/3
61	A2M	c	541	61	-	3/5/27/28	0/3/3/3
11	OMG	AA	2619	11,15	-	1/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1MA	AA	645	11,86	-	0/3/25/26	0/3/3/3
11	OMC	AA	2197	11,87	-	4/9/27/28	0/2/2/2
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
61	4AC	c	1280	61	-	4/11/29/30	0/2/2/2
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
11	OMG	AA	867	11,87	-	2/5/27/28	0/3/3/3
61	4AC	c	1773	61	-	2/11/29/30	0/2/2/2
61	OMU	c	578	61	-	2/9/27/28	0/2/2/2
61	A2M	c	100	86,61	-	1/5/27/28	0/3/3/3
61	MA6	c	1781	61	-	0/7/29/30	0/3/3/3
11	A2M	AA	2640	11	-	0/5/27/28	0/3/3/3
61	B8N	c	1191	61	-	6/16/34/35	0/2/2/2
61	OMG	c	562	7,61	-	1/5/27/28	0/3/3/3
11	1MA	AA	2142	11,86	-	1/3/25/26	0/3/3/3
61	G7M	c	1575	18,61	-	3/3/25/26	0/3/3/3
61	A2M	c	974	61	-	0/5/27/28	0/3/3/3
11	5MC	AA	2278	11,86	-	0/7/25/26	0/2/2/2
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3

The worst 5 of 325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	28	A2M	C3'-C4'	-9.07	1.29	1.53
11	AA	807	A2M	C3'-C4'	-8.89	1.30	1.53
61	c	541	A2M	C3'-C4'	-8.86	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.86	1.30	1.53
61	c	619	A2M	C3'-C4'	-8.86	1.30	1.53

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c	1782	MA6	N1-C6-N6	-13.89	102.43	117.06
61	c	1781	MA6	N1-C6-N6	-13.43	102.92	117.06
11	AA	817	A2M	C5-C6-N6	11.19	137.36	120.35
11	AA	1133	A2M	C5-C6-N6	10.82	136.79	120.35
11	AA	1449	A2M	C5-C6-N6	10.69	136.59	120.35

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 297 ligands modelled in this entry, 291 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
89	GDP	Aa	1001	86	24,30,30	0.93	1 (4%)	30,47,47	1.29	4 (13%)
88	SPD	AA	3614	-	9,9,9	0.33	0	8,8,8	0.94	0
88	SPD	AA	3615	-	9,9,9	0.30	0	8,8,8	0.79	0
91	SO1	Aa	1003	-	35,39,39	1.15	2 (5%)	39,64,64	1.14	3 (7%)
90	PO4	Aa	1002	86	4,4,4	1.02	0	6,6,6	0.51	0
88	SPD	AA	3613	-	9,9,9	0.32	0	8,8,8	0.90	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
89	GDP	Aa	1001	86	-	5/12/32/32	0/3/3/3
88	SPD	AA	3614	-	-	0/7/7/7	-
88	SPD	AA	3615	-	-	3/7/7/7	-
91	SO1	Aa	1003	-	-	10/21/104/104	0/7/5/5
88	SPD	AA	3613	-	-	1/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Aa	1003	SO1	C2-C6	-3.89	1.49	1.55
91	Aa	1003	SO1	C16-C22	-2.41	1.50	1.54
89	Aa	1001	GDP	C6-N1	-2.40	1.34	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	Aa	1001	GDP	PA-O3A-PB	-3.47	120.92	132.83
89	Aa	1001	GDP	C3'-C2'-C1'	2.99	105.48	100.98
91	Aa	1003	SO1	C52-O56-C56	-2.98	108.54	113.67
91	Aa	1003	SO1	C12-C6-C10	-2.64	105.82	107.91
89	Aa	1001	GDP	C8-N7-C5	2.35	107.47	102.99

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

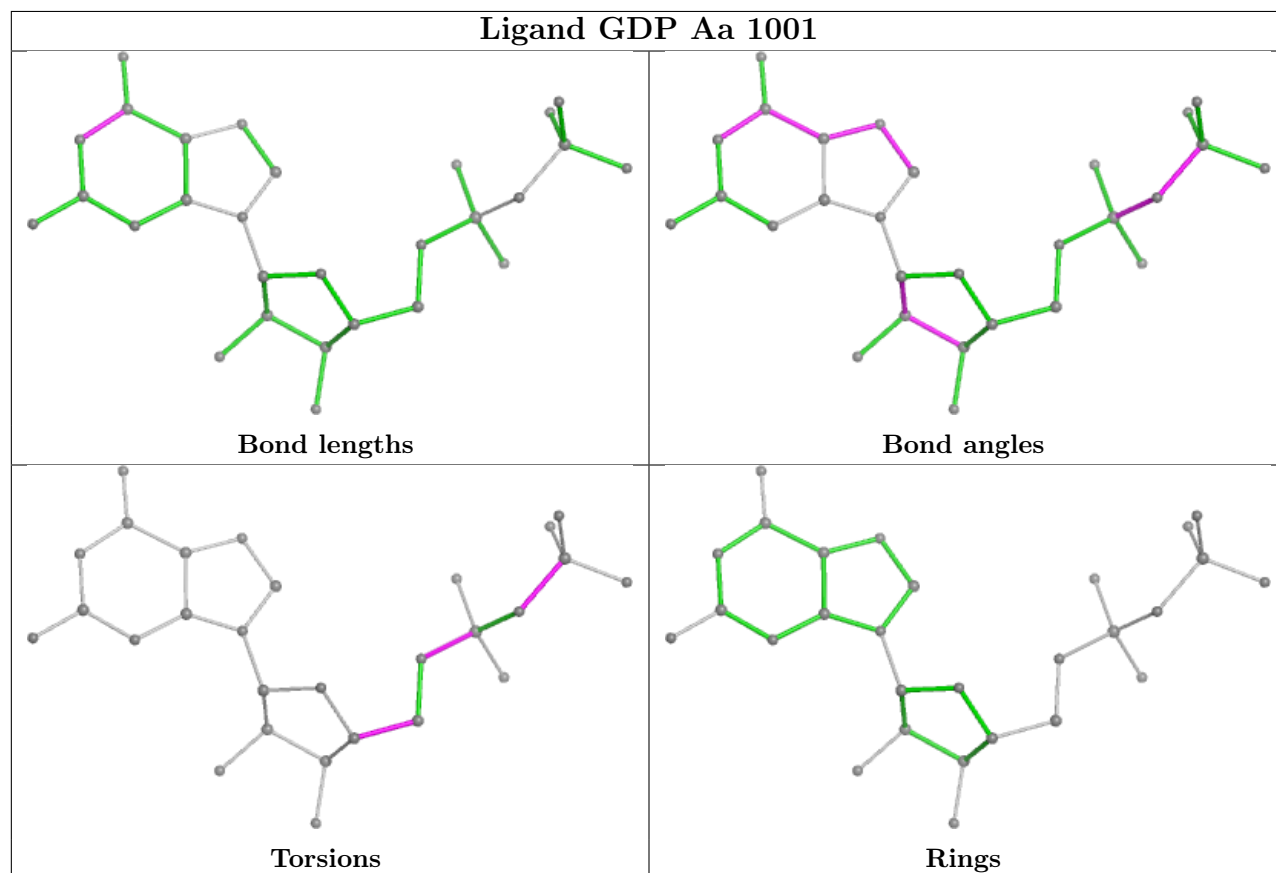
Mol	Chain	Res	Type	Atoms
89	Aa	1001	GDP	O4'-C4'-C5'-O5'
91	Aa	1003	SO1	C2-C1-C5-O14
91	Aa	1003	SO1	C2-C1-C5-O15
91	Aa	1003	SO1	C20-C13-C4-C1
91	Aa	1003	SO1	C21-C13-C4-C1

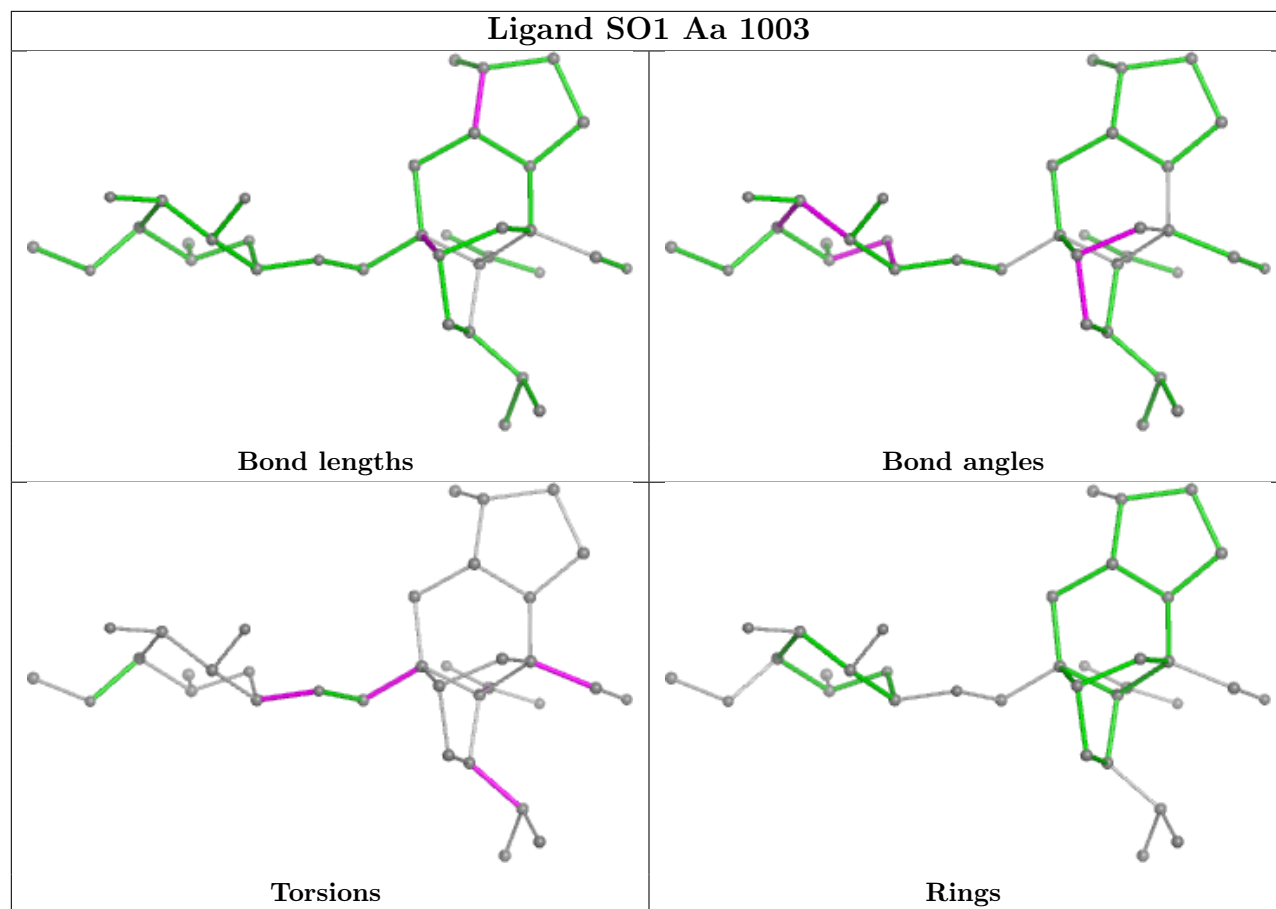
There are no ring outliers.

No monomer is involved in short contacts.

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

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

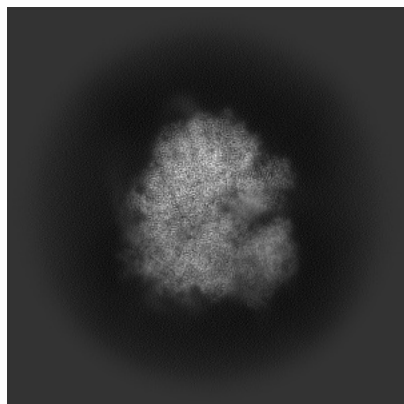
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16609. These allow visual inspection of the internal detail of the map and identification of artifacts.

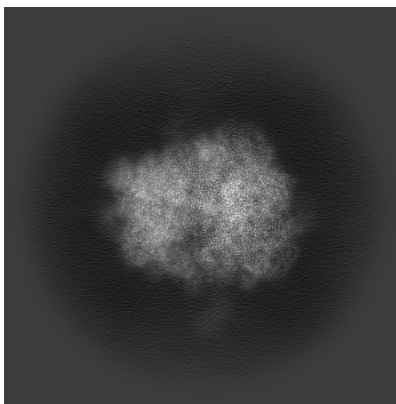
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

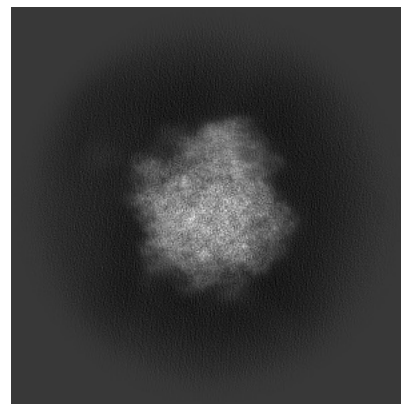
#### 6.1.1 Primary map



X

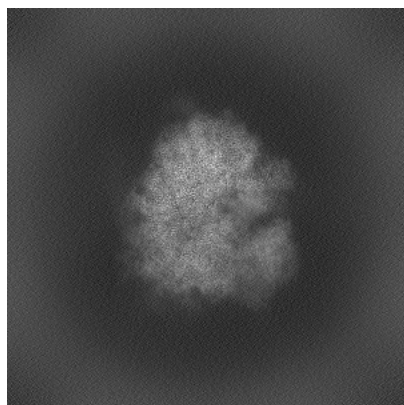


Y

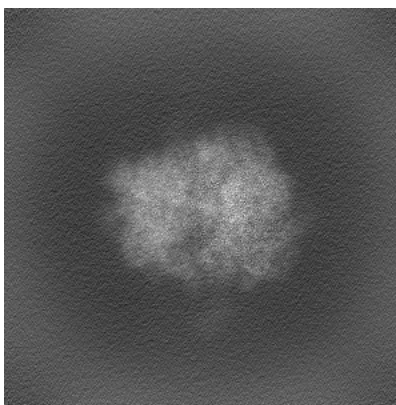


Z

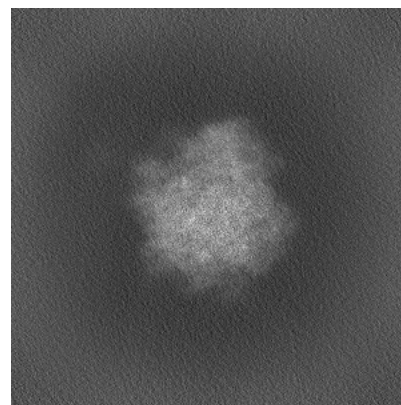
#### 6.1.2 Raw map



X



Y

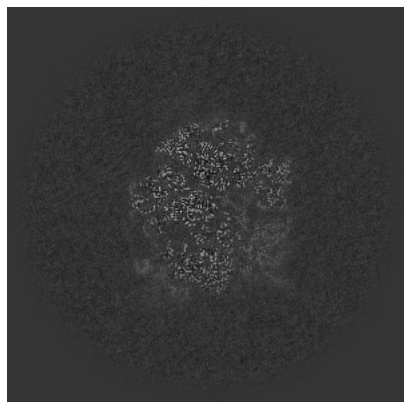


Z

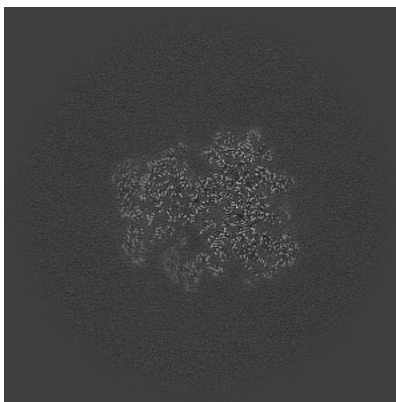
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

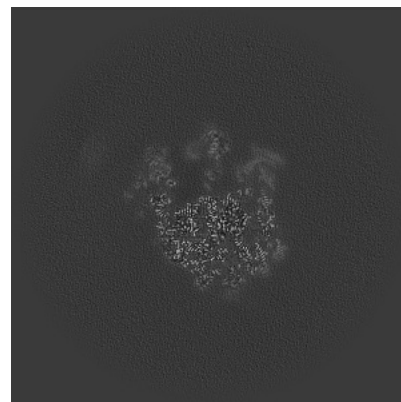
### 6.2.1 Primary map



X Index: 300

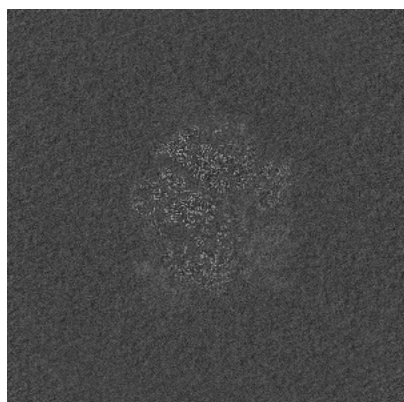


Y Index: 300

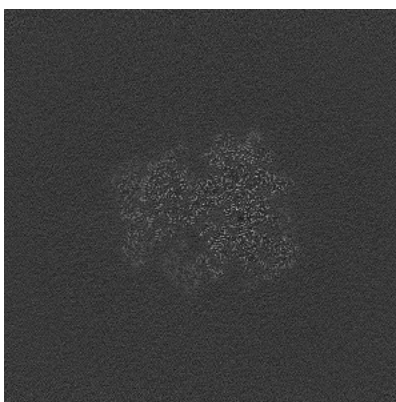


Z Index: 300

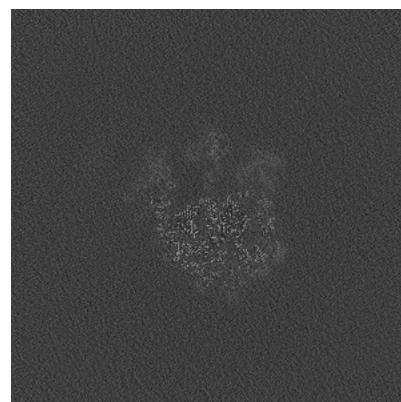
### 6.2.2 Raw map



X Index: 300



Y Index: 300



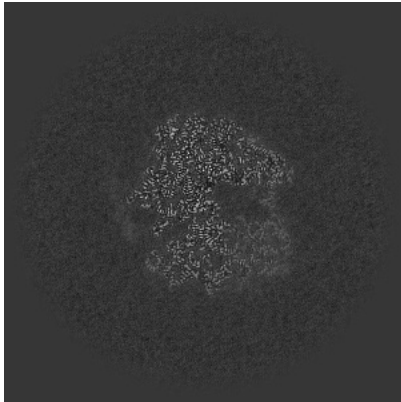
Z Index: 300

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

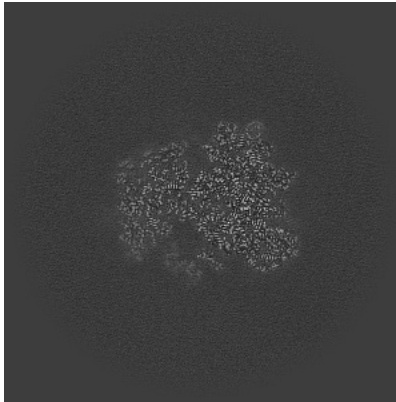


## 6.3 Largest variance slices [i](#)

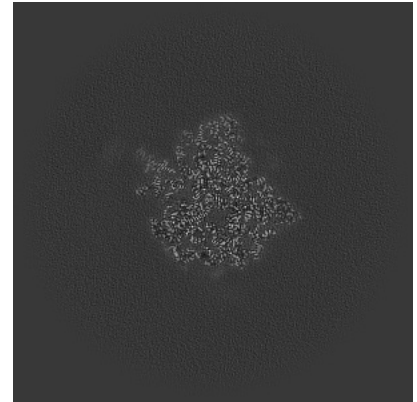
### 6.3.1 Primary map



X Index: 324

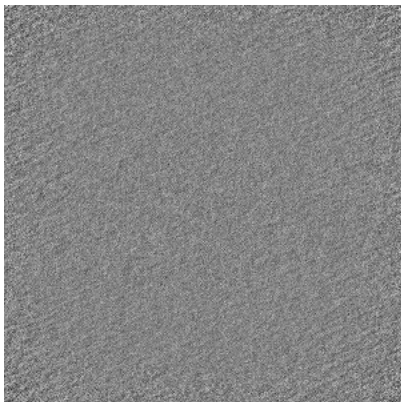


Y Index: 295

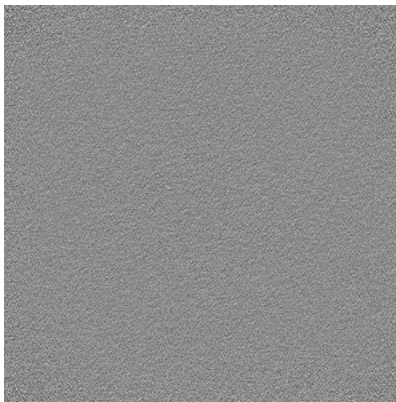


Z Index: 340

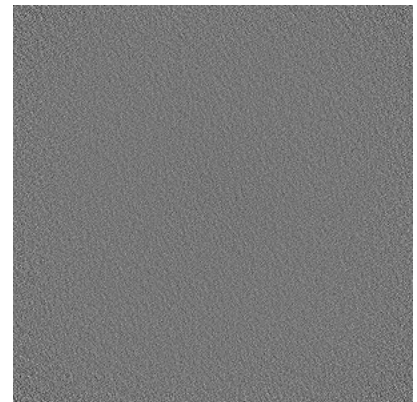
### 6.3.2 Raw map



X Index: 0



Y Index: 0

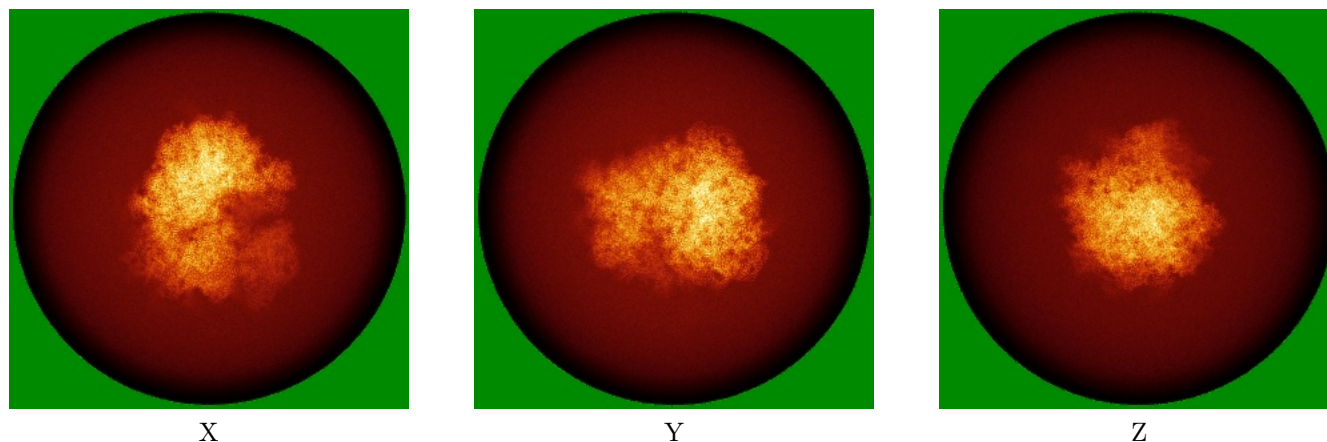


Z Index: 0

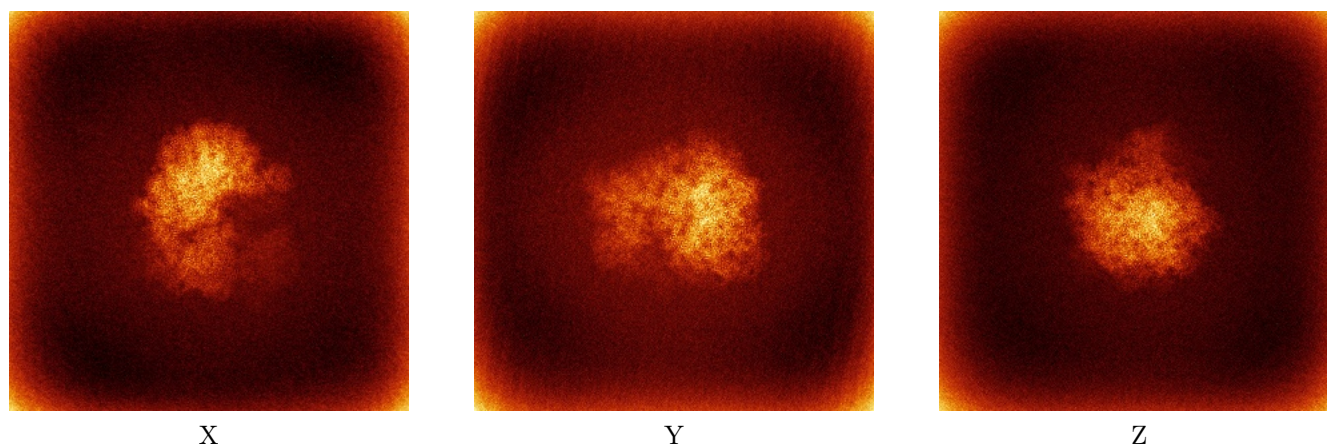
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



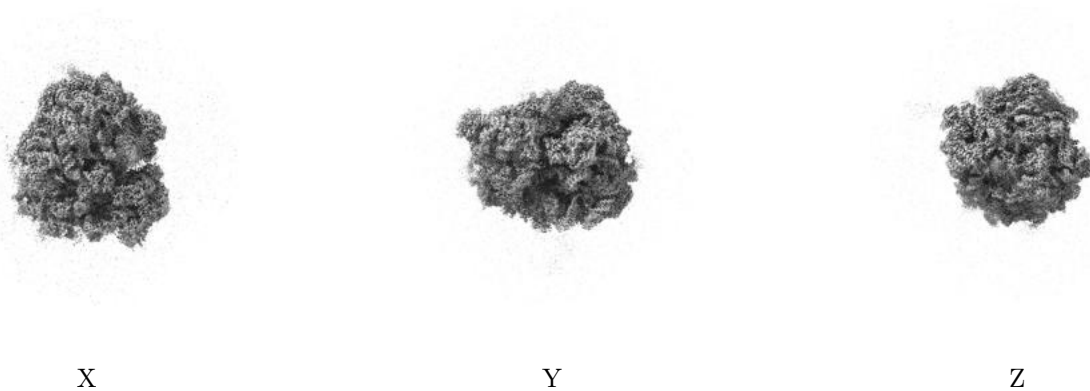
### 6.4.2 Raw map



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.

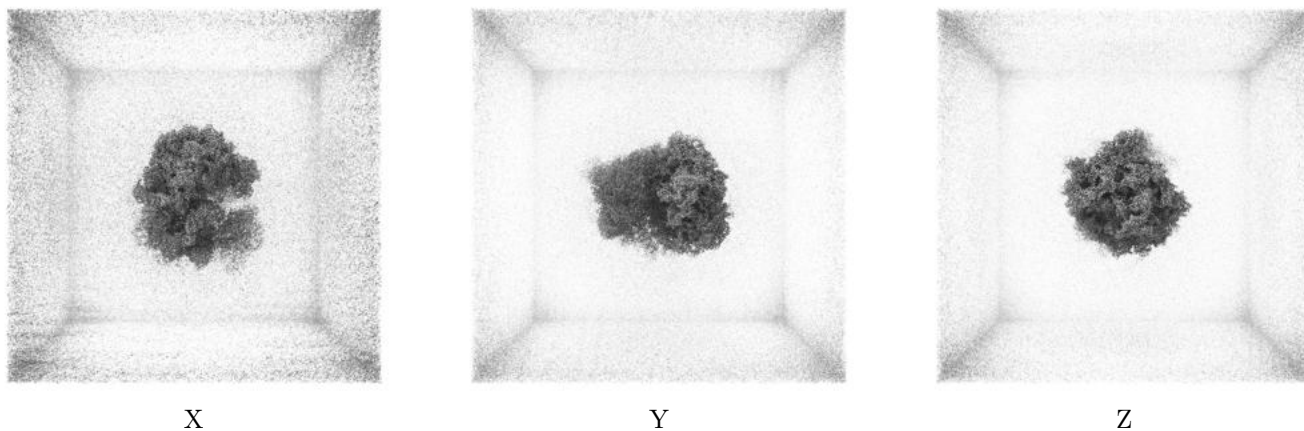
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.161. 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.

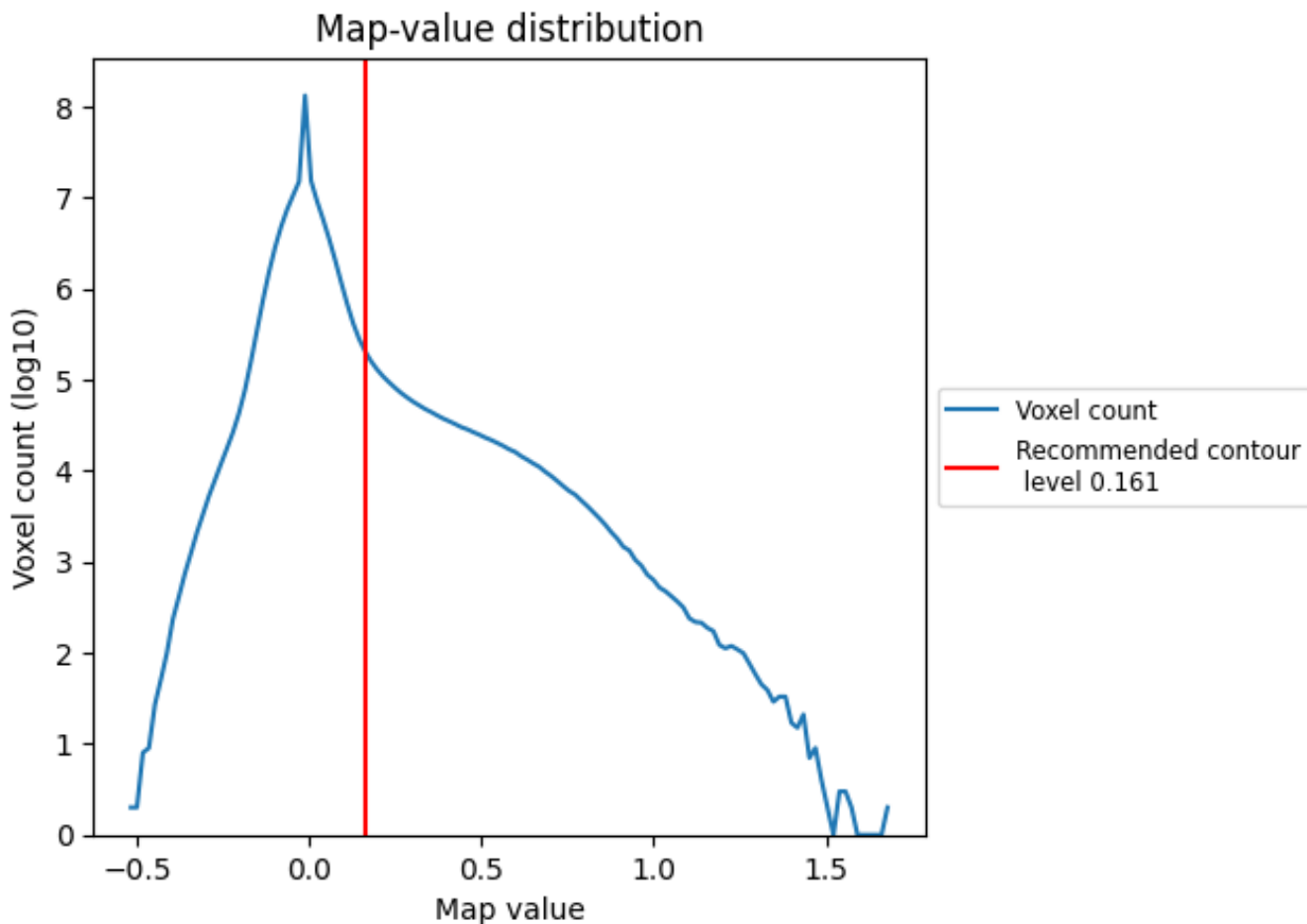
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

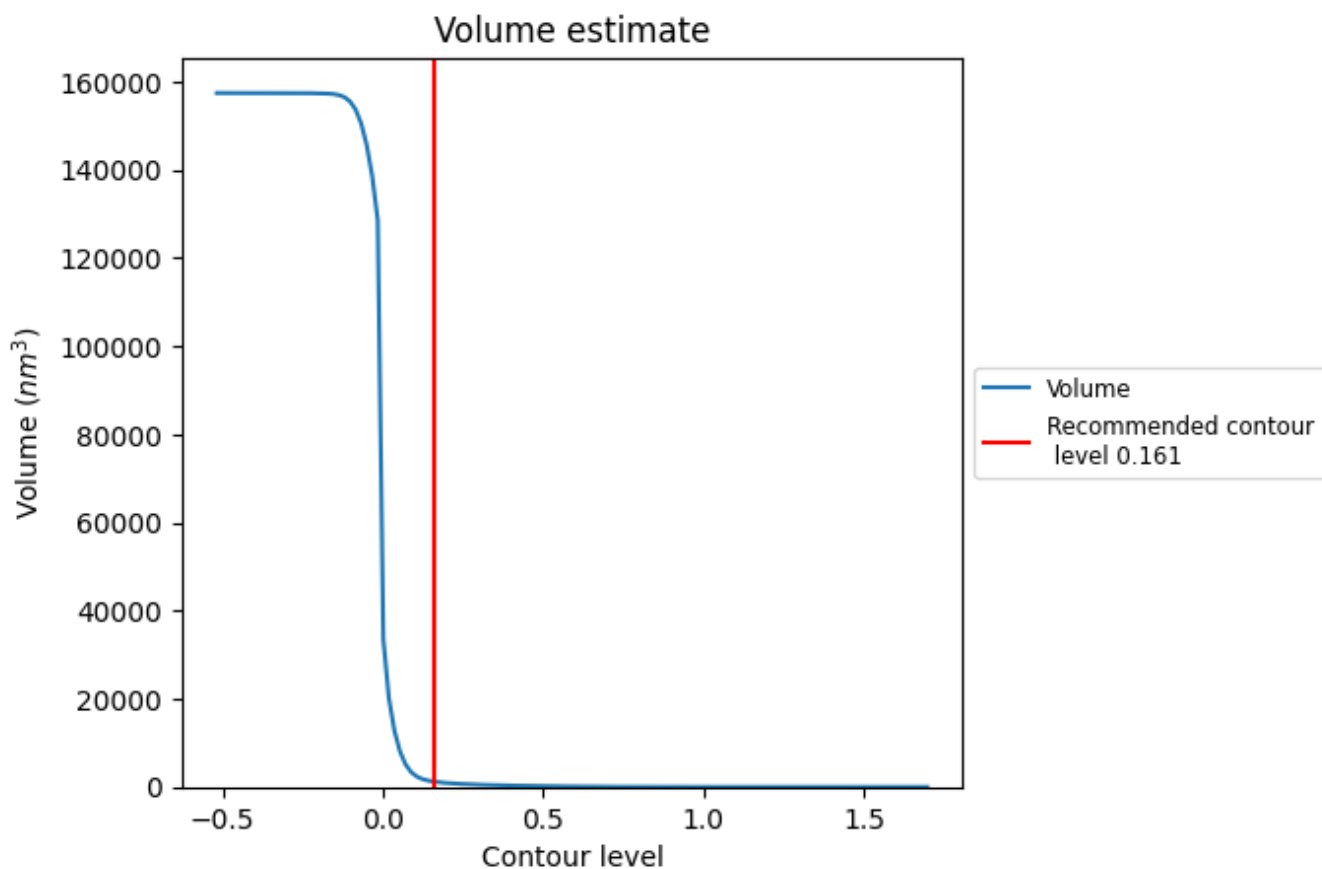
This section contains the results of statistical analysis of the map.

### 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.

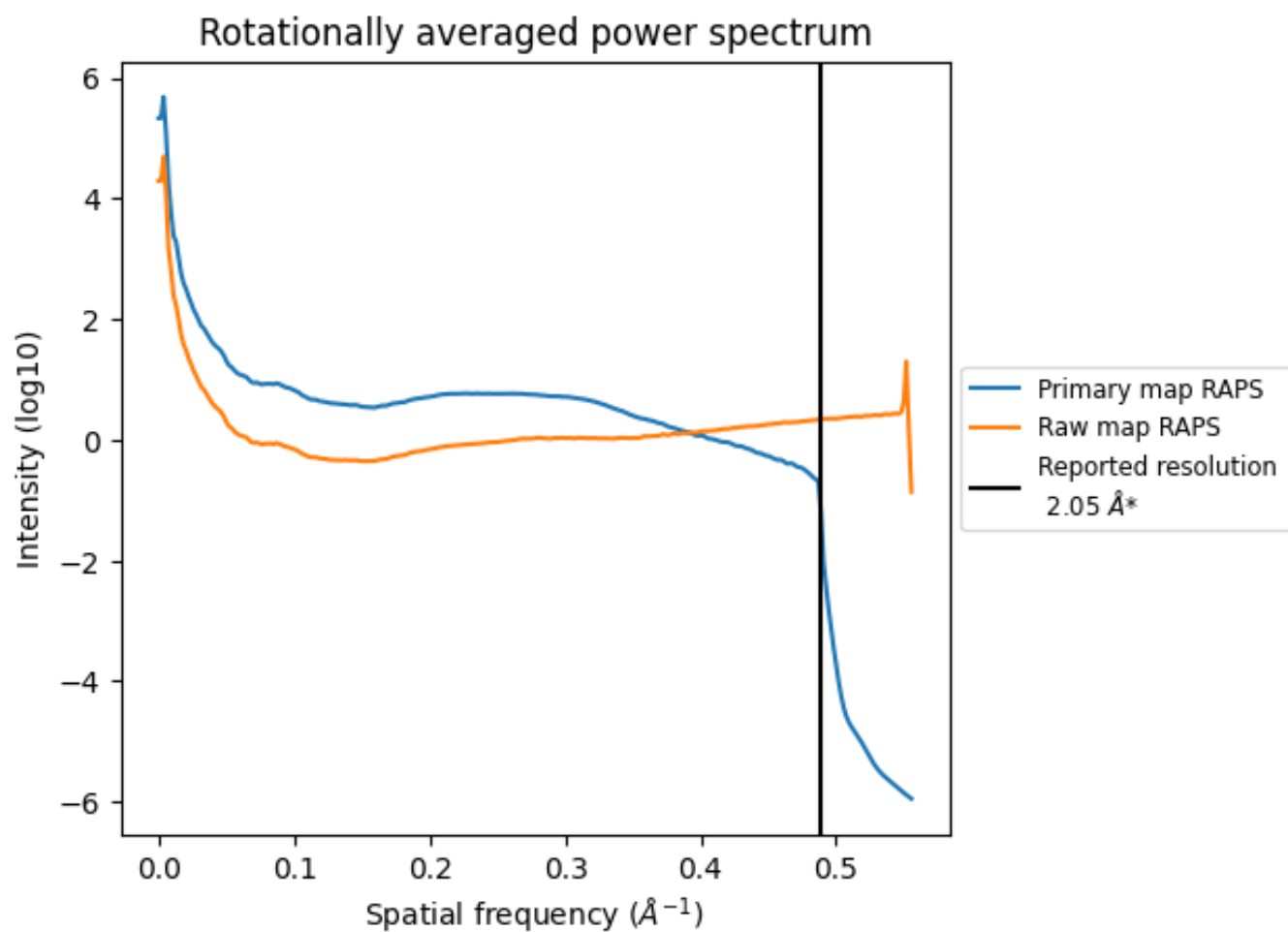
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1195 nm<sup>3</sup>; this corresponds to an approximate mass of 1079 kDa.

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

### 7.3 Rotationally averaged power spectrum i

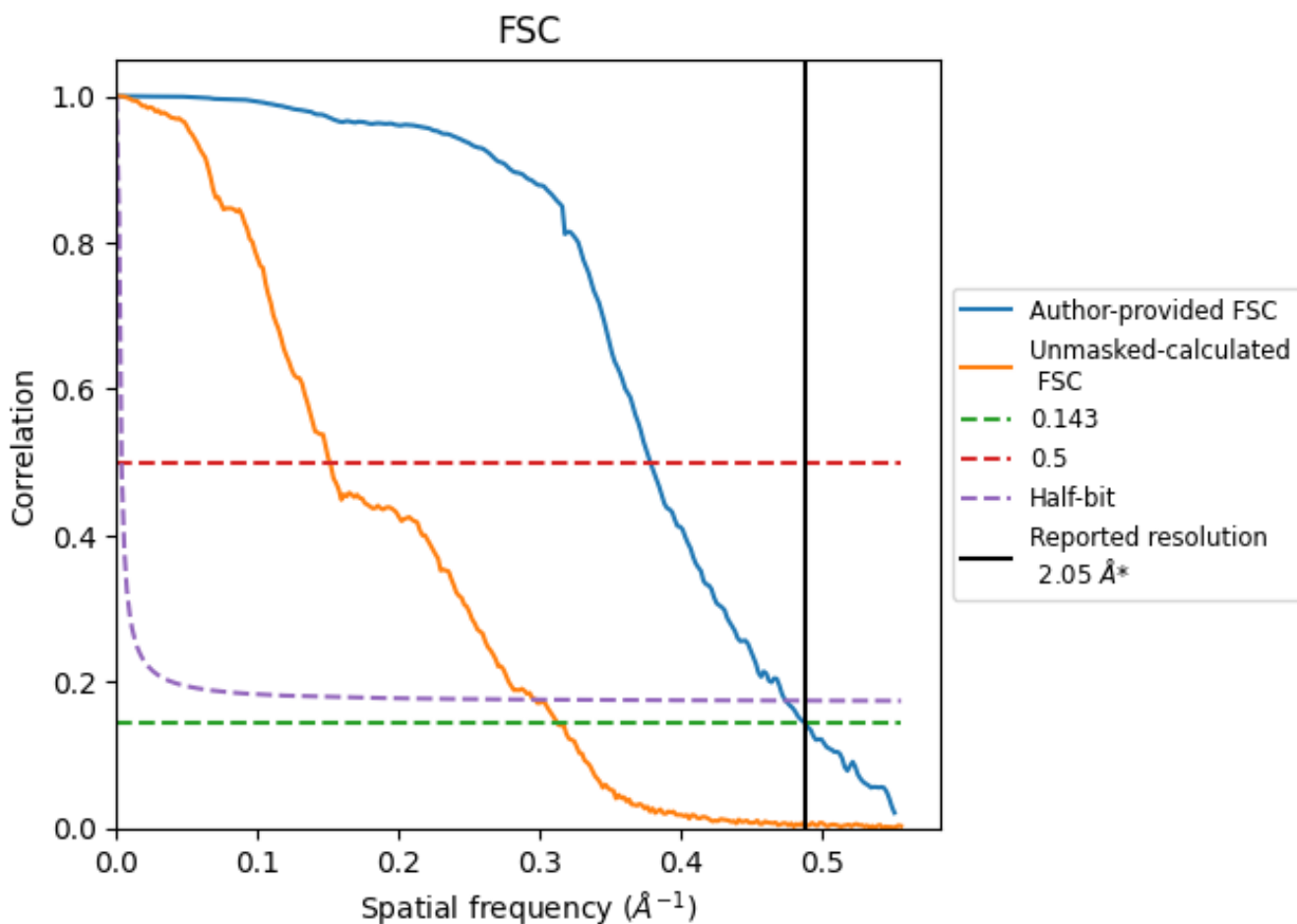


\*Reported resolution corresponds to spatial frequency of 0.488 Å<sup>-1</sup>

## 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 0.488 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.05	-	-
Author-provided FSC curve	2.05	2.65	2.11
Unmasked-calculated*	3.20	6.63	3.37

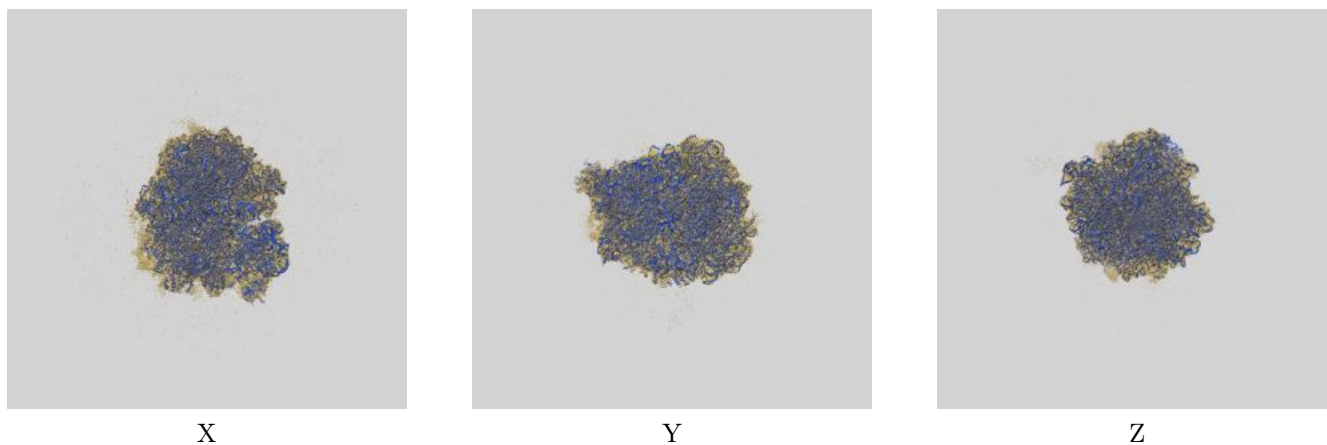
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.05 by more than 10 %



## 9 Map-model fit [i](#)

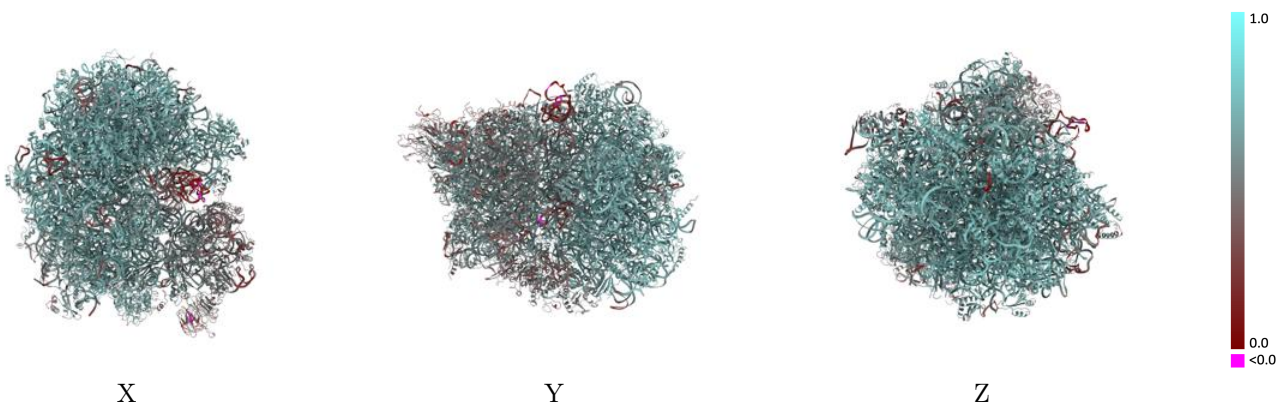
This section contains information regarding the fit between EMDB map EMD-16609 and PDB model 8CEH. Per-residue inclusion information can be found in section 3 on page 25.

### 9.1 Map-model overlay [i](#)



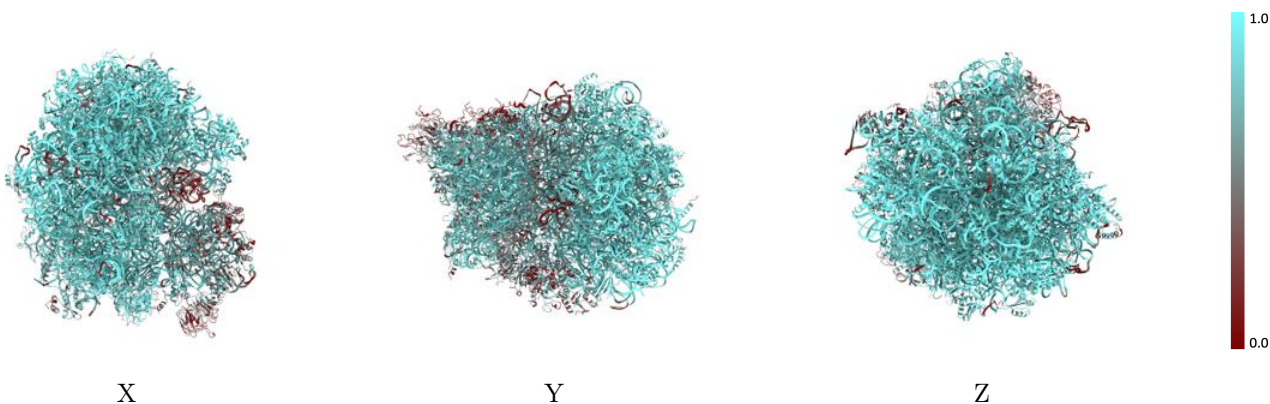
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



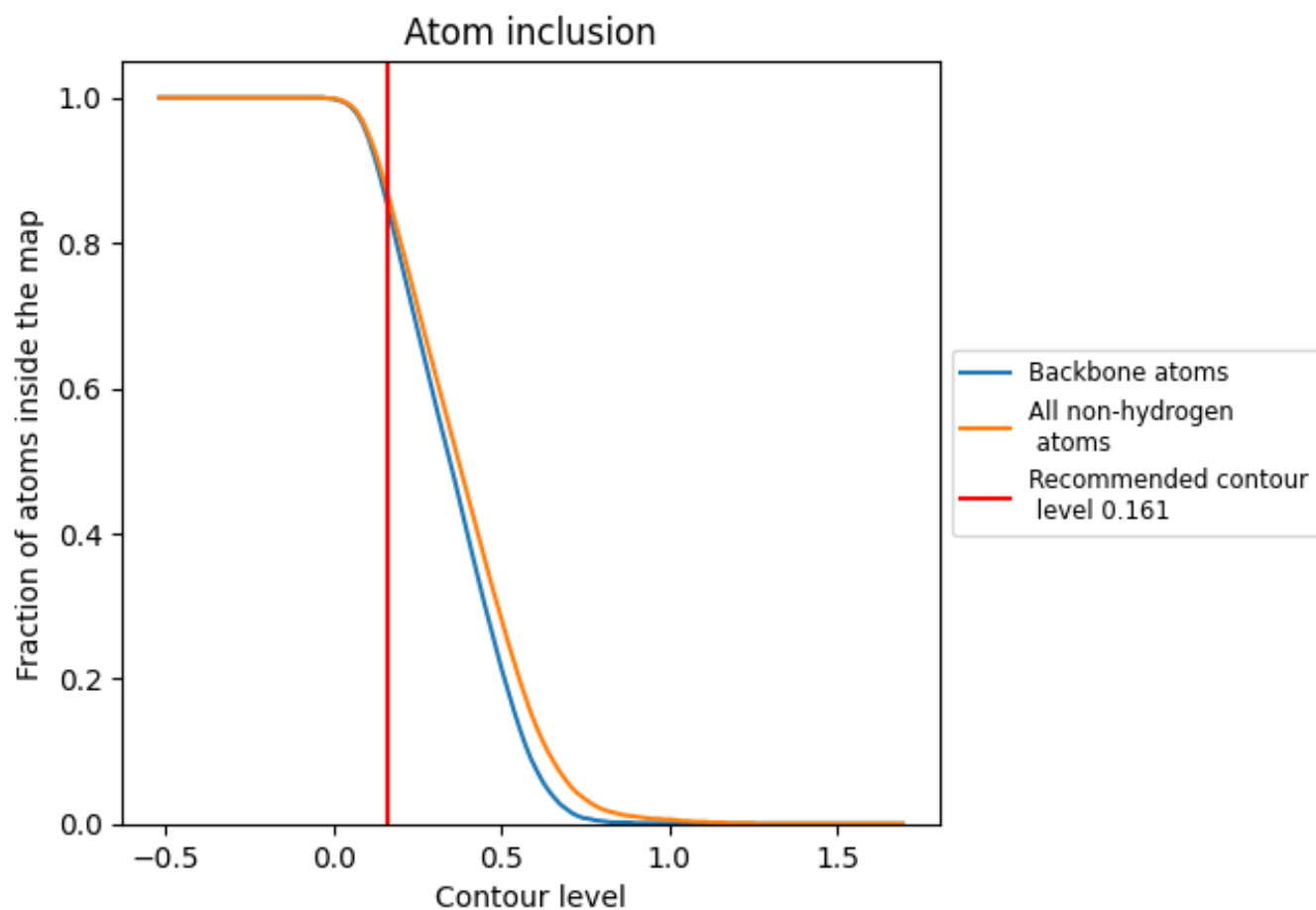
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 87% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.6170
0	 0.7540	 0.5610
1	 0.0770	 0.3350
2	 0.9190	 0.6460
3	 0.8290	 0.6120
4	 0.4760	 0.4890
5	 0.8400	 0.5540
6	 0.7660	 0.5470
7	 0.3680	 0.3870
8	 0.1620	 0.3330
A	 0.9720	 0.6990
AA	 0.9430	 0.6480
Aa	 0.5790	 0.5000
B	 0.9750	 0.7100
BB	 0.9880	 0.6610
Bb	 0.5280	 0.4710
C	 0.9750	 0.7010
CC	 0.9790	 0.6760
Cc	 0.6390	 0.4500
D	 0.9200	 0.6740
DD	 0.5460	 0.5050
Dd	 0.9440	 0.6290
E	 0.9630	 0.6920
EE	 0.9720	 0.7070
Ee	 0.2220	 0.3650
F	 0.9330	 0.6750
FF	 0.9630	 0.6930
G	 0.8690	 0.6200
GG	 0.9640	 0.6970
H	 0.9670	 0.7020
HH	 0.8640	 0.6280
I	 0.9510	 0.6930
II	 0.9290	 0.6700
J	 0.9460	 0.6840
JJ	 0.9570	 0.6890



















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Chain	Atom inclusion	Q-score
K	0.9560	0.6880
KK	0.8840	0.6480
L	0.9320	0.6650
LL	0.9270	0.6690
M	0.9570	0.6890
MM	0.9280	0.6760
N	0.8920	0.6320
NN	0.7960	0.5810
O	0.9360	0.6800
OO	0.9190	0.6680
P	0.9030	0.6550
PP	0.9550	0.6810
Pp	0.4210	0.5790
Q	0.9680	0.7080
QQ	0.9920	0.7100
R	0.9930	0.7180
S	0.9540	0.6890
T	0.9460	0.6700
U	0.8980	0.6410
V	0.9890	0.7080
W	0.8350	0.6320
X	0.9690	0.6830
Y	0.9550	0.6950
Z	0.9430	0.6750
a	0.9300	0.6730
b	0.9400	0.6970
c	0.8830	0.5730
d	0.8700	0.6060
e	0.8680	0.6250
f	0.9160	0.6460
g	0.6420	0.4980
h	0.8810	0.6060
i	0.4930	0.4690
j	0.6650	0.5120
k	0.7110	0.5520
l	0.8730	0.6200
m	0.8680	0.6050
n	0.5600	0.4460
o	0.8940	0.6490
p	0.9300	0.6640
q	0.9360	0.6420
r	0.4970	0.4680

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Chain	Atom inclusion	Q-score
s	 0.6440	 0.5120
t	 0.6260	 0.5000
u	 0.4110	 0.4570
v	 0.5780	 0.4670
w	 0.6060	 0.4890
x	 0.8890	 0.6340
y	 0.9730	 0.6910
z	 0.8740	 0.6230