



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2026 – 02:39 pm BST

PDB ID : 9SCU / pdb_00009scu
EMDB ID : EMD-54774
Title : Cryo-EM structure of the Arabidopsis thaliana 60S ribosomal subunit
Authors : Karki, S.; Lu, X.; Paatero, A.O.; Ruonala, R.; Tranter, D.; Guryanov, S.;
Rehan, S.; Hellmann, E.; Haakonsson, A.; Butcher, S.J.; Huiskonen, J.T.;
Kajander, T.; Helariutta, Y.; Paavilainen, V.O.
Deposited on : 2025-08-12
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

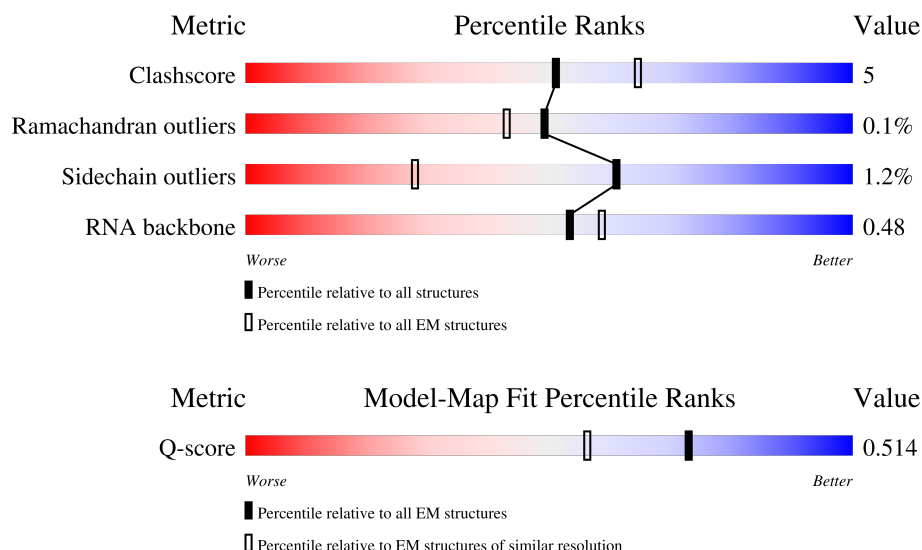
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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




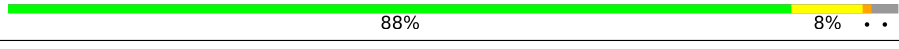
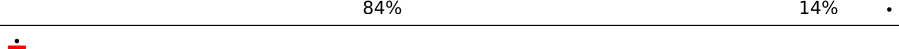
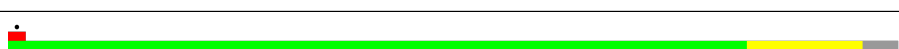



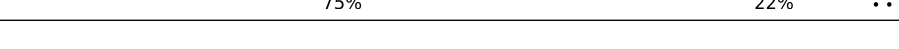



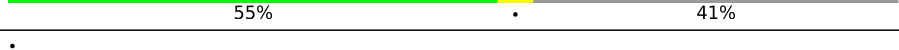

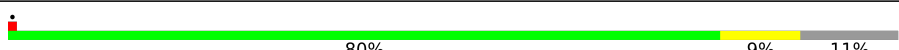


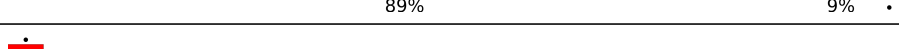







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	5	3381	
2	Ck	69	
3	CA	258	




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	CK	105	
5	Cp	92	
6	Cl	51	
7	CY	146	
8	CL	206	
9	6	121	
10	Cm	128	
11	CZ	135	
12	CM	134	
13	7	164	
14	CN	204	
15	Ca	146	
16	w	124	
17	Cb	83	
18	CO	206	
19	CB	389	
20	CP	176	
21	Cc	112	
22	CQ	187	
23	CC	406	
24	CR	209	
25	Cd	119	
26	CS	217	
27	CD	301	
28	CT	164	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Ce	133	
30	CV	140	
31	CE	233	
32	CW	164	
33	Cf	111	
34	CX	154	
35	CF	242	
36	Cg	120	
37	CG	257	
38	Ch	123	
39	CH	194	
40	Ci	112	
41	CI	221	
42	Cj	95	
43	CJ	182	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 118119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	2953	Total	C	N	O	P	0	0
			63284	28258	11506	20567	2953		

- Molecule 2 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ck	68	Total	C	N	O	S	0	0
			561	359	103	97	2		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2x.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	246	Total	C	N	O	S	0	0
			1891	1185	384	314	8		

- Molecule 4 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CK	81	Total	C	N	O	S	0	0
			649	407	132	108	2		

- Molecule 5 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Cp	89	Total	C	N	O	S	0	0
			697	437	134	120	6		

- Molecule 6 is a protein called Large ribosomal subunit protein eL39z/eL39x.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CY	130	Total	C	N	O	S	0	0
			1062	656	217	186	3		

- Molecule 8 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CL	198	Total	C	N	O	S	0	0
			1607	1017	320	266	4		

- Molecule 9 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	119	Total	C	N	O	P	0	0
			2533	1132	454	829	118		

- Molecule 10 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Cm	52	Total	C	N	O	S	0	0
			431	269	89	66	7		

- Molecule 11 is a protein called Large ribosomal subunit protein eL27x.

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

- Molecule 12 is a protein called Large ribosomal subunit protein eL14z.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CM	131	Total	C	N	O	S	0	0
			1071	685	199	183	4		

- Molecule 13 is a RNA chain called RNA (151-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	151	Total	C	N	O	P	0	0
			3218	1438	579	1051	150		

- Molecule 14 is a protein called Large ribosomal subunit protein eL15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CN	203	Total	C	N	O	S	0	0
			1705	1065	358	279	3		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ca	145	Total	C	N	O	S	0	0
			1155	744	225	183	3		

- Molecule 16 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	w	76	Total	C	N	O	0	0
			475	306	79	90		

- Molecule 17 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cb	49	Total	C	N	O	S	0	0
			346	208	73	64	1		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13w.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CO	204	Total	C	N	O	S	0	0
			1640	1043	316	271	10		

- Molecule 19 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CB	386	Total	C	N	O	S	0	0
			3110	1980	581	532	17		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CP	156	Total	C	N	O	S	0	0
			1253	779	248	222	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL30x.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Cc	89	Total	C	N	O	S	0	0
			683	432	121	125	5		

- Molecule 22 is a protein called Large ribosomal subunit protein eL18y.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CQ	186	Total	C	N	O	S	0	0
			1465	931	282	248	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CC	397	Total	C	N	O	S	0	0
			3087	1950	578	545	14		

- Molecule 24 is a protein called Large ribosomal subunit protein eL19z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CR	169	Total	C	N	O	S	0	0
			1397	872	288	227	10		

- Molecule 25 is a protein called Large ribosomal subunit protein eL31x.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Cd	113	Total	C	N	O	S	0	0
			920	578	177	163	2		

- Molecule 26 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CS	177	Total	C	N	O	S	0	0
			1493	965	275	245	8		

- Molecule 27 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CD	256	Total	C	N	O	S	0	0
			2078	1320	388	366	4		

- Molecule 28 is a protein called Large ribosomal subunit protein eL21x/eL21w.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CT	159	Total	C	N	O	S	0	0
			1281	810	251	216	4		

- Molecule 29 is a protein called Large ribosomal subunit protein eL32z.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CV	129	Total	C	N	O	S	0	0
			976	619	181	168	8		

- Molecule 31 is a protein called Large ribosomal subunit protein eL6x.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CE	180	Total	C	N	O	S	0	0
			1413	914	259	238	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CW	63	Total	C	N	O	S	0	0
			534	345	101	84	4		

- Molecule 33 is a protein called Large ribosomal subunit protein eL33z.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Cf	108	Total	C	N	O	S	0	0
			881	556	170	152	3		

- Molecule 34 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CX	117	Total	C	N	O	S	0	0
			955	615	169	169	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CF	234	Total	C	N	O	S	0	0
			1928	1237	353	334	4		

- Molecule 36 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cg	109	Total	C	N	O	S	0	0
			882	551	184	146	1		

- Molecule 37 is a protein called Large ribosomal subunit protein eL8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CG	231	Total	C	N	O	S	0	0
			1854	1194	335	319	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ch	121	Total	C	N	O	S	0	0
			983	622	192	168	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CH	192	Total	C	N	O	S	0	0
			1528	971	272	279	6		

- Molecule 40 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ci	94	Total	C	N	O	S	0	0
			763	477	162	122	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CI	202	Total	C	N	O	S	0	0
			1627	1033	322	261	11		

- Molecule 42 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cj	88	Total	C	N	O	S	0	0
			714	435	159	114	6		

- Molecule 43 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CJ	170	Total	C	N	O	S	0	0
			1374	869	255	243	7		

- Molecule 44 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
44	5	18	Total	K	0
			18	18	

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	5	32	Total	Mg	0
			32	32	

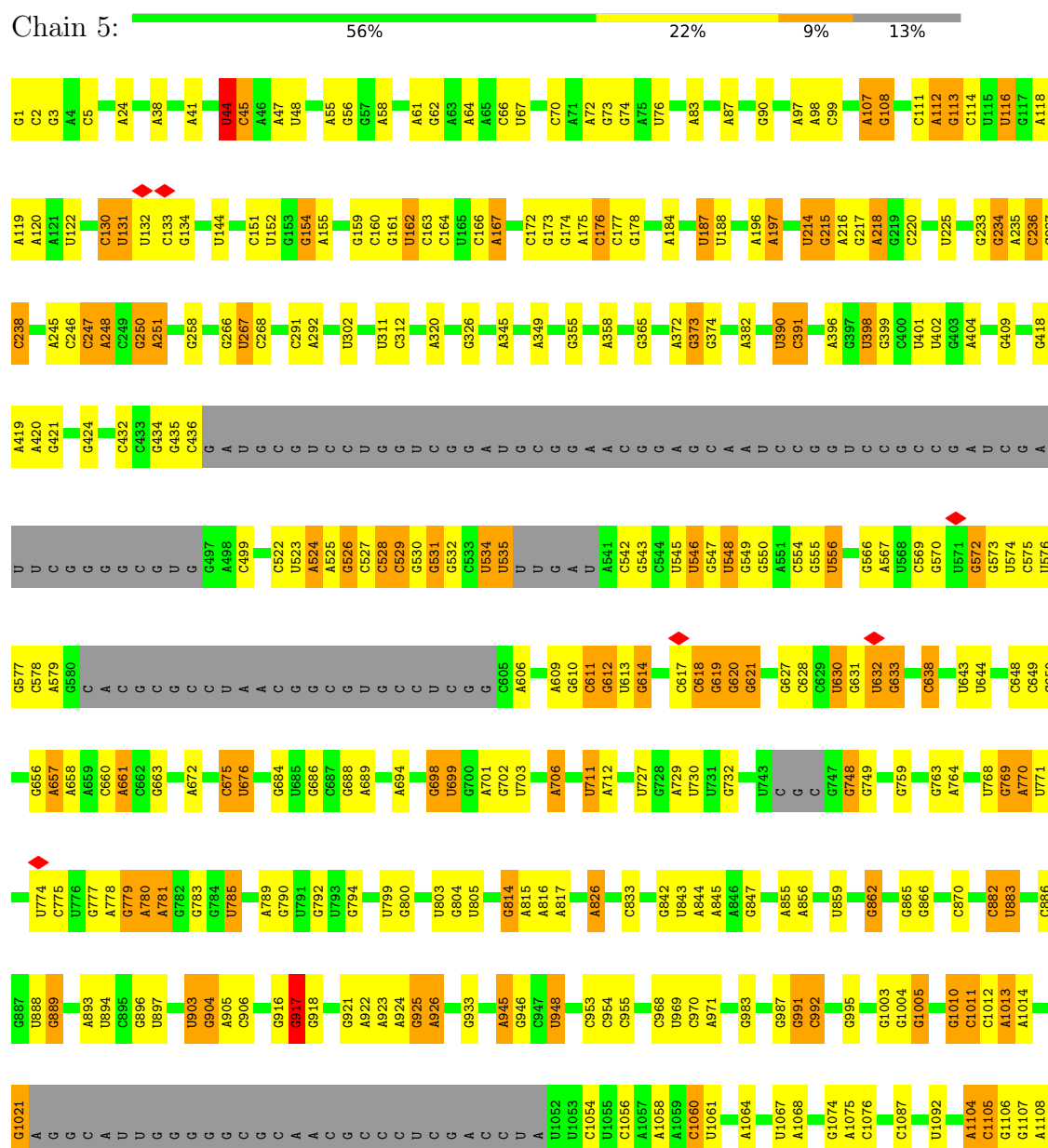
- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	Cp	1	Total	Zn	0
			1	1	

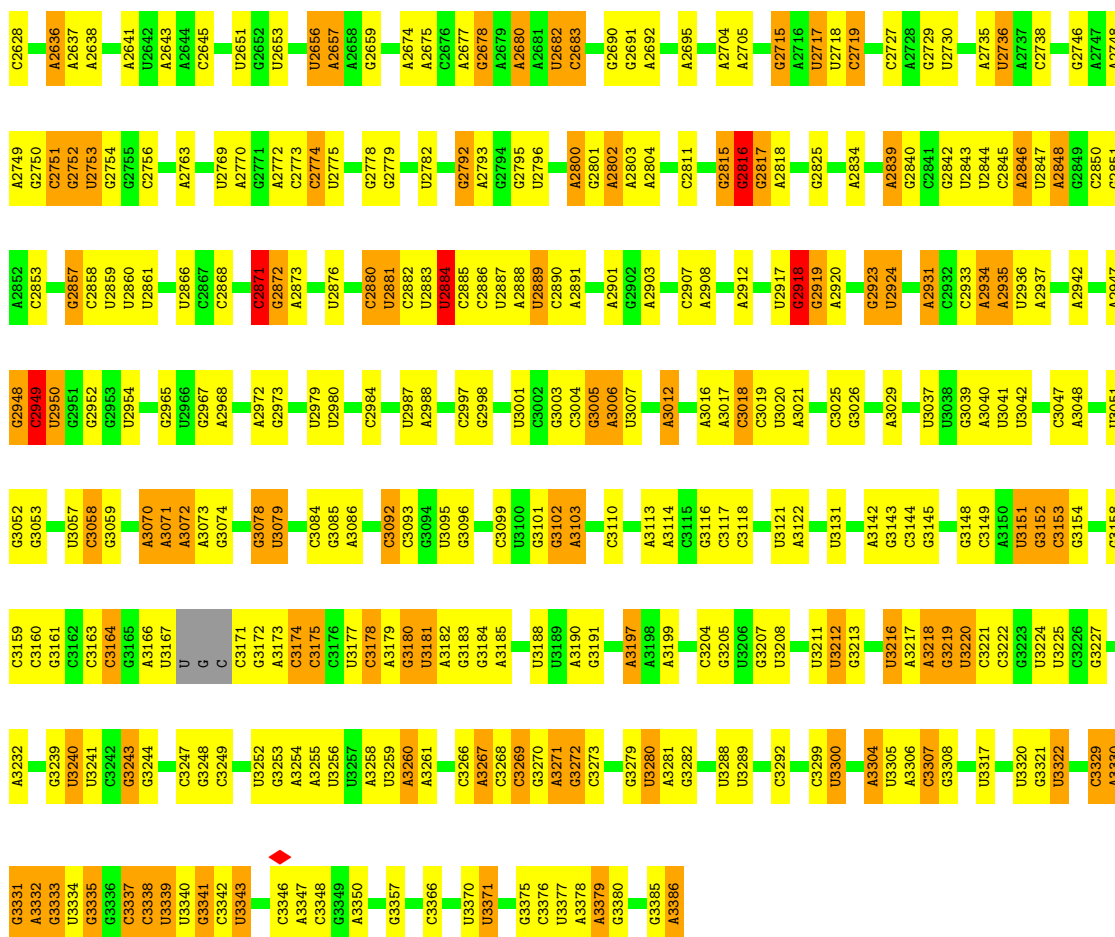
3 Residue-property plots

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

• Molecule 1: 25S RNA

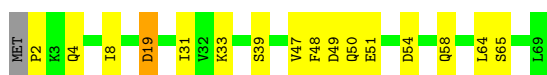






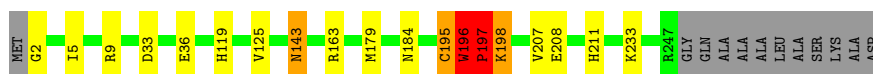
- Molecule 2: Large ribosomal subunit protein eL38z/eL38y

Chain Ck: 75% 22% ..



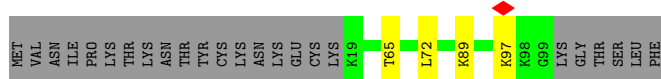
- Molecule 3: Large ribosomal subunit protein uL2x

Chain CA: 88% 5% .. 5%




- Molecule 4: Large ribosomal subunit protein eL42z/eL42y

Chain CK: 73% 23%




- Molecule 5: (thale cress) hypothetical protein

Chain Cp:  88% 8% ..




- Molecule 6: Large ribosomal subunit protein eL39z/eL39x

Chain Cl:  84% 14% .




- Molecule 7: Large ribosomal subunit protein uL24z

Chain CY:  77% 12% 11%



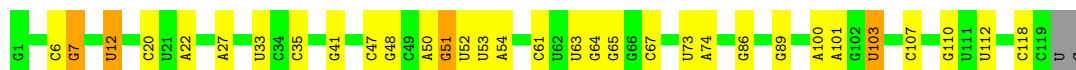
- Molecule 8: Large ribosomal subunit protein eL13z

Chain CL:  83% 13% .



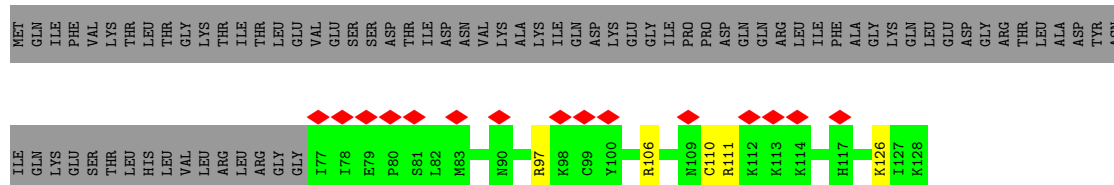
- Molecule 9: RNA (119-MER)

Chain 6:  72% 23% ..




- Molecule 10: Ubiquitin-ribosomal protein eL40z fusion protein

Chain Cm:  12% 37% 59%

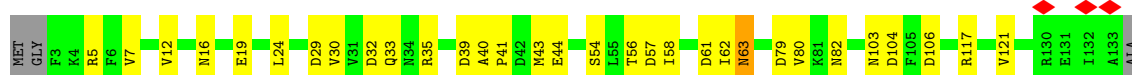
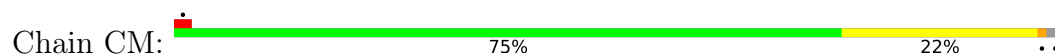


- Molecule 11: Large ribosomal subunit protein eL27x

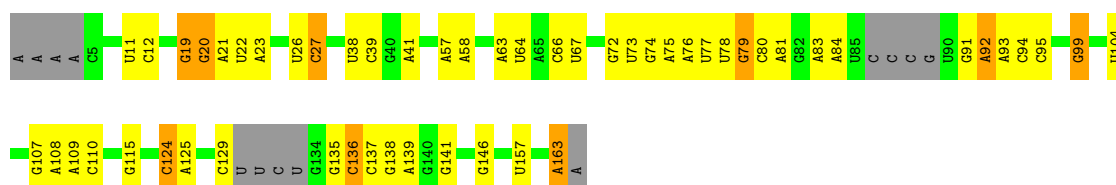
Chain CZ:  85% 14% .



- Molecule 12: Large ribosomal subunit protein eL14z



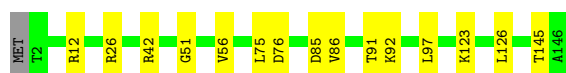
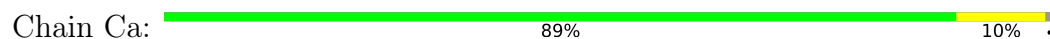
- Molecule 13: RNA (151-MER)



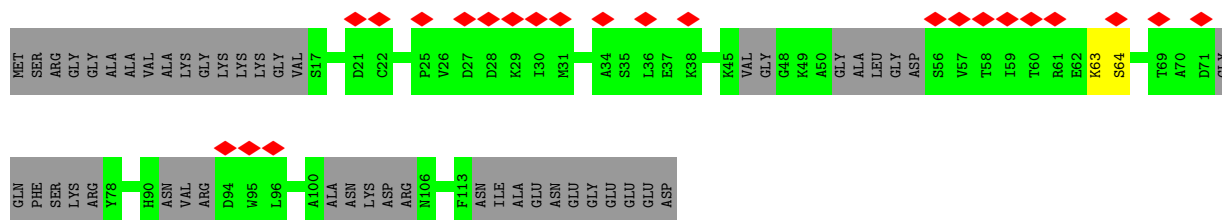
- Molecule 14: Large ribosomal subunit protein eL15y



- Molecule 15: Large ribosomal subunit protein uL15x

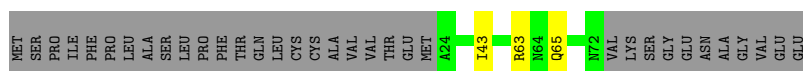


- Molecule 16: Large ribosomal subunit protein eL22z

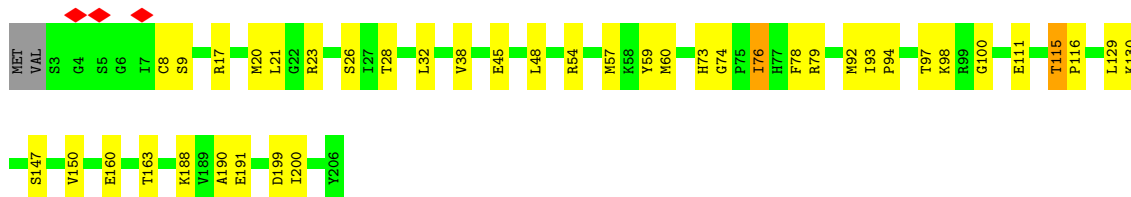
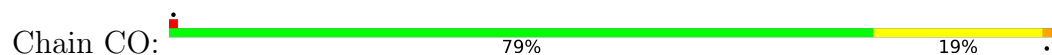


- Molecule 17: 60S ribosomal protein L29





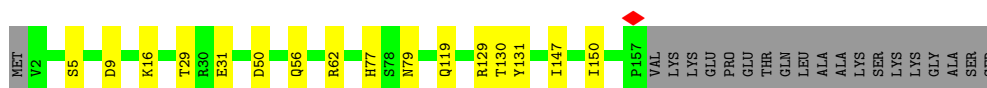
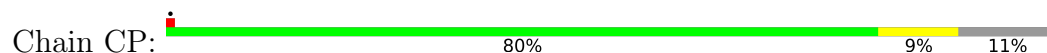
- Molecule 18: Large ribosomal subunit protein uL13w



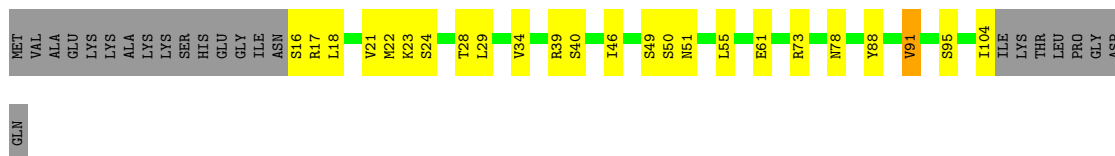
- Molecule 19: Large ribosomal subunit protein uL3z



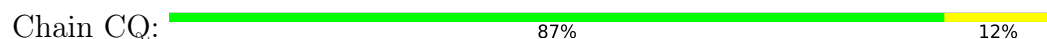
- Molecule 20: Large ribosomal subunit protein uL22z



- Molecule 21: Large ribosomal subunit protein eL30x



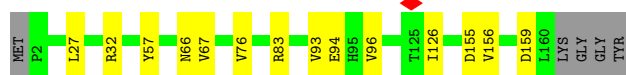
- Molecule 22: Large ribosomal subunit protein eL18y




- Molecule 23: Large ribosomal subunit protein uL4z

- Molecule 28: Large ribosomal subunit protein eL21x/eL21w

Chain CT:  88% 9%




- Molecule 29: Large ribosomal subunit protein eL32z

Chain Ce:  85% 10% 5%



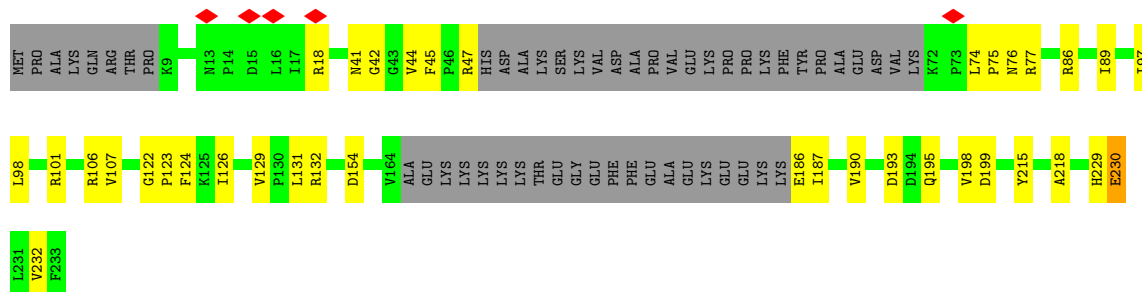
- Molecule 30: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain CV:  81% 11% 8%



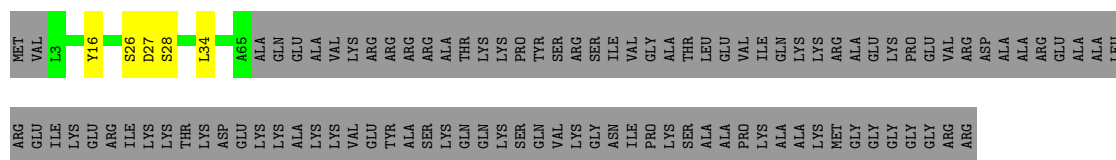
- Molecule 31: Large ribosomal subunit protein eL6x

Chain CE:  61% 15% 23%




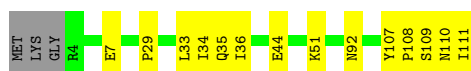
- Molecule 32: Large ribosomal subunit protein eL24z

Chain CW:  35% 62%



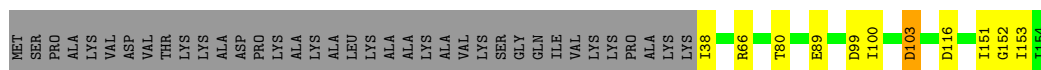
- Molecule 33: Large ribosomal subunit protein eL33z

Chain Cf:  85% 13%



- Molecule 34: Large ribosomal subunit protein uL23y

Chain CX: 69% 6% 24%



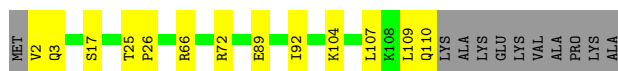
- Molecule 35: Large ribosomal subunit protein uL30y

Chain CF: 83% 13%



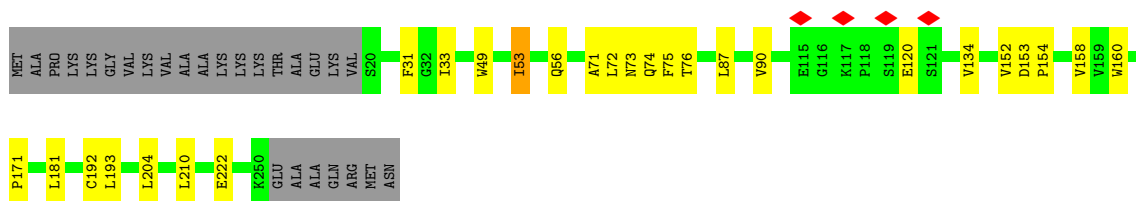
- Molecule 36: Large ribosomal subunit protein eL34z

Chain Cg: 80% 11% 9%



- Molecule 37: Large ribosomal subunit protein eL8z

Chain CG: 79% 10% 10%



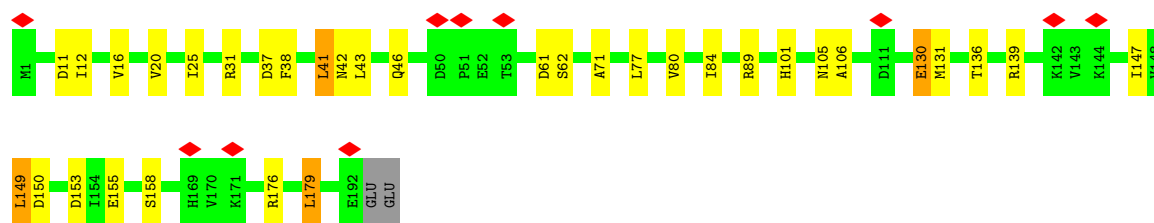
- Molecule 38: Large ribosomal subunit protein uL29x

Chain Ch: 87% 11%



- Molecule 39: Large ribosomal subunit protein uL6z/uL6y

Chain CH: 5% 81% 15%



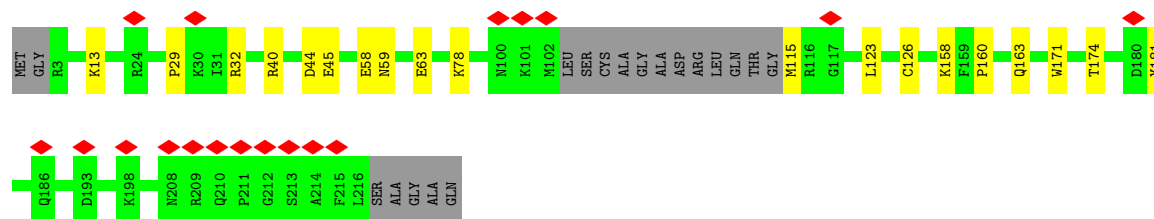
- Molecule 40: Large ribosomal subunit protein eL36y

Chain Ci: 74% 9% 16%



- Molecule 41: Large ribosomal subunit protein uL16y

Chain CI: 8% 83% 9% 9%



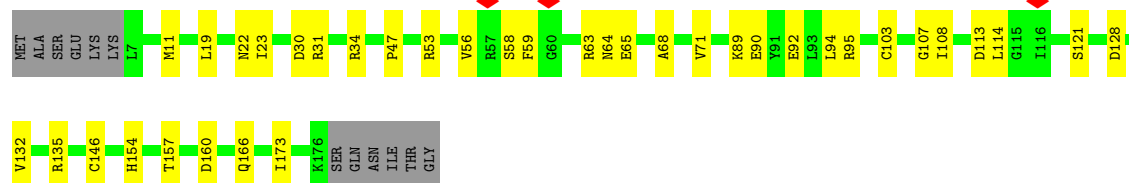
- Molecule 42: Large ribosomal subunit protein eL37z

Chain Cj: 84% 8% 7%



- Molecule 43: Large ribosomal subunit protein uL5z

Chain CJ: 73% 20% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24.512	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.189	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	378.0, 378.0, 378.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, OMG, ZN, OMC, OMU, A2M, K, 5MC, MG, 1MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	5	0.22	0/69543	0.28	0/108431
2	Ck	0.13	0/569	0.25	0/758
3	CA	0.33	1/1936 (0.1%)	0.86	11/2601 (0.4%)
4	CK	0.16	0/661	0.27	0/874
5	Cp	0.40	0/706	0.74	1/936 (0.1%)
6	Cl	0.17	0/456	0.24	0/603
7	CY	0.18	0/1074	0.27	0/1433
8	CL	0.18	0/1639	0.31	0/2197
9	6	0.18	0/2831	0.24	0/4411
10	Cm	0.08	0/437	0.23	0/575
11	CZ	0.16	0/1110	0.25	0/1477
12	CM	0.15	0/1082	0.27	0/1446
13	7	0.21	0/3596	0.26	0/5599
14	CN	0.22	0/1743	0.29	0/2335
15	Ca	0.20	0/1186	0.27	0/1584
16	w	0.08	0/476	0.22	0/651
17	Cb	0.17	0/355	0.29	0/485
18	CO	0.18	0/1669	0.31	0/2232
19	CB	0.18	0/3177	0.29	0/4256
20	CP	0.20	0/1277	0.28	0/1717
21	Cc	0.18	0/693	0.34	0/930
22	CQ	0.20	0/1489	0.33	0/1989
23	CC	0.18	0/3144	0.27	0/4232
24	CR	0.16	0/1416	0.26	0/1869
25	Cd	0.18	0/932	0.28	0/1242
26	CS	0.18	0/1531	0.29	0/2054
27	CD	0.15	0/2117	0.27	0/2840
28	CT	0.18	0/1308	0.26	0/1756
29	Ce	0.17	0/1045	0.25	0/1399
30	CV	0.17	0/992	0.26	0/1334
31	CE	0.12	0/1438	0.26	0/1929
32	CW	0.14	0/547	0.27	0/726

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Cf	0.18	0/901	0.27	0/1209
34	CX	0.17	0/972	0.26	0/1309
35	CF	0.19	0/1962	0.30	0/2621
36	Cg	0.18	0/895	0.28	0/1196
37	CG	0.17	0/1888	0.31	0/2532
38	Ch	0.17	0/992	0.30	0/1316
39	CH	0.13	0/1549	0.29	0/2072
40	Ci	0.15	0/770	0.29	0/1016
41	CI	0.11	0/1665	0.24	0/2228
42	Cj	0.20	0/727	0.28	0/965
43	CJ	0.13	0/1396	0.26	0/1869
All	All	0.21	1/125892 (0.0%)	0.30	12/185234 (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
3	CA	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CA	195	CYS	C-N	9.74	1.53	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CA	196	TRP	O-C-N	-28.23	88.86	121.32
3	CA	196	TRP	N-CA-C	11.88	136.06	109.81
3	CA	197	PRO	N-CA-C	-11.24	89.32	112.47
3	CA	196	TRP	CA-C-N	-10.82	106.31	119.84
3	CA	196	TRP	C-N-CA	-10.82	106.31	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	CA	195	CYS	Mainchain
3	CA	196	TRP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	63284	0	31955	631	0
2	Ck	561	0	606	12	0
3	CA	1891	0	1937	24	0
4	CK	649	0	676	3	0
5	Cp	697	0	737	4	0
6	Cl	444	0	477	5	0
7	CY	1062	0	1142	16	0
8	CL	1607	0	1719	21	0
9	6	2533	0	1286	12	0
10	Cm	431	0	476	5	0
11	CZ	1092	0	1182	13	0
12	CM	1071	0	1160	23	0
13	7	3218	0	1633	30	0
14	CN	1705	0	1765	15	0
15	Ca	1155	0	1207	12	0
16	w	475	0	363	1	0
17	Cb	346	0	281	3	0
18	CO	1640	0	1761	31	0
19	CB	3110	0	3221	30	0
20	CP	1253	0	1271	10	0
21	Cc	683	0	714	13	0
22	CQ	1465	0	1579	18	0
23	CC	3087	0	3239	28	0
24	CR	1397	0	1512	9	0
25	Cd	920	0	975	10	0
26	CS	1493	0	1555	9	0
27	CD	2078	0	2136	29	0
28	CT	1281	0	1335	9	0
29	Ce	1028	0	1105	8	0
30	CV	976	0	1040	11	0
31	CE	1413	0	1524	32	0
32	CW	534	0	557	5	0
33	Cf	881	0	903	10	0
34	CX	955	0	1035	7	0
35	CF	1928	0	2028	20	0
36	Cg	882	0	957	11	0
37	CG	1854	0	1999	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Ch	983	0	1109	11	0
39	CH	1528	0	1613	23	0
40	Ci	763	0	859	8	0
41	CI	1627	0	1684	16	0
42	Cj	714	0	743	7	0
43	CJ	1374	0	1418	25	0
44	5	18	0	0	0	0
45	5	32	0	0	0	0
46	Cp	1	0	0	0	0
All	All	118119	0	86474	1083	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1083 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CA:197:PRO:HD2	3:CA:198:LYS:H	1.00	1.12
1:5:2150:A:OP1	3:CA:197:PRO:O	1.72	1.05
3:CA:196:TRP:O	3:CA:197:PRO:C	1.82	1.00
1:5:3180:G:O2'	1:5:3181:U:O5'	1.78	1.00
3:CA:197:PRO:CD	3:CA:198:LYS:H	1.68	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ck	66/69 (96%)	62 (94%)	4 (6%)	0	100	100
3	CA	244/258 (95%)	230 (94%)	11 (4%)	3 (1%)	10	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CK	79/105 (75%)	75 (95%)	4 (5%)	0	100	100
5	Cp	87/92 (95%)	81 (93%)	6 (7%)	0	100	100
6	Cl	48/51 (94%)	40 (83%)	8 (17%)	0	100	100
7	CY	128/146 (88%)	124 (97%)	4 (3%)	0	100	100
8	CL	196/206 (95%)	184 (94%)	12 (6%)	0	100	100
10	Cm	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
11	CZ	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
12	CM	129/134 (96%)	124 (96%)	5 (4%)	0	100	100
14	CN	201/204 (98%)	185 (92%)	16 (8%)	0	100	100
15	Ca	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
16	w	64/124 (52%)	62 (97%)	2 (3%)	0	100	100
17	Cb	47/83 (57%)	38 (81%)	9 (19%)	0	100	100
18	CO	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
19	CB	384/389 (99%)	362 (94%)	22 (6%)	0	100	100
20	CP	154/176 (88%)	148 (96%)	6 (4%)	0	100	100
21	Cc	87/112 (78%)	76 (87%)	9 (10%)	2 (2%)	5	19
22	CQ	184/187 (98%)	172 (94%)	12 (6%)	0	100	100
23	CC	395/406 (97%)	369 (93%)	26 (7%)	0	100	100
24	CR	167/209 (80%)	160 (96%)	7 (4%)	0	100	100
25	Cd	111/119 (93%)	101 (91%)	10 (9%)	0	100	100
26	CS	175/217 (81%)	167 (95%)	8 (5%)	0	100	100
27	CD	250/301 (83%)	240 (96%)	10 (4%)	0	100	100
28	CT	157/164 (96%)	147 (94%)	10 (6%)	0	100	100
29	Ce	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
30	CV	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
31	CE	174/233 (75%)	165 (95%)	9 (5%)	0	100	100
32	CW	61/164 (37%)	59 (97%)	2 (3%)	0	100	100
33	Cf	106/111 (96%)	102 (96%)	4 (4%)	0	100	100
34	CX	115/154 (75%)	112 (97%)	3 (3%)	0	100	100
35	CF	232/242 (96%)	222 (96%)	10 (4%)	0	100	100
36	Cg	107/120 (89%)	105 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	CG	229/257 (89%)	215 (94%)	14 (6%)	0	100	100
38	Ch	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
39	CH	190/194 (98%)	176 (93%)	14 (7%)	0	100	100
40	Ci	92/112 (82%)	89 (97%)	3 (3%)	0	100	100
41	CI	198/221 (90%)	191 (96%)	7 (4%)	0	100	100
42	Cj	86/95 (90%)	78 (91%)	8 (9%)	0	100	100
43	CJ	168/182 (92%)	163 (97%)	5 (3%)	0	100	100
All	All	6008/6848 (88%)	5686 (95%)	317 (5%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	Cc	91	VAL
3	CA	196	TRP
3	CA	198	LYS
21	Cc	46	ILE
3	CA	197	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ck	64/65 (98%)	63 (98%)	1 (2%)	55	83
3	CA	191/197 (97%)	189 (99%)	2 (1%)	68	89
4	CK	67/93 (72%)	67 (100%)	0	100	100
5	Cp	73/76 (96%)	69 (94%)	4 (6%)	19	50
6	Cl	47/48 (98%)	46 (98%)	1 (2%)	47	77
7	CY	118/133 (89%)	116 (98%)	2 (2%)	53	82
8	CL	170/177 (96%)	166 (98%)	4 (2%)	43	75
10	Cm	48/115 (42%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CZ	116/117 (99%)	116 (100%)	0	100	100
12	CM	115/116 (99%)	114 (99%)	1 (1%)	70	90
14	CN	179/180 (99%)	178 (99%)	1 (1%)	78	93
15	Ca	120/121 (99%)	120 (100%)	0	100	100
16	w	31/104 (30%)	31 (100%)	0	100	100
17	Cb	29/71 (41%)	28 (97%)	1 (3%)	32	66
18	CO	175/177 (99%)	172 (98%)	3 (2%)	53	82
19	CB	327/330 (99%)	321 (98%)	6 (2%)	51	80
20	CP	132/148 (89%)	132 (100%)	0	100	100
21	Cc	77/96 (80%)	75 (97%)	2 (3%)	40	73
22	CQ	156/157 (99%)	155 (99%)	1 (1%)	78	93
23	CC	328/331 (99%)	325 (99%)	3 (1%)	70	90
24	CR	148/179 (83%)	145 (98%)	3 (2%)	48	78
25	Cd	98/104 (94%)	98 (100%)	0	100	100
26	CS	161/198 (81%)	158 (98%)	3 (2%)	50	79
27	CD	217/254 (85%)	215 (99%)	2 (1%)	70	90
28	CT	136/139 (98%)	135 (99%)	1 (1%)	76	92
29	Ce	114/121 (94%)	113 (99%)	1 (1%)	70	90
30	CV	103/110 (94%)	102 (99%)	1 (1%)	68	89
31	CE	151/197 (77%)	149 (99%)	2 (1%)	61	86
32	CW	58/137 (42%)	58 (100%)	0	100	100
33	Cf	95/97 (98%)	95 (100%)	0	100	100
34	CX	108/136 (79%)	106 (98%)	2 (2%)	50	79
35	CF	204/212 (96%)	202 (99%)	2 (1%)	68	89
36	Cg	96/104 (92%)	94 (98%)	2 (2%)	47	77
37	CG	202/221 (91%)	201 (100%)	1 (0%)	81	93
38	Ch	109/110 (99%)	107 (98%)	2 (2%)	51	80
39	CH	173/175 (99%)	169 (98%)	4 (2%)	44	76
40	Ci	81/94 (86%)	79 (98%)	2 (2%)	42	74
41	CI	168/179 (94%)	168 (100%)	0	100	100
42	Cj	74/78 (95%)	74 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	CJ	148/158 (94%)	145 (98%)	3 (2%)	48 78
All	All	5207/5855 (89%)	5144 (99%)	63 (1%)	61 86

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	CQ	187	VAL
39	CH	130	GLU
26	CS	75	GLU
39	CH	41	LEU
40	Ci	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
35	CF	232	ASN
36	Cg	70	ASN
42	Cj	30	GLN
20	CP	90	GLN
19	CB	193	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	2939/3381 (86%)	609 (20%)	72 (2%)
13	7	148/164 (90%)	28 (18%)	1 (0%)
9	6	118/121 (97%)	23 (19%)	0
All	All	3205/3666 (87%)	660 (20%)	73 (2%)

5 of 660 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	C
1	5	3	G
1	5	5	C
1	5	24	A
1	5	38	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	2815	G
1	5	3332	A
1	5	2871	5MC
1	5	3071	A
1	5	1596	G

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

51 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$
1	OMC	5	2294	1	19,22,23	2.98	8 (42%)	26,31,34	1.72	6 (23%)
1	OMG	5	814	1	23,26,27	2.39	9 (39%)	33,38,41	2.52	16 (48%)
1	OMC	5	2683	1	19,22,23	2.98	8 (42%)	26,31,34	1.78	6 (23%)
1	OMC	5	2949	1	19,22,23	2.93	8 (42%)	26,31,34	1.84	6 (23%)
1	OMG	5	2289	1	23,26,27	2.41	8 (34%)	33,38,41	2.52	16 (48%)
1	OMG	5	2918	1	23,26,27	2.40	9 (39%)	33,38,41	2.45	16 (48%)
1	A2M	5	1377	1	22,25,26	3.45	9 (40%)	31,36,39	2.70	11 (35%)
1	OMG	5	2396	1,45	23,26,27	2.37	9 (39%)	33,38,41	2.47	15 (45%)
1	5MC	5	2279	1	18,22,23	3.67	7 (38%)	26,32,35	1.63	6 (23%)
1	OMG	5	2923	1	23,26,27	2.42	9 (39%)	33,38,41	2.52	16 (48%)
1	A2M	5	2322	1	22,25,26	3.45	9 (40%)	31,36,39	2.61	11 (35%)
1	OMU	5	44	1	19,22,23	2.84	6 (31%)	26,31,34	1.83	6 (23%)
1	OMU	5	2651	1	19,22,23	2.87	6 (31%)	26,31,34	1.75	5 (19%)
1	A2M	5	2221	1	22,25,26	3.44	9 (40%)	31,36,39	2.63	12 (38%)
1	OMU	5	676	1	19,22,23	2.84	6 (31%)	26,31,34	1.75	5 (19%)
1	OMU	5	803	1	19,22,23	2.80	6 (31%)	26,31,34	1.75	5 (19%)
1	OMC	5	2198	1,44	19,22,23	2.95	8 (42%)	26,31,34	1.79	3 (11%)
1	UR3	5	2954	1	19,22,23	2.71	8 (42%)	26,32,35	1.31	1 (3%)
1	OMC	5	1447	1	19,22,23	2.90	8 (42%)	26,31,34	1.75	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	5	1855	1	23,26,27	2.39	9 (39%)	33,38,41	2.41	16 (48%)
1	A2M	5	661	1	22,25,26	3.44	9 (40%)	31,36,39	2.68	11 (35%)
1	OMU	5	2422	1	19,22,23	2.84	6 (31%)	26,31,34	1.75	5 (19%)
1	OMC	5	2880	1	19,22,23	2.91	8 (42%)	26,31,34	1.69	6 (23%)
1	OMU	5	48	1	19,22,23	2.79	6 (31%)	26,31,34	1.74	5 (19%)
1	OMU	5	3300	1	19,22,23	2.83	6 (31%)	26,31,34	1.74	5 (19%)
1	OMG	5	2792	1	23,26,27	2.40	8 (34%)	33,38,41	2.46	15 (45%)
1	OMG	5	2125	1	23,26,27	2.41	8 (34%)	33,38,41	2.47	15 (45%)
1	OMU	5	2884	1	19,22,23	2.83	7 (36%)	26,31,34	1.95	8 (30%)
1	5MC	5	2871	1	18,22,23	3.70	8 (44%)	26,32,35	1.62	6 (23%)
1	OMC	5	2366	1	19,22,23	2.93	8 (42%)	26,31,34	1.75	6 (23%)
1	A2M	5	2947	1	22,25,26	3.48	9 (40%)	31,36,39	2.71	12 (38%)
1	1MA	5	657	1	21,25,26	2.81	5 (23%)	31,37,40	3.19	12 (38%)
1	A2M	5	945	1	22,25,26	3.48	9 (40%)	31,36,39	2.66	10 (32%)
1	OMG	5	2392	1	23,26,27	2.40	8 (34%)	33,38,41	2.41	16 (48%)
1	OMC	5	1847	1	19,22,23	2.93	8 (42%)	26,31,34	1.48	4 (15%)
1	OMG	5	2816	1	23,26,27	2.40	8 (34%)	33,38,41	2.45	16 (48%)
1	OMC	5	2338	1	19,22,23	2.92	8 (42%)	26,31,34	1.62	6 (23%)
1	A2M	5	2641	1	22,25,26	3.45	9 (40%)	31,36,39	2.64	10 (32%)
1	A2M	5	1459	1	22,25,26	3.46	9 (40%)	31,36,39	2.69	11 (35%)
1	A2M	5	2127	1	22,25,26	3.42	9 (40%)	31,36,39	2.64	11 (35%)
1	OMG	5	2410	1	23,26,27	2.40	8 (34%)	33,38,41	2.26	13 (39%)
1	OMG	5	917	1	23,26,27	2.44	8 (34%)	33,38,41	2.26	14 (42%)
1	OMU	5	1892	1	19,22,23	2.84	6 (31%)	26,31,34	1.77	5 (19%)
1	OMG	5	1460	1	23,26,27	2.38	9 (39%)	33,38,41	2.35	15 (45%)
1	OMC	5	1860	1	19,22,23	2.92	8 (42%)	26,31,34	1.77	6 (23%)
1	OMC	5	675	1	19,22,23	2.91	8 (42%)	26,31,34	1.61	5 (19%)
1	OMU	5	1067	1	19,22,23	2.85	6 (31%)	26,31,34	1.84	7 (26%)
1	A2M	5	1143	1	22,25,26	3.44	9 (40%)	31,36,39	2.65	10 (32%)
1	OMU	5	2736	1	19,22,23	2.83	6 (31%)	26,31,34	1.72	5 (19%)
1	OMG	5	2620	1	23,26,27	2.39	8 (34%)	33,38,41	2.45	16 (48%)
1	OMU	5	144	1	19,22,23	2.83	6 (31%)	26,31,34	1.76	5 (19%)

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
1	OMC	5	2294	1	-	3/9/27/28	0/2/2/2
1	OMG	5	814	1	-	2/9/27/28	0/3/3/3
1	OMC	5	2683	1	-	3/9/27/28	0/2/2/2
1	OMC	5	2949	1	-	4/9/27/28	0/2/2/2
1	OMG	5	2289	1	-	4/9/27/28	0/3/3/3
1	OMG	5	2918	1	-	3/9/27/28	0/3/3/3
1	A2M	5	1377	1	-	0/9/27/28	0/3/3/3
1	OMG	5	2396	1,45	-	4/9/27/28	0/3/3/3
1	5MC	5	2279	1	-	2/7/25/26	0/2/2/2
1	OMG	5	2923	1	-	3/9/27/28	0/3/3/3
1	A2M	5	2322	1	-	0/9/27/28	0/3/3/3
1	OMU	5	44	1	-	3/9/27/28	0/2/2/2
1	OMU	5	2651	1	-	0/9/27/28	0/2/2/2
1	A2M	5	2221	1	-	3/9/27/28	0/3/3/3
1	OMU	5	676	1	-	2/9/27/28	0/2/2/2
1	OMU	5	803	1	-	2/9/27/28	0/2/2/2
1	OMC	5	2198	1,44	-	3/9/27/28	0/2/2/2
1	UR3	5	2954	1	-	0/7/25/26	0/2/2/2
1	OMC	5	1447	1	-	5/9/27/28	0/2/2/2
1	OMG	5	1855	1	-	2/9/27/28	0/3/3/3
1	A2M	5	661	1	-	3/9/27/28	0/3/3/3
1	OMU	5	2422	1	-	2/9/27/28	0/2/2/2
1	OMC	5	2880	1	-	3/9/27/28	0/2/2/2
1	OMU	5	48	1	-	0/9/27/28	0/2/2/2
1	OMU	5	3300	1	-	2/9/27/28	0/2/2/2
1	OMG	5	2792	1	-	3/9/27/28	0/3/3/3
1	OMG	5	2125	1	-	4/9/27/28	0/3/3/3
1	OMU	5	2884	1	-	1/9/27/28	0/2/2/2
1	5MC	5	2871	1	-	6/7/25/26	0/2/2/2
1	OMC	5	2366	1	-	1/9/27/28	0/2/2/2
1	A2M	5	2947	1	-	1/9/27/28	0/3/3/3
1	1MA	5	657	1	-	2/7/25/26	0/3/3/3
1	A2M	5	945	1	-	3/9/27/28	0/3/3/3
1	OMG	5	2392	1	-	3/9/27/28	0/3/3/3
1	OMC	5	1847	1	-	4/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	5	2816	1	-	2/9/27/28	0/3/3/3
1	OMC	5	2338	1	-	3/9/27/28	0/2/2/2
1	A2M	5	2641	1	-	0/9/27/28	0/3/3/3
1	A2M	5	1459	1	-	0/9/27/28	0/3/3/3
1	A2M	5	2127	1	-	2/9/27/28	0/3/3/3
1	OMG	5	2410	1	-	1/9/27/28	0/3/3/3
1	OMG	5	917	1	-	1/9/27/28	0/3/3/3
1	OMU	5	1892	1	-	0/9/27/28	0/2/2/2
1	OMG	5	1460	1	-	4/9/27/28	0/3/3/3
1	OMC	5	1860	1	-	1/9/27/28	0/2/2/2
1	OMC	5	675	1	-	4/9/27/28	0/2/2/2
1	OMU	5	1067	1	-	0/9/27/28	0/2/2/2
1	A2M	5	1143	1	-	2/9/27/28	0/3/3/3
1	OMU	5	2736	1	-	1/9/27/28	0/2/2/2
1	OMG	5	2620	1	-	4/9/27/28	0/3/3/3
1	OMU	5	144	1	-	3/9/27/28	0/2/2/2

The worst 5 of 397 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2871	5MC	C6-C5	9.53	1.50	1.34
1	5	2279	5MC	C6-C5	9.15	1.49	1.34
1	5	2947	A2M	C2'-C1'	-8.84	1.30	1.53
1	5	1459	A2M	C2'-C1'	-8.78	1.30	1.53
1	5	1143	A2M	C2'-C1'	-8.69	1.30	1.53

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	657	1MA	C1'-N9-C8	-9.46	99.78	126.70
1	5	657	1MA	C1'-N9-C4	8.41	151.50	126.50
1	5	1377	A2M	N6-C6-N1	-7.14	102.71	118.35
1	5	1459	A2M	N6-C6-N1	-7.11	102.78	118.35
1	5	661	A2M	N6-C6-N1	-7.08	102.85	118.35

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	44	OMU	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5	661	A2M	O4'-C4'-C5'-O5'
1	5	661	A2M	C3'-C4'-C5'-O5'
1	5	675	OMC	O4'-C4'-C5'-O5'
1	5	814	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

17 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	2294	OMC	2	0
1	5	2949	OMC	3	0
1	5	2289	OMG	4	0
1	5	2918	OMG	2	0
1	5	2279	5MC	2	0
1	5	2923	OMG	2	0
1	5	44	OMU	2	0
1	5	2198	OMC	1	0
1	5	1855	OMG	2	0
1	5	2884	OMU	1	0
1	5	2871	5MC	4	0
1	5	2392	OMG	3	0
1	5	2816	OMG	2	0
1	5	2410	OMG	2	0
1	5	917	OMG	1	0
1	5	2736	OMU	1	0
1	5	2620	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

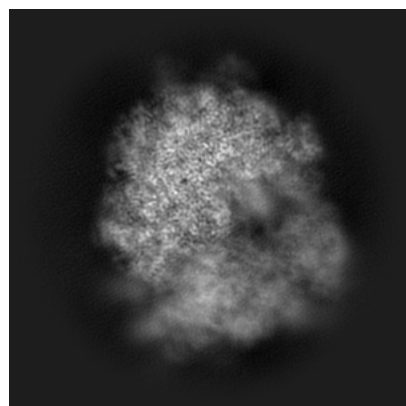
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54774. These allow visual inspection of the internal detail of the map and identification of artifacts.

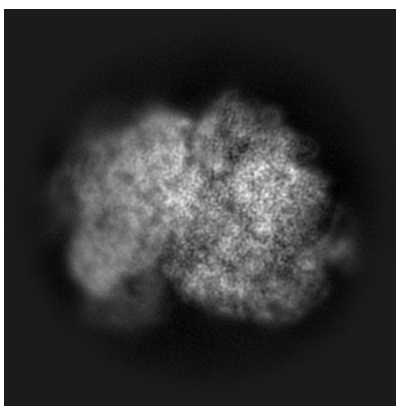
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

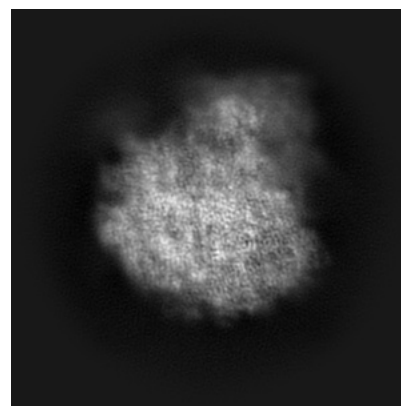
6.1.1 Primary map



X

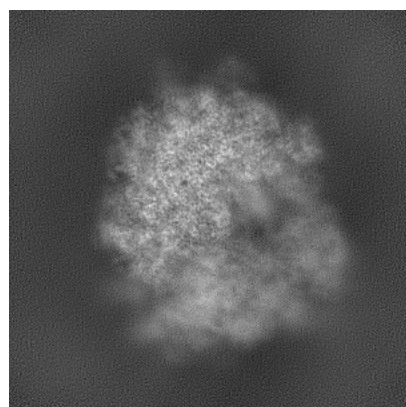


Y

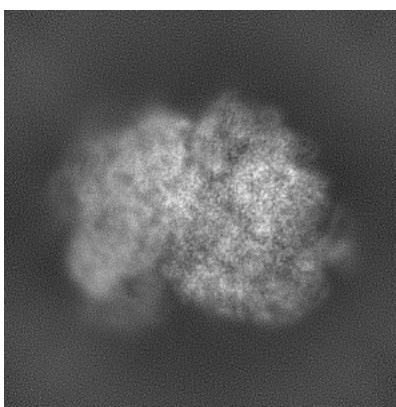


Z

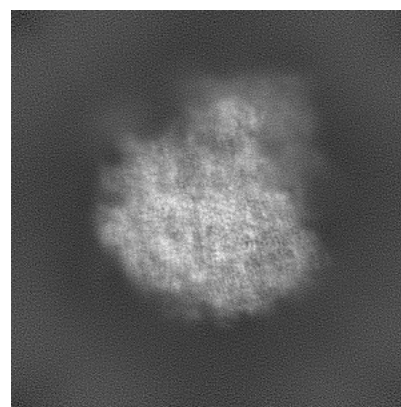
6.1.2 Raw map



X



Y

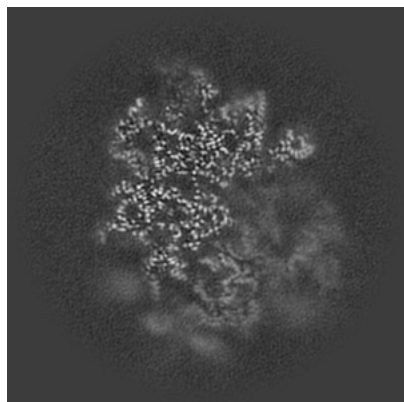


Z

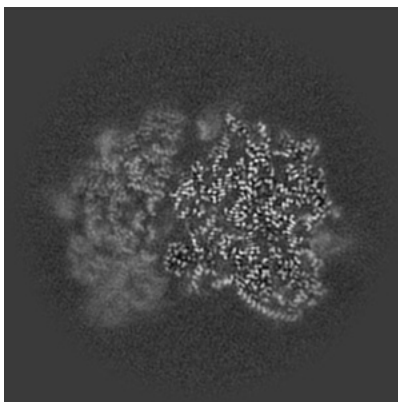
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

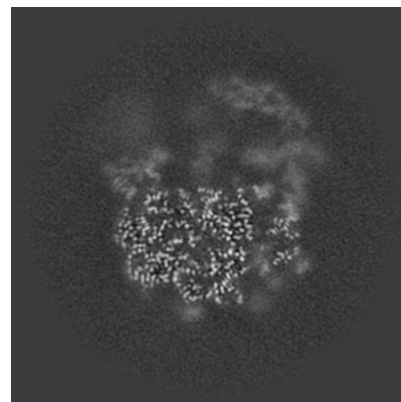
6.2.1 Primary map



X Index: 225

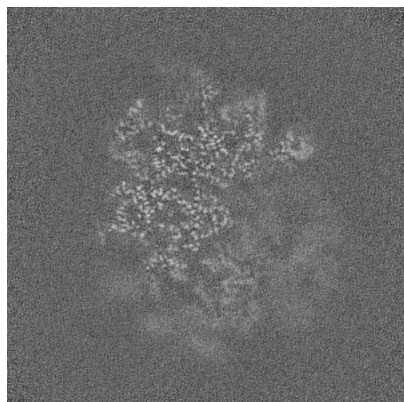


Y Index: 225

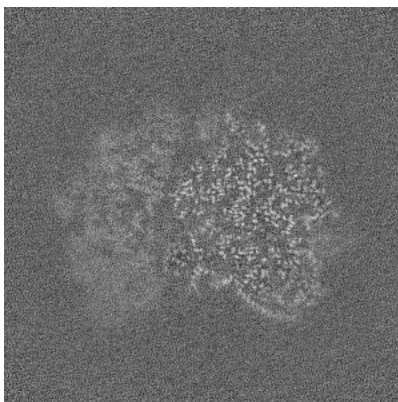


Z Index: 225

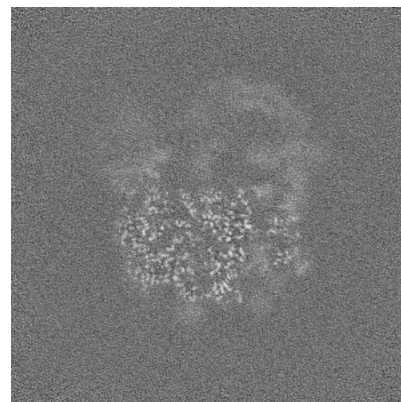
6.2.2 Raw map



X Index: 225



Y Index: 225

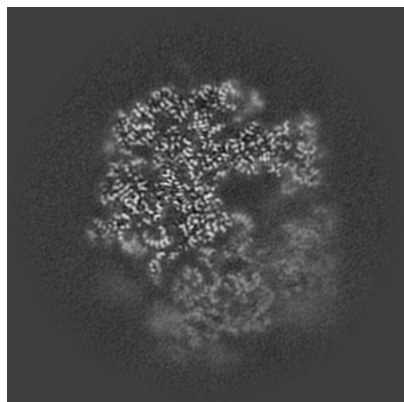


Z Index: 225

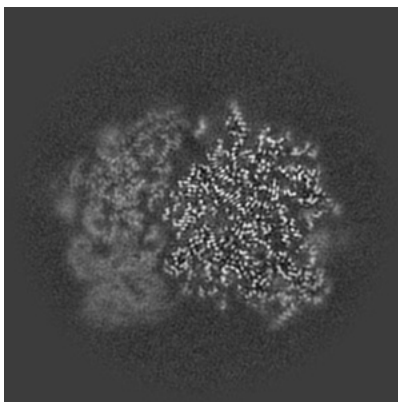
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

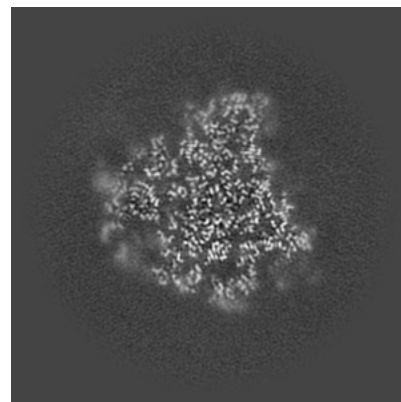
6.3.1 Primary map



X Index: 241

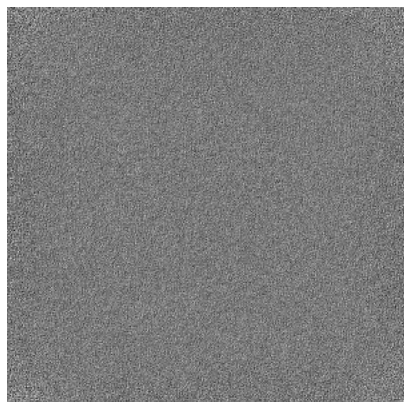


Y Index: 218

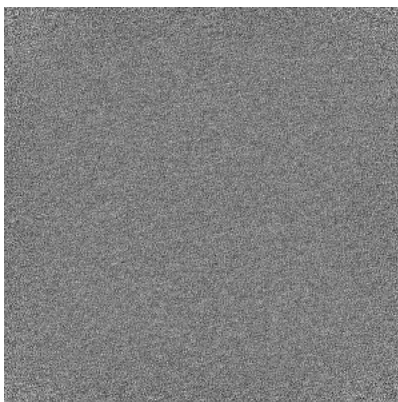


Z Index: 290

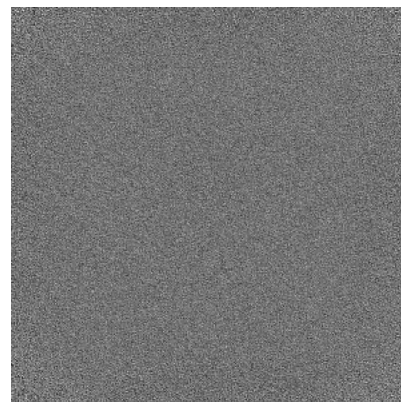
6.3.2 Raw map



X Index: 0



Y Index: 0

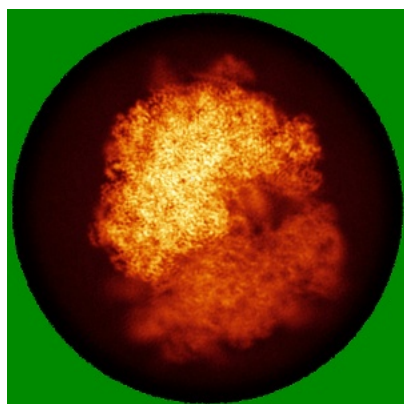


Z Index: 449

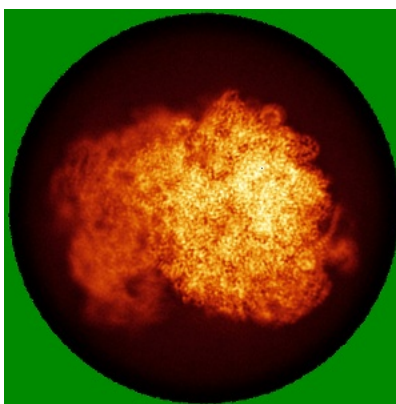
The images above show the largest variance slices of the map in three orthogonal directions.

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

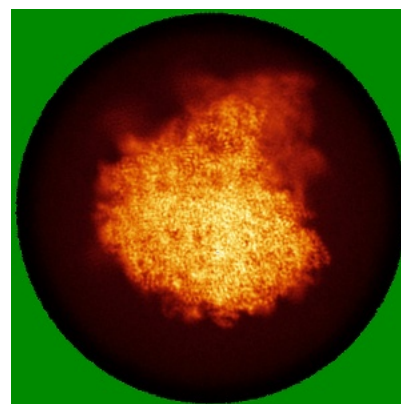
6.4.1 Primary map



X

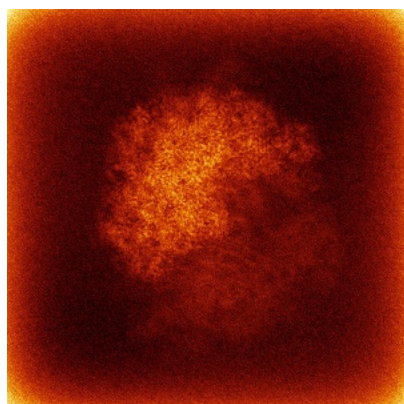


Y

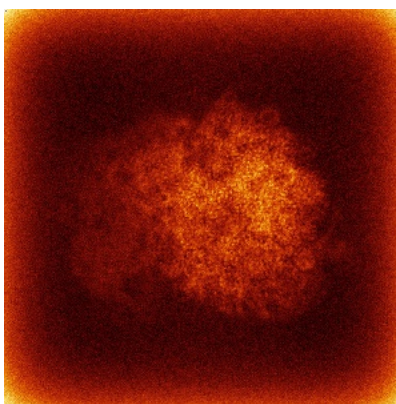


Z

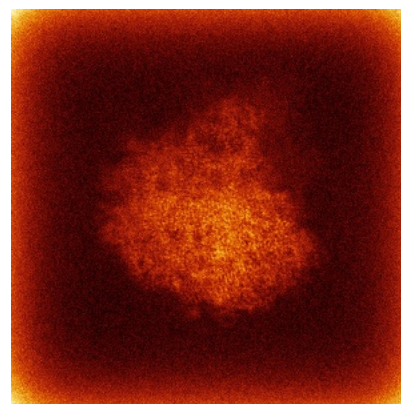
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



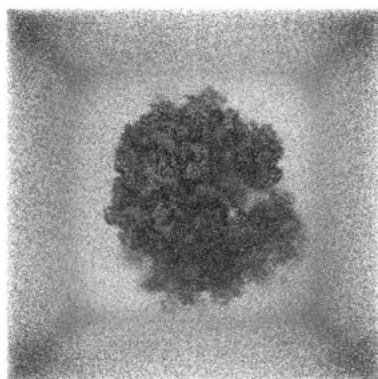
Y



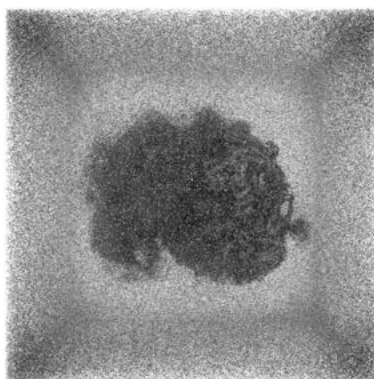
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

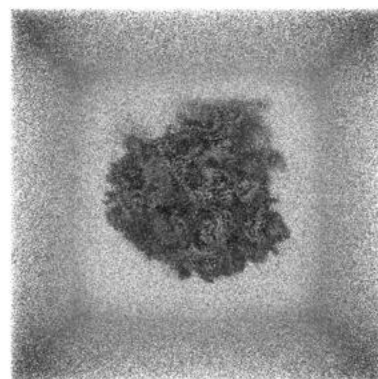
6.5.2 Raw map



X



Y



Z

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

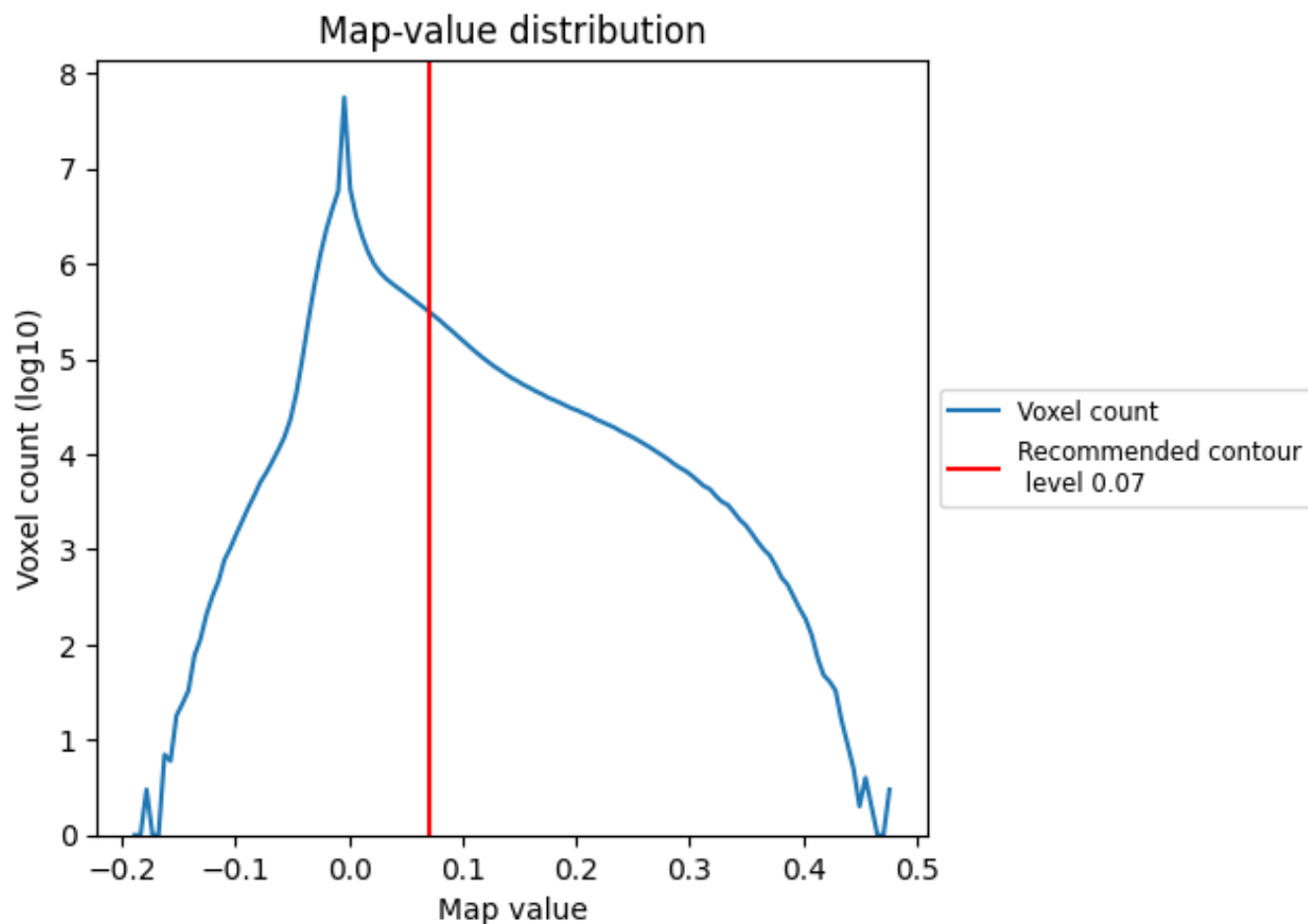
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

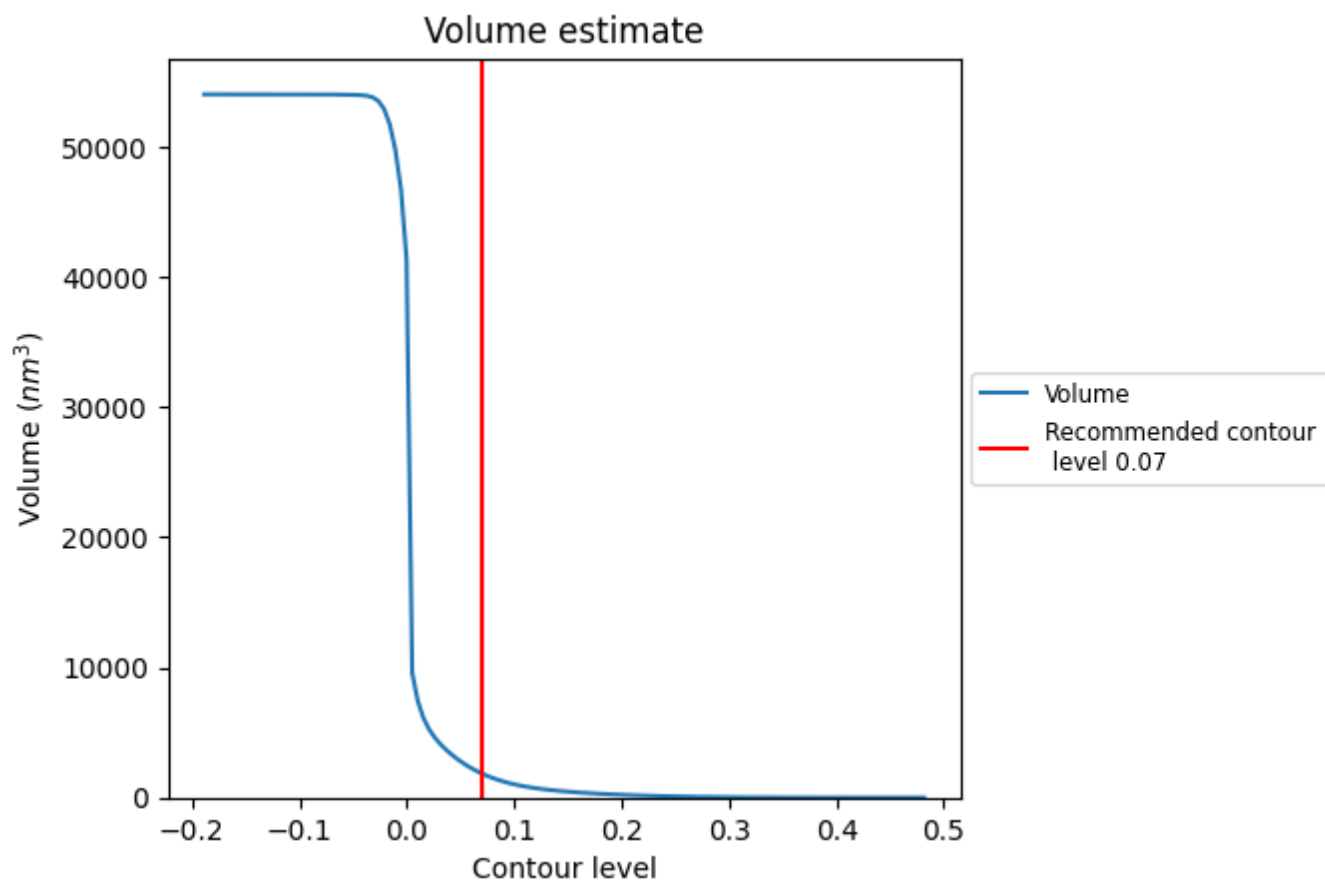
This section contains the results of statistical analysis of the map.

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.

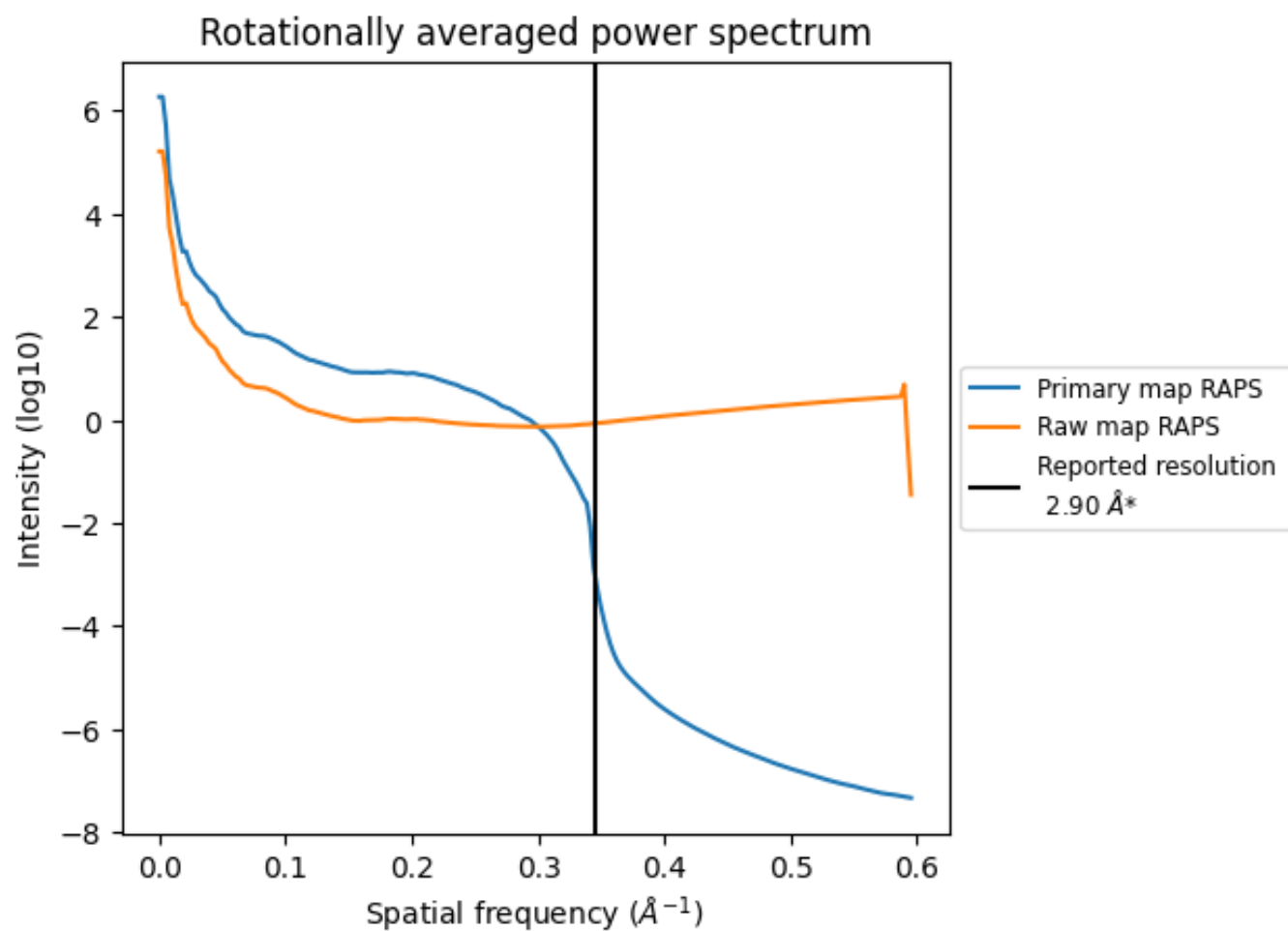
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1842 nm³; this corresponds to an approximate mass of 1664 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

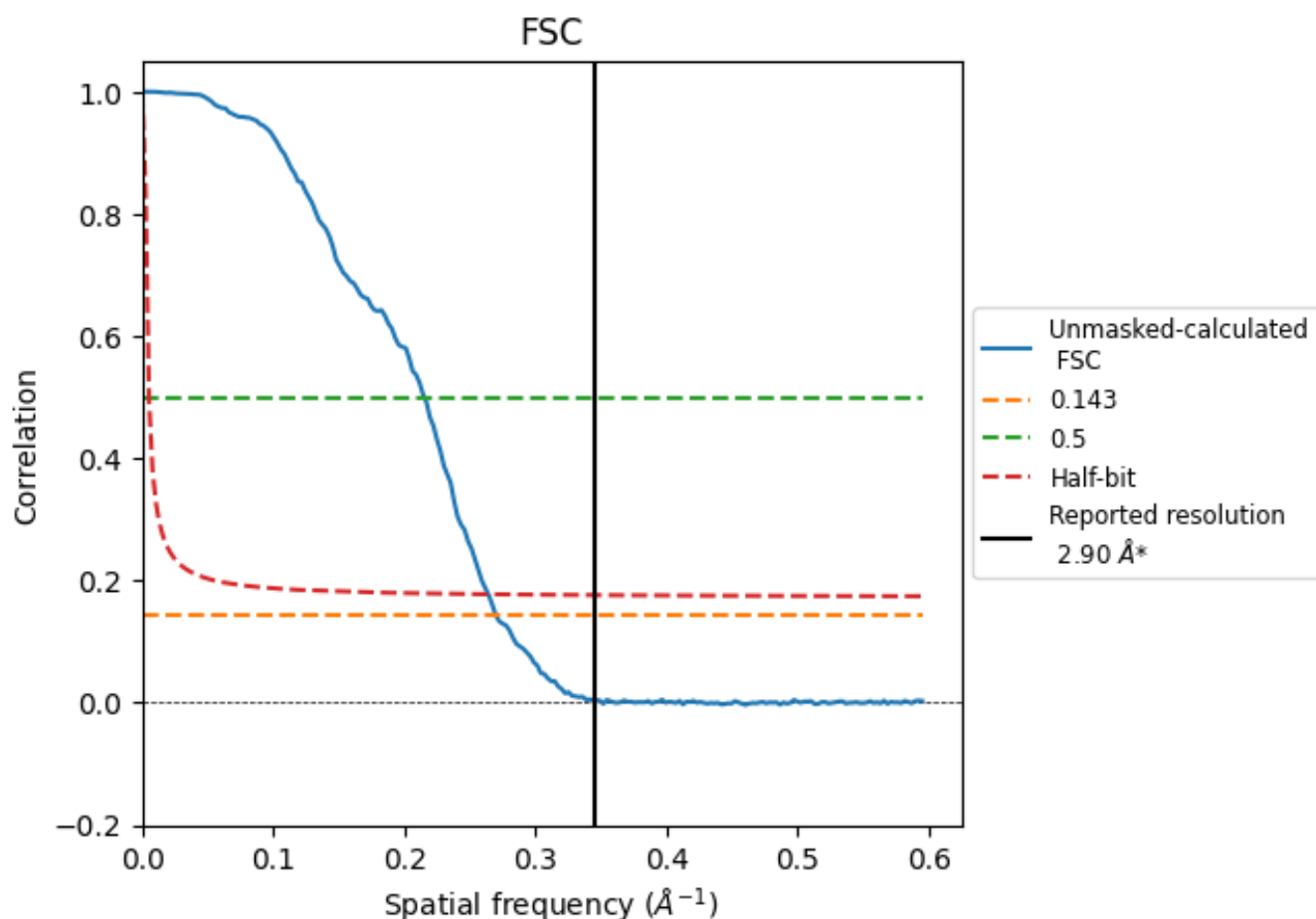


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

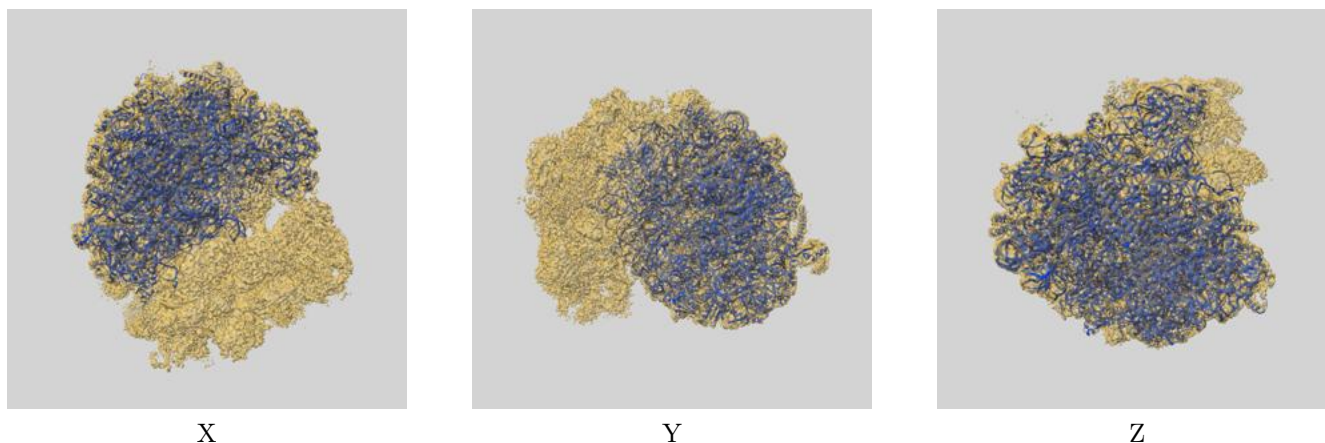
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.64	3.79

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

9 Map-model fit [i](#)

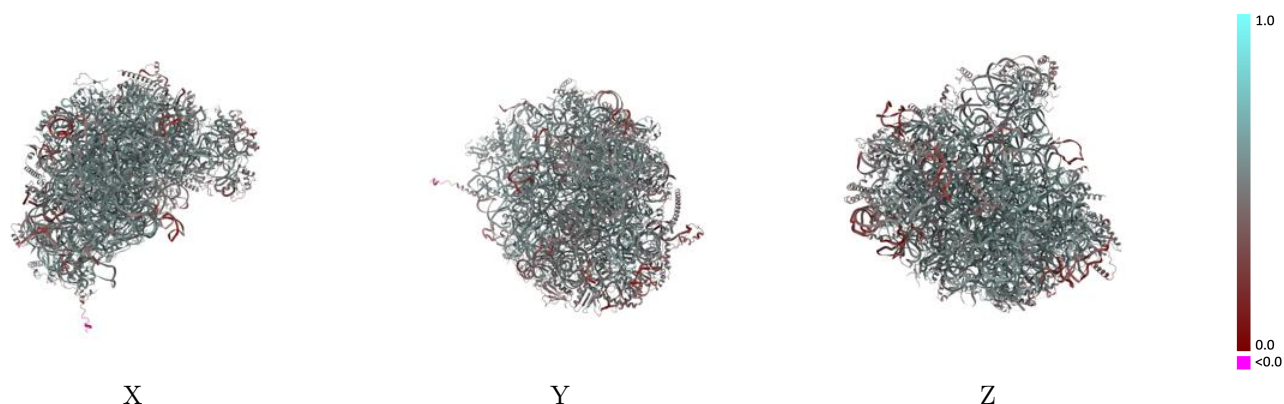
This section contains information regarding the fit between EMDB map EMD-54774 and PDB model 9SCU. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



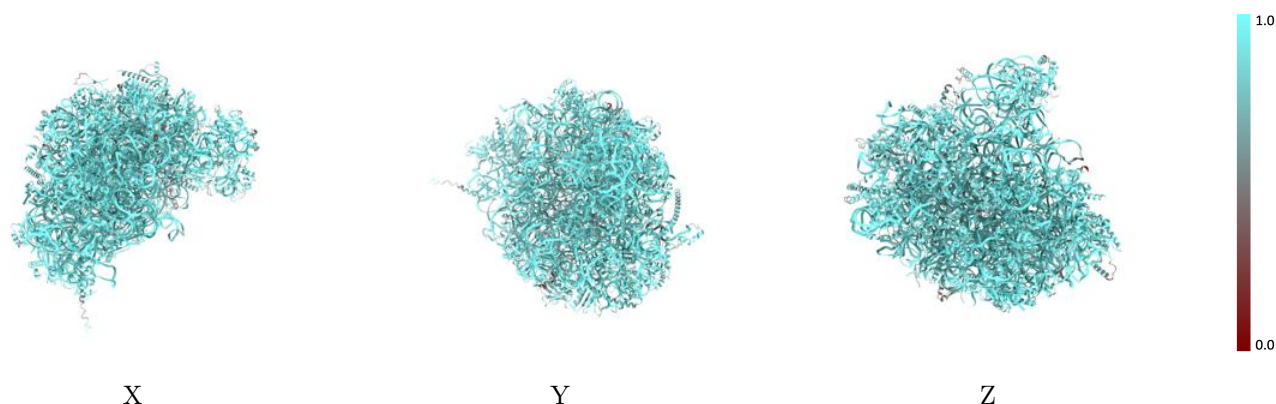
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



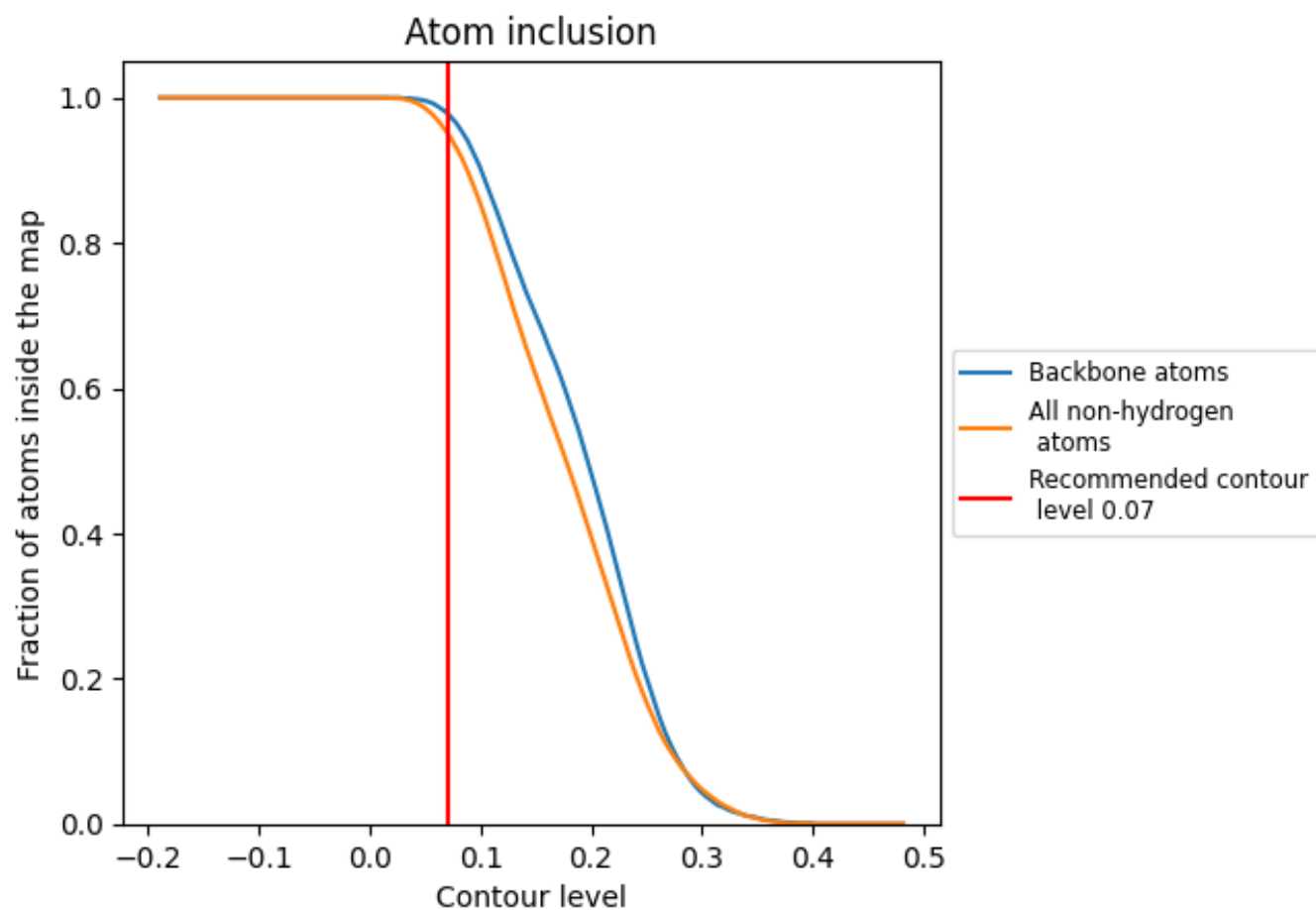
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.5140
5	 0.9820	 0.5080
6	 0.9980	 0.5150
7	 0.9890	 0.5140
CA	 0.9590	 0.5740
CB	 0.9470	 0.5510
CC	 0.9170	 0.5300
CD	 0.8800	 0.4750
CE	 0.8610	 0.4400
CF	 0.9130	 0.5310
CG	 0.8990	 0.5030
CH	 0.7950	 0.4250
CI	 0.8000	 0.4620
CJ	 0.8500	 0.4480
CK	 0.9200	 0.5270
CL	 0.9320	 0.5280
CM	 0.8890	 0.4960
CN	 0.9780	 0.5810
CO	 0.9110	 0.5250
CP	 0.9400	 0.5550
CQ	 0.9620	 0.5620
CR	 0.8850	 0.4860
CS	 0.9430	 0.5390
CT	 0.9290	 0.5380
CV	 0.9210	 0.5540
CW	 0.8980	 0.5280
CX	 0.9230	 0.5410
CY	 0.9400	 0.5380
CZ	 0.9330	 0.5260
Ca	 0.9550	 0.5610
Cb	 0.9680	 0.5430
Cc	 0.9500	 0.5000
Cd	 0.9000	 0.5210
Ce	 0.9370	 0.5510
Cf	 0.9410	 0.5430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Cg	 0.9520	 0.5580
Ch	 0.9200	 0.5150
Ci	 0.9280	 0.5200
Cj	 0.9540	 0.5670
Ck	 0.8990	 0.4830
Cl	 0.9150	 0.5320
Cm	 0.5300	 0.4150
Cp	 0.9250	 0.5260
w	 0.5760	 0.3990