



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:34 AM UTC

PDB ID : 7QCA / pdb_00007qca
EMDB ID : EMD-13892
Title : Spraguea lophii ribosome
Authors : Gil Diez, P.; McLaren, M.; Isupov, M.N.; Daum, B.; Connors, R.; Williams, B.
Deposited on : 2021-11-22
Resolution : 2.79 Å(reported)
Based on initial model : 6RM3

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

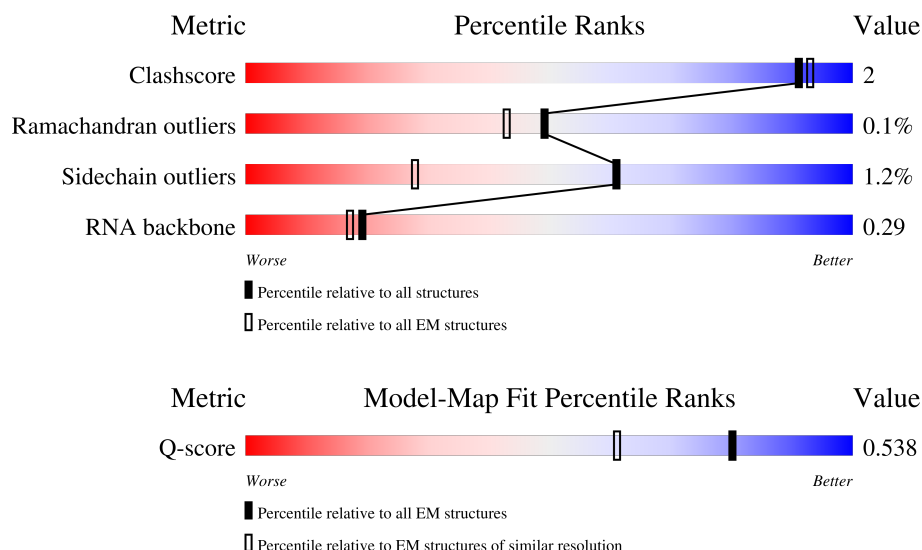
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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.



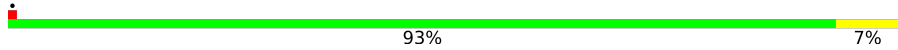
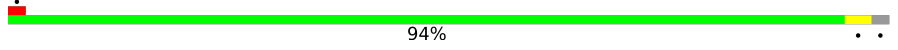
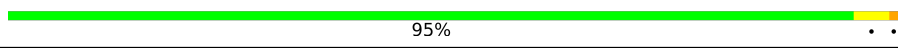
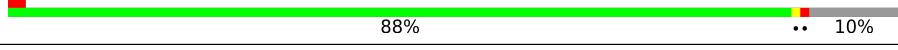
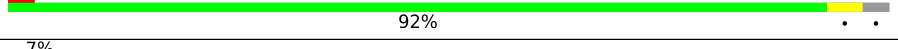
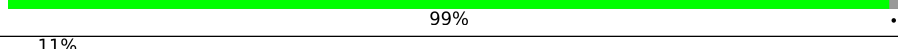
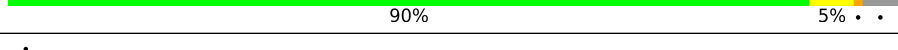
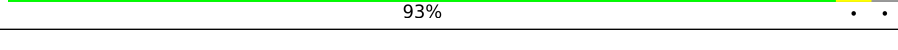
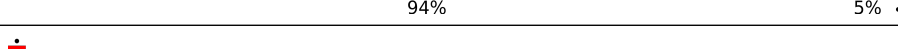
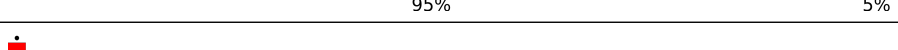
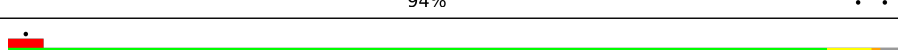
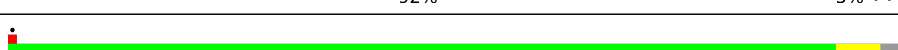
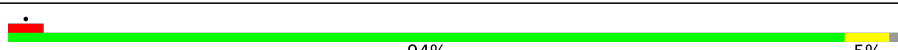
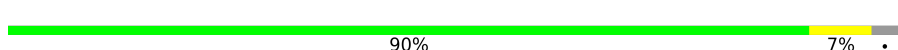
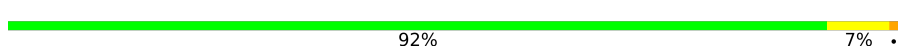
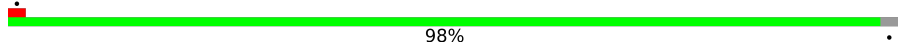
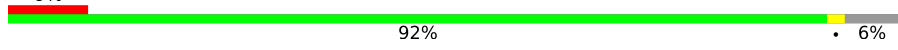
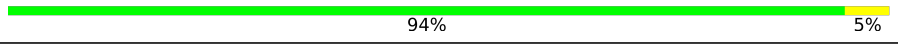
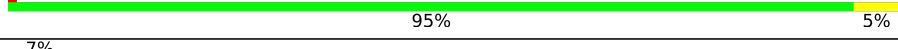
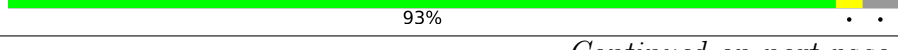
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	L50	2618	
2	L70	119	
3	LA0	246	

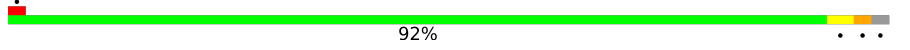
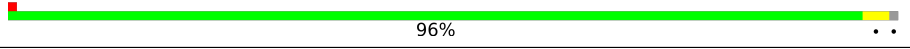
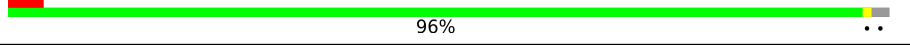
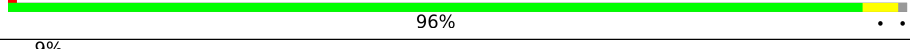
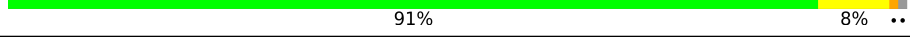
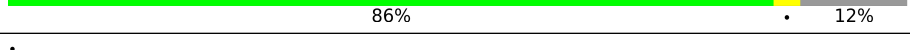
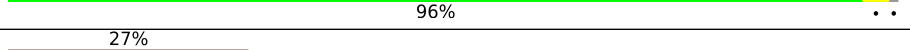
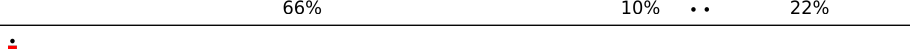
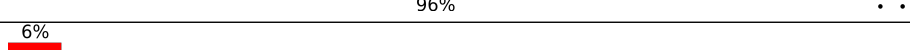
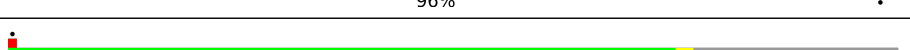
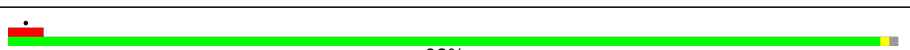
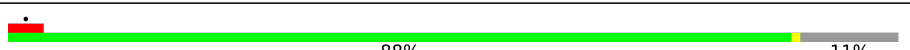
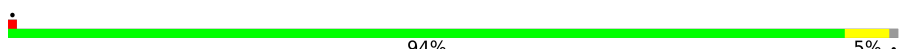
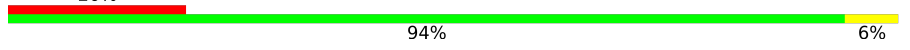
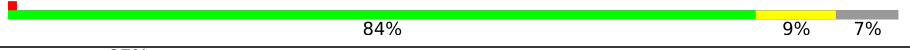
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	LAA	147	
5	LB0	392	
6	LC0	328	
7	LCC	110	
8	LD0	291	
9	LDD	110	
10	LE0	171	
11	LEE	139	
12	LF0	235	
13	LFF	111	
14	LG0	206	
15	LGG	106	
16	LH0	187	
17	LHH	119	
18	LI0	218	
19	LII	98	
20	LJ0	171	
21	LJJ	92	
22	LL0	165	
23	LLL	52	
24	LM0	122	
25	LMM	127	
26	LN0	204	
27	LO0	198	
28	LOO	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LP0	167	
30	LPP	89	
31	LQ0	183	
32	LR0	168	
33	LS0	171	
34	LT0	158	
35	LU0	113	
36	LV0	142	
37	LW0	131	
38	LX0	113	
39	LY0	131	
40	LZ0	153	
41	S60	1368	
42	SA0	233	
43	SAA	102	
44	SB0	230	
45	SBB	82	
46	SC0	248	
47	SCC	65	
48	SD0	242	
49	SDD	65	
50	SE0	280	
51	SEE	60	
52	SF0	195	
53	SFF	150	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SG0	230	
55	SGG	326	
56	SH0	164	
57	SI0	173	
58	SJ0	184	
59	SK0	107	
60	SL0	155	
61	SM0	130	
62	SN0	143	
63	SO0	135	
64	SP0	163	
65	SQ0	143	
66	SR0	120	
67	SS0	160	
68	ST0	143	
69	SU0	119	
70	SV0	67	
71	SW0	128	
72	SX0	141	
73	SY0	146	
74	SZ0	128	

2 Entry composition

There are 77 unique types of molecules in this entry. The entry contains 171001 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 RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L50	2499	Total	C	N	O	P	0	0
			53655	23950	9876	17330	2499		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L70	119	Total	C	N	O	P	0	0
			2542	1136	459	828	119		

- Molecule 3 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA0	245	Total	C	N	O	S	0	0
			1889	1189	361	334	5		

- Molecule 4 is a protein called uL15 LAA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LAA	147	Total	C	N	O	S	0	0
			1167	738	229	194	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB0	383	Total	C	N	O	S	0	0
			3039	1926	559	543	11		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC0	327	Total	C	N	O	S	0	0
			2604	1629	478	485	12		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LCC	99	Total	C	N	O	S	0	0
			781	504	126	148	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD0	281	Total	C	N	O	S	0	0
			2298	1451	410	426	11		

- Molecule 9 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LDD	109	Total	C	N	O	S	0	0
			895	575	163	154	3		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE0	165	Total	C	N	O	S	0	0
			1371	879	227	262	3		

- Molecule 11 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LEE	135	Total	C	N	O	S	0	0
			1090	697	205	182	6		

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LF0	231	Total	C	N	O	S	0	0
			1933	1234	342	350	7		

- Molecule 13 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LFF	111	Total	C	N	O	S	0	0
			893	567	159	162	5		

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG0	199	Total	C	N	O	S	0	0
			1590	1015	275	290	10		

- Molecule 15 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LGG	104	Total	C	N	O	S	0	0
			819	504	169	139	7		

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH0	183	Total	C	N	O	S	0	0
			1477	951	252	266	8		

- Molecule 17 is a protein called Ribosomal L29 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LHH	119	Total	C	N	O	S	0	0
			992	626	188	175	3		

- Molecule 18 is a protein called S60 ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LI0	217	Total	C	N	O	S	0	0
			1750	1096	333	308	13		

- Molecule 19 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LII	97	Total	C	N	O	S	0	0
			784	496	146	136	6		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ0	167	Total	C	N	O	S	0	0
			1332	847	242	236	7		

- Molecule 21 is a protein called eL37 LJJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJJ	89	Total	C	N	O	S	0	0
			701	427	146	118	10		

- Molecule 22 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL0	164	Total	C	N	O	S	0	0
			1353	857	252	232	12		

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LLL	51	Total	C	N	O	S	0	0
			427	272	87	65	3		

- Molecule 24 is a protein called eL14 LM0.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LM0	115	Total	C	N	O	S	0	0
			927	588	151	183	5		

- Molecule 25 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LMM	52	Total	C	N	O	S	0	0
			427	264	89	70	4		

- Molecule 26 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LN0	203	Total	C	N	O	S	0	0
			1688	1055	346	276	11		

- Molecule 27 is a protein called Ribosomal protein L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LO0	198	Total	C	N	O	S	0	0
			1598	1018	286	280	14		

- Molecule 28 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LOO	100	Total	C	N	O	S	0	0
			801	504	163	130	4		

- Molecule 29 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LP0	154	Total	C	N	O	S	0	0
			1238	794	225	213	6		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LPP	87	Total	C	N	O	S	0	0
			684	427	131	116	10		

- Molecule 31 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LQ0	182	Total	C	N	O	S	0	0
			1491	950	270	266	5		

- Molecule 32 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LR0	164	Total	C	N	O	S	0	0
			1336	832	261	236	7		

- Molecule 33 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LS0	170	Total	C	N	O	S	0	0
			1400	898	241	256	5		

- Molecule 34 is a protein called 60s ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LT0	156	Total	C	N	O	S	0	0
			1270	808	233	224	5		

- Molecule 35 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LU0	100	Total	C	N	O	S	0	0
			810	526	135	147	2		

- Molecule 36 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LV0	141	Total	C	N	O	S	0	0
			1057	663	200	189	5		

- Molecule 37 is a protein called Ribosomal protein L24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LW0	102	Total	C	N	O	S	0	0
			832	539	143	147	3		

- Molecule 38 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LX0	112	Total	C	N	O	S	0	0
			874	562	156	155	1		

- Molecule 39 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LY0	131	Total	C	N	O	S	0	0
			1048	658	197	186	7		

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LZ0	118	Total	C	N	O	S	0	0
			963	618	172	169	4		

- Molecule 41 is a RNA chain called RNA SSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S60	1354	Total	C	N	O	P	0	0
			29181	13024	5463	9340	1354		

- Molecule 42 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SA0	220	Total	C	N	O	S	0	0
			1725	1091	292	328	14		

- Molecule 43 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SAA	101	Total	C	N	O	S	0	0
			827	513	163	145	6		

- Molecule 44 is a protein called eS1 SB0.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SB0	204	Total	C	N	O	S	0	0
			1609	1018	286	298	7		

- Molecule 45 is a protein called eS27 SBB.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SBB	81	Total	C	N	O	S	0	0
			627	394	108	116	9		

- Molecule 46 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SC0	226	Total	C	N	O	S	0	0
			1727	1099	300	321	7		

- Molecule 47 is a protein called eS28 SCC.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SCC	62	Total	C	N	O	S	0	0
			476	295	86	91	4		

- Molecule 48 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SD0	216	Total	C	N	O	S	0	0
			1700	1085	300	307	8		

- Molecule 49 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SDD	65	Total	C	N	O	S	0	0
			550	345	102	96	7		

- Molecule 50 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE0	260	Total	C	N	O	S	0	0
			2044	1297	361	379	7		

- Molecule 51 is a protein called eS30 SEE.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SEE	56	Total	C	N	O	S	0	0
			447	284	89	74			

- Molecule 52 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SF0	192	Total	C	N	O	S	0	0
			1509	953	275	275	6		

- Molecule 53 is a protein called Ubiquitin/40s ribosomal protein S27a fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SFF	58	Total	C	N	O	S	0	0
			447	278	81	83	5		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG0	229	Total	C	N	O	S	0	0
			1835	1178	325	328	4		

- Molecule 55 is a protein called Guanine nucleotide binding protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SGG	319	Total	C	N	O	S	0	0
			2478	1558	411	494	15		

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH0	163	Total	C	N	O	S	0	0
			1335	855	219	255	6		

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI0	167	Total	C	N	O	S	0	0
			1347	834	266	240	7		

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SJ0	168	Total	C	N	O	S	0	0
			1379	880	252	243	4		

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SK0	91	Total	C	N	O	S	0	0
			764	490	130	140	4		

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL0	150	Total	C	N	O	S	0	0
			1229	790	217	216	6		

- Molecule 61 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM0	113	Total	C	N	O	S	0	0
			876	553	156	162	5		

- Molecule 62 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN0	142	Total	C	N	O	S	0	0
			1130	728	196	202	4		

- Molecule 63 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO0	129	Total	C	N	O	S	0	0
			983	606	191	183	3		

- Molecule 64 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP0	117	Total	C	N	O	S	0	0
			950	598	172	173	7		

- Molecule 65 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ0	142	Total	C	N	O	S	0	0
			1143	726	204	207	6		

- Molecule 66 is a protein called eS17 SR0.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR0	119	Total	C	N	O	S	0	0
			977	616	172	186	3		

- Molecule 67 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS0	144	Total	C	N	O	S	0	0
			1150	720	220	207	3		

- Molecule 68 is a protein called 40S Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST0	142	Total	C	N	O	S	0	0
			1161	741	208	211	1		

- Molecule 69 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU0	100	Total	C	N	O	S	0	0
			809	515	144	143	7		

- Molecule 70 is a protein called Ribosomal protein S21E.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV0	65	Total	C	N	O	S	0	0
			521	319	96	101	5		

- Molecule 71 is a protein called 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SW0	128	Total	C	N	O	S	0	0
			1022	639	195	180	8		

- Molecule 72 is a protein called uS12 SX0.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX0	140	Total	C	N	O	S	0	0
			1098	692	216	186	4		

- Molecule 73 is a protein called 40s ribosomal protein s24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY0	136	Total	C	N	O	S	0	0
			1118	693	215	204	6		

- Molecule 74 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ0	76	Total	C	N	O	S	0	0
			633	403	116	113	1		

- Molecule 75 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
75	L50	145	Total	K	0
			145	145	
75	LA0	2	Total	K	0
			2	2	
75	LEE	1	Total	K	0
			1	1	
75	LLL	1	Total	K	0
			1	1	
75	LN0	1	Total	K	0
			1	1	
75	S60	44	Total	K	0
			44	44	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
75	SN0	3	Total 3	K 3	0
75	SO0	2	Total 2	K 2	0

- Molecule 76 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
76	L50	104	Total 104	Mg 104	0
76	L70	4	Total 4	Mg 4	0
76	LB0	1	Total 1	Mg 1	0
76	LF0	1	Total 1	Mg 1	0
76	LII	1	Total 1	Mg 1	0
76	LJJ	1	Total 1	Mg 1	0
76	LV0	1	Total 1	Mg 1	0
76	S60	46	Total 46	Mg 46	0
76	SI0	1	Total 1	Mg 1	0

- Molecule 77 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
77	LGG	1	Total 1	Zn 1	0
77	LJJ	1	Total 1	Zn 1	0
77	LMM	1	Total 1	Zn 1	0
77	LOO	1	Total 1	Zn 1	0
77	LPP	1	Total 1	Zn 1	0
77	SAA	1	Total 1	Zn 1	0

Continued on next page...

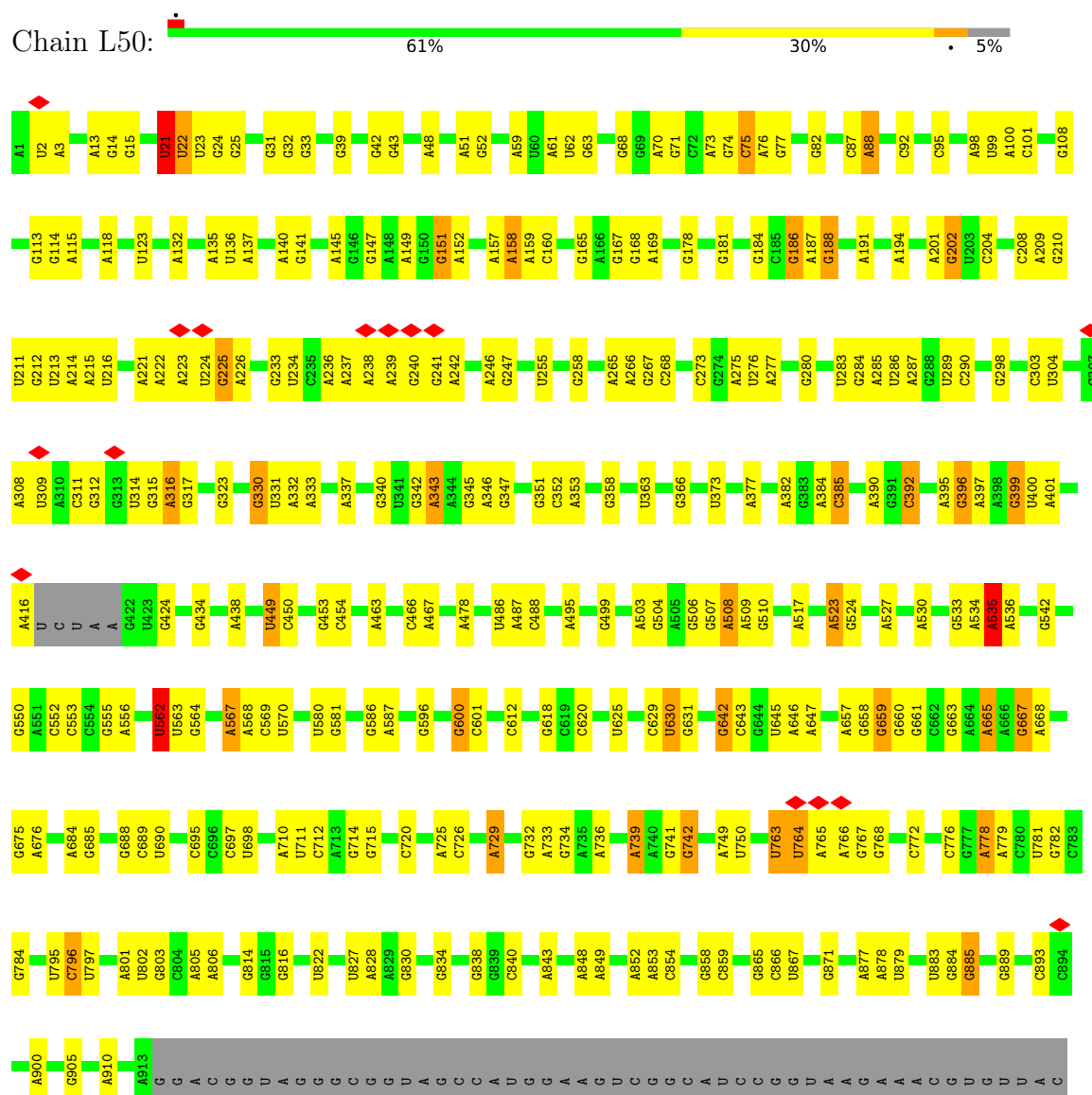
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
77	SBB	1	Total 1	Zn 1	0
77	SDD	1	Total 1	Zn 1	0
77	SFF	1	Total 1	Zn 1	0

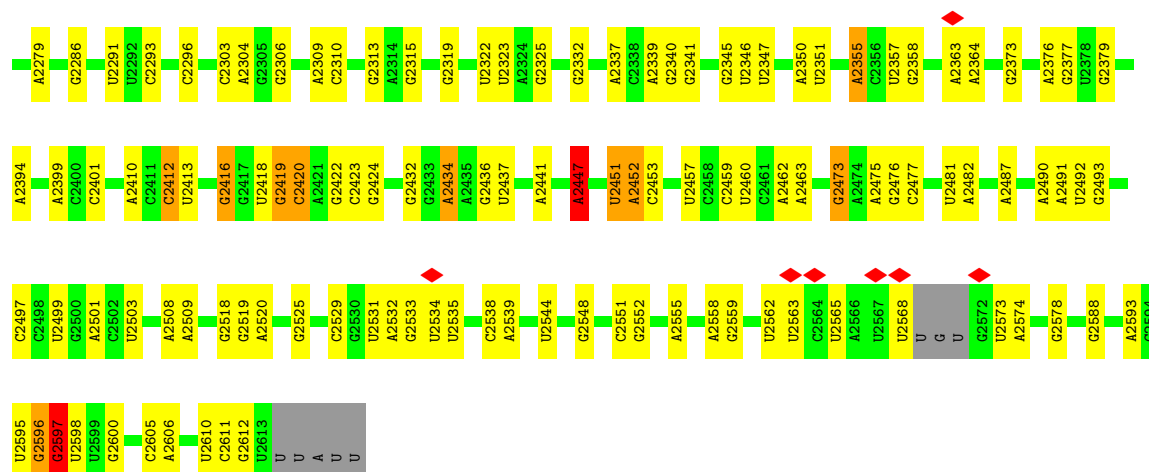
3 Residue-property plots

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

• Molecule 1: RNA 23S

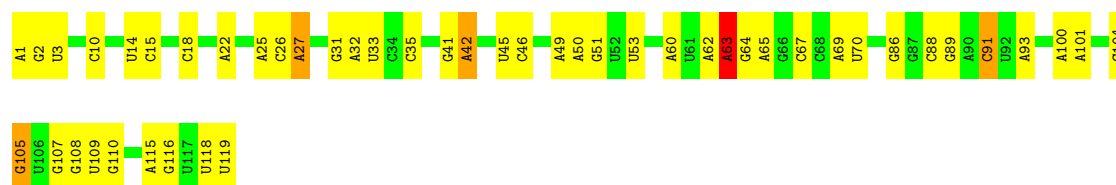






- Molecule 2: RNA 5S

Chain L70: 60% 36% ..



- Molecule 3: 60S ribosomal protein L8

Chain LA0: 97% .



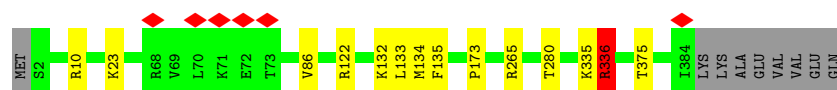
- Molecule 4: uL15 LAA

Chain LAA: 93% 7%



- Molecule 5: 60S ribosomal protein L3

Chain LB0: 94% ..

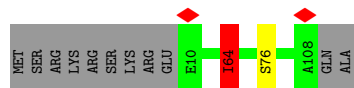


- Molecule 6: 60S ribosomal protein L4

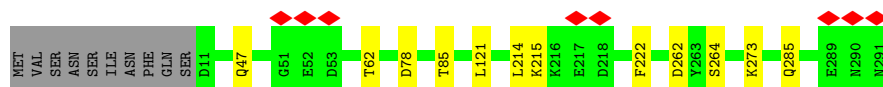
Chain LC0: 95% ..



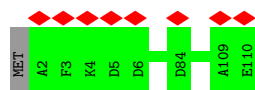
- Molecule 7: 60S ribosomal protein L3



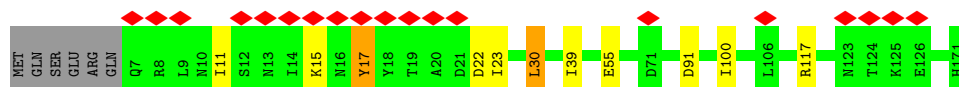
- Molecule 8: 60S ribosomal protein L5



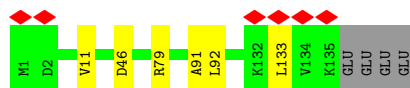
- Molecule 9: 60S ribosomal protein L31



- Molecule 10: 60S ribosomal protein L6



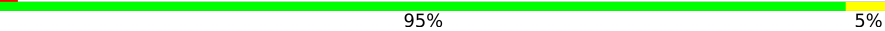
- Molecule 11: 60S ribosomal protein L32



- Molecule 12: 60S ribosomal protein L7

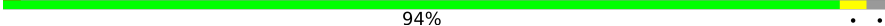


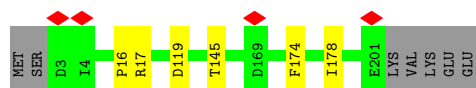
- Molecule 13: 60S ribosomal protein L35a

Chain LFF:  95% 5%

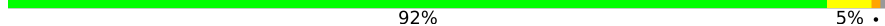


- Molecule 14: 60S ribosomal protein L8

Chain LG0:  94% 5%



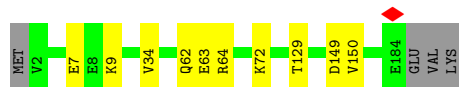
- Molecule 15: Ribosomal protein L34

Chain LGG:  92% 5%

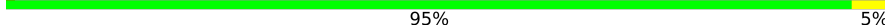


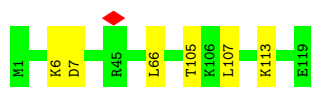
- Molecule 16: 60S ribosomal protein L9

Chain LH0:  93% 5%

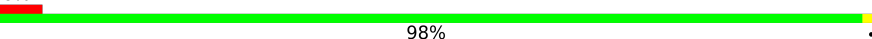


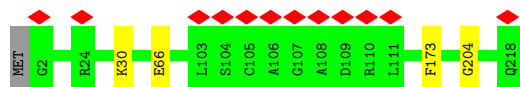
- Molecule 17: Ribosomal L29 protein

Chain LHH:  95% 5%



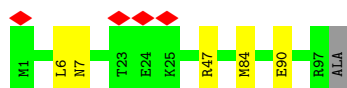
- Molecule 18: S60 ribosomal protein L10

Chain LI0:  98% 6%



- Molecule 19: 60S ribosomal protein L36

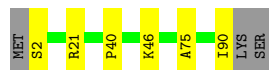
Chain LII:  94% 5%



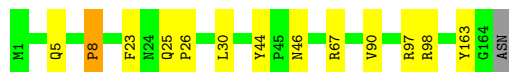
• Molecule 20: 60S ribosomal protein L11

Chain LJ0:  92% 6%

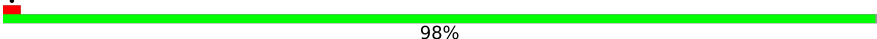
• Molecule 21: eL37 LJJ

Chain LJJ:  90% 7%

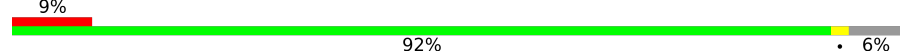
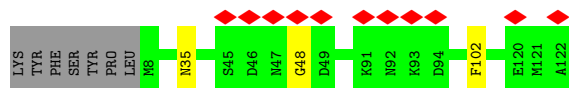
• Molecule 22: 60S ribosomal protein L13

Chain LL0:  92% 7%

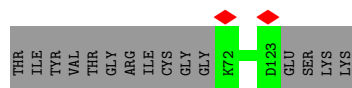
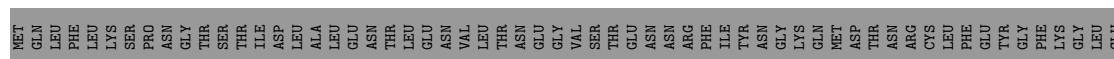
• Molecule 23: 60S ribosomal protein L39

Chain LLL:  98%

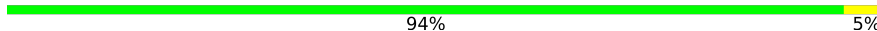
• Molecule 24: eL14 LM0

Chain LM0:  9% 92% 6%

• Molecule 25: Ubiquitin

Chain LMM:  41% 59%

• Molecule 26: Ribosomal protein L15

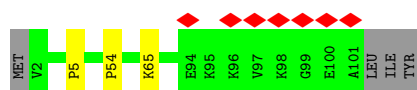
Chain LN0:  94% 5%



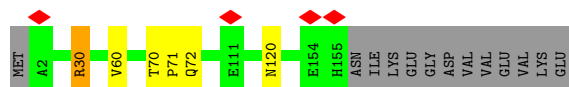
- Molecule 27: Ribosomal protein L13A



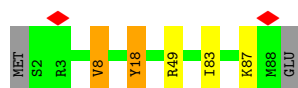
- Molecule 28: 60S ribosomal protein L44



- Molecule 29: 60S ribosomal protein L17



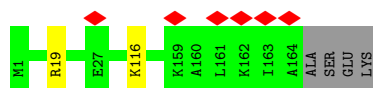
- Molecule 30: 60S ribosomal protein L37a



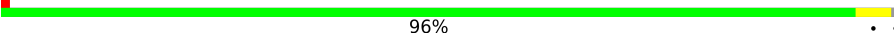
- Molecule 31: 60S ribosomal protein L18

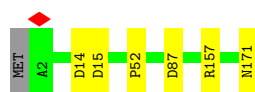


- Molecule 32: 60S ribosomal protein L19



- Molecule 33: 60S ribosomal protein L20

Chain LS0:  96%



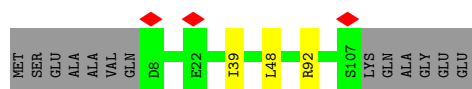
- Molecule 34: 60s ribosomal protein L21

Chain LT0:  9% 91% 8%

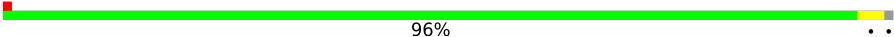


- Molecule 35: 60S ribosomal protein L22

Chain LU0:  86% 12%



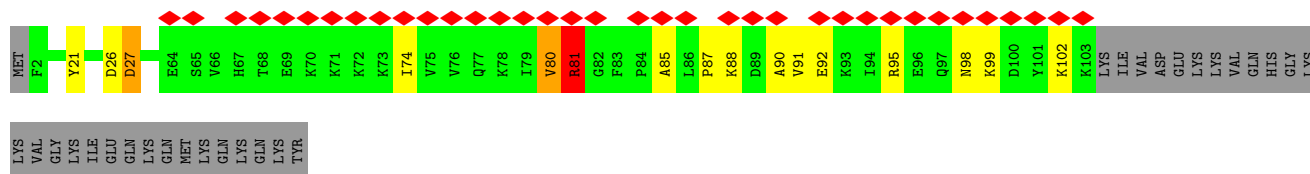
- Molecule 36: Ribosomal protein L23

Chain LV0:  96%

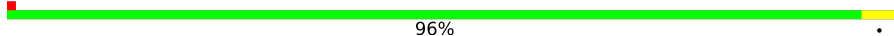


- Molecule 37: Ribosomal protein L24E

Chain LW0:  27% 66% 10% 22%

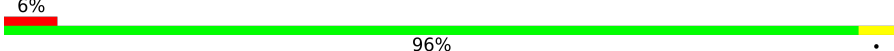


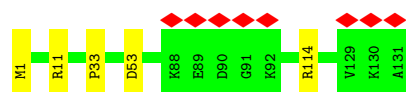
- Molecule 38: 60S ribosomal protein L23a

Chain LX0:  96%

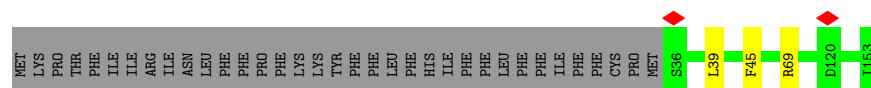
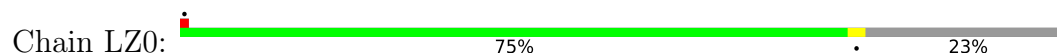


- Molecule 39: 60S ribosomal protein L26

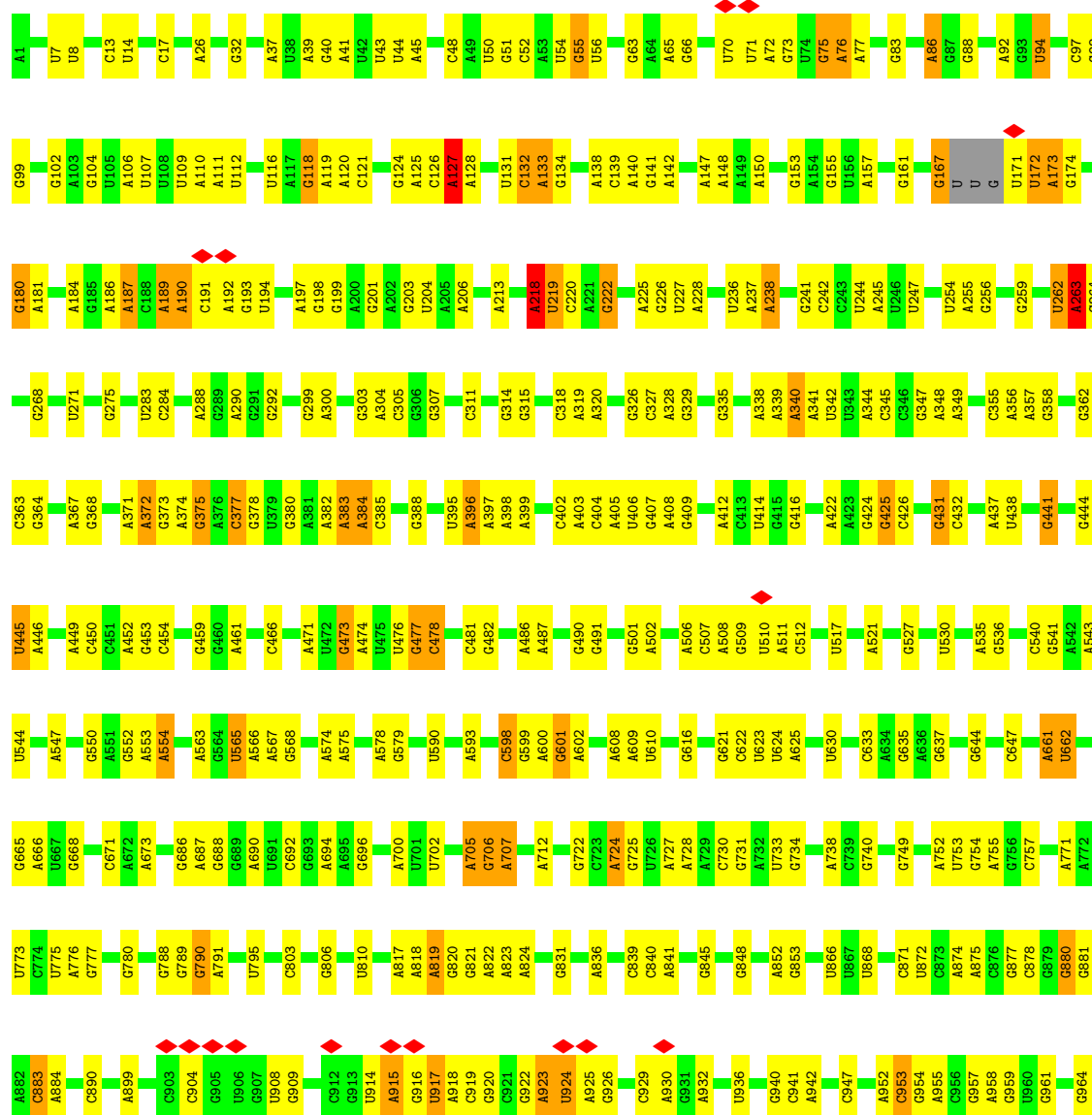
Chain LY0:  6% 96%

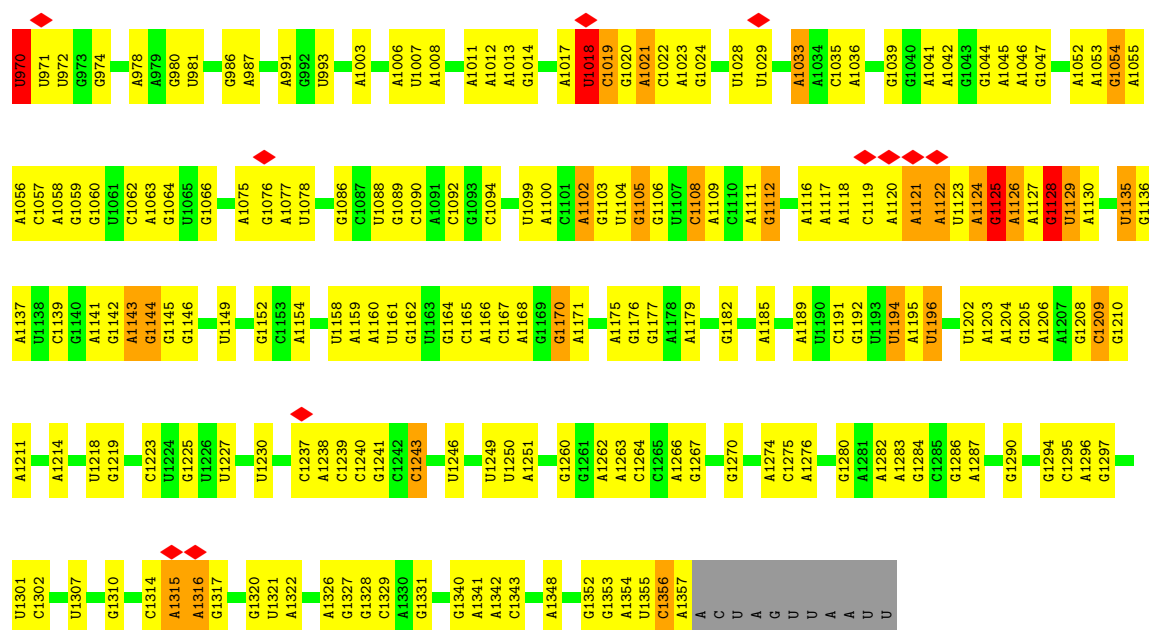


- Molecule 40: 60S ribosomal protein L27



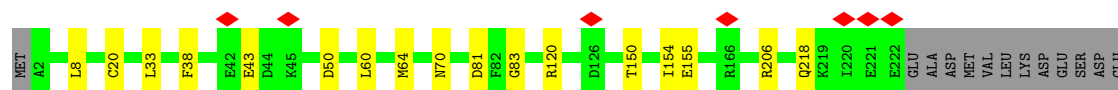
- Molecule 41: RNA SSU





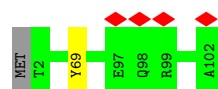
- Molecule 42: 40S ribosomal protein S0

Chain SA0: 87% 7% 6%



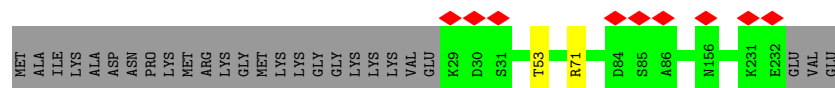
- Molecule 43: 40S ribosomal protein S26

Chain SAA: 98% ..



- Molecule 44: eS1 SB0

Chain SB0: 88% 11%



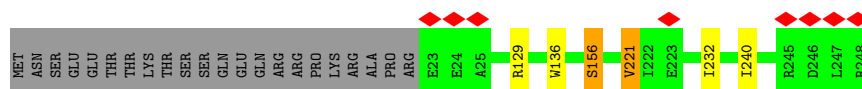
- Molecule 45: eS27 SBB

Chain SBB: 94% 5%



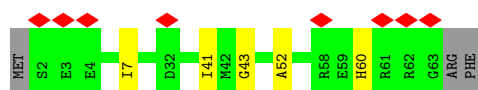
- Molecule 46: 40S ribosomal protein S2

Chain SC0:  89% 9%



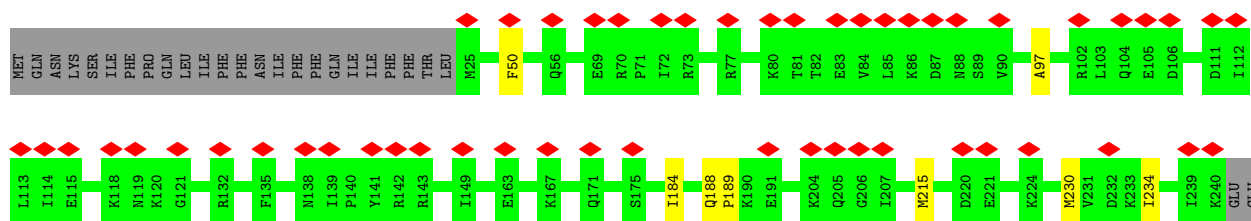
- Molecule 47: eS28 SCC

Chain SCC:  12% 88% 8% 5%

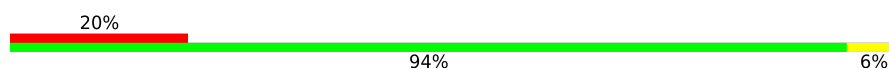


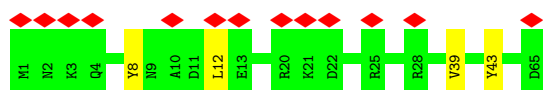
- Molecule 48: 40S ribosomal protein S3

Chain SD0:  21% 86% 11%



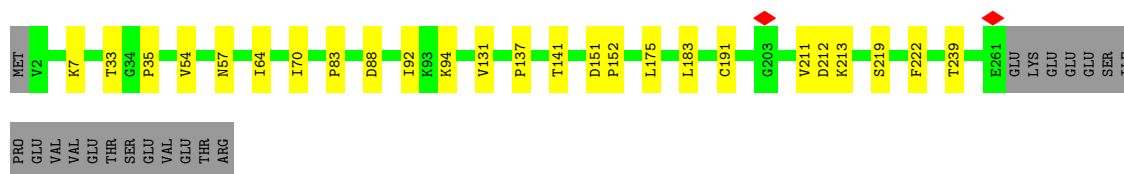
- Molecule 49: 40S ribosomal protein S29

Chain SDD:  20% 94% 6%



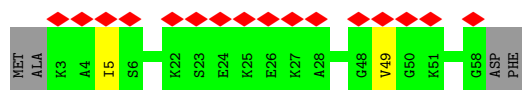
- Molecule 50: 40S ribosomal protein S4

Chain SE0:  84% 9% 7%

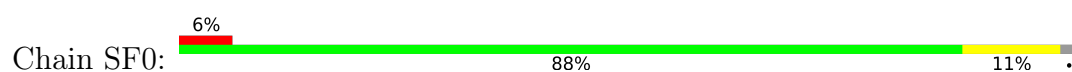


- Molecule 51: eS30 SEE

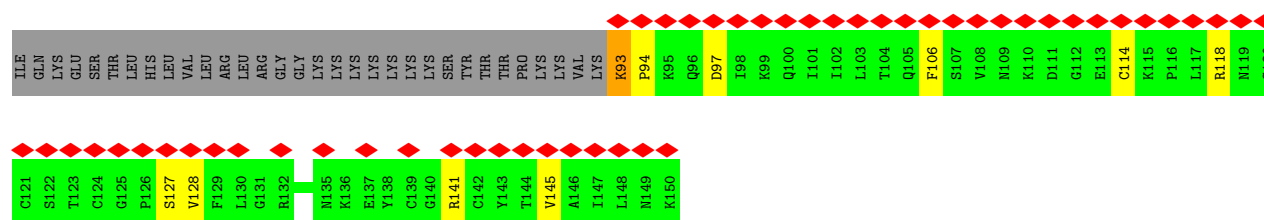
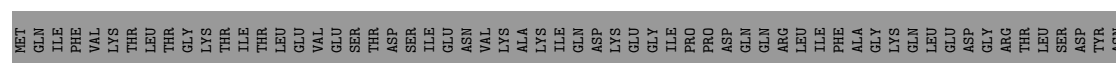
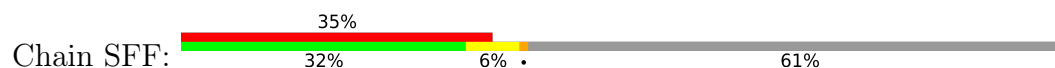
Chain SEE:  27% 90% 7%



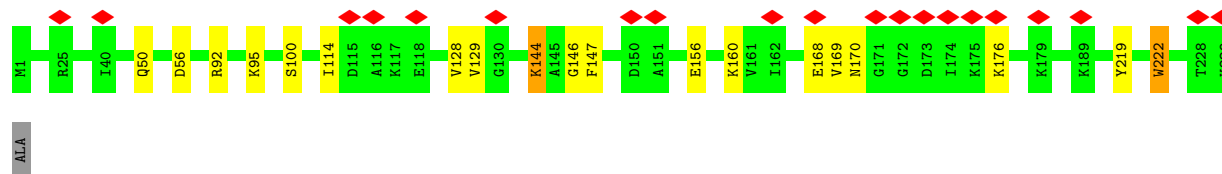
- Molecule 52: 40S ribosomal protein S5



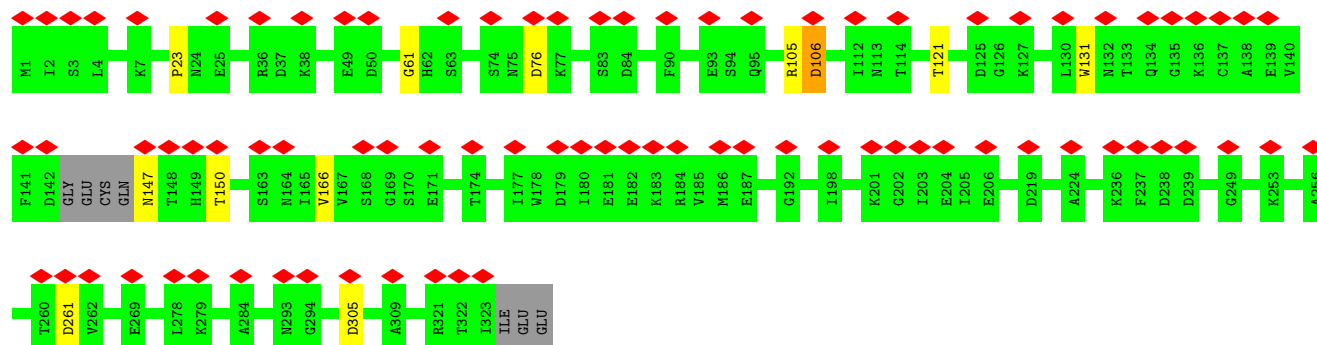
- Molecule 53: Ubiquitin/40s ribosomal protein S27a fusion



- Molecule 54: 40S ribosomal protein S6

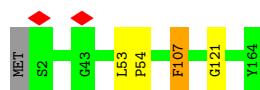


- Molecule 55: Guanine nucleotide binding protein beta subunit

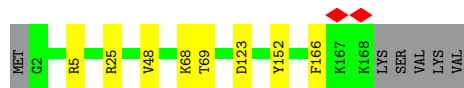


- Molecule 56: 40S ribosomal protein S7





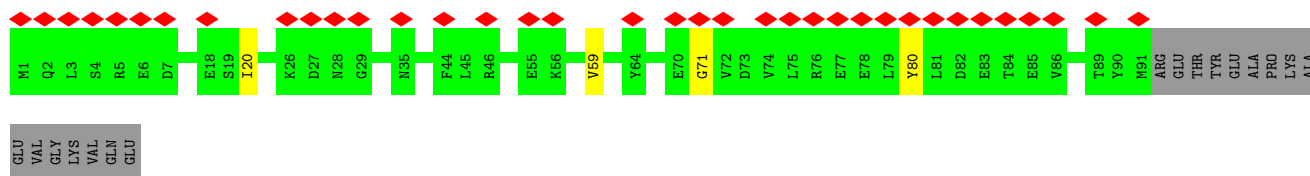
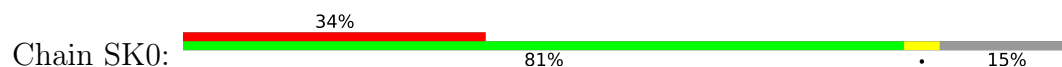
- Molecule 57: 40S ribosomal protein S8



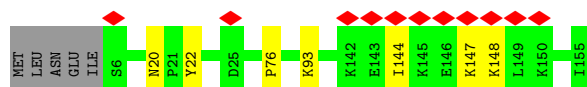
- Molecule 58: 40S ribosomal protein S9



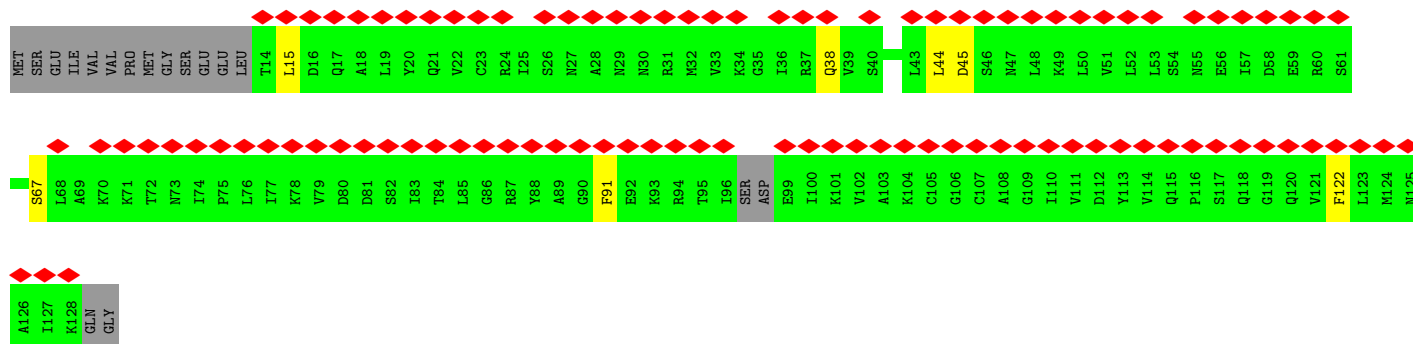
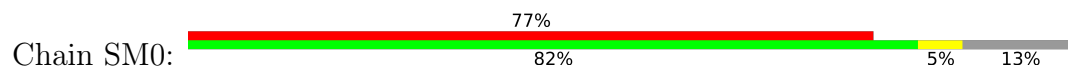
- Molecule 59: 40S ribosomal protein S10



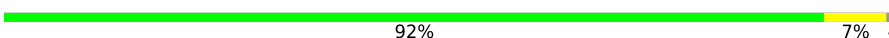
- Molecule 60: 40S ribosomal protein S11

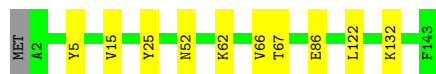


- Molecule 61: 40S ribosomal protein S12



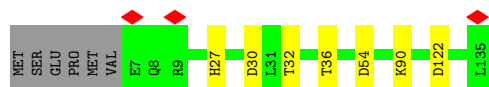
- Molecule 62: 40S ribosomal protein S13

Chain SN0:  92% 7%



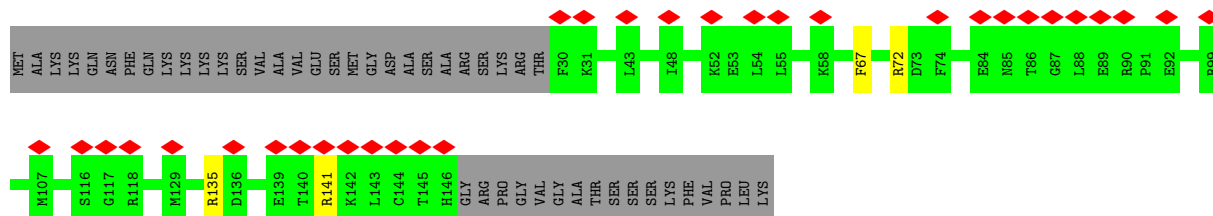
- Molecule 63: 40S ribosomal protein S14

Chain SO0:  90% 5%

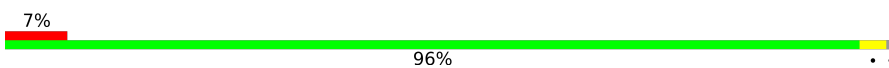


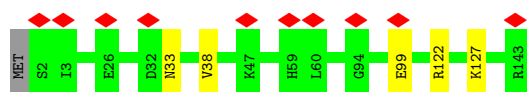
- Molecule 64: Ribosomal protein S19

Chain SP0:  20% 69% 28%

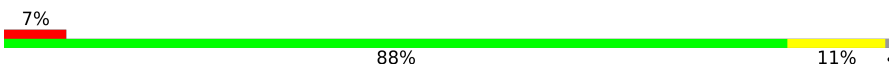


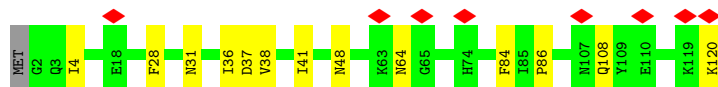
- Molecule 65: 40S ribosomal protein S16

Chain SQ0:  7% 96%



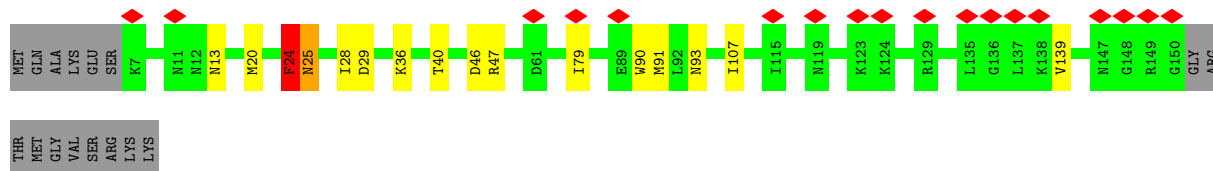
- Molecule 66: eS17 SR0

Chain SR0:  7% 88% 11%

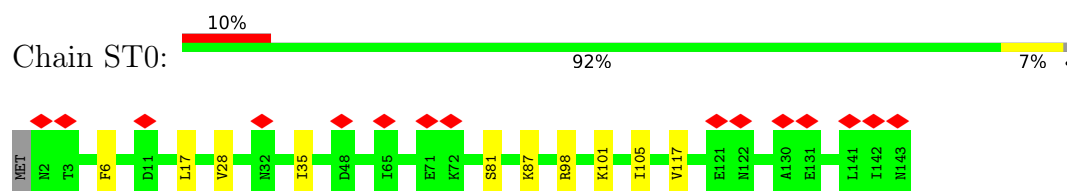


- Molecule 67: 40S ribosomal protein S18

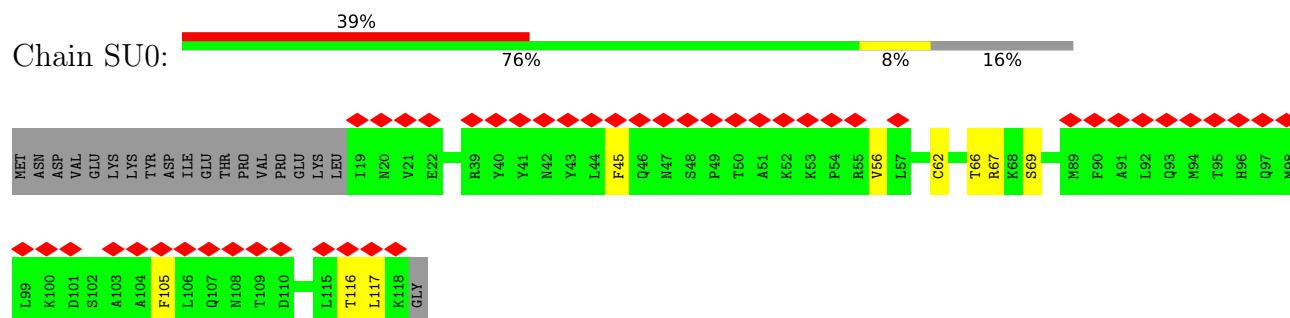
Chain SS0:  11% 80% 9% 10%



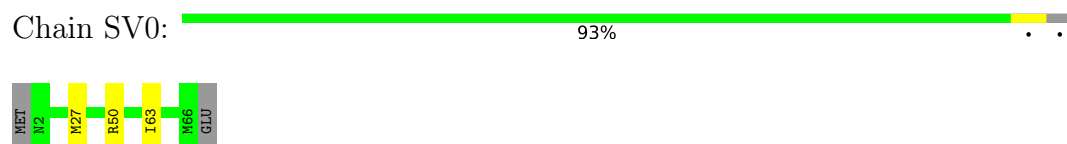
- Molecule 68: 40S Ribosomal protein S19



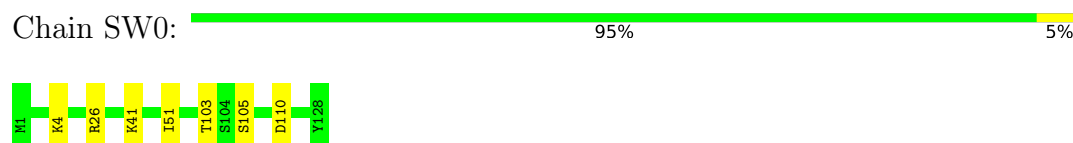
- Molecule 69: 40S ribosomal protein S20



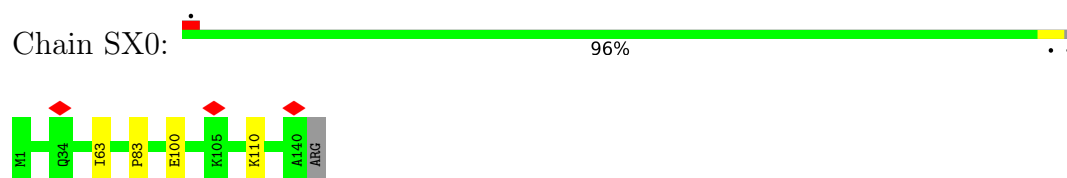
- Molecule 70: Ribosomal protein S21E



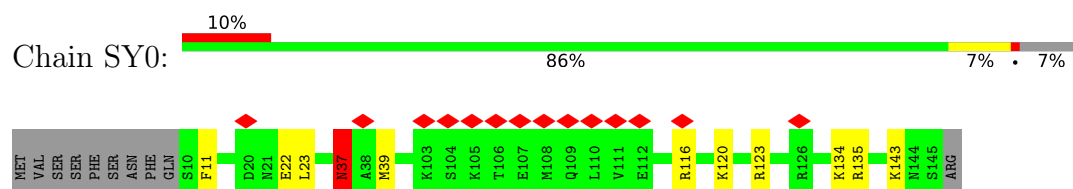
- Molecule 71: 40S ribosomal protein S15A



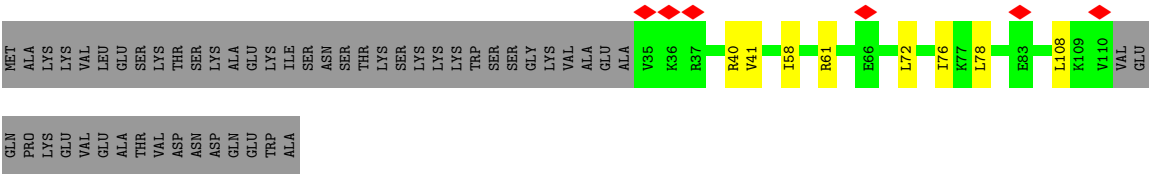
- Molecule 72: uS12 SX0



- Molecule 73: 40s ribosomal protein s24



- Molecule 74: 40S ribosomal protein S25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	285940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS, TFS TALOS	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.5, 41.34	Depositor
Minimum defocus (nm)	1200, 1200	Depositor
Maximum defocus (nm)	2500, 2500	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.403	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.05356	Depositor
Map size ($\text{\AA}$)	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, K

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	L50	0.70	0/60107	1.07	178/93753 (0.2%)
2	L70	0.71	0/2844	1.02	8/4429 (0.2%)
3	LA0	0.54	0/1926	1.05	0/2590
4	LAA	0.55	0/1191	0.94	0/1586
5	LB0	0.52	0/3092	0.99	2/4144 (0.0%)
6	LC0	0.51	0/2646	1.07	3/3555 (0.1%)
7	LCC	0.49	0/794	1.01	0/1067
8	LD0	0.44	0/2328	1.05	3/3098 (0.1%)
9	LDD	0.49	0/913	0.97	0/1223
10	LE0	0.46	0/1394	1.03	3/1875 (0.2%)
11	LEE	0.49	0/1108	1.05	1/1477 (0.1%)
12	LF0	0.48	0/1963	0.99	2/2618 (0.1%)
13	LFF	0.53	0/906	1.02	0/1207
14	LG0	0.47	0/1612	1.05	0/2163
15	LGG	0.49	0/825	1.12	2/1090 (0.2%)
16	LH0	0.48	0/1503	0.95	0/2018
17	LHH	0.44	0/999	1.03	0/1324
18	LI0	0.51	0/1781	0.99	1/2382 (0.0%)
19	LII	0.46	0/790	1.00	0/1041
20	LJ0	0.47	0/1350	1.02	1/1797 (0.1%)
21	LJJ	0.53	0/710	1.14	1/932 (0.1%)
22	LL0	0.48	0/1374	1.12	2/1827 (0.1%)
23	LLL	0.51	0/435	1.02	0/576
24	LM0	0.48	0/935	1.04	0/1251
25	LMM	0.52	0/431	1.04	0/568
26	LN0	0.53	0/1722	1.03	3/2297 (0.1%)
27	LO0	0.49	0/1626	1.03	2/2168 (0.1%)
28	LOO	0.54	0/811	1.01	0/1071
29	LP0	0.54	0/1262	1.11	0/1689
30	LPP	0.53	0/693	1.12	2/918 (0.2%)
31	LQ0	0.47	0/1512	0.99	0/2014
32	LR0	0.49	0/1352	1.04	0/1790

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LS0	0.49	0/1422	0.99	1/1898 (0.1%)
34	LT0	0.50	0/1294	0.98	1/1736 (0.1%)
35	LU0	0.47	0/826	0.99	0/1104
36	LV0	0.55	0/1068	1.03	1/1429 (0.1%)
37	LW0	0.50	0/849	1.14	2/1129 (0.2%)
38	LX0	0.48	0/883	1.03	0/1175
39	LY0	0.49	0/1058	1.08	1/1399 (0.1%)
40	LZ0	0.47	0/976	1.09	2/1302 (0.2%)
41	S60	0.68	0/32725	0.99	61/51066 (0.1%)
42	SA0	0.59	1/1751 (0.1%)	1.01	1/2358 (0.0%)
43	SAA	0.57	0/839	1.06	0/1120
44	SB0	0.50	0/1623	1.01	0/2169
45	SBB	0.57	0/634	0.99	0/844
46	SC0	0.51	0/1751	1.05	2/2359 (0.1%)
47	SCC	0.54	0/480	0.97	2/644 (0.3%)
48	SD0	0.50	0/1721	1.04	0/2304
49	SDD	0.51	0/559	1.00	1/742 (0.1%)
50	SE0	0.54	0/2080	1.07	7/2804 (0.2%)
51	SEE	0.57	0/453	1.10	1/596 (0.2%)
52	SF0	0.50	0/1527	1.09	2/2045 (0.1%)
53	SFF	0.60	0/453	1.00	0/606
54	SG0	0.49	0/1863	1.06	1/2483 (0.0%)
55	SGG	0.58	0/2517	1.05	4/3397 (0.1%)
56	SH0	0.45	0/1356	1.02	1/1820 (0.1%)
57	SI0	0.54	0/1369	1.02	1/1825 (0.1%)
58	SJ0	0.51	0/1403	1.05	0/1880
59	SK0	0.50	0/778	1.07	0/1047
60	SL0	0.54	0/1252	0.99	1/1672 (0.1%)
61	SM0	0.56	0/881	1.15	1/1182 (0.1%)
62	SN0	0.57	0/1154	1.15	2/1557 (0.1%)
63	SO0	0.54	0/993	1.09	1/1326 (0.1%)
64	SP0	0.54	0/964	1.08	0/1289
65	SQ0	0.57	0/1163	1.05	2/1556 (0.1%)
66	SR0	0.56	0/988	1.20	1/1319 (0.1%)
67	SS0	0.56	0/1165	1.12	1/1566 (0.1%)
68	ST0	0.55	0/1181	1.14	1/1585 (0.1%)
69	SU0	0.56	0/824	1.09	4/1110 (0.4%)
70	SV0	0.49	0/525	0.96	0/700
71	SW0	0.51	0/1037	0.99	0/1389
72	SX0	0.55	0/1113	1.05	1/1486 (0.1%)
73	SY0	0.49	0/1131	1.10	1/1503 (0.1%)
74	SZ0	0.57	0/640	1.09	0/855
All	All	0.61	1/182204 (0.0%)	1.04	322/264914 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LC0	0	1
13	LFF	0	1
15	LGG	0	1
66	SR0	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	SA0	20	CYS	C-N	14.48	1.53	1.34

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	1148	A	C4'-C3'-O3'	14.04	130.46	109.40
1	L50	330	G	C2'-C3'-O3'	12.46	132.39	113.70
1	L50	523	A	C1'-C2'-O2'	-12.40	93.19	111.80
41	S60	473	G	C2'-C3'-O3'	11.42	126.63	109.50
1	L50	1808	A	C4'-C3'-O3'	11.35	126.43	109.40
1	L50	1000	G	C1'-C2'-O2'	-11.19	95.02	111.80
1	L50	1018	U	C1'-C2'-O2'	-10.91	95.44	111.80
1	L50	1395	U	C2'-C3'-O3'	10.46	129.39	113.70
1	L50	1733	A	C4'-C3'-O3'	-10.35	97.48	113.00
1	L50	1959	A	C2'-C3'-O3'	10.12	128.88	113.70
41	S60	180	G	C4'-C3'-O3'	10.10	128.16	113.00
1	L50	2452	A	C4'-C3'-O3'	10.00	124.40	109.40
41	S60	565	U	C2'-C3'-O3'	9.97	124.46	109.50
1	L50	1192	A	C4'-C3'-O3'	-9.02	99.47	113.00
1	L50	827	U	C2'-C3'-O3'	-8.93	100.30	113.70
1	L50	2597	G	C2'-C3'-O3'	8.92	127.08	113.70
1	L50	1416	A	C4'-C3'-O3'	-8.85	99.73	113.00
1	L50	95	C	C2'-C3'-O3'	-8.84	100.45	113.70
1	L50	1277	G	C2'-C3'-O3'	8.77	126.86	113.70
41	S60	262	U	C2'-C3'-O3'	8.77	126.85	113.70
1	L50	1192	A	C2'-C3'-O3'	8.52	126.47	113.70
41	S60	127	A	C2'-C3'-O3'	8.51	126.46	113.70
1	L50	600	G	C1'-C2'-O2'	8.50	121.16	108.40
1	L50	600	G	O4'-C1'-C2'	-8.44	99.16	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	S60	383	A	C2'-C3'-O3'	8.41	126.32	113.70
1	L50	1277	G	C4'-C3'-O3'	8.34	125.51	113.00
1	L50	1966	A	C2'-C3'-O3'	8.13	125.90	113.70
2	L70	63	A	C4'-C3'-O3'	8.08	121.52	109.40
1	L50	395	A	C4'-C3'-O3'	-8.07	97.29	109.40
41	S60	262	U	C4'-C3'-O3'	8.04	125.06	113.00
41	S60	598	C	C2'-C3'-O3'	7.99	125.69	113.70
1	L50	1491	U	C4'-C3'-O3'	7.93	121.30	109.40
1	L50	1967	A	C2'-C3'-O3'	7.92	125.58	113.70
41	S60	565	U	C4'-C3'-O3'	7.92	121.27	109.40
1	L50	778	A	C2'-C3'-O3'	-7.77	102.05	113.70
1	L50	1614	G	C1'-C2'-O2'	-7.75	96.77	108.40
1	L50	1394	U	C2'-C3'-O3'	7.71	125.27	113.70
68	ST0	117	VAL	CA-CB-CG1	7.71	123.50	110.40
1	L50	1838	G	O4'-C1'-C2'	-7.53	98.27	105.80
1	L50	21	U	C2'-C3'-O3'	7.53	124.99	113.70
73	SY0	37	ASN	CB-CA-C	7.48	125.30	110.42
1	L50	1585	U	P-O3'-C3'	-7.32	109.22	120.20
1	L50	399	G	C2'-C3'-O3'	7.30	120.45	109.50
41	S60	724	A	C2'-C3'-O3'	-7.30	102.75	113.70
2	L70	45	U	C2'-C3'-O3'	-7.28	102.78	113.70
1	L50	1709	G	C3'-C2'-O2'	-7.26	103.71	114.60
5	LB0	335	LYS	CB-CA-C	7.24	116.99	109.83
1	L50	562	U	P-O5'-C5'	-7.21	110.08	120.90
1	L50	535	A	P-O3'-C3'	7.20	131.00	120.20
1	L50	1837	A	C2'-C3'-O3'	7.16	120.24	109.50
26	LN0	116	PHE	CA-CB-CG	7.14	120.94	113.80
1	L50	1134	A	C2'-C3'-O3'	7.11	124.37	113.70
1	L50	283	U	C4'-C3'-O3'	-7.04	102.44	113.00
1	L50	395	A	C2'-C3'-O3'	7.04	120.05	109.50
1	L50	642	G	C2'-C3'-O3'	-7.00	103.20	113.70
1	L50	1831	G	C2'-C3'-O3'	-6.96	103.25	113.70
55	SGG	166	VAL	CA-CB-CG1	6.95	122.22	110.40
1	L50	1705	U	C4'-C3'-O3'	6.95	119.82	109.40
1	L50	2418	U	C4'-C3'-O3'	-6.95	102.58	113.00
41	S60	109	U	C2'-C3'-O3'	-6.87	103.40	113.70
37	LW0	27	ASP	CB-CA-C	6.84	120.36	110.04
49	SDD	39	VAL	CA-CB-CG1	6.82	122.00	110.40
1	L50	2357	U	C2'-C3'-O3'	-6.81	103.48	113.70
1	L50	14	G	C4'-C3'-O3'	-6.75	102.87	113.00
52	SF0	17	PRO	N-CA-C	6.75	122.77	113.65
1	L50	535	A	C4'-C3'-O3'	6.74	119.52	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	1942	U	C2'-C3'-O3'	6.71	119.57	109.50
41	S60	1135	U	C4'-C3'-O3'	6.67	123.00	113.00
1	L50	1709	G	C1'-C2'-O2'	-6.63	101.86	111.80
1	L50	1000	G	C3'-C2'-O2'	-6.60	104.70	114.60
56	SH0	107	PHE	CA-CB-CG	-6.60	107.20	113.80
51	SEE	49	VAL	CA-CB-CG1	6.54	121.52	110.40
1	L50	2531	U	C4'-C3'-O3'	-6.52	103.21	113.00
1	L50	663	G	C2'-C3'-O3'	-6.51	103.93	113.70
41	S60	1125	G	C2'-C3'-O3'	6.50	123.46	113.70
46	SC0	129	ARG	CB-CA-C	-6.50	98.19	108.91
1	L50	2265	U	C2'-C3'-O3'	-6.48	103.98	113.70
1	L50	562	U	C5'-C4'-C3'	-6.47	106.29	116.00
1	L50	1709	G	C2'-C3'-O3'	-6.46	99.82	109.50
1	L50	1942	U	C1'-C2'-O2'	-6.44	102.14	111.80
1	L50	2451	U	C2'-C3'-O3'	-6.42	104.07	113.70
1	L50	1709	G	C1'-O4'-C4'	-6.40	103.30	109.70
2	L70	91	C	C2'-C3'-O3'	-6.40	104.10	113.70
1	L50	629	C	C4'-C3'-O3'	-6.39	103.42	113.00
40	LZ0	69	ARG	CB-CG-CD	6.37	125.94	111.30
1	L50	2114	G	C4'-C3'-C2'	-6.35	96.25	102.60
72	SX0	83	PRO	N-CA-C	6.34	122.54	113.47
69	SU0	45	PHE	CA-CB-CG	6.34	120.14	113.80
1	L50	1445	U	C4'-C3'-O3'	6.32	118.88	109.40
1	L50	1000	G	C1'-O4'-C4'	-6.32	103.38	109.70
41	S60	1356	C	O5'-P-OP1	-6.31	89.06	108.00
69	SU0	105	PHE	CA-CB-CG	6.28	120.08	113.80
1	L50	1102	G	O4'-C1'-C2'	-6.25	99.55	105.80
6	LC0	223	ASP	CA-CB-CG	6.24	118.84	112.60
8	LD0	78	ASP	CA-CB-CG	6.23	118.83	112.60
63	SO0	54	ASP	CA-CB-CG	6.16	118.76	112.60
1	L50	225	G	C2'-C3'-O3'	6.16	122.94	113.70
1	L50	1835	G	P-O5'-C5'	-6.14	111.69	120.90
12	LF0	193	PHE	CA-CB-CG	6.12	119.92	113.80
1	L50	645	U	C4'-C3'-O3'	6.11	118.57	109.40
6	LC0	57	ARG	CG-CD-NE	-6.09	98.60	112.00
1	L50	115	A	C2'-C3'-O3'	-6.08	104.57	113.70
1	L50	729	A	C1'-C2'-O2'	-6.08	99.29	108.40
26	LN0	131	GLU	CB-CG-CD	6.07	122.92	112.60
1	L50	665	A	C4'-C3'-O3'	6.05	118.47	109.40
1	L50	1098	A	C4'-C3'-O3'	-6.05	103.93	113.00
1	L50	1534	G	C2'-C3'-O3'	-6.04	104.64	113.70
6	LC0	87	ALA	N-CA-C	6.01	118.71	108.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	SE0	151	ASP	CA-CB-CG	6.01	118.61	112.60
22	LL0	67	ARG	CG-CD-NE	6.00	125.20	112.00
41	S60	1102	A	C2'-C3'-O3'	-5.99	104.71	113.70
46	SC0	221	VAL	CA-CB-CG1	5.99	120.58	110.40
1	L50	1212	G	C4'-C3'-O3'	-5.98	104.03	113.00
41	S60	1021	A	C4'-C3'-O3'	-5.97	100.44	109.40
41	S60	118	G	C4'-C3'-O3'	5.96	118.34	109.40
1	L50	2499	U	C2'-C3'-O3'	-5.96	104.76	113.70
54	SG0	56	ASP	CA-CB-CG	5.96	118.56	112.60
1	L50	725	A	O3'-P-O5'	-5.95	95.08	104.00
37	LW0	27	ASP	CA-CB-CG	5.94	118.54	112.60
1	L50	2419	G	C2'-C3'-O3'	5.93	118.40	109.50
1	L50	342	G	C2'-C3'-O3'	-5.93	104.80	113.70
1	L50	1414	U	C2'-C3'-O3'	5.93	118.40	109.50
1	L50	61	A	C4'-C3'-O3'	-5.93	104.11	113.00
41	S60	964	G	C4'-C3'-C2'	-5.92	96.67	102.60
1	L50	1819	A	C2'-C3'-O3'	-5.92	104.82	113.70
41	S60	477	G	C2'-C3'-O3'	-5.91	104.83	113.70
41	S60	993	U	P-O3'-C3'	-5.90	111.34	120.20
1	L50	667	G	C4'-C3'-O3'	5.90	121.84	113.00
5	LB0	336	ARG	CG-CD-NE	5.89	124.96	112.00
1	L50	742	G	C4'-C3'-O3'	-5.87	100.59	109.40
41	S60	1286	G	C4'-C3'-O3'	-5.85	104.23	113.00
61	SM0	91	PHE	CA-CB-CG	5.85	119.65	113.80
1	L50	805	A	C2'-C3'-O3'	-5.85	104.93	113.70
1	L50	552	C	C2'-C3'-O3'	-5.84	104.94	113.70
26	LN0	123	GLN	CB-CA-C	-5.84	97.90	110.45
10	LE0	22	ASP	CA-C-N	5.82	123.91	120.24
10	LE0	22	ASP	C-N-CA	5.82	123.91	120.24
1	L50	805	A	O3'-P-O5'	-5.82	95.27	104.00
41	S60	1112	G	C4'-C3'-C2'	-5.81	96.79	102.60
41	S60	563	A	C2'-C3'-O3'	-5.79	105.01	113.70
1	L50	1074	G	C2'-C3'-O3'	5.78	122.37	113.70
1	L50	1262	A	C4'-C3'-O3'	-5.77	104.34	113.00
1	L50	1967	A	C4'-C3'-O3'	5.76	121.64	113.00
1	L50	280	G	C4'-C3'-C2'	-5.74	96.86	102.60
22	LL0	8	PRO	N-CA-C	5.74	124.29	112.47
41	S60	819	A	P-O3'-C3'	5.74	128.80	120.20
15	LGG	24	ARG	CG-CD-NE	-5.73	99.40	112.00
69	SU0	67	ARG	CG-CD-NE	5.73	124.61	112.00
1	L50	147	G	P-O3'-C3'	-5.71	111.63	120.20
41	S60	1206	A	C2'-C3'-O3'	-5.71	105.14	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	LI0	173	PHE	CA-CB-CG	5.70	119.50	113.80
41	S60	262	U	O4'-C4'-C3'	-5.69	98.31	104.00
1	L50	2074	A	C2'-C3'-O3'	-5.68	105.17	113.70
41	S60	111	A	C2'-C3'-O3'	-5.68	105.18	113.70
1	L50	586	G	C4'-C3'-O3'	5.67	117.91	109.40
1	L50	659	G	C2'-C3'-O3'	5.67	118.01	109.50
1	L50	1317	G	P-O3'-C3'	-5.67	111.69	120.20
1	L50	1192	A	N9-C1'-C2'	5.67	120.50	112.00
1	L50	1303	G	C4'-C3'-C2'	-5.67	96.94	102.60
27	LO0	45	PRO	CB-CA-C	-5.66	103.98	111.23
41	S60	222	G	C4'-C3'-C2'	-5.66	96.94	102.60
1	L50	1627	U	C2'-C3'-O3'	-5.65	105.22	113.70
1	L50	2373	G	C4'-C3'-C2'	-5.64	96.96	102.60
1	L50	1400	A	C2'-C3'-O3'	5.64	117.95	109.50
1	L50	1981	G	C4'-C3'-O3'	-5.63	104.55	113.00
41	S60	970	U	C4'-C3'-O3'	-5.63	104.55	113.00
1	L50	1277	G	C4'-C3'-C2'	-5.63	96.97	102.60
1	L50	884	G	C4'-C3'-O3'	-5.62	104.57	113.00
12	LF0	89	ARG	CB-CG-CD	5.62	124.22	111.30
1	L50	2447	A	P-O5'-C5'	-5.60	112.50	120.90
1	L50	567	A	C2'-C3'-O3'	5.59	117.89	109.50
21	LJJ	21	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	L50	1499	U	C2'-C3'-O3'	5.58	122.08	113.70
41	S60	213	A	P-O3'-C3'	-5.58	111.83	120.20
50	SE0	212	ASP	CA-CB-CG	5.58	118.18	112.60
1	L50	725	A	C2'-C3'-O3'	-5.57	105.34	113.70
41	S60	340	A	C4'-C3'-O3'	-5.57	104.64	113.00
1	L50	2168	G	C2'-C3'-O3'	-5.54	105.38	113.70
1	L50	1684	C	C2'-C3'-O3'	-5.54	105.39	113.70
1	L50	1783	A	P-O3'-C3'	-5.54	111.88	120.20
27	LO0	65	PRO	CB-CA-C	-5.54	103.98	111.85
1	L50	385	C	C2'-C3'-O3'	-5.54	105.39	113.70
1	L50	2012	G	O3'-P-O5'	-5.53	95.70	104.00
52	SF0	17	PRO	CB-CA-C	-5.52	103.60	112.21
39	LY0	53	ASP	CB-CA-C	5.51	120.73	109.76
62	SN0	5	TYR	CB-CA-C	5.50	118.79	109.55
1	L50	151	G	C4'-C3'-O3'	5.50	117.65	109.40
1	L50	814	G	C4'-C3'-O3'	-5.50	104.75	113.00
57	SI0	166	PHE	CA-CB-CG	5.50	119.30	113.80
41	S60	1018	U	C4'-C3'-O3'	5.49	117.63	109.40
41	S60	1128	G	C4'-C3'-O3'	-5.49	104.77	113.00
41	S60	1243	C	C4'-C3'-O3'	-5.47	104.80	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	SCC	60	HIS	CA-C-N	5.47	128.36	120.38
47	SCC	60	HIS	C-N-CA	5.47	128.36	120.38
2	L70	86	G	C4'-C3'-C2'	-5.46	97.14	102.60
1	L50	141	G	O4'-C1'-C2'	-5.45	100.35	105.80
15	LGG	58	ARG	CB-CA-C	5.45	117.28	109.11
2	L70	46	C	P-O3'-C3'	-5.45	112.03	120.20
20	LJ0	115	PRO	N-CA-C	5.44	120.91	113.84
11	LEE	46	ASP	CA-CB-CG	5.43	118.03	112.60
41	S60	263	A	C5'-C4'-C3'	-5.43	107.85	116.00
66	SR0	38	VAL	CA-CB-CG1	5.42	119.62	110.40
42	SA0	50	ASP	CA-CB-CG	5.42	118.02	112.60
1	L50	1007	C	C2'-C3'-O3'	-5.41	105.58	113.70
1	L50	1983	U	C2'-C3'-O3'	-5.41	105.58	113.70
41	S60	109	U	O3'-P-O5'	-5.41	95.89	104.00
41	S60	803	C	C2'-C3'-O3'	-5.41	105.59	113.70
2	L70	31	G	C4'-C3'-O3'	-5.40	104.89	113.00
1	L50	2203	C	C2'-C3'-O3'	-5.40	105.60	113.70
30	LPP	8	VAL	CA-CB-CG1	5.40	119.58	110.40
1	L50	2194	U	C2'-C3'-O3'	-5.40	105.60	113.70
69	SU0	56	VAL	CA-CB-CG1	5.40	119.57	110.40
1	L50	449	U	C4'-C3'-O3'	-5.39	104.91	113.00
41	S60	986	G	C2'-C3'-O3'	-5.39	105.61	113.70
65	SQ0	38	VAL	CA-CB-CG1	5.39	119.57	110.40
41	S60	1042	A	C4'-C3'-O3'	-5.38	104.92	113.00
1	L50	1984	U	C4'-C3'-O3'	-5.37	104.94	113.00
41	S60	1356	C	O4'-C4'-C3'	-5.37	100.73	106.10
1	L50	42	G	C4'-C3'-C2'	-5.37	97.23	102.60
30	LPP	49	ARG	CG-CD-NE	5.37	123.81	112.00
1	L50	1414	U	P-O5'-C5'	-5.36	112.87	120.90
41	S60	1125	G	C3'-C2'-C1'	-5.35	95.95	101.30
1	L50	392	C	C2'-C3'-O3'	-5.35	105.67	113.70
65	SQ0	38	VAL	CB-CA-C	5.35	115.66	110.63
1	L50	342	G	P-O3'-C3'	-5.35	112.17	120.20
1	L50	1942	U	C3'-C2'-O2'	5.35	122.62	114.60
1	L50	75	C	C2'-C3'-O3'	5.35	121.72	113.70
1	L50	2422	G	C2'-C3'-O3'	5.33	121.69	113.70
1	L50	734	G	C4'-C3'-O3'	-5.32	105.02	113.00
2	L70	42	A	C2'-C3'-O3'	-5.32	105.72	113.70
1	L50	630	U	C4'-C3'-O3'	5.32	117.38	109.40
41	S60	822	A	C3'-C2'-O2'	5.32	118.68	110.70
1	L50	535	A	C1'-C2'-O2'	-5.32	103.82	111.80
1	L50	92	C	C2'-C3'-O3'	-5.31	105.73	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	1733	A	N9-C1'-C2'	5.31	119.97	112.00
1	L50	1234	U	N1-C1'-C2'	5.30	119.96	112.00
1	L50	1298	A	C5'-C4'-C3'	-5.30	108.04	116.00
1	L50	2355	A	C4'-C3'-O3'	-5.30	105.05	113.00
50	SE0	239	THR	CA-C-N	5.30	127.64	120.38
50	SE0	239	THR	C-N-CA	5.30	127.64	120.38
1	L50	1432	G	C2'-C3'-O3'	-5.29	105.76	113.70
55	SGG	106	ASP	CA-CB-CG	5.29	117.89	112.60
60	SL0	76	PRO	N-CA-C	5.28	120.71	113.84
1	L50	739	A	C5'-C4'-C3'	-5.28	108.08	116.00
41	S60	1170	G	C1'-O4'-C4'	-5.27	104.63	109.90
1	L50	323	G	C4'-C3'-C2'	-5.27	97.33	102.60
1	L50	337	A	C5'-C4'-C3'	-5.27	108.10	116.00
1	L50	1293	A	C5'-C4'-C3'	-5.27	108.10	116.00
41	S60	601	G	C4'-C3'-C2'	-5.26	97.34	102.60
41	S60	201	G	P-O3'-C3'	-5.25	112.32	120.20
50	SE0	88	ASP	CA-CB-CG	5.25	117.85	112.60
8	LD0	121	LEU	CA-C-N	5.25	127.56	120.38
8	LD0	121	LEU	C-N-CA	5.25	127.56	120.38
62	SN0	86	GLU	CB-CG-CD	5.25	121.52	112.60
1	L50	2457	U	C2'-C3'-O3'	-5.24	105.84	113.70
1	L50	2332	G	C4'-C3'-C2'	-5.24	97.36	102.60
41	S60	692	C	C2'-C3'-O3'	-5.24	105.84	113.70
1	L50	1796	C	C4'-C3'-O3'	-5.24	105.14	113.00
1	L50	1608	U	C4'-C3'-O3'	-5.23	105.15	113.00
1	L50	208	C	C2'-C3'-O3'	5.22	117.34	109.50
1	L50	1602	G	C4'-C3'-C2'	-5.22	97.38	102.60
41	S60	275	G	C4'-C3'-C2'	-5.22	97.38	102.60
1	L50	1182	A	P-O3'-C3'	5.22	128.02	120.20
41	S60	773	U	C2'-C3'-O3'	-5.21	105.89	113.70
1	L50	1608	U	C2'-C3'-O3'	-5.21	105.89	113.70
41	S60	1218	U	C4'-C3'-O3'	-5.20	105.19	113.00
1	L50	596	G	C4'-C3'-C2'	-5.18	97.42	102.60
1	L50	1575	G	C4'-C3'-C2'	-5.18	97.42	102.60
33	LS0	87	ASP	CA-CB-CG	5.18	117.78	112.60
1	L50	1263	A	C3'-C2'-O2'	5.18	118.46	110.70
41	S60	425	G	C2'-C3'-O3'	-5.17	101.74	109.50
1	L50	33	G	C2'-C3'-O3'	-5.17	105.95	113.70
1	L50	690	U	C4'-C3'-C2'	-5.17	97.43	102.60
1	L50	2315	G	C4'-C3'-C2'	-5.17	97.44	102.60
1	L50	1503	A	C4'-C3'-O3'	-5.15	105.27	113.00
10	LE0	91	ASP	CA-CB-CG	5.15	117.75	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	739	A	C2'-C3'-O3'	5.15	121.42	113.70
1	L50	1073	U	C2'-C3'-O3'	-5.15	105.97	113.70
41	S60	263	A	C4'-C3'-O3'	-5.15	105.28	113.00
41	S60	238	A	C4'-C3'-O3'	-5.14	105.28	113.00
55	SGG	23	PRO	N-CA-C	5.14	118.42	111.22
1	L50	149	A	C4'-C3'-O3'	-5.13	105.31	113.00
41	S60	441	G	C4'-C3'-C2'	-5.13	97.47	102.60
41	S60	459	G	C4'-C3'-C2'	-5.12	97.47	102.60
41	S60	883	C	C2'-C3'-O3'	-5.12	106.01	113.70
1	L50	2412	C	P-O5'-C5'	-5.11	113.23	120.90
1	L50	797	U	C5'-C4'-C3'	-5.10	108.35	116.00
1	L50	1187	G	C2'-C3'-O3'	-5.09	106.06	113.70
1	L50	996	A	C1'-C2'-O2'	-5.09	104.17	111.80
34	LT0	15	PHE	CA-CB-CG	5.08	118.88	113.80
1	L50	2341	G	C4'-C3'-C2'	-5.08	97.52	102.60
1	L50	1622	G	C4'-C3'-C2'	-5.07	97.53	102.60
1	L50	1417	A	C4'-C3'-O3'	-5.07	105.40	113.00
1	L50	1101	A	C4'-C3'-O3'	-5.06	101.81	109.40
1	L50	994	A	C2'-C3'-O3'	5.06	117.09	109.50
36	LV0	61	ASP	CA-CB-CG	5.06	117.66	112.60
41	S60	953	C	C4'-C3'-O3'	-5.06	105.41	113.00
41	S60	263	A	P-O5'-C5'	-5.06	113.32	120.90
1	L50	2234	U	C2'-C3'-O3'	5.05	117.08	109.50
40	LZ0	45	PHE	CA-CB-CG	5.05	118.85	113.80
1	L50	697	C	C2'-C3'-O3'	-5.05	106.12	113.70
1	L50	1087	G	C4'-C3'-C2'	-5.05	97.55	102.60
1	L50	2346	U	C4'-C3'-O3'	-5.05	101.82	109.40
1	L50	140	A	O3'-P-O5'	-5.04	96.44	104.00
1	L50	2350	A	C2'-C3'-O3'	-5.04	106.14	113.70
50	SE0	141	THR	CA-C-N	5.04	127.28	120.38
50	SE0	141	THR	C-N-CA	5.04	127.28	120.38
67	SS0	25	ASN	N-CA-C	-5.03	105.80	112.24
41	S60	218	A	C2'-C3'-O3'	5.03	117.05	109.50
1	L50	1162	U	C1'-C2'-O2'	-5.03	100.86	108.40
1	L50	2108	U	C4'-C3'-O3'	-5.03	105.46	113.00
41	S60	1108	C	C4'-C3'-O3'	-5.03	105.46	113.00
1	L50	1977	G	C2'-C3'-O3'	5.02	117.04	109.50
1	L50	2181	A	C4'-C3'-O3'	-5.02	105.46	113.00
2	L70	31	G	P-O3'-C3'	-5.02	112.67	120.20
41	S60	1125	G	C3'-C2'-O2'	5.02	118.23	110.70
55	SGG	261	ASP	CA-CB-CG	5.02	117.62	112.60
1	L50	1338	U	C2'-C3'-O3'	-5.02	106.18	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L50	1773	C	C3'-C2'-O2'	5.02	118.22	110.70
41	S60	1135	U	C2'-C3'-O3'	5.01	121.22	113.70
1	L50	698	U	C4'-C3'-O3'	-5.00	105.49	113.00
1	L50	1835	G	C3'-C2'-C1'	5.00	106.30	101.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LC0	87	ALA	Peptide
13	LFF	101	ILE	Peptide
15	LGG	77	GLY	Peptide
66	SR0	64	ASN	Peptide

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	L50	53655	0	26937	98	0
2	L70	2542	0	1282	8	0
3	LA0	1889	0	1985	3	0
4	LAA	1167	0	1214	5	0
5	LB0	3039	0	3183	5	0
6	LC0	2604	0	2638	11	0
7	LCC	781	0	803	2	0
8	LD0	2298	0	2384	8	0
9	LDD	895	0	948	0	0
10	LE0	1371	0	1389	13	0
11	LEE	1090	0	1173	10	0
12	LF0	1933	0	2011	12	0
13	LFF	893	0	945	3	0
14	LG0	1590	0	1709	5	0
15	LGG	819	0	882	1	0
16	LH0	1477	0	1528	4	0
17	LHH	992	0	1097	5	0
18	LI0	1750	0	1797	2	0
19	LII	784	0	873	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	LJ0	1332	0	1411	6	0
21	LJJ	701	0	753	4	0
22	LL0	1353	0	1433	4	0
23	LLL	427	0	468	0	0
24	LM0	927	0	961	3	0
25	LMM	427	0	461	0	0
26	LN0	1688	0	1752	6	0
27	LO0	1598	0	1681	5	0
28	LOO	801	0	886	3	0
29	LP0	1238	0	1304	3	0
30	LPP	684	0	720	2	0
31	LQ0	1491	0	1587	7	0
32	LR0	1336	0	1430	1	0
33	LS0	1400	0	1450	1	0
34	LT0	1270	0	1321	18	0
35	LU0	810	0	834	1	0
36	LV0	1057	0	1139	2	0
37	LW0	832	0	873	31	0
38	LX0	874	0	956	5	0
39	LY0	1048	0	1135	2	0
40	LZ0	963	0	1022	2	0
41	S60	29181	0	14618	125	0
42	SA0	1725	0	1750	16	0
43	SAA	827	0	859	1	0
44	SB0	1609	0	1728	6	0
45	SBB	627	0	651	3	0
46	SC0	1727	0	1802	4	0
47	SCC	476	0	488	4	0
48	SD0	1700	0	1815	7	0
49	SDD	550	0	542	4	0
50	SE0	2044	0	2116	26	0
51	SEE	447	0	483	1	0
52	SF0	1509	0	1604	21	0
53	SFF	447	0	456	14	0
54	SG0	1835	0	1968	28	0
55	SGG	2478	0	2458	4	0
56	SH0	1335	0	1356	2	0
57	SI0	1347	0	1379	9	0
58	SJ0	1379	0	1436	7	0
59	SK0	764	0	771	2	0
60	SL0	1229	0	1302	5	0
61	SM0	876	0	937	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	SN0	1130	0	1188	8	0
63	SO0	983	0	1028	9	0
64	SP0	950	0	984	4	0
65	SQ0	1143	0	1171	5	0
66	SR0	977	0	1012	12	0
67	SS0	1150	0	1207	21	0
68	ST0	1161	0	1219	11	0
69	SU0	809	0	838	5	0
70	SV0	521	0	525	6	0
71	SW0	1022	0	1052	7	0
72	SX0	1098	0	1183	3	0
73	SY0	1118	0	1166	13	0
74	SZ0	633	0	678	16	0
75	L50	145	0	0	0	0
75	LA0	2	0	0	0	0
75	LEE	1	0	0	0	0
75	LLL	1	0	0	0	0
75	LN0	1	0	0	0	0
75	S60	44	0	0	0	0
75	SN0	3	0	0	0	0
75	SO0	2	0	0	0	0
76	L50	104	0	0	0	0
76	L70	4	0	0	0	0
76	LB0	1	0	0	0	0
76	LF0	1	0	0	0	0
76	LII	1	0	0	0	0
76	LJJ	1	0	0	0	0
76	LV0	1	0	0	0	0
76	S60	46	0	0	0	0
76	SI0	1	0	0	0	0
77	LGG	1	0	0	0	0
77	LJJ	1	0	0	0	0
77	LMM	1	0	0	0	0
77	LOO	1	0	0	0	0
77	LPP	1	0	0	0	0
77	SAA	1	0	0	0	0
77	SBB	1	0	0	0	0
77	SDD	1	0	0	0	0
77	SFF	1	0	0	0	0
All	All	171001	0	132125	490	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 2.

All (490) 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)
52:SF0:90:ILE:HG23	74:SZ0:58:ILE:CD1	1.58	1.33
37:LW0:99:LYS:HA	37:LW0:102:LYS:HE2	1.32	1.09
73:SY0:22:GLU:O	73:SY0:23:LEU:HG	1.54	1.08
74:SZ0:61:ARG:HD3	74:SZ0:76:ILE:HD11	1.36	1.07
34:LT0:126:PRO:HB2	34:LT0:128:LEU:HG	1.34	1.07
1:L50:535:A:O2'	31:LQ0:146:ASN:HB3	1.55	1.06
52:SF0:90:ILE:HG23	74:SZ0:58:ILE:HD11	1.37	1.05
10:LE0:55:GLU:OE2	10:LE0:117:ARG:HG3	1.59	1.02
54:SG0:147:PHE:HZ	54:SG0:160:LYS:HE2	1.22	1.00
41:S60:1315:A:C2	41:S60:1316:A:N6	2.32	0.97
42:SA0:38:PHE:HZ	66:SR0:108:GLN:NE2	1.64	0.95
10:LE0:100:ILE:HD11	24:LM0:102:PHE:HB2	1.49	0.93
41:S60:554:A:N3	71:SW0:103:THR:HG22	1.83	0.93
37:LW0:99:LYS:CA	37:LW0:102:LYS:HE2	2.01	0.90
41:S60:203:G:N3	50:SE0:33:THR:HG21	1.88	0.89
37:LW0:99:LYS:HA	37:LW0:102:LYS:CE	2.04	0.87
41:S60:920:G:H5'	53:SFF:128:VAL:HG13	1.55	0.87
37:LW0:26:ASP:O	37:LW0:27:ASP:OD1	1.94	0.85
52:SF0:90:ILE:CG2	74:SZ0:58:ILE:CD1	2.52	0.85
41:S60:706:G:N3	41:S60:706:G:H2'	1.92	0.85
41:S60:705:A:N3	41:S60:706:G:C6	2.46	0.83
54:SG0:147:PHE:CZ	54:SG0:160:LYS:HE2	2.13	0.83
67:SS0:90:TRP:CZ3	67:SS0:91:MET:HE2	2.14	0.82
74:SZ0:61:ARG:CD	74:SZ0:76:ILE:HD11	2.10	0.82
41:S60:173:A:C8	50:SE0:131:VAL:CG1	2.64	0.80
37:LW0:87:PRO:HD3	54:SG0:169:VAL:HG22	1.63	0.80
53:SFF:93:LYS:HB3	53:SFF:94:PRO:HD2	1.63	0.80
10:LE0:23:ILE:HD11	11:LEE:79:ARG:HH12	1.45	0.79
34:LT0:126:PRO:HB2	34:LT0:128:LEU:CG	2.13	0.78
1:L50:796:C:H5''	34:LT0:131:ARG:H	1.48	0.77
54:SG0:169:VAL:CG1	54:SG0:176:LYS:HE2	2.14	0.76
1:L50:2497:C:H5''	5:LB0:280:THR:HG21	1.68	0.76
54:SG0:170:ASN:HD21	54:SG0:176:LYS:HD3	1.50	0.75
1:L50:883:U:H5''	24:LM0:35:ASN:ND2	2.01	0.75
41:S60:173:A:H8	50:SE0:131:VAL:HG12	1.50	0.75
5:LB0:336:ARG:HG3	5:LB0:336:ARG:HH11	1.51	0.75
52:SF0:90:ILE:HG23	74:SZ0:58:ILE:HD12	1.67	0.74
52:SF0:90:ILE:HG23	74:SZ0:58:ILE:HD13	1.64	0.74
52:SF0:46:ARG:HD3	65:SQ0:122:ARG:HD2	1.69	0.74
41:S60:173:A:C8	50:SE0:131:VAL:HG12	2.23	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LW0:99:LYS:CB	37:LW0:102:LYS:HE2	2.17	0.74
1:L50:883:U:H5''	24:LM0:35:ASN:HD21	1.51	0.74
41:S60:203:G:N3	50:SE0:33:THR:CG2	2.51	0.73
42:SA0:38:PHE:CZ	66:SR0:108:GLN:NE2	2.55	0.73
44:SB0:53:THR:HG22	63:SO0:30:ASP:OD2	1.88	0.73
10:LE0:55:GLU:CD	10:LE0:117:ARG:HG3	2.13	0.72
1:L50:2052:A:H5'	20:LJ0:62:ILE:HD11	1.69	0.72
41:S60:923:A:H4'	41:S60:924:U:H2'	1.72	0.72
67:SS0:20:MET:HG2	67:SS0:29:ASP:HA	1.71	0.72
2:L70:27:A:OP2	8:LD0:62:THR:HG23	1.88	0.72
54:SG0:147:PHE:HZ	54:SG0:160:LYS:CE	2.02	0.71
53:SFF:127:SER:HB3	61:SM0:45:ASP:OD1	1.90	0.71
2:L70:3:U:H3	2:L70:116:G:H1	1.37	0.71
7:LCC:64:ILE:HG22	40:LZ0:39:LEU:HD11	1.72	0.71
41:S60:705:A:C2	41:S60:706:G:O6	2.43	0.71
41:S60:438:U:H4'	72:SX0:110:LYS:HD2	1.72	0.71
41:S60:237:A:H5'	57:SI0:48:VAL:CG1	2.21	0.70
52:SF0:90:ILE:HA	74:SZ0:58:ILE:HD13	1.73	0.70
65:SQ0:33:ASN:HD22	68:ST0:6:PHE:HD2	1.32	0.70
41:S60:1128:G:H5''	68:ST0:98:ARG:HG3	1.72	0.70
2:L70:63:A:H2'	18:LI0:204:GLY:O	1.91	0.70
1:L50:796:C:H5''	34:LT0:131:ARG:N	2.06	0.70
41:S60:237:A:H5'	57:SI0:48:VAL:HG13	1.74	0.69
26:LN0:112:ASN:HD22	26:LN0:112:ASN:H	1.40	0.69
14:LG0:119:ASP:OD1	14:LG0:145:THR:HA	1.92	0.69
44:SB0:53:THR:HG21	63:SO0:32:THR:OG1	1.92	0.69
52:SF0:95:THR:HG21	52:SF0:102:ILE:HG12	1.72	0.69
67:SS0:24:PHE:CZ	67:SS0:107:ILE:HG21	2.27	0.69
41:S60:1315:A:C2	41:S60:1316:A:C6	2.81	0.69
50:SE0:64:ILE:HD12	73:SY0:23:LEU:HD13	1.75	0.69
51:SEE:5:ILE:HD12	72:SX0:63:ILE:HD12	1.74	0.69
41:S60:666:A:OP1	62:SN0:132:LYS:NZ	2.25	0.68
41:S60:173:A:H8	50:SE0:131:VAL:CG1	2.04	0.68
42:SA0:60:LEU:HD21	70:SV0:63:ILE:HD13	1.74	0.68
36:LV0:98:LEU:HD23	37:LW0:21:TYR:HB2	1.75	0.67
41:S60:705:A:C2	41:S60:706:G:C6	2.82	0.67
53:SFF:106:PHE:HZ	61:SM0:44:LEU:HD11	1.58	0.67
42:SA0:70:ASN:HB2	46:SC0:240:ILE:HD11	1.76	0.67
20:LJ0:107:ILE:HD11	20:LJ0:113:TYR:HD1	1.60	0.66
1:L50:2045:C:H5'	20:LJ0:102:GLY:HA3	1.77	0.66
1:L50:2109:G:H5''	1:L50:2109:G:H8	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:SA0:38:PHE:HZ	66:SR0:108:GLN:HE22	1.42	0.66
67:SS0:90:TRP:CH2	67:SS0:91:MET:HE2	2.30	0.65
1:L50:1191:U:H2'	1:L50:1192:A:H5''	1.77	0.65
10:LE0:30:LEU:HD22	11:LEE:11:VAL:CG1	2.26	0.65
37:LW0:99:LYS:HG2	37:LW0:102:LYS:HE2	1.77	0.65
37:LW0:99:LYS:O	37:LW0:102:LYS:HG2	1.96	0.65
44:SB0:71:ARG:HD3	63:SO0:32:THR:HG21	1.78	0.65
1:L50:1018:U:O2'	13:LFF:78:ARG:HD2	1.97	0.65
37:LW0:99:LYS:HA	37:LW0:102:LYS:CD	2.26	0.65
41:S60:1189:A:O2'	52:SF0:74:ASN:ND2	2.29	0.65
65:SQ0:33:ASN:ND2	68:ST0:6:PHE:CD2	2.58	0.65
50:SE0:137:PRO:HG3	54:SG0:222:TRP:HE1	1.63	0.64
1:L50:535:A:O2'	31:LQ0:146:ASN:CB	2.38	0.64
67:SS0:24:PHE:O	67:SS0:25:ASN:CG	2.41	0.64
67:SS0:24:PHE:O	67:SS0:25:ASN:OD1	2.15	0.64
41:S60:661:A:H4'	62:SN0:62:LYS:HE2	1.78	0.64
20:LJ0:107:ILE:HD11	20:LJ0:113:TYR:CD1	2.33	0.64
37:LW0:74:ILE:HG21	54:SG0:114:ILE:HG12	1.80	0.63
34:LT0:5:HIS:HA	34:LT0:9:ARG:HD2	1.80	0.63
74:SZ0:61:ARG:HD3	74:SZ0:76:ILE:CD1	2.23	0.63
67:SS0:24:PHE:CE1	67:SS0:107:ILE:HG21	2.34	0.63
37:LW0:99:LYS:HG2	37:LW0:102:LYS:NZ	2.12	0.63
48:SD0:184:ILE:HD11	48:SD0:230:MET:SD	2.39	0.62
54:SG0:169:VAL:HG11	54:SG0:176:LYS:HE2	1.79	0.62
37:LW0:88:LYS:HD2	54:SG0:128:VAL:HG11	1.82	0.62
41:S60:922:G:C8	61:SM0:38:GLN:NE2	2.69	0.61
2:L70:26:C:OP1	8:LD0:62:THR:HG21	2.01	0.61
73:SY0:116:ARG:CZ	73:SY0:120:LYS:HZ2	2.14	0.61
1:L50:2042:A:H61	1:L50:2054:U:H3	1.48	0.61
37:LW0:99:LYS:HG2	37:LW0:102:LYS:CE	2.31	0.61
41:S60:1315:A:N1	41:S60:1316:A:C6	2.69	0.60
54:SG0:169:VAL:HG12	54:SG0:176:LYS:HE2	1.83	0.60
27:LO0:1:MET:HE3	27:LO0:4:LYS:HD2	1.82	0.60
48:SD0:234:ILE:HG12	66:SR0:41:ILE:HG12	1.83	0.60
21:LJJ:90:ILE:HG22	21:LJJ:90:ILE:O	2.02	0.60
61:SM0:15:LEU:HB3	61:SM0:122:PHE:HE2	1.67	0.60
1:L50:343:A:H1'	19:LII:84:MET:HE3	1.83	0.60
41:S60:705:A:N3	41:S60:706:G:O6	2.35	0.59
54:SG0:170:ASN:HD21	54:SG0:176:LYS:CD	2.15	0.59
12:LF0:115:ASN:HD21	34:LT0:133:PRO:HB2	1.65	0.59
41:S60:403:A:H2'	41:S60:404:C:C6	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LW0:99:LYS:HA	37:LW0:102:LYS:HG2	1.83	0.59
53:SFF:127:SER:CB	61:SM0:45:ASP:OD1	2.51	0.59
10:LE0:23:ILE:CD1	11:LEE:79:ARG:HH12	2.15	0.59
37:LW0:99:LYS:CG	37:LW0:102:LYS:HE2	2.32	0.59
10:LE0:30:LEU:CD2	11:LEE:11:VAL:HG13	2.33	0.59
50:SE0:64:ILE:CD1	73:SY0:23:LEU:HD13	2.33	0.59
1:L50:733:A:O3'	12:LF0:124:LYS:NZ	2.35	0.59
7:LCC:64:ILE:CG2	40:LZ0:39:LEU:HD11	2.33	0.58
41:S60:187:A:H62	41:S60:194:U:H3	1.51	0.58
43:SAA:69:TYR:HE2	63:SO0:90:LYS:O	1.86	0.58
12:LF0:188:LYS:HE3	31:LQ0:2:LEU:HD23	1.85	0.58
41:S60:405:A:H2'	41:S60:406:U:C6	2.38	0.58
41:S60:203:G:C2	50:SE0:33:THR:HG21	2.38	0.58
65:SQ0:33:ASN:ND2	68:ST0:6:PHE:HD2	1.98	0.58
37:LW0:98:ASN:CB	54:SG0:146:GLY:HA3	2.33	0.58
37:LW0:99:LYS:C	37:LW0:102:LYS:HG2	2.29	0.57
41:S60:1122:A:H5''	68:ST0:105:ILE:HD13	1.85	0.57
52:SF0:90:ILE:CG2	74:SZ0:58:ILE:HD11	2.23	0.57
1:L50:2596:G:O2'	5:LB0:173:PRO:HG2	2.04	0.57
41:S60:1168:A:H4'	67:SS0:93:ASN:HD21	1.70	0.57
42:SA0:64:MET:HB3	70:SV0:27:MET:HG2	1.87	0.57
50:SE0:152:PRO:HD2	54:SG0:219:TYR:CE1	2.40	0.57
41:S60:203:G:H21	50:SE0:33:THR:HG21	1.70	0.56
41:S60:1290:G:H8	41:S60:1290:G:H5''	1.70	0.56
41:S60:554:A:N3	71:SW0:103:THR:CG2	2.62	0.56
41:S60:1144:G:C2'	41:S60:1145:G:H5'	2.36	0.56
1:L50:1405:G:H2'	1:L50:1406:G:C8	2.40	0.56
41:S60:1315:A:N1	41:S60:1316:A:N6	2.53	0.56
52:SF0:40:LEU:O	52:SF0:42:HIS:N	2.33	0.56
41:S60:1105:G:H5''	41:S60:1105:G:C8	2.41	0.56
34:LT0:112:ASN:C	34:LT0:112:ASN:HD22	2.12	0.56
67:SS0:20:MET:HE2	67:SS0:29:ASP:OD1	2.06	0.56
41:S60:1129:U:OP1	68:ST0:81:SER:OG	2.17	0.55
54:SG0:170:ASN:HD21	54:SG0:176:LYS:CE	2.19	0.55
1:L50:796:C:H5'	34:LT0:131:ARG:HE	1.70	0.55
41:S60:13:C:O5'	46:SC0:156:SER:HB3	2.06	0.55
33:LS0:14:ASP:CG	33:LS0:15:ASP:H	2.15	0.55
52:SF0:153:THR:HG21	52:SF0:160:LEU:HD13	1.88	0.55
1:L50:1940:C:H2'	1:L50:1941:A:C8	2.42	0.55
4:LAA:70:THR:HG21	19:LII:6:LEU:HG	1.88	0.54
52:SF0:90:ILE:CA	74:SZ0:58:ILE:HD13	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:275:A:N6	6:LC0:163:ILE:CD1	2.71	0.54
10:LE0:30:LEU:HD22	11:LEE:11:VAL:HG13	1.89	0.54
41:S60:171:U:H5'	41:S60:172:U:H2'	1.88	0.54
69:SU0:116:THR:C	69:SU0:117:LEU:HG	2.32	0.54
41:S60:167:G:H21	41:S60:173:A:H2	1.55	0.54
50:SE0:54:VAL:HG22	73:SY0:23:LEU:HD11	1.88	0.54
2:L70:60:A:H5'	8:LD0:273:LYS:HG2	1.88	0.54
48:SD0:188:GLN:N	48:SD0:189:PRO:HD2	2.22	0.54
50:SE0:137:PRO:HG3	54:SG0:222:TRP:NE1	2.23	0.54
67:SS0:24:PHE:CZ	67:SS0:107:ILE:HG12	2.42	0.54
41:S60:1143:A:H5''	67:SS0:36:LYS:HE3	1.90	0.54
41:S60:132:C:H3'	41:S60:133:A:H8	1.72	0.53
67:SS0:13:ASN:HD21	74:SZ0:40:ARG:HG2	1.73	0.53
41:S60:288:A:H5''	57:SI0:25:ARG:NH2	2.23	0.53
1:L50:1169:C:H1'	1:L50:1170:A:H8	1.73	0.53
67:SS0:28:ILE:CD1	67:SS0:40:THR:HB	2.39	0.53
37:LW0:95:ARG:HG2	37:LW0:99:LYS:HE3	1.90	0.53
1:L50:2198:G:H1	1:L50:2226:U:H3	1.54	0.53
47:SCC:43:GLY:HA3	52:SF0:133:SER:OG	2.08	0.53
1:L50:535:A:HO2'	31:LQ0:146:ASN:HB3	1.71	0.53
12:LF0:69:LYS:HD3	34:LT0:141:GLU:HG2	1.91	0.52
1:L50:22:U:OP2	39:LY0:11:ARG:NH1	2.39	0.52
1:L50:796:C:H4'	34:LT0:131:ARG:O	2.10	0.52
37:LW0:99:LYS:HA	37:LW0:102:LYS:CG	2.39	0.52
41:S60:1125:G:H2'	41:S60:1126:A:O4'	2.09	0.52
1:L50:1880:U:H3	1:L50:1938:A:H61	1.56	0.52
3:LA0:89:LEU:HD13	30:LPP:83:ILE:CD1	2.39	0.52
41:S60:203:G:N2	50:SE0:33:THR:HG21	2.25	0.52
6:LC0:308:MET:HE2	12:LF0:148:SER:HB2	1.91	0.52
12:LF0:70:ILE:HG12	34:LT0:144:MET:HG3	1.92	0.52
41:S60:372:A:C4	58:SJ0:2:VAL:HG21	2.45	0.52
67:SS0:24:PHE:CE1	67:SS0:107:ILE:CG2	2.92	0.52
73:SY0:116:ARG:NH1	73:SY0:120:LYS:HZ2	2.07	0.52
1:L50:401:A:N1	6:LC0:80:THR:HG22	2.24	0.52
12:LF0:115:ASN:ND2	34:LT0:133:PRO:HB2	2.24	0.52
47:SCC:41:ILE:HG23	52:SF0:131:ASP:O	2.10	0.52
1:L50:290:C:O3'	39:LY0:33:PRO:HG3	2.09	0.52
41:S60:1126:A:H8	41:S60:1164:G:H21	1.58	0.52
1:L50:555:G:H1'	6:LC0:71:ARG:HH11	1.75	0.52
12:LF0:70:ILE:HG13	34:LT0:144:MET:HE2	1.91	0.52
41:S60:244:U:H2'	41:S60:245:A:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG0:176:LYS:HD2	54:SG0:176:LYS:N	2.25	0.52
10:LE0:11:ILE:HD11	11:LEE:92:LEU:HD23	1.90	0.51
54:SG0:170:ASN:ND2	54:SG0:176:LYS:HD3	2.22	0.51
67:SS0:91:MET:HE3	68:ST0:35:ILE:HD12	1.90	0.51
1:L50:2596:G:H5'	1:L50:2597:G:H5''	1.92	0.51
37:LW0:90:ALA:HB1	54:SG0:168:GLU:HB3	1.92	0.51
73:SY0:22:GLU:C	73:SY0:23:LEU:HG	2.34	0.51
53:SFF:106:PHE:CZ	61:SM0:44:LEU:HD11	2.40	0.51
55:SGG:105:ARG:HH22	66:SR0:37:ASP:HB2	1.74	0.51
58:SJ0:100:GLU:OE1	58:SJ0:103:LEU:HD12	2.11	0.51
1:L50:1131:U:H3	1:L50:1135:G:H1	1.57	0.51
2:L70:27:A:OP2	8:LD0:62:THR:CG2	2.57	0.51
42:SA0:206:ARG:HH21	66:SR0:86:PRO:HG2	1.75	0.51
44:SB0:53:THR:CG2	63:SO0:32:THR:OG1	2.58	0.51
4:LAA:74:ASN:HD22	4:LAA:112:GLY:H	1.59	0.51
37:LW0:99:LYS:CA	37:LW0:102:LYS:HG2	2.40	0.51
1:L50:1942:U:H2'	1:L50:1943:C:C5	2.46	0.51
41:S60:1022:C:OP1	66:SR0:48:ASN:ND2	2.42	0.51
63:SO0:27:HIS:CE1	63:SO0:36:THR:HG23	2.45	0.51
44:SB0:71:ARG:HB3	63:SO0:32:THR:HG21	1.93	0.51
50:SE0:70:ILE:HD13	50:SE0:92:ILE:HG12	1.92	0.50
52:SF0:90:ILE:CG2	74:SZ0:58:ILE:HD13	2.35	0.50
1:L50:2544:U:OP1	5:LB0:375:THR:HG22	2.11	0.50
49:SDD:8:TYR:CD2	64:SP0:72:ARG:HD2	2.46	0.50
1:L50:396:G:N3	1:L50:396:G:H5''	2.26	0.50
3:LA0:88:GLU:HG2	30:LPP:87:LYS:HE2	1.93	0.50
29:LP0:30:ARG:HD3	29:LP0:30:ARG:C	2.36	0.50
67:SS0:46:ASP:OD1	67:SS0:47:ARG:N	2.43	0.50
41:S60:947:C:O2'	69:SU0:69:SER:HB2	2.11	0.50
41:S60:880:G:O6	69:SU0:66:THR:HG22	2.11	0.49
52:SF0:90:ILE:O	52:SF0:94:VAL:HG23	2.12	0.49
41:S60:55:G:H5'	73:SY0:123:ARG:HH11	1.77	0.49
41:S60:1086:G:H5''	64:SP0:141:ARG:HH11	1.77	0.49
1:L50:1328:A:H62	1:L50:1367:A:H61	1.59	0.49
41:S60:139:C:O3'	54:SG0:95:LYS:NZ	2.45	0.49
1:L50:562:U:H5''	1:L50:562:U:H6	1.76	0.49
1:L50:1089:U:H2'	1:L50:1090:A:C8	2.47	0.49
42:SA0:43:GLU:HG2	66:SR0:120:LYS:HE2	1.95	0.49
1:L50:1441:U:H4'	38:LX0:64:ILE:HD11	1.95	0.49
55:SGG:121:THR:HG21	55:SGG:131:TRP:CH2	2.47	0.49
1:L50:2051:C:C6	20:LJ0:56:ILE:HD11	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:1601:A:H4'	3:LA0:170:LEU:O	2.12	0.49
41:S60:915:A:C6	53:SFF:145:VAL:HB	2.47	0.49
50:SE0:92:ILE:HG22	50:SE0:94:LYS:O	2.13	0.49
74:SZ0:41:VAL:HG21	74:SZ0:78:LEU:HD22	1.93	0.49
1:L50:486:U:H2'	1:L50:487:A:C8	2.48	0.49
1:L50:2108:U:H6	1:L50:2108:U:H5''	1.78	0.49
14:LG0:17:ARG:NH1	26:LN0:32:GLN:HE22	2.11	0.49
41:S60:1168:A:C4'	67:SS0:93:ASN:HD21	2.25	0.49
1:L50:2473:G:OP1	16:LH0:72:LYS:HG3	2.12	0.49
48:SD0:50:PHE:HA	59:SK0:59:VAL:HG21	1.95	0.49
41:S60:920:G:C5'	53:SFF:128:VAL:HG13	2.36	0.49
16:LH0:63:GLU:OE2	27:LO0:131:ILE:HG21	2.13	0.48
41:S60:237:A:C5'	57:SI0:48:VAL:HG13	2.43	0.48
41:S60:1144:G:H2'	41:S60:1145:G:H5'	1.95	0.48
44:SB0:71:ARG:HB3	63:SO0:32:THR:CG2	2.43	0.48
16:LH0:7:GLU:OE2	16:LH0:9:LYS:HE3	2.13	0.48
1:L50:2447:A:H5''	1:L50:2447:A:H8	1.79	0.48
41:S60:236:U:O2	57:SI0:5:ARG:NH1	2.46	0.48
41:S60:1165:C:OP1	68:ST0:87:LYS:HE2	2.13	0.48
41:S60:1208:G:C2'	41:S60:1209:C:H5'	2.43	0.48
53:SFF:114:CYS:SG	61:SM0:67:SER:HB2	2.53	0.48
1:L50:1424:A:H5'	15:LGG:77:GLY:HA3	1.94	0.48
10:LE0:23:ILE:HD11	11:LEE:79:ARG:NH1	2.21	0.48
42:SA0:60:LEU:HD11	70:SV0:63:ILE:CD1	2.44	0.48
41:S60:1019:C:H2'	41:S60:1020:G:C8	2.49	0.48
47:SCC:7:ILE:HD13	52:SF0:26:ILE:HD11	1.96	0.48
1:L50:399:G:O6	6:LC0:57:ARG:NH1	2.46	0.48
41:S60:65:A:H62	41:S60:75:G:H21	1.60	0.48
41:S60:377:C:OP1	58:SJ0:150:PRO:HD2	2.13	0.48
41:S60:1128:G:H3'	68:ST0:98:ARG:HE	1.79	0.48
1:L50:1325:G:H22	1:L50:1370:U:H3	1.62	0.48
1:L50:1643:G:H1	1:L50:1672:A:H61	1.62	0.48
41:S60:919:C:OP1	53:SFF:118:ARG:NE	2.44	0.48
42:SA0:155:GLU:O	70:SV0:50:ARG:O	2.32	0.48
45:SBB:24:PHE:CZ	71:SW0:51:ILE:HG23	2.49	0.48
1:L50:1609:G:N2	1:L50:1614:G:O2'	2.47	0.47
41:S60:662:U:H1'	62:SN0:52:ASN:ND2	2.29	0.47
48:SD0:97:ALA:HB1	59:SK0:20:ILE:HD11	1.95	0.47
37:LW0:98:ASN:HB2	54:SG0:146:GLY:HA3	1.96	0.47
46:SC0:136:TRP:HH2	58:SJ0:59:ILE:HG21	1.78	0.47
49:SDD:43:TYR:CE2	69:SU0:62:CYS:HB2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S60:125:A:H2'	41:S60:126:C:C6	2.49	0.47
41:S60:126:C:H2'	41:S60:127:A:C8	2.48	0.47
56:SH0:121:GLY:HA3	71:SW0:41:LYS:HG3	1.96	0.47
8:LD0:215:LYS:HE2	8:LD0:222:PHE:CE2	2.49	0.47
47:SCC:52:ALA:HB2	52:SF0:27:THR:HG21	1.97	0.47
1:L50:2060:A:N3	1:L50:2060:A:H2'	2.29	0.47
41:S60:1194:U:H2'	41:S60:1196:U:C5	2.49	0.47
1:L50:1878:G:H2'	1:L50:1879:A:C8	2.50	0.47
1:L50:2116:A:H2'	1:L50:2117:A:C8	2.49	0.47
41:S60:507:C:H2'	41:S60:508:A:C8	2.50	0.47
41:S60:349:A:OP1	50:SE0:57:ASN:ND2	2.48	0.47
41:S60:404:C:H4'	73:SY0:37:ASN:HA	1.95	0.47
37:LW0:81:ARG:HG2	54:SG0:144:LYS:HG3	1.97	0.47
41:S60:1122:A:C6	68:ST0:101:LYS:HE3	2.50	0.47
13:LFF:20:TYR:C	13:LFF:95:MET:HE2	2.40	0.46
20:LJ0:8:ASN:HD22	20:LJ0:149:GLN:HE22	1.61	0.46
41:S60:396:A:H2'	41:S60:397:A:C8	2.51	0.46
1:L50:303:C:H2'	1:L50:304:U:C6	2.51	0.46
37:LW0:74:ILE:H	54:SG0:50:GLN:HE22	1.64	0.46
41:S60:466:C:H4'	72:SX0:100:GLU:HG2	1.97	0.46
1:L50:1869:A:H5'	26:LN0:24:ARG:HD2	1.97	0.46
41:S60:384:A:C2	58:SJ0:169:ARG:HB2	2.51	0.46
42:SA0:120:ARG:HH11	46:SC0:232:ILE:HG21	1.80	0.46
41:S60:63:G:H2'	41:S60:76:A:C2	2.50	0.46
41:S60:1208:G:H2'	41:S60:1209:C:H5'	1.98	0.46
53:SFF:128:VAL:HG21	53:SFF:141:ARG:HE	1.80	0.46
67:SS0:20:MET:CE	67:SS0:29:ASP:OD1	2.63	0.46
41:S60:1208:G:OP2	65:SQ0:127:LYS:HE3	2.16	0.46
50:SE0:183:LEU:HD22	50:SE0:191:CYS:HB2	1.98	0.46
1:L50:1308:A:H61	1:L50:2434:A:H2	1.63	0.46
10:LE0:39:ILE:HG22	13:LFF:107:ASN:ND2	2.30	0.46
1:L50:2140:A:O2'	1:L50:2141:U:H2'	2.15	0.46
31:LQ0:21:ARG:HB3	31:LQ0:57:THR:HG21	1.98	0.46
22:LL0:25:GLN:HB3	22:LL0:26:PRO:HD3	1.97	0.46
41:S60:244:U:H2'	41:S60:245:A:H8	1.81	0.46
41:S60:517:U:H5'	50:SE0:219:SER:O	2.15	0.46
1:L50:2109:G:H5'	1:L50:2109:G:C8	2.45	0.45
6:LC0:103:VAL:HG13	22:LL0:23:PHE:CZ	2.52	0.45
6:LC0:322:VAL:O	12:LF0:140:ARG:NH2	2.49	0.45
37:LW0:98:ASN:HB3	54:SG0:146:GLY:HA3	1.97	0.45
41:S60:131:U:H2'	41:S60:132:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SS0:24:PHE:CE2	67:SS0:107:ILE:HG12	2.52	0.45
41:S60:1033:A:H5'	66:SR0:4:ILE:HG12	1.96	0.45
4:LAA:127:GLN:HE22	19:LII:7:ASN:H	1.63	0.45
41:S60:705:A:C2	41:S60:706:G:N1	2.83	0.45
41:S60:852:A:H2'	41:S60:853:G:C8	2.52	0.45
41:S60:1165:C:H2'	41:S60:1166:A:C8	2.51	0.45
53:SFF:114:CYS:SG	61:SM0:67:SER:CB	3.05	0.45
2:L70:1:A:H61	2:L70:118:U:H3	1.63	0.45
41:S60:86:A:H1'	50:SE0:7:LYS:HD2	1.97	0.45
61:SM0:15:LEU:C	61:SM0:15:LEU:HD12	2.41	0.45
37:LW0:99:LYS:O	37:LW0:102:LYS:CG	2.63	0.45
42:SA0:60:LEU:HD11	70:SV0:63:ILE:HD11	1.98	0.45
50:SE0:175:LEU:HD22	50:SE0:222:PHE:CD1	2.52	0.45
41:S60:1022:C:H6	66:SR0:28:PHE:CZ	2.35	0.45
62:SN0:66:VAL:HG23	62:SN0:67:THR:HG23	1.97	0.45
73:SY0:116:ARG:CZ	73:SY0:120:LYS:NZ	2.80	0.45
1:L50:1032:A:H8	1:L50:1032:A:H5''	1.82	0.45
41:S60:55:G:H5'	73:SY0:123:ARG:NH1	2.32	0.45
1:L50:188:G:OP2	4:LAA:34:LYS:HG2	2.17	0.44
10:LE0:11:ILE:HD12	11:LEE:91:ALA:HB1	1.99	0.44
29:LP0:70:THR:HG22	29:LP0:72:GLN:H	1.81	0.44
1:L50:202:G:O2'	17:LHH:105:THR:HG22	2.16	0.44
1:L50:2267:C:O2	1:L50:2267:C:O4'	2.33	0.44
6:LC0:328:ILE:HG13	12:LF0:53:ILE:HG22	1.99	0.44
41:S60:478:C:O2	60:SL0:93:LYS:HE2	2.17	0.44
1:L50:2416:G:H5''	1:L50:2416:G:H8	1.82	0.44
41:S60:171:U:H5'	41:S60:172:U:H6	1.82	0.44
41:S60:1124:A:H2'	41:S60:1125:G:C8	2.53	0.44
49:SDD:12:LEU:HD22	64:SP0:72:ARG:HG3	1.98	0.44
37:LW0:95:ARG:O	37:LW0:99:LYS:HG3	2.17	0.44
67:SS0:24:PHE:CE2	67:SS0:79:ILE:HG21	2.53	0.44
1:L50:1885:G:H1	1:L50:1933:C:H42	1.66	0.44
12:LF0:69:LYS:HG3	34:LT0:142:MET:O	2.17	0.44
34:LT0:126:PRO:HB2	34:LT0:128:LEU:CD2	2.47	0.44
35:LU0:39:ILE:HG23	35:LU0:48:LEU:HD21	2.00	0.44
58:SJ0:84:MET:HE2	58:SJ0:84:MET:HA	1.99	0.44
2:L70:70:U:H3	2:L70:105:G:H1	1.65	0.44
17:LHH:113:LYS:HE2	22:LL0:46:ASN:HD22	1.83	0.44
41:S60:661:A:H5'	62:SN0:15:VAL:O	2.17	0.44
1:L50:158:A:N6	1:L50:168:G:H1'	2.32	0.44
1:L50:316:A:OP1	26:LN0:50:MET:HE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S60:662:U:H1'	62:SN0:52:ASN:HD21	1.83	0.44
71:SW0:26:ARG:O	71:SW0:26:ARG:HG2	2.18	0.44
1:L50:2551:C:H2'	1:L50:2552:G:O4'	2.18	0.44
41:S60:1018:U:H4'	41:S60:1019:C:OP2	2.18	0.44
41:S60:431:G:H2'	41:S60:445:U:N3	2.32	0.43
50:SE0:54:VAL:CG2	73:SY0:23:LEU:HD11	2.47	0.43
57:SI0:69:THR:HG21	60:SL0:22:TYR:CE2	2.52	0.43
1:L50:2462:A:H2'	1:L50:2463:A:C8	2.53	0.43
34:LT0:112:ASN:C	34:LT0:112:ASN:ND2	2.76	0.43
52:SF0:98:ASN:HA	74:SZ0:108:LEU:HD11	2.00	0.43
74:SZ0:72:LEU:O	74:SZ0:76:ILE:HG12	2.18	0.43
27:LO0:84:LYS:HE2	27:LO0:89:HIS:CD2	2.54	0.43
41:S60:94:U:H3'	41:S60:263:A:H61	1.83	0.43
41:S60:1149:U:H5''	67:SS0:139:VAL:HG22	2.01	0.43
69:SU0:116:THR:O	69:SU0:117:LEU:HG	2.18	0.43
14:LG0:174:PHE:CE2	14:LG0:178:ILE:HD11	2.53	0.43
26:LN0:14:LYS:HE2	26:LN0:120:TRP:CZ3	2.53	0.43
41:S60:50:U:H2'	41:S60:51:G:C8	2.54	0.43
41:S60:502:A:O3'	71:SW0:4:LYS:NZ	2.51	0.43
41:S60:517:U:C5'	50:SE0:219:SER:O	2.66	0.43
57:SI0:69:THR:HG22	60:SL0:20:ASN:OD1	2.18	0.43
57:SI0:123:ASP:HB2	60:SL0:22:TYR:HE1	1.84	0.43
1:L50:21:U:H5'	1:L50:1087:G:OP1	2.19	0.43
36:LV0:142:TYR:OH	37:LW0:27:ASP:O	2.32	0.43
42:SA0:33:LEU:HD13	42:SA0:150:THR:HA	2.00	0.43
1:L50:555:G:H1'	6:LC0:71:ARG:NH1	2.34	0.43
1:L50:2525:G:H5'	29:LP0:71:PRO:HD3	2.00	0.43
11:LEE:133:LEU:HG	11:LEE:133:LEU:O	2.19	0.43
41:S60:705:A:H2'	41:S60:707:A:N7	2.34	0.43
14:LG0:119:ASP:CG	14:LG0:145:THR:HA	2.44	0.43
54:SG0:144:LYS:C	54:SG0:146:GLY:H	2.27	0.43
55:SGG:105:ARG:NH2	66:SR0:36:ILE:HG22	2.34	0.43
55:SGG:147:ASN:N	55:SGG:147:ASN:HD22	2.17	0.43
41:S60:1166:A:H2'	41:S60:1167:C:C6	2.54	0.43
63:SO0:27:HIS:HE1	63:SO0:36:THR:HG23	1.82	0.43
1:L50:88:A:H5'	21:LJJ:75:ALA:HB2	2.01	0.42
1:L50:1441:U:H4'	38:LX0:64:ILE:CD1	2.49	0.42
62:SN0:122:LEU:HD23	62:SN0:122:LEU:C	2.44	0.42
1:L50:1325:G:H1	1:L50:1370:U:H3	1.67	0.42
1:L50:1875:G:H2'	1:L50:1876:A:C8	2.53	0.42
1:L50:1933:C:H2'	1:L50:1934:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LF0:69:LYS:HD3	34:LT0:141:GLU:CG	2.49	0.42
41:S60:790:G:H5''	41:S60:790:G:H8	1.84	0.42
1:L50:1089:U:H2'	1:L50:1090:A:H8	1.84	0.42
17:LHH:66:LEU:HD12	38:LX0:22:ILE:HD11	2.01	0.42
41:S60:218:A:H4'	41:S60:219:U:H5''	2.00	0.42
41:S60:1035:C:H2'	41:S60:1036:A:C8	2.54	0.42
4:LAA:144:VAL:HG21	22:LL0:163:TYR:O	2.19	0.42
6:LC0:2:SER:O	6:LC0:3:ARG:HG2	2.19	0.42
8:LD0:214:LEU:HD23	8:LD0:214:LEU:HA	1.93	0.42
41:S60:189:A:H2'	41:S60:190:A:H4'	2.01	0.42
57:SI0:68:LYS:HE2	57:SI0:152:TYR:CD2	2.54	0.42
1:L50:145:A:H5''	21:LJJ:46:LYS:HD2	2.01	0.42
5:LB0:265:ARG:NH1	27:LO0:62:SER:OG	2.53	0.42
17:LHH:6:LYS:HG3	17:LHH:7:ASP:OD1	2.19	0.42
41:S60:173:A:N7	50:SE0:131:VAL:CG1	2.82	0.42
41:S60:696:G:H1	41:S60:712:A:H2	1.68	0.42
1:L50:1298:A:H5'	1:L50:1299:A:OP2	2.20	0.42
1:L50:2160:G:H5''	28:LOO:65:LYS:HD2	2.02	0.42
1:L50:2492:U:H2'	1:L50:2493:G:C8	2.55	0.42
1:L50:2170:A:C8	28:LOO:54:PRO:HB3	2.55	0.42
31:LQ0:164:TYR:CE2	31:LQ0:177:ARG:HD2	2.55	0.42
37:LW0:85:ALA:HB1	54:SG0:176:LYS:HG3	2.02	0.42
1:L50:1296:C:H6	1:L50:1296:C:H5''	1.85	0.41
41:S60:375:G:H8	41:S60:375:G:H5''	1.85	0.41
41:S60:1054:G:H2'	41:S60:1055:A:O4'	2.20	0.41
41:S60:1128:G:C5'	68:ST0:98:ARG:HG3	2.47	0.41
42:SA0:218:GLN:HG2	66:SR0:84:PHE:CE1	2.55	0.41
61:SM0:15:LEU:CB	61:SM0:122:PHE:HE2	2.31	0.41
1:L50:2573:U:H2'	1:L50:2574:A:C8	2.55	0.41
1:L50:2610:U:H2'	1:L50:2611:C:C6	2.55	0.41
18:LI0:30:LYS:HE2	18:LI0:66:GLU:HG2	2.02	0.41
49:SDD:12:LEU:HD21	64:SP0:67:PHE:CD2	2.55	0.41
52:SF0:49:THR:O	52:SF0:49:THR:HG22	2.20	0.41
1:L50:222:A:H2'	1:L50:223:A:C8	2.55	0.41
56:SH0:53:LEU:HB3	56:SH0:54:PRO:HD3	2.02	0.41
1:L50:506:G:H2'	1:L50:508:A:N7	2.36	0.41
42:SA0:81:ASP:C	42:SA0:83:GLY:H	2.28	0.41
48:SD0:184:ILE:HD12	48:SD0:215:MET:CE	2.50	0.41
50:SE0:35:PRO:HD2	50:SE0:83:PRO:HG2	2.03	0.41
60:SL0:144:ILE:HD13	60:SL0:147:LYS:HE2	2.03	0.41
1:L50:32:G:H21	1:L50:377:A:H62	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S60:132:C:H3'	41:S60:133:A:C8	2.53	0.41
41:S60:1108:C:H2'	41:S60:1109:A:O4'	2.20	0.41
21:LJJ:40:PRO:O	38:LX0:3:LYS:HE3	2.21	0.41
27:LO0:24:LYS:HA	27:LO0:24:LYS:HD2	1.93	0.41
41:S60:405:A:H2'	41:S60:406:U:H6	1.84	0.41
41:S60:970:U:H5''	41:S60:970:U:H6	1.85	0.41
1:L50:1642:G:H2'	1:L50:1643:G:C8	2.56	0.41
6:LC0:323:GLU:HG2	6:LC0:324:ILE:N	2.36	0.41
10:LE0:17:TYR:CE1	11:LEE:79:ARG:HD3	2.56	0.41
14:LG0:16:PRO:HG2	26:LN0:32:GLN:HE21	1.86	0.41
17:LHH:66:LEU:CD1	38:LX0:22:ILE:HD11	2.51	0.41
37:LW0:80:VAL:O	37:LW0:81:ARG:C	2.63	0.41
41:S60:1121:A:H3'	41:S60:1122:A:H8	1.85	0.41
45:SBB:81:ILE:CD1	62:SN0:25:TYR:HB2	2.51	0.41
48:SD0:184:ILE:HD12	48:SD0:215:MET:HE3	2.03	0.41
1:L50:2211:A:H5''	1:L50:2212:G:N2	2.35	0.41
41:S60:1125:G:C8	41:S60:1125:G:H3'	2.56	0.41
53:SFF:93:LYS:HB3	53:SFF:94:PRO:CD	2.42	0.41
54:SG0:156:GLU:O	54:SG0:160:LYS:HG3	2.20	0.41
1:L50:885:G:H5''	1:L50:885:G:H8	1.86	0.40
42:SA0:60:LEU:CD2	70:SV0:63:ILE:HD13	2.46	0.40
1:L50:885:G:H5''	1:L50:885:G:C8	2.56	0.40
41:S60:132:C:O2	41:S60:132:C:H2'	2.21	0.40
41:S60:552:G:O2'	71:SW0:105:SER:HB3	2.20	0.40
41:S60:917:U:C5	53:SFF:97:ASP:HB3	2.56	0.40
73:SY0:116:ARG:NH2	73:SY0:120:LYS:NZ	2.69	0.40
1:L50:158:A:H61	1:L50:168:G:H1'	1.87	0.40
1:L50:763:U:H2'	1:L50:764:U:O4'	2.22	0.40
8:LD0:47:GLN:HB2	34:LT0:68:ASN:O	2.21	0.40
8:LD0:262:ASP:C	8:LD0:264:SER:H	2.29	0.40
31:LQ0:57:THR:O	31:LQ0:57:THR:HG22	2.22	0.40
1:L50:1344:G:H4'	32:LR0:116:LYS:HD2	2.04	0.40
1:L50:2026:G:C2	28:LOO:5:PRO:HG2	2.55	0.40
16:LH0:129:THR:HG22	16:LH0:150:VAL:HG22	2.04	0.40
1:L50:186:G:H2'	1:L50:187:A:C8	2.56	0.40
1:L50:1133:C:H4'	1:L50:1134:A:H5'	2.02	0.40
1:L50:2420:C:H6	1:L50:2420:C:H2'	1.72	0.40
41:S60:574:A:H1'	45:SBB:67:GLY:CA	2.51	0.40
54:SG0:169:VAL:HG11	54:SG0:176:LYS:HG2	2.04	0.40
58:SJ0:55:LYS:O	58:SJ0:59:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LA0	243/246 (99%)	236 (97%)	7 (3%)	0	100	100
4	LAA	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
5	LB0	381/392 (97%)	372 (98%)	9 (2%)	0	100	100
6	LC0	325/328 (99%)	313 (96%)	11 (3%)	1 (0%)	36	66
7	LCC	97/110 (88%)	94 (97%)	2 (2%)	1 (1%)	12	38
8	LD0	279/291 (96%)	274 (98%)	5 (2%)	0	100	100
9	LDD	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
10	LE0	163/171 (95%)	154 (94%)	9 (6%)	0	100	100
11	LEE	133/139 (96%)	127 (96%)	6 (4%)	0	100	100
12	LF0	229/235 (97%)	224 (98%)	5 (2%)	0	100	100
13	LFF	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
14	LG0	197/206 (96%)	194 (98%)	3 (2%)	0	100	100
15	LGG	102/106 (96%)	96 (94%)	5 (5%)	1 (1%)	12	38
16	LH0	181/187 (97%)	177 (98%)	4 (2%)	0	100	100
17	LHH	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
18	LI0	215/218 (99%)	214 (100%)	1 (0%)	0	100	100
19	LII	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
20	LJ0	165/171 (96%)	156 (94%)	9 (6%)	0	100	100
21	LJJ	87/92 (95%)	86 (99%)	1 (1%)	0	100	100
22	LL0	162/165 (98%)	155 (96%)	6 (4%)	1 (1%)	21	51
23	LLL	49/52 (94%)	48 (98%)	1 (2%)	0	100	100
24	LM0	113/122 (93%)	106 (94%)	6 (5%)	1 (1%)	14	41
25	LMM	50/127 (39%)	50 (100%)	0	0	100	100
26	LN0	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
27	LO0	196/198 (99%)	193 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	LOO	98/104 (94%)	96 (98%)	2 (2%)	0	100	100
29	LP0	152/167 (91%)	145 (95%)	7 (5%)	0	100	100
30	LPP	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	10	34
31	LQ0	180/183 (98%)	175 (97%)	5 (3%)	0	100	100
32	LR0	162/168 (96%)	160 (99%)	2 (1%)	0	100	100
33	LS0	168/171 (98%)	159 (95%)	9 (5%)	0	100	100
34	LT0	154/158 (98%)	145 (94%)	9 (6%)	0	100	100
35	LU0	98/113 (87%)	93 (95%)	5 (5%)	0	100	100
36	LV0	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
37	LW0	100/131 (76%)	94 (94%)	5 (5%)	1 (1%)	12	38
38	LX0	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
39	LY0	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
40	LZ0	116/153 (76%)	116 (100%)	0	0	100	100
42	SA0	218/233 (94%)	206 (94%)	12 (6%)	0	100	100
43	SAA	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
44	SB0	202/230 (88%)	197 (98%)	5 (2%)	0	100	100
45	SBB	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
46	SC0	224/248 (90%)	220 (98%)	4 (2%)	0	100	100
47	SCC	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
48	SD0	214/242 (88%)	212 (99%)	2 (1%)	0	100	100
49	SDD	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
50	SE0	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
51	SEE	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
52	SF0	190/195 (97%)	180 (95%)	10 (5%)	0	100	100
53	SFF	56/150 (37%)	52 (93%)	4 (7%)	0	100	100
54	SG0	227/230 (99%)	213 (94%)	14 (6%)	0	100	100
55	SGG	315/326 (97%)	295 (94%)	19 (6%)	1 (0%)	36	66
56	SH0	161/164 (98%)	156 (97%)	4 (2%)	1 (1%)	21	51
57	SI0	165/173 (95%)	161 (98%)	4 (2%)	0	100	100
58	SJ0	166/184 (90%)	165 (99%)	1 (1%)	0	100	100
59	SK0	89/107 (83%)	84 (94%)	4 (4%)	1 (1%)	11	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	SL0	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
61	SM0	109/130 (84%)	106 (97%)	3 (3%)	0	100	100
62	SN0	140/143 (98%)	134 (96%)	6 (4%)	0	100	100
63	SO0	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
64	SP0	115/163 (71%)	113 (98%)	2 (2%)	0	100	100
65	SQ0	140/143 (98%)	134 (96%)	6 (4%)	0	100	100
66	SR0	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
67	SS0	142/160 (89%)	137 (96%)	4 (3%)	1 (1%)	18	47
68	ST0	140/143 (98%)	140 (100%)	0	0	100	100
69	SU0	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
70	SV0	63/67 (94%)	62 (98%)	1 (2%)	0	100	100
71	SW0	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
72	SX0	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
73	SY0	134/146 (92%)	122 (91%)	10 (8%)	2 (2%)	8	28
74	SZ0	74/128 (58%)	69 (93%)	5 (7%)	0	100	100
All	All	10483/11325 (93%)	10120 (96%)	350 (3%)	13 (0%)	49	77

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LGG	78	GLY
73	SY0	134	LYS
30	LPP	18	TYR
37	LW0	81	ARG
67	SS0	24	PHE
73	SY0	37	ASN
55	SGG	61	GLY
24	LM0	48	GLY
56	SH0	107	PHE
59	SK0	71	GLY
7	LCC	64	ILE
22	LL0	8	PRO
6	LC0	297	ILE

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	
3	LA0	202/203 (100%)	199 (98%)	3 (2%)	57	84
4	LAA	123/123 (100%)	119 (97%)	4 (3%)	33	69
5	LB0	328/336 (98%)	319 (97%)	9 (3%)	39	74
6	LC0	277/278 (100%)	274 (99%)	3 (1%)	65	87
7	LCC	87/97 (90%)	85 (98%)	2 (2%)	44	78
8	LD0	251/261 (96%)	249 (99%)	2 (1%)	73	90
9	LDD	99/100 (99%)	99 (100%)	0	100	100
10	LE0	153/159 (96%)	150 (98%)	3 (2%)	48	80
11	LEE	118/122 (97%)	118 (100%)	0	100	100
12	LF0	212/216 (98%)	211 (100%)	1 (0%)	81	93
13	LFF	98/98 (100%)	98 (100%)	0	100	100
14	LG0	183/190 (96%)	183 (100%)	0	100	100
15	LGG	88/90 (98%)	86 (98%)	2 (2%)	44	78
16	LH0	165/169 (98%)	161 (98%)	4 (2%)	43	77
17	LHH	110/110 (100%)	109 (99%)	1 (1%)	70	89
18	LI0	188/189 (100%)	188 (100%)	0	100	100
19	LII	84/84 (100%)	82 (98%)	2 (2%)	43	77
20	LJ0	146/149 (98%)	144 (99%)	2 (1%)	59	85
21	LJJ	78/81 (96%)	77 (99%)	1 (1%)	61	86
22	LL0	148/149 (99%)	142 (96%)	6 (4%)	27	62
23	LLL	46/47 (98%)	46 (100%)	0	100	100
24	LM0	110/117 (94%)	110 (100%)	0	100	100
25	LMM	46/112 (41%)	46 (100%)	0	100	100
26	LN0	175/176 (99%)	171 (98%)	4 (2%)	44	78
27	LO0	178/178 (100%)	177 (99%)	1 (1%)	78	92
28	LOO	85/89 (96%)	85 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	LP0	135/147 (92%)	132 (98%)	3 (2%)	45	78
30	LPP	75/77 (97%)	73 (97%)	2 (3%)	39	74
31	LQ0	165/166 (99%)	165 (100%)	0	100	100
32	LR0	142/145 (98%)	141 (99%)	1 (1%)	76	91
33	LS0	155/156 (99%)	152 (98%)	3 (2%)	50	81
34	LT0	140/142 (99%)	138 (99%)	2 (1%)	59	85
35	LU0	89/98 (91%)	88 (99%)	1 (1%)	65	87
36	LV0	113/114 (99%)	112 (99%)	1 (1%)	70	89
37	LW0	93/120 (78%)	89 (96%)	4 (4%)	26	60
38	LX0	92/93 (99%)	91 (99%)	1 (1%)	65	87
39	LY0	116/116 (100%)	114 (98%)	2 (2%)	53	83
40	LZ0	106/141 (75%)	106 (100%)	0	100	100
42	SA0	194/206 (94%)	192 (99%)	2 (1%)	68	88
43	SAA	92/93 (99%)	92 (100%)	0	100	100
44	SB0	182/203 (90%)	182 (100%)	0	100	100
45	SBB	72/73 (99%)	71 (99%)	1 (1%)	59	85
46	SC0	187/209 (90%)	185 (99%)	2 (1%)	65	87
47	SCC	51/54 (94%)	51 (100%)	0	100	100
48	SD0	189/215 (88%)	189 (100%)	0	100	100
49	SDD	57/57 (100%)	57 (100%)	0	100	100
50	SE0	231/251 (92%)	229 (99%)	2 (1%)	70	89
51	SEE	44/47 (94%)	44 (100%)	0	100	100
52	SF0	167/170 (98%)	163 (98%)	4 (2%)	43	77
53	SFF	52/136 (38%)	51 (98%)	1 (2%)	50	81
54	SG0	199/200 (100%)	194 (98%)	5 (2%)	42	76
55	SGG	282/288 (98%)	278 (99%)	4 (1%)	59	85
56	SH0	153/154 (99%)	153 (100%)	0	100	100
57	SI0	147/153 (96%)	147 (100%)	0	100	100
58	SJ0	152/165 (92%)	150 (99%)	2 (1%)	61	86
59	SK0	86/99 (87%)	85 (99%)	1 (1%)	63	87
60	SL0	140/145 (97%)	139 (99%)	1 (1%)	76	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	SM0	99/114 (87%)	99 (100%)	0	100	100
62	SN0	126/127 (99%)	126 (100%)	0	100	100
63	SO0	102/108 (94%)	101 (99%)	1 (1%)	68	88
64	SP0	107/144 (74%)	106 (99%)	1 (1%)	70	89
65	SQ0	120/121 (99%)	119 (99%)	1 (1%)	73	90
66	SR0	110/111 (99%)	109 (99%)	1 (1%)	70	89
67	SS0	125/138 (91%)	124 (99%)	1 (1%)	73	90
68	ST0	129/130 (99%)	127 (98%)	2 (2%)	55	83
69	SU0	92/110 (84%)	92 (100%)	0	100	100
70	SV0	61/63 (97%)	61 (100%)	0	100	100
71	SW0	111/111 (100%)	110 (99%)	1 (1%)	70	89
72	SX0	115/116 (99%)	115 (100%)	0	100	100
73	SY0	126/136 (93%)	121 (96%)	5 (4%)	28	63
74	SZ0	73/118 (62%)	73 (100%)	0	100	100
All	All	9372/10003 (94%)	9264 (99%)	108 (1%)	61	87

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LA0	44	GLU
3	LA0	189	ARG
3	LA0	222	VAL
4	LAA	22	VAL
4	LAA	26	ARG
4	LAA	39	LYS
4	LAA	54	ARG
5	LB0	10	ARG
5	LB0	23	LYS
5	LB0	86	VAL
5	LB0	122	ARG
5	LB0	132	LYS
5	LB0	133	LEU
5	LB0	134	MET
5	LB0	135	PHE
5	LB0	336	ARG
6	LC0	103	VAL
6	LC0	207	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	LC0	328	ILE
7	LCC	64	ILE
7	LCC	76	SER
8	LD0	85	THR
8	LD0	285	GLN
10	LE0	15	LYS
10	LE0	17	TYR
10	LE0	30	LEU
12	LF0	42	ARG
15	LGG	32	PHE
15	LGG	101	MET
16	LH0	34	VAL
16	LH0	62	GLN
16	LH0	64	ARG
16	LH0	149	ASP
17	LHH	107	LEU
19	LII	47	ARG
19	LII	90	GLU
20	LJ0	106	HIS
20	LJ0	144	ARG
21	LJJ	2	SER
22	LL0	5	GLN
22	LL0	30	LEU
22	LL0	44	TYR
22	LL0	90	VAL
22	LL0	97	ARG
22	LL0	98	ARG
26	LN0	65	ARG
26	LN0	112	ASN
26	LN0	135	VAL
26	LN0	155	VAL
27	LO0	105	ASP
29	LP0	30	ARG
29	LP0	60	VAL
29	LP0	120	ASN
30	LPP	8	VAL
30	LPP	18	TYR
32	LR0	19	ARG
33	LS0	52	PRO
33	LS0	157	ARG
33	LS0	171	ASN
34	LT0	55	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	LT0	112	ASN
35	LU0	92	ARG
36	LV0	28	LEU
37	LW0	80	VAL
37	LW0	81	ARG
37	LW0	91	VAL
37	LW0	92	GLU
38	LX0	40	HIS
39	LY0	1	MET
39	LY0	114	ARG
42	SA0	8	LEU
42	SA0	154	ILE
45	SBB	58	CYS
46	SC0	156	SER
46	SC0	221	VAL
50	SE0	211	VAL
50	SE0	213	LYS
52	SF0	18	TYR
52	SF0	61	GLU
52	SF0	92	GLU
52	SF0	97	GLN
53	SFF	93	LYS
54	SG0	92	ARG
54	SG0	100	SER
54	SG0	129	VAL
54	SG0	144	LYS
54	SG0	222	TRP
55	SGG	76	ASP
55	SGG	106	ASP
55	SGG	150	THR
55	SGG	305	ASP
58	SJ0	62	ASP
58	SJ0	130	GLN
59	SK0	80	TYR
60	SL0	148	LYS
63	SO0	122	ASP
64	SP0	135	ARG
65	SQ0	99	GLU
66	SR0	31	ASN
67	SS0	24	PHE
68	ST0	17	LEU
68	ST0	28	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	SW0	110	ASP
73	SY0	11	PHE
73	SY0	37	ASN
73	SY0	39	MET
73	SY0	135	ARG
73	SY0	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L50	2494/2618 (95%)	748 (29%)	102 (4%)
2	L70	118/119 (99%)	36 (30%)	4 (3%)
41	S60	1352/1368 (98%)	512 (37%)	65 (4%)
All	All	3964/4105 (96%)	1296 (32%)	171 (4%)

All (1296) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L50	2	U
1	L50	3	A
1	L50	13	A
1	L50	15	G
1	L50	21	U
1	L50	22	U
1	L50	23	U
1	L50	24	G
1	L50	25	G
1	L50	31	G
1	L50	39	G
1	L50	43	G
1	L50	48	A
1	L50	51	A
1	L50	52	G
1	L50	59	A
1	L50	62	U
1	L50	63	G
1	L50	68	G
1	L50	70	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	71	G
1	L50	73	A
1	L50	74	G
1	L50	75	C
1	L50	76	A
1	L50	77	G
1	L50	82	G
1	L50	87	C
1	L50	88	A
1	L50	98	A
1	L50	99	U
1	L50	100	A
1	L50	101	C
1	L50	108	G
1	L50	113	G
1	L50	114	G
1	L50	118	A
1	L50	123	U
1	L50	132	A
1	L50	135	A
1	L50	136	U
1	L50	137	A
1	L50	151	G
1	L50	152	A
1	L50	157	A
1	L50	158	A
1	L50	159	A
1	L50	160	C
1	L50	165	G
1	L50	167	G
1	L50	169	A
1	L50	178	G
1	L50	181	G
1	L50	184	G
1	L50	186	G
1	L50	188	G
1	L50	191	A
1	L50	194	A
1	L50	201	A
1	L50	202	G
1	L50	204	C
1	L50	209	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	210	G
1	L50	211	U
1	L50	212	G
1	L50	213	U
1	L50	214	A
1	L50	215	A
1	L50	216	U
1	L50	221	A
1	L50	224	U
1	L50	225	G
1	L50	226	A
1	L50	233	G
1	L50	234	U
1	L50	237	A
1	L50	238	A
1	L50	239	A
1	L50	240	G
1	L50	241	G
1	L50	242	A
1	L50	246	A
1	L50	247	G
1	L50	255	U
1	L50	258	G
1	L50	265	A
1	L50	266	A
1	L50	267	G
1	L50	268	C
1	L50	273	C
1	L50	276	U
1	L50	277	A
1	L50	284	G
1	L50	285	A
1	L50	286	U
1	L50	287	A
1	L50	289	U
1	L50	298	G
1	L50	309	U
1	L50	311	C
1	L50	312	G
1	L50	314	U
1	L50	315	G
1	L50	316	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	317	G
1	L50	330	G
1	L50	331	U
1	L50	332	A
1	L50	333	A
1	L50	340	G
1	L50	343	A
1	L50	345	G
1	L50	346	A
1	L50	347	G
1	L50	352	C
1	L50	353	A
1	L50	358	G
1	L50	366	G
1	L50	373	U
1	L50	382	A
1	L50	384	A
1	L50	385	C
1	L50	390	A
1	L50	392	C
1	L50	396	G
1	L50	397	A
1	L50	400	U
1	L50	416	A
1	L50	434	G
1	L50	438	A
1	L50	449	U
1	L50	450	C
1	L50	453	G
1	L50	454	C
1	L50	467	A
1	L50	478	A
1	L50	488	C
1	L50	495	A
1	L50	499	G
1	L50	503	A
1	L50	504	G
1	L50	507	G
1	L50	508	A
1	L50	509	A
1	L50	510	G
1	L50	517	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	523	A
1	L50	524	G
1	L50	527	A
1	L50	530	A
1	L50	533	G
1	L50	534	A
1	L50	535	A
1	L50	536	A
1	L50	542	G
1	L50	553	C
1	L50	556	A
1	L50	562	U
1	L50	563	U
1	L50	564	G
1	L50	567	A
1	L50	568	A
1	L50	569	C
1	L50	570	U
1	L50	580	U
1	L50	581	G
1	L50	587	A
1	L50	601	C
1	L50	612	C
1	L50	618	G
1	L50	620	C
1	L50	625	U
1	L50	630	U
1	L50	631	G
1	L50	642	G
1	L50	643	C
1	L50	646	A
1	L50	647	A
1	L50	658	G
1	L50	659	G
1	L50	660	G
1	L50	661	G
1	L50	665	A
1	L50	667	G
1	L50	668	A
1	L50	675	G
1	L50	676	A
1	L50	684	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	685	G
1	L50	688	G
1	L50	689	C
1	L50	695	C
1	L50	710	A
1	L50	711	U
1	L50	714	G
1	L50	715	G
1	L50	720	C
1	L50	726	C
1	L50	729	A
1	L50	732	G
1	L50	736	A
1	L50	739	A
1	L50	741	G
1	L50	742	G
1	L50	749	A
1	L50	750	U
1	L50	763	U
1	L50	764	U
1	L50	765	A
1	L50	766	A
1	L50	767	G
1	L50	768	G
1	L50	772	C
1	L50	776	C
1	L50	778	A
1	L50	779	A
1	L50	781	U
1	L50	782	G
1	L50	784	G
1	L50	795	U
1	L50	796	C
1	L50	801	A
1	L50	802	U
1	L50	803	G
1	L50	806	A
1	L50	816	G
1	L50	822	U
1	L50	828	A
1	L50	830	G
1	L50	834	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	838	G
1	L50	840	C
1	L50	843	A
1	L50	848	A
1	L50	849	A
1	L50	852	A
1	L50	853	A
1	L50	854	C
1	L50	858	G
1	L50	859	C
1	L50	865	G
1	L50	866	C
1	L50	867	U
1	L50	871	G
1	L50	877	A
1	L50	878	A
1	L50	879	U
1	L50	885	G
1	L50	889	G
1	L50	893	C
1	L50	900	A
1	L50	905	G
1	L50	910	A
1	L50	980	A
1	L50	990	U
1	L50	998	U
1	L50	1001	A
1	L50	1002	U
1	L50	1010	A
1	L50	1017	A
1	L50	1018	U
1	L50	1021	G
1	L50	1022	A
1	L50	1023	U
1	L50	1024	G
1	L50	1030	U
1	L50	1032	A
1	L50	1033	G
1	L50	1034	C
1	L50	1037	G
1	L50	1050	U
1	L50	1053	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1055	A
1	L50	1056	C
1	L50	1061	G
1	L50	1062	A
1	L50	1070	G
1	L50	1075	A
1	L50	1082	G
1	L50	1085	G
1	L50	1087	G
1	L50	1089	U
1	L50	1090	A
1	L50	1096	A
1	L50	1099	G
1	L50	1100	C
1	L50	1102	G
1	L50	1105	C
1	L50	1111	G
1	L50	1117	A
1	L50	1118	G
1	L50	1120	G
1	L50	1121	A
1	L50	1123	A
1	L50	1124	A
1	L50	1130	C
1	L50	1131	U
1	L50	1133	C
1	L50	1134	A
1	L50	1135	G
1	L50	1136	C
1	L50	1142	A
1	L50	1144	A
1	L50	1148	A
1	L50	1149	G
1	L50	1150	G
1	L50	1151	A
1	L50	1155	G
1	L50	1163	U
1	L50	1169	C
1	L50	1170	A
1	L50	1171	U
1	L50	1172	A
1	L50	1173	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1175	A
1	L50	1177	G
1	L50	1181	G
1	L50	1182	A
1	L50	1183	G
1	L50	1189	U
1	L50	1191	U
1	L50	1192	A
1	L50	1193	A
1	L50	1194	G
1	L50	1196	G
1	L50	1213	A
1	L50	1217	A
1	L50	1218	A
1	L50	1221	A
1	L50	1224	A
1	L50	1231	U
1	L50	1232	G
1	L50	1233	A
1	L50	1235	A
1	L50	1236	U
1	L50	1237	U
1	L50	1243	G
1	L50	1247	G
1	L50	1250	C
1	L50	1252	G
1	L50	1254	C
1	L50	1256	U
1	L50	1257	A
1	L50	1264	C
1	L50	1267	G
1	L50	1268	U
1	L50	1269	A
1	L50	1270	U
1	L50	1274	C
1	L50	1277	G
1	L50	1278	U
1	L50	1282	C
1	L50	1283	A
1	L50	1284	C
1	L50	1296	C
1	L50	1299	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1304	A
1	L50	1305	A
1	L50	1308	A
1	L50	1309	C
1	L50	1317	G
1	L50	1318	U
1	L50	1327	A
1	L50	1332	G
1	L50	1333	A
1	L50	1340	A
1	L50	1341	G
1	L50	1342	A
1	L50	1346	A
1	L50	1350	U
1	L50	1355	C
1	L50	1356	G
1	L50	1361	G
1	L50	1362	G
1	L50	1374	U
1	L50	1375	G
1	L50	1384	U
1	L50	1385	G
1	L50	1386	A
1	L50	1387	G
1	L50	1395	U
1	L50	1396	G
1	L50	1402	G
1	L50	1411	C
1	L50	1412	C
1	L50	1414	U
1	L50	1416	A
1	L50	1427	A
1	L50	1429	A
1	L50	1430	U
1	L50	1431	G
1	L50	1432	G
1	L50	1440	G
1	L50	1447	C
1	L50	1449	A
1	L50	1450	A
1	L50	1453	G
1	L50	1454	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1455	A
1	L50	1457	C
1	L50	1458	A
1	L50	1466	A
1	L50	1467	A
1	L50	1468	G
1	L50	1474	G
1	L50	1475	A
1	L50	1479	U
1	L50	1485	G
1	L50	1486	G
1	L50	1488	U
1	L50	1489	G
1	L50	1490	U
1	L50	1491	U
1	L50	1492	U
1	L50	1499	U
1	L50	1513	G
1	L50	1524	G
1	L50	1527	U
1	L50	1533	C
1	L50	1534	G
1	L50	1535	G
1	L50	1536	G
1	L50	1538	G
1	L50	1547	G
1	L50	1554	U
1	L50	1555	G
1	L50	1556	U
1	L50	1557	G
1	L50	1563	A
1	L50	1564	U
1	L50	1565	U
1	L50	1566	G
1	L50	1568	G
1	L50	1569	A
1	L50	1571	A
1	L50	1573	G
1	L50	1574	G
1	L50	1575	G
1	L50	1583	A
1	L50	1591	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1592	U
1	L50	1602	G
1	L50	1610	A
1	L50	1611	A
1	L50	1612	G
1	L50	1613	A
1	L50	1614	G
1	L50	1617	A
1	L50	1619	G
1	L50	1624	G
1	L50	1626	G
1	L50	1638	G
1	L50	1643	G
1	L50	1644	U
1	L50	1645	C
1	L50	1646	G
1	L50	1649	A
1	L50	1651	A
1	L50	1653	G
1	L50	1665	A
1	L50	1668	A
1	L50	1674	G
1	L50	1675	G
1	L50	1680	A
1	L50	1682	G
1	L50	1685	G
1	L50	1686	G
1	L50	1689	G
1	L50	1692	A
1	L50	1693	C
1	L50	1697	G
1	L50	1698	A
1	L50	1699	C
1	L50	1705	U
1	L50	1708	G
1	L50	1709	G
1	L50	1710	U
1	L50	1711	A
1	L50	1717	A
1	L50	1718	C
1	L50	1720	C
1	L50	1724	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1733	A
1	L50	1735	G
1	L50	1739	A
1	L50	1742	C
1	L50	1743	G
1	L50	1746	U
1	L50	1749	A
1	L50	1751	G
1	L50	1755	U
1	L50	1760	A
1	L50	1770	U
1	L50	1772	U
1	L50	1797	A
1	L50	1799	U
1	L50	1800	U
1	L50	1801	C
1	L50	1808	A
1	L50	1809	A
1	L50	1810	C
1	L50	1811	G
1	L50	1820	C
1	L50	1821	G
1	L50	1822	G
1	L50	1828	G
1	L50	1832	A
1	L50	1833	A
1	L50	1835	G
1	L50	1836	A
1	L50	1837	A
1	L50	1838	G
1	L50	1839	A
1	L50	1846	U
1	L50	1854	A
1	L50	1858	U
1	L50	1860	G
1	L50	1868	A
1	L50	1869	A
1	L50	1870	G
1	L50	1872	U
1	L50	1873	G
1	L50	1874	U
1	L50	1881	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1883	A
1	L50	1885	G
1	L50	1887	G
1	L50	1888	A
1	L50	1931	C
1	L50	1934	C
1	L50	1935	A
1	L50	1937	G
1	L50	1938	A
1	L50	1939	U
1	L50	1940	C
1	L50	1941	A
1	L50	1942	U
1	L50	1943	C
1	L50	1946	G
1	L50	1949	A
1	L50	1950	C
1	L50	1955	G
1	L50	1956	U
1	L50	1957	U
1	L50	1958	U
1	L50	1959	A
1	L50	1960	A
1	L50	1961	G
1	L50	1963	A
1	L50	1966	A
1	L50	1967	A
1	L50	1968	G
1	L50	1973	G
1	L50	1977	G
1	L50	1978	G
1	L50	1985	G
1	L50	1991	G
1	L50	1995	G
1	L50	1997	A
1	L50	2007	A
1	L50	2008	A
1	L50	2011	A
1	L50	2013	A
1	L50	2015	C
1	L50	2016	G
1	L50	2019	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2020	U
1	L50	2022	G
1	L50	2023	A
1	L50	2027	A
1	L50	2030	G
1	L50	2031	U
1	L50	2032	A
1	L50	2036	A
1	L50	2037	C
1	L50	2039	G
1	L50	2042	A
1	L50	2043	G
1	L50	2045	C
1	L50	2046	G
1	L50	2047	A
1	L50	2048	G
1	L50	2049	A
1	L50	2052	A
1	L50	2057	U
1	L50	2059	U
1	L50	2060	A
1	L50	2061	G
1	L50	2062	A
1	L50	2063	G
1	L50	2065	A
1	L50	2067	A
1	L50	2073	U
1	L50	2075	A
1	L50	2076	A
1	L50	2077	G
1	L50	2078	A
1	L50	2085	G
1	L50	2087	G
1	L50	2093	G
1	L50	2096	C
1	L50	2097	U
1	L50	2098	A
1	L50	2099	C
1	L50	2108	U
1	L50	2109	G
1	L50	2110	A
1	L50	2111	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2114	G
1	L50	2122	G
1	L50	2124	C
1	L50	2130	G
1	L50	2131	A
1	L50	2136	A
1	L50	2140	A
1	L50	2141	U
1	L50	2142	A
1	L50	2145	A
1	L50	2146	G
1	L50	2149	A
1	L50	2150	C
1	L50	2152	U
1	L50	2160	G
1	L50	2162	G
1	L50	2164	G
1	L50	2167	A
1	L50	2168	G
1	L50	2169	A
1	L50	2170	A
1	L50	2171	A
1	L50	2177	C
1	L50	2178	C
1	L50	2185	A
1	L50	2189	C
1	L50	2211	A
1	L50	2212	G
1	L50	2213	A
1	L50	2217	C
1	L50	2221	G
1	L50	2224	G
1	L50	2228	U
1	L50	2229	U
1	L50	2234	U
1	L50	2235	C
1	L50	2239	G
1	L50	2240	A
1	L50	2241	U
1	L50	2243	U
1	L50	2253	C
1	L50	2254	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2255	A
1	L50	2256	G
1	L50	2257	C
1	L50	2260	G
1	L50	2262	C
1	L50	2266	G
1	L50	2272	G
1	L50	2275	G
1	L50	2279	A
1	L50	2286	G
1	L50	2291	U
1	L50	2293	C
1	L50	2296	C
1	L50	2303	C
1	L50	2304	A
1	L50	2306	G
1	L50	2309	A
1	L50	2310	C
1	L50	2313	G
1	L50	2319	G
1	L50	2322	U
1	L50	2323	U
1	L50	2325	G
1	L50	2337	A
1	L50	2339	A
1	L50	2340	G
1	L50	2345	G
1	L50	2347	U
1	L50	2351	U
1	L50	2355	A
1	L50	2358	G
1	L50	2364	A
1	L50	2376	A
1	L50	2377	G
1	L50	2379	G
1	L50	2394	A
1	L50	2399	A
1	L50	2401	C
1	L50	2410	A
1	L50	2412	C
1	L50	2413	U
1	L50	2416	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2419	G
1	L50	2420	C
1	L50	2423	C
1	L50	2424	G
1	L50	2432	G
1	L50	2434	A
1	L50	2436	G
1	L50	2437	U
1	L50	2441	A
1	L50	2447	A
1	L50	2451	U
1	L50	2452	A
1	L50	2453	C
1	L50	2459	C
1	L50	2460	U
1	L50	2473	G
1	L50	2475	A
1	L50	2476	G
1	L50	2477	C
1	L50	2482	A
1	L50	2487	A
1	L50	2490	A
1	L50	2491	A
1	L50	2501	A
1	L50	2503	U
1	L50	2508	A
1	L50	2509	A
1	L50	2518	G
1	L50	2519	G
1	L50	2520	A
1	L50	2529	C
1	L50	2532	A
1	L50	2533	G
1	L50	2534	U
1	L50	2535	U
1	L50	2538	C
1	L50	2539	A
1	L50	2548	G
1	L50	2555	A
1	L50	2558	A
1	L50	2559	G
1	L50	2562	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	2563	U
1	L50	2565	U
1	L50	2568	U
1	L50	2578	G
1	L50	2588	G
1	L50	2593	A
1	L50	2595	U
1	L50	2596	G
1	L50	2597	G
1	L50	2598	U
1	L50	2600	G
1	L50	2605	C
1	L50	2606	A
1	L50	2612	G
2	L70	2	G
2	L70	10	C
2	L70	14	U
2	L70	15	C
2	L70	18	C
2	L70	22	A
2	L70	25	A
2	L70	27	A
2	L70	32	A
2	L70	33	U
2	L70	35	C
2	L70	41	G
2	L70	42	A
2	L70	49	A
2	L70	50	A
2	L70	51	G
2	L70	53	U
2	L70	63	A
2	L70	64	G
2	L70	65	A
2	L70	67	C
2	L70	69	A
2	L70	88	C
2	L70	89	G
2	L70	91	C
2	L70	93	A
2	L70	100	A
2	L70	101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L70	104	C
2	L70	105	G
2	L70	107	G
2	L70	108	G
2	L70	109	U
2	L70	110	G
2	L70	115	A
2	L70	119	U
41	S60	7	U
41	S60	8	U
41	S60	14	U
41	S60	17	C
41	S60	26	A
41	S60	32	G
41	S60	37	A
41	S60	39	A
41	S60	40	G
41	S60	41	A
41	S60	43	U
41	S60	44	U
41	S60	45	A
41	S60	48	C
41	S60	52	C
41	S60	54	U
41	S60	55	G
41	S60	56	U
41	S60	66	G
41	S60	70	U
41	S60	71	U
41	S60	72	A
41	S60	73	G
41	S60	75	G
41	S60	76	A
41	S60	77	A
41	S60	83	G
41	S60	86	A
41	S60	88	G
41	S60	92	A
41	S60	94	U
41	S60	97	C
41	S60	98	G
41	S60	99	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	102	G
41	S60	104	G
41	S60	106	A
41	S60	107	U
41	S60	110	A
41	S60	112	U
41	S60	116	U
41	S60	118	G
41	S60	119	A
41	S60	120	A
41	S60	121	C
41	S60	124	G
41	S60	127	A
41	S60	128	A
41	S60	132	C
41	S60	133	A
41	S60	134	G
41	S60	138	A
41	S60	140	A
41	S60	141	G
41	S60	142	A
41	S60	147	A
41	S60	148	A
41	S60	150	A
41	S60	153	G
41	S60	155	G
41	S60	157	A
41	S60	161	G
41	S60	167	G
41	S60	172	U
41	S60	173	A
41	S60	174	G
41	S60	180	G
41	S60	181	A
41	S60	184	A
41	S60	186	A
41	S60	187	A
41	S60	189	A
41	S60	190	A
41	S60	191	C
41	S60	192	A
41	S60	193	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	197	A
41	S60	198	G
41	S60	199	G
41	S60	204	U
41	S60	206	A
41	S60	219	U
41	S60	220	C
41	S60	222	G
41	S60	226	G
41	S60	227	U
41	S60	228	A
41	S60	238	A
41	S60	241	G
41	S60	242	C
41	S60	247	U
41	S60	254	U
41	S60	255	A
41	S60	256	G
41	S60	259	G
41	S60	262	U
41	S60	263	A
41	S60	264	C
41	S60	268	G
41	S60	271	U
41	S60	283	U
41	S60	284	C
41	S60	290	A
41	S60	292	G
41	S60	299	G
41	S60	300	A
41	S60	303	G
41	S60	304	A
41	S60	305	C
41	S60	307	G
41	S60	311	C
41	S60	314	G
41	S60	315	G
41	S60	318	C
41	S60	319	A
41	S60	320	A
41	S60	326	G
41	S60	327	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	328	A
41	S60	329	G
41	S60	335	G
41	S60	338	A
41	S60	339	A
41	S60	340	A
41	S60	341	A
41	S60	342	U
41	S60	344	A
41	S60	345	C
41	S60	347	G
41	S60	348	A
41	S60	355	C
41	S60	356	A
41	S60	357	A
41	S60	358	G
41	S60	362	G
41	S60	363	C
41	S60	364	G
41	S60	367	A
41	S60	368	G
41	S60	371	A
41	S60	372	A
41	S60	373	G
41	S60	374	A
41	S60	375	G
41	S60	377	C
41	S60	378	G
41	S60	380	G
41	S60	382	A
41	S60	383	A
41	S60	384	A
41	S60	385	C
41	S60	388	G
41	S60	395	U
41	S60	396	A
41	S60	398	A
41	S60	399	A
41	S60	402	C
41	S60	407	G
41	S60	408	A
41	S60	409	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	412	A
41	S60	414	U
41	S60	416	G
41	S60	422	A
41	S60	424	G
41	S60	425	G
41	S60	426	C
41	S60	431	G
41	S60	432	C
41	S60	437	A
41	S60	441	G
41	S60	444	G
41	S60	445	U
41	S60	446	A
41	S60	449	A
41	S60	450	C
41	S60	452	A
41	S60	453	G
41	S60	454	C
41	S60	461	A
41	S60	471	A
41	S60	473	G
41	S60	474	A
41	S60	476	U
41	S60	477	G
41	S60	478	C
41	S60	481	C
41	S60	482	G
41	S60	486	A
41	S60	487	A
41	S60	490	G
41	S60	491	G
41	S60	501	G
41	S60	506	A
41	S60	509	G
41	S60	510	U
41	S60	511	A
41	S60	512	C
41	S60	521	A
41	S60	527	G
41	S60	530	U
41	S60	535	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	536	G
41	S60	540	C
41	S60	541	G
41	S60	543	A
41	S60	544	U
41	S60	547	A
41	S60	550	G
41	S60	553	A
41	S60	554	A
41	S60	565	U
41	S60	566	A
41	S60	567	A
41	S60	568	G
41	S60	575	A
41	S60	578	A
41	S60	579	G
41	S60	590	U
41	S60	593	A
41	S60	598	C
41	S60	599	G
41	S60	600	A
41	S60	601	G
41	S60	602	A
41	S60	608	A
41	S60	609	A
41	S60	610	U
41	S60	616	G
41	S60	621	G
41	S60	622	C
41	S60	623	U
41	S60	624	U
41	S60	625	A
41	S60	630	U
41	S60	633	C
41	S60	635	G
41	S60	637	G
41	S60	644	G
41	S60	647	C
41	S60	661	A
41	S60	662	U
41	S60	665	G
41	S60	668	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	671	C
41	S60	673	A
41	S60	686	G
41	S60	687	A
41	S60	688	G
41	S60	690	A
41	S60	694	A
41	S60	700	A
41	S60	702	U
41	S60	705	A
41	S60	706	G
41	S60	707	A
41	S60	722	G
41	S60	724	A
41	S60	725	G
41	S60	727	A
41	S60	728	A
41	S60	730	C
41	S60	731	G
41	S60	733	U
41	S60	734	G
41	S60	738	A
41	S60	740	G
41	S60	749	G
41	S60	752	A
41	S60	753	U
41	S60	754	G
41	S60	755	A
41	S60	757	C
41	S60	771	A
41	S60	775	U
41	S60	776	A
41	S60	777	G
41	S60	780	G
41	S60	788	G
41	S60	789	G
41	S60	790	G
41	S60	791	A
41	S60	795	U
41	S60	806	G
41	S60	810	U
41	S60	817	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	818	A
41	S60	820	G
41	S60	821	G
41	S60	823	A
41	S60	824	A
41	S60	831	G
41	S60	836	A
41	S60	839	C
41	S60	840	C
41	S60	841	A
41	S60	845	G
41	S60	848	G
41	S60	866	U
41	S60	868	U
41	S60	871	C
41	S60	872	U
41	S60	874	A
41	S60	875	A
41	S60	877	G
41	S60	878	C
41	S60	880	G
41	S60	881	G
41	S60	883	C
41	S60	884	A
41	S60	890	C
41	S60	899	A
41	S60	904	C
41	S60	908	U
41	S60	909	G
41	S60	915	A
41	S60	916	G
41	S60	917	U
41	S60	918	A
41	S60	923	A
41	S60	924	U
41	S60	925	A
41	S60	926	G
41	S60	929	C
41	S60	930	A
41	S60	932	A
41	S60	936	U
41	S60	940	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	941	C
41	S60	942	A
41	S60	952	A
41	S60	953	C
41	S60	955	A
41	S60	957	G
41	S60	958	A
41	S60	959	G
41	S60	961	G
41	S60	968	C
41	S60	970	U
41	S60	971	U
41	S60	972	U
41	S60	974	G
41	S60	978	A
41	S60	980	G
41	S60	981	U
41	S60	987	A
41	S60	991	A
41	S60	1003	A
41	S60	1006	A
41	S60	1007	U
41	S60	1008	A
41	S60	1011	A
41	S60	1012	A
41	S60	1013	A
41	S60	1014	G
41	S60	1017	A
41	S60	1018	U
41	S60	1019	C
41	S60	1021	A
41	S60	1023	A
41	S60	1024	G
41	S60	1028	U
41	S60	1029	U
41	S60	1033	A
41	S60	1039	G
41	S60	1041	A
41	S60	1044	G
41	S60	1045	A
41	S60	1046	A
41	S60	1047	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	1052	A
41	S60	1053	A
41	S60	1054	G
41	S60	1056	A
41	S60	1057	C
41	S60	1058	A
41	S60	1059	G
41	S60	1060	G
41	S60	1062	C
41	S60	1063	A
41	S60	1064	G
41	S60	1066	G
41	S60	1075	A
41	S60	1076	G
41	S60	1077	A
41	S60	1078	U
41	S60	1088	U
41	S60	1089	G
41	S60	1090	C
41	S60	1092	C
41	S60	1094	C
41	S60	1099	U
41	S60	1100	A
41	S60	1102	A
41	S60	1103	G
41	S60	1104	U
41	S60	1105	G
41	S60	1106	G
41	S60	1111	A
41	S60	1112	G
41	S60	1116	A
41	S60	1117	A
41	S60	1118	A
41	S60	1119	C
41	S60	1120	A
41	S60	1121	A
41	S60	1122	A
41	S60	1123	U
41	S60	1124	A
41	S60	1125	G
41	S60	1126	A
41	S60	1127	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	1128	G
41	S60	1129	U
41	S60	1130	A
41	S60	1135	U
41	S60	1136	G
41	S60	1137	A
41	S60	1139	C
41	S60	1141	A
41	S60	1142	G
41	S60	1143	A
41	S60	1144	G
41	S60	1146	G
41	S60	1152	G
41	S60	1154	A
41	S60	1158	U
41	S60	1159	A
41	S60	1160	A
41	S60	1161	U
41	S60	1162	G
41	S60	1170	G
41	S60	1171	A
41	S60	1175	A
41	S60	1176	G
41	S60	1177	G
41	S60	1179	A
41	S60	1182	G
41	S60	1185	A
41	S60	1191	C
41	S60	1192	G
41	S60	1194	U
41	S60	1195	A
41	S60	1196	U
41	S60	1202	U
41	S60	1203	A
41	S60	1204	A
41	S60	1205	G
41	S60	1209	C
41	S60	1210	G
41	S60	1211	A
41	S60	1214	A
41	S60	1219	G
41	S60	1223	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	1225	G
41	S60	1227	U
41	S60	1230	U
41	S60	1237	C
41	S60	1238	A
41	S60	1239	C
41	S60	1240	C
41	S60	1241	G
41	S60	1243	C
41	S60	1246	U
41	S60	1249	U
41	S60	1250	U
41	S60	1251	A
41	S60	1260	G
41	S60	1262	A
41	S60	1263	A
41	S60	1264	C
41	S60	1266	A
41	S60	1267	G
41	S60	1270	G
41	S60	1274	A
41	S60	1275	C
41	S60	1276	A
41	S60	1280	G
41	S60	1282	A
41	S60	1283	A
41	S60	1284	G
41	S60	1287	A
41	S60	1294	G
41	S60	1295	C
41	S60	1296	A
41	S60	1297	G
41	S60	1301	U
41	S60	1302	C
41	S60	1307	U
41	S60	1310	G
41	S60	1314	C
41	S60	1315	A
41	S60	1316	A
41	S60	1317	G
41	S60	1320	G
41	S60	1322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	1326	A
41	S60	1327	G
41	S60	1328	G
41	S60	1329	C
41	S60	1331	G
41	S60	1340	G
41	S60	1341	A
41	S60	1342	A
41	S60	1343	C
41	S60	1348	A
41	S60	1352	G
41	S60	1353	G
41	S60	1354	A
41	S60	1355	U
41	S60	1356	C
41	S60	1357	A

All (171) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L50	2	U
1	L50	3	A
1	L50	21	U
1	L50	22	U
1	L50	73	A
1	L50	75	C
1	L50	135	A
1	L50	211	U
1	L50	214	A
1	L50	225	G
1	L50	236	A
1	L50	265	A
1	L50	276	U
1	L50	308	A
1	L50	330	G
1	L50	351	G
1	L50	363	U
1	L50	396	G
1	L50	424	G
1	L50	463	A
1	L50	466	C
1	L50	523	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	535	A
1	L50	550	G
1	L50	563	U
1	L50	567	A
1	L50	600	G
1	L50	657	A
1	L50	659	G
1	L50	667	G
1	L50	710	A
1	L50	712	C
1	L50	732	G
1	L50	741	G
1	L50	778	A
1	L50	782	G
1	L50	853	A
1	L50	996	A
1	L50	1000	G
1	L50	1008	U
1	L50	1017	A
1	L50	1018	U
1	L50	1032	A
1	L50	1061	G
1	L50	1089	U
1	L50	1134	A
1	L50	1148	A
1	L50	1172	A
1	L50	1182	A
1	L50	1256	U
1	L50	1277	G
1	L50	1384	U
1	L50	1394	U
1	L50	1395	U
1	L50	1449	A
1	L50	1454	U
1	L50	1474	G
1	L50	1485	G
1	L50	1491	U
1	L50	1564	U
1	L50	1596	A
1	L50	1611	A
1	L50	1644	U
1	L50	1697	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L50	1709	G
1	L50	1717	A
1	L50	1743	G
1	L50	1749	A
1	L50	1798	U
1	L50	1800	U
1	L50	1808	A
1	L50	1809	A
1	L50	1835	G
1	L50	1838	G
1	L50	1931	C
1	L50	1942	U
1	L50	1945	C
1	L50	1959	A
1	L50	1966	A
1	L50	1967	A
1	L50	2015	C
1	L50	2036	A
1	L50	2051	C
1	L50	2060	A
1	L50	2075	A
1	L50	2212	G
1	L50	2240	A
1	L50	2254	U
1	L50	2255	A
1	L50	2347	U
1	L50	2351	U
1	L50	2363	A
1	L50	2419	G
1	L50	2420	C
1	L50	2447	A
1	L50	2452	A
1	L50	2476	G
1	L50	2481	U
1	L50	2519	G
1	L50	2532	A
1	L50	2596	G
1	L50	2597	G
2	L70	32	A
2	L70	41	G
2	L70	62	A
2	L70	109	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	71	U
41	S60	76	A
41	S60	118	G
41	S60	127	A
41	S60	180	G
41	S60	186	A
41	S60	190	A
41	S60	191	C
41	S60	218	A
41	S60	225	A
41	S60	226	G
41	S60	256	G
41	S60	262	U
41	S60	283	U
41	S60	303	G
41	S60	328	A
41	S60	339	A
41	S60	355	C
41	S60	372	A
41	S60	383	A
41	S60	407	G
41	S60	408	A
41	S60	424	G
41	S60	425	G
41	S60	445	U
41	S60	473	G
41	S60	509	G
41	S60	511	A
41	S60	553	A
41	S60	565	U
41	S60	598	C
41	S60	661	A
41	S60	724	A
41	S60	753	U
41	S60	776	A
41	S60	788	G
41	S60	819	A
41	S60	877	G
41	S60	914	U
41	S60	917	U
41	S60	923	A
41	S60	924	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S60	954	G
41	S60	970	U
41	S60	980	G
41	S60	1007	U
41	S60	1018	U
41	S60	1021	A
41	S60	1045	A
41	S60	1057	C
41	S60	1077	A
41	S60	1088	U
41	S60	1089	G
41	S60	1103	G
41	S60	1105	G
41	S60	1125	G
41	S60	1135	U
41	S60	1141	A
41	S60	1143	A
41	S60	1176	G
41	S60	1195	A
41	S60	1314	C
41	S60	1321	U
41	S60	1328	G
41	S60	1356	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 368 ligands modelled in this entry, 368 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.

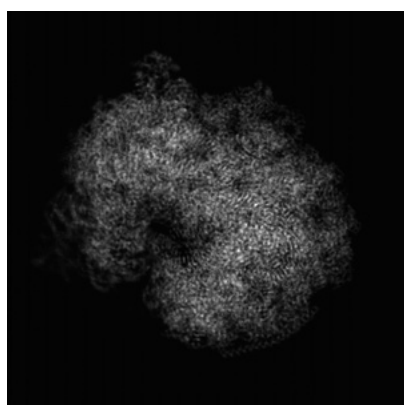
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13892. These allow visual inspection of the internal detail of the map and identification of artifacts.

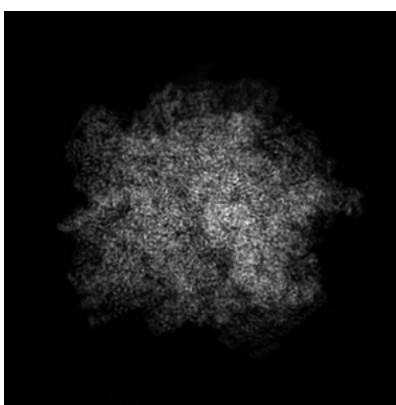
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

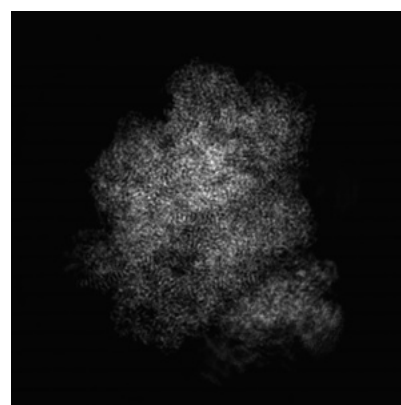
6.1.1 Primary map



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: 160



Y Index: 160



Z Index: 160

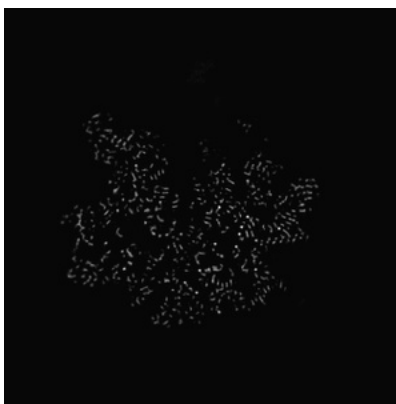
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 164



Y Index: 170

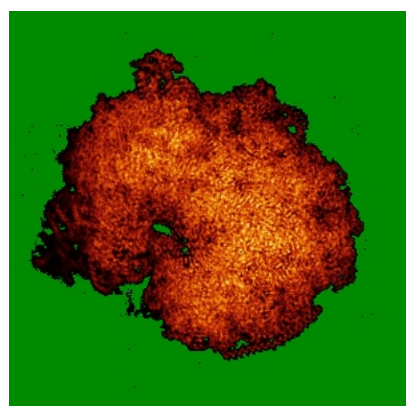


Z Index: 185

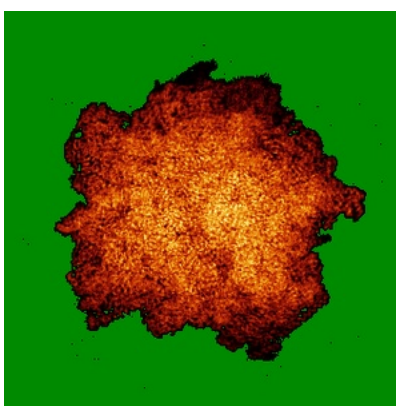
The images above show the largest variance slices of the map in three orthogonal directions.

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

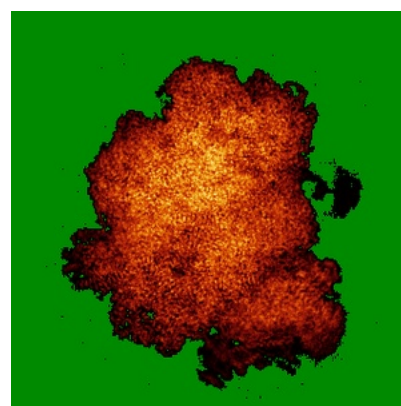
6.4.1 Primary map



X



Y

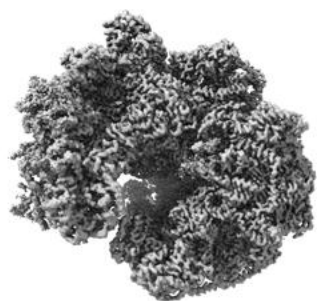


Z

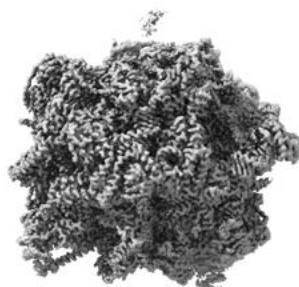
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.05356. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

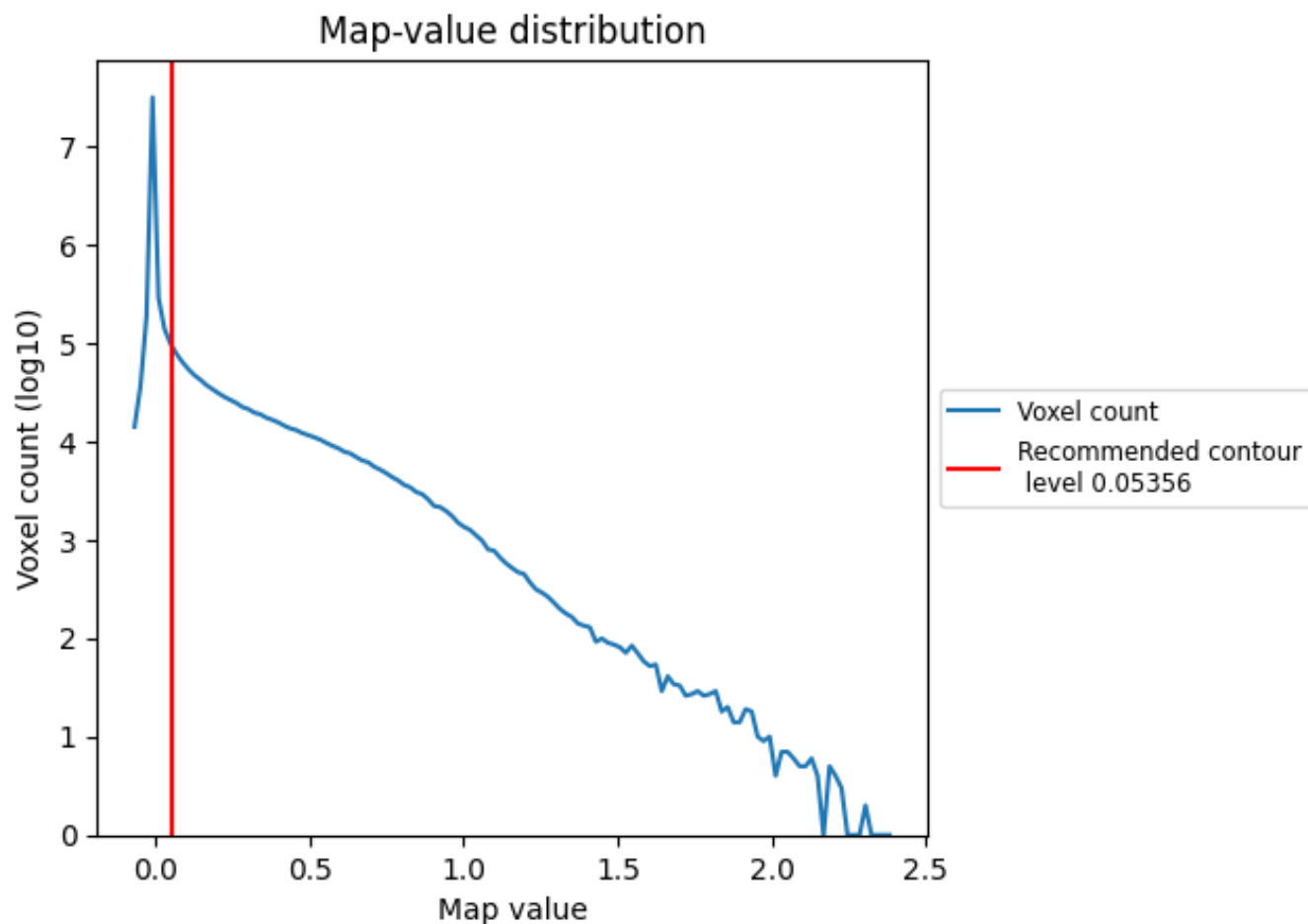
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

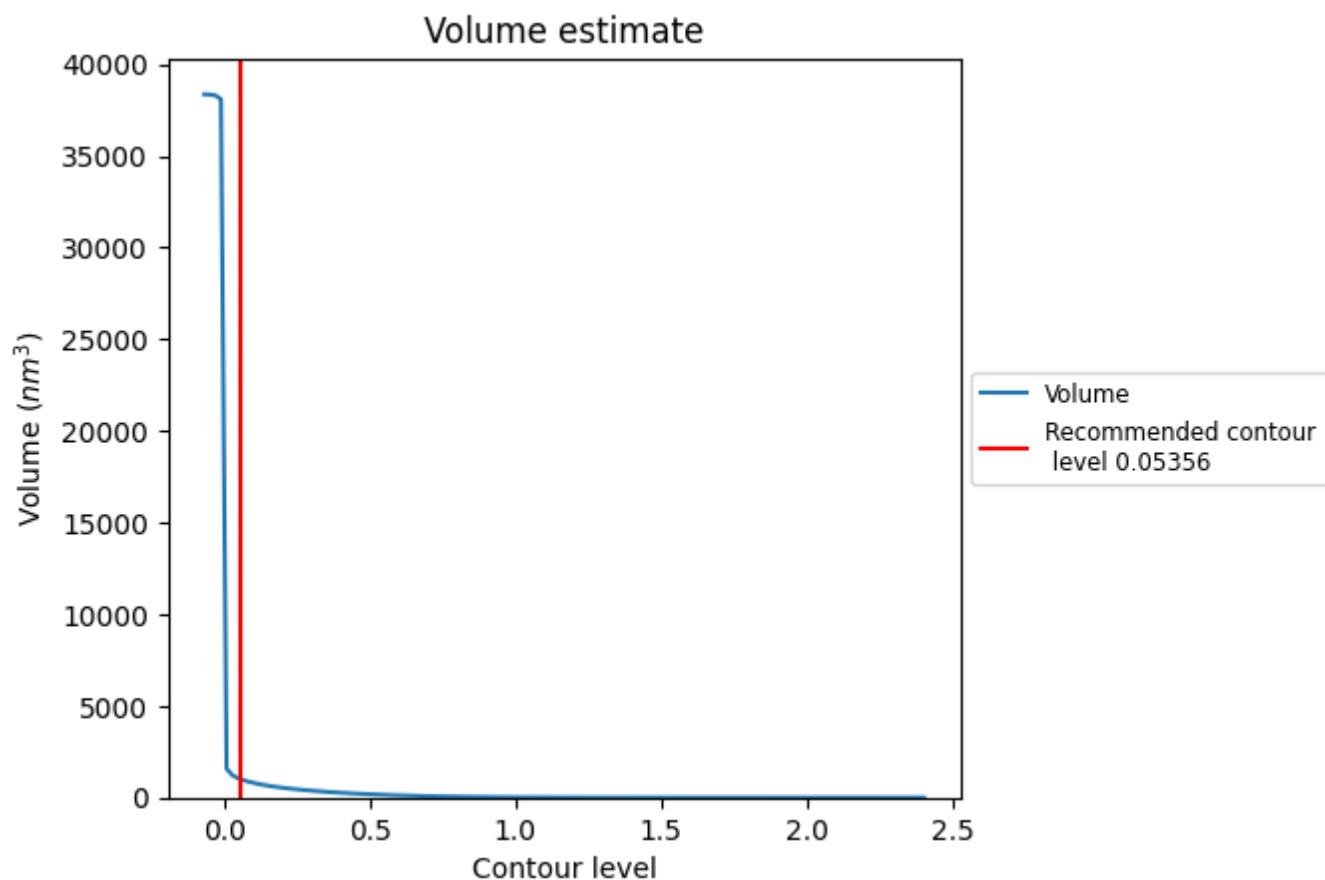
This section contains the results of statistical analysis of the map.

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.

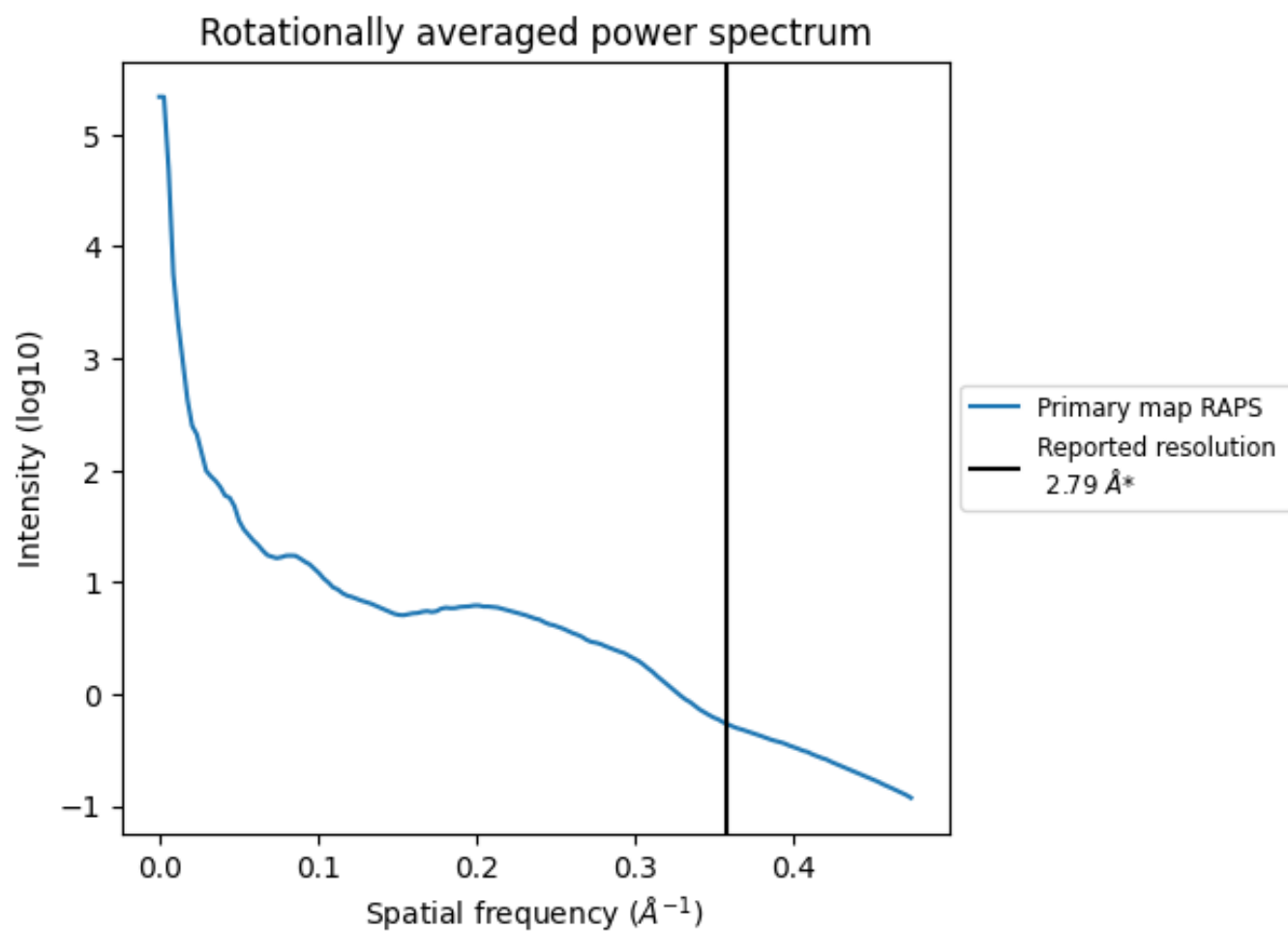
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1025 nm³; this corresponds to an approximate mass of 926 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 ⓘ

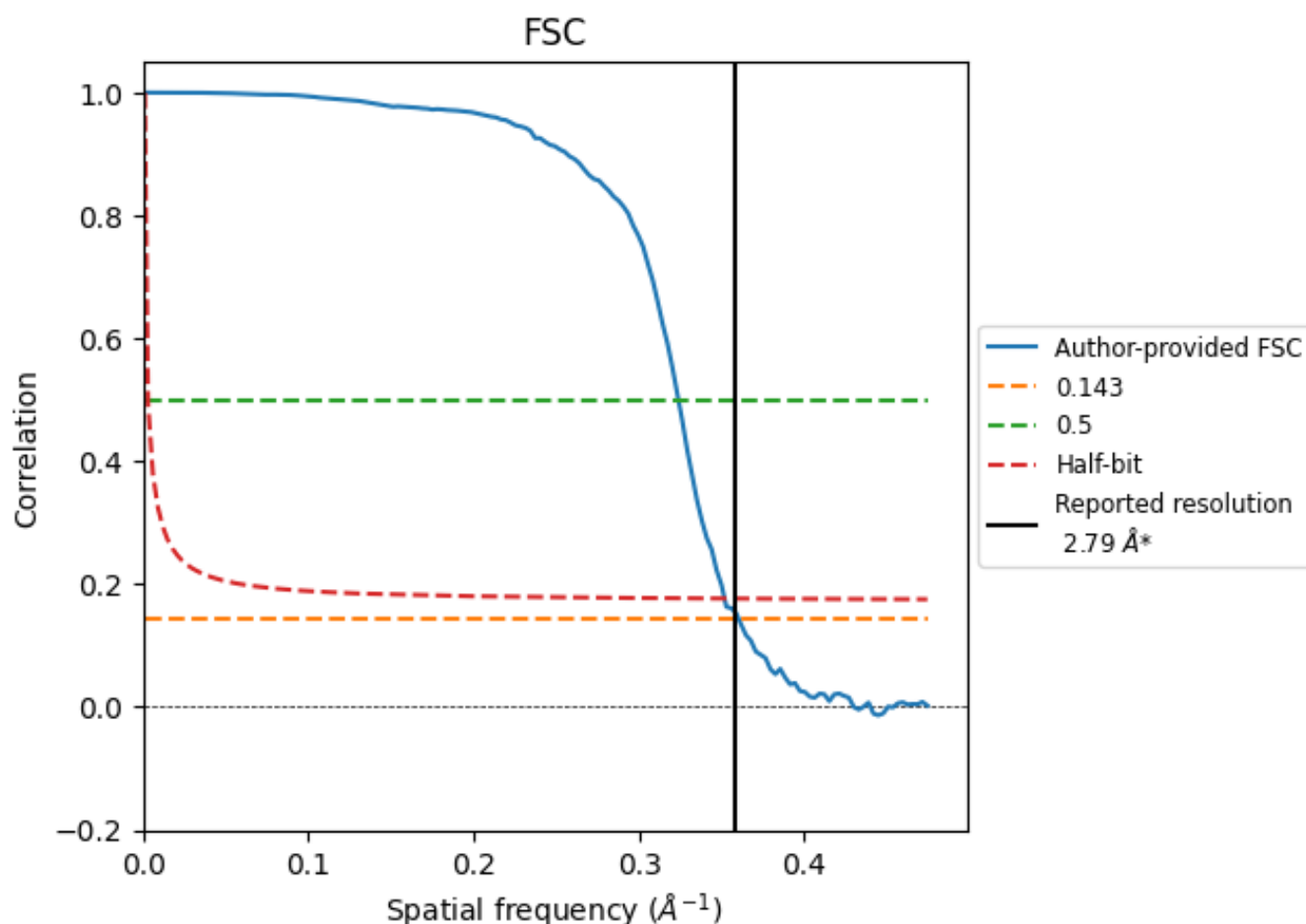


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

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 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

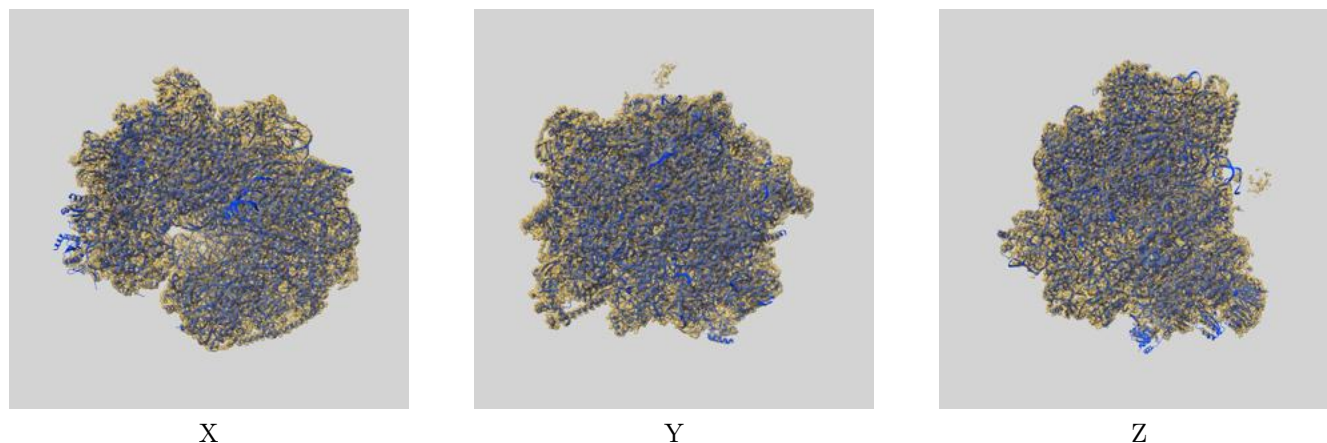
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.78	3.09	2.84
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

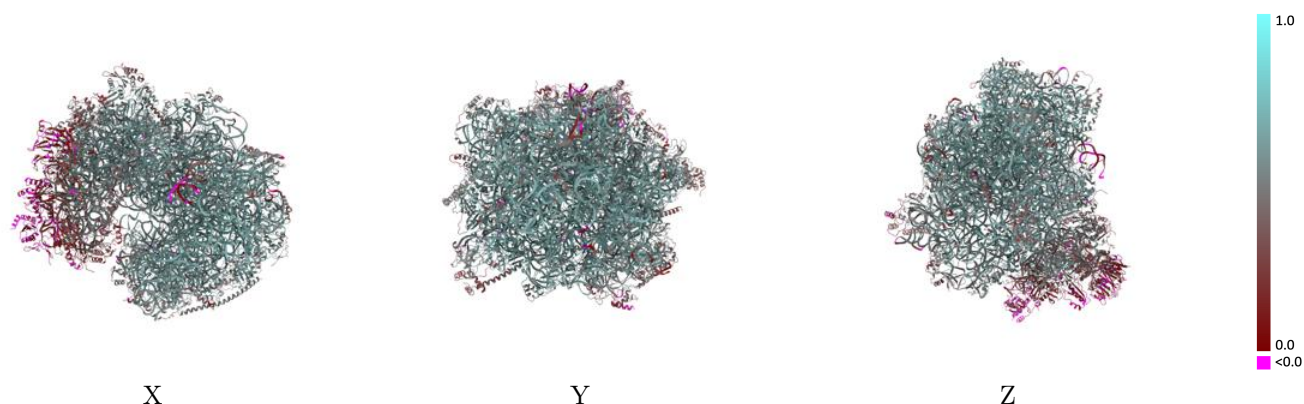
This section contains information regarding the fit between EMDB map EMD-13892 and PDB model 7QCA. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



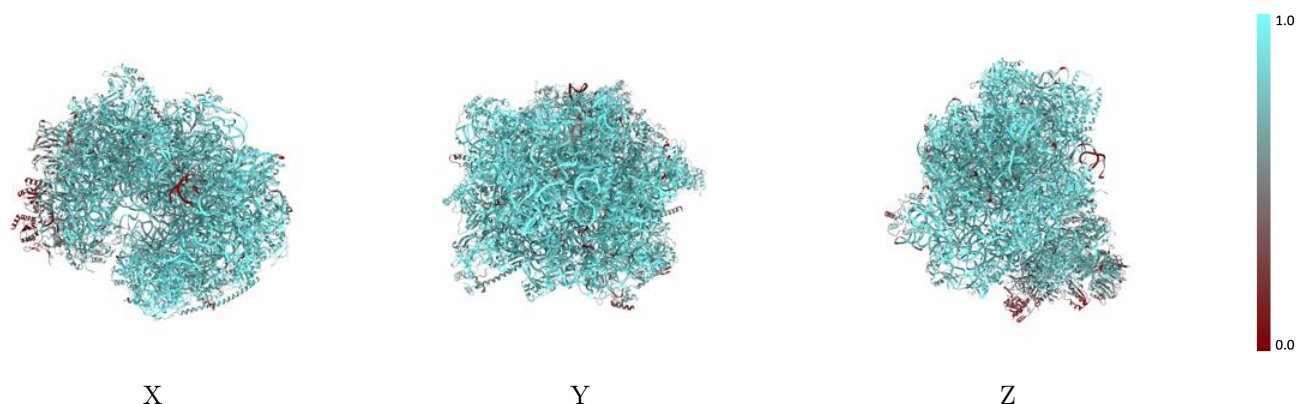
The images above show the 3D surface view of the map at the recommended contour level 0.05356 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



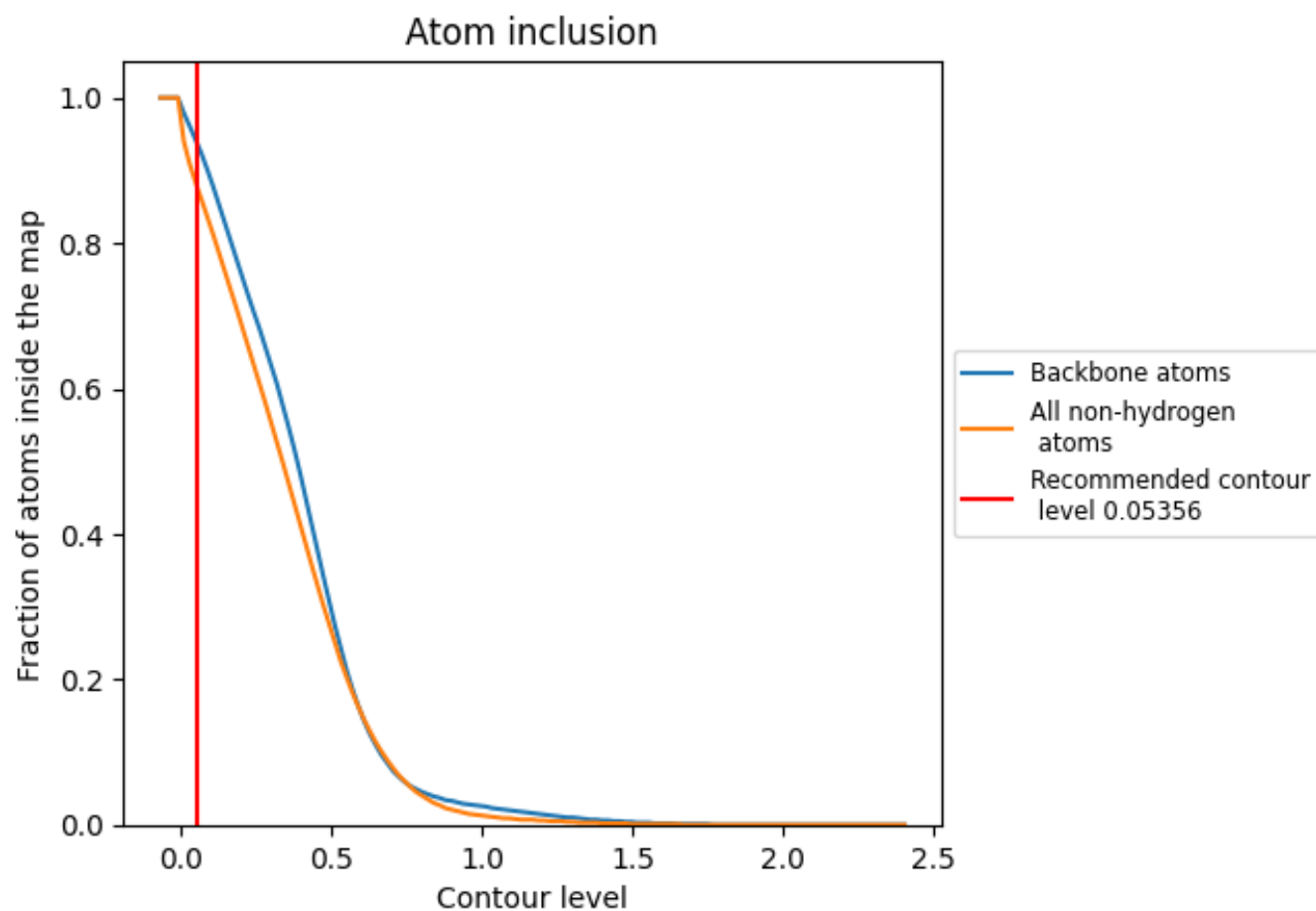
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05356).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.05356) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5380
L50	 0.9570	 0.6180
L70	 0.9820	 0.6100
LA0	 0.9150	 0.6140
LAA	 0.9390	 0.6260
LB0	 0.9020	 0.5950
LC0	 0.8950	 0.5850
LCC	 0.8850	 0.5500
LD0	 0.8320	 0.5000
LDD	 0.8410	 0.5610
LE0	 0.6950	 0.4160
LEE	 0.8720	 0.5690
LF0	 0.8880	 0.5650
LFF	 0.8920	 0.5860
LG0	 0.8530	 0.5190
LGG	 0.8770	 0.5700
LH0	 0.8930	 0.5730
LHH	 0.8600	 0.5520
LI0	 0.8710	 0.5640
LII	 0.8250	 0.5130
LJ0	 0.8050	 0.4680
LJJ	 0.9200	 0.6250
LL0	 0.8890	 0.5740
LLL	 0.9220	 0.6080
LM0	 0.7640	 0.4460
LMM	 0.8680	 0.5660
LN0	 0.9730	 0.6600
LO0	 0.8700	 0.5570
LOO	 0.8520	 0.5540
LP0	 0.8920	 0.5830
LPP	 0.9140	 0.6080
LQ0	 0.8870	 0.5790
LR0	 0.8420	 0.5420
LS0	 0.8810	 0.5620
LT0	 0.8270	 0.5340



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LU0	 0.8100	 0.4960
LV0	 0.9070	 0.6030
LW0	 0.5830	 0.4010
LX0	 0.8620	 0.5650
LY0	 0.8200	 0.5360
LZ0	 0.8150	 0.4790
S60	 0.9330	 0.5490
SA0	 0.7810	 0.4370
SAA	 0.8700	 0.5430
SB0	 0.8290	 0.5060
SBB	 0.8770	 0.5250
SC0	 0.8400	 0.5030
SCC	 0.6750	 0.4050
SD0	 0.5730	 0.2460
SDD	 0.6060	 0.2920
SE0	 0.8340	 0.5000
SEE	 0.6120	 0.4200
SF0	 0.7490	 0.4160
SFF	 0.1090	 0.0310
SG0	 0.7030	 0.4000
SGG	 0.5550	 0.1570
SH0	 0.8180	 0.4420
SI0	 0.8880	 0.5450
SJ0	 0.8680	 0.5180
SK0	 0.4450	 0.1240
SL0	 0.8350	 0.5200
SM0	 0.1140	 0.0140
SN0	 0.9130	 0.5590
SO0	 0.8820	 0.5480
SP0	 0.5180	 0.1740
SQ0	 0.7360	 0.3400
SR0	 0.6850	 0.2960
SS0	 0.6410	 0.2850
ST0	 0.6950	 0.2540
SU0	 0.4050	 0.1760
SV0	 0.8430	 0.4920
SW0	 0.9330	 0.5830
SX0	 0.8450	 0.5300
SY0	 0.6700	 0.3780
SZ0	 0.6590	 0.2470