



## Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 03:39 pm BST

PDB ID : 9RG7 / pdb\_00009rg7  
EMDB ID : EMD-53944  
Title : In vitro reconstituted NAA40-NAC bound 80S  
Authors : Guan, D.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2025-06-05  
Resolution : 2.72 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

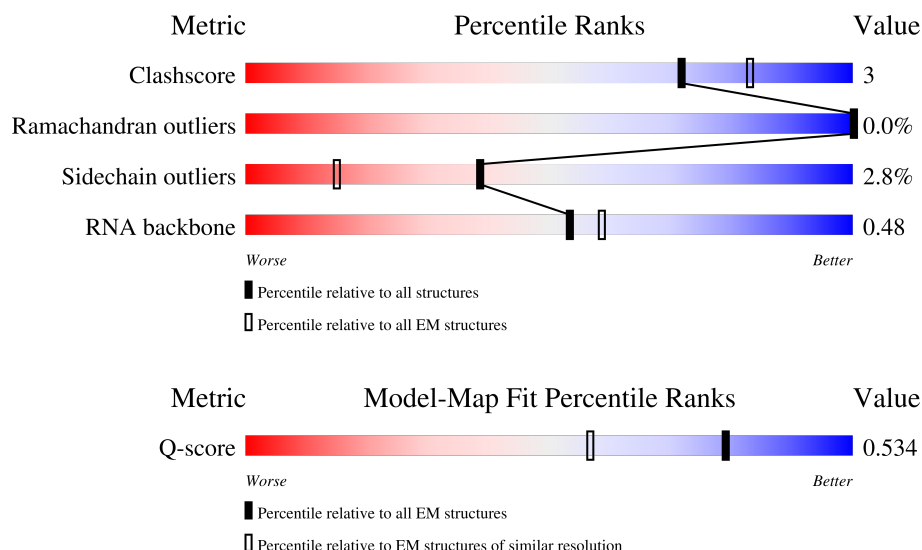
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 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	10355 ( 2.22 - 3.22 )

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

Mol	Chain	Length	Quality of chain
1	LA	257	
2	NA	215	
3	SA	295	

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Mol	Chain	Length	Quality of chain
4	LB	403	
5	NB	206	
6	SB	264	
7	L5	5070	
8	L7	121	
9	L8	157	
10	LC	427	
11	LD	297	
12	LE	288	
13	LF	248	
14	LG	266	
15	LH	192	
16	LI	214	
17	LJ	178	
18	LL	211	
19	LM	215	
20	LN	204	
21	LO	203	
22	LP	184	
23	LQ	188	
24	LR	196	
25	LS	176	
26	LT	160	
27	LU	128	
28	LV	140	







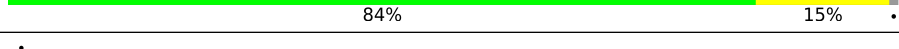
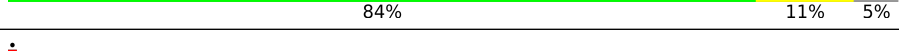
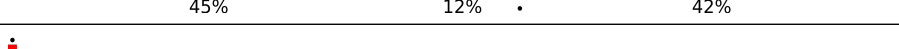

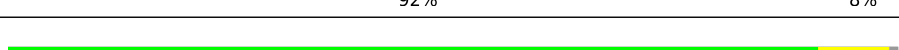
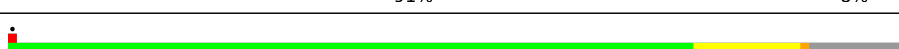
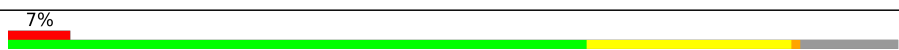

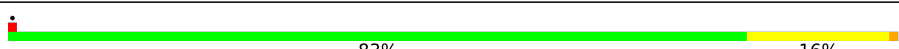





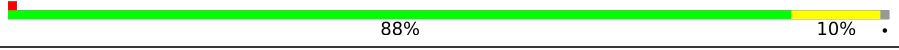
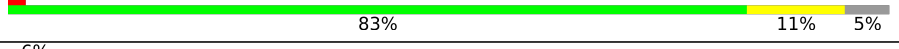
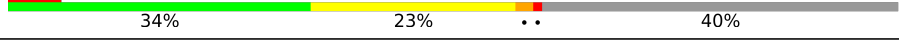


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Mol	Chain	Length	Quality of chain
29	LW	157	
30	LX	156	
31	LY	145	
32	LZ	136	
33	La	148	
34	Lb	159	
35	Lc	115	
36	Ld	125	
37	Le	135	
38	Lf	110	
39	Lg	117	
40	Lh	123	
41	Li	105	
42	Lj	97	
43	Lk	70	
44	Ll	51	
45	Lm	128	
46	Ln	25	
47	Lo	106	
48	Lp	92	
49	Lr	137	
50	Ls	317	
51	Lt	165	
52	N4	237	
53	S2	1869	




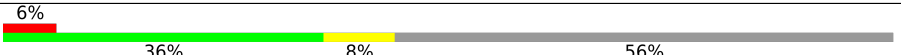

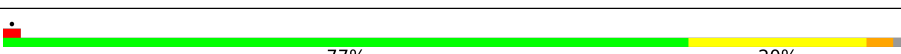
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Mol	Chain	Length	Quality of chain
54	SC	293	
55	SD	243	
56	SE	263	
57	SF	204	
58	SG	249	
59	SH	194	
60	SI	208	
61	SJ	194	
62	SK	165	
63	SL	158	
64	SM	132	
65	SN	151	
66	SO	151	
67	SP	145	
68	SQ	146	
69	SR	135	
70	SS	152	
71	ST	145	
72	SU	119	
73	SV	83	
74	SW	130	
75	SX	143	
76	SY	133	
77	SZ	125	
78	Sa	115	

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Mol	Chain	Length	Quality of chain
79	Sb	84	 87% 12% .
80	Sc	69	 6% 75% 16% . 7%
81	Sd	56	 88% 9% . .
82	Se	133	 6% 36% 8% 56%
83	Sf	156	 15% 38% 5% 57%
84	Sg	317	 77% 20% . .

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 219040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	NA	108	Total	C	N	O	S	0	0
			841	524	153	160	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 4 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 5 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	NB	106	Total	C	N	O	S	0	0
			821	514	153	151	3		

- Molecule 6 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SB	221	Total	C	N	O	S	0	0
			1791	1135	323	319	14		

- Molecule 7 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L5	3669	Total	C	N	O	P	0	0
			78658	35027	14397	25566	3668		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 9 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 10 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 12 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	221	Total	C	N	O	S	0	0
			1774	1142	336	292	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 14 is a protein called 60S ribosomal protein L7a.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 15 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 16 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

- Molecule 17 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 18 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	207	Total	C	N	O	S	0	0
			1673	1046	346	277	4		

- Molecule 19 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 20 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 21 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 22 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 23 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 26 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LU	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 30 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 31 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 33 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 34 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lb	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

- Molecule 35 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 36 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 37 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 38 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 39 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 40 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 41 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 42 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 43 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 44 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 45 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 46 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 47 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 48 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 49 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 50 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 51 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 52 is a protein called N-alpha-acetyltransferase 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	N4	223	Total	C	N	O	S	0	0
			1809	1136	317	341	15		

- Molecule 53 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S2	1719	Total	C	N	O	P	0	0
			36456	16264	6516	11958	1718		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

- Molecule 54 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 55 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 56 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 57 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 58 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 59 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 60 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 61 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 62 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 63 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 64 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SM	122	Total	C	N	O		0	0
			604	359	122	123			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 65 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 66 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 67 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SP	129	Total	C	N	O	S	0	0
			1061	672	202	180	7		

- Molecule 68 is a protein called 40S ribosomal protein S16.



Mol	Chain	Residues	Atoms					AltConf	Trace
68	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 69 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 70 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 71 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 72 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 73 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 74 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SY	126	Total	C	N	O	S	0	0
			1027	648	201	173	5		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 79 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 80 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 81 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 83 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 84 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).


Mol	Chain	Residues	Atoms		AltConf
85	LA	1	Total	Mg	0
			1	1	
85	L5	210	Total	Mg	0
			210	210	
85	L7	3	Total	Mg	0
			3	3	
85	L8	6	Total	Mg	0
			6	6	
85	LI	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	2	Total	Mg	0
			2	2	
85	Lg	1	Total	Mg	0
			1	1	
85	S2	30	Total	Mg	0
			30	30	
85	SG	1	Total	Mg	0
			1	1	

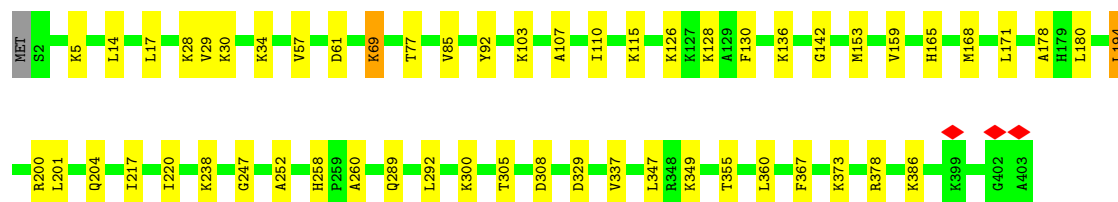
- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	Lg	1	Total 1	Zn 1	0
86	Lj	1	Total 1	Zn 1	0
86	Lm	1	Total 1	Zn 1	0
86	Lo	1	Total 1	Zn 1	0
86	Lp	1	Total 1	Zn 1	0
86	Sa	1	Total 1	Zn 1	0
86	Sd	1	Total 1	Zn 1	0
86	Sf	1	Total 1	Zn 1	0



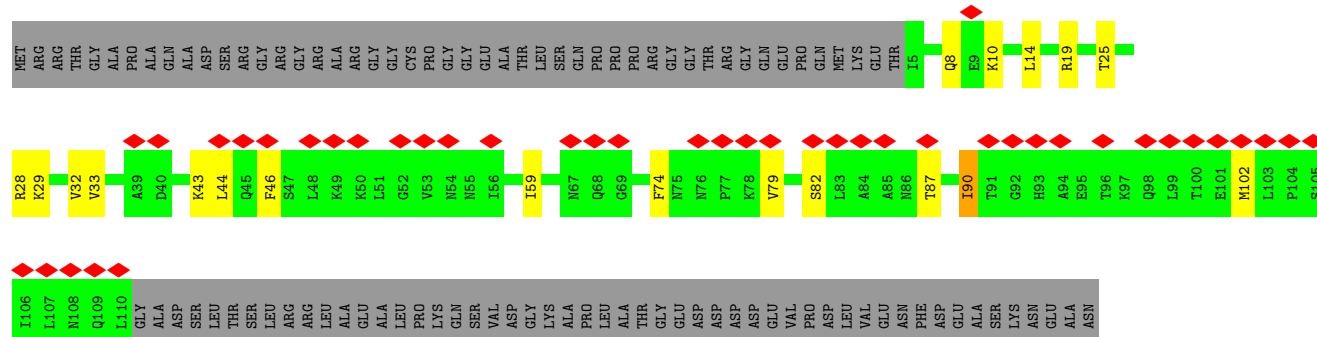
- Molecule 4: 60S ribosomal protein L3

Chain LB:  86% 13%




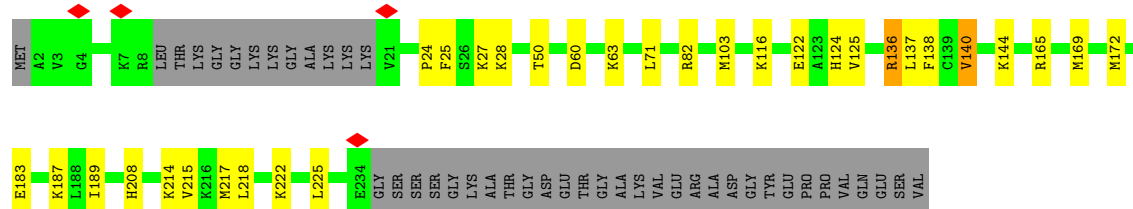
- Molecule 5: Transcription factor BTF3

Chain NB:  21% 42% 9% 49%



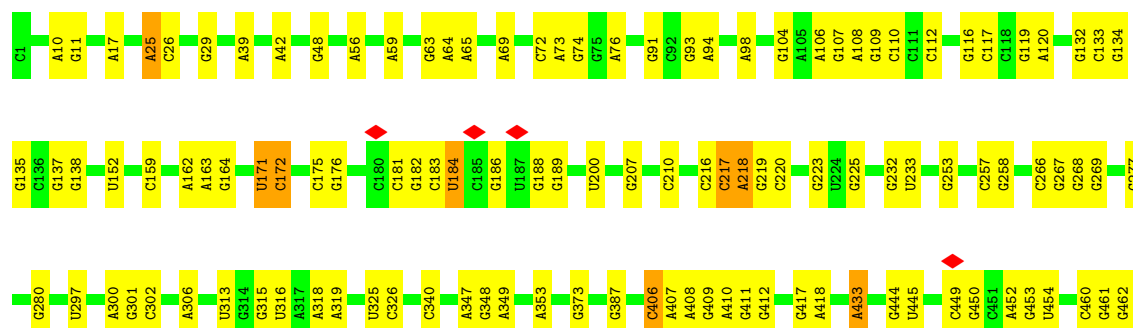
- Molecule 6: 40S ribosomal protein S3a

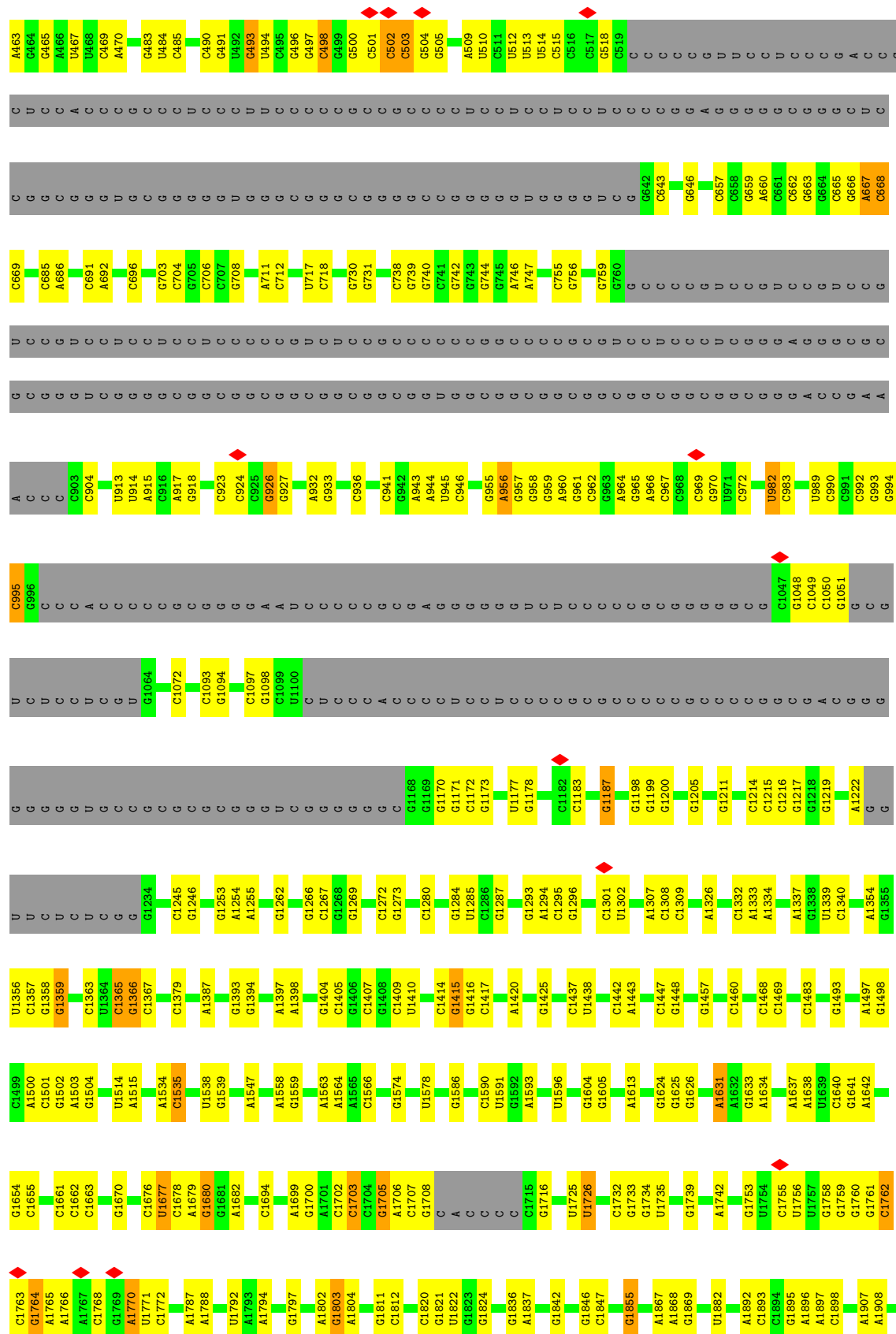
Chain SB:  72% 11% 16%



- Molecule 7: 28S rRNA

Chain L5:  51% 20% 28%










C4906	A5014	G4617	G4785	G	G4222	G4109	A	A3876	C3708	G
G4907	G5015	G4618	G4769	G	G4225	G4110	G	A3877	U3709	C
A5016	G	A4626	U4770	G	G4226	U4111	G	C3877	G3710	G
G4910	A	U4627	C4771	A	G4228	C4114	U	G3878	A3711	C
A4911	G	C4505	C4506	G	U4229	G4115	G	G3879	A3712	U
G4912	C	A4635	A4507	G	A4233	C4116	G	G3880	U3713	C
G4913	C	U4636	C4508	G	A4233	U4117	G	G3881	G3714	G
C4914	C	G4637	A4512	G	G4238	U4118	A	G3885		
	C	G4652	A4513	G	A4239	C4119	G	G3886	A3717	C
C4924	G		C4519	C	G4240	G4122	C	C3887	A3719	G
U4925	U	A4656	U4657	C	G4241	A4127	C	U3892	G3720	G
	C	U4657	C4670	G	U4242	A4139	C	G3897	A3727	C
C4928	U	C4671	A4672	C	A4251	C4140	C	U3898	A3719	G
C4929	C	G4679	G4679	C	G4254	G4141	G	G3900	A3732	C
A4934	C	U4672	C4672	C	A4255	C4142	G	A3901	A3733	G
C4935	C	G4679	U4530	C	G4258	C4143	U	G3906	U3734	C
G4936	C	G4679	U4531	C	C4259	C4144	C	A3905	G3735	G
	C	A4684	C4537	C	U4260	C4145	A	A3906	G3736	G
C4940	C	U4685	C4537	G	C4261	G4146	A	G3907	U3616	C
G4941	G	G4686	U4538	G	C4261	G4147	C	A3908	A3737	C
A4943	C	A4687	C4545	C	A4388	C4148	C	C3909	G3617	G
C4944	C	A4691	A4548	C	A4389	C4149	C	G3910	C3618	C
	C	U4699	C4549	C	G4391	G4150	C	C3911	G3619	U
G4949	C	A4700	C4560	C	A4268	C4159	C		G3750	U
U4950	C	A4708	C4567	C	A4273	C4160	C	U3915	G3753	C
C4951	C	U4709	A4568	C	A4274	G4161	G	G3916	A3630	C
	C	G4719	C4573	C	G4275	C4162	U	A3917	A3635	C
G4954	C	C4720	C4575	C	G4277	U4163	C	A3760	A3635	C
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G4960	C	G4734	U4579	C	A4279	G4169	C	A3774	A3648	C
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A4968	C	G4737	A4584	C	A4281	C4171	C	G3776	U3645	G
	C	C4741	U4585	C	A4282	G4177	C	G3777	A3646	G
U4973	C	G4742	C4590	C	G4283	C4183	C	A3784	A3647	C
C4974	C	A4743	U4591	C	G4291	G4184	C	A3785	A3648	C
G4975	C	G4744	C4592	C	C4294	C4188	C	U3786	A3652	C
U4976	C	G4745	U4593	C	U4302	U4189	C	G3811	A3653	G
A4979	C	G4750	C4595	C	G4305	G4190	C	A3948	A3656	G
	C	G4754	U4595	C	G4309	G4191	C	A3949	U3657	U
U4985	C	C4757	C4600	C	C4314	G4196	C	U3950	U3814	U
U4988	C	U4757	U4601	C	C4319	G4201	C	G3951		C
U4989	C	G4758	A4602	C	G4320	U4202	C	A3954	A3662	C
C4990	C	G4759	A4611	C	G4321	A4203	C	U3818	A3663	G
U4991	C	G4760	C4612	C	G4322	C4103	C	G3819	C3664	G
G4992	C	G4761		C	G4329	A4105	C	G3955	G3665	C
G4993	C	A4762		C	G4330	G4106	C	U3838	G3672	C
	C			C		U4107	C	G3839	G3673	C
U5006	C			C		C4109	C	U3840	G3674	C
A5007	C			C		C4109	C			
C5008	C			C		C4103	C	A3861	G3674	G
G5009	C			C		G4104	C	A3862		C
	C			C		A4105	C	G3884	G3685	C
C5013	C			C		G4106	C	A3867		U
	C			C		G4107	C	G3868	U3707	C
	C			C		G4108	C			C

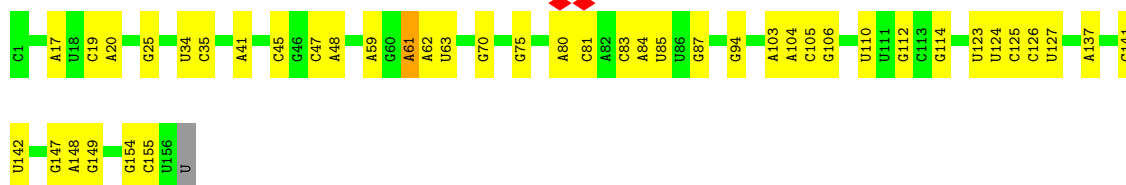
- Molecule 8: 5S rRNA

Chain L7:  84% 14% ..




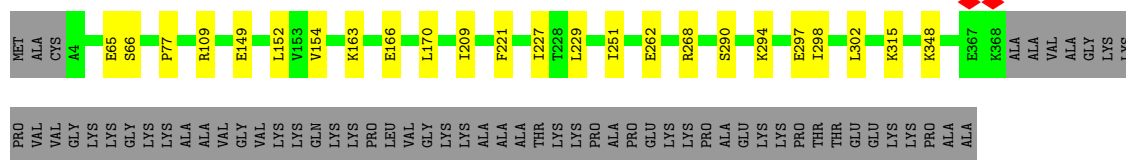
- Molecule 9: 5.8S rRNA

Chain L8:  72% 27% ..




- Molecule 10: 60S ribosomal protein L4

Chain LC:  80% 6% 15%



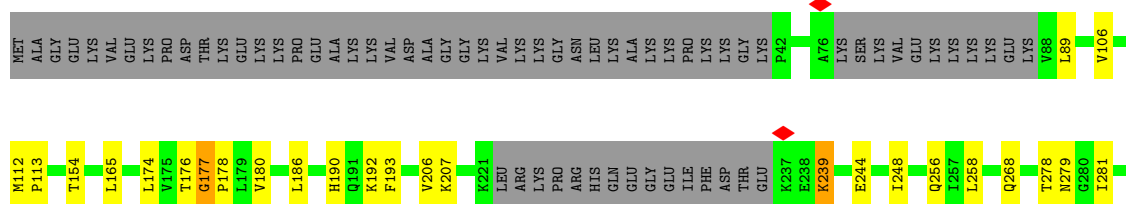
- Molecule 11: 60S ribosomal protein L5

Chain LD:  86% 12% .




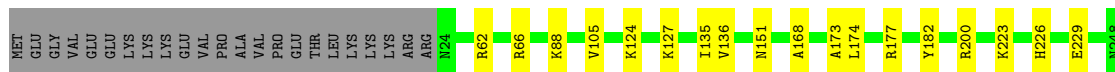
- Molecule 12: Large ribosomal subunit protein eL6

Chain LE:  68% 8% 23%



F288


- Molecule 13: Large ribosomal subunit protein uL30

Chain LF:  83% 7% 9%


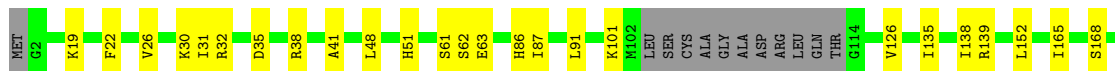
- Molecule 14: 60S ribosomal protein L7a

Chain LG:  82% 8% 9%


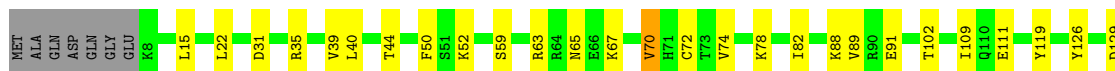
- Molecule 15: 60S ribosomal protein L9

Chain LH:  83% 16% .

- Molecule 16: 60S ribosomal protein L10

Chain LI:  81% 13% 6%

- Molecule 17: 60S ribosomal protein L11

Chain LJ:  78% 18% . .



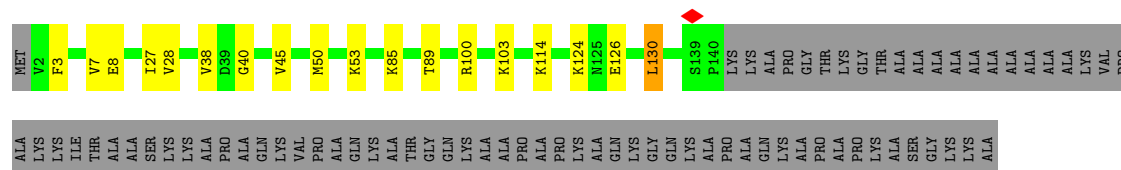
- Molecule 18: Large ribosomal subunit protein eL13

Chain LL: 91% 8%



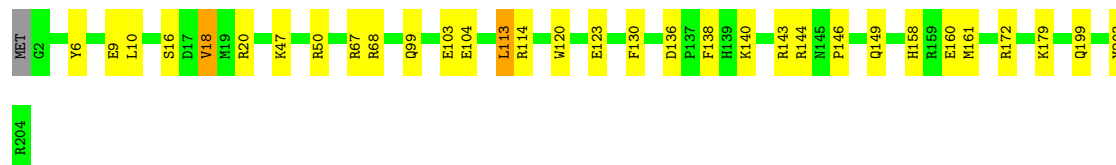
- Molecule 19: 60S ribosomal protein L14

Chain LM: 56% 8% 35%



- Molecule 20: 60S ribosomal protein L15

Chain LN: 84% 15%



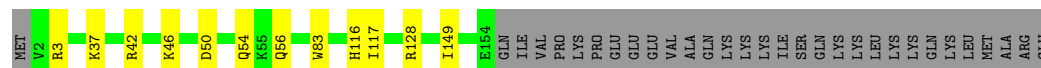
- Molecule 21: 60S ribosomal protein L13a

Chain LO: 93% 5%



- Molecule 22: 60S ribosomal protein L17

Chain LP: 77% 7% 17%

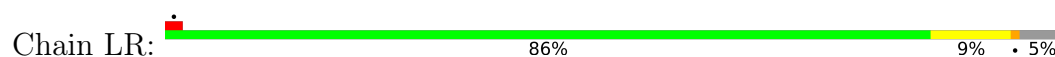


- Molecule 23: 60S ribosomal protein L18

Chain LQ: 95%



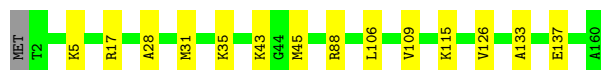
- Molecule 24: 60S ribosomal protein L19



- Molecule 25: 60S ribosomal protein L18a



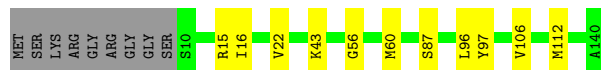
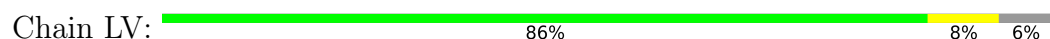
- Molecule 26: 60S ribosomal protein L21



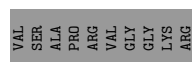
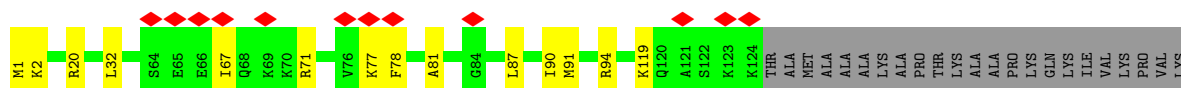
- Molecule 27: 60S ribosomal protein L22



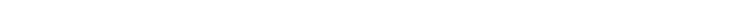
- Molecule 28: 60S ribosomal protein L23

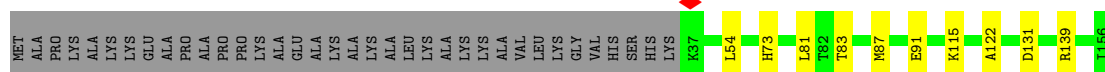


- Molecule 29: 60S ribosomal protein L24



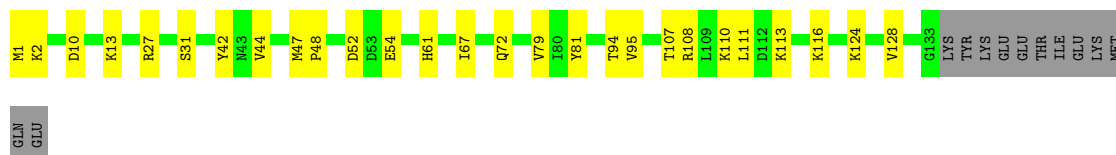
- Molecule 30: 60S ribosomal protein L23a

Chain LX:  71% 6% 23%



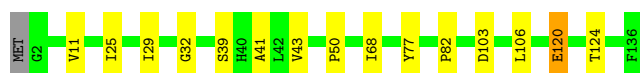
- Molecule 31: 60S ribosomal protein L26

Chain LY: 



- Molecule 32: 60S ribosomal protein L27

Chain LZ:  88% 10% ..



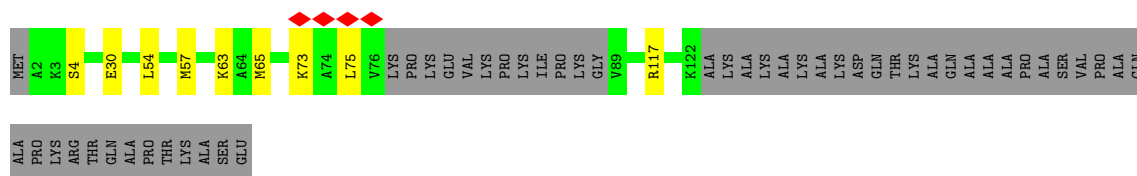
- Molecule 33: 60S ribosomal protein L27a

Chain La:  89% 11%



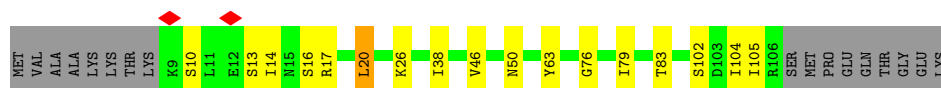
- Molecule 34: 60S ribosomal protein L29

Chain Lb:  63% 6% 31%




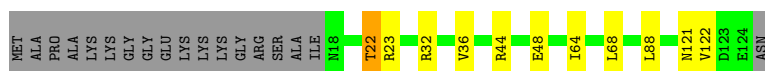
- Molecule 35: 60S ribosomal protein L30

Chain Lc:  70% 14% 15%



- Molecule 36: 60S ribosomal protein L31

Chain Ld:  77% 8% 14%



- Molecule 37: 60S ribosomal protein L32

Chain Le: 89% 6% 5%



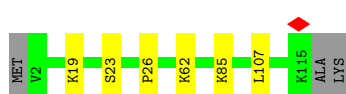
- Molecule 38: 60S ribosomal protein L35a

Chain Lf: 91% 8% .



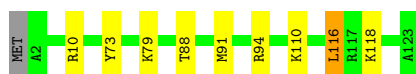
- Molecule 39: 60S ribosomal protein L34

Chain Lg: 92% 5% .



- Molecule 40: 60S ribosomal protein L35

Chain Lh: 92% 7% ..



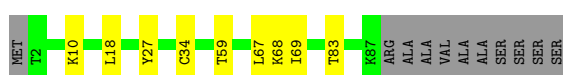
- Molecule 41: 60S ribosomal protein L36

Chain Li: 92% 5% .



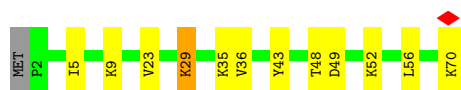
- Molecule 42: Large ribosomal subunit protein eL37

Chain Lj: 79% 9% 11%



- Molecule 43: 60S ribosomal protein L38

Chain Lk: 81% 16% ..



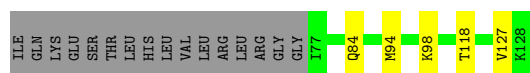
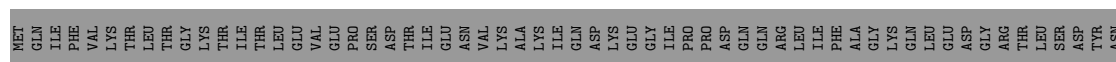
- Molecule 44: 60S ribosomal protein L39

Chain Ll: 78% 16% . .



- Molecule 45: Large ribosomal subunit protein eL40

Chain Lm: 37% . 59%



- Molecule 46: 60S ribosomal protein L41

Chain Ln: 84% 12% .



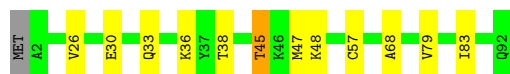
- Molecule 47: 60S ribosomal protein L36a

Chain Lo: 86% 13% .



- Molecule 48: 60S ribosomal protein L37a

Chain Lp: 86% 12% . .



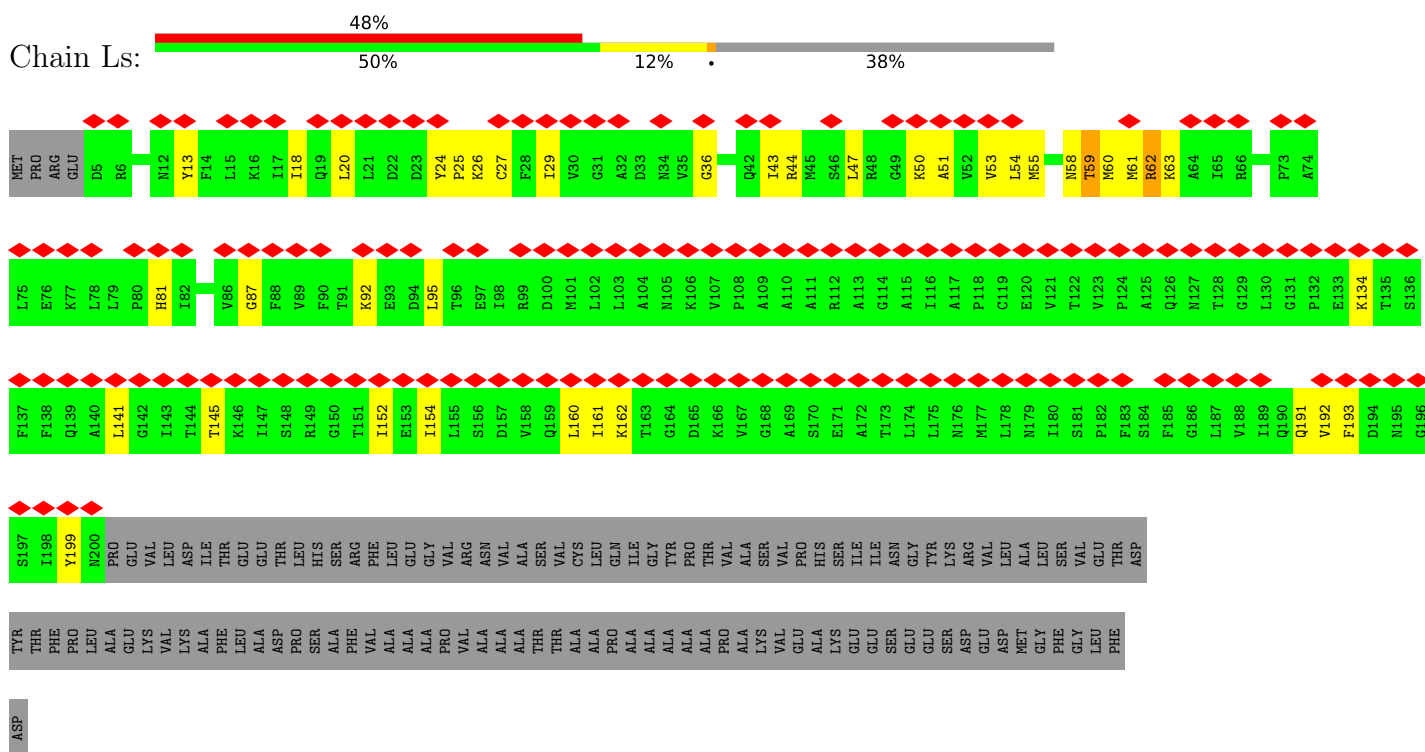
- Molecule 49: 60S ribosomal protein L28

Chain Lr: 85% 6% 9%

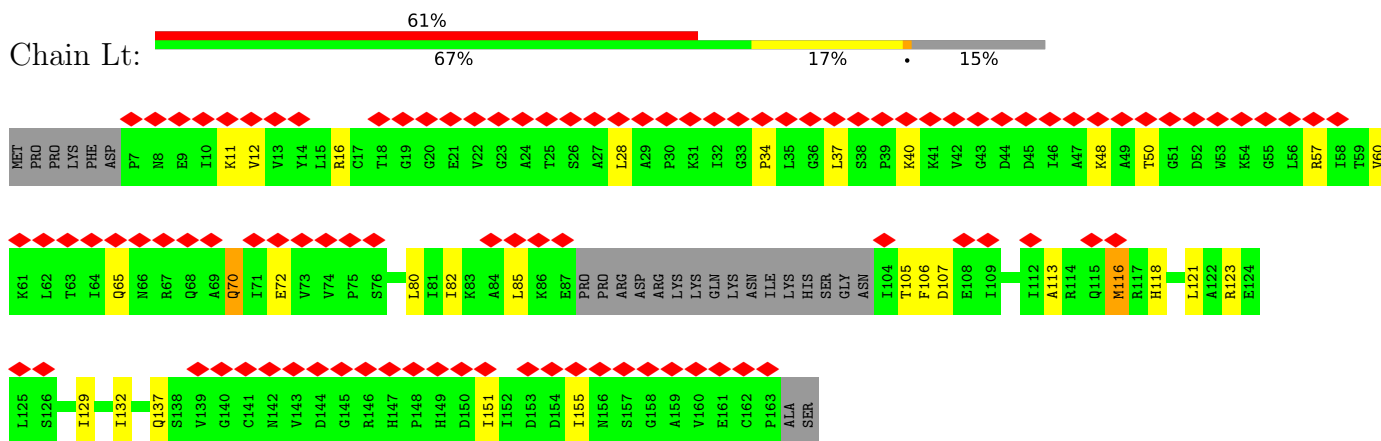


- Molecule 50: 60S acidic ribosomal protein P0

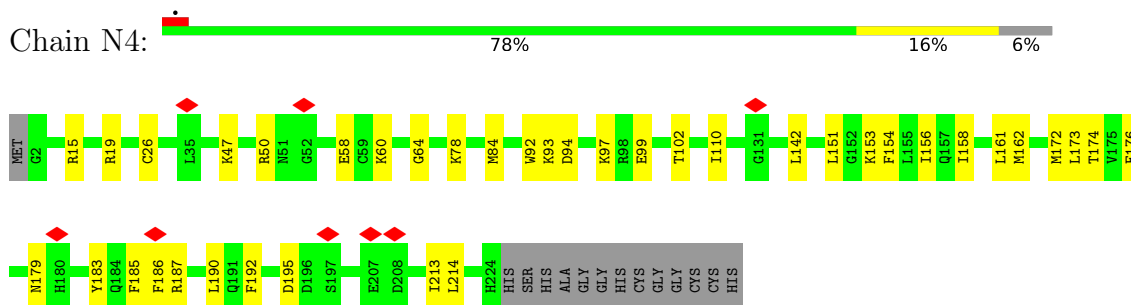




- Molecule 51: Large ribosomal subunit protein uL11



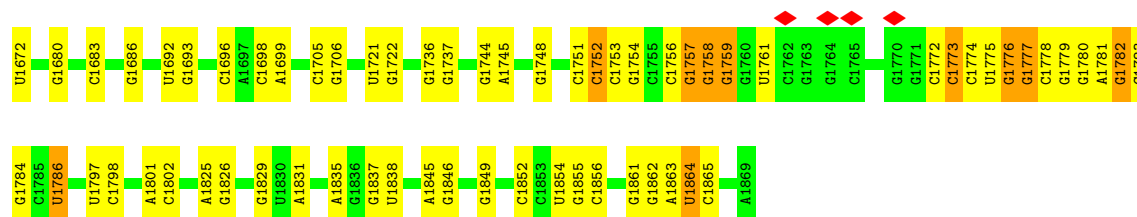
- Molecule 52: N-alpha-acetyltransferase 40



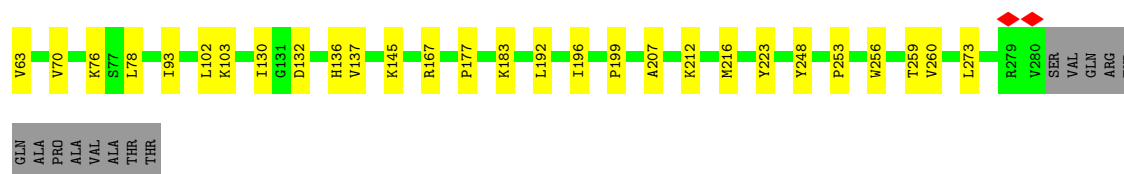
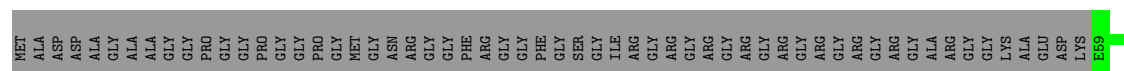
- Molecule 53: 18S rRNA



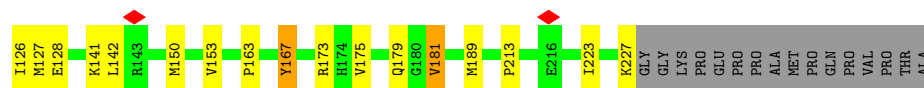
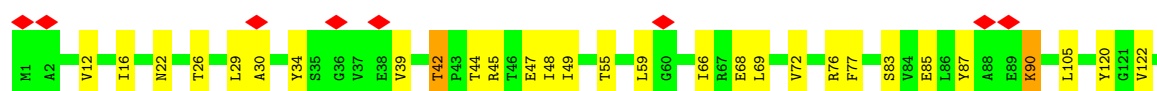
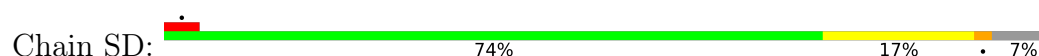
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A1569	C1436	C1309	C1219	A1028	U917	A811	C	G673	A549	C409	A302	C	U115	C4
G1570	C1437	U1310	G1221	A1037	A920	G821	U	U678	A554	A433	G308	C	U116	U5
A1579	A1438	G1312	G1224	G1037	G921	U822	G	U681	U562	C434	C	C	U121	G6
A1580	A1439	A1313	G1227	A1060	A922	A830	C	C687	G563	G438	C311	C	G126	C17
U1585	U1457	U1319	A1228	C1067	G925	U837	C	U688	G564	A448	G312	C	C	C18
U1586	G1458	G1320	G1229	A1080	G928	U889	C	U689	G565	A449	C319	G	C129	U26
U1587	U1462	G1324	U1232	A1083	G929	U890	C	G690	C567	C450	C	U	G130	A27
A1588	U1463	U1333	G1233	A1084	C930	C835	C	G691	C568	G451	C322	C	C133	U28
C1593	C1468	C1337	U1239	C1085	G933	G836	G	A	A576	G452	C324	A	C134	G29
A1594	G1475	G1338	U1242	C1089	G934	A837	C	G	C579	A455	C325	G	U135	G33
U1598	A1476	C1341	U1243	G1089	U940	C838	C	C	C	C456	C326	C	C136	U34
G1600	U1477	U1342	U1244	C1098	U943	C840	C	C	C583	A464	G327	C	U143	C35
A1601	U1477	U1343	G1245	C1099	A944	G841	C	C	G584	A465	U328	U	U144	G41
G1606	A1487	G1348	A1251	A1100	U947	C842	C	G	G588	A466	G329	C	U145	A42
C1618	C1488	U1371	C1252	U1101	C948	A847	C	G	G589	G471	G330	C	U146	U43
U1621	A1489	U1372	A1253	G1102	C949	C851	C	C	A591	C472	G332	C	A147	A44
G1622	G1495	C1373	G1256	C1109	A955	G852	C	G	C592	G474	G333	C	G155	A45
A1623	U1496	C1374	G1257	U1115	A963	G860	C	G	A604	G482	A339	G	U160	A46
A1630	G1497	G1375	A1258	C1116	A964	A861	C	U	C614	A485	G347	C	U161	U51
U1631	A1498	A1378	C1275	C1117	U965	A862	C	C	G623	A486	G351	C	C162	G52
G1632	U1504	U1382	U1263	G1121	G971	A870	C	C	U627	U487	A360	C	U163	G56
A1633	U1505	A1383	C1264	C1122	A981	G873	C	G	A628	U488	U361	C	G167	U57
A1634	G1507	C1384	G1275	A1133	G982	A875	C	C	G	C492	A362	C	A171	C58
C1644	U1508	G1394	C1277	C1138	A990	G878	C	G	U631	A493	A364	C	A175	U59
U1645	U1509	U1397	A1278	G1144	G991	G880	C	A	C638	C502	U367	G	C182	G65
C1646	C1513	G1396	C1283	A1145	A992	C879	C	G	C639	A508	U368	G	U198	G66
G1647	G1514	U1401	C1284	A1146	A996	A886	C	C	A640	G509	C369	C	C199	G67
U1649	G1520	A1402	G1285	C1153	A997	U887	C	A	U642	C517	G370	C	G200	A68
A1650	C1521	C1403	G1286	U1154	A998	U888	C	C	A643	A525	A371	G	C201	G71
A1651	A1522	U1404	G1289	U1172	C999	U889	C	C	G644	A526	U375	C	C202	C72
U1653	A1533	A1405	U1290	C1000	G1000	U890	C	A	U649	C527	A376	C	G203	C73
G1654	G1536	U1406	G1294	A1001	U1002	G891	C	C	A650	C528	U377	C	G204	G74
U1655	A1537	U1407	A1293	A1189	U1007	G895	C	C	A655	A529	U378	C	U210	G75
G1656	G1546	C1415	A1295	A1190	C1007	U896	C	G	G656	C	C379	C	G211	U76
C1660	U1661	C1419	G1298	A1195	A1008	U897	C	C	C	G535	G383	G	C	A91
U1662	G1550	G1420	C1301	U1201	A1009	U898	C	C	C660	A536	U384	C	U220	A102
A1663	U1551	A1421	U1301	U1202	G1010	U899	C	G	C	C385	G385	C	A221	A103
A1664	G1552	G1422	G1302	G1203	A1011	C900	C	U	C	C386	C386	C	U222	A104
G1665	C1553	C1423	C1303	A1204	A1012	A904	C	C	C663	U541	C387	U	C223	U105
U1668	A1556	G1428	U1364	G1207	U1013	G907	C	C	A664	U542	C391	C	A224	C106
G1669	C1557	C1433	C1305	C1215	U1016	A908	C	C	A668	A545	A392	U	G225	A107
C1670	U1560	C1434	U1307	A1217	U1017	A913	C	G	A669	G546	C400	C	A	G108
G1671					A1023		C	C	A671	G547	G291	C	A	U112
											A292	C	A	G113



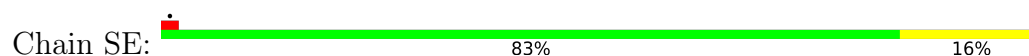
• Molecule 54: 40S ribosomal protein S2



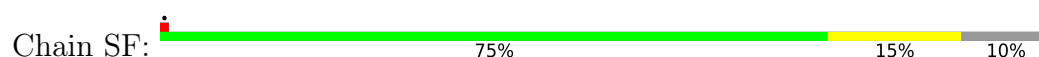
• Molecule 55: 40S ribosomal protein S3

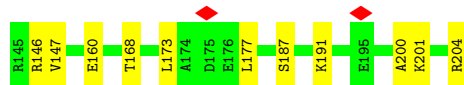


• Molecule 56: Small ribosomal subunit protein eS4, X isoform

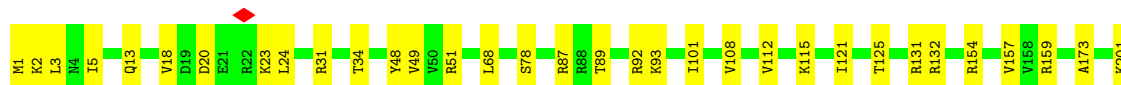
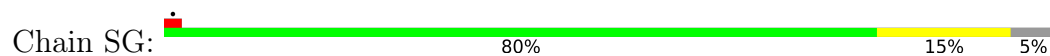


• Molecule 57: 40S ribosomal protein S5

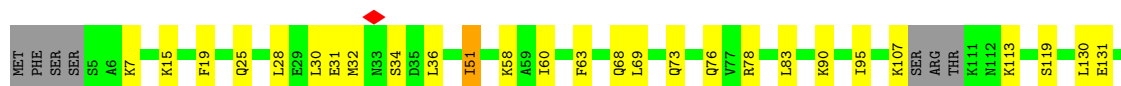
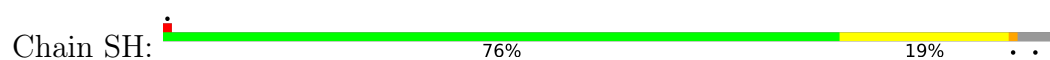




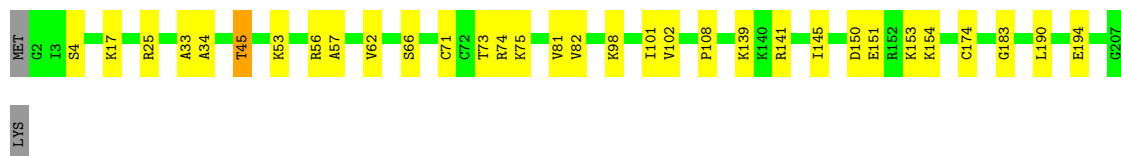
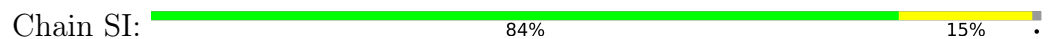
- Molecule 58: 40S ribosomal protein S6



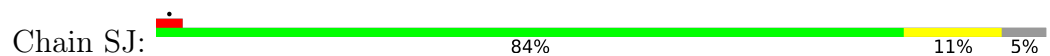
- Molecule 59: 40S ribosomal protein S7



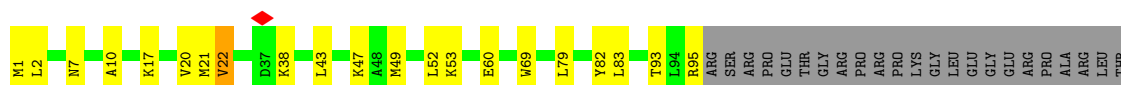
- Molecule 60: 40S ribosomal protein S8



- Molecule 61: 40S ribosomal protein S9



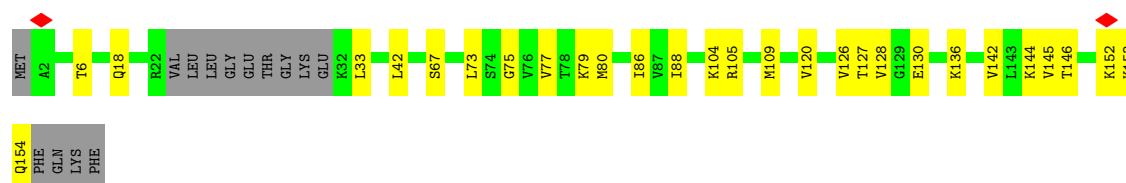
- Molecule 62: 40S ribosomal protein S10



ARG GLY GLU ALA ASP ARG ASP THR TYR ARG ARG SER SER ALA VAL PRO PRO GLY ALA ASP LYS LYS ALA GLU GLY ALA GLY ALA GLY SER SER THR THR PHE GLN PHE ARG GLY PHE GLY ARG GLY ARG GLN PRO PRO GLN

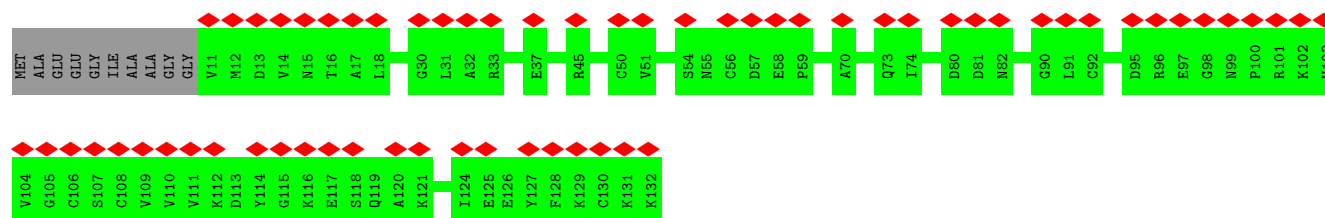
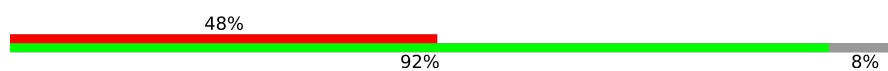
• Molecule 63: 40S ribosomal protein S11

Chain SL:



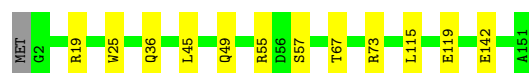
• Molecule 64: 40S ribosomal protein S12

Chain SM:



• Molecule 65: 40S ribosomal protein S13

Chain SN:



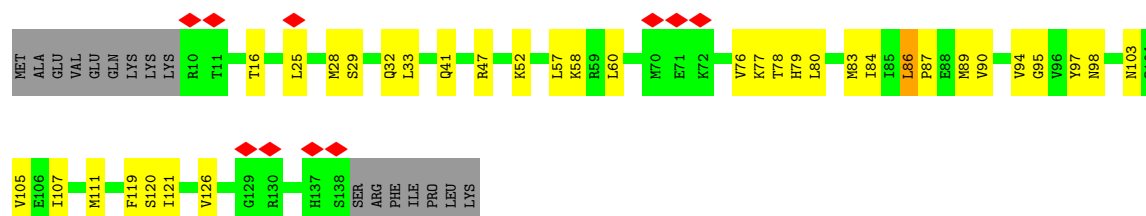
• Molecule 66: 40S ribosomal protein S14

Chain SO:

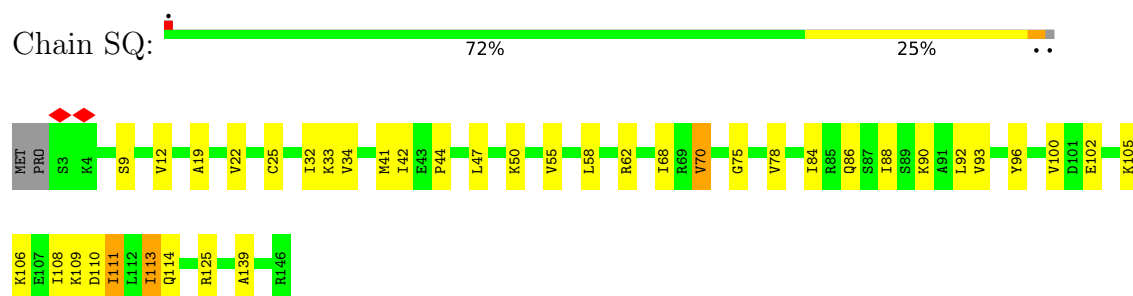


• Molecule 67: 40S ribosomal protein S15

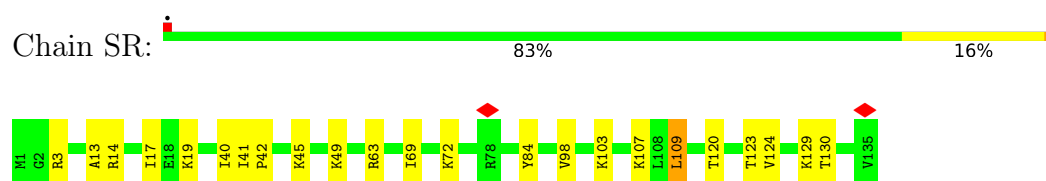
Chain SP:



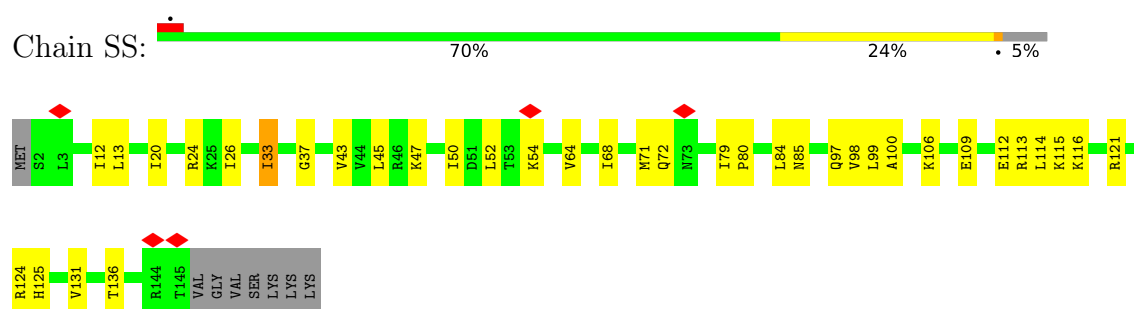
- Molecule 68: 40S ribosomal protein S16



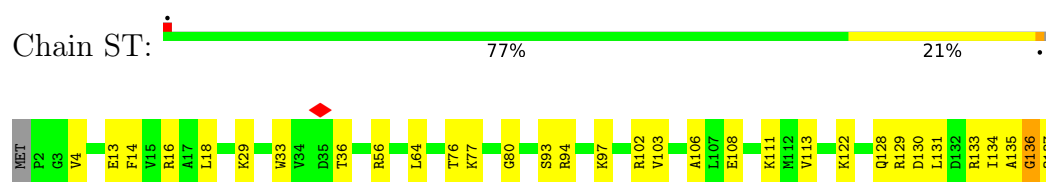
- Molecule 69: 40S ribosomal protein S17



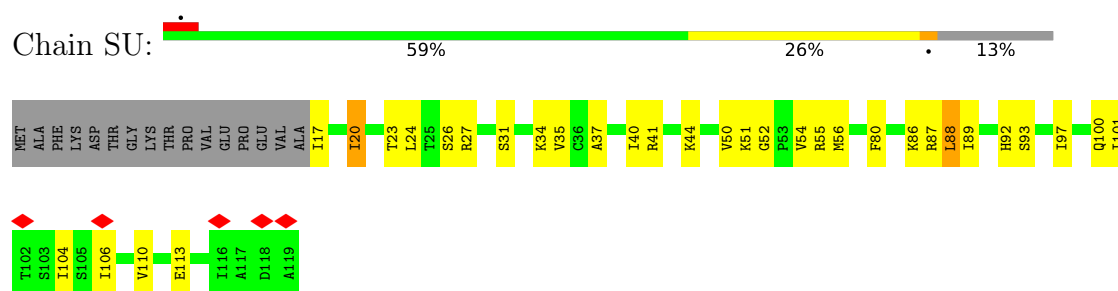
- Molecule 70: 40S ribosomal protein S18



- Molecule 71: 40S ribosomal protein S19



- Molecule 72: 40S ribosomal protein S20




- Molecule 73: 40S ribosomal protein S21

Chain SV:  90% 10%



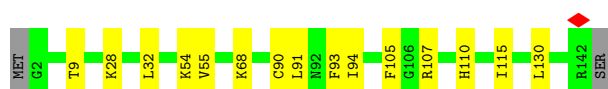
- Molecule 74: 40S ribosomal protein S15a

Chain SW:  85% 14%




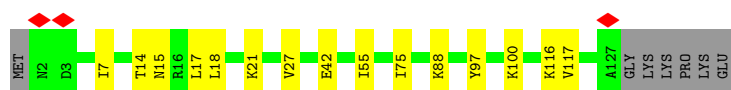
- Molecule 75: 40S ribosomal protein S23

Chain SX:  88% 10%

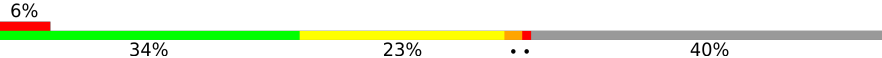


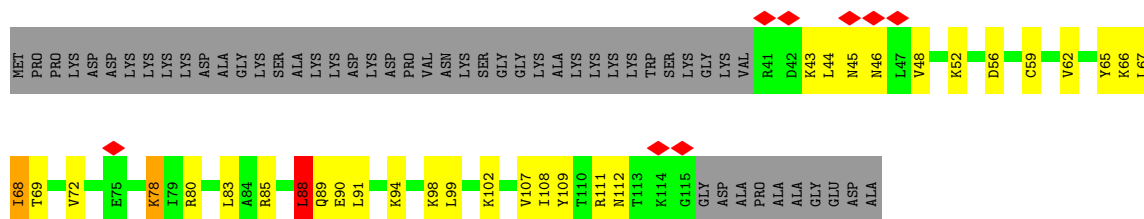
- Molecule 76: 40S ribosomal protein S24

Chain SY:  83% 11% 5%




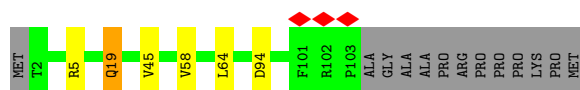
- Molecule 77: 40S ribosomal protein S25

Chain SZ:  6% 34% 23% 40%



- Molecule 78: 40S ribosomal protein S26

Chain Sa:  83% 11%

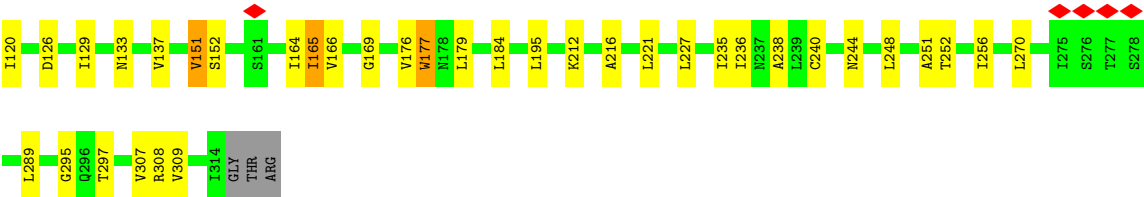


- Molecule 79: 40S ribosomal protein S27

Chain Sb:  87% 12%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.822	Depositor
Minimum map value	-2.416	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	465.28, 465.28, 465.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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, MLZ, ZN

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	LA	0.31	0/1936	0.49	0/2596
2	NA	0.18	0/845	0.56	0/1128
3	SA	0.25	0/1778	0.54	0/2416
4	LB	0.29	0/3306	0.49	0/4424
5	NB	0.26	0/829	0.69	1/1112 (0.1%)
6	SB	0.21	0/1817	0.49	0/2428
7	L5	0.33	0/87990	0.38	2/137262 (0.0%)
8	L7	0.31	0/2861	0.34	0/4459
9	L8	0.32	0/3701	0.34	0/5766
10	LC	0.29	0/2962	0.47	0/3977
11	LD	0.25	0/2428	0.46	0/3252
12	LE	0.25	0/1808	0.48	2/2425 (0.1%)
13	LF	0.29	0/1905	0.44	0/2539
14	LG	0.26	0/1960	0.53	0/2637
15	LH	0.26	0/1537	0.45	0/2066
16	LI	0.26	0/1677	0.43	0/2237
17	LJ	0.28	0/1394	0.65	2/1863 (0.1%)
18	LL	0.26	0/1704	0.44	0/2282
19	LM	0.25	0/1161	0.41	0/1554
20	LN	0.34	0/1746	0.43	0/2338
21	LO	0.30	0/1682	0.43	0/2250
22	LP	0.30	0/1268	0.46	0/1701
23	LQ	0.30	0/1537	0.41	0/2052
24	LR	0.27	0/1582	0.45	0/2091
25	LS	0.27	0/1493	0.41	0/2003
26	LT	0.27	0/1326	0.38	0/1770
27	LU	0.26	0/830	0.58	1/1114 (0.1%)
28	LV	0.29	0/993	0.46	0/1332
29	LW	0.25	0/1030	0.50	1/1364 (0.1%)
30	LX	0.25	0/1002	0.41	0/1345
31	LY	0.26	0/1123	0.43	0/1493
32	LZ	0.25	0/1130	0.40	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	La	0.29	0/1191	0.42	0/1591
34	Lb	0.26	0/895	0.49	0/1182
35	Lc	0.28	0/774	0.51	0/1038
36	Ld	0.26	0/903	0.44	0/1216
37	Le	0.30	0/1071	0.45	0/1429
38	Lf	0.30	0/895	0.40	0/1198
39	Lg	0.29	0/916	0.45	0/1220
40	Lh	0.24	0/1023	0.43	0/1351
41	Li	0.23	0/843	0.47	0/1115
42	Lj	0.34	0/720	0.53	0/952
43	Lk	0.27	0/575	0.53	1/761 (0.1%)
44	Ll	0.32	0/454	0.39	0/599
45	Lm	0.24	0/425	0.40	0/561
46	Ln	0.20	0/231	0.40	0/294
47	Lo	0.26	0/876	0.42	0/1156
48	Lp	0.28	0/718	0.43	0/953
49	Lr	0.28	0/1017	0.42	0/1364
50	Ls	0.19	0/1519	0.55	0/2052
51	Lt	0.21	0/1058	0.69	2/1430 (0.1%)
52	N4	0.20	0/1846	0.58	0/2476
53	S2	0.22	0/40751	0.34	0/63496
54	SC	0.24	0/1762	0.52	0/2381
55	SD	0.26	0/1793	0.70	4/2414 (0.2%)
56	SE	0.21	0/2118	0.48	0/2849
57	SF	0.23	0/1481	0.61	1/1988 (0.1%)
58	SG	0.23	0/1946	0.58	1/2590 (0.0%)
59	SH	0.26	0/1519	0.65	0/2033
60	SI	0.24	0/1715	0.49	1/2287 (0.0%)
61	SJ	0.21	0/1550	0.47	0/2069
62	SK	0.29	0/823	0.86	0/1111
63	SL	0.23	0/1202	0.40	0/1606
64	SM	0.09	0/603	0.26	0/837
65	SN	0.25	0/1232	0.44	0/1656
66	SO	0.23	0/1023	0.52	1/1372 (0.1%)
67	SP	0.27	0/1082	0.75	0/1446
68	SQ	0.25	0/1160	0.68	0/1553
69	SR	0.30	0/1105	0.75	1/1484 (0.1%)
70	SS	0.30	0/1208	0.79	1/1618 (0.1%)
71	ST	0.29	0/1131	0.75	4/1515 (0.3%)
72	SU	0.29	0/827	0.80	0/1110
73	SV	0.22	0/643	0.48	1/860 (0.1%)
74	SW	0.25	0/1051	0.43	0/1406
75	SX	0.20	0/1116	0.39	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SY	0.25	0/1044	0.61	0/1388
77	SZ	0.33	0/604	1.06	2/810 (0.2%)
78	Sa	0.28	0/836	0.59	1/1121 (0.1%)
79	Sb	0.24	0/665	0.51	0/891
80	Sc	0.28	0/508	0.71	2/680 (0.3%)
81	Sd	0.31	0/470	0.73	0/623
82	Se	0.19	0/465	0.45	0/612
83	Sf	0.24	0/560	0.67	1/745 (0.1%)
84	Sg	0.21	0/2493	0.62	2/3394 (0.1%)
All	All	0.28	0/234777	0.44	35/344156 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	LE	0	1
27	LU	0	1
51	Lt	0	1
59	SH	0	1
62	SK	0	1
72	SU	0	1
77	SZ	0	1
84	Sg	0	1
All	All	0	8

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	NB	8	GLN	CA-CB-CG	7.14	128.38	114.10
55	SD	128	GLU	CA-CB-CG	6.54	127.17	114.10
51	Lt	37	LEU	CA-CB-CG	6.37	138.59	116.30
55	SD	127	MET	CA-C-N	-6.12	113.06	122.60
55	SD	127	MET	C-N-CA	-6.12	113.06	122.60
70	SS	113	ARG	CA-CB-CG	6.04	126.18	114.10
71	ST	137	GLN	CA-CB-CG	6.02	126.14	114.10
7	L5	417	G	O4'-C1'-N9	6.01	117.22	108.20
84	Sg	42	MET	CA-CB-CG	5.97	126.05	114.10
60	SI	139	LYS	CA-CB-CG	5.90	125.91	114.10
77	SZ	52	LYS	CA-CB-CG	5.73	125.56	114.10

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	SG	223	LYS	CB-CG-CD	5.65	124.30	111.30
17	LJ	88	LYS	CB-CG-CD	5.62	124.24	111.30
17	LJ	91	GLU	CA-CB-CG	5.58	125.26	114.10
84	Sg	5	MET	CB-CG-SD	5.47	129.10	112.70
57	SF	94	LYS	CB-CG-CD	5.45	123.83	111.30
71	ST	111	LYS	CA-CB-CG	5.40	124.91	114.10
80	Sc	40	ARG	CA-CB-CG	5.32	124.73	114.10
29	LW	91	MET	CA-CB-CG	5.25	124.59	114.10
51	Lt	116	MET	CA-CB-CG	5.24	124.58	114.10
71	ST	136	GLY	CA-C-N	-5.23	111.38	121.58
71	ST	136	GLY	C-N-CA	-5.23	111.38	121.58
69	SR	109	LEU	CA-CB-CG	5.21	134.55	116.30
77	SZ	88	LEU	CA-CB-CG	5.19	134.46	116.30
66	SO	116	LEU	CA-CB-CG	5.17	134.39	116.30
27	LU	67	LYS	CB-CG-CD	5.14	123.13	111.30
55	SD	90	LYS	CB-CG-CD	5.14	123.13	111.30
43	Lk	29	LYS	CB-CG-CD	5.12	123.06	111.30
83	Sf	90	LYS	CB-CG-CD	5.10	123.02	111.30
12	LE	207	LYS	CB-CG-CD	5.06	122.94	111.30
78	Sa	19	GLN	CB-CG-CD	5.05	121.19	112.60
7	L5	406	C	C2'-C3'-O3'	5.04	121.27	113.70
12	LE	239	LYS	CA-CB-CG	5.04	124.18	114.10
73	SV	11	LEU	CA-CB-CG	5.04	133.93	116.30
80	Sc	7	GLN	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	LE	177	GLY	Peptide
27	LU	107	LYS	Peptide
51	Lt	118	HIS	Peptide
59	SH	32	MET	Peptide
62	SK	17	LYS	Peptide
72	SU	106	ILE	Peptide
77	SZ	78	LYS	Peptide
84	Sg	179	LEU	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	LA	1898	0	1993	15	0
2	NA	841	0	898	17	0
3	SA	1741	0	1746	19	0
4	LB	3238	0	3376	31	0
5	NB	821	0	867	10	0
6	SB	1791	0	1870	16	0
7	L5	78658	0	39747	270	0
8	L7	2561	0	1295	5	0
9	L8	3314	0	1683	12	0
10	LC	2908	0	3082	13	0
11	LD	2382	0	2410	20	0
12	LE	1774	0	1930	17	0
13	LF	1870	0	1996	12	0
14	LG	1927	0	2074	16	0
15	LH	1518	0	1601	16	0
16	LI	1639	0	1687	14	0
17	LJ	1371	0	1412	17	0
18	LL	1673	0	1779	9	0
19	LM	1138	0	1204	11	0
20	LN	1701	0	1749	21	0
21	LO	1650	0	1794	8	0
22	LP	1242	0	1269	5	0
23	LQ	1513	0	1628	3	0
24	LR	1566	0	1729	10	0
25	LS	1453	0	1490	13	0
26	LT	1298	0	1366	11	0
27	LU	816	0	842	4	0
28	LV	979	0	1039	6	0
29	LW	1015	0	1079	9	0
30	LX	985	0	1066	4	0
31	LY	1106	0	1192	13	0
32	LZ	1107	0	1182	8	0
33	La	1162	0	1213	7	0
34	Lb	882	0	959	6	0
35	Lc	764	0	804	10	0
36	Ld	888	0	930	6	0
37	Le	1053	0	1147	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lf	876	0	912	5	0
39	Lg	906	0	998	5	0
40	Lh	1015	0	1148	6	0
41	Li	832	0	917	2	0
42	Lj	705	0	737	5	0
43	Lk	569	0	637	9	0
44	Ll	444	0	483	7	0
45	Lm	430	0	466	2	0
46	Ln	230	0	276	2	0
47	Lo	862	0	929	8	0
48	Lp	708	0	756	8	0
49	Lr	1002	0	1068	4	0
50	Ls	1496	0	1540	24	0
51	Lt	1046	0	1076	17	0
52	N4	1809	0	1764	25	0
53	S2	36456	0	18381	174	0
54	SC	1725	0	1813	13	0
55	SD	1765	0	1865	29	0
56	SE	2076	0	2177	22	0
57	SF	1461	0	1511	19	0
58	SG	1923	0	2089	25	0
59	SH	1497	0	1590	23	0
60	SI	1686	0	1772	18	0
61	SJ	1525	0	1640	13	0
62	SK	799	0	823	15	0
63	SL	1182	0	1253	12	0
64	SM	604	0	281	0	0
65	SN	1208	0	1294	6	0
66	SO	1010	0	1034	7	0
67	SP	1061	0	1107	25	0
68	SQ	1142	0	1213	22	0
69	SR	1090	0	1149	12	0
70	SS	1190	0	1249	20	0
71	ST	1112	0	1146	19	0
72	SU	817	0	882	22	0
73	SV	636	0	637	3	0
74	SW	1034	0	1080	12	0
75	SX	1098	0	1167	8	0
76	SY	1027	0	1093	9	0
77	SZ	598	0	656	17	0
78	Sa	821	0	870	4	0
79	Sb	651	0	672	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Sc	506	0	536	6	0
81	Sd	459	0	448	4	0
82	Se	459	0	503	7	0
83	Sf	548	0	551	5	0
84	Sg	2436	0	2393	38	0
85	L5	210	0	0	0	0
85	L7	3	0	0	0	0
85	L8	6	0	0	0	0
85	LA	1	0	0	0	0
85	LI	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	2	0	0	0	0
85	Lg	1	0	0	0	0
85	S2	30	0	0	0	0
85	SG	1	0	0	0	0
86	Lg	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
86	Sd	1	0	0	0	0
86	Sf	1	0	0	0	0
All	All	219040	0	163710	1280	0

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

All (1280) 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)
53:S2:1756:C:N4	53:S2:1776:G:H22	1.53	1.06
53:S2:1756:C:H42	53:S2:1776:G:N2	1.52	1.06
7:L5:1762:C:N4	7:L5:1770:A:C2	2.35	0.94
7:L5:1996:C:H42	7:L5:2000:G:N2	1.73	0.86
7:L5:2557:G:H1	7:L5:2570:U:H3	1.19	0.86
7:L5:1996:C:H42	7:L5:2000:G:H22	1.25	0.83
7:L5:1762:C:N4	7:L5:1770:A:H2	1.77	0.83
59:SH:30:LEU:O	59:SH:34:SER:HB3	1.79	0.83
7:L5:184:U:H3	7:L5:253:G:H21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SU:24:LEU:O	72:SU:86:LYS:HA	1.86	0.76
7:L5:1996:C:N4	7:L5:2000:G:H22	1.85	0.74
53:S2:1756:C:H42	53:S2:1776:G:H22	0.79	0.73
7:L5:4139:G:H21	7:L5:4140:C:H41	1.36	0.73
53:S2:1463:U:H3'	69:SR:63:ARG:HH22	1.53	0.73
51:Lt:113:ALA:HA	51:Lt:116:MET:HE3	1.71	0.72
55:SD:163:PRO:O	55:SD:167:TYR:HB2	1.89	0.72
55:SD:16:ILE:HD11	81:Sd:22:ARG:HD2	1.71	0.71
7:L5:1976:G:H1	7:L5:1990:A:H61	1.37	0.71
53:S2:940:U:H3	53:S2:1002:U:H3	1.39	0.70
53:S2:563:G:H1	53:S2:592:C:H5	1.40	0.70
17:LJ:63:ARG:HH12	47:Lo:104:ILE:HB	1.56	0.69
77:SZ:46:ASN:H	77:SZ:78:LYS:HE3	1.57	0.68
7:L5:1732:C:H5''	26:LT:43:LYS:HD2	1.76	0.68
53:S2:1748:G:H1	53:S2:1786:U:H3	1.42	0.67
10:LC:163:LYS:HB2	10:LC:166:GLU:HG3	1.75	0.67
53:S2:1751:C:H42	53:S2:1782:G:H21	1.41	0.67
39:Lg:85:LYS:H	39:Lg:85:LYS:HE2	1.59	0.67
53:S2:1401:A:H4'	72:SU:52:GLY:HA3	1.76	0.67
53:S2:1324:G:H1	53:S2:1504:U:H3	1.41	0.67
4:LB:153:MET:HB2	4:LB:194:LEU:HD11	1.77	0.67
62:SK:7:ASN:HA	62:SK:38:LYS:HZ1	1.59	0.67
53:S2:928:G:H1	53:S2:1013:U:H3	1.43	0.67
53:S2:925:G:H1	53:S2:1017:U:H3	1.41	0.66
28:LV:43:LYS:HG3	28:LV:60:MET:HG2	1.77	0.66
57:SF:35:LEU:HD21	57:SF:146:ARG:HE	1.59	0.66
15:LH:48:LEU:HD11	15:LH:56:ARG:HD3	1.76	0.66
7:L5:4093:G:N1	7:L5:4114:C:C2	2.65	0.65
7:L5:2469:C:H5	7:L5:2471:G:H1	1.43	0.65
60:SI:150:ASP:HA	60:SI:153:LYS:HG3	1.78	0.65
7:L5:2458:C:H5''	20:LN:67:ARG:HD2	1.79	0.65
3:SA:38:ILE:HD12	3:SA:47:TYR:HB3	1.77	0.65
16:LI:87:ILE:HG12	16:LI:138:ILE:HG12	1.77	0.65
56:SE:31:PRO:HG3	56:SE:43:PRO:HG3	1.79	0.65
7:L5:1762:C:N3	7:L5:1770:A:N1	2.44	0.65
20:LN:158:HIS:HB3	20:LN:161:MET:HB2	1.78	0.65
62:SK:53:LYS:HE3	62:SK:60:GLU:HB3	1.78	0.65
7:L5:4691:A:H4'	15:LH:71:ARG:HG2	1.79	0.65
50:Ls:29:ILE:HB	50:Ls:191:GLN:HB2	1.79	0.65
44:Ll:9:ILE:HD12	44:Ll:51:LEU:HD11	1.79	0.64
67:SP:103:ASN:HD21	67:SP:120:SER:HA	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:851:C:H5''	53:S2:852:G:H5'	1.80	0.64
6:SB:137:LEU:HG	6:SB:215:VAL:HG22	1.80	0.63
6:SB:144:LYS:HD3	6:SB:208:HIS:HB3	1.78	0.63
7:L5:4891:G:H1	7:L5:4928:C:H5	1.45	0.63
53:S2:323:C:H2'	53:S2:327:G:H22	1.63	0.63
67:SP:25:LEU:HA	67:SP:28:MET:HG2	1.80	0.63
55:SD:29:LEU:HB2	55:SD:34:TYR:HB2	1.81	0.63
72:SU:17:ILE:HD11	72:SU:92:HIS:HB3	1.81	0.63
7:L5:493:G:O6	7:L5:660:A:N1	2.32	0.62
70:SS:71:MET:HE1	70:SS:99:LEU:HD13	1.81	0.62
72:SU:54:VAL:HB	72:SU:88:LEU:HD23	1.81	0.62
50:Ls:27:CYS:HB2	50:Ls:193:PHE:HB3	1.81	0.62
59:SH:140:VAL:HG21	59:SH:193:GLN:HE21	1.65	0.62
66:SO:33:ILE:HG12	66:SO:42:VAL:HG12	1.81	0.62
56:SE:100:ARG:HB2	56:SE:114:ILE:HD13	1.82	0.62
75:SX:68:LYS:HB3	75:SX:91:LEU:HD13	1.81	0.62
35:Lc:20:LEU:HB3	35:Lc:102:SER:HB2	1.81	0.62
54:SC:167:ARG:HB3	54:SC:177:PRO:HB2	1.81	0.62
7:L5:4277:G:H5''	26:LT:17:ARG:HG2	1.82	0.62
59:SH:63:PHE:HA	59:SH:95:ILE:O	2.00	0.62
7:L5:1940:G:H22	7:L5:4434:C:H5''	1.65	0.61
53:S2:201:C:H3'	53:S2:202:G:H21	1.65	0.61
53:S2:508:A:H3'	53:S2:509:G:H8	1.64	0.61
84:Sg:118:ARG:HE	84:Sg:119:GLN:HG2	1.64	0.61
14:LG:38:ASN:HB3	14:LG:43:GLN:HG2	1.83	0.61
19:LM:40:GLY:HA3	19:LM:45:VAL:HB	1.83	0.61
76:SY:88:LYS:HB3	76:SY:97:TYR:HE2	1.66	0.61
7:L5:4093:G:H22	7:L5:4114:C:N4	1.99	0.61
53:S2:566:U:H3	53:S2:584:G:H1	1.49	0.61
7:L5:408:A:H4'	7:L5:409:G:H3'	1.83	0.60
7:L5:4093:G:N1	7:L5:4114:C:N3	2.48	0.60
53:S2:1752:C:H42	53:S2:1778:C:H42	1.48	0.60
55:SD:42:THR:HG23	55:SD:44:THR:H	1.66	0.60
51:Lt:123:ARG:HD3	51:Lt:129:ILE:HD11	1.83	0.60
72:SU:40:ILE:HG23	72:SU:50:VAL:HG21	1.84	0.60
3:SA:126:ASP:O	3:SA:130:ASP:HB2	2.01	0.60
17:LJ:78:LYS:HE2	17:LJ:78:LYS:H	1.67	0.60
52:N4:186:PHE:HA	52:N4:190:LEU:HD12	1.82	0.60
84:Sg:129:ILE:HD11	84:Sg:151:VAL:HG11	1.84	0.60
4:LB:378:ARG:HG2	29:LW:32:LEU:HD21	1.83	0.59
7:L5:2611:A:H5'	7:L5:2688:G:H4'	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LG:209:SER:HA	14:LG:212:LYS:HG3	1.84	0.59
52:N4:99:GLU:HA	52:N4:102:THR:HG22	1.83	0.59
4:LB:107:ALA:HB2	4:LB:201:LEU:HD22	1.84	0.59
56:SE:31:PRO:HA	56:SE:81:THR:HG22	1.84	0.59
77:SZ:91:LEU:HA	77:SZ:94:LYS:HZ3	1.67	0.59
7:L5:2020:U:H2'	7:L5:2021:G:H8	1.66	0.59
51:Lt:12:VAL:HB	51:Lt:65:GLN:HB3	1.83	0.59
53:S2:1650:A:H5''	68:SQ:139:ALA:HB2	1.85	0.59
62:SK:60:GLU:HB2	62:SK:69:TRP:HD1	1.68	0.59
4:LB:305:THR:HG22	4:LB:308:ASP:HB2	1.83	0.59
7:L5:1959:U:H4'	7:L5:1960:A:H5''	1.85	0.59
9:L8:45:C:H4'	44:Ll:11:ARG:HD2	1.83	0.59
59:SH:131:GLU:HG3	59:SH:139:ILE:HD12	1.85	0.59
3:SA:37:TYR:HA	3:SA:53:ARG:HD2	1.85	0.58
7:L5:2101:C:H2'	7:L5:2102:G:H8	1.68	0.58
63:SL:75:GLY:HA3	63:SL:88:ILE:HD12	1.84	0.58
17:LJ:119:TYR:HB3	70:SS:12:ILE:HG12	1.84	0.58
20:LN:16:SER:O	20:LN:20:ARG:HB2	2.04	0.58
60:SI:45:THR:HG23	60:SI:53:LYS:HG3	1.86	0.58
4:LB:168:MET:HG3	4:LB:178:ALA:HA	1.83	0.58
50:Ls:81:HIS:HB3	50:Ls:191:GLN:HG3	1.85	0.58
84:Sg:11:LEU:HB3	84:Sg:307:VAL:O	2.03	0.58
35:Lc:13:SER:O	35:Lc:17:ARG:HD2	2.04	0.58
11:LD:62:CYS:HB3	11:LD:105:LEU:HD22	1.84	0.58
53:S2:1630:A:H5''	70:SS:37:GLY:H	1.69	0.58
79:Sb:64:CYS:HA	79:Sb:72:ARG:O	2.04	0.58
7:L5:3717:A:H2'	7:L5:3718:A:C8	2.39	0.57
68:SQ:110:ASP:HA	68:SQ:113:ILE:HG22	1.85	0.57
80:Sc:18:LEU:HD21	80:Sc:31:ARG:HG3	1.86	0.57
63:SL:80:MET:HE2	63:SL:86:ILE:HG21	1.86	0.57
68:SQ:58:LEU:HD21	68:SQ:108:ILE:HG23	1.86	0.57
70:SS:47:LYS:HE3	70:SS:79:ILE:HG22	1.85	0.57
3:SA:122:LEU:HD13	3:SA:142:LEU:HD21	1.85	0.57
50:Ls:58:ASN:HA	50:Ls:61:MET:HG2	1.86	0.57
2:NA:178:VAL:HG13	2:NA:192:ARG:HH22	1.70	0.57
53:S2:547:G:H1'	53:S2:549:C:H41	1.69	0.57
2:NA:190:VAL:HG11	2:NA:213:LEU:HD22	1.87	0.57
3:SA:205:ARG:HH12	69:SR:84:TYR:HB3	1.69	0.57
55:SD:39:VAL:HG22	55:SD:48:ILE:HD12	1.87	0.57
12:LE:206:VAL:HG13	12:LE:256:GLN:HB2	1.86	0.57
55:SD:227:LYS:HD2	84:Sg:184:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SH:58:LYS:O	59:SH:90:LYS:HA	2.05	0.57
28:LV:96:LEU:HD13	29:LW:20:ARG:HD2	1.87	0.57
29:LW:77:LYS:HE2	53:S2:1778:C:H5''	1.87	0.57
31:LY:54:GLU:HG3	31:LY:108:ARG:HG2	1.87	0.57
33:La:72:THR:HG22	33:La:110:LYS:HB3	1.87	0.57
55:SD:45:ARG:HH12	55:SD:85:GLU:HB3	1.69	0.57
20:LN:9:GLU:HB2	41:Li:44:ILE:HG13	1.85	0.57
22:LP:116:HIS:HB3	22:LP:149:ILE:HB	1.86	0.57
27:LU:20:LYS:HG2	27:LU:73:THR:HG22	1.85	0.57
53:S2:1017:U:H5'	65:SN:55:ARG:HD3	1.87	0.57
7:L5:4281:A:H2'	7:L5:4282:A:H2'	1.85	0.56
62:SK:82:TYR:HD2	62:SK:83:LEU:HD22	1.70	0.56
32:LZ:50:PRO:HD3	32:LZ:68:ILE:HG12	1.86	0.56
53:S2:874:G:H2'	53:S2:875:A:H8	1.69	0.56
72:SU:80:PHE:HB3	81:Sd:52:PHE:HB3	1.88	0.56
28:LV:16:ILE:HD11	28:LV:56:GLY:HA3	1.88	0.56
38:Lf:71:TRP:HB2	38:Lf:89:ARG:HE	1.70	0.56
43:Lk:29:LYS:HE2	43:Lk:29:LYS:H	1.69	0.56
47:Lo:33:LEU:HA	47:Lo:38:LYS:HG2	1.87	0.56
63:SL:18:GLN:HB3	63:SL:33:LEU:HD11	1.85	0.56
20:LN:140:LYS:HG3	20:LN:144:ARG:HH21	1.69	0.56
26:LT:115:LYS:HD2	26:LT:126:VAL:HG21	1.86	0.56
53:S2:681:U:H4'	75:SX:9:THR:HG22	1.87	0.56
77:SZ:65:TYR:HA	77:SZ:111:ARG:HH21	1.69	0.56
7:L5:667:A:H5''	7:L5:668:C:H5''	1.86	0.56
31:LY:31:SER:HA	31:LY:48:PRO:HA	1.87	0.56
68:SQ:9:SER:HA	68:SQ:25:CYS:O	2.06	0.56
71:ST:13:GLU:HA	71:ST:16:ARG:HB2	1.88	0.56
84:Sg:7:LEU:HD21	84:Sg:308:ARG:HG2	1.87	0.56
11:LD:223:PHE:HB3	11:LD:226:TYR:HB2	1.88	0.56
17:LJ:40:LEU:HD12	17:LJ:70:VAL:HG22	1.87	0.56
36:Ld:64:ILE:HG23	36:Ld:68:LEU:HD23	1.88	0.56
53:S2:649:U:H2'	53:S2:650:A:H8	1.71	0.56
69:SR:45:LYS:HE3	69:SR:49:LYS:HE2	1.87	0.56
67:SP:52:LYS:HE2	67:SP:80:LEU:HD11	1.86	0.55
53:S2:1420:G:H21	53:S2:1421:A:H1'	1.72	0.55
66:SO:98:ARG:HB3	66:SO:132:VAL:HG23	1.88	0.55
7:L5:2517:A:H5'	39:Lg:62:LYS:HD3	1.88	0.55
53:S2:1293:A:H1'	83:Sf:138:ARG:HH12	1.71	0.55
56:SE:197:ASN:HB3	56:SE:209:HIS:HB2	1.88	0.55
13:LF:105:VAL:HG13	13:LF:136:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LN:138:PHE:HA	20:LN:143:ARG:HD2	1.87	0.55
4:LB:128:LYS:HG3	7:L5:4966:A:H5'	1.89	0.55
10:LC:152:LEU:HD23	10:LC:251:ILE:HG12	1.89	0.55
72:SU:97:ILE:HA	72:SU:100:GLN:HG3	1.87	0.55
77:SZ:99:LEU:HD21	77:SZ:102:LYS:HB2	1.89	0.55
7:L5:4363:A:H5''	47:Lo:36:GLN:HG2	1.87	0.55
70:SS:26:ILE:HD11	70:SS:54:LYS:HG3	1.88	0.55
4:LB:247:GLY:HA2	7:L5:2838:G:H5'	1.88	0.55
62:SK:21:MET:HB3	62:SK:69:TRP:HE3	1.71	0.55
13:LF:182:TYR:HB3	13:LF:200:ARG:HG3	1.89	0.55
65:SN:25:TRP:HE1	79:Sb:84:HIS:HB3	1.71	0.55
80:Sc:9:ILE:HD11	80:Sc:57:THR:HB	1.89	0.55
7:L5:4530:U:H2'	7:L5:4531:U:H2'	1.90	0.54
53:S2:1864:U:H3'	78:Sa:5:ARG:HH21	1.70	0.54
7:L5:1994:C:H1'	51:Lt:132:ILE:HA	1.90	0.54
2:NA:111:VAL:HG22	2:NA:122:VAL:HG22	1.88	0.54
7:L5:1976:G:H1	7:L5:1990:A:N6	2.03	0.54
21:LO:61:ARG:HA	21:LO:70:PRO:HD2	1.89	0.54
63:SL:126:VAL:HG12	63:SL:145:VAL:HG22	1.88	0.54
15:LH:92:MET:HE2	15:LH:179:ILE:HG22	1.89	0.54
54:SC:102:LEU:HG	54:SC:130:ILE:HG12	1.89	0.54
84:Sg:87:LEU:HD11	84:Sg:111:VAL:HG11	1.89	0.54
43:Lk:23:VAL:HG22	43:Lk:36:VAL:HG22	1.88	0.54
66:SO:45:THR:HG22	66:SO:52:THR:HA	1.89	0.54
7:L5:4274:A:H2'	7:L5:4275:G:C8	2.43	0.54
11:LD:55:VAL:HG11	11:LD:158:LYS:HE3	1.88	0.54
74:SW:18:GLU:HG2	74:SW:69:LEU:HB3	1.89	0.54
7:L5:4279:A:H5'	7:L5:4281:A:H1'	1.88	0.54
5:NB:10:LYS:H	5:NB:10:LYS:HE2	1.72	0.54
53:S2:1394:G:H21	53:S2:1475:G:H1'	1.73	0.54
53:S2:1550:G:H3'	53:S2:1579:A:H61	1.73	0.54
53:S2:1618:C:H5''	67:SP:47:ARG:HH21	1.72	0.54
83:Sf:89:LYS:HG2	83:Sf:91:ASN:H	1.72	0.54
2:NA:96:ILE:HB	2:NA:104:PHE:HB2	1.90	0.54
2:NA:98:LYS:HB3	2:NA:102:ILE:HB	1.90	0.54
84:Sg:22:ALA:HB3	84:Sg:32:LEU:HB2	1.90	0.54
84:Sg:30:MET:HG2	84:Sg:42:MET:HE3	1.89	0.54
4:LB:85:VAL:HG22	4:LB:204:GLN:HG2	1.89	0.54
7:L5:460:C:H2'	7:L5:461:G:H8	1.73	0.54
14:LG:154:LEU:HB3	14:LG:204:PHE:HB2	1.89	0.54
53:S2:1692:U:H2'	53:S2:1693:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:207:VAL:HG13	1:LA:208:GLU:HG3	1.90	0.53
7:L5:1500:A:H5''	7:L5:1501:C:H5''	1.90	0.53
7:L5:4092:G:H3'	7:L5:4093:G:H21	1.73	0.53
17:LJ:89:VAL:HG11	17:LJ:109:ILE:HG23	1.90	0.53
35:Lc:38:ILE:HG21	35:Lc:63:TYR:HB3	1.89	0.53
47:Lo:22:LYS:HZ1	47:Lo:78:ARG:HH22	1.56	0.53
53:S2:933:G:H22	78:Sa:19:GLN:NE2	2.06	0.53
7:L5:4769:G:H5''	21:LO:176:ARG:HD3	1.90	0.53
68:SQ:19:ALA:HB2	68:SQ:75:GLY:HA3	1.91	0.53
44:Ll:23:ILE:HD12	44:Ll:27:ILE:HD11	1.89	0.53
7:L5:1363:C:H3'	18:LL:36:ARG:HH22	1.73	0.53
7:L5:2107:C:H2'	7:L5:2108:G:H8	1.74	0.53
37:Le:89:LEU:HD13	37:Le:118:LEU:HD22	1.90	0.53
84:Sg:152:SER:H	84:Sg:169:GLY:HA2	1.74	0.53
84:Sg:216:ALA:HB2	84:Sg:236:ILE:HG12	1.90	0.53
52:N4:179:ASN:O	52:N4:183:TYR:HB2	2.09	0.53
69:SR:14:ARG:HG2	69:SR:69:ILE:HD11	1.90	0.53
72:SU:40:ILE:HD11	72:SU:89:ILE:HD12	1.90	0.53
7:L5:496:G:H2'	7:L5:498:C:H5''	1.91	0.53
11:LD:272:SER:HB3	11:LD:275:GLN:HG3	1.89	0.53
52:N4:15:ARG:HE	52:N4:19:ARG:HH12	1.56	0.53
2:NA:101:ASN:HB3	2:NA:131:LEU:HB3	1.90	0.53
53:S2:1144:A:H2'	53:S2:1145:A:C8	2.43	0.53
71:ST:77:LYS:HB2	71:ST:94:ARG:HH21	1.73	0.53
84:Sg:236:ILE:HA	84:Sg:252:THR:HG22	1.89	0.53
12:LE:165:LEU:HD12	12:LE:174:LEU:HG	1.90	0.52
25:LS:47:PHE:HE1	25:LS:125:GLN:HG2	1.74	0.52
50:Ls:44:ARG:HE	50:Ls:53:VAL:HG13	1.73	0.52
53:S2:1310:U:H5''	83:Sf:130:VAL:HG11	1.91	0.52
77:SZ:68:ILE:HG13	77:SZ:109:TYR:HB2	1.90	0.52
7:L5:1187:G:H1'	11:LD:275:GLN:HE21	1.74	0.52
46:Ln:10:MET:HE2	53:S2:1172:U:H5''	1.91	0.52
53:S2:928:G:H2'	53:S2:929:G:C8	2.44	0.52
77:SZ:69:THR:HB	77:SZ:72:VAL:HG22	1.89	0.52
4:LB:168:MET:HA	4:LB:171:LEU:HD12	1.90	0.52
63:SL:73:LEU:HD12	63:SL:109:MET:HE1	1.91	0.52
7:L5:1762:C:H5''	7:L5:1764:G:H1	1.75	0.52
19:LM:3:PHE:H	25:LS:175:PHE:HZ	1.56	0.52
35:Lc:38:ILE:HD11	35:Lc:46:VAL:HG21	1.92	0.52
75:SX:28:LYS:O	75:SX:32:LEU:HB2	2.10	0.52
52:N4:58:GLU:HG3	52:N4:110:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SG:227:GLN:HA	58:SG:230:LYS:HG2	1.91	0.52
6:SB:124:HIS:HA	6:SB:137:LEU:O	2.08	0.52
31:LY:10:ASP:HB3	31:LY:13:LYS:HB2	1.90	0.52
53:S2:860:G:H21	74:SW:107:SER:HB2	1.74	0.52
7:L5:137:G:H2'	7:L5:138:G:H8	1.74	0.52
53:S2:1228:A:H2'	53:S2:1229:G:H8	1.74	0.52
55:SD:76:ARG:HB2	62:SK:22:VAL:HG21	1.92	0.52
59:SH:19:PHE:HZ	59:SH:60:ILE:HD12	1.74	0.52
3:SA:84:GLN:HE22	3:SA:101:GLY:HA2	1.75	0.52
7:L5:1245:C:H2'	7:L5:1246:G:H8	1.75	0.52
7:L5:3736:A:H2'	7:L5:3737:A:C8	2.45	0.52
57:SF:78:MET:HG3	57:SF:79:HIS:HA	1.92	0.52
57:SF:200:ALA:O	57:SF:204:ARG:HB2	2.10	0.52
58:SG:78:SER:HB3	58:SG:92:ARG:HG2	1.91	0.52
67:SP:80:LEU:HB2	67:SP:83:MET:HE1	1.91	0.52
4:LB:136:LYS:HB2	4:LB:142:GLY:HA3	1.91	0.52
7:L5:4238:G:H2'	7:L5:4239:A:C8	2.45	0.52
15:LH:50:LYS:HA	15:LH:53:LYS:HZ2	1.73	0.52
55:SD:66:ILE:HA	55:SD:69:LEU:HD12	1.91	0.52
24:LR:135:LYS:HG2	24:LR:139:MET:HE2	1.91	0.51
61:SJ:127:ARG:HD3	82:Se:31:ARG:HD3	1.91	0.51
53:S2:145:G:H2'	53:S2:146:G:C8	2.45	0.51
1:LA:137:ILE:HD11	1:LA:149:LYS:HB2	1.91	0.51
7:L5:4093:G:H22	7:L5:4114:C:H42	1.58	0.51
7:L5:4611:A:H2	15:LH:120:GLU:HG2	1.75	0.51
84:Sg:106:LYS:HE2	84:Sg:126:ASP:HA	1.93	0.51
7:L5:3868:G:H22	7:L5:3900:G:H1'	1.75	0.51
7:L5:5006:U:H4'	7:L5:5007:A:H5'	1.91	0.51
53:S2:1454:A:H5''	69:SR:3:ARG:HD2	1.93	0.51
58:SG:34:THR:O	58:SG:51:ARG:HA	2.11	0.51
48:Lp:47:MET:HE2	48:Lp:57:CYS:HB2	1.92	0.51
3:SA:207:PRO:HA	3:SA:210:ILE:HG22	1.93	0.51
7:L5:4699:U:H1'	7:L5:4700:A:H5''	1.92	0.51
7:L5:4942:C:H4'	12:LE:154:THR:HG23	1.92	0.51
32:LZ:41:ALA:HB2	32:LZ:77:TYR:HE1	1.75	0.51
58:SG:159:ARG:HE	58:SG:173:ALA:HB2	1.74	0.51
62:SK:1:MET:HE3	62:SK:47:LYS:HD2	1.92	0.51
7:L5:2745:A:H2'	7:L5:2746:A:C8	2.46	0.51
51:Lt:121:LEU:HB3	51:Lt:123:ARG:HB3	1.92	0.51
10:LC:209:ILE:HB	10:LC:229:LEU:HD13	1.92	0.51
84:Sg:256:ILE:HB	84:Sg:270:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:NB:79:VAL:HG22	5:NB:90:ILE:HG22	1.93	0.51
6:SB:24:PRO:HA	6:SB:27:LYS:HD2	1.93	0.51
28:LV:87:SER:HA	28:LV:97:TYR:HB3	1.91	0.51
52:N4:187:ARG:HD3	52:N4:214:LEU:HD11	1.91	0.51
7:L5:217:C:H3'	7:L5:218:A:H2'	1.92	0.51
52:N4:156:ILE:HD13	52:N4:190:LEU:HD13	1.93	0.51
52:N4:176:PHE:HB2	52:N4:179:ASN:HB2	1.92	0.51
53:S2:107:A:H2'	53:S2:108:G:C8	2.46	0.51
57:SF:38:TYR:CD2	57:SF:144:LEU:HB2	2.46	0.51
68:SQ:102:GLU:HA	68:SQ:105:LYS:HB3	1.92	0.51
72:SU:31:SER:HA	72:SU:34:LYS:HE2	1.92	0.51
72:SU:56:MET:SD	72:SU:88:LEU:HD21	2.51	0.51
84:Sg:31:ILE:HG13	84:Sg:45:LEU:HD11	1.91	0.51
3:SA:24:HIS:HA	3:SA:49:ILE:HB	1.93	0.50
12:LE:165:LEU:HD11	12:LE:176:THR:HG22	1.93	0.50
53:S2:1239:U:H3	53:S2:1242:U:H5''	1.76	0.50
7:L5:1332:C:H2'	7:L5:1333:A:H8	1.75	0.50
25:LS:15:ARG:HB3	25:LS:27:LEU:HD23	1.93	0.50
35:Lc:20:LEU:HD13	35:Lc:102:SER:HA	1.92	0.50
43:Lk:49:ASP:HB2	43:Lk:52:LYS:HG3	1.93	0.50
53:S2:1293:A:H1'	83:Sf:138:ARG:HH22	1.76	0.50
53:S2:1513:C:H2'	53:S2:1514:G:H8	1.76	0.50
71:ST:128:GLN:HA	71:ST:131:LEU:HB2	1.92	0.50
7:L5:3720:G:H22	7:L5:3733:A:H2	1.59	0.50
36:Ld:36:VAL:HG21	36:Ld:44:ARG:HG2	1.94	0.50
69:SR:13:ALA:O	69:SR:17:ILE:HD12	2.11	0.50
54:SC:196:ILE:HB	54:SC:223:TYR:HB2	1.94	0.50
55:SD:105:LEU:HB3	55:SD:122:VAL:HG21	1.93	0.50
67:SP:57:LEU:HD21	67:SP:86:LEU:HD23	1.94	0.50
71:ST:18:LEU:HD13	71:ST:134:ILE:HG21	1.94	0.50
3:SA:124:VAL:HG21	3:SA:134:LEU:HD21	1.93	0.50
11:LD:204:VAL:O	11:LD:208:MET:HG3	2.12	0.50
55:SD:76:ARG:HG3	55:SD:77:PHE:CD2	2.47	0.50
50:Ls:59:THR:HA	50:Ls:62:ARG:HE	1.77	0.50
84:Sg:80:SER:HB3	84:Sg:90:TRP:HE1	1.77	0.50
1:LA:117:GLU:HG2	1:LA:124:GLY:H	1.75	0.50
13:LF:226:HIS:HB3	13:LF:229:GLU:HG3	1.94	0.50
6:SB:165:ARG:HG2	6:SB:169:MET:HE2	1.94	0.50
7:L5:1811:G:H21	34:Lb:57:MET:HE1	1.77	0.50
9:L8:154:G:H5''	14:LG:89:ARG:HH12	1.77	0.50
35:Lc:10:SER:O	35:Lc:14:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SU:35:VAL:HG21	72:SU:110:VAL:HG11	1.93	0.50
7:L5:4238:G:H2'	7:L5:4239:A:H8	1.77	0.50
53:S2:1277:C:H2'	53:S2:1278:A:C8	2.47	0.50
67:SP:29:SER:O	67:SP:33:LEU:HB2	2.12	0.50
68:SQ:90:LYS:HA	68:SQ:93:VAL:HG22	1.93	0.50
77:SZ:98:LYS:HZ3	77:SZ:112:ASN:HA	1.77	0.50
1:LA:147:ARG:HG3	1:LA:157:VAL:HG22	1.94	0.49
2:NA:85:LEU:HD22	2:NA:86:ARG:H	1.77	0.49
7:L5:347:A:H2'	7:L5:348:G:C8	2.47	0.49
53:S2:448:A:H5''	60:SI:25:ARG:HA	1.93	0.49
53:S2:1277:C:H2'	53:S2:1278:A:H8	1.75	0.49
59:SH:51:ILE:HG21	59:SH:179:LYS:HG3	1.94	0.49
84:Sg:166:VAL:HG22	84:Sg:176:VAL:HG22	1.94	0.49
30:LX:122:ALA:HB3	30:LX:139:ARG:HG2	1.94	0.49
53:S2:1115:U:H3	53:S2:1118:C:H42	1.60	0.49
67:SP:79:HIS:HA	67:SP:97:TYR:HB2	1.94	0.49
71:ST:130:ASP:HA	71:ST:133:ARG:HB2	1.93	0.49
4:LB:373:LYS:HG2	7:L5:4627:U:H5''	1.94	0.49
7:L5:691:C:H2'	7:L5:692:A:C8	2.47	0.49
7:L5:1942:A:H2'	7:L5:1943:A:C8	2.47	0.49
7:L5:2521:G:H4'	39:Lg:26:PRO:HD2	1.94	0.49
7:L5:4992:G:H2'	7:L5:4993:G:C8	2.47	0.49
29:LW:90:ILE:O	29:LW:94:ARG:HG2	2.13	0.49
11:LD:208:MET:HB2	11:LD:233:PRO:HG3	1.94	0.49
19:LM:38:VAL:HG21	19:LM:50:MET:HE3	1.94	0.49
51:Lt:50:THR:HG21	51:Lt:72:GLU:HB2	1.95	0.49
7:L5:4537:C:H2'	7:L5:4538:G:C8	2.48	0.49
53:S2:527:C:H2'	53:S2:528:A:H8	1.77	0.49
53:S2:562:U:H4'	61:SJ:132:GLN:HB3	1.94	0.49
62:SK:82:TYR:CD2	62:SK:83:LEU:HD22	2.47	0.49
24:LR:183:GLU:HA	24:LR:186:LYS:HG2	1.94	0.49
77:SZ:48:VAL:HA	77:SZ:83:LEU:HD11	1.94	0.49
10:LC:290:SER:O	10:LC:294:LYS:HG2	2.11	0.49
31:LY:52:ASP:HB2	31:LY:110:LYS:HG3	1.93	0.49
36:Ld:32:ARG:HB3	36:Ld:48:GLU:HG3	1.94	0.49
53:S2:367:U:H4'	53:S2:371:A:C8	2.48	0.49
53:S2:1397:U:H3	68:SQ:12:VAL:HA	1.78	0.49
70:SS:112:GLU:HA	70:SS:115:LYS:HB3	1.94	0.49
7:L5:300:A:H2'	7:L5:301:G:H8	1.77	0.49
7:L5:433:A:C2	7:L5:3867:A:H4'	2.48	0.49
7:L5:1802:A:H5''	7:L5:1803:G:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lc:104:ILE:HG23	35:Lc:105:ILE:HG13	1.95	0.49
53:S2:1228:A:H2'	53:S2:1229:G:C8	2.48	0.49
7:L5:493:G:H1	7:L5:660:A:H2	1.61	0.49
7:L5:1308:C:H2'	7:L5:1309:C:C6	2.48	0.49
7:L5:2303:C:H5''	37:Le:104:SER:HB3	1.95	0.49
84:Sg:244:ASN:HD21	84:Sg:295:GLY:HA3	1.78	0.49
9:L8:19:C:H2'	9:L8:20:A:C8	2.48	0.49
20:LN:120:TRP:HZ2	20:LN:123:GLU:HG2	1.78	0.49
22:LP:42:ARG:O	22:LP:46:LYS:HG2	2.12	0.49
56:SE:57:THR:HG22	56:SE:59:ASP:H	1.78	0.49
56:SE:152:PRO:HG2	58:SG:216:ARG:HG3	1.95	0.49
6:SB:60:ASP:HA	6:SB:63:LYS:HG3	1.94	0.48
7:L5:4743:G:H2'	7:L5:4744:A:H8	1.76	0.48
53:S2:944:A:H5''	66:SO:134:PRO:HB3	1.95	0.48
56:SE:188:ASN:HB3	56:SE:191:ARG:HD3	1.95	0.48
60:SI:101:ILE:HD12	60:SI:190:LEU:HD11	1.96	0.48
60:SI:141:ARG:HB2	60:SI:145:ILE:HD11	1.95	0.48
12:LE:180:VAL:HG21	12:LE:258:LEU:HD11	1.95	0.48
18:LL:25:TRP:HE1	20:LN:199:GLN:HG3	1.79	0.48
32:LZ:103:ASP:HB3	32:LZ:106:LEU:HD12	1.94	0.48
53:S2:1401:A:H2'	53:S2:1402:A:C8	2.48	0.48
59:SH:168:HIS:HE1	59:SH:169:LYS:HE2	1.78	0.48
70:SS:13:LEU:HB2	70:SS:20:ILE:HB	1.95	0.48
5:NB:74:PHE:HE1	5:NB:90:ILE:HD13	1.77	0.48
7:L5:1339:U:H2'	7:L5:1340:C:C6	2.49	0.48
53:S2:793:G:H2'	53:S2:794:A:H8	1.77	0.48
53:S2:1551:U:H4'	53:S2:1552:G:C5	2.48	0.48
57:SF:61:PHE:HE1	57:SF:144:LEU:HD22	1.78	0.48
7:L5:1332:C:H2'	7:L5:1333:A:C8	2.49	0.48
7:L5:3880:G:H2'	7:L5:3881:G:C8	2.49	0.48
7:L5:4685:U:H2'	7:L5:4686:G:C8	2.48	0.48
53:S2:562:U:H2'	53:S2:563:G:C8	2.49	0.48
53:S2:1759:G:H21	53:S2:1773:C:H4'	1.77	0.48
56:SE:11:ARG:HA	56:SE:28:ALA:HB2	1.96	0.48
70:SS:80:PRO:HG2	71:ST:36:THR:HG21	1.96	0.48
76:SY:7:ILE:HG12	76:SY:27:VAL:HG12	1.94	0.48
76:SY:15:ASN:HD21	76:SY:18:LEU:HD13	1.78	0.48
13:LF:173:ALA:O	13:LF:177:ARG:HG3	2.13	0.48
53:S2:1415:C:H4'	71:ST:129:ARG:CZ	2.43	0.48
53:S2:1779:G:H2'	53:S2:1780:G:C8	2.49	0.48
70:SS:106:LYS:HA	70:SS:109:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Sg:164:ILE:HG21	84:Sg:221:LEU:HD12	1.95	0.48
25:LS:147:ASP:HB3	25:LS:150:ILE:HB	1.95	0.48
53:S2:981:A:H2'	53:S2:982:G:C8	2.48	0.48
58:SG:121:ILE:HD12	58:SG:121:ILE:H	1.78	0.48
68:SQ:106:LYS:HA	68:SQ:109:LYS:HB3	1.94	0.48
7:L5:2495:U:H2'	7:L5:2496:G:C8	2.49	0.48
7:L5:4618:G:H5''	28:LV:15:ARG:HB2	1.95	0.48
44:Ll:12:PHE:CD2	44:Ll:51:LEU:HD13	2.49	0.48
4:LB:69:LYS:HB2	4:LB:69:LYS:HE2	1.53	0.48
25:LS:69:GLU:HB2	25:LS:101:THR:HG23	1.96	0.48
28:LV:106:VAL:HG12	28:LV:112:MET:HA	1.96	0.48
50:Ls:50:LYS:HG2	50:Ls:51:ALA:H	1.78	0.48
53:S2:916:A:C6	65:SN:73:ARG:HD2	2.49	0.48
55:SD:68:GLU:HG3	62:SK:93:THR:HB	1.95	0.48
57:SF:173:LEU:HD13	57:SF:177:LEU:HD13	1.95	0.48
58:SG:48:TYR:HE1	58:SG:121:ILE:HD11	1.78	0.48
84:Sg:79:LEU:HD22	84:Sg:120:ILE:HD12	1.96	0.48
7:L5:4591:U:H2'	7:L5:4592:C:C6	2.49	0.48
11:LD:220:LYS:HD3	11:LD:227:ILE:HD13	1.96	0.48
68:SQ:33:LYS:HA	68:SQ:33:LYS:HD3	1.69	0.48
71:ST:80:GLY:HA3	71:ST:93:SER:O	2.14	0.48
76:SY:88:LYS:HB3	76:SY:97:TYR:CE2	2.48	0.48
84:Sg:70:VAL:HG12	84:Sg:79:LEU:HB3	1.95	0.48
84:Sg:238:ALA:HB3	84:Sg:251:ALA:HB3	1.96	0.48
2:NA:80:MET:HE3	2:NA:83:LEU:HD21	1.95	0.48
7:L5:2789:A:H1'	44:Ll:45:ARG:HH22	1.79	0.48
7:L5:2870:A:H2'	7:L5:2871:A:C8	2.49	0.48
53:S2:1651:A:H2'	53:S2:1652:G:H8	1.79	0.48
53:S2:1845:A:H2'	53:S2:1846:G:C8	2.48	0.48
68:SQ:42:ILE:HG22	68:SQ:44:PRO:HD2	1.96	0.48
1:LA:245:ARG:HG2	7:L5:3747:A:C8	2.49	0.47
3:SA:89:LYS:HE2	3:SA:201:LEU:HG	1.96	0.47
7:L5:171:U:H3'	7:L5:172:C:H4'	1.95	0.47
7:L5:2101:C:H2'	7:L5:2102:G:C8	2.48	0.47
7:L5:4101:C:N4	7:L5:4107:G:O6	2.47	0.47
7:L5:4258:C:H2'	7:L5:4259:C:H6	1.79	0.47
7:L5:4743:G:H2'	7:L5:4744:A:C8	2.49	0.47
17:LJ:159:LYS:O	17:LJ:163:MET:HG3	2.14	0.47
33:La:131:ARG:O	33:La:135:GLU:HG3	2.14	0.47
42:Lj:68:LYS:HG3	42:Lj:69:ILE:HD13	1.96	0.47
53:S2:525:A:H2'	53:S2:526:A:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SH:139:ILE:HG23	59:SH:156:VAL:HG13	1.96	0.47
62:SK:10:ALA:HB3	62:SK:38:LYS:HZ3	1.79	0.47
70:SS:26:ILE:HD12	70:SS:26:ILE:H	1.79	0.47
71:ST:14:PHE:HE2	71:ST:135:ALA:HB2	1.79	0.47
2:NA:85:LEU:HD12	2:NA:112:TYR:HB3	1.96	0.47
21:LO:34:VAL:HG22	21:LO:103:LYS:HB2	1.94	0.47
57:SF:28:VAL:HG22	57:SF:110:GLN:HB2	1.95	0.47
58:SG:31:ARG:HG2	58:SG:101:ILE:HD13	1.96	0.47
62:SK:43:LEU:O	62:SK:47:LYS:HG2	2.15	0.47
65:SN:19:ARG:HA	65:SN:19:ARG:HD2	1.75	0.47
6:SB:71:LEU:HD21	6:SB:189:ILE:HD12	1.95	0.47
11:LD:232:THR:H	11:LD:235:MET:HE1	1.79	0.47
50:Ls:43:ILE:O	50:Ls:47:LEU:HB2	2.14	0.47
52:N4:172:MET:HG2	52:N4:213:ILE:HD11	1.96	0.47
53:S2:375:U:H2'	53:S2:376:A:C8	2.49	0.47
53:S2:1203:G:H2'	53:S2:1204:A:C8	2.49	0.47
70:SS:64:VAL:O	70:SS:68:ILE:HD12	2.13	0.47
43:Lk:5:ILE:HD11	43:Lk:43:TYR:HB3	1.97	0.47
49:Lr:97:ILE:HD13	49:Lr:107:ARG:HA	1.96	0.47
53:S2:1218:C:H2'	53:S2:1219:C:H6	1.79	0.47
58:SG:2:LYS:HB2	58:SG:108:VAL:HG22	1.96	0.47
67:SP:58:LYS:HE3	67:SP:58:LYS:HB3	1.71	0.47
7:L5:755:C:H2'	7:L5:756:G:H8	1.79	0.47
7:L5:1762:C:C4	7:L5:1770:A:N1	2.82	0.47
7:L5:3641:U:H5	7:L5:3646:A:N7	2.13	0.47
7:L5:3727:A:H2'	7:L5:3728:A:C8	2.50	0.47
15:LH:7:ASN:HD22	15:LH:56:ARG:HH11	1.62	0.47
44:Ll:43:HIS:HB3	44:Ll:46:ARG:HG3	1.95	0.47
51:Lt:82:ILE:HG21	51:Lt:137:GLN:HG3	1.97	0.47
58:SG:3:LEU:HB3	58:SG:5:ILE:HD11	1.96	0.47
7:L5:268:G:H2'	7:L5:269:G:H8	1.79	0.47
7:L5:4219:A:H2'	7:L5:4220:A:C8	2.49	0.47
15:LH:76:HIS:O	15:LH:80:MET:HG3	2.14	0.47
18:LL:163:LYS:HA	18:LL:163:LYS:HD2	1.65	0.47
31:LY:2:LYS:HB3	31:LY:2:LYS:HE3	1.70	0.47
53:S2:1536:G:H2'	53:S2:1537:A:H8	1.78	0.47
83:Sf:89:LYS:HE3	83:Sf:92:LYS:HD3	1.95	0.47
7:L5:490:C:H2'	7:L5:491:G:H8	1.79	0.47
7:L5:1468:C:H2'	7:L5:1469:C:C6	2.50	0.47
16:LI:61:SER:HA	16:LI:126:VAL:HG12	1.97	0.47
29:LW:78:PHE:HB3	58:SG:131:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Lt:11:LYS:HD2	51:Lt:11:LYS:HA	1.65	0.47
53:S2:640:A:H2'	53:S2:641:A:C8	2.49	0.47
62:SK:49:MET:HA	62:SK:52:LEU:HG	1.97	0.47
72:SU:101:ILE:HA	72:SU:104:ILE:HG13	1.96	0.47
78:Sa:45:VAL:HG11	78:Sa:64:LEU:HD22	1.96	0.47
7:L5:717:U:H2'	7:L5:718:C:C6	2.49	0.47
7:L5:4601:U:H2'	7:L5:4602:A:H8	1.80	0.47
10:LC:154:VAL:HG21	10:LC:170:LEU:HD11	1.96	0.47
20:LN:99:GLN:O	20:LN:103:GLU:HG3	2.15	0.47
40:Lh:91:MET:HA	40:Lh:94:ARG:HB2	1.96	0.47
48:Lp:36:LYS:HE2	48:Lp:48:LYS:HB2	1.96	0.47
51:Lt:65:GLN:HA	51:Lt:70:GLN:HA	1.97	0.47
55:SD:76:ARG:HG3	55:SD:77:PHE:HD2	1.80	0.47
59:SH:160:LYS:HD2	59:SH:191:GLU:HA	1.95	0.47
67:SP:87:PRO:HA	67:SP:90:VAL:HG23	1.96	0.47
74:SW:14:ILE:HD11	74:SW:27:ILE:HD11	1.95	0.47
6:SB:183:GLU:HG3	6:SB:187:LYS:HE3	1.96	0.47
24:LR:105:LEU:HD22	24:LR:135:LYS:HG3	1.96	0.47
50:Ls:25:PRO:HB2	50:Ls:26:LYS:HD2	1.96	0.47
53:S2:996:A:H2'	53:S2:997:A:C8	2.49	0.47
57:SF:53:ALA:HB1	68:SQ:125:ARG:HH22	1.80	0.47
7:L5:257:C:H2'	7:L5:258:G:H8	1.80	0.47
7:L5:1907:A:H4'	13:LF:223:LYS:HE3	1.97	0.47
25:LS:96:GLU:HB3	25:LS:142:VAL:HG21	1.97	0.47
36:Ld:32:ARG:HD3	36:Ld:48:GLU:HB3	1.97	0.47
50:Ls:192:VAL:HB	50:Ls:199:TYR:HB2	1.96	0.47
53:S2:377:G:H5'	60:SI:98:LYS:HB3	1.96	0.47
80:Sc:46:VAL:HG21	80:Sc:50:VAL:HG21	1.96	0.47
1:LA:172:GLY:HA3	48:Lp:68:ALA:H	1.80	0.46
7:L5:313:U:H5''	20:LN:179:LYS:HE3	1.97	0.46
7:L5:1994:C:H2'	7:L5:1995:G:H8	1.79	0.46
13:LF:127:LYS:HB2	26:LT:133:ALA:HB3	1.96	0.46
53:S2:102:A:H4'	53:S2:104:A:C8	2.50	0.46
53:S2:1736:G:H2'	53:S2:1737:G:C8	2.50	0.46
60:SI:34:ALA:HB2	60:SI:56:ARG:HD2	1.98	0.46
20:LN:113:LEU:HD22	20:LN:136:ASP:HA	1.96	0.46
53:S2:1536:G:H2'	53:S2:1537:A:C8	2.50	0.46
61:SJ:160:SER:HB3	61:SJ:163:SER:HB2	1.97	0.46
68:SQ:34:VAL:HA	68:SQ:70:VAL:HG22	1.97	0.46
7:L5:461:G:H2'	7:L5:462:G:H8	1.80	0.46
7:L5:1460:C:H5''	23:LQ:144:LYS:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L5:1604:G:H2'	7:L5:1605:G:C8	2.51	0.46
7:L5:3684:G:H2'	7:L5:3685:C:C6	2.50	0.46
7:L5:3910:C:H2'	7:L5:3911:C:C6	2.51	0.46
7:L5:4302:U:H4'	26:LT:5:LYS:HD2	1.97	0.46
7:L5:4593:C:H2'	7:L5:4594:U:H6	1.80	0.46
53:S2:1098:C:H2'	53:S2:1099:G:C8	2.50	0.46
55:SD:22:ASN:O	55:SD:26:THR:HG23	2.15	0.46
3:SA:76:VAL:HG12	3:SA:123:VAL:HB	1.97	0.46
17:LJ:15:LEU:HD23	17:LJ:134:LEU:HD13	1.97	0.46
53:S2:639:C:H2'	53:S2:640:A:H8	1.80	0.46
53:S2:1298:G:H4'	67:SP:78:THR:HA	1.98	0.46
55:SD:49:ILE:HG12	55:SD:87:TYR:HB2	1.98	0.46
57:SF:22:LYS:HB3	57:SF:22:LYS:HE2	1.71	0.46
57:SF:39:ILE:HG21	57:SF:113:VAL:HG22	1.96	0.46
59:SH:7:LYS:HA	59:SH:7:LYS:HD3	1.71	0.46
60:SI:57:ALA:HB2	60:SI:183:GLY:HA2	1.98	0.46
67:SP:60:LEU:HD13	67:SP:89:MET:HG3	1.97	0.46
71:ST:128:GLN:HE21	71:ST:129:ARG:HH12	1.63	0.46
81:Sd:3:HIS:HB3	81:Sd:6:LEU:HG	1.97	0.46
10:LC:294:LYS:HE3	10:LC:294:LYS:HB3	1.72	0.46
13:LF:62:ARG:O	13:LF:66:ARG:HG2	2.15	0.46
55:SD:175:VAL:O	55:SD:181:VAL:HA	2.15	0.46
60:SI:17:LYS:HA	60:SI:17:LYS:HD2	1.76	0.46
9:L8:41:A:H4'	42:Lj:59:THR:HG23	1.97	0.46
10:LC:66:SER:HA	10:LC:77:PRO:HA	1.98	0.46
14:LG:165:GLU:HA	14:LG:168:VAL:HG22	1.97	0.46
53:S2:1037:G:H4'	53:S2:1845:A:H4'	1.98	0.46
55:SD:142:LEU:HD13	55:SD:150:MET:HG3	1.98	0.46
63:SL:120:VAL:HG22	63:SL:145:VAL:HG11	1.96	0.46
68:SQ:68:ILE:HG21	68:SQ:88:ILE:HG22	1.98	0.46
84:Sg:73:SER:H	84:Sg:117:ASN:HD21	1.61	0.46
4:LB:130:PHE:H	7:L5:4727:A:H5'	1.81	0.46
6:SB:136:ARG:HB2	6:SB:218:LEU:HD11	1.96	0.46
7:L5:318:A:H2'	7:L5:319:A:C8	2.51	0.46
12:LE:278:THR:HB	12:LE:281:ILE:HG12	1.97	0.46
49:Lr:101:LYS:HE2	49:Lr:101:LYS:HB2	1.77	0.46
55:SD:141:LYS:HD2	55:SD:179:GLN:HB3	1.97	0.46
58:SG:1:MET:HE3	58:SG:1:MET:HB2	1.84	0.46
66:SO:78:ALA:HB3	66:SO:118:ALA:HB3	1.98	0.46
6:SB:225:LEU:HD12	14:LG:264:LYS:HA	1.98	0.46
7:L5:746:A:H2'	7:L5:747:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L5:1365:C:H5	7:L5:1366:G:H21	1.64	0.46
26:LT:28:ALA:HA	26:LT:31:MET:HB2	1.97	0.46
52:N4:153:LYS:HG3	52:N4:185:PHE:HE1	1.81	0.46
54:SC:212:LYS:O	54:SC:216:MET:HG3	2.16	0.46
55:SD:55:THR:H	55:SD:90:LYS:NZ	2.14	0.46
55:SD:213:PRO:HG3	69:SR:19:LYS:HZ3	1.80	0.46
68:SQ:32:ILE:HG13	68:SQ:68:ILE:HB	1.97	0.46
70:SS:24:ARG:HD3	70:SS:24:ARG:HA	1.80	0.46
3:SA:85:ARG:O	3:SA:89:LYS:HG2	2.16	0.46
30:LX:73:HIS:HB2	30:LX:115:LYS:HZ3	1.80	0.46
32:LZ:25:ILE:HA	32:LZ:43:VAL:HG12	1.97	0.46
54:SC:70:VAL:HG21	54:SC:93:ILE:HG23	1.98	0.46
56:SE:72:ILE:HG12	56:SE:90:ILE:HG12	1.97	0.46
61:SJ:29:LEU:HB3	82:Se:42:PHE:HE2	1.80	0.46
75:SX:107:ARG:HB3	75:SX:110:HIS:HB3	1.98	0.46
7:L5:93:G:H2'	7:L5:94:A:C8	2.51	0.46
14:LG:165:GLU:HB3	20:LN:10:LEU:HD23	1.98	0.46
33:La:43:ILE:O	33:La:47:LYS:HB2	2.16	0.46
50:Ls:55:MET:HB3	50:Ls:87:GLY:HA2	1.97	0.46
50:Ls:63:LYS:HA	50:Ls:63:LYS:HD3	1.78	0.46
53:S2:639:C:H2'	53:S2:640:A:C8	2.50	0.46
57:SF:122:ARG:HG2	57:SF:146:ARG:NH1	2.30	0.46
59:SH:30:LEU:O	59:SH:34:SER:CB	2.58	0.46
60:SI:151:GLU:HA	60:SI:154:LYS:NZ	2.31	0.46
71:ST:80:GLY:CA	71:ST:93:SER:O	2.64	0.46
77:SZ:102:LYS:HA	77:SZ:107:VAL:HG23	1.98	0.46
7:L5:1914:C:H4'	21:LO:89:PRO:HD3	1.98	0.45
7:L5:4309:G:H5'	7:L5:4338:G:H5''	1.98	0.45
7:L5:4967:A:H2'	7:L5:4968:A:C8	2.51	0.45
15:LH:44:GLU:HB3	15:LH:58:ASP:HB2	1.97	0.45
15:LH:91:LYS:HG2	15:LH:145:ILE:HD13	1.97	0.45
32:LZ:11:VAL:HG12	32:LZ:82:PRO:HA	1.97	0.45
32:LZ:29:ILE:HG22	32:LZ:32:GLY:H	1.80	0.45
43:Lk:35:LYS:HA	43:Lk:43:TYR:O	2.16	0.45
59:SH:25:GLN:HA	59:SH:28:LEU:HD12	1.98	0.45
74:SW:111:MET:HE1	74:SW:119:LYS:HD2	1.98	0.45
84:Sg:36:ARG:HG2	84:Sg:65:PHE:HB3	1.98	0.45
7:L5:2667:C:O4'	24:LR:96:MET:HG3	2.16	0.45
8:L7:74:A:H61	8:L7:100:A:H3'	1.81	0.45
15:LH:18:ILE:HG12	15:LH:27:VAL:HG22	1.98	0.45
44:Ll:28:ARG:H	44:Ll:28:ARG:HG2	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:N4:142:LEU:HD21	52:N4:151:LEU:HB3	1.97	0.45
53:S2:223:C:H2'	53:S2:224:A:C8	2.51	0.45
53:S2:385:G:H3'	63:SL:136:LYS:HB2	1.99	0.45
58:SG:20:ASP:HB3	58:SG:23:LYS:HD2	1.98	0.45
77:SZ:56:ASP:HA	77:SZ:59:CYS:HB2	1.98	0.45
16:LI:19:LYS:HE2	16:LI:26:VAL:HB	1.98	0.45
53:S2:1705:C:H2'	53:S2:1706:G:C8	2.52	0.45
53:S2:1854:U:H2'	53:S2:1855:G:H8	1.81	0.45
55:SD:42:THR:HG22	55:SD:45:ARG:H	1.80	0.45
7:L5:162:A:H2'	7:L5:163:A:C8	2.52	0.45
7:L5:3656:A:H2'	7:L5:3657:U:H6	1.82	0.45
11:LD:164:LYS:HA	11:LD:167:VAL:HG22	1.99	0.45
16:LI:30:LYS:HG2	16:LI:63:GLU:HG3	1.98	0.45
56:SE:87:MET:HG3	56:SE:100:ARG:HH11	1.81	0.45
57:SF:44:LYS:HE2	57:SF:44:LYS:HB2	1.82	0.45
57:SF:187:SER:O	57:SF:191:LYS:HG2	2.17	0.45
61:SJ:55:LYS:HE3	61:SJ:55:LYS:HB2	1.69	0.45
12:LE:176:THR:HB	12:LE:186:LEU:HD13	1.98	0.45
12:LE:278:THR:HG22	12:LE:279:ASN:H	1.81	0.45
15:LH:15:ASN:HD21	15:LH:85:THR:HG22	1.80	0.45
31:LY:124:LYS:O	31:LY:128:VAL:HG23	2.17	0.45
39:Lg:19:LYS:HA	39:Lg:19:LYS:HD3	1.72	0.45
52:N4:195:ASP:HB3	52:N4:213:ILE:HG23	1.97	0.45
53:S2:455:A:H2'	53:S2:456:C:H6	1.81	0.45
53:S2:1099:G:H22	53:S2:1133:A:H2	1.63	0.45
53:S2:1217:A:H2'	53:S2:1218:C:C6	2.51	0.45
56:SE:19:MET:SD	56:SE:108:ARG:HD2	2.57	0.45
63:SL:77:VAL:HG11	63:SL:80:MET:HE3	1.98	0.45
71:ST:108:GLU:HG2	71:ST:113:VAL:HG23	1.99	0.45
17:LJ:50:PHE:HB2	17:LJ:67:LYS:HZ2	1.82	0.45
20:LN:104:GLU:HA	20:LN:160:GLU:HG3	1.98	0.45
24:LR:126:LYS:HG2	24:LR:131:VAL:HG21	1.98	0.45
24:LR:178:GLN:HA	24:LR:181:LYS:HG2	1.99	0.45
33:La:36:GLY:HA3	33:La:40:HIS:CE1	2.52	0.45
53:S2:540:U:H2'	53:S2:541:U:H6	1.82	0.45
53:S2:1777:G:H2'	53:S2:1778:C:C6	2.52	0.45
76:SY:14:THR:HG22	76:SY:21:LYS:HE2	1.98	0.45
7:L5:2411:C:H2'	7:L5:2412:A:C8	2.52	0.45
17:LJ:31:ASP:O	17:LJ:35:ARG:HG3	2.17	0.45
51:Lt:151:ILE:O	51:Lt:155:ILE:HB	2.16	0.45
53:S2:167:G:N2	58:SG:132:ARG:HH22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:525:A:H2'	53:S2:526:A:C8	2.52	0.45
74:SW:55:ASP:HB3	79:Sb:25:VAL:HG22	1.98	0.45
7:L5:25:A:H2'	7:L5:26:C:H6	1.82	0.45
7:L5:1969:G:H4'	50:Ls:36:GLY:HA2	1.98	0.45
7:L5:2261:G:H4'	12:LE:112:MET:HE1	1.98	0.45
7:L5:4108:G:H2'	7:L5:4109:G:C8	2.52	0.45
36:Ld:22:THR:HA	36:Ld:88:LEU:O	2.16	0.45
53:S2:455:A:H2'	53:S2:456:C:C6	2.51	0.45
54:SC:199:PRO:HG3	61:SJ:58:ARG:HH11	1.81	0.45
68:SQ:50:LYS:HD3	68:SQ:50:LYS:HA	1.77	0.45
14:LG:37:LYS:HB3	14:LG:37:LYS:HE2	1.78	0.45
15:LH:106:GLN:HB2	15:LH:111:LEU:HB3	1.97	0.45
19:LM:126:GLU:HB3	21:LO:181:ALA:HB1	1.98	0.45
32:LZ:120:GLU:O	32:LZ:124:THR:HG23	2.17	0.45
35:Lc:50:ASN:ND2	35:Lc:76:GLY:H	2.14	0.45
52:N4:158:ILE:O	52:N4:162:MET:HG2	2.16	0.45
53:S2:210:U:H2'	53:S2:211:G:H8	1.81	0.45
53:S2:379:C:H5'	60:SI:33:ALA:HA	1.98	0.45
65:SN:115:LEU:O	65:SN:119:GLU:HG3	2.16	0.45
77:SZ:85:ARG:HA	77:SZ:88:LEU:HD23	1.99	0.45
82:Se:12:VAL:HA	82:Se:15:GLN:HG2	1.98	0.45
2:NA:179:LYS:HA	2:NA:179:LYS:HD2	1.82	0.45
53:S2:115:U:H2'	53:S2:116:U:C6	2.52	0.45
53:S2:220:U:H2'	53:S2:221:A:H8	1.82	0.45
58:SG:18:VAL:HG21	58:SG:24:LEU:HD11	1.99	0.45
3:SA:134:LEU:HD22	3:SA:144:THR:HG21	1.97	0.44
7:L5:490:C:H2'	7:L5:491:G:C8	2.52	0.44
12:LE:177:GLY:HA2	12:LE:178:PRO:HD3	1.87	0.44
12:LE:190:HIS:HB3	12:LE:193:PHE:HD2	1.82	0.44
12:LE:239:LYS:HE2	12:LE:239:LYS:N	2.32	0.44
16:LI:212:LEU:HD23	16:LI:212:LEU:HA	1.82	0.44
17:LJ:22:LEU:HA	17:LJ:129:ASP:O	2.17	0.44
52:N4:94:ASP:HA	52:N4:97:LYS:HG2	1.98	0.44
55:SD:26:THR:O	55:SD:30:ALA:HB2	2.17	0.44
56:SE:92:ILE:HG21	76:SY:17:LEU:HD11	1.99	0.44
1:LA:178:PRO:HD2	48:Lp:26:VAL:HG12	1.98	0.44
5:NB:29:LYS:HA	27:LU:115:PHE:HD1	1.82	0.44
6:SB:138:PHE:HD2	6:SB:214:LYS:HB3	1.81	0.44
8:L7:112:U:H2'	8:L7:113:G:H8	1.82	0.44
11:LD:125:VAL:HG11	11:LD:199:ILE:HG21	1.99	0.44
31:LY:67:ILE:HG12	31:LY:107:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Ls:95:LEU:HD13	50:Ls:192:VAL:HG11	1.99	0.44
53:S2:162:C:H5''	58:SG:87:ARG:HH22	1.82	0.44
59:SH:113:LYS:HB3	59:SH:113:LYS:HE3	1.67	0.44
72:SU:55:ARG:HE	72:SU:87:ARG:CZ	2.30	0.44
1:LA:112:ILE:HG13	48:Lp:79:VAL:HG22	1.99	0.44
2:NA:183:LEU:HD11	52:N4:154:PHE:HE1	1.83	0.44
4:LB:29:VAL:HA	4:LB:220:ILE:HD13	1.99	0.44
7:L5:4239:A:H2'	7:L5:4240:G:C8	2.53	0.44
25:LS:30:MET:HE2	25:LS:30:MET:HB3	1.77	0.44
29:LW:71:ARG:HA	29:LW:71:ARG:HD3	1.80	0.44
53:S2:1568:C:H2'	53:S2:1569:A:C8	2.52	0.44
54:SC:137:VAL:HG23	54:SC:216:MET:HB2	2.00	0.44
71:ST:29:LYS:HE3	71:ST:106:ALA:HB2	2.00	0.44
80:Sc:34:PHE:HB2	80:Sc:40:ARG:HH21	1.82	0.44
84:Sg:68:ASP:HB3	84:Sg:111:VAL:HG22	2.00	0.44
7:L5:956:A:H8	7:L5:957:G:C8	2.36	0.44
7:L5:1535:C:H5''	42:Lj:10:LYS:HB2	1.99	0.44
7:L5:4742:G:H2'	7:L5:4743:G:H8	1.81	0.44
16:LI:31:ILE:HG22	16:LI:62:SER:HB2	2.00	0.44
18:LL:79:GLU:O	18:LL:83:VAL:HG23	2.18	0.44
53:S2:91:A:H61	58:SG:89:THR:HG22	1.82	0.44
2:NA:121:ILE:HG13	5:NB:44:LEU:HD22	2.00	0.44
7:L5:223:G:H4'	7:L5:225:G:N7	2.33	0.44
7:L5:1855:G:OP1	34:Lb:4:SER:HB2	2.18	0.44
7:L5:4169:G:H4'	7:L5:4171:C:C2	2.52	0.44
7:L5:4761:G:H2'	7:L5:4762:A:H8	1.83	0.44
19:LM:124:LYS:HB2	19:LM:124:LYS:HE3	1.67	0.44
53:S2:17:C:H2'	53:S2:18:C:C6	2.53	0.44
53:S2:1402:A:H5''	72:SU:51:LYS:HE2	1.99	0.44
53:S2:1513:C:H2'	53:S2:1514:G:C8	2.52	0.44
57:SF:87:LEU:HD21	68:SQ:47:LEU:HD23	1.99	0.44
67:SP:76:VAL:O	67:SP:94:VAL:HA	2.17	0.44
84:Sg:42:MET:SD	84:Sg:57:ARG:HB2	2.57	0.44
7:L5:1415:G:H2'	7:L5:1416:G:H8	1.83	0.44
7:L5:1933:G:H2'	7:L5:1934:A:C8	2.53	0.44
7:L5:4594:U:H2'	7:L5:4595:G:H8	1.81	0.44
7:L5:4761:G:H2'	7:L5:4762:A:C8	2.53	0.44
26:LT:88:ARG:HH22	34:Lb:30:GLU:CD	2.25	0.44
43:Lk:29:LYS:HE2	43:Lk:29:LYS:N	2.31	0.44
50:Ls:134:LYS:H	50:Ls:134:LYS:HG2	1.52	0.44
51:Lt:34:PRO:HG3	51:Lt:40:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:1593:C:H2'	53:S2:1594:A:C8	2.53	0.44
59:SH:130:LEU:HD21	59:SH:156:VAL:HG21	2.00	0.44
69:SR:72:LYS:N	69:SR:72:LYS:HE2	2.33	0.44
70:SS:114:LEU:HD11	70:SS:121:ARG:HB2	1.98	0.44
75:SX:130:LEU:HD23	75:SX:130:LEU:HA	1.83	0.44
7:L5:1846:G:H2'	7:L5:1847:C:C6	2.53	0.44
7:L5:2411:C:H2'	7:L5:2412:A:H8	1.82	0.44
14:LG:131:LYS:HD2	14:LG:131:LYS:HA	1.77	0.44
20:LN:47:LYS:HD2	20:LN:50:ARG:HH11	1.82	0.44
29:LW:119:LYS:HD3	29:LW:119:LYS:HA	1.81	0.44
52:N4:60:LYS:HE3	52:N4:64:GLY:HA3	2.00	0.44
53:S2:1520:G:H5'	70:SS:136:THR:HG22	1.99	0.44
57:SF:201:LYS:HD3	57:SF:204:ARG:NH2	2.33	0.44
60:SI:174:CYS:HB2	60:SI:190:LEU:HD21	1.98	0.44
67:SP:90:VAL:HA	67:SP:107:ILE:HG21	2.00	0.44
71:ST:56:ARG:HG3	71:ST:103:VAL:HG21	2.00	0.44
82:Se:51:LYS:HA	82:Se:51:LYS:HD2	1.79	0.44
84:Sg:11:LEU:CB	84:Sg:307:VAL:O	2.64	0.44
5:NB:43:LYS:HD2	5:NB:46:PHE:CE2	2.53	0.44
7:L5:2103:G:H2'	7:L5:2104:G:H8	1.81	0.44
34:Lb:117:ARG:HA	34:Lb:117:ARG:HD3	1.65	0.44
76:SY:55:ILE:HG23	76:SY:75:ILE:HG13	2.00	0.44
77:SZ:48:VAL:HG13	77:SZ:83:LEU:HD11	1.99	0.44
7:L5:1307:A:H2'	7:L5:1308:C:C6	2.53	0.44
7:L5:1725:U:H2'	7:L5:1726:U:H6	1.83	0.44
7:L5:3917:A:H2'	7:L5:3918:G:H8	1.83	0.44
7:L5:4389:C:H2'	7:L5:4390:A:H8	1.83	0.44
9:L8:148:A:H2'	9:L8:149:G:C8	2.53	0.44
9:L8:154:G:H3'	14:LG:89:ARG:HH22	1.83	0.44
10:LC:221:PHE:HB3	10:LC:227:ILE:HG21	1.99	0.44
14:LG:80:ILE:HD11	20:LN:18:VAL:HG23	2.00	0.44
19:LM:7:VAL:HG13	19:LM:27:ILE:HD13	2.00	0.44
23:LQ:9:LYS:HA	23:LQ:9:LYS:HD3	1.74	0.44
35:Lc:26:LYS:HB2	35:Lc:26:LYS:HE3	1.75	0.44
50:Ls:13:TYR:HE1	50:Ls:54:LEU:HD21	1.82	0.44
68:SQ:108:ILE:HA	68:SQ:111:ILE:HG22	2.00	0.44
5:NB:19:ARG:HD3	5:NB:19:ARG:HA	1.79	0.43
7:L5:2870:A:H2'	7:L5:2871:A:H8	1.81	0.43
53:S2:106:C:H2'	53:S2:107:A:H8	1.83	0.43
53:S2:391:C:H2'	53:S2:392:A:H8	1.83	0.43
53:S2:508:A:H3'	53:S2:509:G:C8	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:1010:G:H2'	53:S2:1011:A:C8	2.52	0.43
53:S2:1405:A:H2'	53:S2:1406:G:O4'	2.18	0.43
61:SJ:60:LEU:HD22	61:SJ:70:ARG:HA	1.99	0.43
71:ST:33:TRP:HZ2	71:ST:102:ARG:HG3	1.83	0.43
7:L5:300:A:H2'	7:L5:301:G:C8	2.52	0.43
7:L5:1363:C:H3'	18:LL:36:ARG:NH2	2.33	0.43
10:LC:348:LYS:HB3	10:LC:348:LYS:HE3	1.81	0.43
11:LD:60:ILE:HB	11:LD:80:ALA:HB2	1.99	0.43
26:LT:106:LEU:HA	26:LT:109:VAL:HG22	2.00	0.43
31:LY:61:HIS:CE1	52:N4:15:ARG:HD2	2.53	0.43
45:Lm:98:MLZ:HD3	45:Lm:118:THR:HG21	1.99	0.43
53:S2:1652:G:H1	53:S2:1672:U:H3	1.65	0.43
56:SE:67:GLN:HB3	56:SE:69:PHE:CE2	2.53	0.43
57:SF:78:MET:HE2	57:SF:78:MET:HB2	1.92	0.43
60:SI:74:ARG:HD2	60:SI:108:PRO:HB3	2.01	0.43
7:L5:10:A:H2'	7:L5:11:G:C8	2.53	0.43
7:L5:418:A:C2	9:L8:17:A:H1'	2.54	0.43
20:LN:146:PRO:HA	20:LN:149:GLN:HG3	1.99	0.43
40:Lh:10:ARG:HA	40:Lh:10:ARG:HD3	1.86	0.43
49:Lr:122:LYS:HE3	49:Lr:122:LYS:HB2	1.75	0.43
53:S2:28:U:H2'	53:S2:29:G:H8	1.83	0.43
53:S2:51:U:H2'	53:S2:52:G:C8	2.54	0.43
53:S2:502:C:O4'	56:SE:66:MET:HG3	2.18	0.43
84:Sg:133:ASN:HD21	84:Sg:137:VAL:HG22	1.83	0.43
1:LA:122:ASP:HB2	1:LA:125:LYS:HE2	2.01	0.43
7:L5:1097:C:H2'	7:L5:1098:G:H8	1.83	0.43
7:L5:3732:A:H2'	7:L5:3733:A:C8	2.54	0.43
7:L5:4459:U:H2'	7:L5:4460:U:C6	2.53	0.43
21:LO:180:GLN:HE22	21:LO:183:LYS:NZ	2.16	0.43
30:LX:81:LEU:HG	30:LX:83:THR:HG23	2.01	0.43
53:S2:833:C:H2'	53:S2:834:C:C6	2.53	0.43
53:S2:1580:A:C8	72:SU:56:MET:HG2	2.53	0.43
67:SP:94:VAL:HG12	67:SP:107:ILE:HD11	2.01	0.43
75:SX:32:LEU:HD12	75:SX:32:LEU:HA	1.88	0.43
79:Sb:5:LYS:HE3	79:Sb:7:LEU:HD23	2.01	0.43
4:LB:238:LYS:HE2	4:LB:238:LYS:HB2	1.67	0.43
6:SB:82:ARG:HG3	6:SB:103:MET:HE2	2.01	0.43
7:L5:502:C:H3'	7:L5:503:C:H3'	2.00	0.43
7:L5:1093:C:H2'	7:L5:1094:G:H8	1.83	0.43
7:L5:2568:C:H2'	7:L5:2569:G:C8	2.53	0.43
7:L5:3707:U:H2'	7:L5:3708:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L5:4321:U:H2'	7:L5:4322:G:C8	2.53	0.43
19:LM:85:LYS:O	19:LM:89:THR:HG23	2.18	0.43
29:LW:81:ALA:HB2	29:LW:87:LEU:HD13	2.00	0.43
50:Ls:20:LEU:HD12	50:Ls:20:LEU:HA	1.89	0.43
53:S2:220:U:H2'	53:S2:221:A:C8	2.54	0.43
53:S2:375:U:H2'	53:S2:376:A:H8	1.84	0.43
53:S2:528:A:H2'	53:S2:529:A:C8	2.53	0.43
53:S2:535:G:H2'	53:S2:536:A:H8	1.83	0.43
53:S2:1757:G:H8	53:S2:1758:G:H1'	1.83	0.43
55:SD:55:THR:O	55:SD:59:LEU:HD22	2.19	0.43
63:SL:127:THR:HB	63:SL:144:LYS:HG2	2.01	0.43
70:SS:33:ILE:HD11	70:SS:100:ALA:HB2	2.01	0.43
76:SY:21:LYS:HE2	76:SY:21:LYS:HB3	1.77	0.43
82:Se:18:LYS:HE2	82:Se:18:LYS:N	2.34	0.43
84:Sg:20:GLN:HG2	84:Sg:69:VAL:H	1.84	0.43
2:NA:205:ASP:HB3	2:NA:208:ASN:OD1	2.18	0.43
4:LB:28:LYS:HD3	4:LB:30:LYS:HG3	2.00	0.43
12:LE:192:LYS:HD3	38:Lf:107:PRO:HB3	2.00	0.43
22:LP:37:LYS:HG3	22:LP:117:ILE:HG22	2.00	0.43
25:LS:70:LYS:HD3	25:LS:70:LYS:HA	1.83	0.43
27:LU:22:THR:HA	27:LU:70:ILE:O	2.18	0.43
52:N4:78:LYS:HA	52:N4:92:TRP:HH2	1.83	0.43
74:SW:3:ARG:HD3	74:SW:6:VAL:HG12	2.00	0.43
84:Sg:17:TRP:HB2	84:Sg:36:ARG:HD2	2.01	0.43
4:LB:5:LYS:HB3	4:LB:5:LYS:HE2	1.84	0.43
7:L5:1563:A:H2'	7:L5:1564:A:C8	2.54	0.43
14:LG:99:ALA:HB1	14:LG:136:LEU:HD11	2.00	0.43
30:LX:83:THR:O	30:LX:87:MET:HG2	2.18	0.43
36:Ld:23:ARG:HG2	36:Ld:121:ASN:HA	2.00	0.43
45:Lm:94:MET:HE3	45:Lm:94:MET:HB3	1.80	0.43
53:S2:528:A:H2'	53:S2:529:A:H8	1.84	0.43
67:SP:111:MET:HG3	67:SP:119:PHE:HZ	1.83	0.43
7:L5:469:C:H2'	7:L5:470:A:H8	1.84	0.43
7:L5:1442:C:H2'	7:L5:1443:A:C8	2.53	0.43
7:L5:1726:U:H5'	13:LF:135:ILE:HD11	1.99	0.43
7:L5:1867:A:H2'	7:L5:1868:A:C8	2.54	0.43
7:L5:2611:A:H2'	7:L5:2612:G:C8	2.54	0.43
7:L5:3664:G:H2'	7:L5:3665:G:H8	1.83	0.43
19:LM:100:ARG:HA	19:LM:103:LYS:HE2	2.00	0.43
31:LY:72:GLN:HB3	31:LY:81:TYR:HB2	2.01	0.43
52:N4:172:MET:HA	52:N4:214:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SP:29:SER:H	67:SP:32:GLN:NE2	2.17	0.43
69:SR:41:ILE:HA	69:SR:42:PRO:HD3	1.92	0.43
79:Sb:36:LYS:HE2	79:Sb:36:LYS:HB2	1.76	0.43
80:Sc:18:LEU:HB2	80:Sc:29:GLN:HB3	2.00	0.43
7:L5:1788:A:H2'	16:LI:22:PHE:CZ	2.53	0.43
9:L8:141:C:H2'	9:L8:142:U:C6	2.53	0.43
11:LD:238:GLU:O	11:LD:242:LYS:HG3	2.18	0.43
33:La:71:PRO:HG2	33:La:108:TYR:HA	2.01	0.43
53:S2:77:A:P	58:SG:154:ARG:HH22	2.42	0.43
55:SD:68:GLU:O	55:SD:72:VAL:HG23	2.19	0.43
77:SZ:45:ASN:HB2	77:SZ:80:ARG:HH21	1.83	0.43
2:NA:94:VAL:HB	2:NA:106:ILE:HB	2.00	0.43
4:LB:217:ILE:HD12	4:LB:347:LEU:HB3	2.01	0.43
7:L5:162:A:H2'	7:L5:163:A:H8	1.84	0.43
7:L5:1733:G:N3	7:L5:4214:A:H2'	2.34	0.43
7:L5:2520:C:H2'	7:L5:2521:G:H8	1.84	0.43
7:L5:4260:U:H2'	7:L5:4261:C:C6	2.53	0.43
7:L5:4507:A:H2'	7:L5:4508:C:C6	2.54	0.43
16:LI:51:HIS:CD2	16:LI:168:SER:HB2	2.53	0.43
21:LO:177:LEU:HD23	21:LO:177:LEU:HA	1.90	0.43
32:LZ:39:SER:HB3	32:LZ:77:TYR:CD2	2.54	0.43
34:Lb:73:LYS:HA	34:Lb:73:LYS:HD3	1.72	0.43
53:S2:862:A:C8	74:SW:107:SER:HA	2.54	0.43
53:S2:1256:G:H1	81:Sd:31:ILE:HG23	1.84	0.43
67:SP:41:GLN:HB3	67:SP:84:ILE:HD13	2.01	0.43
70:SS:84:LEU:HD22	70:SS:97:GLN:HB2	2.01	0.43
82:Se:27:LYS:H	82:Se:27:LYS:HG2	1.64	0.43
6:SB:28:LYS:HA	6:SB:50:THR:HA	2.01	0.42
7:L5:4578:G:H2'	7:L5:4579:U:C6	2.54	0.42
7:L5:4594:U:H2'	7:L5:4595:G:C8	2.54	0.42
9:L8:47:C:H1'	9:L8:61:A:H2'	2.01	0.42
9:L8:106:G:H4'	9:L8:137:A:H5'	2.00	0.42
11:LD:156:GLY:HA2	11:LD:181:PRO:HG3	2.01	0.42
12:LE:112:MET:HG3	12:LE:113:PRO:HD2	2.01	0.42
17:LJ:44:THR:HG21	17:LJ:72:CYS:SG	2.59	0.42
19:LM:53:LYS:HB3	19:LM:53:LYS:HE3	1.66	0.42
22:LP:54:GLN:HA	22:LP:83:TRP:CD1	2.53	0.42
25:LS:47:PHE:CE1	25:LS:125:GLN:HG2	2.54	0.42
53:S2:527:C:H2'	53:S2:528:A:C8	2.54	0.42
53:S2:649:U:H2'	53:S2:650:A:C8	2.50	0.42
53:S2:1801:A:H2'	53:S2:1802:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SP:107:ILE:HA	67:SP:111:MET:HE1	1.99	0.42
72:SU:55:ARG:HE	72:SU:87:ARG:NH1	2.16	0.42
76:SY:21:LYS:HG3	76:SY:75:ILE:HB	2.00	0.42
1:LA:3:ARG:HD2	1:LA:208:GLU:HG2	2.01	0.42
4:LB:103:LYS:HA	4:LB:103:LYS:HD3	1.75	0.42
7:L5:1593:A:H5''	7:L5:2839:U:H5''	2.02	0.42
7:L5:1682:A:H5''	18:LL:3:PRO:O	2.19	0.42
7:L5:4504:C:H2'	7:L5:4505:C:C6	2.54	0.42
10:LC:298:ILE:O	10:LC:302:LEU:HG	2.20	0.42
16:LI:32:ARG:HA	16:LI:32:ARG:HD2	1.83	0.42
53:S2:5:U:H2'	53:S2:6:G:H8	1.83	0.42
53:S2:907:G:H2'	53:S2:908:A:C8	2.54	0.42
53:S2:1298:G:H1'	67:SP:79:HIS:HB2	2.00	0.42
55:SD:173:ARG:HD3	55:SD:173:ARG:HA	1.82	0.42
58:SG:51:ARG:HB3	58:SG:112:VAL:HG23	2.01	0.42
60:SI:190:LEU:HD22	60:SI:194:GLU:HG2	2.00	0.42
63:SL:128:VAL:HG12	63:SL:142:VAL:HA	2.01	0.42
2:NA:85:LEU:HD21	2:NA:115:PRO:HD3	2.00	0.42
7:L5:1662:C:H2'	7:L5:1663:C:C6	2.53	0.42
10:LC:163:LYS:HB3	10:LC:163:LYS:HE3	1.75	0.42
24:LR:133:LYS:HA	24:LR:133:LYS:HD3	1.84	0.42
35:Lc:79:ILE:O	35:Lc:83:THR:HG23	2.19	0.42
51:Lt:57:ARG:NH1	51:Lt:80:LEU:HB3	2.34	0.42
53:S2:1736:G:H2'	53:S2:1737:G:H8	1.85	0.42
67:SP:121:ILE:HD13	67:SP:121:ILE:HA	1.92	0.42
84:Sg:195:LEU:HD13	84:Sg:195:LEU:HA	1.89	0.42
7:L5:1177:U:H2'	7:L5:1178:G:H8	1.84	0.42
7:L5:1356:U:H2'	7:L5:1357:C:C6	2.54	0.42
7:L5:2520:C:H2'	7:L5:2521:G:C8	2.54	0.42
7:L5:4593:C:H2'	7:L5:4594:U:C6	2.54	0.42
20:LN:99:GLN:HG3	20:LN:130:PHE:CD1	2.54	0.42
50:Ls:24:TYR:HA	50:Ls:25:PRO:HD3	1.91	0.42
53:S2:933:G:H22	78:Sa:19:GLN:HE22	1.66	0.42
54:SC:145:LYS:HE2	54:SC:145:LYS:HB2	1.77	0.42
72:SU:20:ILE:HD11	72:SU:93:SER:HB3	2.01	0.42
7:L5:1333:A:H2'	7:L5:1334:A:C8	2.54	0.42
7:L5:1952:G:H4'	25:LS:93:MET:HE3	2.00	0.42
7:L5:1994:C:H2'	7:L5:1995:G:C8	2.54	0.42
7:L5:2485:U:H4'	7:L5:2486:G:N2	2.35	0.42
7:L5:3656:A:H2'	7:L5:3657:U:C6	2.54	0.42
7:L5:4159:C:H2'	7:L5:4160:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L7:58:A:H2'	8:L7:59:G:C8	2.54	0.42
11:LD:235:MET:HE3	11:LD:235:MET:H	1.83	0.42
16:LI:38:ARG:HG2	16:LI:41:ALA:HB2	2.01	0.42
16:LI:91:LEU:HD12	16:LI:135:ILE:HG23	2.02	0.42
17:LJ:164:ARG:NH1	17:LJ:164:ARG:HB2	2.35	0.42
31:LY:111:LEU:HB3	31:LY:116:LYS:HE3	2.00	0.42
52:N4:173:LEU:HD22	52:N4:174:THR:H	1.84	0.42
53:S2:948:C:H2'	53:S2:949:G:H8	1.84	0.42
53:S2:1656:G:H1	53:S2:1668:U:H3	1.66	0.42
68:SQ:62:ARG:HA	68:SQ:62:ARG:CZ	2.49	0.42
70:SS:98:VAL:HG21	70:SS:106:LYS:HD3	2.01	0.42
72:SU:26:SER:HB3	72:SU:110:VAL:HG22	2.01	0.42
72:SU:40:ILE:HG22	72:SU:44:LYS:NZ	2.34	0.42
4:LB:14:LEU:HB3	4:LB:17:LEU:HD22	2.01	0.42
6:SB:125:VAL:HG11	6:SB:172:MET:HB2	2.01	0.42
7:L5:325:U:H2'	7:L5:326:C:C6	2.54	0.42
7:L5:1097:C:H2'	7:L5:1098:G:C8	2.53	0.42
7:L5:2568:C:H2'	7:L5:2569:G:H8	1.83	0.42
7:L5:4274:A:H2'	7:L5:4275:G:H8	1.81	0.42
12:LE:244:GLU:O	12:LE:248:ILE:HD12	2.19	0.42
17:LJ:22:LEU:HD11	17:LJ:82:ILE:HG21	2.01	0.42
38:Lf:52:LYS:HB2	38:Lf:52:LYS:HE2	1.90	0.42
60:SI:66:SER:HA	60:SI:73:THR:HA	2.02	0.42
60:SI:81:VAL:HG22	60:SI:102:VAL:HG12	2.00	0.42
70:SS:124:ARG:HB2	70:SS:131:VAL:HG12	2.01	0.42
75:SX:90:CYS:HA	75:SX:93:PHE:CD2	2.54	0.42
7:L5:1177:U:H2'	7:L5:1178:G:C8	2.55	0.42
7:L5:1794:A:H5''	7:L5:4214:A:H61	1.85	0.42
7:L5:2362:U:H2'	7:L5:2363:A:H8	1.85	0.42
7:L5:3652:A:H2'	7:L5:3653:A:C5	2.54	0.42
24:LR:182:GLU:HA	24:LR:185:ILE:HG12	2.02	0.42
48:Lp:83:ILE:HD13	48:Lp:83:ILE:HA	1.91	0.42
56:SE:84:ALA:HB1	56:SE:101:LEU:HD13	2.01	0.42
69:SR:103:LYS:O	69:SR:107:LYS:HG2	2.20	0.42
74:SW:46:TYR:HB3	74:SW:69:LEU:HD13	2.02	0.42
77:SZ:66:LYS:HE2	77:SZ:66:LYS:HB2	1.95	0.42
84:Sg:17:TRP:H	84:Sg:36:ARG:HB2	1.84	0.42
84:Sg:165:ILE:HG23	84:Sg:177:TRP:HD1	1.84	0.42
84:Sg:212:LYS:HD2	84:Sg:235:ILE:HD12	2.02	0.42
3:SA:52:LYS:HB2	69:SR:109:LEU:HD23	2.01	0.42
4:LB:110:ILE:HG22	4:LB:115:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L5:1677:U:H4'	7:L5:1680:G:C2	2.54	0.42
7:L5:1702:C:C6	7:L5:1703:C:H1'	2.55	0.42
7:L5:3612:C:H1'	7:L5:5016:A:C8	2.55	0.42
7:L5:3774:A:H2'	7:L5:3775:A:C8	2.55	0.42
7:L5:4188:U:H2'	7:L5:4189:U:C6	2.55	0.42
7:L5:4389:C:H2'	7:L5:4390:A:C8	2.54	0.42
7:L5:4935:C:H2'	7:L5:4936:G:C8	2.54	0.42
11:LD:208:MET:HE2	11:LD:233:PRO:HG3	2.01	0.42
13:LF:88:LYS:HE3	13:LF:88:LYS:HB2	1.88	0.42
14:LG:58:PRO:HD2	14:LG:61:ILE:HD12	2.01	0.42
15:LH:101:ILE:HG23	15:LH:114:ILE:HG23	2.02	0.42
33:La:2:PRO:HG2	33:La:5:LEU:HD12	2.02	0.42
53:S2:35:C:H5''	53:S2:579:C:H5''	2.02	0.42
53:S2:71:G:H2'	53:S2:72:C:H4'	2.01	0.42
53:S2:329:G:H2'	53:S2:330:G:C8	2.55	0.42
57:SF:115:ALA:O	57:SF:119:SER:HB2	2.19	0.42
68:SQ:47:LEU:HD21	68:SQ:78:VAL:HG22	2.01	0.42
6:SB:25:PHE:HA	6:SB:28:LYS:HG3	2.01	0.42
7:L5:116:G:H2'	7:L5:117:C:C6	2.55	0.42
7:L5:2714:G:H2'	7:L5:2715:G:H8	1.85	0.42
16:LI:35:ASP:HB3	16:LI:86:HIS:HE2	1.84	0.42
39:Lg:107:LEU:HD12	39:Lg:107:LEU:HA	1.91	0.42
50:Ls:18:ILE:HD13	50:Ls:18:ILE:HA	1.94	0.42
53:S2:929:G:H2'	53:S2:930:C:O4'	2.19	0.42
58:SG:93:LYS:HE3	58:SG:93:LYS:HB3	1.80	0.42
72:SU:37:ALA:O	72:SU:41:ARG:HB2	2.19	0.42
84:Sg:78:ALA:HB2	84:Sg:92:LEU:HD21	2.01	0.42
3:SA:5:LEU:HD13	73:SV:41:LYS:HA	2.01	0.42
4:LB:165:HIS:HB3	4:LB:180:LEU:HD12	2.02	0.42
4:LB:252:ALA:HB3	7:L5:4457:U:H1'	2.01	0.42
5:NB:59:ILE:HG21	5:NB:79:VAL:HG21	2.01	0.42
7:L5:1245:C:H2'	7:L5:1246:G:C8	2.55	0.42
7:L5:2292:C:H2'	7:L5:2293:U:C6	2.55	0.42
7:L5:5057:C:H2'	7:L5:5058:A:C8	2.54	0.42
25:LS:25:PRO:HA	25:LS:26:PRO:HD3	1.93	0.42
49:Lr:35:ARG:HG2	49:Lr:37:SER:HB2	2.02	0.42
53:S2:1201:U:H2'	53:S2:1202:U:C6	2.55	0.42
55:SD:12:VAL:O	55:SD:16:ILE:HG22	2.20	0.42
61:SJ:112:THR:O	61:SJ:116:LYS:HG2	2.20	0.42
70:SS:45:LEU:HD12	70:SS:45:LEU:HA	1.81	0.42
71:ST:4:VAL:HG21	71:ST:136:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:ST:76:THR:HG21	71:ST:97:LYS:HG2	2.02	0.42
84:Sg:22:ALA:HB1	84:Sg:71:ILE:HD11	2.01	0.42
3:SA:125:THR:HG23	3:SA:175:TRP:HE1	1.84	0.41
7:L5:318:A:H2'	7:L5:319:A:H8	1.85	0.41
25:LS:2:LYS:HE2	25:LS:35:PRO:HD3	2.01	0.41
25:LS:78:PHE:O	25:LS:96:GLU:HA	2.20	0.41
37:Le:19:LYS:HB3	37:Le:19:LYS:HE3	1.84	0.41
42:Lj:67:LEU:HD23	42:Lj:67:LEU:HA	1.82	0.41
50:Ls:162:LYS:HA	50:Ls:162:LYS:HD3	1.63	0.41
53:S2:1457:U:H2'	53:S2:1458:G:C8	2.55	0.41
53:S2:1671:G:H2'	53:S2:1672:U:H6	1.85	0.41
70:SS:125:HIS:CD2	70:SS:131:VAL:HG11	2.54	0.41
84:Sg:227:LEU:HD23	84:Sg:227:LEU:HA	1.81	0.41
1:LA:199:VAL:HG21	7:L5:1631:A:N7	2.35	0.41
3:SA:8:LEU:HD11	73:SV:39:VAL:HG21	2.02	0.41
7:L5:3664:G:H2'	7:L5:3665:G:C8	2.55	0.41
7:L5:3923:A:H2'	7:L5:3924:C:C6	2.54	0.41
7:L5:4584:A:H2'	7:L5:4585:U:O4'	2.20	0.41
7:L5:4861:G:H2'	7:L5:4862:G:H8	1.85	0.41
34:Lb:63:LYS:HE3	34:Lb:63:LYS:HB3	1.93	0.41
43:Lk:9:LYS:H	43:Lk:9:LYS:HG2	1.63	0.41
48:Lp:38:THR:HA	48:Lp:45:THR:HA	2.02	0.41
50:Ls:145:THR:HG23	50:Ls:154:ILE:HG13	2.02	0.41
53:S2:1289:U:H4'	62:SK:2:LEU:HG	2.02	0.41
59:SH:28:LEU:O	59:SH:31:GLU:HG2	2.21	0.41
60:SI:141:ARG:H	60:SI:141:ARG:HG2	1.72	0.41
67:SP:77:LYS:HA	67:SP:95:GLY:O	2.18	0.41
67:SP:97:TYR:HD1	67:SP:98:ASN:H	1.68	0.41
7:L5:444:G:H2'	7:L5:445:U:C6	2.55	0.41
7:L5:1468:C:H2'	7:L5:1469:C:H6	1.85	0.41
7:L5:4242:U:H3	7:L5:4281:A:H2	1.68	0.41
7:L5:4742:G:H2'	7:L5:4743:G:C8	2.56	0.41
9:L8:70:G:H5''	31:LY:27:ARG:CZ	2.49	0.41
16:LI:152:LEU:HB3	16:LI:165:ILE:HD12	2.01	0.41
24:LR:104:ARG:O	24:LR:108:ARG:HG3	2.20	0.41
29:LW:2:LYS:HE3	29:LW:2:LYS:HB2	1.66	0.41
46:Ln:10:MET:HE1	46:Ln:17:ARG:NH1	2.35	0.41
53:S2:77:A:H5'	58:SG:154:ARG:HH12	1.85	0.41
53:S2:1797:U:H2'	53:S2:1798:C:C6	2.55	0.41
54:SC:253:PRO:HA	54:SC:256:TRP:CD1	2.55	0.41
61:SJ:66:LYS:HA	61:SJ:66:LYS:HD3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SJ:86:VAL:HG13	61:SJ:104:ASP:HB2	2.02	0.41
66:SO:124:MET:HE3	66:SO:124:MET:HB2	1.70	0.41
77:SZ:67:LEU:HD13	77:SZ:72:VAL:HG21	2.02	0.41
4:LB:77:THR:HG21	4:LB:337:VAL:HG22	2.01	0.41
7:L5:1558:A:H2'	7:L5:1559:G:C8	2.55	0.41
7:L5:1655:C:H3'	33:La:26:ARG:HH12	1.86	0.41
7:L5:1811:G:H2'	7:L5:1812:C:H6	1.85	0.41
7:L5:1824:G:H5''	26:LT:35:LYS:HE2	2.02	0.41
7:L5:2539:C:H2'	7:L5:2540:C:C6	2.56	0.41
7:L5:4611:A:H2'	7:L5:4612:C:H6	1.85	0.41
17:LJ:52:LYS:HA	17:LJ:67:LYS:HA	2.02	0.41
50:Ls:25:PRO:HD2	50:Ls:92:LYS:HA	2.03	0.41
51:Lt:105:THR:HG22	51:Lt:107:ASP:HB2	2.03	0.41
53:S2:874:G:H2'	53:S2:875:A:C8	2.53	0.41
53:S2:1298:G:H21	67:SP:52:LYS:NZ	2.18	0.41
53:S2:1779:G:H2'	53:S2:1780:G:H8	1.85	0.41
54:SC:183:LYS:HE2	74:SW:95:PRO:HA	2.02	0.41
59:SH:69:LEU:HD23	59:SH:69:LEU:HA	1.89	0.41
80:Sc:66:ARG:NE	80:Sc:66:ARG:H	2.18	0.41
7:L5:175:C:H2'	7:L5:176:G:H8	1.85	0.41
7:L5:711:A:H2'	7:L5:712:C:C6	2.54	0.41
7:L5:1538:U:H2'	7:L5:1539:G:H8	1.86	0.41
7:L5:1739:G:H5''	8:L7:102:U:H1'	2.03	0.41
7:L5:1811:G:H2'	7:L5:1812:C:C6	2.56	0.41
18:LL:177:LYS:HE2	18:LL:177:LYS:HB2	1.89	0.41
40:Lh:116:LEU:H	40:Lh:116:LEU:HD12	1.86	0.41
43:Lk:56:LEU:HA	43:Lk:56:LEU:HD12	1.83	0.41
47:Lo:23:VAL:HG22	47:Lo:70:LEU:HD23	2.01	0.41
47:Lo:35:ALA:O	47:Lo:39:ARG:HG3	2.21	0.41
50:Ls:145:THR:HG22	50:Ls:152:ILE:HG22	2.02	0.41
53:S2:1406:G:H2'	53:S2:1407:U:C6	2.56	0.41
1:LA:46:LYS:HA	1:LA:46:LYS:HD2	1.86	0.41
7:L5:29:G:H5''	20:LN:172:ARG:HG2	2.02	0.41
7:L5:926:G:H2'	7:L5:927:G:H8	1.85	0.41
7:L5:994:G:H2'	7:L5:995:C:H4'	2.03	0.41
13:LF:174:LEU:HD23	13:LF:177:ARG:HH12	1.85	0.41
17:LJ:39:VAL:HG21	17:LJ:126:TYR:HD1	1.84	0.41
26:LT:45:MET:HB2	26:LT:45:MET:HE3	1.85	0.41
52:N4:93:LYS:HA	52:N4:93:LYS:HD3	1.81	0.41
56:SE:39:ARG:H	56:SE:39:ARG:HG2	1.67	0.41
63:SL:152:LYS:HE2	63:SL:152:LYS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Sg:5:MET:HE3	84:Sg:5:MET:HA	2.02	0.41
4:LB:34:LYS:HB3	4:LB:34:LYS:HE3	1.77	0.41
4:LB:126:LYS:HB2	4:LB:128:LYS:HG2	2.01	0.41
7:L5:1705:G:H2'	7:L5:1706:A:O4'	2.21	0.41
7:L5:2864:A:H2'	7:L5:2865:U:C6	2.56	0.41
15:LH:54:ARG:HE	15:LH:54:ARG:HB2	1.52	0.41
43:Lk:70:LYS:HD2	43:Lk:70:LYS:HA	1.96	0.41
47:Lo:93:LEU:HD23	47:Lo:93:LEU:HA	1.94	0.41
52:N4:47:LYS:HA	52:N4:47:LYS:HD2	1.72	0.41
53:S2:4:C:H4'	54:SC:207:ALA:HB2	2.02	0.41
53:S2:964:A:H2'	53:S2:965:U:H6	1.85	0.41
55:SD:189:MET:HE3	55:SD:189:MET:HB2	1.91	0.41
59:SH:107:LYS:HD3	59:SH:107:LYS:HA	1.80	0.41
74:SW:86:LEU:O	74:SW:90:GLN:HG3	2.20	0.41
77:SZ:44:LEU:HD23	77:SZ:44:LEU:HA	1.89	0.41
2:NA:110:ASP:HB2	2:NA:123:PHE:HD2	1.86	0.41
7:L5:4294:C:O3'	47:Lo:13:LYS:HE2	2.21	0.41
7:L5:4344:U:H2'	7:L5:4345:C:C6	2.56	0.41
7:L5:4906:C:H2'	7:L5:4907:G:H8	1.85	0.41
48:Lp:30:GLU:HA	48:Lp:33:GLN:HG2	2.02	0.41
51:Lt:85:LEU:HD13	51:Lt:106:PHE:HB2	2.03	0.41
53:S2:1454:A:H2	53:S2:1476:A:H1'	1.86	0.41
53:S2:1556:A:H8	53:S2:1557:C:C6	2.39	0.41
56:SE:104:ASP:HB3	56:SE:110:ALA:HB2	2.03	0.41
60:SI:62:VAL:HG21	60:SI:75:LYS:HE2	2.03	0.41
82:Se:2:VAL:HG22	82:Se:4:GLY:H	1.86	0.41
4:LB:57:VAL:HB	4:LB:367:PHE:HB3	2.03	0.41
4:LB:258:HIS:HA	4:LB:260:ALA:N	2.36	0.41
5:NB:43:LYS:HA	5:NB:46:PHE:CZ	2.56	0.41
6:SB:122:GLU:HG2	6:SB:140:VAL:HG23	2.03	0.41
7:L5:460:C:H2'	7:L5:461:G:C8	2.54	0.41
7:L5:662:C:H2'	7:L5:663:G:C8	2.55	0.41
7:L5:2566:G:H2'	7:L5:2567:G:H8	1.85	0.41
7:L5:3861:A:H2'	7:L5:3862:A:C8	2.56	0.41
10:LC:315:LYS:HG3	13:LF:168:ALA:HB1	2.01	0.41
11:LD:67:ALA:HB1	26:LT:31:MET:HE2	2.03	0.41
12:LE:258:LEU:HD23	12:LE:258:LEU:HA	1.94	0.41
13:LF:124:LYS:HB3	13:LF:124:LYS:HE2	1.92	0.41
14:LG:95:LEU:HD23	14:LG:184:ILE:HD12	2.03	0.41
16:LI:48:LEU:O	16:LI:139:ARG:HA	2.21	0.41
17:LJ:159:LYS:HG3	17:LJ:163:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LM:130:LEU:HD21	21:LO:180:GLN:HG3	2.02	0.41
31:LY:47:MET:HE3	31:LY:47:MET:HB3	1.91	0.41
40:Lh:88:THR:OG1	40:Lh:91:MET:HG2	2.21	0.41
51:Lt:48:LYS:HA	51:Lt:48:LYS:HD2	1.74	0.41
52:N4:162:MET:HE3	52:N4:162:MET:HB3	1.80	0.41
53:S2:433:A:H2'	53:S2:434:G:C8	2.56	0.41
53:S2:746:C:H2'	53:S2:747:U:C6	2.56	0.41
53:S2:796:G:H2'	53:S2:797:C:O4'	2.20	0.41
53:S2:895:G:H3'	53:S2:896:U:H4'	2.02	0.41
53:S2:1189:A:H2'	53:S2:1190:A:C8	2.56	0.41
53:S2:1337:C:H2'	53:S2:1338:G:H8	1.86	0.41
53:S2:1477:U:H5'	69:SR:3:ARG:HH21	1.85	0.41
54:SC:183:LYS:HG3	74:SW:95:PRO:HA	2.02	0.41
55:SD:122:VAL:O	55:SD:126:ILE:HG12	2.20	0.41
57:SF:28:VAL:HG21	57:SF:109:LEU:HB2	2.02	0.41
57:SF:35:LEU:HD12	57:SF:147:VAL:HG23	2.02	0.41
58:SG:48:TYR:CE1	58:SG:121:ILE:HD11	2.55	0.41
58:SG:201:LYS:HB3	58:SG:201:LYS:HE2	1.85	0.41
59:SH:68:GLN:H	59:SH:68:GLN:HG2	1.70	0.41
59:SH:73:GLN:HA	59:SH:76:GLN:HB2	2.03	0.41
59:SH:83:LEU:HD23	59:SH:83:LEU:HA	1.89	0.41
61:SJ:91:LYS:HD2	61:SJ:96:TYR:CE2	2.56	0.41
63:SL:153:LYS:HA	63:SL:153:LYS:HD3	1.98	0.41
73:SV:70:LEU:O	73:SV:74:LYS:HG3	2.21	0.41
74:SW:20:ARG:HA	74:SW:20:ARG:HD2	1.88	0.41
75:SX:94:ILE:HD13	75:SX:94:ILE:HA	1.95	0.41
2:NA:108:LYS:HD3	2:NA:108:LYS:HA	1.81	0.41
5:NB:82:SER:HB3	5:NB:87:THR:O	2.21	0.41
7:L5:302:C:OP1	20:LN:68:ARG:HB2	2.21	0.41
7:L5:462:G:H2'	7:L5:463:A:C8	2.55	0.41
7:L5:1359:G:H4'	20:LN:203:TYR:HB2	2.02	0.41
7:L5:2342:G:H5''	10:LC:109:ARG:HH21	1.86	0.41
7:L5:4745:G:H1	7:L5:4955:A:H61	1.67	0.41
12:LE:89:LEU:HD12	12:LE:89:LEU:HA	1.87	0.41
15:LH:141:LYS:HE2	15:LH:141:LYS:HB2	1.85	0.41
42:Lj:27:TYR:HA	42:Lj:34:CYS:HA	2.02	0.41
52:N4:192:PHE:HB3	52:N4:214:LEU:HG	2.03	0.41
53:S2:943:U:H2'	53:S2:944:A:H8	1.86	0.41
53:S2:1653:U:H2'	53:S2:1654:G:C8	2.56	0.41
59:SH:36:LEU:HD21	59:SH:78:ARG:HE	1.86	0.41
66:SO:103:ASN:HB2	66:SO:142:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:ST:64:LEU:HD23	71:ST:64:LEU:HA	1.84	0.41
72:SU:40:ILE:C	72:SU:44:LYS:HZ2	2.29	0.41
4:LB:92:TYR:HB2	4:LB:159:VAL:HB	2.03	0.40
7:L5:106:A:H2'	7:L5:107:G:O4'	2.21	0.40
7:L5:1907:A:H2'	7:L5:1908:A:C8	2.56	0.40
7:L5:2386:U:H5''	24:LR:24:LEU:HD12	2.03	0.40
7:L5:2632:U:H2'	7:L5:2633:U:C6	2.56	0.40
7:L5:4736:C:H2'	7:L5:4737:G:H8	1.85	0.40
7:L5:4929:C:H5''	19:LM:114:LYS:HD3	2.02	0.40
7:L5:4954:G:H2'	7:L5:4955:A:C8	2.56	0.40
11:LD:208:MET:HB3	11:LD:219:TYR:HE1	1.86	0.40
14:LG:177:MET:HE2	14:LG:177:MET:HB2	1.86	0.40
20:LN:6:TYR:CZ	41:Li:40:VAL:HG22	2.57	0.40
52:N4:158:ILE:HD12	52:N4:161:LEU:HB2	2.03	0.40
56:SE:107:GLY:HA2	56:SE:189:LEU:HG	2.03	0.40
56:SE:141:THR:HG22	56:SE:160:ILE:HD11	2.02	0.40
61:SJ:131:ARG:HD2	61:SJ:131:ARG:HA	1.78	0.40
72:SU:23:THR:OG1	72:SU:113:GLU:HB3	2.21	0.40
1:LA:234:LYS:HG2	1:LA:238:ILE:HG12	2.03	0.40
4:LB:349:LYS:HB3	4:LB:349:LYS:HE3	1.92	0.40
4:LB:355:THR:HA	4:LB:360:LEU:HD11	2.02	0.40
7:L5:982:U:H2'	7:L5:983:C:C6	2.56	0.40
7:L5:2264:C:H2'	7:L5:2265:G:O4'	2.21	0.40
7:L5:2765:A:H2'	7:L5:2766:A:C8	2.56	0.40
7:L5:3917:A:H2'	7:L5:3918:G:C8	2.56	0.40
15:LH:51:LYS:HD3	15:LH:51:LYS:HA	1.80	0.40
27:LU:21:PHE:HA	27:LU:108:GLU:O	2.21	0.40
40:Lh:73:TYR:HB3	40:Lh:79:LYS:HG3	2.03	0.40
53:S2:1007:C:H2'	53:S2:1008:A:C8	2.56	0.40
53:S2:1010:G:H2'	53:S2:1011:A:H8	1.87	0.40
53:S2:1232:U:H2'	53:S2:1233:G:H8	1.85	0.40
53:S2:1244:U:H2'	53:S2:1245:G:H8	1.86	0.40
53:S2:1670:C:H2'	53:S2:1671:G:C8	2.56	0.40
54:SC:132:ASP:OD1	54:SC:136:HIS:HB2	2.21	0.40
1:LA:49:ILE:HD11	1:LA:75:LEU:HD11	2.03	0.40
7:L5:1503:A:H4'	7:L5:1504:G:H5'	2.02	0.40
7:L5:4611:A:H2'	7:L5:4612:C:C6	2.57	0.40
7:L5:4966:A:H2'	7:L5:4967:A:O4'	2.21	0.40
8:L7:55:A:H4'	17:LJ:155:HIS:HB2	2.02	0.40
9:L8:154:G:H5''	14:LG:89:ARG:NH1	2.37	0.40
11:LD:5:LYS:HB3	11:LD:5:LYS:HE3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LD:36:LEU:HD22	11:LD:50:ARG:HD2	2.03	0.40
22:LP:50:ASP:HB3	22:LP:56:GLN:HG3	2.03	0.40
53:S2:540:U:H2'	53:S2:541:U:C6	2.57	0.40
53:S2:1319:U:H2'	53:S2:1320:G:C8	2.57	0.40
53:S2:1457:U:H2'	53:S2:1458:G:H8	1.85	0.40
56:SE:102:ILE:HD11	56:SE:239:PRO:HD3	2.02	0.40
56:SE:256:LEU:HD13	56:SE:256:LEU:HA	1.95	0.40
62:SK:60:GLU:HB2	62:SK:69:TRP:CD1	2.52	0.40
65:SN:45:LEU:HB3	65:SN:49:GLN:HB2	2.03	0.40
1:LA:233:ARG:HB2	7:L5:4184:G:H5'	2.04	0.40
3:SA:145:ILE:HG12	3:SA:159:ILE:HB	2.04	0.40
7:L5:3932:U:H2'	7:L5:3933:G:C8	2.56	0.40
23:LQ:179:GLY:HA2	23:LQ:186:TYR:CE2	2.57	0.40
31:LY:1:MET:HE3	31:LY:2:LYS:H	1.87	0.40
53:S2:386:C:H2'	53:S2:387:C:C6	2.56	0.40
56:SE:44:LEU:HD13	56:SE:72:ILE:HD11	2.04	0.40
58:SG:48:TYR:HD2	58:SG:48:TYR:HA	1.82	0.40
62:SK:95:ARG:HD2	62:SK:95:ARG:HA	1.91	0.40
68:SQ:84:ILE:O	68:SQ:88:ILE:HG13	2.21	0.40
68:SQ:86:GLN:O	68:SQ:90:LYS:HG3	2.20	0.40
71:ST:122:LYS:HB2	71:ST:122:LYS:HE2	1.79	0.40
84:Sg:240:CYS:SG	84:Sg:289:LEU:HD13	2.61	0.40
3:SA:42:LYS:HG3	3:SA:46:ILE:O	2.21	0.40
7:L5:163:A:H2'	7:L5:164:G:C8	2.57	0.40
7:L5:1538:U:H2'	7:L5:1539:G:C8	2.57	0.40
7:L5:1895:G:H2'	7:L5:1896:A:O4'	2.21	0.40
7:L5:2372:U:H2'	7:L5:2373:C:C6	2.56	0.40
18:LL:127:PHE:HB2	40:Lh:118:LYS:HB3	2.04	0.40
18:LL:177:LYS:HB3	18:LL:180:ALA:HB3	2.03	0.40
38:Lf:33:VAL:HG13	38:Lf:38:GLU:HB3	2.02	0.40
38:Lf:41:PHE:HE1	38:Lf:110:ILE:HD13	1.86	0.40
50:Ls:160:LEU:HG	50:Ls:161:ILE:HG13	2.03	0.40
51:Lt:16:ARG:HD2	51:Lt:28:LEU:HD12	2.02	0.40
51:Lt:57:ARG:HH11	51:Lt:80:LEU:HB3	1.86	0.40
53:S2:1101:U:H2'	53:S2:1102:G:C8	2.56	0.40
55:SD:45:ARG:HG2	55:SD:83:SER:HA	2.03	0.40
58:SG:49:VAL:HG12	58:SG:115:LYS:HG2	2.04	0.40
59:SH:15:LYS:HB2	59:SH:15:LYS:HE2	1.82	0.40
61:SJ:65:GLU:HG3	61:SJ:66:LYS:NZ	2.36	0.40
67:SP:80:LEU:H	67:SP:80:LEU:HD12	1.87	0.40
77:SZ:90:GLU:HG3	77:SZ:94:LYS:HZ2	1.87	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	
1	LA	246/257 (96%)	235 (96%)	11 (4%)	0	100	100
2	NA	104/215 (48%)	102 (98%)	2 (2%)	0	100	100
3	SA	219/295 (74%)	211 (96%)	8 (4%)	0	100	100
4	LB	400/403 (99%)	381 (95%)	19 (5%)	0	100	100
5	NB	104/206 (50%)	95 (91%)	9 (9%)	0	100	100
6	SB	217/264 (82%)	212 (98%)	5 (2%)	0	100	100
10	LC	363/427 (85%)	348 (96%)	14 (4%)	1 (0%)	36	59
11	LD	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
12	LE	215/288 (75%)	201 (94%)	14 (6%)	0	100	100
13	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
14	LG	239/266 (90%)	229 (96%)	10 (4%)	0	100	100
15	LH	188/192 (98%)	175 (93%)	13 (7%)	0	100	100
16	LI	198/214 (92%)	194 (98%)	4 (2%)	0	100	100
17	LJ	169/178 (95%)	166 (98%)	3 (2%)	0	100	100
18	LL	205/211 (97%)	195 (95%)	8 (4%)	2 (1%)	12	30
19	LM	137/215 (64%)	134 (98%)	3 (2%)	0	100	100
20	LN	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
21	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
22	LP	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
23	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
24	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
25	LS	173/176 (98%)	166 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
27	LU	98/128 (77%)	97 (99%)	1 (1%)	0	100	100
28	LV	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
29	LW	122/157 (78%)	117 (96%)	5 (4%)	0	100	100
30	LX	118/156 (76%)	115 (98%)	3 (2%)	0	100	100
31	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
32	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
33	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
34	Lb	105/159 (66%)	101 (96%)	4 (4%)	0	100	100
35	Lc	96/115 (84%)	96 (100%)	0	0	100	100
36	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
37	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
38	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
39	Lg	112/117 (96%)	112 (100%)	0	0	100	100
40	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
41	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
42	Lj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
43	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
44	Ll	48/51 (94%)	48 (100%)	0	0	100	100
45	Lm	49/128 (38%)	49 (100%)	0	0	100	100
46	Ln	22/25 (88%)	22 (100%)	0	0	100	100
47	Lo	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
48	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
49	Lr	123/137 (90%)	123 (100%)	0	0	100	100
50	Ls	194/317 (61%)	181 (93%)	13 (7%)	0	100	100
51	Lt	137/165 (83%)	115 (84%)	22 (16%)	0	100	100
52	N4	221/237 (93%)	211 (96%)	10 (4%)	0	100	100
54	SC	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
55	SD	225/243 (93%)	212 (94%)	13 (6%)	0	100	100
56	SE	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
57	SF	180/204 (88%)	171 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
59	SH	182/194 (94%)	176 (97%)	6 (3%)	0	100	100
60	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
61	SJ	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
62	SK	93/165 (56%)	84 (90%)	9 (10%)	0	100	100
63	SL	140/158 (89%)	134 (96%)	6 (4%)	0	100	100
64	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
65	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
66	SO	133/151 (88%)	123 (92%)	9 (7%)	1 (1%)	16	35
67	SP	127/145 (88%)	121 (95%)	6 (5%)	0	100	100
68	SQ	142/146 (97%)	131 (92%)	11 (8%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	4 (3%)	1 (1%)	16	35
70	SS	142/152 (93%)	127 (89%)	15 (11%)	0	100	100
71	ST	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
72	SU	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
73	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
74	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
75	SX	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
76	SY	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
77	SZ	73/125 (58%)	59 (81%)	14 (19%)	0	100	100
78	Sa	100/115 (87%)	97 (97%)	3 (3%)	0	100	100
79	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
80	Sc	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
81	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
82	Se	56/133 (42%)	55 (98%)	1 (2%)	0	100	100
83	Sf	65/156 (42%)	56 (86%)	9 (14%)	0	100	100
84	Sg	311/317 (98%)	282 (91%)	29 (9%)	0	100	100
All	All	12034/13902 (87%)	11554 (96%)	475 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
66	SO	138	ASP

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Mol	Chain	Res	Type
18	LL	97	SER
10	LC	149	GLU
18	LL	136	LYS
69	SR	129	LYS

### 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	
1	LA	190/199 (96%)	188 (99%)	2 (1%)	65	84
2	NA	95/183 (52%)	93 (98%)	2 (2%)	47	73
3	SA	183/243 (75%)	178 (97%)	5 (3%)	39	68
4	LB	348/349 (100%)	339 (97%)	9 (3%)	40	69
5	NB	90/165 (54%)	83 (92%)	7 (8%)	11	28
6	SB	200/231 (87%)	195 (98%)	5 (2%)	42	69
10	LC	304/348 (87%)	300 (99%)	4 (1%)	61	81
11	LD	246/250 (98%)	239 (97%)	7 (3%)	38	67
12	LE	195/252 (77%)	193 (99%)	2 (1%)	68	85
13	LF	194/215 (90%)	193 (100%)	1 (0%)	81	91
14	LG	203/223 (91%)	199 (98%)	4 (2%)	48	74
15	LH	169/171 (99%)	164 (97%)	5 (3%)	36	64
16	LI	172/181 (95%)	169 (98%)	3 (2%)	53	77
17	LJ	144/149 (97%)	137 (95%)	7 (5%)	22	47
18	LL	173/177 (98%)	168 (97%)	5 (3%)	37	65
19	LM	118/161 (73%)	115 (98%)	3 (2%)	42	69
20	LN	171/172 (99%)	168 (98%)	3 (2%)	51	76
21	LO	173/174 (99%)	170 (98%)	3 (2%)	53	77
22	LP	134/163 (82%)	132 (98%)	2 (2%)	57	79
23	LQ	164/165 (99%)	160 (98%)	4 (2%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	LR	166/175 (95%)	162 (98%)	4 (2%)	43	70
25	LS	156/157 (99%)	151 (97%)	5 (3%)	34	62
26	LT	139/140 (99%)	138 (99%)	1 (1%)	76	89
27	LU	90/115 (78%)	87 (97%)	3 (3%)	33	61
28	LV	101/107 (94%)	100 (99%)	1 (1%)	68	85
29	LW	103/126 (82%)	101 (98%)	2 (2%)	50	75
30	LX	108/133 (81%)	105 (97%)	3 (3%)	38	67
31	LY	123/135 (91%)	117 (95%)	6 (5%)	22	47
32	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	86
33	La	120/121 (99%)	117 (98%)	3 (2%)	42	69
34	Lb	89/126 (71%)	86 (97%)	3 (3%)	32	60
35	Lc	83/97 (86%)	81 (98%)	2 (2%)	43	70
36	Ld	98/110 (89%)	96 (98%)	2 (2%)	48	74
37	Le	114/121 (94%)	110 (96%)	4 (4%)	32	59
38	Lf	88/89 (99%)	87 (99%)	1 (1%)	65	84
39	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	85
40	Lh	109/110 (99%)	107 (98%)	2 (2%)	51	76
41	Li	86/89 (97%)	83 (96%)	3 (4%)	32	59
42	Lj	73/80 (91%)	71 (97%)	2 (3%)	39	68
43	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	78
44	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	52
45	Lm	47/115 (41%)	45 (96%)	2 (4%)	26	52
46	Ln	23/24 (96%)	22 (96%)	1 (4%)	26	52
47	Lo	93/94 (99%)	91 (98%)	2 (2%)	45	72
48	Lp	74/75 (99%)	73 (99%)	1 (1%)	59	80
49	Lr	109/121 (90%)	107 (98%)	2 (2%)	51	76
50	Ls	162/258 (63%)	158 (98%)	4 (2%)	42	69
51	Lt	112/137 (82%)	110 (98%)	2 (2%)	51	76
52	N4	195/204 (96%)	192 (98%)	3 (2%)	57	79
54	SC	188/225 (84%)	179 (95%)	9 (5%)	23	48
55	SD	190/202 (94%)	183 (96%)	7 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	SE	224/225 (100%)	216 (96%)	8 (4%)	31	58
57	SF	156/170 (92%)	154 (99%)	2 (1%)	61	81
58	SG	207/218 (95%)	203 (98%)	4 (2%)	50	75
59	SH	166/174 (95%)	162 (98%)	4 (2%)	43	70
60	SI	178/180 (99%)	174 (98%)	4 (2%)	45	72
61	SJ	161/168 (96%)	157 (98%)	4 (2%)	42	69
62	SK	86/136 (63%)	83 (96%)	3 (4%)	32	59
63	SL	130/142 (92%)	121 (93%)	9 (7%)	14	33
65	SN	130/131 (99%)	126 (97%)	4 (3%)	35	63
66	SO	105/119 (88%)	99 (94%)	6 (6%)	18	41
67	SP	115/130 (88%)	111 (96%)	4 (4%)	32	59
68	SQ	119/121 (98%)	109 (92%)	10 (8%)	10	24
69	SR	122/122 (100%)	116 (95%)	6 (5%)	22	47
70	SS	125/132 (95%)	118 (94%)	7 (6%)	19	42
71	ST	113/115 (98%)	113 (100%)	0	100	100
72	SU	94/107 (88%)	91 (97%)	3 (3%)	34	62
73	SV	67/67 (100%)	64 (96%)	3 (4%)	24	50
74	SW	112/113 (99%)	109 (97%)	3 (3%)	39	68
75	SX	113/115 (98%)	109 (96%)	4 (4%)	32	59
76	SY	109/115 (95%)	105 (96%)	4 (4%)	30	57
77	SZ	66/103 (64%)	60 (91%)	6 (9%)	9	21
78	Sa	89/98 (91%)	87 (98%)	2 (2%)	45	72
79	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	55
80	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	76
81	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	53
82	Se	47/104 (45%)	46 (98%)	1 (2%)	47	73
83	Sf	60/140 (43%)	58 (97%)	2 (3%)	33	61
84	Sg	272/275 (99%)	259 (95%)	13 (5%)	23	48
All	All	10377/11695 (89%)	10087 (97%)	290 (3%)	38	67

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LA	4	VAL
1	LA	32	VAL
2	NA	207	VAL
2	NA	212	GLU
3	SA	46	ILE
3	SA	87	VAL
3	SA	88	LEU
3	SA	144	THR
3	SA	201	LEU
4	LB	61	ASP
4	LB	69	LYS
4	LB	194	LEU
4	LB	200	ARG
4	LB	289	GLN
4	LB	292	LEU
4	LB	300	LYS
4	LB	329	ASP
4	LB	386	LYS
5	NB	14	LEU
5	NB	25	THR
5	NB	28	ARG
5	NB	32	VAL
5	NB	33	VAL
5	NB	90	ILE
5	NB	102	MET
6	SB	116	LYS
6	SB	136	ARG
6	SB	140	VAL
6	SB	217	MET
6	SB	222	LYS
10	LC	65	GLU
10	LC	262	GLU
10	LC	268	ARG
10	LC	297	GLU
11	LD	7	VAL
11	LD	116	ASP
11	LD	128	ASP
11	LD	138	GLN
11	LD	157	ASN
11	LD	229	ASN
11	LD	292	GLU
12	LE	106	VAL
12	LE	268	GLN

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Mol	Chain	Res	Type
13	LF	151	ASN
14	LG	43	GLN
14	LG	112	GLN
14	LG	135	VAL
14	LG	206	GLN
15	LH	9	THR
15	LH	46	SER
15	LH	121	LYS
15	LH	187	VAL
15	LH	188	GLN
16	LI	101	LYS
16	LI	203	ARG
16	LI	208	LYS
17	LJ	59	SER
17	LJ	65	ASN
17	LJ	70	VAL
17	LJ	74	VAL
17	LJ	102	THR
17	LJ	111	GLU
17	LJ	132	VAL
18	LL	59	VAL
18	LL	93	THR
18	LL	106	SER
18	LL	122	SER
18	LL	126	LEU
19	LM	8	GLU
19	LM	28	VAL
19	LM	130	LEU
20	LN	18	VAL
20	LN	113	LEU
20	LN	114	ARG
21	LO	4	VAL
21	LO	165	LYS
21	LO	183	LYS
22	LP	3	ARG
22	LP	128	ARG
23	LQ	5	ILE
23	LQ	14	ARG
23	LQ	41	SER
23	LQ	68	ARG
24	LR	3	MET
24	LR	122	SER

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Mol	Chain	Res	Type
24	LR	144	LYS
24	LR	186	LYS
25	LS	16	CYS
25	LS	49	SER
25	LS	62	VAL
25	LS	164	LYS
25	LS	173	ASN
26	LT	137	GLU
27	LU	68	SER
27	LU	72	VAL
27	LU	75	GLU
28	LV	22	VAL
29	LW	1	MET
29	LW	67	ILE
30	LX	54	LEU
30	LX	91	GLU
30	LX	131	ASP
31	LY	42	TYR
31	LY	44	VAL
31	LY	79	VAL
31	LY	94	THR
31	LY	95	VAL
31	LY	113	LYS
32	LZ	120	GLU
33	La	16	SER
33	La	56	VAL
33	La	103	VAL
34	Lb	54	LEU
34	Lb	65	MET
34	Lb	75	LEU
35	Lc	16	SER
35	Lc	20	LEU
36	Ld	22	THR
36	Ld	122	VAL
37	Le	17	THR
37	Le	86	GLU
37	Le	94	SER
37	Le	102	ASN
38	Lf	25	THR
39	Lg	23	SER
40	Lh	110	LYS
40	Lh	116	LEU

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Mol	Chain	Res	Type
41	Li	64	SER
41	Li	74	LYS
41	Li	86	LYS
42	Lj	18	LEU
42	Lj	83	THR
43	Lk	48	THR
44	Ll	11	ARG
44	Ll	27	ILE
45	Lm	84	GLN
45	Lm	127	VAL
46	Ln	20	MET
47	Lo	2	VAL
47	Lo	100	LYS
48	Lp	45	THR
49	Lr	5	LEU
49	Lr	111	ILE
50	Ls	59	THR
50	Ls	60	MET
50	Ls	62	ARG
50	Ls	141	LEU
51	Lt	60	VAL
51	Lt	70	GLN
52	N4	26	CYS
52	N4	50	ARG
52	N4	84	MET
54	SC	63	VAL
54	SC	76	LYS
54	SC	78	LEU
54	SC	103	LYS
54	SC	192	LEU
54	SC	248	TYR
54	SC	259	THR
54	SC	260	VAL
54	SC	273	LEU
55	SD	42	THR
55	SD	47	GLU
55	SD	120	TYR
55	SD	153	VAL
55	SD	167	TYR
55	SD	181	VAL
55	SD	223	ILE
56	SE	19	MET

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Mol	Chain	Res	Type
56	SE	79	ASP
56	SE	111	VAL
56	SE	115	THR
56	SE	217	SER
56	SE	236	ILE
56	SE	247	THR
56	SE	248	ILE
57	SF	160	GLU
57	SF	168	THR
58	SG	13	GLN
58	SG	68	LEU
58	SG	125	THR
58	SG	157	VAL
59	SH	51	ILE
59	SH	119	SER
59	SH	138	GLU
59	SH	166	VAL
60	SI	4	SER
60	SI	45	THR
60	SI	71	CYS
60	SI	82	VAL
61	SJ	61	LEU
61	SJ	79	ARG
61	SJ	102	ILE
61	SJ	141	VAL
62	SK	20	VAL
62	SK	22	VAL
62	SK	79	LEU
63	SL	6	THR
63	SL	42	LEU
63	SL	67	SER
63	SL	79	LYS
63	SL	104	LYS
63	SL	105	ARG
63	SL	130	GLU
63	SL	146	THR
63	SL	154	GLN
65	SN	36	GLN
65	SN	57	SER
65	SN	67	THR
65	SN	142	GLU
66	SO	83	GLN

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Mol	Chain	Res	Type
66	SO	91	THR
66	SO	107	THR
66	SO	114	SER
66	SO	138	ASP
66	SO	151	LEU
67	SP	16	THR
67	SP	86	LEU
67	SP	105	VAL
67	SP	126	VAL
68	SQ	22	VAL
68	SQ	41	MET
68	SQ	55	VAL
68	SQ	70	VAL
68	SQ	92	LEU
68	SQ	96	TYR
68	SQ	100	VAL
68	SQ	111	ILE
68	SQ	113	ILE
68	SQ	114	GLN
69	SR	40	ILE
69	SR	98	VAL
69	SR	120	THR
69	SR	123	THR
69	SR	124	VAL
69	SR	130	THR
70	SS	33	ILE
70	SS	43	VAL
70	SS	50	ILE
70	SS	52	LEU
70	SS	72	GLN
70	SS	85	ASN
70	SS	116	LYS
72	SU	20	ILE
72	SU	27	ARG
72	SU	88	LEU
73	SV	9	VAL
73	SV	42	VAL
73	SV	79	VAL
74	SW	25	VAL
74	SW	74	VAL
74	SW	80	ASP
75	SX	54	LYS

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Mol	Chain	Res	Type
75	SX	55	VAL
75	SX	105	PHE
75	SX	115	ILE
76	SY	42	GLU
76	SY	100	LYS
76	SY	116	LYS
76	SY	117	VAL
77	SZ	43	LYS
77	SZ	62	VAL
77	SZ	68	ILE
77	SZ	88	LEU
77	SZ	89	GLN
77	SZ	108	ILE
78	Sa	58	VAL
78	Sa	94	ASP
79	Sb	3	LEU
79	Sb	56	CYS
79	Sb	57	VAL
80	Sc	11	LEU
81	Sd	31	ILE
81	Sd	55	LEU
82	Se	43	VAL
83	Sf	102	VAL
83	Sf	113	LYS
84	Sg	7	LEU
84	Sg	10	THR
84	Sg	24	THR
84	Sg	41	ILE
84	Sg	71	ILE
84	Sg	90	TRP
84	Sg	109	LEU
84	Sg	151	VAL
84	Sg	165	ILE
84	Sg	177	TRP
84	Sg	248	LEU
84	Sg	297	THR
84	Sg	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
2	NA	69	GLN

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Mol	Chain	Res	Type
3	SA	36	GLN
3	SA	50	ASN
5	NB	86	ASN
6	SB	76	ASN
6	SB	92	GLN
10	LC	89	GLN
10	LC	286	ASN
10	LC	329	ASN
11	LD	138	GLN
11	LD	157	ASN
11	LD	225	GLN
11	LD	250	ASN
11	LD	267	ASN
11	LD	275	GLN
11	LD	291	GLN
13	LF	63	GLN
13	LF	126	ASN
13	LF	239	GLN
14	LG	66	GLN
15	LH	102	ASN
16	LI	73	ASN
16	LI	130	HIS
17	LJ	98	ASN
19	LM	34	ASN
19	LM	44	GLN
20	LN	149	GLN
20	LN	156	HIS
21	LO	180	GLN
22	LP	34	GLN
22	LP	133	HIS
23	LQ	160	HIS
24	LR	178	GLN
26	LT	54	HIS
28	LV	27	ASN
29	LW	50	ASN
30	LX	73	HIS
31	LY	18	HIS
31	LY	56	GLN
31	LY	72	GLN
33	La	19	HIS
33	La	60	HIS
33	La	67	GLN

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Mol	Chain	Res	Type
33	La	120	GLN
34	Lb	6	ASN
35	Lc	72	HIS
37	Le	52	GLN
38	Lf	21	GLN
38	Lf	80	ASN
39	Lg	14	ASN
40	Lh	65	GLN
41	Li	15	HIS
42	Lj	66	HIS
44	Ll	25	GLN
44	Ll	33	ASN
47	Lo	19	GLN
49	Lr	41	ASN
49	Lr	85	ASN
50	Ls	159	GLN
50	Ls	190	GLN
50	Ls	191	GLN
52	N4	184	GLN
52	N4	191	GLN
55	SD	22	ASN
55	SD	207	HIS
56	SE	197	ASN
56	SE	209	HIS
57	SF	29	GLN
57	SF	118	ASN
58	SG	110	ASN
59	SH	44	ASN
60	SI	7	ASN
60	SI	52	ASN
61	SJ	75	ASN
63	SL	11	GLN
63	SL	19	ASN
63	SL	94	HIS
65	SN	58	HIS
66	SO	103	ASN
66	SO	113	GLN
67	SP	46	ASN
67	SP	103	ASN
67	SP	114	HIS
68	SQ	97	GLN
70	SS	11	HIS

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Mol	Chain	Res	Type
70	SS	17	ASN
71	ST	128	GLN
74	SW	91	ASN
75	SX	39	ASN
77	SZ	89	GLN
77	SZ	106	GLN
78	Sa	19	GLN
78	Sa	86	ASN
84	Sg	51	ASN
84	Sg	76	GLN
84	Sg	117	ASN
84	Sg	187	ASN
84	Sg	196	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	S2	1696/1869 (90%)	346 (20%)	5 (0%)
7	L5	3657/5070 (72%)	760 (20%)	19 (0%)
8	L7	119/121 (98%)	11 (9%)	0
9	L8	155/157 (98%)	29 (18%)	0
All	All	5627/7217 (77%)	1146 (20%)	24 (0%)

All (1146) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	L5	17	A
7	L5	25	A
7	L5	39	A
7	L5	42	A
7	L5	48	G
7	L5	56	A
7	L5	59	A
7	L5	63	G
7	L5	64	A
7	L5	65	A
7	L5	69	A
7	L5	72	C
7	L5	73	A
7	L5	74	G
7	L5	76	A

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Mol	Chain	Res	Type
7	L5	91	G
7	L5	98	A
7	L5	104	G
7	L5	108	A
7	L5	109	G
7	L5	110	C
7	L5	112	C
7	L5	119	G
7	L5	120	A
7	L5	132	G
7	L5	133	C
7	L5	134	G
7	L5	135	G
7	L5	152	U
7	L5	159	C
7	L5	171	U
7	L5	172	C
7	L5	181	C
7	L5	182	G
7	L5	183	C
7	L5	184	U
7	L5	186	G
7	L5	188	G
7	L5	189	G
7	L5	200	U
7	L5	207	G
7	L5	210	C
7	L5	216	C
7	L5	217	C
7	L5	218	A
7	L5	219	G
7	L5	220	C
7	L5	232	G
7	L5	233	U
7	L5	266	C
7	L5	267	G
7	L5	277	G
7	L5	280	G
7	L5	297	U
7	L5	306	A
7	L5	315	G
7	L5	316	U

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Mol	Chain	Res	Type
7	L5	340	C
7	L5	349	A
7	L5	353	A
7	L5	373	G
7	L5	387	G
7	L5	407	A
7	L5	410	A
7	L5	411	G
7	L5	412	G
7	L5	433	A
7	L5	449	C
7	L5	450	G
7	L5	452	A
7	L5	453	G
7	L5	454	U
7	L5	465	G
7	L5	467	U
7	L5	483	G
7	L5	484	U
7	L5	485	C
7	L5	493	G
7	L5	494	U
7	L5	497	G
7	L5	498	C
7	L5	500	G
7	L5	501	C
7	L5	502	C
7	L5	503	C
7	L5	504	G
7	L5	505	G
7	L5	509	A
7	L5	510	U
7	L5	512	U
7	L5	513	U
7	L5	514	U
7	L5	515	C
7	L5	518	G
7	L5	643	C
7	L5	646	G
7	L5	657	C
7	L5	659	G
7	L5	665	C

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Mol	Chain	Res	Type
7	L5	666	G
7	L5	667	A
7	L5	668	C
7	L5	669	C
7	L5	685	C
7	L5	686	A
7	L5	696	C
7	L5	703	G
7	L5	704	C
7	L5	706	C
7	L5	708	G
7	L5	730	G
7	L5	731	G
7	L5	738	C
7	L5	739	G
7	L5	740	G
7	L5	742	G
7	L5	744	G
7	L5	759	G
7	L5	904	C
7	L5	913	U
7	L5	914	U
7	L5	915	A
7	L5	917	A
7	L5	918	G
7	L5	923	C
7	L5	924	C
7	L5	926	G
7	L5	932	A
7	L5	933	G
7	L5	936	C
7	L5	941	C
7	L5	943	A
7	L5	944	A
7	L5	945	U
7	L5	946	C
7	L5	956	A
7	L5	958	G
7	L5	959	G
7	L5	960	A
7	L5	961	G
7	L5	962	C

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Mol	Chain	Res	Type
7	L5	964	A
7	L5	965	G
7	L5	966	A
7	L5	967	C
7	L5	969	C
7	L5	970	G
7	L5	972	C
7	L5	982	U
7	L5	989	U
7	L5	990	C
7	L5	992	C
7	L5	993	G
7	L5	995	C
7	L5	1048	G
7	L5	1049	C
7	L5	1050	C
7	L5	1051	G
7	L5	1072	C
7	L5	1170	G
7	L5	1171	G
7	L5	1172	C
7	L5	1173	G
7	L5	1183	C
7	L5	1187	G
7	L5	1198	G
7	L5	1199	G
7	L5	1200	G
7	L5	1205	G
7	L5	1211	G
7	L5	1214	C
7	L5	1215	C
7	L5	1216	C
7	L5	1217	G
7	L5	1219	G
7	L5	1222	A
7	L5	1253	G
7	L5	1254	A
7	L5	1255	A
7	L5	1262	G
7	L5	1266	G
7	L5	1267	C
7	L5	1269	G

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Mol	Chain	Res	Type
7	L5	1272	C
7	L5	1273	G
7	L5	1280	C
7	L5	1284	G
7	L5	1285	U
7	L5	1287	G
7	L5	1293	G
7	L5	1294	A
7	L5	1295	C
7	L5	1296	G
7	L5	1301	C
7	L5	1302	U
7	L5	1326	A
7	L5	1337	A
7	L5	1354	A
7	L5	1358	G
7	L5	1359	G
7	L5	1365	C
7	L5	1366	G
7	L5	1367	C
7	L5	1379	C
7	L5	1387	A
7	L5	1393	G
7	L5	1394	G
7	L5	1397	A
7	L5	1398	A
7	L5	1404	G
7	L5	1405	C
7	L5	1407	C
7	L5	1409	C
7	L5	1410	U
7	L5	1414	C
7	L5	1415	G
7	L5	1417	C
7	L5	1420	A
7	L5	1425	G
7	L5	1437	C
7	L5	1438	U
7	L5	1447	C
7	L5	1448	G
7	L5	1457	G
7	L5	1483	C

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Mol	Chain	Res	Type
7	L5	1493	G
7	L5	1497	A
7	L5	1498	G
7	L5	1502	G
7	L5	1514	U
7	L5	1515	A
7	L5	1534	A
7	L5	1535	C
7	L5	1547	A
7	L5	1566	C
7	L5	1574	G
7	L5	1578	U
7	L5	1586	G
7	L5	1591	U
7	L5	1596	U
7	L5	1613	A
7	L5	1624	G
7	L5	1625	G
7	L5	1626	G
7	L5	1631	A
7	L5	1633	G
7	L5	1634	A
7	L5	1637	A
7	L5	1638	A
7	L5	1640	C
7	L5	1641	G
7	L5	1642	A
7	L5	1654	G
7	L5	1661	C
7	L5	1670	G
7	L5	1676	C
7	L5	1677	U
7	L5	1678	C
7	L5	1679	A
7	L5	1680	G
7	L5	1694	C
7	L5	1699	A
7	L5	1700	G
7	L5	1703	C
7	L5	1705	G
7	L5	1707	C
7	L5	1708	G

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Mol	Chain	Res	Type
7	L5	1716	G
7	L5	1726	U
7	L5	1734	G
7	L5	1735	U
7	L5	1742	A
7	L5	1753	G
7	L5	1755	C
7	L5	1756	U
7	L5	1758	G
7	L5	1759	G
7	L5	1760	G
7	L5	1761	G
7	L5	1762	C
7	L5	1763	C
7	L5	1764	G
7	L5	1765	A
7	L5	1766	A
7	L5	1768	C
7	L5	1770	A
7	L5	1771	U
7	L5	1772	C
7	L5	1787	A
7	L5	1792	U
7	L5	1797	G
7	L5	1803	G
7	L5	1804	A
7	L5	1820	C
7	L5	1821	G
7	L5	1822	U
7	L5	1836	G
7	L5	1837	A
7	L5	1842	G
7	L5	1855	G
7	L5	1869	G
7	L5	1882	U
7	L5	1892	A
7	L5	1893	C
7	L5	1897	A
7	L5	1898	C
7	L5	1918	U
7	L5	1919	G
7	L5	1920	C

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Mol	Chain	Res	Type
7	L5	1921	C
7	L5	1922	G
7	L5	1925	G
7	L5	1928	C
7	L5	1930	U
7	L5	1931	C
7	L5	1932	A
7	L5	1936	C
7	L5	1948	G
7	L5	1951	G
7	L5	1959	U
7	L5	1960	A
7	L5	1961	G
7	L5	1962	A
7	L5	1972	G
7	L5	1974	U
7	L5	1975	G
7	L5	1978	C
7	L5	1980	U
7	L5	1983	A
7	L5	1984	A
7	L5	1985	G
7	L5	1986	U
7	L5	1987	C
7	L5	1988	G
7	L5	1990	A
7	L5	1992	U
7	L5	1993	C
7	L5	1997	U
7	L5	1998	A
7	L5	2001	G
7	L5	2002	A
7	L5	2003	G
7	L5	2004	U
7	L5	2017	A
7	L5	2018	C
7	L5	2024	G
7	L5	2026	A
7	L5	2033	A
7	L5	2034	G
7	L5	2044	U
7	L5	2046	G

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Mol	Chain	Res	Type
7	L5	2048	U
7	L5	2052	G
7	L5	2055	G
7	L5	2056	G
7	L5	2069	A
7	L5	2084	C
7	L5	2085	G
7	L5	2089	G
7	L5	2090	U
7	L5	2092	G
7	L5	2094	G
7	L5	2095	A
7	L5	2096	G
7	L5	2098	G
7	L5	2099	G
7	L5	2101	C
7	L5	2112	G
7	L5	2250	C
7	L5	2252	G
7	L5	2253	A
7	L5	2256	C
7	L5	2258	C
7	L5	2261	G
7	L5	2270	G
7	L5	2289	C
7	L5	2300	A
7	L5	2301	G
7	L5	2306	G
7	L5	2313	A
7	L5	2314	G
7	L5	2316	G
7	L5	2333	G
7	L5	2342	G
7	L5	2345	G
7	L5	2348	G
7	L5	2349	A
7	L5	2351	C
7	L5	2360	A
7	L5	2389	A
7	L5	2395	A
7	L5	2397	G
7	L5	2402	G

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Mol	Chain	Res	Type
7	L5	2412	A
7	L5	2417	A
7	L5	2421	G
7	L5	2425	U
7	L5	2440	U
7	L5	2441	C
7	L5	2442	G
7	L5	2447	U
7	L5	2450	G
7	L5	2469	C
7	L5	2471	G
7	L5	2475	G
7	L5	2478	C
7	L5	2479	G
7	L5	2483	G
7	L5	2484	A
7	L5	2485	U
7	L5	2487	G
7	L5	2488	C
7	L5	2489	C
7	L5	2490	U
7	L5	2491	C
7	L5	2494	U
7	L5	2495	U
7	L5	2503	G
7	L5	2504	C
7	L5	2505	C
7	L5	2506	G
7	L5	2513	A
7	L5	2514	G
7	L5	2519	U
7	L5	2520	C
7	L5	2529	A
7	L5	2537	A
7	L5	2544	G
7	L5	2546	G
7	L5	2547	G
7	L5	2553	A
7	L5	2554	U
7	L5	2555	G
7	L5	2559	G
7	L5	2560	C

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Mol	Chain	Res	Type
7	L5	2565	A
7	L5	2573	A
7	L5	2583	C
7	L5	2587	A
7	L5	2589	C
7	L5	2601	A
7	L5	2618	G
7	L5	2627	C
7	L5	2653	C
7	L5	2662	G
7	L5	2669	C
7	L5	2670	C
7	L5	2673	G
7	L5	2675	G
7	L5	2676	A
7	L5	2687	U
7	L5	2694	G
7	L5	2695	A
7	L5	2696	A
7	L5	2707	U
7	L5	2709	C
7	L5	2710	C
7	L5	2711	G
7	L5	2721	G
7	L5	2724	G
7	L5	2726	G
7	L5	2738	C
7	L5	2739	C
7	L5	2742	G
7	L5	2743	A
7	L5	2746	A
7	L5	2754	G
7	L5	2756	G
7	L5	2761	U
7	L5	2763	U
7	L5	2769	U
7	L5	2770	C
7	L5	2787	A
7	L5	2788	U
7	L5	2790	U
7	L5	2814	C
7	L5	2826	U

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Mol	Chain	Res	Type
7	L5	2827	G
7	L5	2838	G
7	L5	2842	G
7	L5	2846	G
7	L5	2848	G
7	L5	2855	G
7	L5	2876	G
7	L5	2877	G
7	L5	2892	C
7	L5	2894	A
7	L5	2900	U
7	L5	2902	G
7	L5	2903	G
7	L5	2904	U
7	L5	2905	C
7	L5	2906	G
7	L5	2907	G
7	L5	2908	U
7	L5	3585	G
7	L5	3590	G
7	L5	3591	C
7	L5	3594	C
7	L5	3595	U
7	L5	3596	A
7	L5	3597	G
7	L5	3604	A
7	L5	3615	G
7	L5	3616	U
7	L5	3618	C
7	L5	3619	G
7	L5	3626	G
7	L5	3630	A
7	L5	3635	A
7	L5	3644	U
7	L5	3646	A
7	L5	3648	A
7	L5	3662	A
7	L5	3672	G
7	L5	3673	C
7	L5	3674	G
7	L5	3710	G
7	L5	3714	G

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Mol	Chain	Res	Type
7	L5	3727	A
7	L5	3729	U
7	L5	3735	G
7	L5	3750	G
7	L5	3753	G
7	L5	3759	A
7	L5	3760	A
7	L5	3761	C
7	L5	3776	G
7	L5	3777	G
7	L5	3784	A
7	L5	3786	U
7	L5	3811	G
7	L5	3814	U
7	L5	3817	A
7	L5	3818	U
7	L5	3819	G
7	L5	3838	U
7	L5	3839	G
7	L5	3840	U
7	L5	3867	A
7	L5	3877	A
7	L5	3878	C
7	L5	3879	G
7	L5	3885	G
7	L5	3887	C
7	L5	3892	U
7	L5	3897	G
7	L5	3898	G
7	L5	3901	A
7	L5	3905	A
7	L5	3906	A
7	L5	3907	G
7	L5	3908	A
7	L5	3915	U
7	L5	3930	U
7	L5	3938	G
7	L5	3939	G
7	L5	3948	C
7	L5	3949	A
7	L5	3950	U
7	L5	3951	G

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Mol	Chain	Res	Type
7	L5	3955	G
7	L5	4064	C
7	L5	4065	G
7	L5	4076	G
7	L5	4086	G
7	L5	4091	G
7	L5	4093	G
7	L5	4095	G
7	L5	4097	G
7	L5	4099	G
7	L5	4102	C
7	L5	4104	G
7	L5	4106	G
7	L5	4107	G
7	L5	4108	G
7	L5	4111	U
7	L5	4114	C
7	L5	4115	G
7	L5	4116	C
7	L5	4117	U
7	L5	4119	C
7	L5	4122	G
7	L5	4127	A
7	L5	4139	G
7	L5	4140	C
7	L5	4141	G
7	L5	4142	C
7	L5	4143	G
7	L5	4144	C
7	L5	4146	G
7	L5	4148	C
7	L5	4150	G
7	L5	4160	C
7	L5	4162	C
7	L5	4163	U
7	L5	4168	G
7	L5	4170	A
7	L5	4177	C
7	L5	4183	G
7	L5	4184	G
7	L5	4191	G
7	L5	4196	G

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Mol	Chain	Res	Type
7	L5	4201	G
7	L5	4203	A
7	L5	4222	G
7	L5	4225	G
7	L5	4228	G
7	L5	4229	U
7	L5	4233	A
7	L5	4242	U
7	L5	4251	A
7	L5	4254	G
7	L5	4255	A
7	L5	4265	U
7	L5	4268	A
7	L5	4273	A
7	L5	4283	G
7	L5	4291	G
7	L5	4305	G
7	L5	4314	C
7	L5	4319	C
7	L5	4329	G
7	L5	4330	G
7	L5	4332	C
7	L5	4338	G
7	L5	4349	C
7	L5	4350	C
7	L5	4371	G
7	L5	4373	G
7	L5	4376	A
7	L5	4377	G
7	L5	4378	A
7	L5	4379	A
7	L5	4380	A
7	L5	4387	C
7	L5	4391	G
7	L5	4394	A
7	L5	4405	G
7	L5	4422	A
7	L5	4426	C
7	L5	4430	G
7	L5	4444	C
7	L5	4448	G
7	L5	4449	A

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Mol	Chain	Res	Type
7	L5	4453	C
7	L5	4464	A
7	L5	4475	G
7	L5	4488	A
7	L5	4491	G
7	L5	4500	U
7	L5	4512	U
7	L5	4513	A
7	L5	4519	C
7	L5	4524	G
7	L5	4525	C
7	L5	4528	G
7	L5	4545	G
7	L5	4548	A
7	L5	4549	G
7	L5	4560	C
7	L5	4567	G
7	L5	4569	U
7	L5	4573	G
7	L5	4575	G
7	L5	4584	A
7	L5	4590	A
7	L5	4600	G
7	L5	4617	G
7	L5	4626	A
7	L5	4627	U
7	L5	4635	A
7	L5	4636	U
7	L5	4637	G
7	L5	4652	G
7	L5	4656	A
7	L5	4657	U
7	L5	4670	C
7	L5	4672	A
7	L5	4679	G
7	L5	4684	A
7	L5	4687	A
7	L5	4700	A
7	L5	4708	A
7	L5	4709	U
7	L5	4719	G
7	L5	4720	C

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Mol	Chain	Res	Type
7	L5	4734	A
7	L5	4741	C
7	L5	4742	G
7	L5	4745	G
7	L5	4750	G
7	L5	4754	G
7	L5	4757	C
7	L5	4759	C
7	L5	4761	G
7	L5	4765	G
7	L5	4771	C
7	L5	4772	C
7	L5	4775	C
7	L5	4859	C
7	L5	4867	G
7	L5	4870	G
7	L5	4871	C
7	L5	4873	G
7	L5	4874	A
7	L5	4875	G
7	L5	4882	U
7	L5	4883	C
7	L5	4889	G
7	L5	4895	C
7	L5	4896	G
7	L5	4899	G
7	L5	4900	C
7	L5	4901	G
7	L5	4910	G
7	L5	4911	A
7	L5	4912	G
7	L5	4914	C
7	L5	4924	C
7	L5	4925	U
7	L5	4928	C
7	L5	4934	A
7	L5	4940	C
7	L5	4941	G
7	L5	4943	A
7	L5	4944	C
7	L5	4949	G
7	L5	4951	G

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Mol	Chain	Res	Type
7	L5	4955	A
7	L5	4960	G
7	L5	4966	A
7	L5	4973	U
7	L5	4974	C
7	L5	4975	G
7	L5	4976	U
7	L5	4979	A
7	L5	4985	U
7	L5	4988	U
7	L5	4989	U
7	L5	4991	U
7	L5	5009	G
7	L5	5013	C
7	L5	5014	A
7	L5	5017	G
7	L5	5022	U
7	L5	5025	C
7	L5	5026	U
7	L5	5027	C
7	L5	5028	G
7	L5	5029	C
7	L5	5030	U
7	L5	5034	A
7	L5	5041	G
7	L5	5050	C
7	L5	5054	C
7	L5	5055	G
7	L5	5058	A
7	L5	5061	A
7	L5	5069	U
8	L7	24	C
8	L7	33	U
8	L7	38	U
8	L7	42	A
8	L7	53	U
8	L7	54	A
8	L7	64	G
8	L7	97	G
8	L7	100	A
8	L7	110	G
8	L7	111	C

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Mol	Chain	Res	Type
9	L8	25	G
9	L8	34	U
9	L8	35	C
9	L8	48	A
9	L8	59	A
9	L8	61	A
9	L8	62	A
9	L8	63	U
9	L8	75	G
9	L8	80	A
9	L8	81	C
9	L8	83	C
9	L8	84	A
9	L8	85	U
9	L8	87	G
9	L8	94	G
9	L8	103	A
9	L8	104	A
9	L8	105	C
9	L8	110	U
9	L8	112	G
9	L8	114	G
9	L8	123	U
9	L8	124	U
9	L8	125	C
9	L8	126	C
9	L8	127	U
9	L8	147	G
9	L8	155	C
53	S2	4	C
53	S2	17	C
53	S2	26	U
53	S2	33	G
53	S2	41	G
53	S2	42	A
53	S2	44	U
53	S2	45	A
53	S2	46	A
53	S2	56	G
53	S2	58	C
53	S2	59	U
53	S2	62	G

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Mol	Chain	Res	Type
53	S2	65	C
53	S2	67	C
53	S2	68	A
53	S2	72	C
53	S2	73	C
53	S2	74	G
53	S2	75	G
53	S2	76	U
53	S2	103	A
53	S2	113	G
53	S2	114	G
53	S2	115	U
53	S2	116	U
53	S2	121	U
53	S2	126	G
53	S2	129	C
53	S2	130	G
53	S2	143	U
53	S2	147	A
53	S2	155	G
53	S2	160	U
53	S2	162	C
53	S2	163	U
53	S2	171	A
53	S2	175	A
53	S2	182	C
53	S2	198	U
53	S2	200	G
53	S2	203	G
53	S2	204	G
53	S2	292	A
53	S2	295	C
53	S2	302	A
53	S2	308	G
53	S2	311	C
53	S2	312	G
53	S2	319	C
53	S2	322	C
53	S2	323	C
53	S2	324	C
53	S2	325	C
53	S2	326	C

*Continued on next page...*

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Mol	Chain	Res	Type
53	S2	328	U
53	S2	329	G
53	S2	332	G
53	S2	333	G
53	S2	339	A
53	S2	347	G
53	S2	351	G
53	S2	360	A
53	S2	362	C
53	S2	364	A
53	S2	368	U
53	S2	369	C
53	S2	370	G
53	S2	383	G
53	S2	385	G
53	S2	386	C
53	S2	400	C
53	S2	407	G
53	S2	408	A
53	S2	409	C
53	S2	438	G
53	S2	448	A
53	S2	449	A
53	S2	450	C
53	S2	452	G
53	S2	464	A
53	S2	466	G
53	S2	471	G
53	S2	472	C
53	S2	473	A
53	S2	474	G
53	S2	482	G
53	S2	485	A
53	S2	487	U
53	S2	488	U
53	S2	492	C
53	S2	493	A
53	S2	517	C
53	S2	540	U
53	S2	541	U
53	S2	542	U
53	S2	545	A

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Mol	Chain	Res	Type
53	S2	547	G
53	S2	548	C
53	S2	554	A
53	S2	555	A
53	S2	563	G
53	S2	564	A
53	S2	568	C
53	S2	576	A
53	S2	583	C
53	S2	588	G
53	S2	589	G
53	S2	591	U
53	S2	604	A
53	S2	614	C
53	S2	623	G
53	S2	627	U
53	S2	628	A
53	S2	631	U
53	S2	638	C
53	S2	643	A
53	S2	644	G
53	S2	655	A
53	S2	656	G
53	S2	660	C
53	S2	663	C
53	S2	664	A
53	S2	668	A
53	S2	669	A
53	S2	671	A
53	S2	672	A
53	S2	673	G
53	S2	678	U
53	S2	687	C
53	S2	688	U
53	S2	689	U
53	S2	690	G
53	S2	749	U
53	S2	751	G
53	S2	752	G
53	S2	753	C
53	S2	791	C
53	S2	792	C

*Continued on next page...*

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Mol	Chain	Res	Type
53	S2	797	C
53	S2	801	U
53	S2	808	A
53	S2	811	A
53	S2	821	G
53	S2	822	U
53	S2	830	A
53	S2	836	G
53	S2	837	A
53	S2	838	G
53	S2	839	C
53	S2	840	C
53	S2	842	C
53	S2	847	A
53	S2	870	A
53	S2	873	G
53	S2	878	G
53	S2	880	G
53	S2	886	A
53	S2	888	U
53	S2	889	U
53	S2	891	G
53	S2	896	U
53	S2	897	U
53	S2	898	U
53	S2	900	C
53	S2	904	A
53	S2	913	A
53	S2	917	U
53	S2	920	A
53	S2	922	A
53	S2	933	G
53	S2	934	G
53	S2	955	A
53	S2	963	A
53	S2	971	G
53	S2	990	A
53	S2	992	A
53	S2	999	G
53	S2	1001	A
53	S2	1016	U
53	S2	1017	U

*Continued on next page...*

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Mol	Chain	Res	Type
53	S2	1023	A
53	S2	1027	A
53	S2	1028	A
53	S2	1060	A
53	S2	1067	C
53	S2	1080	A
53	S2	1083	A
53	S2	1085	C
53	S2	1089	G
53	S2	1109	C
53	S2	1115	U
53	S2	1116	C
53	S2	1118	C
53	S2	1121	G
53	S2	1133	A
53	S2	1138	C
53	S2	1153	C
53	S2	1154	U
53	S2	1195	A
53	S2	1207	G
53	S2	1215	C
53	S2	1216	C
53	S2	1217	A
53	S2	1221	G
53	S2	1224	G
53	S2	1227	G
53	S2	1242	U
53	S2	1243	U
53	S2	1251	A
53	S2	1253	A
53	S2	1256	G
53	S2	1257	G
53	S2	1259	A
53	S2	1263	U
53	S2	1264	C
53	S2	1274	G
53	S2	1275	G
53	S2	1283	C
53	S2	1285	G
53	S2	1286	G
53	S2	1290	G
53	S2	1294	G

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Mol	Chain	Res	Type
53	S2	1295	A
53	S2	1301	A
53	S2	1302	G
53	S2	1303	C
53	S2	1305	C
53	S2	1306	U
53	S2	1308	U
53	S2	1312	G
53	S2	1313	A
53	S2	1333	U
53	S2	1341	C
53	S2	1342	U
53	S2	1343	U
53	S2	1348	G
53	S2	1371	U
53	S2	1372	U
53	S2	1373	C
53	S2	1375	G
53	S2	1378	A
53	S2	1382	A
53	S2	1384	C
53	S2	1397	U
53	S2	1398	G
53	S2	1404	U
53	S2	1415	C
53	S2	1421	A
53	S2	1423	C
53	S2	1428	G
53	S2	1433	C
53	S2	1434	C
53	S2	1435	C
53	S2	1436	C
53	S2	1438	A
53	S2	1439	A
53	S2	1454	A
53	S2	1462	U
53	S2	1463	U
53	S2	1468	C
53	S2	1487	A
53	S2	1489	A
53	S2	1490	G
53	S2	1495	G

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Mol	Chain	Res	Type
53	S2	1497	G
53	S2	1498	A
53	S2	1505	U
53	S2	1507	G
53	S2	1508	A
53	S2	1509	U
53	S2	1520	G
53	S2	1521	C
53	S2	1522	A
53	S2	1533	A
53	S2	1537	A
53	S2	1546	G
53	S2	1552	G
53	S2	1553	C
53	S2	1557	C
53	S2	1560	U
53	S2	1570	G
53	S2	1579	A
53	S2	1580	A
53	S2	1585	U
53	S2	1587	G
53	S2	1588	A
53	S2	1598	G
53	S2	1600	G
53	S2	1601	A
53	S2	1606	G
53	S2	1621	U
53	S2	1623	A
53	S2	1632	G
53	S2	1634	A
53	S2	1644	C
53	S2	1646	C
53	S2	1648	G
53	S2	1660	C
53	S2	1661	A
53	S2	1663	A
53	S2	1664	A
53	S2	1665	G
53	S2	1680	G
53	S2	1683	C
53	S2	1686	G
53	S2	1696	C

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Mol	Chain	Res	Type
53	S2	1698	C
53	S2	1699	A
53	S2	1721	U
53	S2	1722	G
53	S2	1744	G
53	S2	1745	A
53	S2	1752	C
53	S2	1753	C
53	S2	1754	G
53	S2	1757	G
53	S2	1758	G
53	S2	1759	G
53	S2	1761	U
53	S2	1772	C
53	S2	1773	C
53	S2	1774	C
53	S2	1775	U
53	S2	1776	G
53	S2	1777	G
53	S2	1781	A
53	S2	1782	G
53	S2	1783	C
53	S2	1784	G
53	S2	1786	U
53	S2	1825	A
53	S2	1826	G
53	S2	1829	G
53	S2	1831	A
53	S2	1835	A
53	S2	1837	G
53	S2	1838	U
53	S2	1849	G
53	S2	1852	C
53	S2	1856	C
53	S2	1861	G
53	S2	1862	G
53	S2	1863	A
53	S2	1864	U
53	S2	1865	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	L5	218	A
7	L5	406	C
7	L5	504	G
7	L5	914	U
7	L5	955	G
7	L5	1198	G
7	L5	1590	C
7	L5	1633	G
7	L5	1977	C
7	L5	2033	A
7	L5	2675	G
7	L5	2760	G
7	L5	2786	C
7	L5	3614	G
7	L5	3673	C
7	L5	3876	A
7	L5	4378	A
7	L5	4699	U
7	L5	4913	G
53	S2	112	U
53	S2	291	G
53	S2	563	G
53	S2	688	U
53	S2	1434	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
45	MLZ	Lm	98	45	8,9,10	0.81	0	4,9,11	0.67	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	MLZ	Lm	98	45	-	0/7/8/10	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	Lm	98	MLZ	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 265 ligands modelled in this entry, 265 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

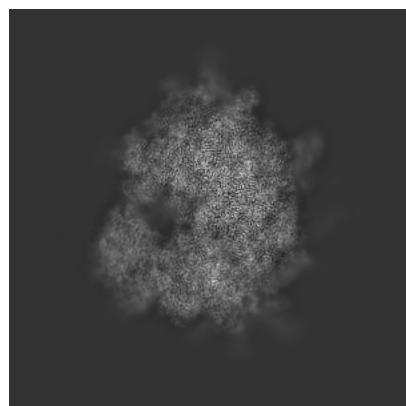
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53944. These allow visual inspection of the internal detail of the map and identification of artifacts.

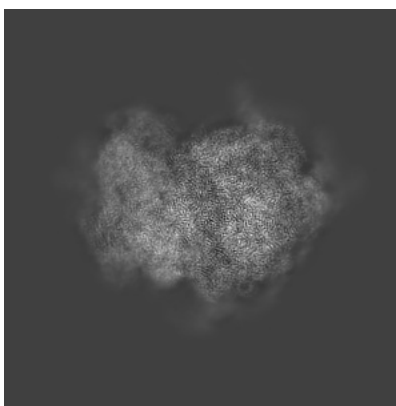
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

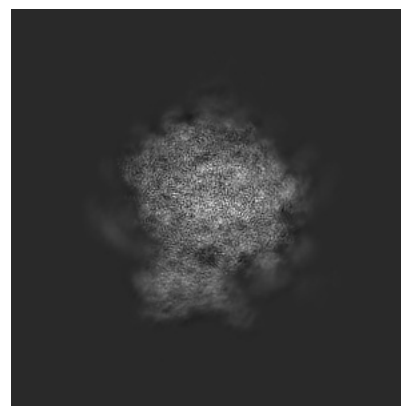
#### 6.1.1 Primary map



X

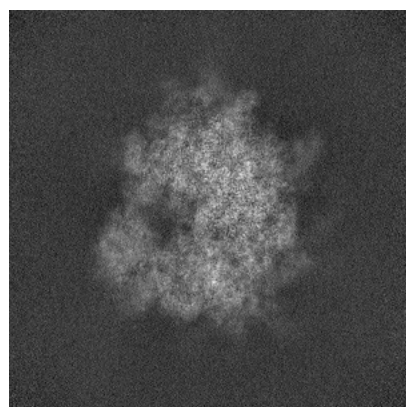


Y

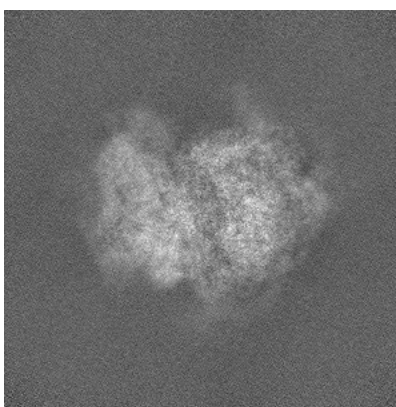


Z

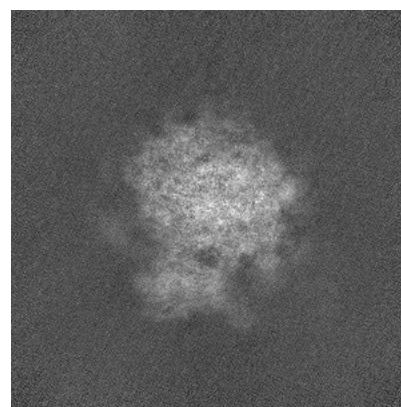
#### 6.1.2 Raw map



X



Y

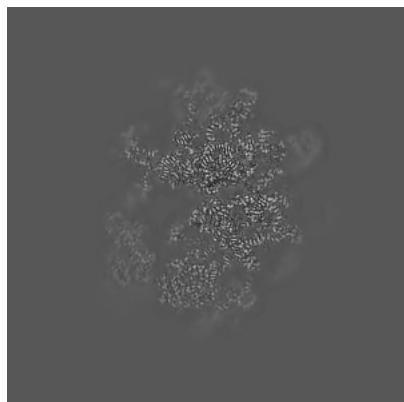


Z

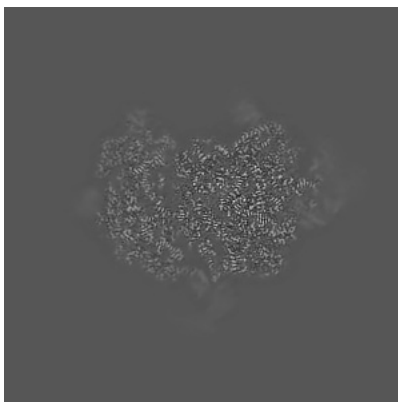
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

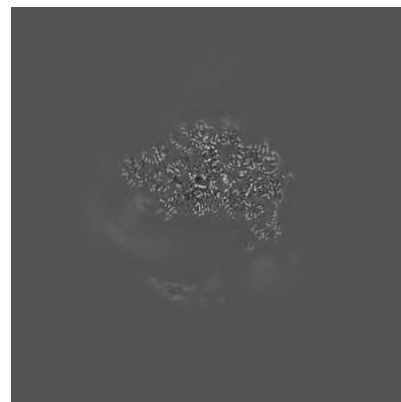
### 6.2.1 Primary map



X Index: 320

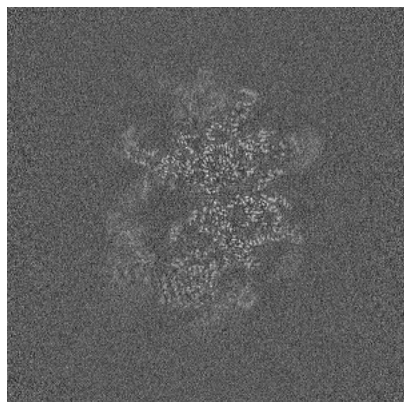


Y Index: 320

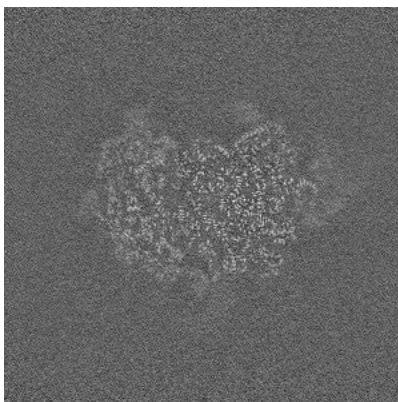


Z Index: 320

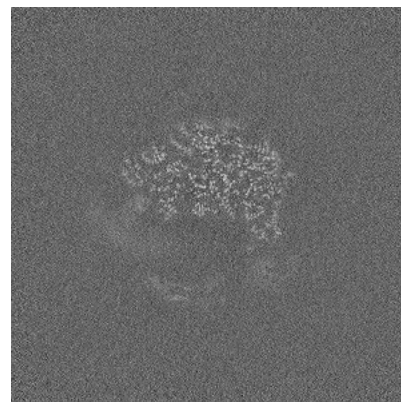
### 6.2.2 Raw map



X Index: 320



Y Index: 320



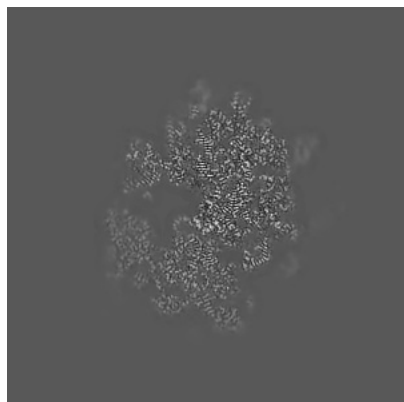
Z Index: 320

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

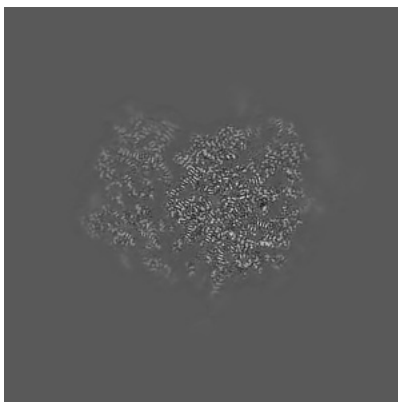


## 6.3 Largest variance slices [i](#)

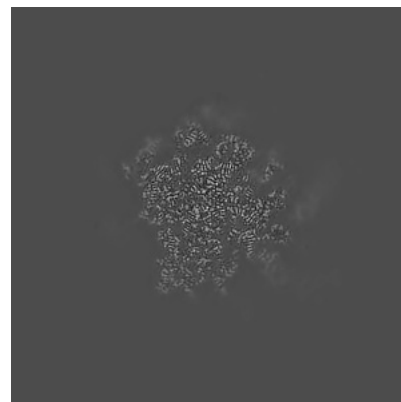
### 6.3.1 Primary map



X Index: 299

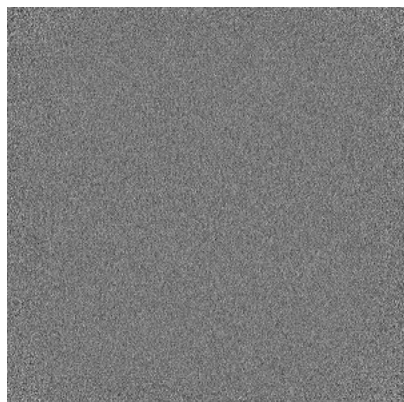


Y Index: 339

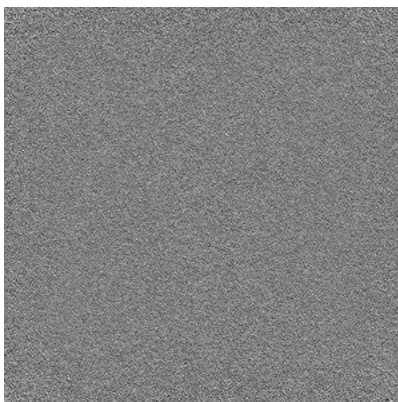


Z Index: 385

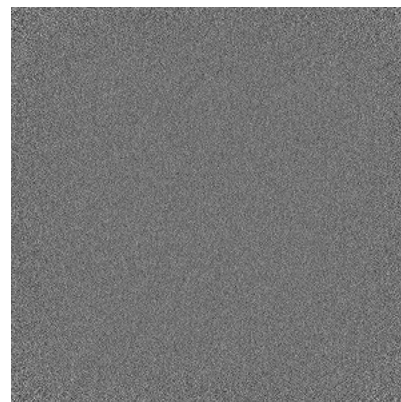
### 6.3.2 Raw map



X Index: 0



Y Index: 0



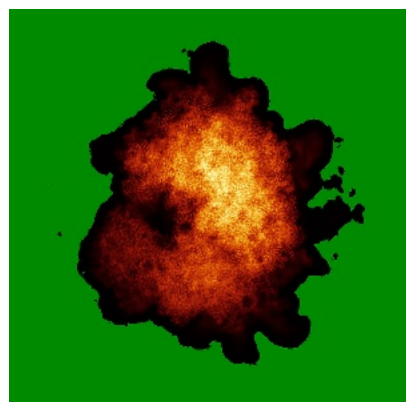
Z Index: 0

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

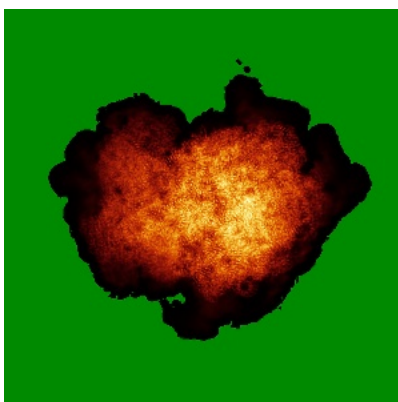


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

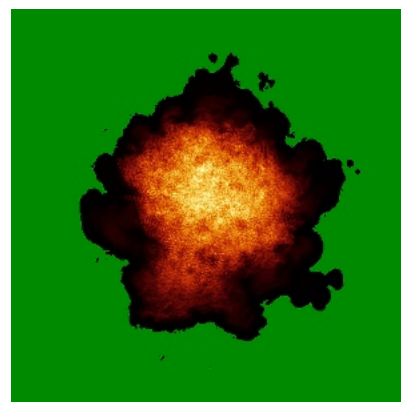
### 6.4.1 Primary map



X

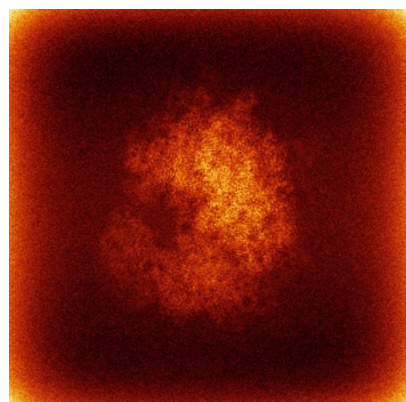


Y

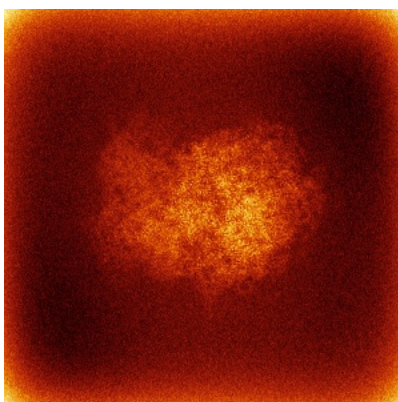


Z

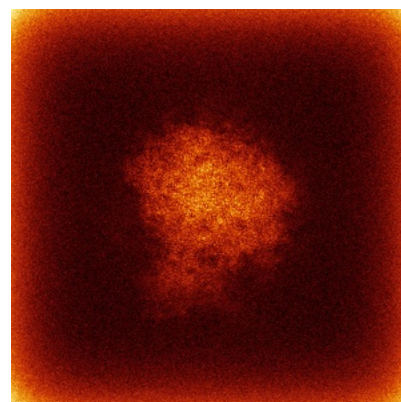
### 6.4.2 Raw map



X



Y

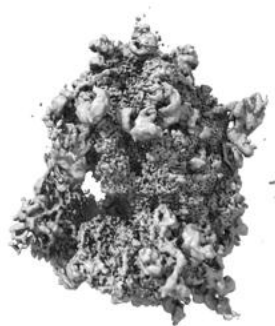


Z

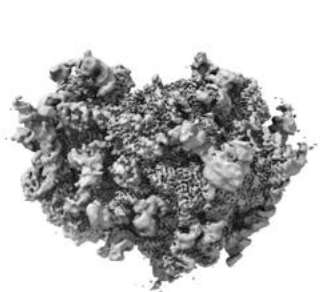
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



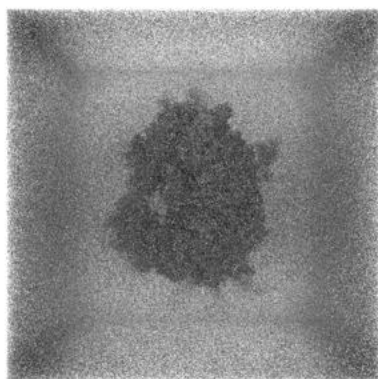
Y



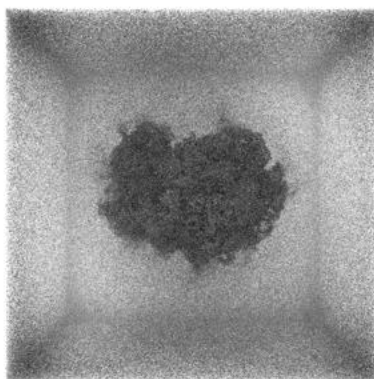
Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

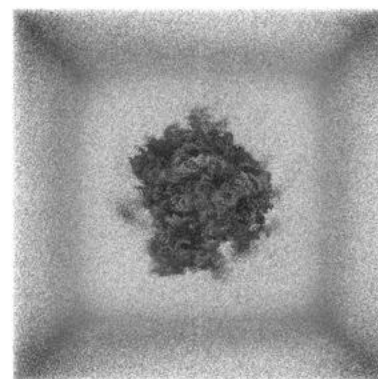
### 6.5.2 Raw map



X



Y



Z

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

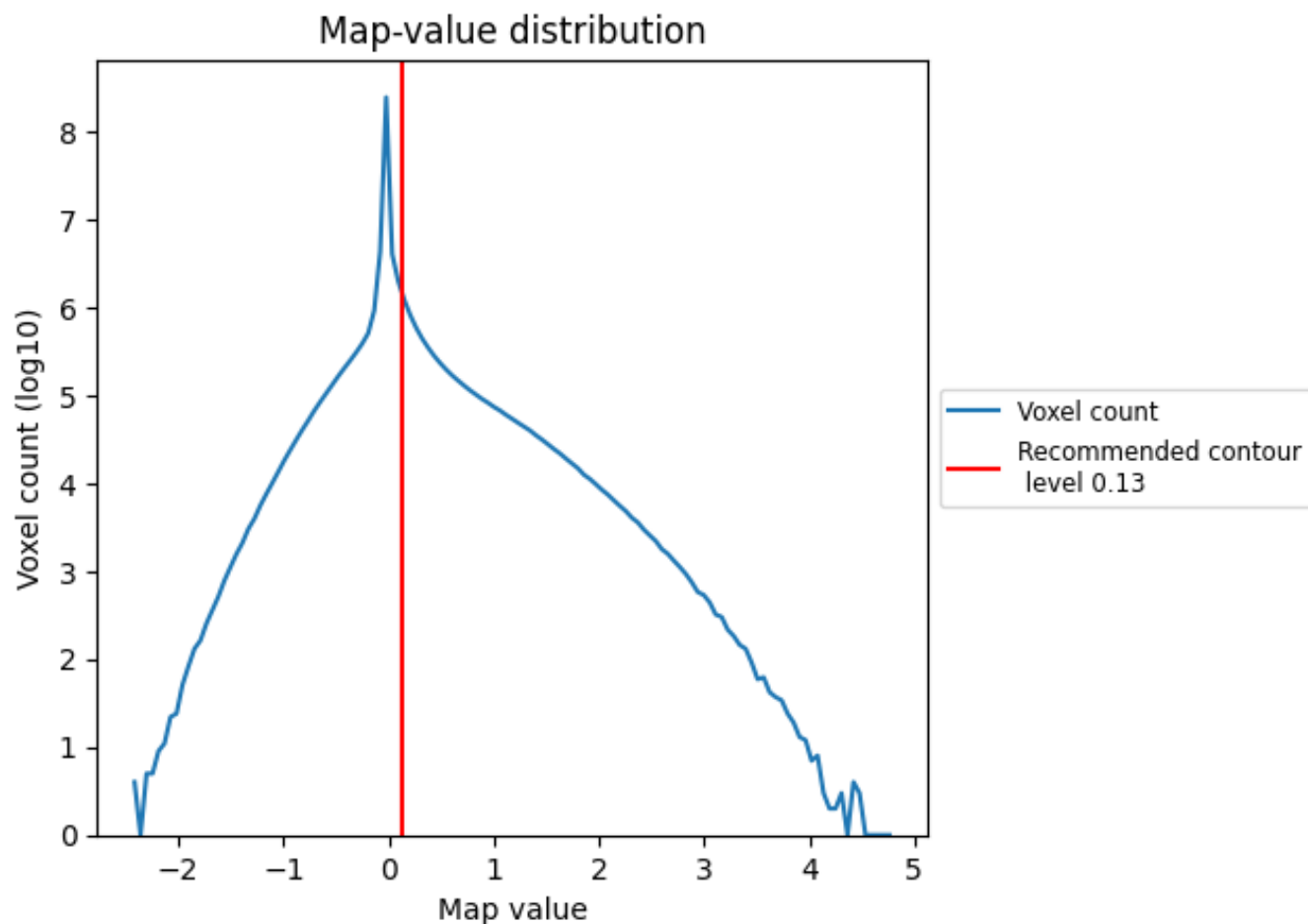
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

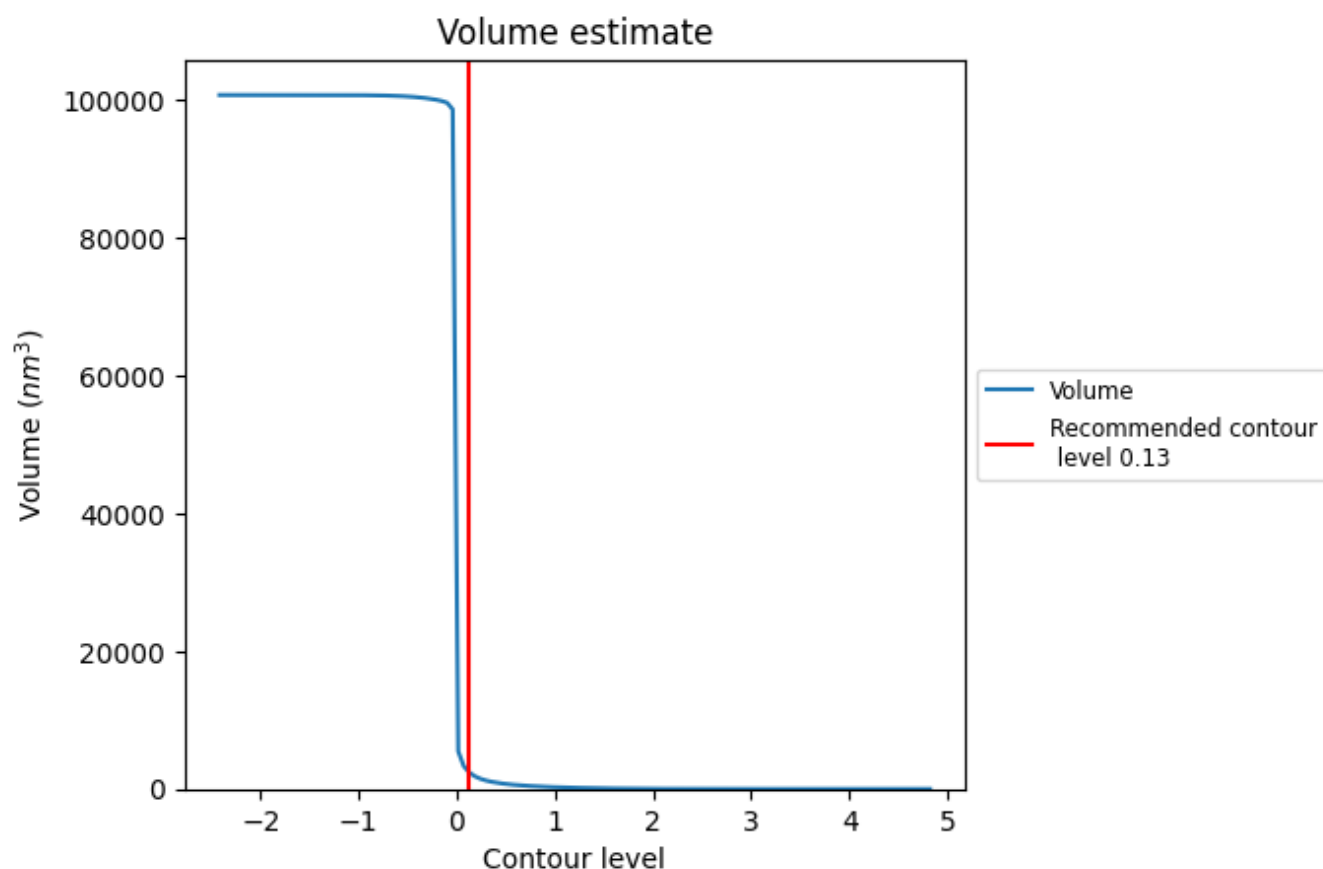
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

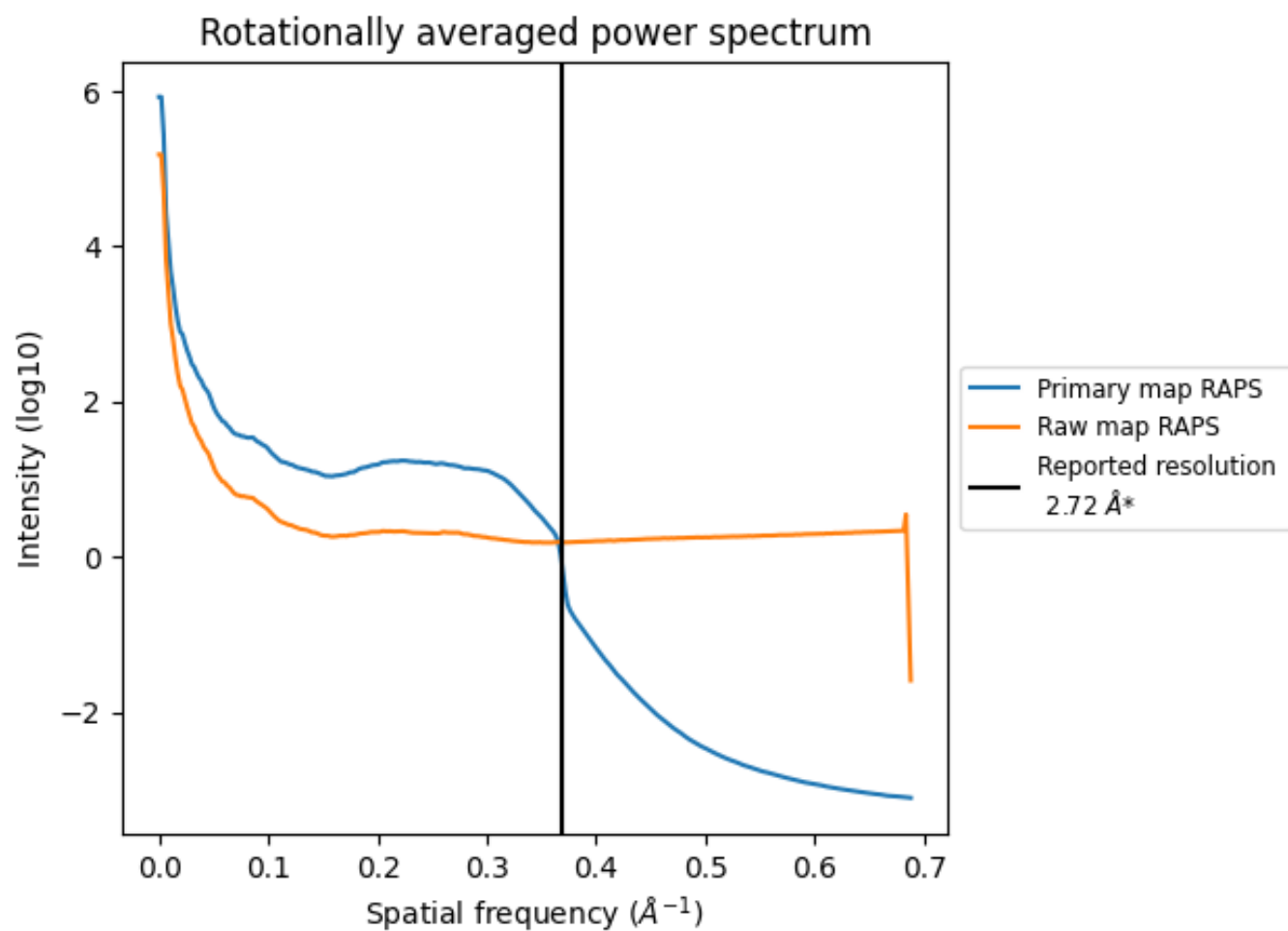
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2367  $\text{nm}^3$ ; this corresponds to an approximate mass of 2138 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 ⓘ

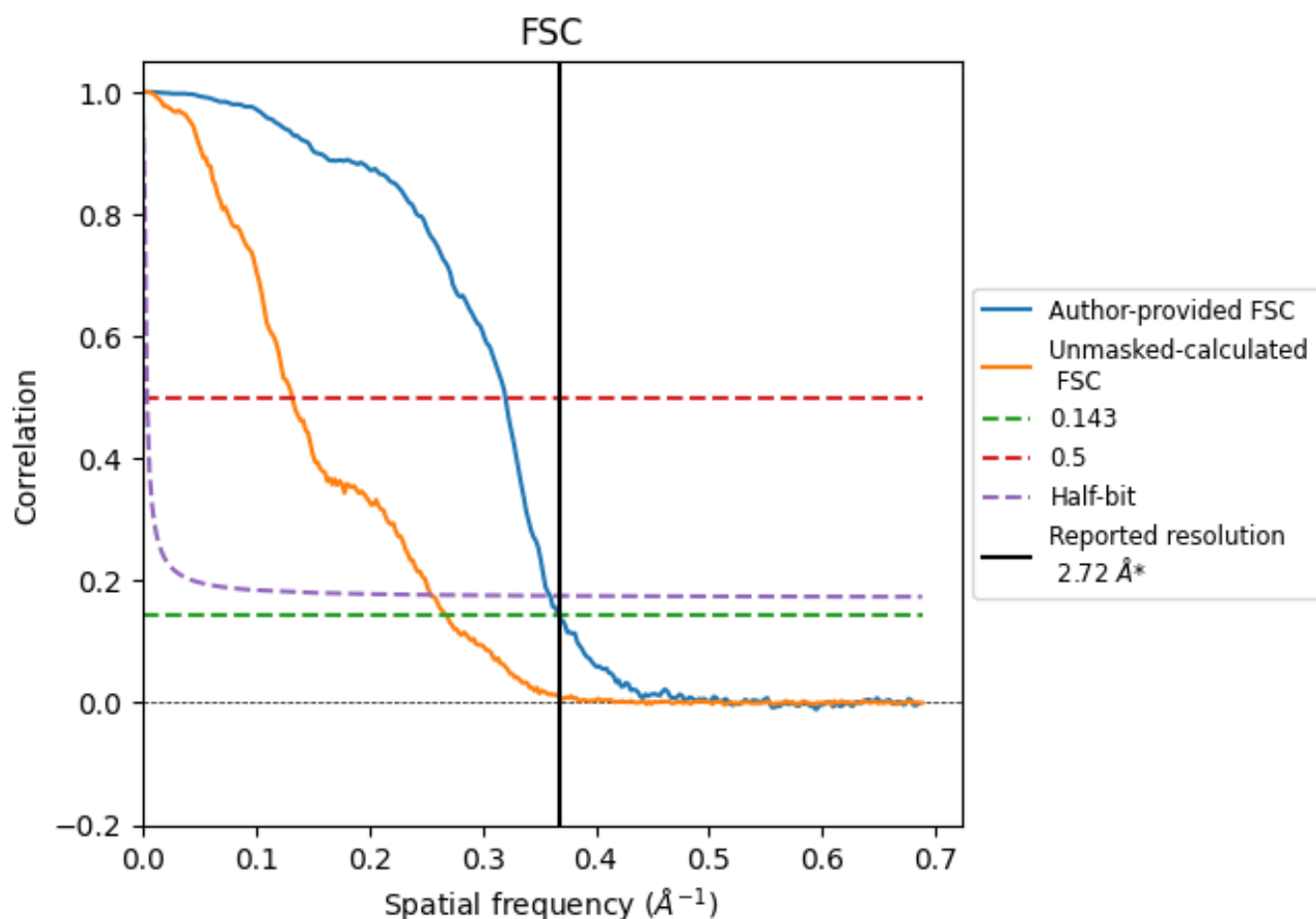


\*Reported resolution corresponds to spatial frequency of 0.368  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.368  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

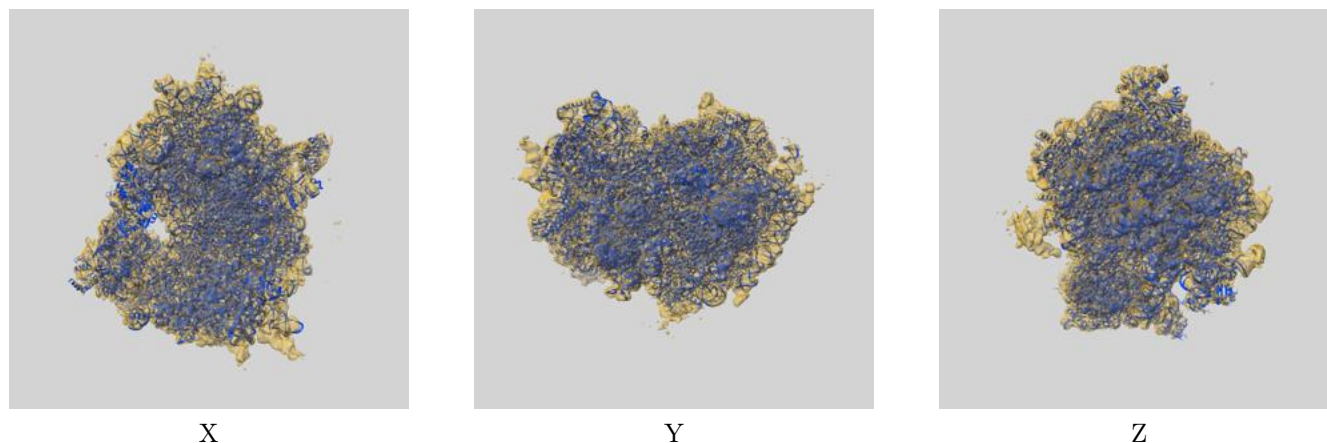
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.12	2.78
Unmasked-calculated*	3.73	7.56	3.93

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 2.72 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-53944 and PDB model 9RG7. Per-residue inclusion information can be found in section [3](#) on page [21](#).

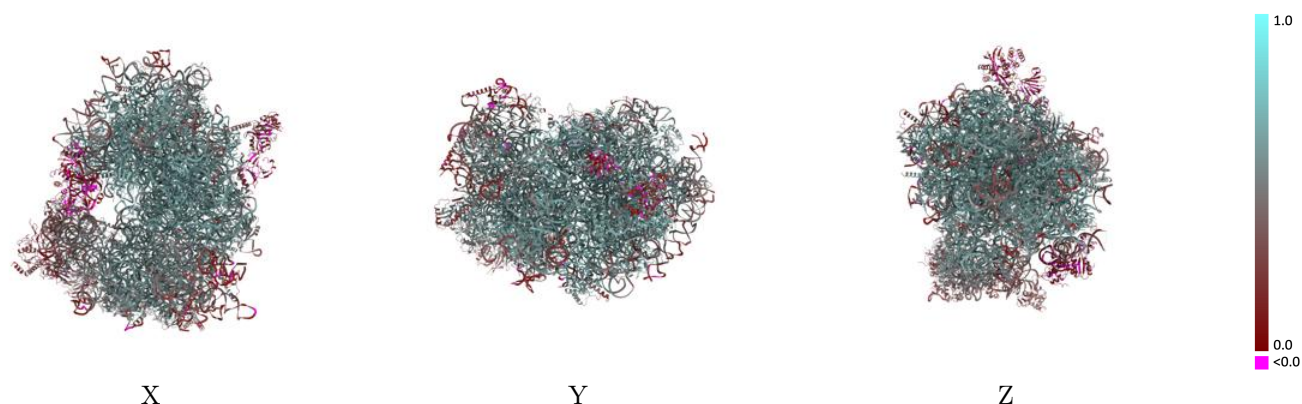
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

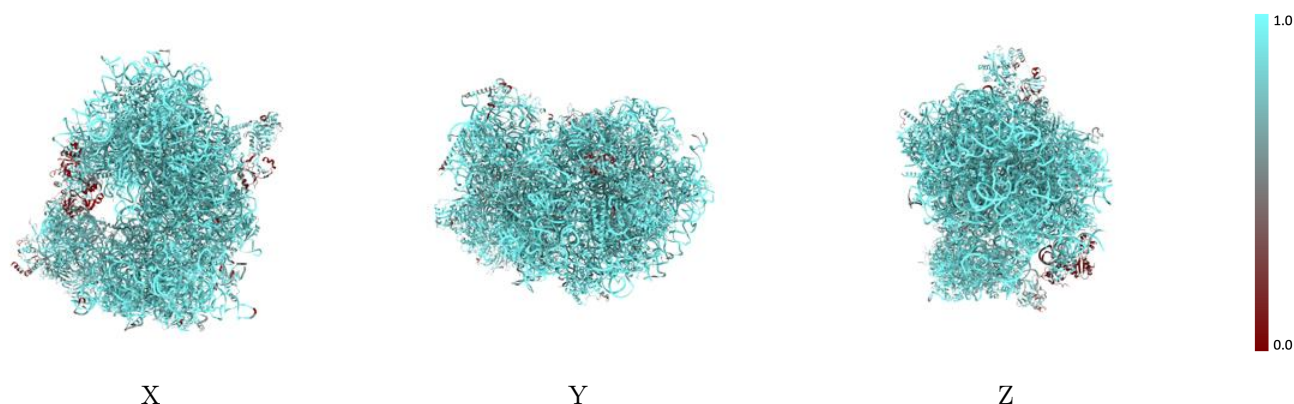


## 9.2 Q-score mapped to coordinate model [i](#)



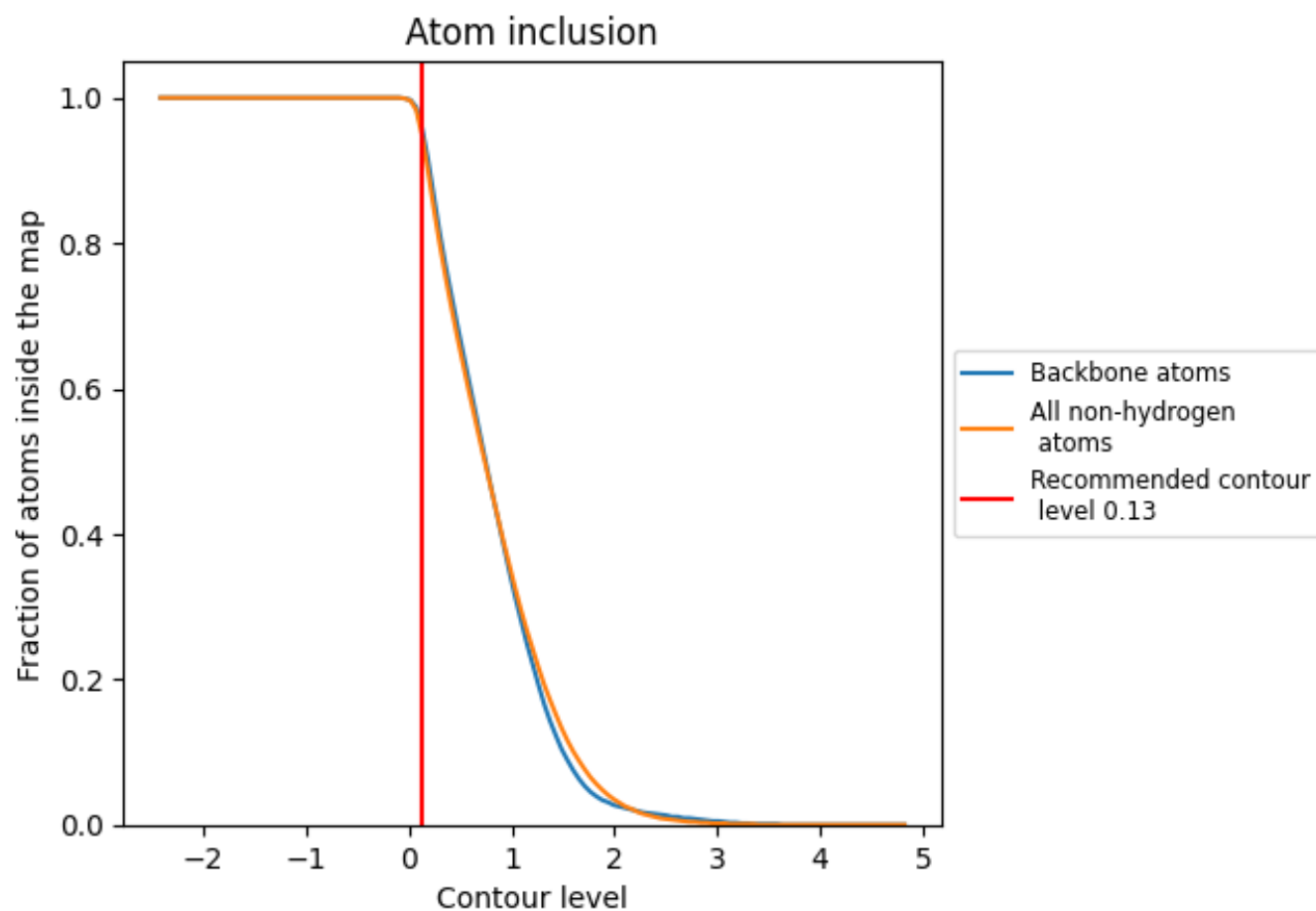
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.5340
L5	 0.9750	 0.5660
L7	 0.9970	 0.6200
L8	 0.9790	 0.6030
LA	 0.9910	 0.6550
LB	 0.9800	 0.6260
LC	 0.9780	 0.6300
LD	 0.9750	 0.5700
LE	 0.9750	 0.5800
LF	 0.9870	 0.6360
LG	 0.9230	 0.5390
LH	 0.9750	 0.5940
LI	 0.9800	 0.6120
LJ	 0.9390	 0.5140
LL	 0.9780	 0.6040
LM	 0.9740	 0.6050
LN	 0.9960	 0.6560
LO	 0.9880	 0.6360
LP	 0.9880	 0.6440
LQ	 0.9910	 0.6520
LR	 0.9430	 0.5840
LS	 0.9910	 0.6420
LT	 0.9700	 0.6090
LU	 0.9470	 0.5400
LV	 0.9840	 0.6280
LW	 0.8170	 0.4230
LX	 0.9730	 0.6060
LY	 0.9790	 0.6170
LZ	 0.9870	 0.6110
La	 0.9900	 0.6460
Lb	 0.9210	 0.5330
Lc	 0.9680	 0.6070
Ld	 0.9690	 0.6040
Le	 0.9920	 0.6500
Lf	 0.9930	 0.6570



















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Chain	Atom inclusion	Q-score
Lg	 0.9680	 0.6120
Lh	 0.9730	 0.6000
Li	 0.9670	 0.5810
Lj	 0.9910	 0.6470
Lk	 0.9370	 0.5340
Ll	 0.9930	 0.6400
Lm	 0.9640	 0.6050
Ln	 0.8280	 0.5350
Lo	 0.9590	 0.6070
Lp	 0.9780	 0.6270
Lr	 0.9840	 0.6310
Ls	 0.2110	 0.0890
Lt	 0.2720	 0.0700
N4	 0.8380	 0.1820
NA	 0.5260	 0.1200
NB	 0.5500	 0.2060
S2	 0.9690	 0.4980
SA	 0.9400	 0.5250
SB	 0.9370	 0.5360
SC	 0.9620	 0.5560
SD	 0.8420	 0.3770
SE	 0.9420	 0.5330
SF	 0.8780	 0.4040
SG	 0.8940	 0.4270
SH	 0.9050	 0.4590
SI	 0.9440	 0.5360
SJ	 0.9340	 0.5170
SK	 0.8280	 0.3070
SL	 0.9490	 0.5720
SM	 0.4620	 0.2250
SN	 0.9740	 0.5890
SO	 0.9410	 0.5530
SP	 0.7940	 0.2940
SQ	 0.8950	 0.3960
SR	 0.8990	 0.4360
SS	 0.8480	 0.3220
ST	 0.8940	 0.3700
SU	 0.8510	 0.3630
SV	 0.9440	 0.5220
SW	 0.9720	 0.5910
SX	 0.9540	 0.5700
SY	 0.9200	 0.4650

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Chain	Atom inclusion	Q-score
SZ	 0.7980	 0.2670
Sa	 0.9330	 0.5460
Sb	 0.9360	 0.5290
Sc	 0.9010	 0.4180
Sd	 0.9160	 0.4210
Se	 0.8360	 0.4520
Sf	 0.5750	 0.1840
Sg	 0.8720	 0.2870