



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:28 PM UTC

PDB ID : 9I2D / pdb_00009i2d
EMDB ID : EMD-52581
Title : NMT1-NAC bound human RNC with 10 amino acid ARF1-linker
Authors : Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2025-01-20
Resolution : 2.19 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

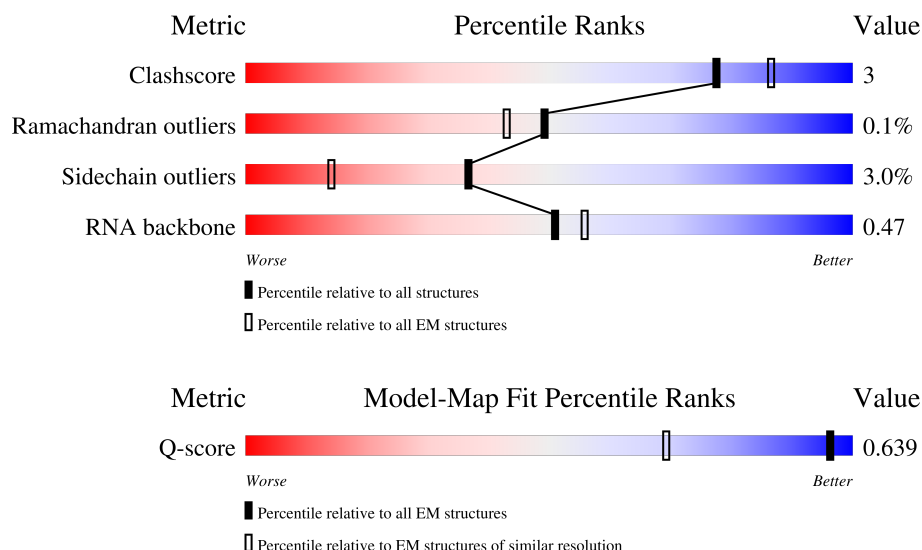
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

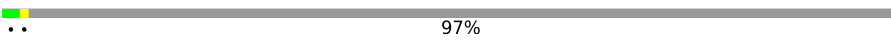


The reported resolution of this entry is 2.19 Å.

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	2745 (1.70 - 2.69)

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

Mol	Chain	Length	Quality of chain
1	CM	409	 97%
2	CP	75	 27% 64% 36%
3	CR	437	 27% 85% 8% 5%

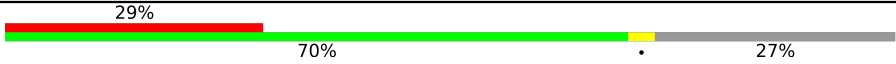

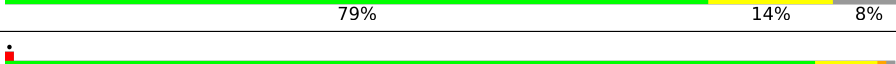
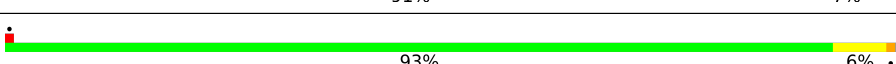


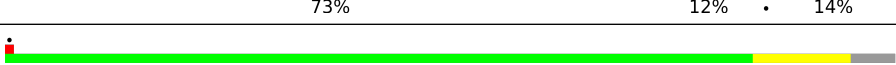
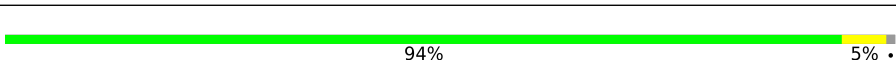

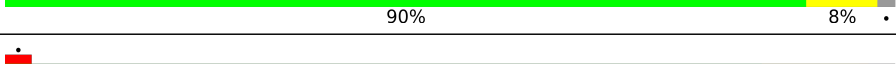
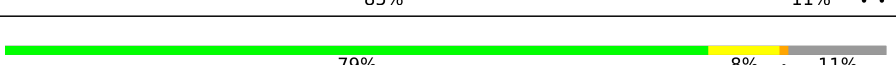

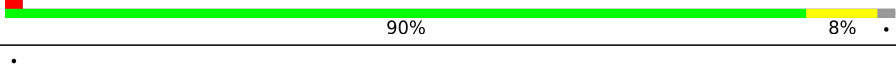

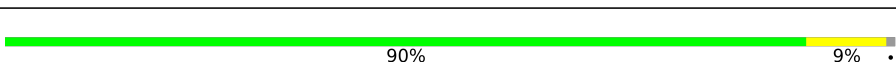
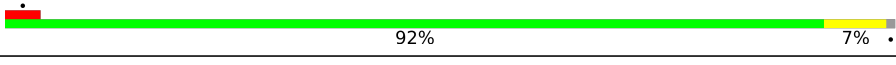
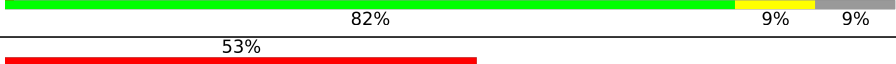






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Mol	Chain	Length	Quality of chain
4	CZ	55	
5	L5	5070	
6	L7	121	
7	L8	157	
8	LA	257	
9	LB	403	
10	LC	427	
11	LD	297	
12	LE	288	
13	LF	248	
14	LG	266	
15	LH	192	
16	LI	214	
17	LJ	178	
18	LL	211	
19	LM	215	
20	LN	204	
21	LO	203	
22	LP	184	
23	LQ	188	
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	NA	215	
53	NB	162	




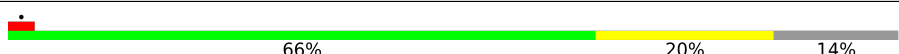
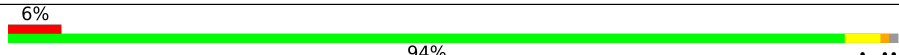
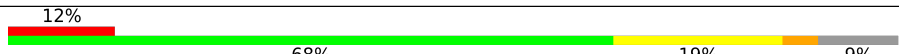

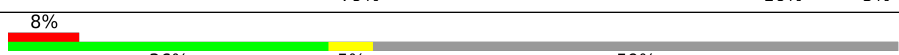

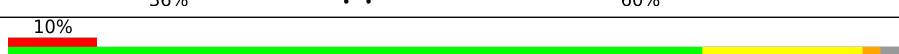
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Mol	Chain	Length	Quality of chain
54	NM	496	
55	S2	1869	
56	SA	295	
57	SB	264	
58	SC	293	
59	SD	243	
60	SE	263	
61	SF	204	
62	SG	249	
63	SH	194	
64	SI	208	
65	SJ	194	
66	SK	165	
67	SL	158	
68	SM	132	
69	SN	151	
70	SO	151	
71	SP	145	
72	SQ	146	
73	SR	135	
74	SS	152	
75	ST	145	
76	SU	119	
77	SV	83	
78	SW	130	

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Mol	Chain	Length	Quality of chain
79	SX	143	
80	SY	133	
81	SZ	125	
82	Sa	115	
83	Sb	84	
84	Sc	69	
85	Sd	56	
86	Se	133	
87	Sf	156	
88	Sg	317	

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 222256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called CMV-staller mRNA with 18aa ARF1-linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CM	12	Total	C	N	O	P	0	0
			247	111	37	87	12		

- Molecule 2 is a RNA chain called prolyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CP	75	Total	C	N	O	P	0	0
			1602	713	284	530	75		

- Molecule 3 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CR	414	Total	C	N	O	S	0	0
			3269	2080	557	621	11		

- Molecule 4 is a protein called nascent polypeptide 10aa ARF1-linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CZ	54	Total	C	N	O	S	0	0
			333	211	58	62	2		

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	3648	Total	C	N	O	P	0	0
			78199	34823	14307	25422	3647		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 7 is a RNA chain called 5.8S rRNA.

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

- Molecule 8 is a protein called 60S ribosomal protein L8.

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

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	395	Total	C	N	O	S	0	0
			3183	2027	597	545	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	364	Total	C	N	O	S	0	0
			2884	1814	576	479	15		

- 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
			2361	1496	430	421	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	219	Total	C	N	O	S	0	0
			1754	1129	334	287	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	229	Total	C	N	O	S	0	0
			1818	1157	351	306	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
			1510	950	282	272	6		

- Molecule 16 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	207	Total	C	N	O	S	0	0
			1666	1059	323	270	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LJ	169	Total	C	N	O	S	0	0
			1329	841	250	232	6		

- Molecule 18 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	205	Total	C	N	O	S	0	0
			1630	1020	340	266	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
			1122	720	216	179	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	200	Total	C	N	O	S	0	0
			1633	1053	318	257	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
			1234	771	240	214	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
			1502	939	313	245	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LR	176	Total	C	N	O	S	0	0
			1452	898	318	227	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
			1452	925	283	234	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
			1282	813	250	213	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LU	101	Total	C	N	O	S	0	0
			806	520	141	143	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
			971	613	183	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	115	Total	C	N	O	S	0	0
			808	506	160	139	3		

- 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
			981	627	184	169	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	134	Total	C	N	O	S	0	0
			1111	697	225	186	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
			1154	731	236	184	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lb	75	Total	C	N	O	S	0	0
			590	367	123	97	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lc	97	Total	C	N	O	S	0	0
			742	473	130	133	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
			874	554	171	147	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
			1049	664	215	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
			872	552	173	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
			889	557	184	142	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lh	121	Total	C	N	O	S	0	0
			1006	635	203	167	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
			813	510	176	123	4		

- Molecule 42 is a protein called 60S ribosomal protein L37.

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
			542	350	100	91	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 Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lm	52	Total	C	N	O	S	0	0
			425	264	90	65	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
			696	440	135	114	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
			997	618	207	168	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ls	212	Total	C	N	O	S	0	0
			1640	1042	284	305	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lt	160	Total	C	N	O	S	0	0
			1208	749	226	229	4		

- Molecule 52 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	NA	67	Total	C	N	O	S	0	0
			531	335	97	98	1		

- Molecule 53 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	NB	124	Total	C	N	O	S	0	0
			963	597	175	188	3		

- Molecule 54 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	NM	393	Total	C	N	O	S	3	0
			3209	2075	544	573	17		

- Molecule 55 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S2	1713	Total	C	N	O	P	0	0
			36562	16320	6565	11965	1712		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	140	C	U	conflict	GB 151415227

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SA	216	Total	C	N	O	S	0	0
			1671	1068	297	298	8		

- Molecule 57 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SB	213	Total	C	N	O	S	0	0
			1718	1092	308	304	14		

- Molecule 58 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SC	219	Total	C	N	O	S	0	0
			1661	1076	284	291	10		

- Molecule 59 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SD	223	Total	C	N	O	S	0	0
			1594	1023	291	273	7		

- Molecule 60 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SE	262	Total	C	N	O	S	0	0
			1972	1270	370	324	8		

- Molecule 61 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SF	181	Total	C	N	O	S	0	0
			1403	879	269	248	7		

- Molecule 62 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SG	231	Total	C	N	O	S	0	0
			1634	1026	332	269	7		

- Molecule 63 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SH	183	Total	C	N	O		0	0
			1274	819	242	213			

- Molecule 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SI	206	Total	C	N	O	S	0	0
			1574	989	308	272	5		

- Molecule 65 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SJ	179	Total	C	N	O	S	0	0
			1431	915	290	224	2		

- Molecule 66 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	96	Total	C	N	O	S	0	0
			726	479	127	115	5		

- Molecule 67 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SL	144	Total	C	N	O	S	0	0
			1143	730	213	194	6		

- Molecule 68 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 69 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SN	150	Total	C	N	O	S	0	0
			1182	758	226	197	1		

- Molecule 70 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SO	134	Total	C	N	O	S	0	0
			969	596	194	173	6		

- Molecule 71 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SP	129	Total	C	N	O	S	0	0
			990	626	190	168	6		

- Molecule 72 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SQ	142	Total	C	N	O	S	0	0
			1075	689	204	179	3		

- Molecule 73 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SR	131	Total	C	N	O	S	0	0
			942	600	179	159	4		

- Molecule 74 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SS	141	Total	C	N	O	S	0	0
			1130	712	232	185	1		

- Molecule 75 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	ST	143	Total	C	N	O	S	0	0
			1081	679	210	189	3		

- Molecule 76 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SU	101	Total	C	N	O	S	0	0
			713	447	137	125	4		

- Molecule 77 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SV	83	Total	C	N	O	S	0	0
			618	385	115	113	5		

- Molecule 78 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SW	129	Total	C	N	O	S	0	0
			1026	655	193	172	6		

- Molecule 79 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SX	141	Total	C	N	O	S	0	0
			1078	682	212	181	3		

- Molecule 80 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SY	123	Total	C	N	O	S	0	0
			927	588	183	152	4		

- Molecule 81 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SZ	75	Total	C	N	O	S	0	0
			559	361	105	92	1		

- Molecule 82 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	99	Total	C	N	O	S	0	0
			781	487	165	124	5		

- Molecule 83 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	83	Total	C	N	O	S	0	0
			618	386	118	107	7		

- Molecule 84 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sc	63	Total	C	N	O	S	0	0
			472	289	92	89	2		

- Molecule 85 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	53	Total	C	N	O	S	0	0
			433	271	87	70	5		

- Molecule 86 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Se	55	Total	C	N	O	S	0	0
			416	254	93	68	1		

- Molecule 87 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 88 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Sg	308	Total	C	N	O	S	0	0
			2180	1393	381	395	11		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	CM	1	Total	Mg	0
			1	1	
89	L5	127	Total	Mg	0
			127	127	
89	L7	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
89	L8	3	Total 3	Mg 3	0
89	LA	1	Total 1	Mg 1	0
89	LC	1	Total 1	Mg 1	0
89	LN	1	Total 1	Mg 1	0
89	LP	1	Total 1	Mg 1	0
89	LV	1	Total 1	Mg 1	0
89	S2	52	Total 52	Mg 52	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	L5	3	Total 3	O 3	0
91	L7	1	Total 1	O 1	0

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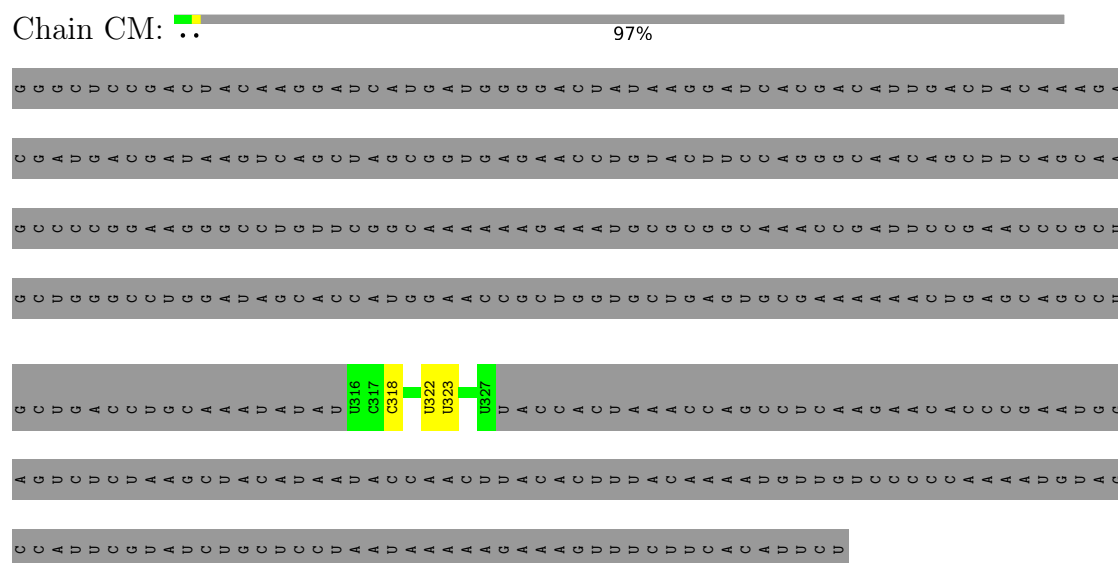
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	LI	1	Total 1	O 1	0
91	LN	1	Total 1	O 1	0
91	La	1	Total 1	O 1	0
91	Li	1	Total 1	O 1	0
91	S2	3	Total 3	O 3	0

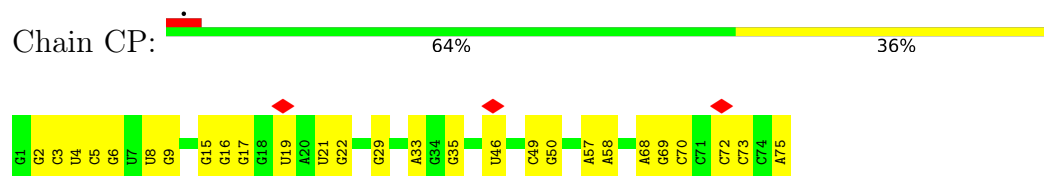
3 Residue-property plots

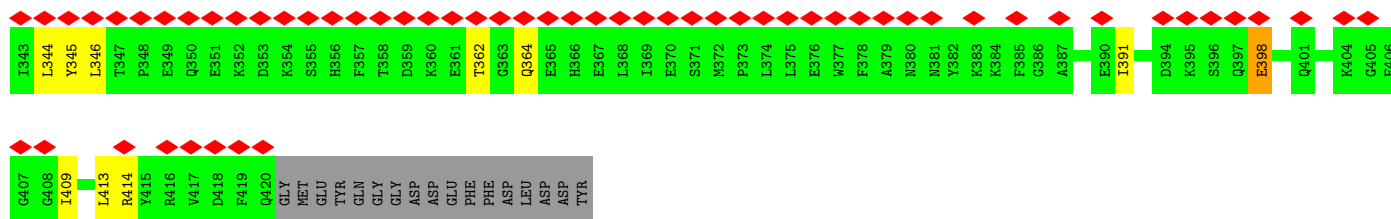
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: CMV-staller mRNA with 18aa ARF1-linker

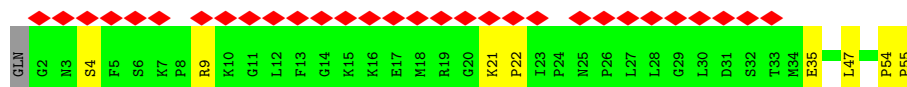
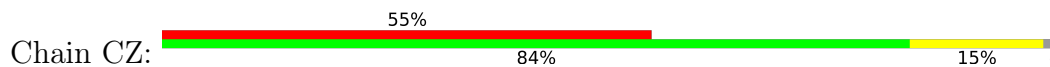


- Molecule 2: prolyl-tRNA

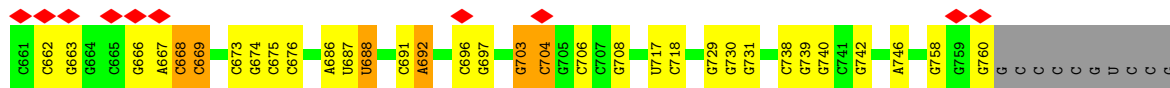
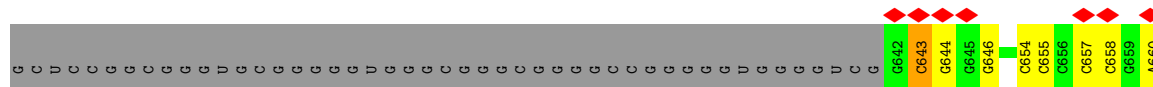
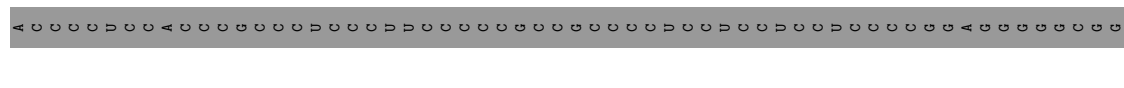
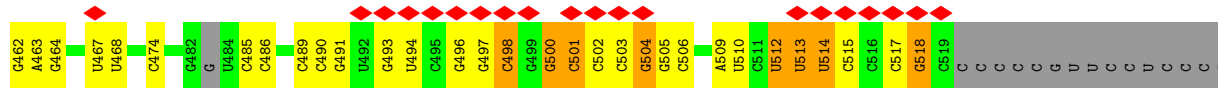
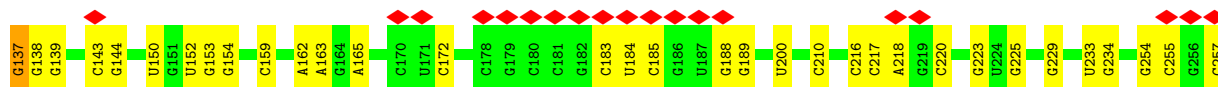




- Molecule 4: nascent polypeptide 10aa ARF1-linker

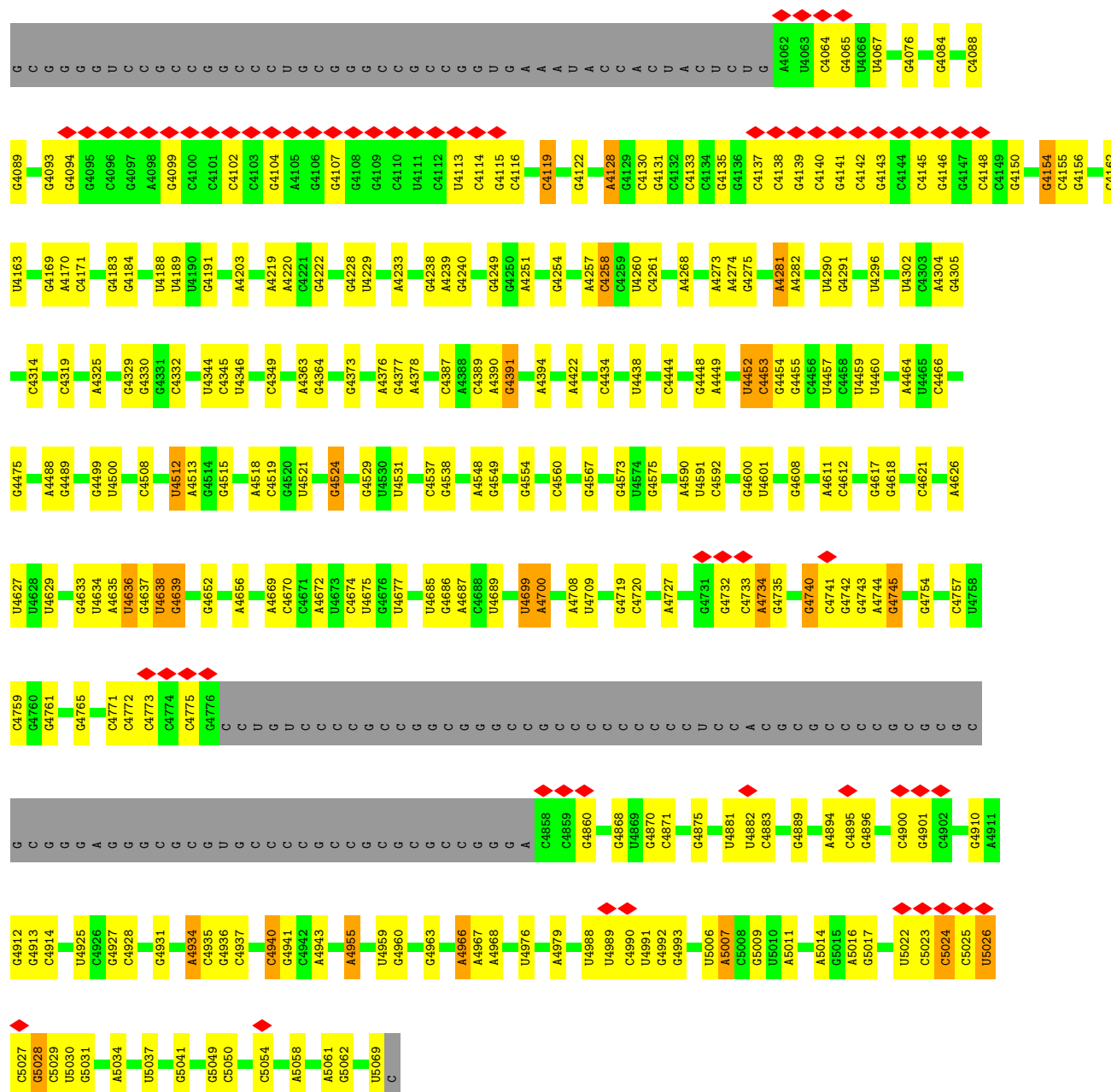


- Molecule 5: 28S rRNA



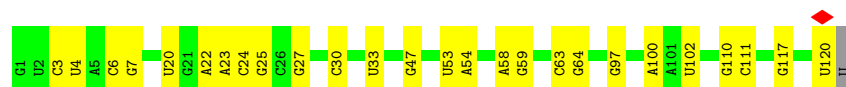






• Molecule 6: 5S rRNA

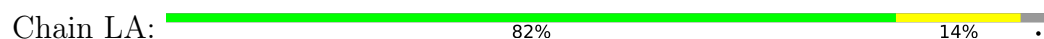
Chain L7: 78% 21%



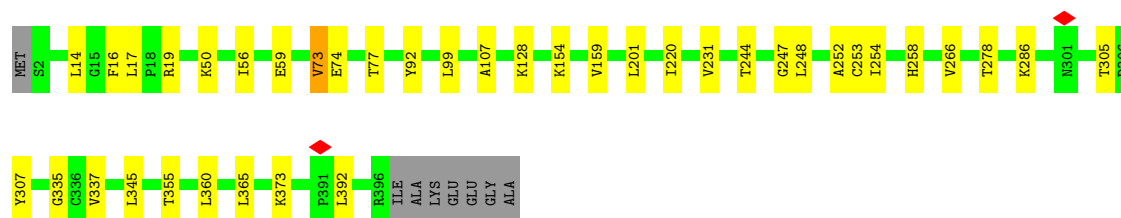
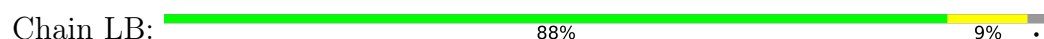
• Molecule 7: 5.8S rRNA

Chain L8: 6% 71% 26%

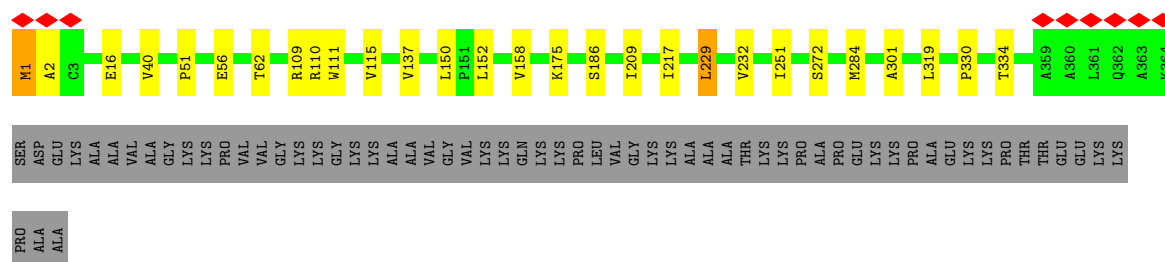
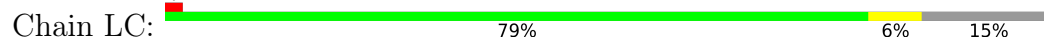
- Molecule 8: 60S ribosomal protein L8



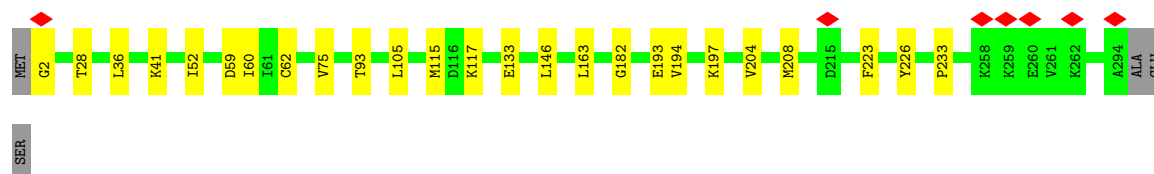
- Molecule 9: 60S ribosomal protein L3



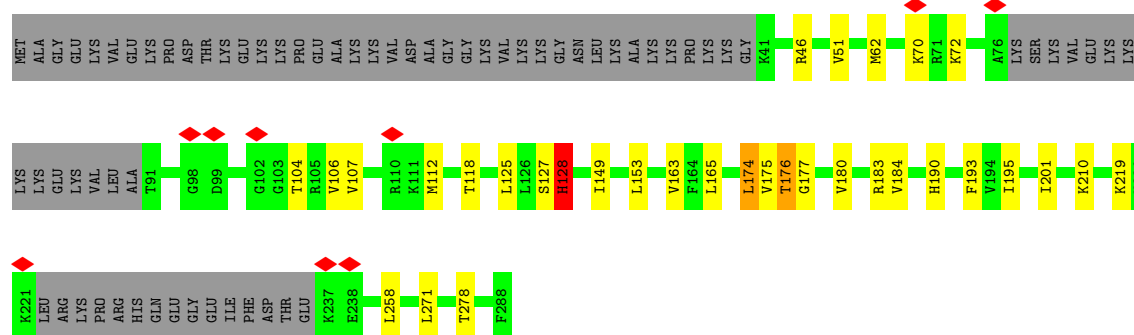
- Molecule 10: 60S ribosomal protein L4



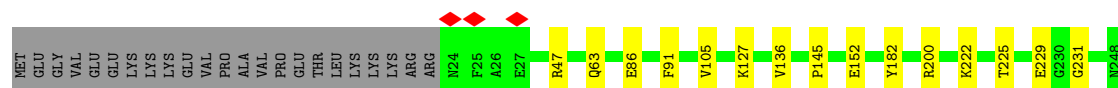
- Molecule 11: 60S ribosomal protein L5

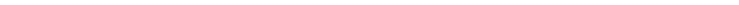


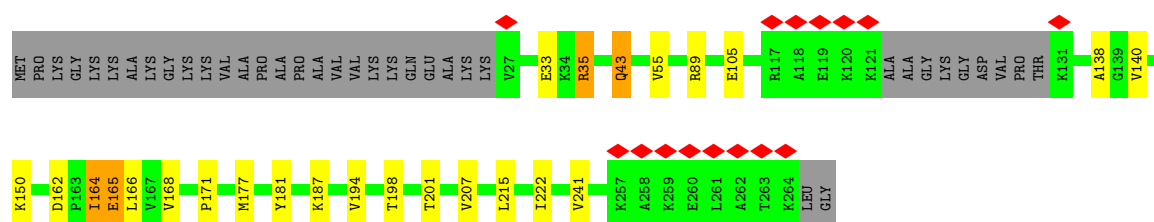
- Chain LE: 



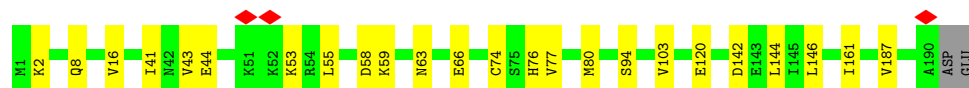
- Chain LF: 85% 6% 9%



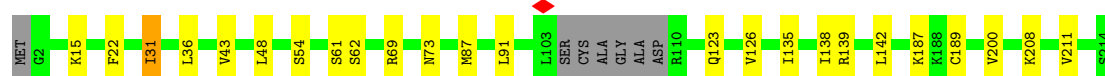
- Chain LG:  6% 77% 8% 14%




- Chain LH: 86% 12%



- Chain LI: 86% 11% .



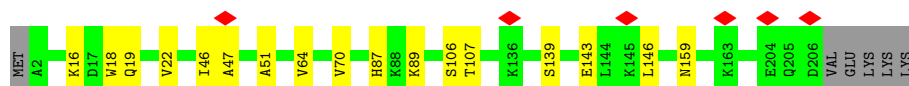
- 

Chain LJ:  88% 7% 5%



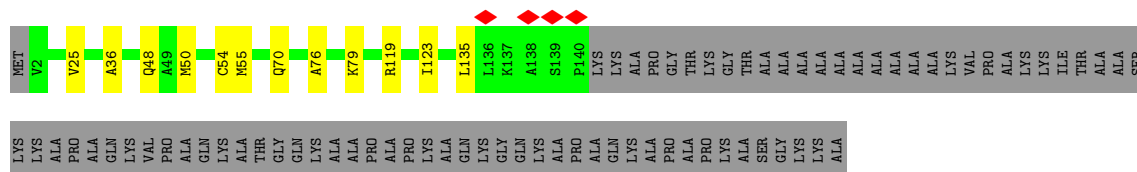
- Molecule 18: 60S ribosomal protein L13

Chain LL:  89% 8% .




- Molecule 19: 60S ribosomal protein L14

Chain LM:  59% 6% 35%



- Molecule 20: 60S ribosomal protein L15

Chain LN:  88% 11%




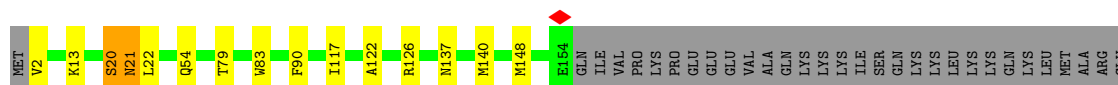
- Molecule 21: 60S ribosomal protein L13a

Chain LO:  88% 10% ..



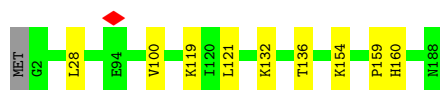
- Molecule 22: 60S ribosomal protein L17

Chain LP:  75% 7% 17%

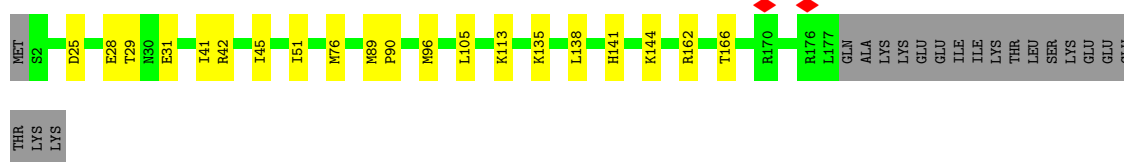
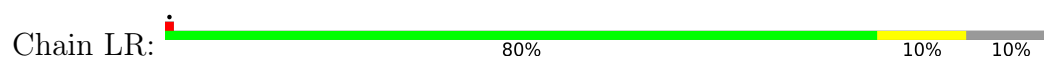


- Molecule 23: 60S ribosomal protein L18

Chain LQ:  95% 5% .



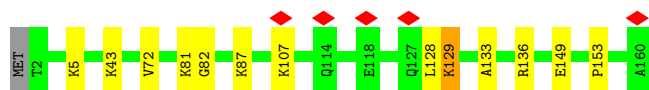
- Molecule 24: 60S ribosomal protein L19



- Molecule 25: 60S ribosomal protein L18a



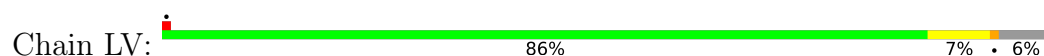
- Molecule 26: 60S ribosomal protein L21



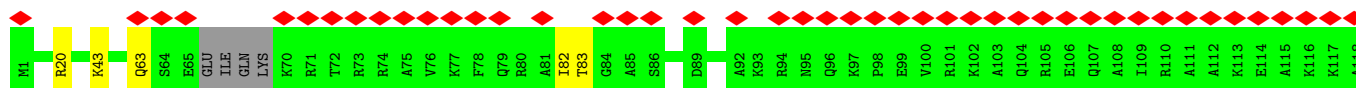
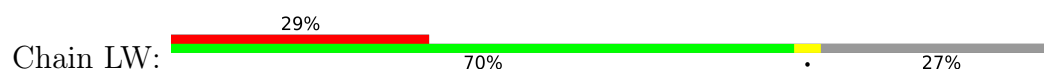
- Molecule 27: 60S ribosomal protein L22



- Molecule 28: 60S ribosomal protein L23



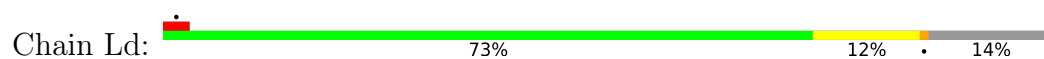
- Molecule 29: 60S ribosomal protein L24



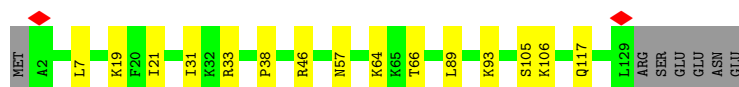
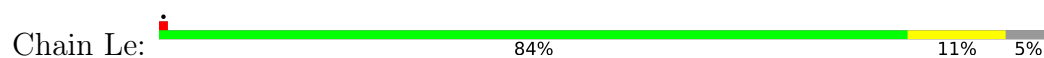




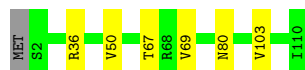
- Molecule 36: 60S ribosomal protein L31



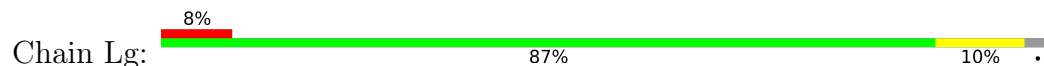
- Molecule 37: 60S ribosomal protein L32



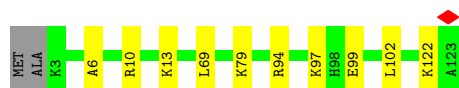
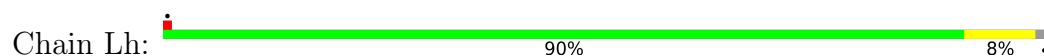
- Molecule 38: 60S ribosomal protein L35a



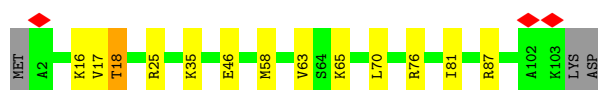
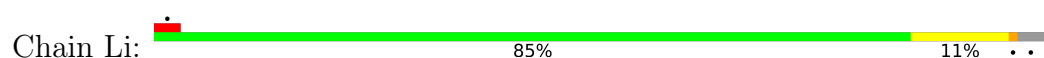
- Molecule 39: 60S ribosomal protein L34




- Molecule 40: 60S ribosomal protein L35



- Molecule 41: 60S ribosomal protein L36




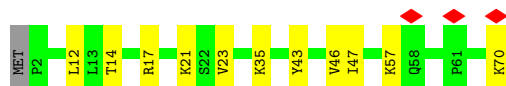
- Molecule 42: 60S ribosomal protein L37

Chain Lj:  79% 8% 11%



- Molecule 43: 60S ribosomal protein L38

Chain Lk:  83% 16%




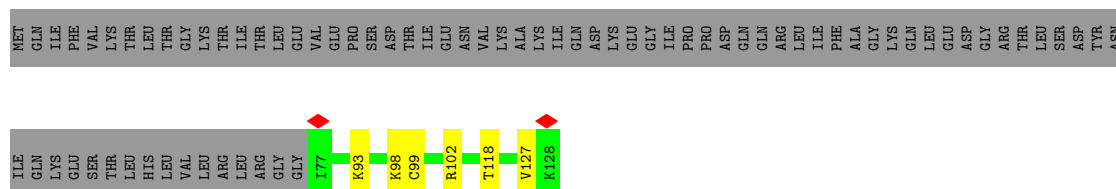
- Molecule 44: 60S ribosomal protein L39

Chain Ll:  90% 8%



- Molecule 45: Ubiquitin-60S ribosomal protein L40

Chain Lm:  36% 5% 59%



- Molecule 46: 60S ribosomal protein L41

Chain Ln:  92% 7% 1%



- Molecule 47: 60S ribosomal protein L36a

Chain Lo:  90% 9% 1%

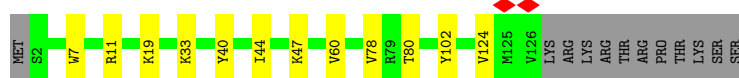
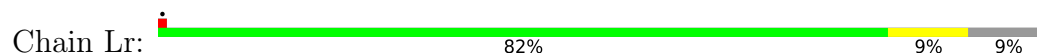


- Molecule 48: 60S ribosomal protein L37a

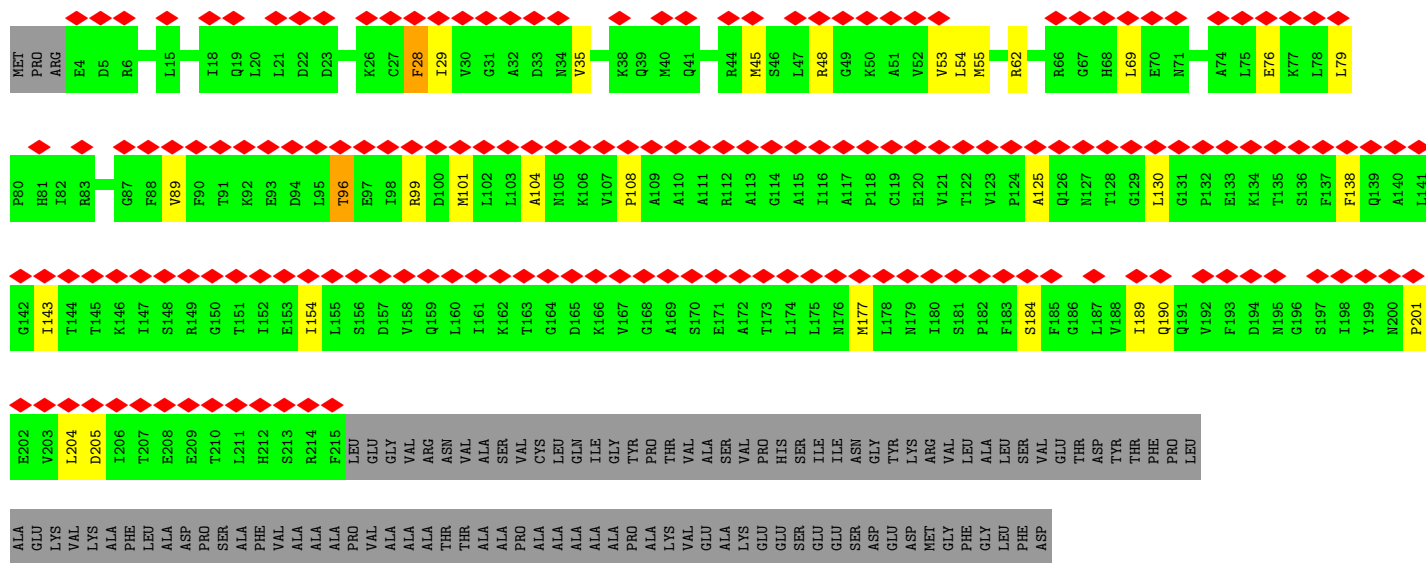
Chain Lp:  92% 7% 1%



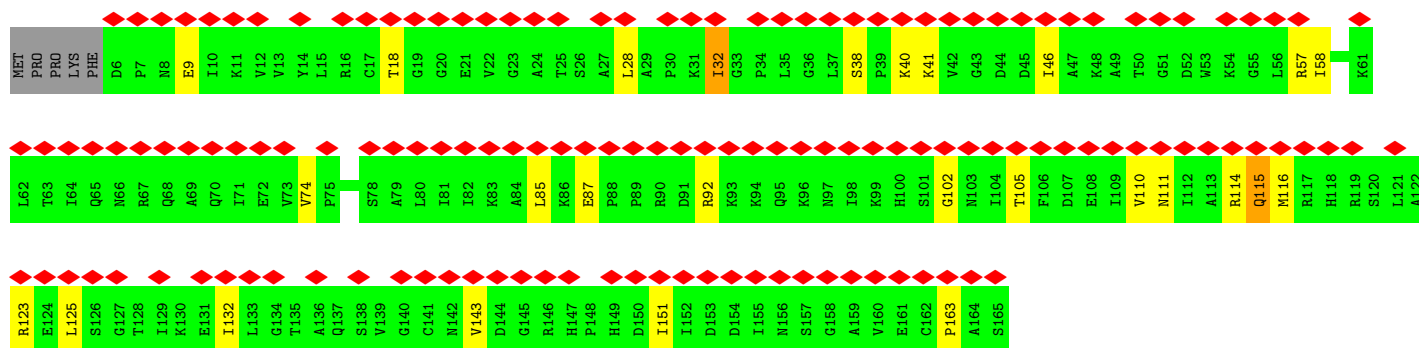
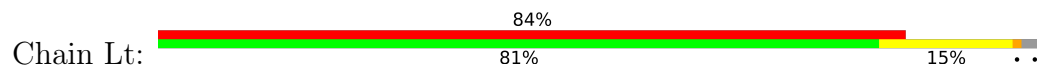
- Molecule 49: 60S ribosomal protein L28



- Molecule 50: 60S acidic ribosomal protein P0

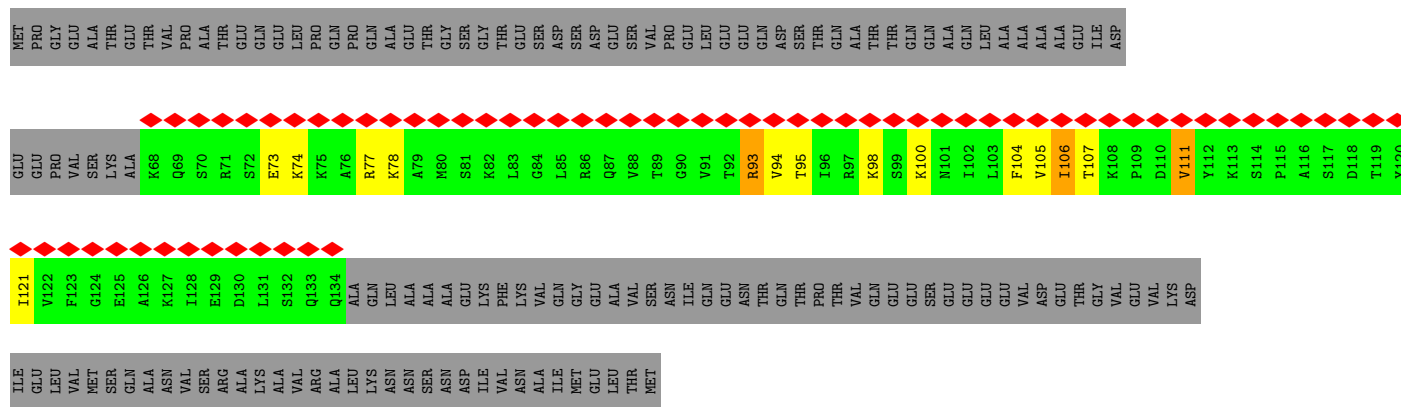


- Molecule 51: Large ribosomal subunit protein uL11

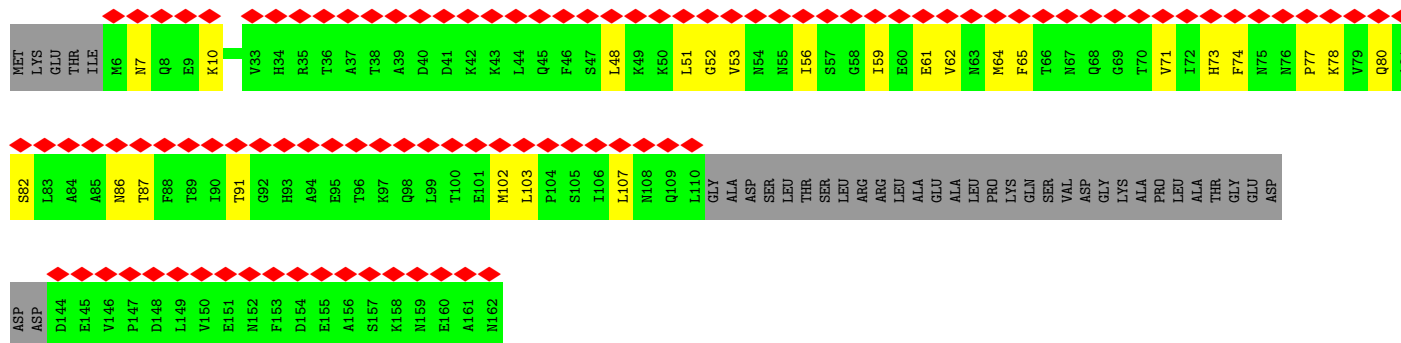


- Molecule 52: Nascent polypeptide-associated complex subunit alpha

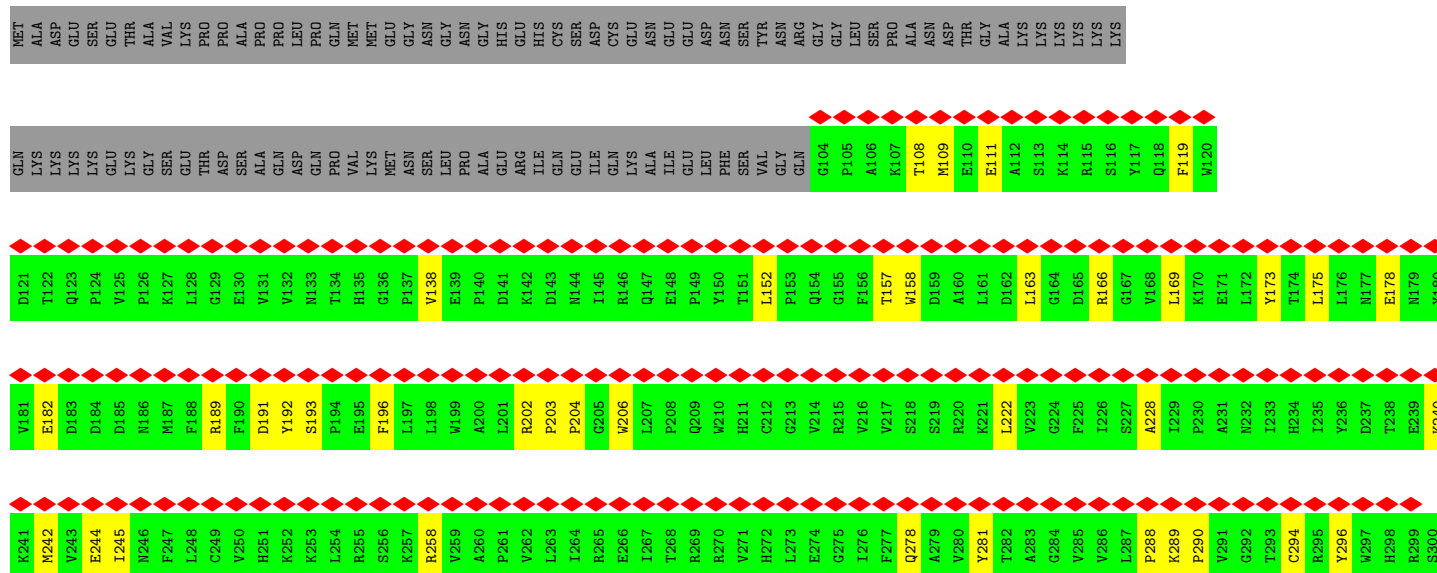
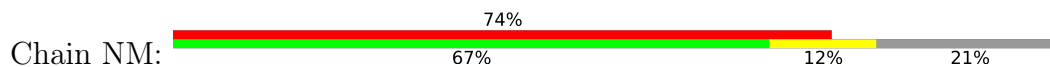


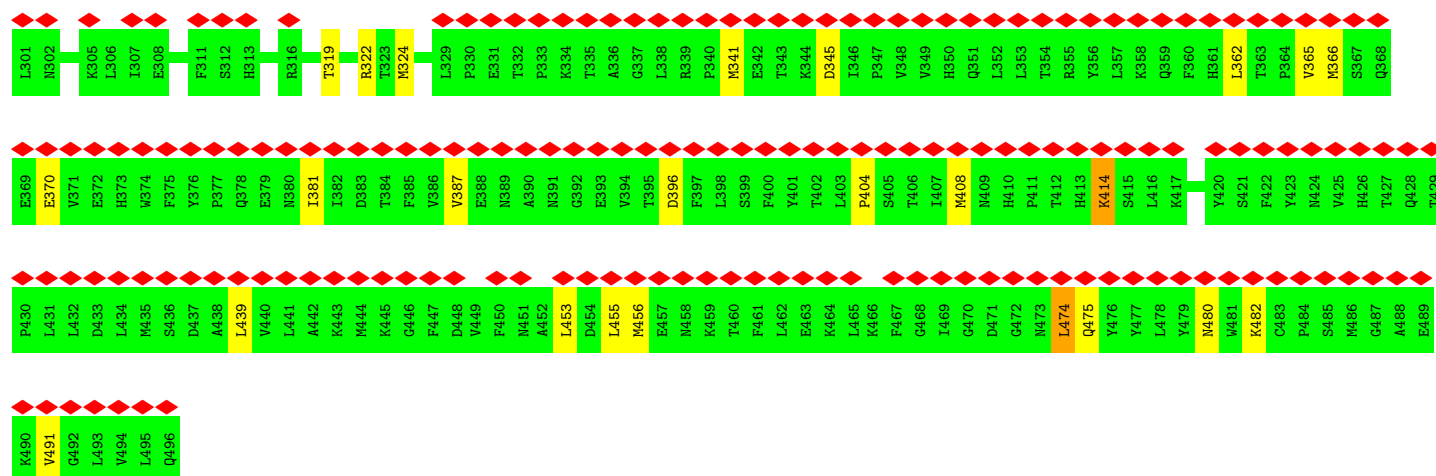


• Molecule 53: Isoform 2 of Transcription factor BTF3

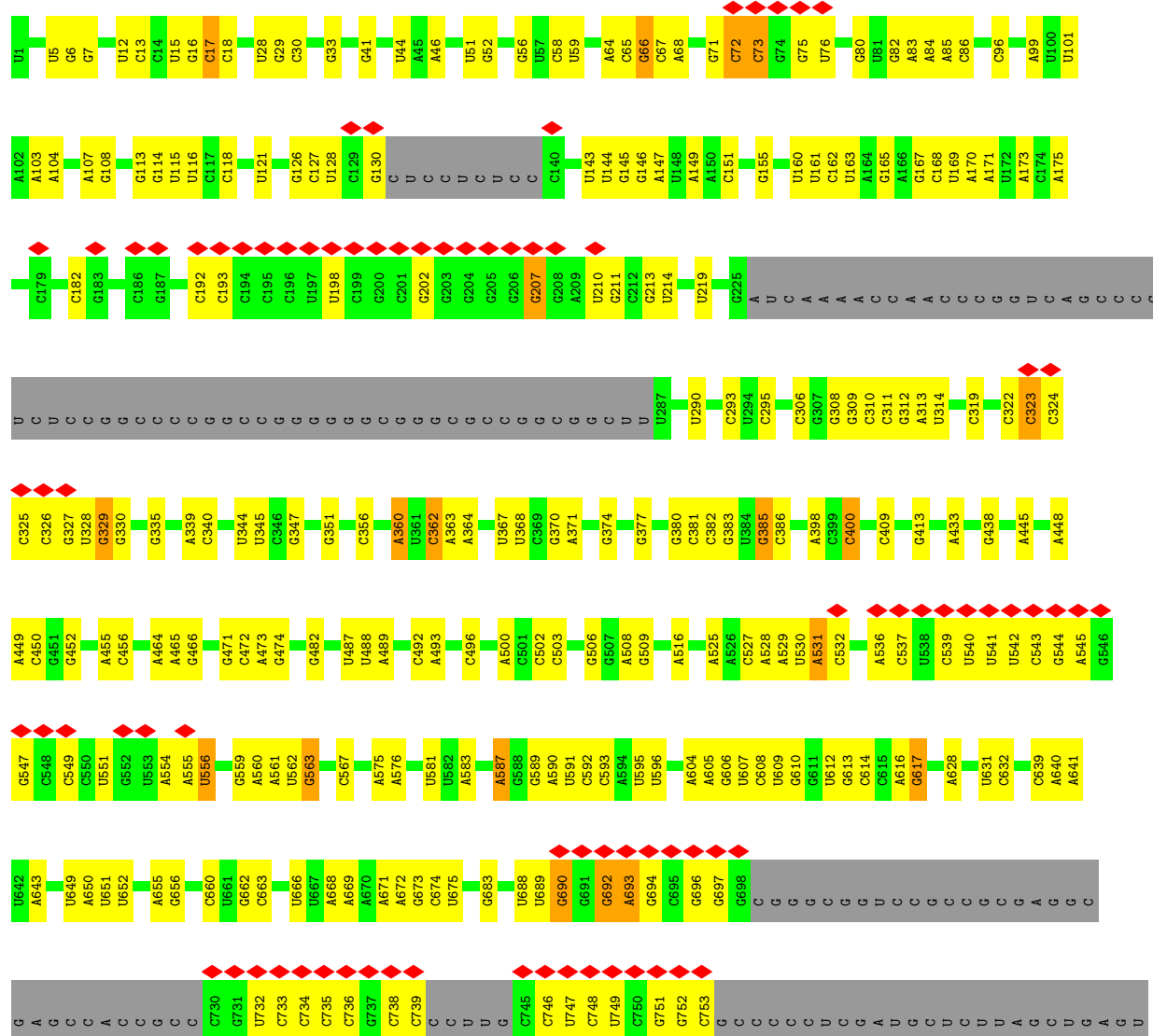


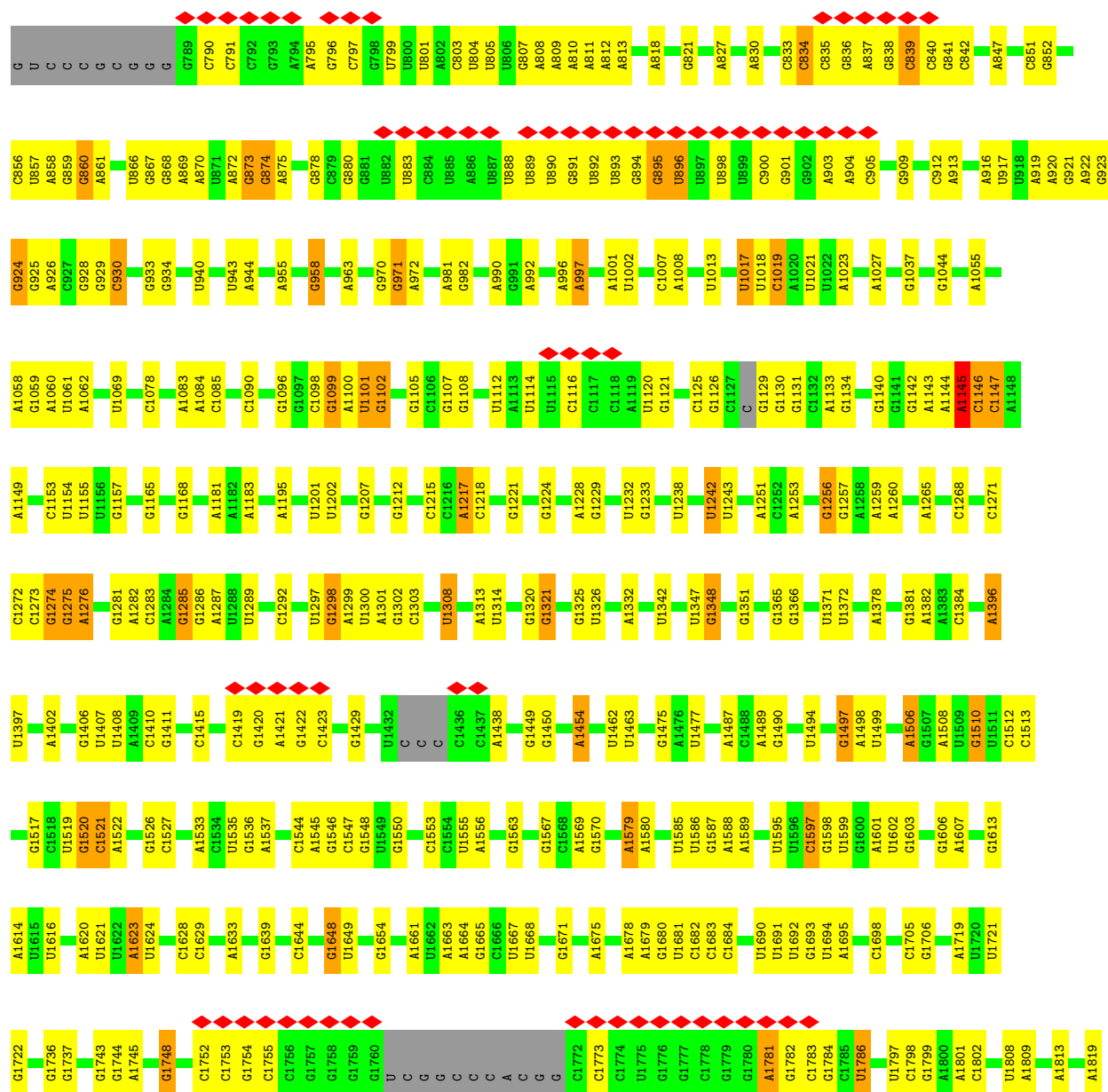
• Molecule 54: Glycylpeptide N-tetradecanoyltransferase 1



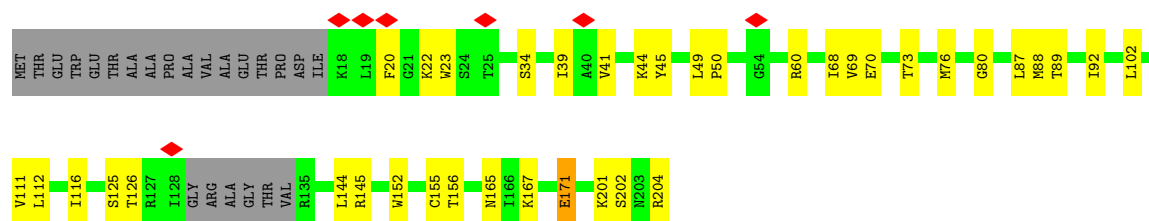


• Molecule 55: 18S rRNA

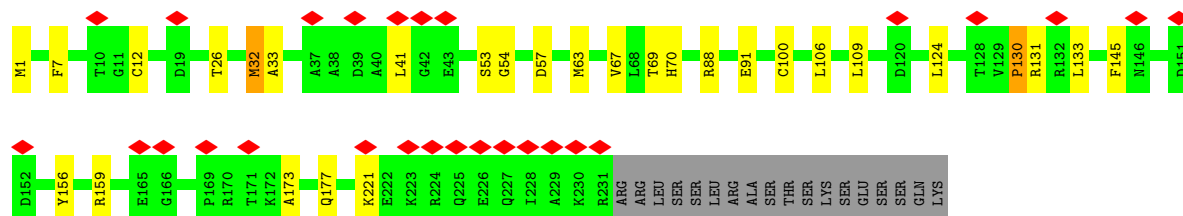
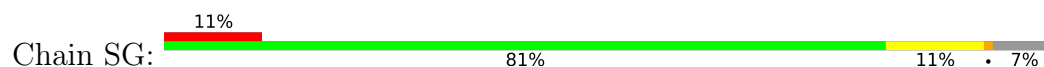




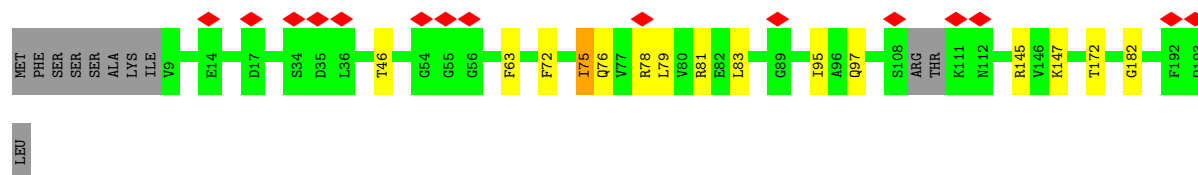
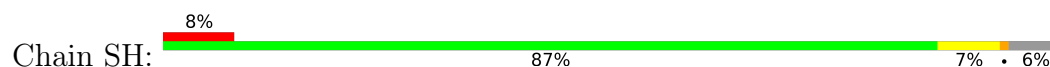
Chain SF: 



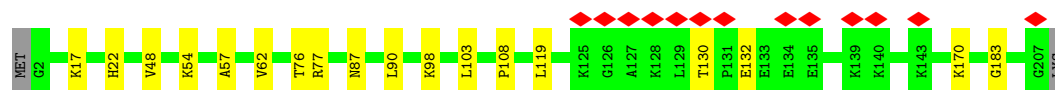
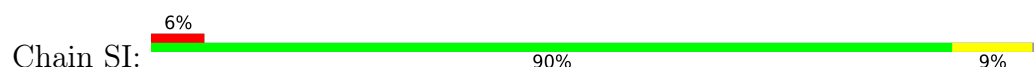
• Molecule 62: 40S ribosomal protein S6



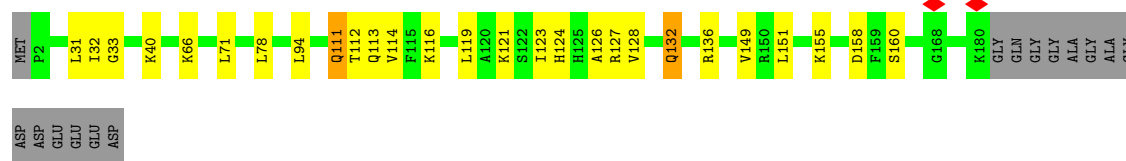
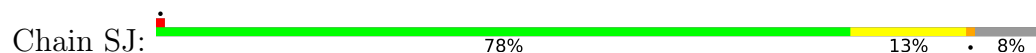
• Molecule 63: 40S ribosomal protein S7



• Molecule 64: 40S ribosomal protein S8

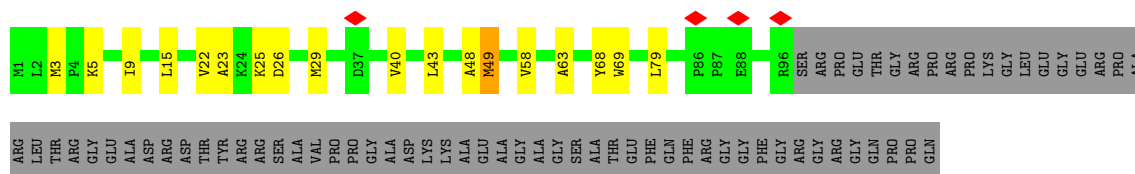


• Molecule 65: 40S ribosomal protein S9



• Molecule 66: 40S ribosomal protein S10





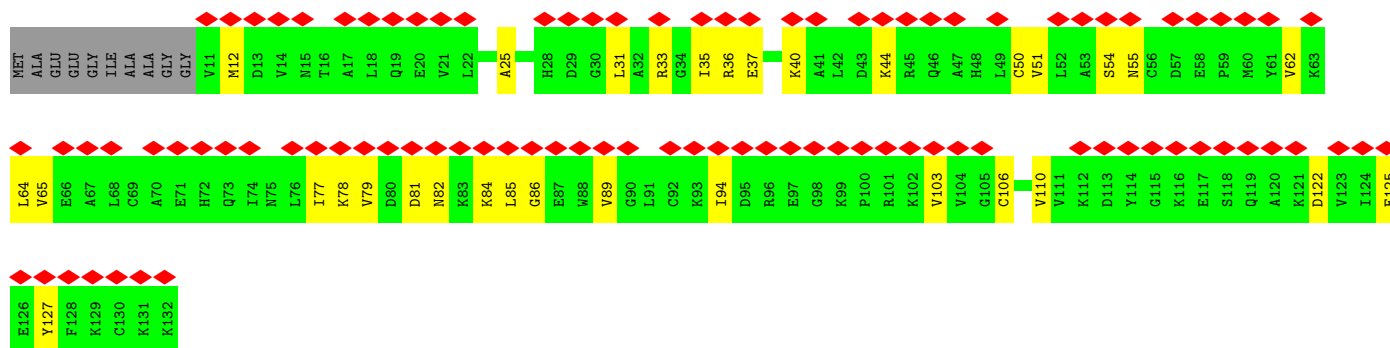
- Molecule 67: 40S ribosomal protein S11

Chain SL: 78% 13% 9%



- Molecule 68: 40S ribosomal protein S12

Chain SM: 72% 68% 24% 8%



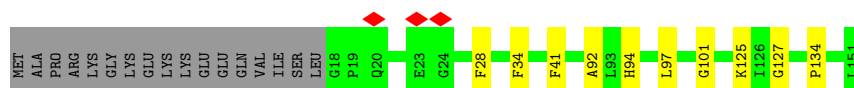
- Molecule 69: 40S ribosomal protein S13

Chain SN: 95%



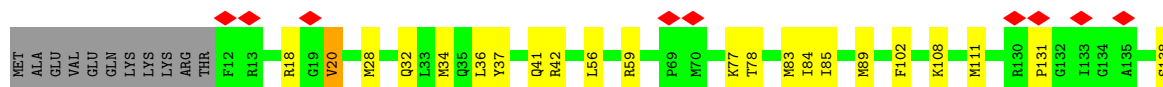
- Molecule 70: 40S ribosomal protein S14

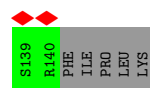
Chain SO: 82% 7% 11%



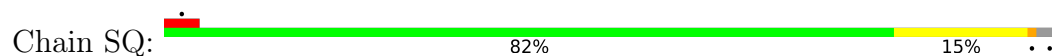
- Molecule 71: 40S ribosomal protein S15

Chain SP: 8% 74% 14% 11%

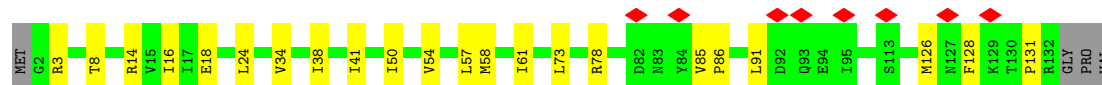
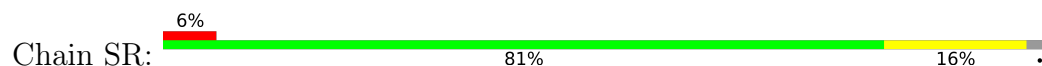




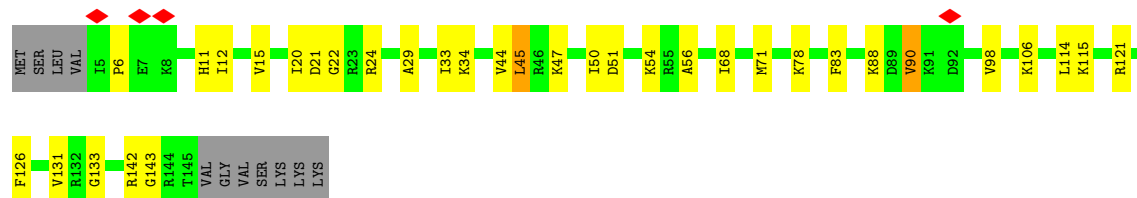
- Molecule 72: 40S ribosomal protein S16



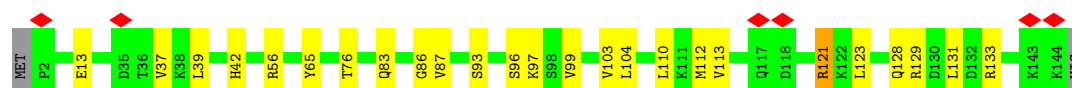
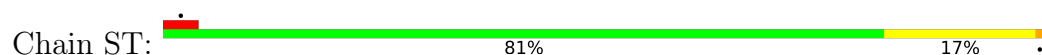
- Molecule 73: 40S ribosomal protein S17



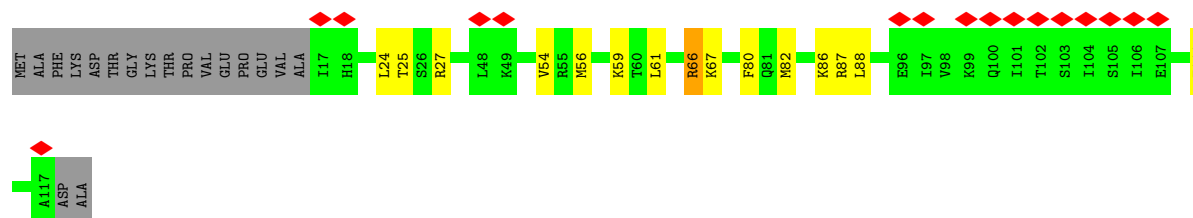
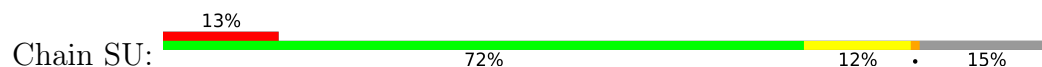
- Molecule 74: 40S ribosomal protein S18




- Molecule 75: 40S ribosomal protein S19



- Molecule 76: 40S ribosomal protein S20



- Molecule 77: 40S ribosomal protein S21

Chain SV:  90% 7%



- Molecule 78: 40S ribosomal protein S15a

Chain SW:  89% 10%




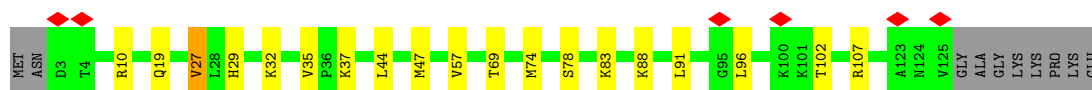
- Molecule 79: 40S ribosomal protein S23

Chain SX:  90% 8%



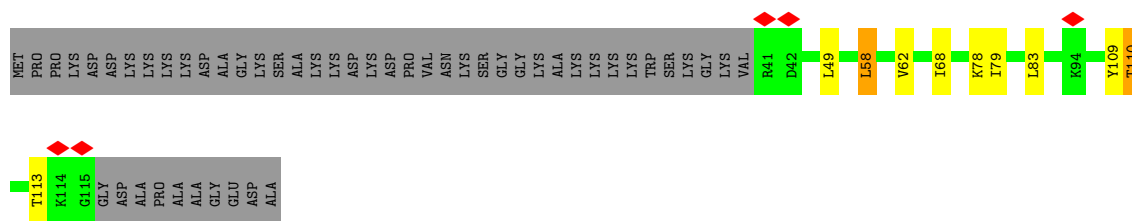
- Molecule 80: 40S ribosomal protein S24

Chain SY:  5% 78% 14% 8%



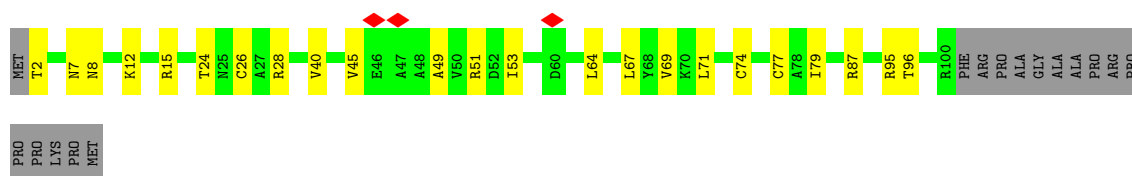
- Molecule 81: 40S ribosomal protein S25

Chain SZ:  52% 6% 40%

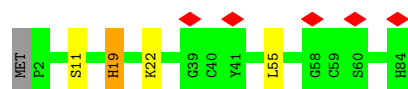


- Molecule 82: 40S ribosomal protein S26

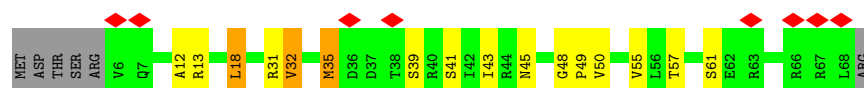
Chain Sa:  66% 20% 14%



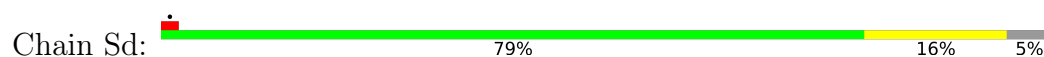
- Molecule 83: 40S ribosomal protein S27



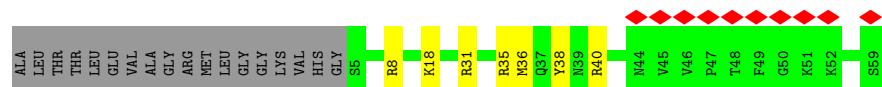
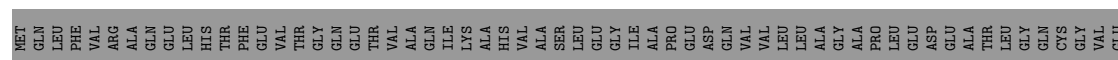
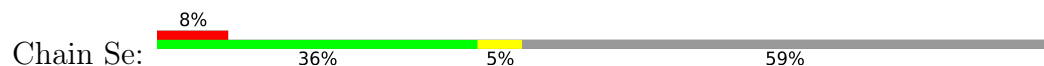
- Molecule 84: 40S ribosomal protein S28



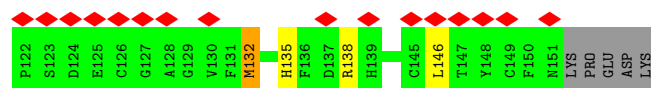
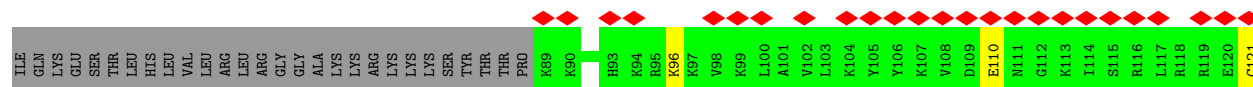
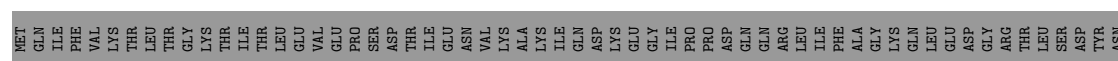
- Molecule 85: 40S ribosomal protein S29



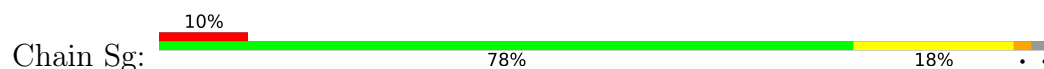
- Molecule 86: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

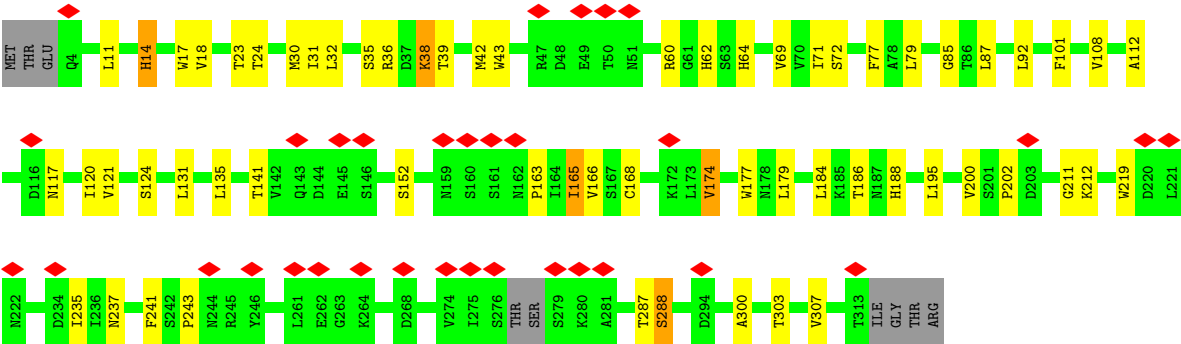


- Molecule 87: Ubiquitin



- Molecule 88: Receptor of activated protein C kinase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163265	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	6.307	Depositor
Minimum map value	-3.076	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.35	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: ZN, LYO, MG

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	CM	0.36	0/273	0.52	0/421
2	CP	0.27	0/1789	0.48	0/2788
3	CR	0.21	0/3311	0.47	1/4452 (0.0%)
4	CZ	0.25	0/338	0.54	0/463
5	L5	0.34	0/87471	0.44	4/136443 (0.0%)
6	L7	0.33	0/2858	0.39	0/4455
7	L8	0.33	0/3701	0.41	0/5766
8	LA	0.36	0/1936	0.70	4/2596 (0.2%)
9	LB	0.30	0/3251	0.54	0/4352
10	LC	0.31	0/2938	0.57	2/3947 (0.1%)
11	LD	0.29	0/2407	0.56	0/3227
12	LE	0.31	0/1788	0.62	4/2399 (0.2%)
13	LF	0.32	0/1905	0.56	0/2539
14	LG	0.29	0/1849	0.61	3/2496 (0.1%)
15	LH	0.29	0/1529	0.53	0/2058
16	LI	0.29	0/1705	0.57	1/2277 (0.0%)
17	LJ	0.27	0/1352	0.57	0/1813
18	LL	0.28	0/1661	0.54	0/2229
19	LM	0.27	0/1145	0.51	0/1536
20	LN	0.32	0/1746	0.53	0/2338
21	LO	0.31	0/1665	0.53	1/2229 (0.0%)
22	LP	0.32	0/1260	0.53	0/1692
23	LQ	0.30	0/1526	0.56	0/2038
24	LR	0.27	0/1468	0.50	0/1945
25	LS	0.30	0/1492	0.51	0/2003
26	LT	0.30	0/1310	0.60	0/1752
27	LU	0.22	0/820	0.53	1/1102 (0.1%)
28	LV	0.32	0/985	0.58	0/1323
29	LW	0.27	0/820	0.50	0/1104
30	LX	0.29	0/998	0.52	0/1341
31	LY	0.34	0/1128	0.57	0/1500
32	LZ	0.29	0/1130	0.51	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	La	0.32	0/1183	0.57	0/1582
34	Lb	0.31	0/600	0.60	0/796
35	Lc	0.29	0/752	0.50	0/1011
36	Ld	0.27	0/889	0.50	0/1198
37	Le	0.31	0/1067	0.59	0/1425
38	Lf	0.34	0/891	0.65	0/1194
39	Lg	0.29	0/899	0.54	0/1200
40	Lh	0.26	0/1014	0.47	0/1340
41	Li	0.23	0/824	0.45	0/1093
42	Lj	0.35	0/720	0.58	0/952
43	Lk	0.28	0/548	0.58	0/730
44	Ll	0.32	0/454	0.55	0/599
45	Lm	0.28	0/431	0.49	0/570
46	Ln	0.34	0/231	0.52	0/294
47	Lo	0.32	0/876	0.56	0/1156
48	Lp	0.31	0/706	0.56	0/939
49	Lr	0.34	0/1012	0.57	0/1358
50	Ls	0.19	0/1666	0.54	0/2250
51	Lt	0.28	0/1224	0.71	2/1651 (0.1%)
52	NA	0.31	0/536	0.72	1/715 (0.1%)
53	NB	0.30	0/972	0.76	0/1304
54	NM	0.21	0/3299	0.59	1/4483 (0.0%)
55	S2	0.33	0/40882	0.47	4/63715 (0.0%)
56	SA	0.31	0/1708	0.59	2/2324 (0.1%)
57	SB	0.26	0/1745	0.50	0/2337
58	SC	0.29	0/1697	0.53	0/2301
59	SD	0.23	0/1620	0.48	0/2198
60	SE	0.26	0/2014	0.52	0/2726
61	SF	0.30	0/1423	0.64	3/1913 (0.2%)
62	SG	0.21	0/1657	0.49	0/2247
63	SH	0.23	0/1295	0.52	1/1763 (0.1%)
64	SI	0.26	0/1603	0.47	0/2161
65	SJ	0.24	0/1456	0.47	0/1957
66	SK	0.25	0/750	0.54	0/1026
67	SL	0.29	0/1163	0.52	1/1562 (0.1%)
68	SM	0.26	0/960	0.70	1/1286 (0.1%)
69	SN	0.27	0/1206	0.47	0/1626
70	SO	0.31	0/982	0.66	0/1320
71	SP	0.22	0/1010	0.47	0/1362
72	SQ	0.27	0/1093	0.58	0/1470
73	SR	0.25	0/955	0.59	0/1294
74	SS	0.26	0/1148	0.63	0/1542
75	ST	0.24	0/1100	0.46	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SU	0.25	0/722	0.54	0/983
77	SV	0.24	0/625	0.45	0/837
78	SW	0.30	0/1043	0.55	0/1396
79	SX	0.30	0/1096	0.69	4/1467 (0.3%)
80	SY	0.28	0/944	0.53	0/1271
81	SZ	0.25	0/565	0.55	0/764
82	Sa	0.32	0/794	0.66	2/1065 (0.2%)
83	Sb	0.31	0/632	0.68	2/851 (0.2%)
84	Sc	0.27	0/474	0.64	0/638
85	Sd	0.30	0/443	0.54	0/589
86	Se	0.23	0/420	0.52	0/554
87	Sf	0.28	0/525	0.69	1/695 (0.1%)
88	Sg	0.22	0/2235	0.57	0/3068
All	All	0.31	0/238334	0.49	46/349758 (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
4	CZ	0	1
9	LB	0	1
12	LE	0	2
18	LL	0	1
38	Lf	0	1
39	Lg	0	1
54	NM	0	1
56	SA	0	1
62	SG	0	1
74	SS	0	2
All	All	0	12

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	S2	1145	A	O4'-C1'-N9	10.53	124.29	108.50
79	SX	11	ARG	N-CA-C	-7.66	104.54	114.04
61	SF	88	MET	CG-SD-CE	-7.35	84.74	100.90
83	Sb	19	HIS	CA-C-N	6.91	134.74	121.54
83	Sb	19	HIS	C-N-CA	6.91	134.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	SF	88	MET	CA-CB-CG	6.70	127.50	114.10
14	LG	164	ILE	CA-C-N	6.63	133.98	122.32
14	LG	164	ILE	C-N-CA	6.63	133.98	122.32
51	Lt	40	LYS	CA-CB-CG	6.30	126.71	114.10
79	SX	8	ARG	CA-CB-CG	6.06	126.21	114.10
16	LI	187	LYS	CA-CB-CG	6.03	126.15	114.10
12	LE	177	GLY	N-CA-C	-5.97	100.16	112.34
67	SL	4	ILE	N-CA-C	-5.92	107.15	112.12
21	LO	110	PRO	N-CA-C	5.79	117.76	110.70
61	SF	88	MET	N-CA-CB	-5.76	101.36	109.94
12	LE	128	HIS	CA-CB-CG	5.74	119.54	113.80
87	Sf	110	GLU	CA-CB-CG	5.66	125.42	114.10
8	LA	171	GLY	CA-C-N	5.59	131.14	120.07
8	LA	171	GLY	C-N-CA	5.59	131.14	120.07
52	NA	93	ARG	CA-CB-CG	5.55	125.21	114.10
63	SH	75	ILE	CB-CA-C	5.52	117.99	111.59
5	L5	406	C	C2'-C3'-O3'	5.47	121.91	113.70
56	SA	192	GLU	CA-C-N	-5.43	105.09	121.98
56	SA	192	GLU	C-N-CA	-5.43	105.09	121.98
10	LC	109	ARG	CA-C-N	5.40	131.85	121.54
10	LC	109	ARG	C-N-CA	5.40	131.85	121.54
12	LE	210	LYS	CA-CB-CG	5.38	124.85	114.10
54	NM	414	LYS	CA-CB-CG	5.37	124.85	114.10
5	L5	417	G	O4'-C1'-N9	5.36	116.24	108.20
82	Sa	7	ASN	CA-C-N	-5.36	115.18	123.17
82	Sa	7	ASN	C-N-CA	-5.36	115.18	123.17
55	S2	958	G	O4'-C1'-N9	5.35	116.53	108.50
8	LA	113	VAL	CA-C-N	-5.33	113.96	122.17
8	LA	113	VAL	C-N-CA	-5.33	113.96	122.17
14	LG	165	GLU	N-CA-C	-5.31	101.23	108.24
5	L5	2117	G	P-O3'-C3'	5.29	128.13	120.20
55	S2	1860	A	P-O3'-C3'	5.27	128.11	120.20
55	S2	1860	A	C2'-C3'-O3'	5.21	117.32	109.50
3	CR	329	MET	CA-CB-CG	5.20	124.51	114.10
68	SM	12	MET	CB-CG-SD	5.15	128.14	112.70
12	LE	127	SER	N-CA-C	5.11	119.23	113.15
51	Lt	9	GLU	CA-CB-CG	5.10	124.29	114.10
5	L5	1552	G	O4'-C1'-N9	5.09	115.83	108.20
79	SX	9	THR	CA-C-N	5.06	131.20	121.54
79	SX	9	THR	C-N-CA	5.06	131.20	121.54
27	LU	108	GLU	CA-CB-CG	5.05	124.20	114.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	CZ	9	ARG	Mainchain
9	LB	335	GLY	Peptide
12	LE	176	THR	Peptide
12	LE	278	THR	Peptide
18	LL	47	ALA	Peptide
38	Lf	103	VAL	Peptide
39	Lg	52	ARG	Peptide
54	NM	365	VAL	Peptide
56	SA	195	TRP	Peptide
62	SG	32	MET	Peptide
74	SS	11	HIS	Peptide
74	SS	88	LYS	Peptide

5.2 Too-close contacts [i](#)

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	CM	247	0	128	1	0
2	CP	1602	0	809	1	0
3	CR	3269	0	3312	25	0
4	CZ	333	0	280	3	0
5	L5	78199	0	39524	246	0
6	L7	2558	0	1296	6	0
7	L8	3314	0	1683	12	0
8	LA	1898	0	1993	20	0
9	LB	3183	0	3316	24	0
10	LC	2884	0	3050	13	0
11	LD	2361	0	2378	14	0
12	LE	1754	0	1899	14	0
13	LF	1870	0	1996	8	0
14	LG	1818	0	1911	11	0
15	LH	1510	0	1579	12	0
16	LI	1666	0	1711	12	0
17	LJ	1329	0	1348	7	0
18	LL	1630	0	1715	7	0
19	LM	1122	0	1174	5	0
20	LN	1701	0	1749	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	LO	1633	0	1771	13	0
22	LP	1234	0	1254	8	0
23	LQ	1502	0	1616	5	0
24	LR	1452	0	1580	9	0
25	LS	1452	0	1490	6	0
26	LT	1282	0	1336	9	0
27	LU	806	0	826	9	0
28	LV	971	0	1023	7	0
29	LW	808	0	726	3	0
30	LX	981	0	1055	5	0
31	LY	1111	0	1194	10	0
32	LZ	1107	0	1182	6	0
33	La	1154	0	1198	5	0
34	Lb	590	0	613	6	0
35	Lc	742	0	774	7	0
36	Ld	874	0	918	8	0
37	Le	1049	0	1136	7	0
38	Lf	872	0	901	2	0
39	Lg	889	0	968	6	0
40	Lh	1006	0	1132	7	0
41	Li	813	0	887	7	0
42	Lj	705	0	737	6	0
43	Lk	542	0	590	4	0
44	Ll	444	0	483	2	0
45	Lm	425	0	462	2	0
46	Ln	230	0	276	1	0
47	Lo	862	0	929	4	0
48	Lp	696	0	744	4	0
49	Lr	997	0	1054	4	0
50	Ls	1640	0	1687	15	0
51	Lt	1208	0	1257	13	0
52	NA	531	0	573	11	0
53	NB	963	0	982	13	0
54	NM	3209	0	3185	37	0
55	S2	36562	0	18473	173	0
56	SA	1671	0	1672	22	0
57	SB	1718	0	1786	18	0
58	SC	1661	0	1710	12	0
59	SD	1594	0	1568	17	0
60	SE	1972	0	2012	12	0
61	SF	1403	0	1421	23	0
62	SG	1634	0	1568	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	SH	1274	0	1196	10	0
64	SI	1574	0	1540	12	0
65	SJ	1431	0	1497	16	0
66	SK	726	0	674	10	0
67	SL	1143	0	1177	11	0
68	SM	950	0	987	16	0
69	SN	1182	0	1249	4	0
70	SO	969	0	982	5	0
71	SP	990	0	974	15	0
72	SQ	1075	0	1110	13	0
73	SR	942	0	913	13	0
74	SS	1130	0	1167	22	0
75	ST	1081	0	1093	12	0
76	SU	713	0	692	11	0
77	SV	618	0	617	6	0
78	SW	1026	0	1072	7	0
79	SX	1078	0	1130	7	0
80	SY	927	0	914	10	0
81	SZ	559	0	594	6	0
82	Sa	781	0	831	11	0
83	Sb	618	0	604	2	0
84	Sc	472	0	484	9	0
85	Sd	433	0	415	6	0
86	Se	416	0	439	6	0
87	Sf	515	0	521	5	0
88	Sg	2180	0	1968	29	0
89	CM	1	0	0	0	0
89	L5	127	0	0	0	0
89	L7	3	0	0	0	0
89	L8	3	0	0	0	0
89	LA	1	0	0	0	0
89	LC	1	0	0	0	0
89	LN	1	0	0	0	0
89	LP	1	0	0	0	0
89	LV	1	0	0	0	0
89	S2	52	0	0	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Sd	1	0	0	0	0
90	Sf	1	0	0	0	0
91	L5	3	0	0	0	0
91	L7	1	0	0	0	0
91	LI	1	0	0	0	0
91	LN	1	0	0	0	0
91	La	1	0	0	0	0
91	Li	1	0	0	0	0
91	S2	3	0	0	0	0
All	All	22256	0	164440	1133	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 (1133) 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)
55:S2:1748:G:H1	55:S2:1786:U:H3	1.09	0.98
3:CR:329:MET:O	3:CR:346:LEU:HB2	1.69	0.93
5:L5:3751:G:H21	5:L5:3775:A:H8	1.25	0.85
1:CM:322:U:H3	2:CP:33:A:H61	1.24	0.83
24:LR:141:HIS:HA	24:LR:144:LYS:HE2	1.60	0.81
7:L8:55:U:H3	7:L8:62:A:H2	1.29	0.80
8:LA:117:GLU:HB2	8:LA:162:ASN:HB2	1.63	0.80
55:S2:1348:G:H1	55:S2:1381:G:H22	1.24	0.79
5:L5:1443:A:N6	5:L5:2103:G:C6	2.51	0.78
6:L7:30:C:H5	6:L7:47:G:H1	1.32	0.77
52:NA:73:GLU:HB2	53:NB:86:ASN:HD21	1.48	0.77
55:S2:1107:G:H1	55:S2:1125:C:H5	1.33	0.76
55:S2:529:A:H61	55:S2:556:U:H3	1.31	0.76
55:S2:1098:C:H5	55:S2:1134:G:H1	1.29	0.76
5:L5:5027:C:H42	64:SI:170:LYS:HE2	1.51	0.76
55:S2:1649:U:H3	55:S2:1675:A:H2	1.31	0.76
5:L5:2611:A:H5'	5:L5:2688:G:H4'	1.69	0.75
55:S2:925:G:H1	55:S2:1017:U:H3	1.36	0.73
51:Lt:28:LEU:O	51:Lt:32:ILE:HB	1.88	0.73
34:Lb:53:GLY:O	34:Lb:57:MET:HB2	1.88	0.73
55:S2:928:G:H1	55:S2:1013:U:H3	1.35	0.72
5:L5:4626:A:H62	5:L5:4669:A:H2	1.37	0.72
5:L5:468:U:H3	5:L5:688:U:H3	1.36	0.72
36:Ld:29:ILE:HG13	36:Ld:84:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S2:563:G:H1	55:S2:592:C:H5	1.39	0.71
55:S2:923:G:H1	55:S2:1019:C:H5	1.39	0.71
5:L5:2469:C:H5	5:L5:2471:G:H1	1.38	0.70
55:S2:1265:A:H2	55:S2:1517:G:H22	1.40	0.70
68:SM:33:ARG:H	68:SM:37:GLU:HB2	1.56	0.70
55:S2:192:C:H41	55:S2:207:G:H21	1.41	0.69
88:Sg:87:LEU:HB2	88:Sg:101:PHE:HB2	1.75	0.69
5:L5:4302:U:H4'	26:LT:5:LYS:HG2	1.74	0.68
55:S2:1616:U:H3	55:S2:1620:A:H2	1.40	0.68
59:SD:8:LYS:HG2	76:SU:61:LEU:HD21	1.74	0.67
27:LU:65:ARG:HH21	27:LU:67:LYS:HA	1.59	0.67
82:Sa:51:ARG:HH12	84:Sc:39:SER:HB2	1.60	0.66
16:LI:48:LEU:O	16:LI:139:ARG:HA	1.96	0.66
55:S2:433:A:H5''	64:SI:22:HIS:HB3	1.77	0.66
63:SH:72:PHE:O	63:SH:75:ILE:O	2.14	0.66
57:SB:34:LYS:O	57:SB:98:THR:HB	1.95	0.66
65:SJ:111:GLN:HE21	65:SJ:123:ILE:HG13	1.62	0.65
55:S2:1308:U:H1'	87:Sf:135:HIS:HE1	1.60	0.65
52:NA:93:ARG:HH21	52:NA:107:THR:HG22	1.63	0.64
88:Sg:72:SER:HB2	88:Sg:117:ASN:HD21	1.62	0.64
54:NM:278:GLN:HG3	54:NM:480:ASN:HB3	1.80	0.64
9:LB:305:THR:HG23	9:LB:307:TYR:H	1.63	0.64
66:SK:3:MET:HE1	66:SK:48:ALA:HB2	1.78	0.64
55:S2:1276:A:H62	55:S2:1321:G:H8	1.46	0.63
55:S2:1347:U:H2'	55:S2:1348:G:C8	2.33	0.63
57:SB:152:LYS:HB2	73:SR:131:PRO:HB3	1.81	0.63
58:SC:78:LEU:HD12	58:SC:81:ILE:HD11	1.80	0.63
76:SU:25:THR:HG22	76:SU:86:LYS:HG3	1.80	0.63
55:S2:1679:A:H2'	61:SF:60:ARG:HD3	1.80	0.63
55:S2:617:G:H4'	79:SX:88:ASP:HB3	1.79	0.63
56:SA:89:LYS:HD2	56:SA:201:LEU:HG	1.80	0.63
26:LT:82:GLY:HA3	34:Lb:16:TRP:HB2	1.81	0.63
52:NA:93:ARG:HH11	52:NA:95:THR:HG22	1.64	0.63
5:L5:4128:A:H2	5:L5:4156:G:H21	1.44	0.63
81:SZ:68:ILE:HB	81:SZ:109:TYR:HB2	1.80	0.63
35:Lc:48:LEU:HD21	35:Lc:60:ILE:HG21	1.82	0.62
68:SM:55:ASN:HB2	68:SM:82:ASN:HB2	1.82	0.62
3:CR:318:GLU:HG3	3:CR:319:ILE:HG13	1.80	0.62
60:SE:185:GLY:H	60:SE:189:LEU:HG	1.65	0.62
28:LV:13:LYS:HD2	28:LV:128:LEU:HD11	1.82	0.61
5:L5:958:G:H21	12:LE:125:LEU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S2:1228:A:H2'	55:S2:1229:G:C8	2.35	0.61
56:SA:137:ALA:HB1	56:SA:142:LEU:HB3	1.82	0.61
5:L5:4745:G:H1	5:L5:4955:A:H61	1.49	0.61
52:NA:98:LYS:HD3	52:NA:104:PHE:HD2	1.65	0.61
51:Lt:18:THR:HA	51:Lt:57:ARG:HA	1.82	0.61
5:L5:1443:A:N6	5:L5:2103:G:N1	2.48	0.61
56:SA:81:ASN:HA	56:SA:84:GLN:HG3	1.83	0.61
88:Sg:11:LEU:HB2	88:Sg:307:VAL:HB	1.81	0.61
56:SA:198:MET:HG2	56:SA:200:ASP:H	1.66	0.60
56:SA:84:GLN:HB3	56:SA:100:ALA:HB1	1.82	0.60
55:S2:1454:A:H5''	73:SR:3:ARG:HD2	1.84	0.60
53:NB:78:LYS:HG3	53:NB:91:THR:HG22	1.84	0.59
74:SS:44:VAL:HG11	74:SS:71:MET:HG3	1.83	0.59
5:L5:3717:A:H2'	5:L5:3718:A:C8	2.38	0.59
63:SH:63:PHE:HA	63:SH:95:ILE:O	2.02	0.59
9:LB:107:ALA:HB2	9:LB:201:LEU:HG	1.84	0.59
54:NM:191:ASP:HB3	54:NM:404:PRO:HB2	1.85	0.59
55:S2:165:G:H4'	62:SG:53:SER:HB3	1.85	0.58
8:LA:181:LYS:HB2	8:LA:184:ARG:HG3	1.85	0.58
74:SS:12:ILE:HG22	74:SS:21:ASP:HA	1.84	0.58
5:L5:1940:G:H22	5:L5:4434:C:H5''	1.67	0.58
75:ST:96:SER:HB3	75:ST:99:VAL:HB	1.85	0.58
5:L5:496:G:H2'	5:L5:498:C:H5''	1.84	0.58
5:L5:4274:A:H2'	5:L5:4275:G:C8	2.39	0.58
55:S2:1550:G:H3'	55:S2:1579:A:H61	1.67	0.58
68:SM:54:SER:HB3	68:SM:78:LYS:HD2	1.86	0.58
5:L5:418:A:N6	7:L8:16:G:H1'	2.18	0.58
56:SA:184:ARG:HD3	56:SA:191:ARG:HD3	1.85	0.58
75:ST:110:LEU:HB3	75:ST:112:MET:HG3	1.86	0.58
5:L5:1574:G:HO2'	5:L5:1575:A:H8	1.51	0.58
57:SB:198:GLU:HG2	57:SB:210:VAL:HB	1.85	0.58
3:CR:145:LYS:HG2	3:CR:162:GLN:HG2	1.84	0.58
84:Sc:18:LEU:HD11	84:Sc:43:ILE:HD12	1.86	0.58
54:NM:203:PRO:HD2	54:NM:206:TRP:HB3	1.86	0.57
55:S2:587:A:H5'	55:S2:592:C:H42	1.69	0.57
54:NM:182:GLU:HG2	54:NM:189:ARG:HE	1.69	0.57
71:SP:18:ARG:HD3	74:SS:90:VAL:HA	1.85	0.57
5:L5:2607:C:H5'	24:LR:96:MET:HE1	1.86	0.57
28:LV:45:ILE:HG21	28:LV:53:PRO:HB3	1.85	0.57
11:LD:223:PHE:HB3	11:LD:226:TYR:HB2	1.86	0.57
20:LN:138:PHE:HA	20:LN:143:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:703:G:H2'	5:L5:704:C:H4'	1.87	0.57
53:NB:48:LEU:HA	53:NB:51:LEU:HB2	1.87	0.57
54:NM:119:PHE:HB2	54:NM:258:ARG:HH22	1.70	0.57
55:S2:1017:U:H5'	69:SN:55:ARG:HD3	1.86	0.57
62:SG:54:GLY:HA2	62:SG:63:MET:HE2	1.86	0.57
74:SS:115:LYS:HD2	74:SS:126:PHE:HB2	1.87	0.57
75:ST:123:LEU:HD21	75:ST:131:LEU:HD22	1.87	0.57
12:LE:190:HIS:HB3	12:LE:193:PHE:HD2	1.70	0.57
5:L5:1503:A:H4'	5:L5:1504:G:H5'	1.87	0.56
55:S2:1860:A:H3'	82:Sa:8:ASN:HB3	1.86	0.56
55:S2:895:G:H8	55:S2:896:U:H4'	1.70	0.56
3:CR:317:VAL:HA	3:CR:413:LEU:HA	1.86	0.56
5:L5:2838:G:H5'	9:LB:247:GLY:HA2	1.87	0.56
13:LF:182:TYR:HB3	13:LF:200:ARG:HG3	1.87	0.56
54:NM:453:LEU:HD12	54:NM:455:LEU:HD22	1.86	0.56
55:S2:1536:G:H2'	55:S2:1537:A:C8	2.39	0.56
70:SO:34:PHE:HB3	70:SO:41:PHE:HB2	1.86	0.56
5:L5:4537:C:H2'	5:L5:4538:G:C8	2.40	0.56
55:S2:666:U:H3	55:S2:1145:A:H61	1.53	0.56
31:LY:38:LEU:HA	31:LY:41:LYS:HB3	1.88	0.56
72:SQ:58:LEU:HB3	72:SQ:62:ARG:HD2	1.87	0.56
5:L5:137:G:H2'	5:L5:138:G:H8	1.69	0.56
5:L5:1828:C:H1'	34:Lb:57:MET:HE2	1.88	0.56
21:LO:61:ARG:HA	21:LO:70:PRO:HD2	1.88	0.56
54:NM:163:LEU:HD11	54:NM:202:ARG:HG3	1.87	0.56
5:L5:518:G:H1	5:L5:643:C:H2'	1.71	0.56
88:Sg:195:LEU:HA	88:Sg:211:GLY:HA3	1.87	0.56
24:LR:105:LEU:HD22	24:LR:135:LYS:HG2	1.87	0.55
88:Sg:163:PRO:HB2	88:Sg:179:LEU:HD12	1.87	0.55
5:L5:2337:C:H4'	49:Lr:19:LYS:HB2	1.89	0.55
5:L5:4130:C:H5	5:L5:4154:G:H22	1.54	0.55
43:Lk:14:THR:HA	43:Lk:17:ARG:HD3	1.88	0.55
3:CR:84:LEU:HD13	71:SP:131:PRO:HA	1.88	0.55
74:SS:45:LEU:HG	74:SS:50:ILE:HD11	1.87	0.55
76:SU:27:ARG:HD2	76:SU:82:MET:HE2	1.88	0.55
80:SY:102:THR:HG23	80:SY:107:ARG:HH11	1.70	0.55
5:L5:1553:A:N6	5:L5:1574:G:H1'	2.21	0.55
45:Lm:98:LYS:HG3	45:Lm:118:THR:HG21	1.87	0.55
55:S2:66:G:H21	55:S2:82:G:H21	1.55	0.55
55:S2:690:G:H8	63:SH:182:GLY:HA3	1.71	0.55
55:S2:1748:G:O6	55:S2:1786:U:O4	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:NM:175:LEU:HD22	54:NM:222:LEU:HG	1.87	0.55
74:SS:51:ASP:HB3	74:SS:54:LYS:HG3	1.89	0.55
80:SY:91:LEU:HB3	80:SY:96:LEU:HD22	1.88	0.55
65:SJ:127:ARG:HD2	86:SE:31:ARG:HD3	1.89	0.55
64:SI:76:THR:HG22	64:SI:108:PRO:HG2	1.89	0.55
70:SO:92:ALA:HB2	70:SO:125:LYS:HB2	1.88	0.55
5:L5:5011:A:H62	5:L5:5037:U:H3	1.55	0.55
9:LB:244:THR:HB	9:LB:248:LEU:HD12	1.89	0.55
13:LF:222:LYS:HB3	13:LF:231:GLY:HA2	1.89	0.55
55:S2:996:A:H2'	55:S2:997:A:C8	2.41	0.55
68:SM:86:GLY:HA2	68:SM:106:CYS:HB3	1.89	0.55
5:L5:1332:C:H2'	5:L5:1333:A:H8	1.70	0.54
55:S2:1752:C:H42	55:S2:1781:A:H2	1.55	0.54
5:L5:4128:A:H8	14:LG:35:ARG:H	1.55	0.54
5:L5:4740:G:O6	5:L5:4959:U:O2	2.25	0.54
57:SB:183:GLU:HA	57:SB:186:ASN:HB2	1.89	0.54
5:L5:4618:G:H5''	28:LV:15:ARG:HB2	1.88	0.54
16:LI:189:CYS:HA	16:LI:200:VAL:HG22	1.88	0.54
36:Ld:22:THR:HG22	36:Ld:122:VAL:HB	1.90	0.54
36:Ld:64:ILE:HG23	36:Ld:68:LEU:HD23	1.90	0.54
55:S2:528:A:H2'	55:S2:529:A:C8	2.41	0.54
57:SB:144:LYS:HG3	57:SB:208:HIS:HB3	1.89	0.54
72:SQ:89:SER:HB3	72:SQ:112:LEU:HD13	1.90	0.54
9:LB:56:ILE:O	9:LB:73:VAL:HA	2.08	0.54
60:SE:180:LEU:HA	60:SE:194:VAL:HA	1.89	0.54
5:L5:4457:U:H1'	9:LB:252:ALA:HB3	1.88	0.54
11:LD:62:CYS:HB3	11:LD:105:LEU:HD22	1.90	0.54
55:S2:374:G:H1'	67:SL:83:GLN:HE21	1.71	0.54
78:SW:14:ILE:HG13	78:SW:27:ILE:HD11	1.90	0.54
60:SE:105:THR:HG23	60:SE:245:ARG:HA	1.88	0.54
63:SH:145:ARG:HG3	63:SH:147:LYS:HG2	1.90	0.54
73:SR:57:LEU:O	73:SR:61:ILE:HG13	2.08	0.54
5:L5:4992:G:H2'	5:L5:4993:G:C8	2.43	0.53
74:SS:98:VAL:HG11	74:SS:106:LYS:HG3	1.90	0.53
5:L5:1308:C:H2'	5:L5:1309:C:C6	2.44	0.53
20:LN:178:HIS:HA	20:LN:181:HIS:CE1	2.43	0.53
5:L5:1175:A:H2	5:L5:1185:G:H22	1.57	0.53
16:LI:36:LEU:HD11	16:LI:69:ARG:HD2	1.90	0.53
56:SA:77:ILE:HG12	56:SA:99:ILE:HB	1.91	0.53
61:SF:102:LEU:HD22	81:SZ:110:THR:HG21	1.90	0.53
62:SG:32:MET:HB2	62:SG:100:CYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LU:63:ILE:HG12	27:LU:72:VAL:HG22	1.90	0.53
75:ST:76:THR:HG21	75:ST:97:LYS:HG3	1.90	0.53
5:L5:4940:C:H3'	12:LE:219:LYS:HZ3	1.73	0.53
32:LZ:50:PRO:HD3	32:LZ:68:ILE:HG12	1.90	0.53
54:NM:228:ALA:HA	54:NM:244:GLU:O	2.07	0.53
50:Ls:138:PHE:HB2	50:Ls:143:ILE:HB	1.90	0.53
55:S2:981:A:H2'	55:S2:982:G:C8	2.44	0.53
51:Lt:111:ASN:HA	51:Lt:114:ARG:HD2	1.90	0.53
52:NA:94:VAL:HB	52:NA:106:ILE:HG23	1.90	0.53
66:SK:63:ALA:HB2	66:SK:68:TYR:HE1	1.72	0.53
74:SS:15:VAL:HB	74:SS:68:ILE:HD11	1.91	0.53
5:L5:512:U:H2'	5:L5:513:U:H4'	1.91	0.53
10:LC:158:VAL:HG12	10:LC:217:ILE:HD12	1.91	0.53
54:NM:192:TYR:HD1	54:NM:196:PHE:HE2	1.56	0.53
58:SC:69:LEU:HD11	58:SC:273:LEU:HD11	1.91	0.53
59:SD:210:ILE:HG12	73:SR:16:ILE:HG22	1.91	0.53
81:SZ:58:LEU:HD12	81:SZ:62:VAL:HG21	1.91	0.53
88:Sg:38:LYS:HE3	88:Sg:64:HIS:H	1.74	0.53
12:LE:149:ILE:HD12	12:LE:271:LEU:HD21	1.91	0.53
17:LJ:15:LEU:HD13	17:LJ:134:LEU:HD13	1.90	0.53
64:SI:87:ASN:HB3	64:SI:90:LEU:HG	1.91	0.53
5:L5:1755:C:H1'	11:LD:2:GLY:HA3	1.91	0.52
54:NM:294:CYS:HB3	54:NM:453:LEU:HD21	1.90	0.52
55:S2:640:A:H2'	55:S2:641:A:C8	2.45	0.52
61:SF:87:LEU:HD11	72:SQ:47:LEU:HD11	1.90	0.52
9:LB:254:ILE:HG23	9:LB:266:VAL:HG11	1.91	0.52
52:NA:93:ARG:HG3	53:NB:65:PHE:HE1	1.74	0.52
8:LA:137:ILE:HD11	8:LA:149:LYS:HB2	1.91	0.52
10:LC:110:ARG:HA	20:LN:204:ARG:HH21	1.74	0.52
72:SQ:24:HIS:CE1	72:SQ:69:ARG:HB2	2.44	0.52
55:S2:1839:U:H2'	55:S2:1840:U:C6	2.45	0.52
71:SP:85:ILE:HA	71:SP:89:MET:HE2	1.91	0.52
3:CR:362:THR:HG23	3:CR:364:GLN:H	1.74	0.52
5:L5:1942:A:H2'	5:L5:1943:A:C8	2.44	0.52
65:SJ:78:LEU:HD11	65:SJ:94:LEU:HB3	1.92	0.52
8:LA:108:PRO:HG3	48:Lp:90:LYS:HG3	1.91	0.52
13:LF:91:PHE:HB2	13:LF:145:PRO:HG3	1.91	0.52
63:SH:79:LEU:O	63:SH:83:LEU:HB2	2.10	0.52
72:SQ:10:VAL:O	72:SQ:24:HIS:HA	2.09	0.52
17:LJ:125:ILE:HD11	74:SS:12:ILE:HD11	1.92	0.52
54:NM:152:LEU:HD13	54:NM:157:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S2:146:G:H22	55:S2:175:A:H1'	1.75	0.52
55:S2:562:U:H2'	55:S2:563:G:C8	2.45	0.52
55:S2:1606:G:H1'	55:S2:1633:A:N6	2.25	0.52
55:S2:1683:C:H2'	55:S2:1684:C:H6	1.75	0.52
63:SH:72:PHE:O	63:SH:75:ILE:C	2.53	0.52
5:L5:1097:C:H2'	5:L5:1098:G:H8	1.75	0.52
51:Lt:110:VAL:HG11	51:Lt:163:PRO:HG2	1.91	0.52
55:S2:1407:U:H2'	55:S2:1408:U:C6	2.44	0.52
57:SB:52:THR:HG23	57:SB:57:ILE:HA	1.91	0.52
5:L5:3946:G:H21	5:L5:3947:A:H62	1.57	0.52
55:S2:1597:C:H4'	55:S2:1603:G:C6	2.45	0.52
78:SW:86:LEU:HD21	78:SW:113:HIS:HB2	1.92	0.52
87:Sf:96:LYS:H	87:Sf:96:LYS:HD2	1.74	0.52
5:L5:3946:G:H22	5:L5:4067:U:H3	1.58	0.51
55:S2:323:C:H2'	55:S2:327:G:H22	1.75	0.51
72:SQ:16:LYS:H	72:SQ:19:ALA:HB3	1.75	0.51
5:L5:3641:U:H5	5:L5:3646:A:N7	2.08	0.51
55:S2:455:A:H2'	55:S2:456:C:C6	2.45	0.51
55:S2:616:A:H5'	86:Se:8:ARG:HG3	1.93	0.51
59:SD:178:ARG:HH22	59:SD:179:GLN:HE21	1.58	0.51
5:L5:1332:C:H2'	5:L5:1333:A:C8	2.45	0.51
5:L5:2520:C:H2'	5:L5:2521:G:C8	2.45	0.51
35:Lc:21:VAL:HG11	35:Lc:96:ILE:HD12	1.93	0.51
5:L5:3923:A:H2'	5:L5:3924:C:C6	2.46	0.51
12:LE:165:LEU:HD12	12:LE:174:LEU:HD13	1.91	0.51
53:NB:62:VAL:HG22	53:NB:74:PHE:HB2	1.93	0.51
55:S2:1101:U:H2'	55:S2:1102:G:C8	2.46	0.51
55:S2:1536:G:H2'	55:S2:1537:A:H8	1.73	0.51
68:SM:81:ASP:HB3	68:SM:84:LYS:HB2	1.92	0.51
5:L5:3937:C:H1'	20:LN:125:SER:HB3	1.92	0.51
16:LI:61:SER:HA	16:LI:126:VAL:HG12	1.92	0.51
51:Lt:143:VAL:HG13	51:Lt:151:ILE:HD12	1.91	0.51
55:S2:377:G:H5'	64:SI:98:LYS:HB3	1.93	0.51
56:SA:183:LEU:HB3	56:SA:189:ILE:HG12	1.91	0.51
58:SC:183:LYS:HA	58:SC:195:LEU:O	2.10	0.51
12:LE:153:LEU:HD11	12:LE:195:ILE:HG13	1.93	0.51
15:LH:2:LYS:HE3	15:LH:63:ASN:HB3	1.92	0.51
55:S2:1866:A:H4'	82:Sa:95:ARG:HD3	1.93	0.51
73:SR:41:ILE:HD13	73:SR:50:ILE:HD12	1.92	0.51
5:L5:2373:C:H5'	36:Ld:46:LEU:HD22	1.93	0.51
78:SW:32:LYS:O	78:SW:36:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SH:46:THR:HG21	63:SH:97:GLN:HG3	1.93	0.51
5:L5:1645:C:H2'	5:L5:1646:A:C8	2.45	0.51
5:L5:4699:U:H1'	5:L5:4700:A:H5''	1.92	0.51
25:LS:80:ILE:HG12	25:LS:129:VAL:HG13	1.92	0.51
50:Ls:48:ARG:HH12	51:Lt:123:ARG:HA	1.74	0.51
82:Sa:12:LYS:HG3	82:Sa:15:ARG:HB2	1.93	0.51
19:LM:36:ALA:HB3	19:LM:55:MET:HE1	1.93	0.51
61:SF:50:PRO:HB3	61:SF:69:VAL:HG13	1.93	0.51
68:SM:79:VAL:HG11	68:SM:85:LEU:HB2	1.93	0.51
76:SU:80:PHE:HB3	85:Sd:52:PHE:HB3	1.92	0.51
54:NM:455:LEU:HG	54:NM:456:MET:SD	2.51	0.50
55:S2:1512:C:H5''	85:Sd:8:TRP:HZ3	1.75	0.50
55:S2:385:G:H3'	67:SL:136:LYS:HB2	1.93	0.50
55:S2:649:U:H5''	79:SX:108:LYS:HD2	1.93	0.50
56:SA:134:LEU:HD11	56:SA:144:THR:HG21	1.93	0.50
5:L5:1994:C:H2'	5:L5:1995:G:H8	1.74	0.50
22:LP:54:GLN:HA	22:LP:83:TRP:CD1	2.47	0.50
55:S2:663:C:H4'	58:SC:227:ARG:HH22	1.76	0.50
59:SD:7:LYS:HD2	76:SU:25:THR:HG21	1.92	0.50
88:Sg:17:TRP:HB2	88:Sg:36:ARG:HD2	1.93	0.50
5:L5:1174:G:H1	5:L5:1186:U:H3	1.58	0.50
21:LO:36:VAL:HG21	21:LO:108:ILE:HG23	1.94	0.50
27:LU:23:LEU:HD23	27:LU:110:TYR:HB2	1.93	0.50
46:Ln:1:MET:HE3	55:S2:1851:A:H5'	1.94	0.50
50:Ls:101:MET:HA	50:Ls:104:ALA:HB3	1.93	0.50
27:LU:80:LYS:HZ1	27:LU:109:SER:H	1.59	0.50
39:Lg:42:PRO:HB2	39:Lg:53:LEU:HD12	1.92	0.50
66:SK:26:ASP:HB3	66:SK:29:MET:HG2	1.94	0.50
5:L5:1339:U:H2'	5:L5:1340:C:C6	2.46	0.50
55:S2:1679:A:C8	61:SF:60:ARG:HB2	2.46	0.50
5:L5:4611:A:H2	15:LH:120:GLU:HG2	1.77	0.50
5:L5:4627:U:H4'	9:LB:373:LYS:HE2	1.94	0.50
18:LL:46:ILE:HD11	18:LL:51:ALA:HA	1.93	0.50
28:LV:43:LYS:HG3	28:LV:60:MET:HG2	1.93	0.50
50:Ls:29:ILE:HG22	50:Ls:190:GLN:HB2	1.93	0.50
54:NM:178:GLU:HA	54:NM:189:ARG:HH12	1.77	0.50
57:SB:150:ILE:HG21	73:SR:128:PHE:HD2	1.77	0.50
60:SE:229:GLY:HA2	60:SE:235:TRP:CD1	2.46	0.50
5:L5:4239:A:H2'	5:L5:4240:G:C8	2.47	0.50
55:S2:943:U:H2'	55:S2:944:A:H8	1.76	0.50
62:SG:12:CYS:HB3	62:SG:124:LEU:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Sg:23:THR:HG23	88:Sg:31:ILE:HG22	1.92	0.50
55:S2:955:A:N6	55:S2:971:G:H1'	2.26	0.50
5:L5:2640:G:H2'	5:L5:2641:A:C8	2.47	0.49
59:SD:163:PRO:O	59:SD:167:TYR:HB2	2.11	0.49
76:SU:56:MET:HB2	76:SU:86:LYS:HB3	1.94	0.49
88:Sg:39:THR:HG22	88:Sg:60:ARG:HG3	1.94	0.49
5:L5:325:U:H2'	5:L5:326:C:C6	2.47	0.49
30:LX:73:HIS:ND1	30:LX:115:LYS:HD3	2.26	0.49
41:Li:63:VAL:HG23	41:Li:65:LYS:HG3	1.94	0.49
52:NA:93:ARG:HH22	52:NA:105:VAL:HB	1.77	0.49
55:S2:1396:A:H4'	55:S2:1396:A:OP1	2.11	0.49
58:SC:125:LYS:HD3	58:SC:127:PHE:CZ	2.47	0.49
50:Ls:101:MET:HE3	50:Ls:101:MET:H	1.77	0.49
55:S2:1217:A:H2'	55:S2:1218:C:C6	2.46	0.49
15:LH:59:LYS:HE3	15:LH:66:GLU:HB3	1.95	0.49
68:SM:36:ARG:HH22	68:SM:40:LYS:HZ1	1.60	0.49
70:SO:28:PHE:HA	70:SO:92:ALA:O	2.12	0.49
5:L5:2765:A:H2'	5:L5:2766:A:C8	2.48	0.49
5:L5:3748:A:H5''	8:LA:243:THR:HB	1.95	0.49
56:SA:24:HIS:HB3	56:SA:51:LEU:HD21	1.95	0.49
70:SO:101:GLY:HA3	70:SO:134:PRO:HG2	1.94	0.49
5:L5:257:C:H2'	5:L5:258:G:C8	2.48	0.49
5:L5:3932:U:H2'	5:L5:3933:G:C8	2.48	0.49
31:LY:10:ASP:HB3	31:LY:13:LYS:HB2	1.94	0.49
42:Lj:28:HIS:CE1	42:Lj:31:LYS:HD3	2.47	0.49
30:LX:91:GLU:HG3	54:NM:322:ARG:HE	1.76	0.49
31:LY:22:PRO:O	31:LY:26:ARG:HB2	2.13	0.49
64:SI:48:VAL:HG11	64:SI:54:LYS:HD2	1.93	0.49
5:L5:3868:G:H22	5:L5:3900:G:H1'	1.77	0.49
7:L8:82:A:H62	7:L8:84:A:H3'	1.78	0.49
16:LI:31:ILE:HG22	16:LI:62:SER:HB2	1.95	0.49
59:SD:76:ARG:HB2	66:SK:22:VAL:HG11	1.95	0.49
64:SI:103:LEU:HD22	64:SI:170:LYS:HG3	1.95	0.49
80:SY:27:VAL:HG22	80:SY:29:HIS:HD2	1.77	0.49
84:Sc:32:VAL:O	84:Sc:41:SER:HA	2.13	0.49
10:LC:209:ILE:HB	10:LC:229:LEU:HD13	1.94	0.49
66:SK:23:ALA:HB3	66:SK:69:TRP:HZ3	1.78	0.49
5:L5:4139:G:H4'	5:L5:4146:G:H22	1.78	0.49
5:L5:4689:U:H5	5:L5:4699:U:O4	1.96	0.49
7:L8:16:G:HO2'	7:L8:17:A:H8	1.61	0.49
54:NM:362:LEU:HB3	54:NM:491:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SF:41:VAL:HG11	61:SF:68:ILE:HG22	1.93	0.49
65:SJ:32:ILE:HD11	65:SJ:40:LYS:HG3	1.94	0.49
65:SJ:112:THR:O	65:SJ:116:LYS:HG2	2.12	0.49
88:Sg:174:VAL:HG22	88:Sg:188:HIS:HB2	1.95	0.49
5:L5:4088:C:H2'	5:L5:4089:G:C8	2.48	0.48
21:LO:175:MET:HE3	21:LO:179:LYS:HD3	1.94	0.48
32:LZ:100:VAL:HG13	32:LZ:107:LYS:HG2	1.95	0.48
54:NM:341:MET:HE2	54:NM:345:ASP:HB2	1.94	0.48
55:S2:107:A:H2'	55:S2:108:G:C8	2.48	0.48
5:L5:3619:G:H22	5:L5:3624:A:H1'	1.78	0.48
21:LO:194:GLU:O	21:LO:198:THR:HG23	2.13	0.48
54:NM:387:VAL:HB	54:NM:396:ASP:HB2	1.95	0.48
62:SG:159:ARG:HH11	62:SG:173:ALA:HB2	1.77	0.48
3:CR:110:VAL:HB	71:SP:138:SER:HB2	1.95	0.48
19:LM:50:MET:HB3	19:LM:55:MET:HE2	1.95	0.48
62:SG:67:VAL:HG12	62:SG:69:THR:HG22	1.95	0.48
79:SX:100:VAL:HG12	79:SX:125:VAL:HA	1.96	0.48
88:Sg:108:VAL:HA	88:Sg:124:SER:HB3	1.94	0.48
4:CZ:54:PRO:HA	4:CZ:55:PRO:HD3	1.68	0.48
5:L5:4459:U:H2'	5:L5:4460:U:C6	2.48	0.48
8:LA:120:PRO:HA	8:LA:162:ASN:HB3	1.94	0.48
48:Lp:46:LYS:HB3	48:Lp:46:LYS:HE3	1.64	0.48
80:SY:27:VAL:HG13	80:SY:69:THR:HB	1.95	0.48
3:CR:322:VAL:O	3:CR:391:ILE:HA	2.14	0.48
5:L5:1662:C:H2'	5:L5:1663:C:C6	2.48	0.48
5:L5:4093:G:H2'	5:L5:4094:G:C8	2.49	0.48
8:LA:28:ARG:HB2	8:LA:123:ARG:HG3	1.95	0.48
11:LD:204:VAL:O	11:LD:208:MET:HG3	2.13	0.48
15:LH:55:LEU:HD23	15:LH:77:VAL:HG11	1.95	0.48
56:SA:33:GLN:HB2	56:SA:154:LEU:HD11	1.95	0.48
57:SB:60:ASP:HA	57:SB:63:LYS:HD2	1.94	0.48
65:SJ:66:LYS:HA	65:SJ:71:LEU:HD11	1.94	0.48
65:SJ:136:ARG:HD3	65:SJ:160:SER:HA	1.95	0.48
4:CZ:54:PRO:HD2	5:L5:4531:U:H4'	1.94	0.48
5:L5:4629:U:H3	5:L5:4669:A:H62	1.62	0.48
55:S2:66:G:N2	55:S2:82:G:H21	2.11	0.48
55:S2:857:U:H2'	55:S2:858:A:C8	2.48	0.48
55:S2:1648:G:H5''	72:SQ:125:ARG:HB2	1.94	0.48
56:SA:134:LEU:HD12	56:SA:134:LEU:HA	1.71	0.48
57:SB:225:LEU:O	57:SB:229:MET:HG2	2.13	0.48
75:ST:104:LEU:HD22	75:ST:121:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:SY:37:LYS:HD2	80:SY:57:VAL:HG23	1.94	0.48
80:SY:44:LEU:HD12	80:SY:47:MET:HE3	1.95	0.48
45:Lm:93:LYS:HD2	45:Lm:102:ARG:HG2	1.95	0.48
55:S2:527:C:H2'	55:S2:528:A:C8	2.48	0.48
55:S2:921:G:C2	83:Sb:22:LYS:HG3	2.49	0.48
55:S2:1845:A:H2'	55:S2:1846:G:C8	2.49	0.48
75:ST:39:LEU:O	75:ST:96:SER:HB2	2.14	0.48
5:L5:1307:A:H2'	5:L5:1308:C:C6	2.48	0.48
5:L5:3707:U:H2'	5:L5:3708:C:C6	2.48	0.48
5:L5:4119:C:H5	39:Lg:100:GLN:HG2	1.78	0.48
29:LW:83:THR:HA	62:SG:131:ARG:HB3	1.95	0.48
55:S2:508:A:H3'	55:S2:509:G:H8	1.79	0.48
58:SC:196:ILE:HB	58:SC:223:TYR:HB2	1.95	0.48
60:SE:137:PRO:HB2	60:SE:150:PRO:HD2	1.96	0.48
55:S2:1129:G:H5'	83:Sb:19:HIS:HB2	1.96	0.48
5:L5:2864:A:H2'	5:L5:2865:U:C6	2.49	0.48
5:L5:4274:A:H2'	5:L5:4275:G:H8	1.78	0.48
24:LR:105:LEU:HD23	24:LR:138:LEU:HD23	1.96	0.48
54:Nm:290:PRO:HB3	54:Nm:475:GLN:HB3	1.96	0.48
57:SB:137:LEU:HG	57:SB:215:VAL:HG22	1.95	0.48
88:Sg:165:ILE:HG13	88:Sg:177:TRP:HB2	1.96	0.48
5:L5:501:C:H42	5:L5:506:C:H41	1.62	0.47
55:S2:928:G:H2'	55:S2:929:G:C8	2.48	0.47
55:S2:1348:G:H22	55:S2:1381:G:N2	2.12	0.47
55:S2:1544:C:H2'	55:S2:1545:A:H5''	1.95	0.47
59:SD:138:VAL:HG22	59:SD:184:ILE:HD13	1.95	0.47
74:SS:33:ILE:HD13	74:SS:71:MET:HE1	1.95	0.47
87:Sf:121:CYS:HB2	87:Sf:146:LEU:HD11	1.96	0.47
5:L5:2483:G:H2'	5:L5:2484:A:C8	2.49	0.47
5:L5:4260:U:H2'	5:L5:4261:C:C6	2.48	0.47
47:Lo:70:LEU:O	47:Lo:80:LYS:HA	2.14	0.47
54:Nm:288:PRO:HA	54:Nm:289:LYS:HA	1.64	0.47
55:S2:527:C:H2'	55:S2:528:A:H8	1.78	0.47
68:SM:40:LYS:O	68:SM:44:LYS:HB2	2.14	0.47
88:Sg:112:ALA:HB3	88:Sg:121:VAL:HG12	1.96	0.47
5:L5:153:G:H2'	5:L5:154:G:H8	1.79	0.47
5:L5:3736:A:H2'	5:L5:3737:A:C8	2.48	0.47
40:Lh:6:ALA:O	40:Lh:10:ARG:HG2	2.15	0.47
55:S2:1623:A:O5'	74:SS:133:GLY:HA3	2.15	0.47
60:SE:17:HIS:HB2	60:SE:108:ARG:HA	1.96	0.47
61:SF:22:LYS:HG3	61:SF:23:TRP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:424:U:H2'	5:L5:425:U:C6	2.49	0.47
5:L5:1604:G:H2'	5:L5:1605:G:C8	2.50	0.47
7:L8:28:C:H4'	10:LC:51:PRO:HG2	1.95	0.47
8:LA:80:GLU:HB2	8:LA:170:ALA:HA	1.96	0.47
10:LC:40:VAL:HG22	10:LC:115:VAL:HG11	1.96	0.47
28:LV:96:LEU:HD23	29:LW:20:ARG:HB3	1.96	0.47
55:S2:1692:U:H2'	55:S2:1693:G:C8	2.50	0.47
71:SP:28:MET:HE3	71:SP:32:GLN:HG2	1.97	0.47
80:SY:83:LYS:HE3	80:SY:96:LEU:HD11	1.95	0.47
5:L5:452:A:H4'	5:L5:453:G:H5'	1.95	0.47
5:L5:3726:A:H2'	5:L5:3727:A:C8	2.49	0.47
5:L5:4727:A:H4'	9:LB:128:LYS:O	2.14	0.47
53:NB:7:ASN:H	53:NB:10:LYS:HE2	1.79	0.47
60:SE:36:HIS:CG	60:SE:85:GLY:HA3	2.49	0.47
74:SS:78:LYS:HA	74:SS:78:LYS:HD3	1.70	0.47
42:Lj:34:CYS:HB3	42:Lj:39:TYR:H	1.79	0.47
70:SO:94:HIS:HA	70:SO:127:GLY:O	2.13	0.47
5:L5:4169:G:H4'	5:L5:4171:C:C2	2.49	0.47
5:L5:4363:A:H5''	47:Lo:36:GLN:HG2	1.97	0.47
5:L5:4499:G:C2	5:L5:4529:G:H1'	2.49	0.47
5:L5:4518:A:P	9:LB:258:HIS:HB2	2.55	0.47
9:LB:392:LEU:HA	9:LB:392:LEU:HD12	1.76	0.47
39:Lg:83:CYS:SG	39:Lg:86:CYS:HB2	2.55	0.47
54:Nm:245:ILE:HB	54:Nm:281:TYR:HB3	1.95	0.47
55:S2:5:U:H2'	55:S2:6:G:H8	1.79	0.47
55:S2:382:C:H2'	55:S2:383:G:H8	1.80	0.47
55:S2:1298:G:H5''	71:SP:102:PHE:CZ	2.50	0.47
55:S2:1606:G:H5''	75:ST:86:GLY:C	2.39	0.47
62:SG:7:PHE:HB3	62:SG:12:CYS:HB2	1.97	0.47
65:SJ:155:LYS:HA	65:SJ:155:LYS:HD3	1.69	0.47
67:SL:88:ILE:HD11	67:SL:109:MET:HE2	1.97	0.47
68:SM:62:VAL:HA	68:SM:65:VAL:HG12	1.97	0.47
87:Sf:121:CYS:HB3	87:Sf:132:MET:HE1	1.96	0.47
6:L7:58:A:H2'	6:L7:59:G:C8	2.50	0.47
27:LU:80:LYS:HD2	27:LU:108:GLU:HA	1.95	0.47
62:SG:88:ARG:HB3	62:SG:91:GLU:HB2	1.96	0.47
63:SH:79:LEU:H	63:SH:79:LEU:HD23	1.80	0.47
10:LC:284:MET:HE3	23:LQ:28:LEU:HD23	1.97	0.47
24:LR:25:ASP:HB3	24:LR:28:GLU:HB2	1.97	0.47
55:S2:1351:G:H4'	56:SA:110:ASN:HA	1.97	0.47
55:S2:1801:A:H2'	55:S2:1802:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SU:54:VAL:HB	76:SU:88:LEU:HB2	1.97	0.47
82:Sa:45:VAL:HB	82:Sa:49:ALA:HB3	1.97	0.47
5:L5:1348:U:H2'	5:L5:1349:G:H8	1.79	0.47
5:L5:4524:G:N3	9:LB:252:ALA:HB1	2.29	0.47
54:NM:296:TYR:CD2	54:NM:453:LEU:HD23	2.50	0.47
67:SL:66:VAL:HG11	67:SL:141:ASN:HD22	1.78	0.47
5:L5:1836:G:H4'	26:LT:129:LYS:HD3	1.97	0.46
5:L5:2411:C:H2'	5:L5:2412:A:C8	2.50	0.46
5:L5:2539:C:H2'	5:L5:2540:C:C6	2.50	0.46
5:L5:2744:A:H2'	5:L5:2745:A:C8	2.51	0.46
7:L8:148:A:H2'	7:L8:149:G:C8	2.50	0.46
15:LH:53:LYS:HA	15:LH:53:LYS:HD3	1.65	0.46
33:La:37:GLY:H	33:La:41:HIS:HB2	1.80	0.46
54:NM:366:MET:HE1	54:NM:370:GLU:HB3	1.97	0.46
55:S2:367:U:H4'	55:S2:371:A:C8	2.50	0.46
3:CR:17:ILE:O	3:CR:21:ILE:HG12	2.15	0.46
53:NB:61:GLU:HG2	53:NB:73:HIS:CE1	2.50	0.46
55:S2:1217:A:H2'	55:S2:1218:C:H6	1.81	0.46
55:S2:1256:G:H8	85:Sd:29:GLY:HA2	1.81	0.46
82:Sa:53:ILE:HD11	82:Sa:64:LEU:HD11	1.96	0.46
5:L5:2411:C:H2'	5:L5:2412:A:H8	1.79	0.46
5:L5:2554:U:O2	5:L5:2764:A:N7	2.48	0.46
8:LA:101:VAL:HG22	8:LA:165:VAL:HG22	1.98	0.46
15:LH:103:VAL:HG11	15:LH:144:LEU:HD21	1.96	0.46
22:LP:20:SER:O	22:LP:22:LEU:HG	2.16	0.46
5:L5:513:U:H3'	5:L5:514:U:H4'	1.98	0.46
5:L5:2293:U:H2'	5:L5:2294:G:C8	2.50	0.46
5:L5:2664:G:H4'	5:L5:2677:G:H4'	1.98	0.46
55:S2:72:C:H1'	55:S2:73:C:H2'	1.98	0.46
55:S2:1275:G:H5''	55:S2:1506:A:H61	1.79	0.46
68:SM:36:ARG:HH11	68:SM:36:ARG:HA	1.81	0.46
73:SR:34:VAL:O	73:SR:38:ILE:HG13	2.15	0.46
77:SV:62:MET:HE2	77:SV:64:GLU:HG3	1.97	0.46
84:Sc:12:ALA:HB1	84:Sc:32:VAL:HB	1.97	0.46
5:L5:99:A:H4'	20:LN:181:HIS:CE1	2.51	0.46
7:L8:19:C:H2'	7:L8:20:A:C8	2.49	0.46
41:Li:35:LYS:HB2	41:Li:35:LYS:HE3	1.75	0.46
55:S2:851:C:H5''	55:S2:852:G:H5'	1.96	0.46
59:SD:64:ARG:O	59:SD:68:GLU:HG2	2.15	0.46
75:ST:56:ARG:HG3	75:ST:103:VAL:HG21	1.98	0.46
5:L5:3910:C:H2'	5:L5:3911:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4508:C:N3	5:L5:4512:U:H5	2.14	0.46
11:LD:41:LYS:HA	11:LD:41:LYS:HD3	1.68	0.46
50:Ls:125:ALA:HA	50:Ls:154:ILE:HG23	1.98	0.46
55:S2:803:C:H5	55:S2:860:G:H1	1.64	0.46
55:S2:866:U:H2'	55:S2:867:G:C8	2.51	0.46
5:L5:1994:C:H2'	5:L5:1995:G:C8	2.49	0.46
5:L5:3880:G:H2'	5:L5:3881:G:C8	2.51	0.46
5:L5:4325:A:N3	11:LD:36:LEU:HB3	2.31	0.46
27:LU:47:ILE:HD12	27:LU:63:ILE:HD11	1.98	0.46
41:Li:16:LYS:HA	41:Li:16:LYS:HD3	1.69	0.46
50:Ls:96:THR:HA	50:Ls:204:LEU:HD11	1.98	0.46
58:SC:73:MET:HE3	58:SC:73:MET:HB3	1.76	0.46
84:Sc:18:LEU:HD21	84:Sc:31:ARG:HB2	1.98	0.46
5:L5:1834:U:C2	26:LT:128:LEU:HD12	2.50	0.46
7:L8:106:G:H4'	7:L8:137:A:H5'	1.98	0.46
23:LQ:159:PRO:HA	23:LQ:160:HIS:HA	1.67	0.46
30:LX:64:SER:HB2	40:Lh:69:LEU:HD13	1.98	0.46
55:S2:1348:G:H5'	58:SC:145:LYS:HE3	1.97	0.46
61:SF:39:ILE:HG23	61:SF:68:ILE:HD13	1.97	0.46
67:SL:126:VAL:HG12	67:SL:145:VAL:HG22	1.98	0.46
71:SP:18:ARG:H	71:SP:18:ARG:HG2	1.55	0.46
73:SR:16:ILE:HD12	73:SR:24:LEU:HD11	1.97	0.46
11:LD:60:ILE:HD11	11:LD:93:THR:HA	1.97	0.46
18:LL:87:HIS:HE1	18:LL:89:LYS:HD2	1.80	0.46
55:S2:171:A:H5'	62:SG:177:GLN:HG2	1.97	0.46
55:S2:1201:U:H2'	55:S2:1202:U:C6	2.51	0.46
3:CR:318:GLU:HB3	3:CR:414:ARG:HG3	1.96	0.46
9:LB:154:LYS:HE2	9:LB:154:LYS:HB2	1.76	0.46
25:LS:45:TRP:CD1	25:LS:56:LYS:HD3	2.52	0.46
54:Nm:408:MET:HE3	54:Nm:408:MET:H	1.80	0.46
55:S2:15:U:H2'	55:S2:16:G:O4'	2.16	0.46
55:S2:1238:U:O2	55:S2:1242:U:H5	1.98	0.46
5:L5:46:U:H5''	18:LL:16:LYS:HG3	1.99	0.45
5:L5:268:G:H2'	5:L5:269:G:H8	1.80	0.45
24:LR:89:MET:HE3	24:LR:90:PRO:HD2	1.97	0.45
47:Lo:63:THR:OG1	47:Lo:87:ARG:HG3	2.15	0.45
49:Lr:33:LYS:HD2	49:Lr:40:TYR:CE2	2.51	0.45
50:Ls:99:ARG:HH22	50:Ls:205:ASP:HA	1.82	0.45
51:Lt:116:MET:HE2	51:Lt:116:MET:HB3	1.70	0.45
52:NA:74:LYS:HA	52:NA:77:ARG:HG3	1.97	0.45
64:SI:57:ALA:HB2	64:SI:183:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sa:26:CYS:SG	82:Sa:28:ARG:HB2	2.56	0.45
3:CR:19:LYS:HA	3:CR:19:LYS:HD3	1.73	0.45
5:L5:229:G:H5''	31:LY:11:ARG:HG3	1.97	0.45
7:L8:141:C:H2'	7:L8:142:U:C6	2.51	0.45
9:LB:92:TYR:HB3	9:LB:99:LEU:HD22	1.97	0.45
42:Lj:48:ASN:HA	42:Lj:54:LYS:HE2	1.97	0.45
43:Lk:35:LYS:HA	43:Lk:43:TYR:O	2.16	0.45
71:SP:59:ARG:HE	71:SP:59:ARG:HB3	1.62	0.45
74:SS:22:GLY:HA2	74:SS:56:ALA:HB3	1.98	0.45
5:L5:1097:C:H2'	5:L5:1098:G:C8	2.51	0.45
5:L5:4130:C:H41	5:L5:4154:G:H1	1.63	0.45
53:NB:80:GLN:HE22	53:NB:82:SER:HB2	1.80	0.45
55:S2:104:A:H62	55:S2:356:C:H5	1.65	0.45
88:Sg:32:LEU:HD21	88:Sg:42:MET:HG2	1.98	0.45
5:L5:2520:C:H2'	5:L5:2521:G:H8	1.81	0.45
5:L5:4591:U:H2'	5:L5:4592:C:C6	2.51	0.45
5:L5:4967:A:H2'	5:L5:4968:A:C8	2.51	0.45
17:LJ:85:LYS:HE2	17:LJ:85:LYS:HB3	1.66	0.45
18:LL:146:LEU:HD11	40:Lh:122:LYS:HG2	1.99	0.45
52:NA:77:ARG:NH1	52:NA:78:LYS:HB3	2.32	0.45
55:S2:874:G:H2'	55:S2:875:A:H8	1.82	0.45
55:S2:1037:G:H4'	55:S2:1845:A:H4'	1.97	0.45
63:SH:63:PHE:HB3	63:SH:97:GLN:HG2	1.97	0.45
5:L5:150:U:H3	14:LG:162:ASP:HB2	1.82	0.45
5:L5:433:A:C2	5:L5:3867:A:H4'	2.52	0.45
14:LG:138:ALA:HB2	14:LG:194:VAL:HG11	1.98	0.45
21:LO:186:GLU:HA	21:LO:189:ILE:HG22	1.97	0.45
55:S2:656:G:H5'	55:S2:662:G:N2	2.32	0.45
55:S2:683:G:H4'	78:SW:4:MET:HG2	1.99	0.45
55:S2:1347:U:H2'	55:S2:1348:G:H8	1.77	0.45
55:S2:1628:C:H2'	55:S2:1629:C:C6	2.52	0.45
59:SD:8:LYS:HD2	76:SU:59:LYS:HD3	1.99	0.45
88:Sg:30:MET:HE3	88:Sg:30:MET:HB3	1.81	0.45
5:L5:258:G:H2'	5:L5:259:C:C6	2.51	0.45
5:L5:411:G:H4'	5:L5:412:G:H5''	1.98	0.45
5:L5:1077:C:H4'	5:L5:1215:C:C4	2.52	0.45
5:L5:1333:A:H2'	5:L5:1334:A:C8	2.52	0.45
5:L5:2461:G:H5'	20:LN:104:GLU:OE1	2.17	0.45
5:L5:4389:C:H2'	5:L5:4390:A:C8	2.51	0.45
19:LM:76:ALA:HA	19:LM:79:LYS:HE2	1.97	0.45
22:LP:54:GLN:HG2	22:LP:83:TRP:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Le:7:LEU:HB2	37:Le:93:LYS:HB3	1.98	0.45
37:Le:106:LYS:HE2	37:Le:106:LYS:HB3	1.57	0.45
54:NM:453:LEU:HB3	54:NM:455:LEU:HD22	1.98	0.45
65:SJ:114:VAL:HG23	65:SJ:126:ALA:HB1	1.98	0.45
88:Sg:72:SER:HB2	88:Sg:117:ASN:ND2	2.31	0.45
5:L5:1461:C:H2'	5:L5:1462:A:C8	2.52	0.45
50:Ls:28:PHE:HB3	50:Ls:89:VAL:HB	1.98	0.45
55:S2:804:U:H2'	55:S2:805:U:C6	2.51	0.45
19:LM:119:ARG:HA	21:LO:189:ILE:HD11	1.98	0.45
55:S2:1325:G:H1'	55:S2:1510:G:H5''	1.98	0.45
57:SB:124:HIS:HA	57:SB:137:LEU:O	2.17	0.45
5:L5:662:C:H2'	5:L5:663:G:C8	2.52	0.45
5:L5:3612:C:H1'	5:L5:5016:A:C8	2.52	0.45
14:LG:165:GLU:HA	14:LG:168:VAL:HG22	1.97	0.45
18:LL:19:GLN:HA	18:LL:22:VAL:HG23	1.99	0.45
25:LS:30:MET:HE2	25:LS:30:MET:HB3	1.81	0.45
51:Lt:111:ASN:O	51:Lt:115:GLN:HG2	2.16	0.45
85:Sd:21:CYS:HB2	85:Sd:39:CYS:HB3	1.99	0.45
3:CR:42:LYS:HB2	3:CR:42:LYS:HE2	1.73	0.45
5:L5:4621:C:OP1	28:LV:48:ARG:HD2	2.17	0.45
8:LA:5:ILE:HG12	8:LA:8:GLN:HB2	1.98	0.45
13:LF:105:VAL:HG13	13:LF:136:VAL:HG12	1.98	0.45
26:LT:107:LYS:HB3	26:LT:107:LYS:HE3	1.74	0.45
31:LY:116:LYS:O	31:LY:120:GLU:HG2	2.17	0.45
55:S2:1512:C:H2'	55:S2:1513:C:C6	2.52	0.45
69:SN:64:ARG:HD3	69:SN:70:LYS:HD3	1.99	0.45
74:SS:24:ARG:HB2	74:SS:29:ALA:HB2	1.99	0.45
81:SZ:78:LYS:HD3	81:SZ:78:LYS:HA	1.81	0.45
81:SZ:79:ILE:HG23	81:SZ:83:LEU:HD23	1.99	0.45
3:CR:330:ARG:NH1	3:CR:344:LEU:H	2.14	0.44
5:L5:93:G:H2'	5:L5:94:A:C8	2.52	0.44
5:L5:453:G:H4'	5:L5:454:U:H5'	1.99	0.44
8:LA:103:PRO:HA	8:LA:163:ARG:HA	1.99	0.44
9:LB:50:LYS:HB2	9:LB:345:LEU:HD11	1.99	0.44
37:Le:64:LYS:HB2	37:Le:64:LYS:HE2	1.82	0.44
55:S2:64:A:H2	55:S2:83:A:H62	1.64	0.44
61:SF:41:VAL:HA	61:SF:45:TYR:HB2	1.99	0.44
61:SF:44:LYS:HE2	61:SF:44:LYS:HB3	1.87	0.44
61:SF:89:THR:HA	61:SF:92:ILE:HD12	1.98	0.44
88:Sg:168:CYS:HB2	88:Sg:195:LEU:HG	1.98	0.44
3:CR:278:VAL:HA	3:CR:281:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LM:123:ILE:HD12	21:LO:182:GLU:HG3	1.98	0.44
21:LO:79:ILE:HG21	21:LO:138:LEU:HD11	1.98	0.44
32:LZ:41:ALA:HB2	32:LZ:77:TYR:HE1	1.83	0.44
58:SC:192:LEU:HB3	58:SC:227:ARG:HB3	1.98	0.44
63:SH:78:ARG:HD2	63:SH:81:ARG:HE	1.81	0.44
5:L5:1788:A:H2'	16:LI:22:PHE:CZ	2.53	0.44
5:L5:2745:A:H2'	5:L5:2746:A:C8	2.52	0.44
49:Lr:7:TRP:CE2	49:Lr:11:ARG:HG3	2.53	0.44
55:S2:674:C:H2'	55:S2:675:U:C6	2.51	0.44
55:S2:916:A:C5	69:SN:73:ARG:HD3	2.53	0.44
59:SD:66:ILE:HD11	59:SD:86:LEU:HB3	1.99	0.44
59:SD:137:VAL:HG22	59:SD:151:LYS:HG3	1.99	0.44
65:SJ:113:GLN:HG3	65:SJ:149:VAL:HG21	1.99	0.44
73:SR:16:ILE:HD11	73:SR:54:VAL:HG21	1.98	0.44
79:SX:41:PHE:HZ	79:SX:102:VAL:HG12	1.83	0.44
5:L5:1345:A:H2'	5:L5:1346:C:C6	2.52	0.44
5:L5:1685:G:H5''	5:L5:1685:G:H8	1.83	0.44
5:L5:1846:G:H2'	5:L5:1847:C:C6	2.52	0.44
6:L7:6:C:H4'	11:LD:52:ILE:HD13	1.98	0.44
8:LA:158:ILE:HB	8:LA:162:ASN:HD21	1.81	0.44
14:LG:140:VAL:HG21	14:LG:166:LEU:O	2.17	0.44
38:Lf:50:VAL:HG22	38:Lf:69:VAL:HG22	1.98	0.44
55:S2:1736:G:H2'	55:S2:1737:G:C8	2.53	0.44
61:SF:167:LYS:HG2	61:SF:171:GLU:HG3	1.99	0.44
5:L5:1812:C:H5''	34:Lb:56:LYS:HD2	2.00	0.44
11:LD:146:LEU:HB2	11:LD:163:LEU:HD12	1.99	0.44
55:S2:839:C:H41	80:SY:10:ARG:HA	1.83	0.44
55:S2:1667:U:H2'	55:S2:1668:U:C6	2.53	0.44
60:SE:45:ILE:HD12	60:SE:80:ILE:HD11	1.99	0.44
10:LC:152:LEU:HD23	10:LC:251:ILE:HG12	1.99	0.44
27:LU:56:LEU:HD23	27:LU:56:LEU:HA	1.81	0.44
71:SP:34:MET:HB3	71:SP:42:ARG:HG3	2.00	0.44
71:SP:56:LEU:HD23	71:SP:83:MET:HG2	2.00	0.44
3:CR:19:LYS:HZ3	3:CR:22:LYS:HE3	1.83	0.44
5:L5:4966:A:H2'	5:L5:4967:A:O4'	2.18	0.44
16:LI:54:SER:HB2	16:LI:135:ILE:HD11	1.99	0.44
22:LP:22:LEU:HB3	22:LP:90:PHE:CE2	2.53	0.44
24:LR:42:ARG:HA	24:LR:45:ILE:HD12	2.00	0.44
24:LR:76:MET:HE3	24:LR:76:MET:HB3	1.81	0.44
35:Lc:65:MET:HE3	35:Lc:65:MET:HB3	1.80	0.44
53:NB:56:ILE:HD11	53:NB:59:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sa:74:CYS:SG	82:Sa:77:CYS:HB2	2.57	0.44
88:Sg:188:HIS:HB3	88:Sg:219:TRP:CH2	2.53	0.44
5:L5:4188:U:H2'	5:L5:4189:U:C6	2.52	0.44
12:LE:183:ARG:HD2	12:LE:183:ARG:HA	1.81	0.44
30:LX:39:LYS:HB2	30:LX:39:LYS:HE2	1.77	0.44
55:S2:1512:C:H2'	55:S2:1513:C:H6	1.83	0.44
67:SL:80:MET:HE2	67:SL:80:MET:HB3	1.67	0.44
86:Se:36:MET:HG2	86:Se:40:ARG:NH1	2.33	0.44
5:L5:153:G:H2'	5:L5:154:G:C8	2.53	0.44
5:L5:3923:A:H2'	5:L5:3924:C:H6	1.83	0.44
9:LB:77:THR:HG21	9:LB:337:VAL:HG22	1.98	0.44
12:LE:46:ARG:HB2	12:LE:62:MET:HE1	2.00	0.44
20:LN:31:ARG:HD3	20:LN:124:ASP:OD2	2.18	0.44
55:S2:29:G:H2'	55:S2:30:C:C6	2.53	0.44
57:SB:125:VAL:HG21	57:SB:172:MET:HB3	1.99	0.44
73:SR:14:ARG:O	73:SR:18:GLU:HG3	2.17	0.44
88:Sg:24:THR:HB	88:Sg:71:ILE:HG21	1.98	0.44
5:L5:500:G:H1'	5:L5:504:G:H3'	1.99	0.43
5:L5:1786:A:H2'	5:L5:1789:C:C5	2.53	0.43
5:L5:3861:A:H2'	5:L5:3862:A:C8	2.53	0.43
5:L5:4281:A:O2'	5:L5:4282:A:H2'	2.17	0.43
20:LN:135:ILE:HG23	20:LN:142:ILE:HD13	2.00	0.43
27:LU:67:LYS:HE2	27:LU:67:LYS:HB2	1.73	0.43
55:S2:1007:C:H2'	55:S2:1008:A:C8	2.53	0.43
61:SF:70:GLU:HA	61:SF:73:THR:HG22	2.00	0.43
75:ST:42:HIS:HB2	75:ST:83:GLN:HA	1.99	0.43
77:SV:55:ILE:HG21	77:SV:65:SER:HB2	1.99	0.43
88:Sg:31:ILE:HG13	88:Sg:43:TRP:HB2	2.00	0.43
5:L5:3684:G:H2'	5:L5:3685:C:C6	2.53	0.43
10:LC:150:LEU:HA	10:LC:150:LEU:HD12	1.68	0.43
11:LD:182:GLY:HA2	11:LD:194:VAL:HB	2.00	0.43
38:Lf:36:ARG:HB2	38:Lf:80:ASN:HA	2.00	0.43
55:S2:1520:G:H5''	55:S2:1521:C:H5	1.82	0.43
72:SQ:34:VAL:HG13	72:SQ:42:ILE:HD11	1.99	0.43
82:Sa:24:THR:HG21	82:Sa:71:LEU:HA	1.99	0.43
5:L5:4521:U:H1'	9:LB:253:CYS:SG	2.59	0.43
14:LG:150:LYS:HE3	14:LG:177:MET:HE3	2.01	0.43
16:LI:87:MET:HE3	16:LI:87:MET:HB2	1.64	0.43
21:LO:130:LYS:HB2	21:LO:133:ARG:HG2	1.98	0.43
34:Lb:13:SER:HA	34:Lb:16:TRP:CE2	2.53	0.43
67:SL:104:LYS:NZ	79:SX:8:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SM:25:ALA:HB1	68:SM:31:LEU:HD21	1.98	0.43
5:L5:23:C:H2'	5:L5:24:G:O4'	2.19	0.43
5:L5:3934:G:H2'	5:L5:3935:C:C6	2.54	0.43
31:LY:30:MET:HB3	31:LY:101:PRO:HG2	2.01	0.43
39:Lg:69:LYS:HG2	39:Lg:73:HIS:CD2	2.53	0.43
40:Lh:99:GLU:HA	40:Lh:102:LEU:HD12	2.00	0.43
55:S2:17:C:H2'	55:S2:18:C:C6	2.54	0.43
55:S2:1705:C:H2'	55:S2:1706:G:C8	2.54	0.43
86:Se:18:LYS:HA	86:Se:18:LYS:HD3	1.83	0.43
88:Sg:79:LEU:HD22	88:Sg:120:ILE:HD12	1.98	0.43
12:LE:180:VAL:HG11	12:LE:258:LEU:HD11	2.00	0.43
15:LH:8:GLN:HG2	15:LH:74:CYS:SG	2.59	0.43
18:LL:18:TRP:CD1	18:LL:18:TRP:H	2.36	0.43
20:LN:124:ASP:HB3	20:LN:127:TYR:H	1.83	0.43
51:Lt:38:SER:HB2	51:Lt:41:LYS:HB3	2.00	0.43
55:S2:329:G:H2'	55:S2:330:G:C8	2.53	0.43
55:S2:940:U:H3	55:S2:1002:U:H3	1.65	0.43
3:CR:329:MET:HE1	3:CR:331:TYR:CG	2.53	0.43
55:S2:692:G:H2'	55:S2:693:A:C4	2.53	0.43
55:S2:1365:G:H2'	55:S2:1366:G:C8	2.53	0.43
59:SD:105:LEU:HB2	59:SD:122:VAL:HG21	2.00	0.43
60:SE:125:LYS:HG2	60:SE:142:HIS:HB3	2.01	0.43
67:SL:104:LYS:HZ3	79:SX:8:ARG:HD2	1.83	0.43
84:Sc:13:ARG:H	84:Sc:35:MET:HG3	1.83	0.43
5:L5:262:G:H2'	5:L5:263:G:H8	1.83	0.43
5:L5:1971:C:H5	5:L5:2000:G:H2'	1.83	0.43
5:L5:2090:U:H4'	5:L5:2091:C:H3'	2.01	0.43
5:L5:4238:G:H2'	5:L5:4239:A:C8	2.53	0.43
29:LW:82:ILE:O	62:SG:130:PRO:HB2	2.19	0.43
36:Ld:25:TYR:O	36:Ld:85:ARG:HD2	2.18	0.43
48:Lp:6:LYS:HD3	48:Lp:7:LYS:HE2	2.00	0.43
51:Lt:85:LEU:HD11	51:Lt:102:GLY:H	1.84	0.43
53:NB:107:LEU:H	53:NB:107:LEU:HD23	1.84	0.43
55:S2:1298:G:H4'	71:SP:78:THR:HA	2.00	0.43
55:S2:1690:U:H2'	55:S2:1691:U:C6	2.54	0.43
56:SA:8:LEU:HD11	77:SV:39:VAL:HG21	2.00	0.43
65:SJ:128:VAL:HG22	65:SJ:132:GLN:HE22	1.84	0.43
71:SP:20:VAL:HG11	71:SP:36:LEU:HD21	2.00	0.43
3:CR:398:GLU:H	3:CR:398:GLU:HG2	1.66	0.43
5:L5:1468:C:H2'	5:L5:1469:C:C6	2.53	0.43
55:S2:344:U:H2'	55:S2:345:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S2:924:G:OP1	69:SN:3:ARG:HA	2.19	0.43
5:L5:1617:G:H1'	5:L5:2513:A:N6	2.33	0.43
5:L5:2676:A:H8	5:L5:2676:A:OP2	2.01	0.43
5:L5:2705:G:H1	5:L5:2710:C:H5	1.67	0.43
5:L5:3652:A:H2'	5:L5:3653:A:C5	2.53	0.43
21:LO:177:LEU:HD23	21:LO:177:LEU:HA	1.85	0.43
35:Lc:36:LYS:HE2	35:Lc:36:LYS:HB2	1.76	0.43
50:Ls:108:PRO:HA	50:Ls:184:SER:HA	2.00	0.43
55:S2:16:G:H2'	55:S2:17:C:C6	2.54	0.43
56:SA:123:VAL:HA	56:SA:145:ILE:O	2.19	0.43
62:SG:57:ASP:HA	62:SG:106:LEU:HA	1.99	0.43
64:SI:119:LEU:HD23	64:SI:119:LEU:HA	1.93	0.43
78:SW:83:LEU:HD11	78:SW:120:HIS:HA	2.00	0.43
79:SX:3:LYS:H	79:SX:3:LYS:HG2	1.63	0.43
5:L5:1461:C:H2'	5:L5:1462:A:H8	1.84	0.43
33:La:3:SER:HA	33:La:6:ARG:HG3	2.00	0.43
60:SE:18:TRP:HH2	60:SE:31:PRO:HD3	1.84	0.43
3:CR:87:LYS:HB3	3:CR:87:LYS:HE3	1.57	0.42
5:L5:1515:A:H2'	5:L5:1516:G:O4'	2.19	0.42
5:L5:4453:C:H2'	5:L5:4454:G:O4'	2.18	0.42
5:L5:5026:U:H1'	5:L5:5027:C:H5	1.84	0.42
13:LF:127:LYS:HB2	26:LT:133:ALA:HB3	2.01	0.42
22:LP:21:ASN:HB3	22:LP:122:ALA:HB1	2.00	0.42
41:Li:76:ARG:HA	41:Li:76:ARG:HD3	1.88	0.42
50:Ls:130:LEU:HD11	50:Ls:177:MET:HE3	2.01	0.42
54:Nm:414:LYS:N	54:Nm:414:LYS:HE2	2.33	0.42
88:Sg:42:MET:HE2	88:Sg:92:LEU:HD22	2.00	0.42
5:L5:966:A:H5''	5:L5:2092:G:H22	1.83	0.42
5:L5:4088:C:H2'	5:L5:4089:G:H8	1.83	0.42
5:L5:4934:A:H2'	5:L5:4935:C:C6	2.53	0.42
37:Le:19:LYS:HE3	37:Le:19:LYS:HB3	1.90	0.42
37:Le:21:ILE:HD11	37:Le:33:ARG:NH2	2.34	0.42
53:NB:59:ILE:HG22	53:NB:77:PRO:HD2	2.01	0.42
61:SF:145:ARG:HB2	84:Sc:48:GLY:HA3	2.01	0.42
75:ST:13:GLU:H	75:ST:13:GLU:HG2	1.66	0.42
76:SU:66:ARG:HA	76:SU:66:ARG:HD2	1.92	0.42
77:SV:58:ALA:O	77:SV:62:MET:HG3	2.19	0.42
5:L5:2123:C:H1'	12:LE:72:LYS:HD2	2.00	0.42
5:L5:4344:U:H2'	5:L5:4345:C:C6	2.55	0.42
5:L5:4967:A:H2'	5:L5:4968:A:H8	1.84	0.42
10:LC:301:ALA:HB1	23:LQ:132:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LD:193:GLU:O	11:LD:197:LYS:HG2	2.19	0.42
12:LE:165:LEU:HD11	12:LE:176:THR:HG22	2.01	0.42
14:LG:207:VAL:HG21	14:LG:215:LEU:HD13	2.01	0.42
23:LQ:154:LYS:HB3	23:LQ:154:LYS:HE3	1.88	0.42
44:Ll:34:LYS:HB2	44:Ll:34:LYS:HE3	1.64	0.42
51:Lt:85:LEU:HD22	51:Lt:87:GLU:HB2	2.01	0.42
54:Nm:152:LEU:HD11	54:Nm:158:TRP:CD1	2.55	0.42
66:SK:15:LEU:HD23	66:SK:79:LEU:HD11	2.00	0.42
3:CR:14:ILE:HG12	3:CR:117:PHE:CG	2.54	0.42
4:CZ:4:SER:H	54:Nm:474:LEU:HD21	1.85	0.42
5:L5:223:G:H4'	5:L5:225:G:N7	2.34	0.42
5:L5:2732:G:H2'	5:L5:2733:C:C6	2.54	0.42
5:L5:3727:A:H2'	5:L5:3728:A:C8	2.54	0.42
7:L8:141:C:H5''	20:LN:60:VAL:HG11	2.02	0.42
14:LG:164:ILE:HG23	20:LN:22:LEU:HD21	2.02	0.42
30:LX:122:ALA:HB3	30:LX:139:ARG:HG2	2.01	0.42
31:LY:27:ARG:HB2	31:LY:75:ARG:CZ	2.49	0.42
35:Lc:47:ILE:HB	35:Lc:94:LEU:HG	2.01	0.42
43:Lk:21:LYS:HA	43:Lk:21:LYS:HD3	1.83	0.42
54:Nm:138:VAL:HG22	54:Nm:482:LYS:HG3	2.01	0.42
55:S2:1274:G:OP2	55:S2:1275:G:H5'	2.19	0.42
68:SM:50:CYS:HB2	68:SM:110:VAL:HG22	2.01	0.42
71:SP:108:LYS:HB2	71:SP:111:MET:HG3	2.00	0.42
74:SS:106:LYS:HA	74:SS:106:LYS:HD3	1.90	0.42
75:ST:65:TYR:HE1	75:ST:128:GLN:HG3	1.83	0.42
88:Sg:288:SER:O	88:Sg:300:ALA:HA	2.19	0.42
3:CR:28:ARG:HD3	3:CR:28:ARG:HA	1.81	0.42
5:L5:267:G:H2'	5:L5:268:G:H8	1.84	0.42
5:L5:3612:C:H1'	5:L5:5016:A:H8	1.83	0.42
5:L5:4638:U:H2'	5:L5:4639:G:N3	2.35	0.42
15:LH:76:HIS:O	15:LH:80:MET:HG3	2.19	0.42
21:LO:189:ILE:HD12	21:LO:189:ILE:HA	1.83	0.42
72:SQ:86:GLN:HE22	72:SQ:122:ALA:HA	1.84	0.42
5:L5:106:A:H2'	5:L5:107:G:O4'	2.20	0.42
5:L5:1346:C:H2'	5:L5:1347:G:H8	1.84	0.42
5:L5:2705:G:H22	5:L5:2710:C:H5	1.68	0.42
5:L5:3911:C:H2'	5:L5:3912:U:C6	2.55	0.42
5:L5:3932:U:H2'	5:L5:3933:G:H8	1.83	0.42
5:L5:4743:G:H2'	5:L5:4744:A:C8	2.54	0.42
7:L8:140:C:H2'	7:L8:141:C:C6	2.55	0.42
10:LC:1:MET:HB2	10:LC:2:ALA:H	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LD:117:LYS:HA	11:LD:117:LYS:HD3	1.84	0.42
15:LH:94:SER:HB2	15:LH:142:ASP:HB3	2.02	0.42
20:LN:84:PRO:HA	20:LN:87:HIS:CG	2.54	0.42
22:LP:20:SER:HB3	22:LP:21:ASN:H	1.68	0.42
37:Le:38:PRO:HG2	37:Le:46:ARG:HB3	2.02	0.42
48:Lp:3:LYS:HE3	48:Lp:3:LYS:HB2	1.78	0.42
55:S2:51:U:H2'	55:S2:52:G:C8	2.55	0.42
55:S2:118:C:H1'	55:S2:445:A:C5	2.53	0.42
56:SA:119:PRO:HG2	56:SA:142:LEU:HD21	2.01	0.42
56:SA:123:VAL:HG12	56:SA:145:ILE:HB	2.02	0.42
72:SQ:134:GLY:HA3	72:SQ:140:ARG:HA	2.01	0.42
76:SU:24:LEU:HB2	76:SU:87:ARG:HB2	2.01	0.42
5:L5:4389:C:H2'	5:L5:4390:A:H8	1.83	0.42
8:LA:192:LYS:HE2	8:LA:192:LYS:HB3	1.88	0.42
16:LI:87:MET:HG2	16:LI:138:ILE:HG12	2.01	0.42
31:LY:35:SER:O	31:LY:39:ARG:HB2	2.19	0.42
36:Ld:44:ARG:O	36:Ld:48:GLU:HG2	2.20	0.42
55:S2:1098:C:H2'	55:S2:1099:G:C8	2.54	0.42
55:S2:1839:U:H1'	55:S2:1863:A:H2	1.85	0.42
55:S2:1863:A:H8	82:Sa:79:ILE:HG21	1.85	0.42
61:SF:112:LEU:O	61:SF:116:ILE:HG12	2.20	0.42
65:SJ:33:GLY:HA3	86:Se:38:TYR:CG	2.55	0.42
71:SP:41:GLN:HG3	71:SP:84:ILE:HD12	2.01	0.42
82:Sa:40:VAL:HB	82:Sa:69:VAL:HG22	2.02	0.42
88:Sg:85:GLY:HA2	88:Sg:108:VAL:HG23	2.02	0.42
5:L5:4258:C:H5'	17:LJ:68:ILE:HD11	2.01	0.42
5:L5:5006:U:H4'	5:L5:5007:A:H5'	2.00	0.42
8:LA:248:GLY:HA2	55:S2:1044:G:C6	2.54	0.42
9:LB:16:PHE:HB2	9:LB:19:ARG:HH21	1.85	0.42
15:LH:41:ILE:HG22	15:LH:43:VAL:HG13	2.02	0.42
15:LH:44:GLU:HG3	15:LH:58:ASP:HB2	2.02	0.42
33:La:7:LYS:HE2	33:La:7:LYS:HB3	1.77	0.42
36:Ld:36:VAL:HG21	36:Ld:44:ARG:HG2	2.02	0.42
52:NA:100:LYS:HA	52:NA:100:LYS:HD3	1.75	0.42
55:S2:1499:U:H4'	59:SD:176:LEU:HD13	2.00	0.42
61:SF:201:LYS:HA	61:SF:204:ARG:HG3	2.00	0.42
68:SM:51:VAL:HG22	68:SM:77:ILE:HB	2.02	0.42
68:SM:94:ILE:HD12	68:SM:94:ILE:HA	1.88	0.42
5:L5:2412:A:H2'	5:L5:2413:U:C6	2.54	0.42
5:L5:3599:A:H2'	5:L5:3600:G:C8	2.54	0.42
7:L8:6:C:H2'	7:L8:7:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:355:THR:HA	9:LB:360:LEU:HD11	2.01	0.42
17:LJ:19:LYS:HG2	17:LJ:133:VAL:HB	2.02	0.42
18:LL:107:THR:HB	41:Li:18:THR:HG23	2.01	0.42
20:LN:120:TRP:HZ2	20:LN:123:GLU:HB2	1.85	0.42
42:Lj:27:TYR:HA	42:Lj:34:CYS:HA	2.02	0.42
50:Ls:45:MET:HE2	50:Ls:45:MET:HA	2.01	0.42
54:NM:108:THR:HG23	54:NM:111:GLU:H	1.84	0.42
55:S2:1406:G:H2'	55:S2:1407:U:C6	2.54	0.42
57:SB:182:LYS:HB3	57:SB:182:LYS:HE3	1.83	0.42
58:SC:195:LEU:HD12	58:SC:224:THR:HG22	2.01	0.42
61:SF:49:LEU:HD12	72:SQ:50:LYS:HG2	2.01	0.42
74:SS:20:ILE:HD11	74:SS:33:ILE:HG13	2.01	0.42
5:L5:1278:C:H2'	5:L5:1279:A:O4'	2.20	0.42
5:L5:1811:G:H2'	5:L5:1812:C:C6	2.55	0.42
5:L5:2020:U:H2'	5:L5:2021:G:H8	1.84	0.42
5:L5:4390:A:H2'	5:L5:4391:G:O4'	2.20	0.42
13:LF:225:THR:HB	13:LF:229:GLU:HG3	2.02	0.42
14:LG:187:LYS:HG3	14:LG:198:THR:HG23	2.02	0.42
21:LO:179:LYS:HA	21:LO:179:LYS:HD2	1.75	0.42
28:LV:67:LYS:HB2	28:LV:67:LYS:HE3	1.74	0.42
54:NM:166:ARG:HA	54:NM:169:LEU:HG	2.02	0.42
55:S2:169:U:H1'	62:SG:133:LEU:HD12	2.01	0.42
55:S2:803:C:H5	55:S2:860:G:H22	1.68	0.42
65:SJ:151:LEU:HD23	65:SJ:151:LEU:HA	1.92	0.42
74:SS:6:PRO:HD3	81:SZ:49:LEU:HB3	2.01	0.42
78:SW:12:LYS:HA	78:SW:12:LYS:HD3	1.85	0.42
80:SY:88:LYS:HA	80:SY:91:LEU:HD12	2.02	0.42
5:L5:490:C:H2'	5:L5:491:G:C8	2.55	0.41
5:L5:1567:U:H2'	5:L5:1568:C:C6	2.54	0.41
5:L5:2542:G:H2'	5:L5:2543:A:C8	2.55	0.41
5:L5:3775:A:H5'	5:L5:3776:G:OP2	2.20	0.41
5:L5:3848:U:H2'	5:L5:3849:A:C8	2.55	0.41
8:LA:247:ARG:HD3	55:S2:1069:U:H4'	2.01	0.41
55:S2:1232:U:H2'	55:S2:1233:G:C8	2.55	0.41
5:L5:462:G:H2'	5:L5:463:A:C8	2.54	0.41
5:L5:717:U:H2'	5:L5:718:C:C6	2.54	0.41
5:L5:1194:G:H2'	5:L5:1195:G:C8	2.54	0.41
5:L5:4148:C:H5''	32:LZ:59:LYS:NZ	2.35	0.41
6:L7:7:G:OP2	11:LD:28:THR:HG22	2.20	0.41
39:Lg:69:LYS:HZ3	39:Lg:69:LYS:HG3	1.78	0.41
49:Lr:47:LYS:HB3	49:Lr:102:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S2:833:C:H2'	55:S2:834:C:C6	2.55	0.41
55:S2:1146:C:H2'	55:S2:1147:C:O2	2.20	0.41
57:SB:129:THR:HB	57:SB:180:ASP:HA	2.02	0.41
75:ST:129:ARG:HD3	75:ST:133:ARG:NH2	2.35	0.41
5:L5:2487:G:H22	5:L5:2492:C:H1'	1.85	0.41
12:LE:70:LYS:HE3	12:LE:70:LYS:HB3	1.90	0.41
15:LH:146:LEU:HD13	15:LH:146:LEU:HA	1.92	0.41
22:LP:126:ARG:HB2	22:LP:140:MET:HE1	2.01	0.41
35:Lc:18:LEU:HD12	35:Lc:18:LEU:HA	1.87	0.41
52:NA:111:VAL:HA	52:NA:121:ILE:O	2.19	0.41
53:NB:52:GLY:HA3	53:NB:82:SER:HA	2.02	0.41
55:S2:929:G:H2'	55:S2:930:C:O4'	2.20	0.41
60:SE:208:VAL:HG11	60:SE:225:ILE:HG13	2.01	0.41
61:SF:76:MET:HG2	61:SF:155:CYS:SG	2.61	0.41
88:Sg:212:LYS:HD3	88:Sg:235:ILE:HD11	2.01	0.41
3:CR:226:LEU:O	3:CR:253:LEU:HA	2.20	0.41
5:L5:3871:A:H2'	5:L5:3872:A:C8	2.54	0.41
16:LI:91:LEU:HD12	16:LI:91:LEU:HA	1.92	0.41
42:Lj:21:ARG:NH2	42:Lj:39:TYR:HA	2.36	0.41
55:S2:28:U:H2'	55:S2:29:G:H8	1.84	0.41
55:S2:115:U:H2'	55:S2:116:U:C6	2.55	0.41
55:S2:1808:U:H2'	55:S2:1809:A:C8	2.55	0.41
56:SA:122:LEU:O	56:SA:144:THR:HA	2.20	0.41
61:SF:152:TRP:O	61:SF:156:THR:HG23	2.21	0.41
64:SI:17:LYS:HB3	64:SI:17:LYS:HE3	1.90	0.41
66:SK:5:LYS:O	66:SK:9:ILE:HD12	2.20	0.41
73:SR:85:VAL:HG23	73:SR:86:PRO:HD3	2.02	0.41
3:CR:330:ARG:NH2	3:CR:332:VAL:HA	2.35	0.41
5:L5:668:C:O2'	5:L5:669:C:H5''	2.19	0.41
5:L5:2800:G:H1'	42:Lj:9:GLY:HA3	2.03	0.41
5:L5:4219:A:H2'	5:L5:4220:A:C8	2.55	0.41
11:LD:208:MET:HE2	11:LD:233:PRO:HD3	2.03	0.41
25:LS:127:MET:HG2	26:LT:153:PRO:HG2	2.01	0.41
31:LY:2:LYS:HE3	31:LY:2:LYS:HB3	1.86	0.41
55:S2:147:A:N6	55:S2:173:A:H61	2.18	0.41
55:S2:530:U:H2'	55:S2:531:A:H8	1.85	0.41
61:SF:76:MET:HB3	61:SF:76:MET:HE3	1.76	0.41
62:SG:145:PHE:CE2	62:SG:156:TYR:HB3	2.56	0.41
74:SS:34:LYS:HB3	74:SS:34:LYS:HE2	1.83	0.41
3:CR:328:ILE:HD11	3:CR:345:TYR:HB2	2.03	0.41
5:L5:1266:G:H4'	5:L5:2121:C:H41	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1397:A:C8	33:La:114:LYS:HD2	2.55	0.41
5:L5:1802:A:H5''	5:L5:1803:G:H5'	2.01	0.41
5:L5:2461:G:H2'	5:L5:2462:C:C6	2.55	0.41
5:L5:2864:A:H2'	5:L5:2865:U:H6	1.86	0.41
5:L5:4611:A:H2'	5:L5:4612:C:H6	1.86	0.41
53:NB:102:MET:HE2	53:NB:102:MET:HA	2.03	0.41
54:NM:240:LYS:HG3	54:NM:242:MET:SD	2.61	0.41
57:SB:85:LYS:HB3	57:SB:101:HIS:HB3	2.03	0.41
59:SD:177:LEU:HD12	59:SD:182:LEU:HD13	2.03	0.41
60:SE:29:PRO:HG2	60:SE:46:ILE:HG22	2.02	0.41
5:L5:1504:G:H2'	5:L5:1505:C:C6	2.55	0.41
5:L5:4685:U:H2'	5:L5:4686:G:C8	2.56	0.41
8:LA:175:ILE:H	8:LA:175:ILE:HG13	1.70	0.41
9:LB:56:ILE:HD13	9:LB:365:LEU:HD22	2.02	0.41
21:LO:47:PHE:CE1	21:LO:140:ARG:HD3	2.56	0.41
25:LS:147:ASP:HB3	25:LS:150:ILE:HB	2.02	0.41
55:S2:5:U:H2'	55:S2:6:G:C8	2.56	0.41
55:S2:360:A:C2	55:S2:362:C:H2'	2.56	0.41
55:S2:363:A:N6	55:S2:400:C:H1'	2.36	0.41
59:SD:172:VAL:HG22	59:SD:185:LYS:HG3	2.01	0.41
65:SJ:124:HIS:CE1	86:Se:35:ARG:HB2	2.56	0.41
67:SL:20:LYS:HE2	67:SL:20:LYS:HB3	1.92	0.41
88:Sg:14:HIS:CE1	88:Sg:35:SER:HB2	2.55	0.41
88:Sg:77:PHE:HD2	88:Sg:77:PHE:HA	1.77	0.41
5:L5:10:A:H2'	5:L5:11:G:C8	2.56	0.41
5:L5:3685:C:H5'	8:LA:193:ARG:CZ	2.50	0.41
5:L5:4454:G:H2'	5:L5:4455:G:C8	2.56	0.41
33:La:8:THR:HG23	33:La:17:HIS:NE2	2.36	0.41
34:Lb:40:LEU:HD12	34:Lb:40:LEU:HA	1.94	0.41
40:Lh:13:LYS:H	40:Lh:13:LYS:HG2	1.73	0.41
55:S2:12:U:H2'	55:S2:13:C:C6	2.56	0.41
55:S2:639:C:H2'	55:S2:640:A:C8	2.56	0.41
55:S2:921:G:C6	78:SW:28:ARG:HG3	2.55	0.41
55:S2:943:U:H2'	55:S2:944:A:C8	2.55	0.41
67:SL:59:LYS:HB2	67:SL:112:HIS:NE2	2.35	0.41
74:SS:47:LYS:HA	74:SS:47:LYS:HD2	1.90	0.41
76:SU:67:LYS:HA	85:Sd:44:ARG:HD2	2.02	0.41
5:L5:162:A:H2'	5:L5:163:A:C8	2.56	0.41
5:L5:1348:U:H2'	5:L5:1349:G:C8	2.55	0.41
5:L5:4488:A:H4'	5:L5:4489:G:C8	2.55	0.41
5:L5:4524:G:C2	9:LB:252:ALA:HB1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4935:C:H2'	5:L5:4936:G:C8	2.56	0.41
6:L7:24:C:H2'	6:L7:25:G:O4'	2.21	0.41
8:LA:77:ILE:HD12	8:LA:128:ARG:HB2	2.03	0.41
9:LB:14:LEU:HD22	9:LB:17:LEU:HD11	2.02	0.41
9:LB:220:ILE:HG12	9:LB:278:THR:HG23	2.01	0.41
10:LC:175:LYS:HB3	10:LC:175:LYS:HE3	1.90	0.41
10:LC:330:PRO:HG3	13:LF:47:ARG:NH2	2.36	0.41
24:LR:166:THR:HG21	55:S2:873:G:H5''	2.01	0.41
27:LU:45:GLU:H	27:LU:45:GLU:HG2	1.76	0.41
41:Li:70:LEU:HB2	41:Li:87:ARG:NH1	2.36	0.41
50:Ls:62:ARG:HG2	50:Ls:79:LEU:HD22	2.03	0.41
54:NM:109:MET:HE3	54:NM:109:MET:HA	2.03	0.41
55:S2:1058:A:H2'	55:S2:1059:G:C8	2.56	0.41
55:S2:1102:G:H1	55:S2:1130:G:H1	1.67	0.41
55:S2:1285:G:H5'	68:SM:35:ILE:HG23	2.03	0.41
55:S2:1292:C:H42	87:Sf:138:ARG:HH21	1.68	0.41
55:S2:1606:G:HO2'	55:S2:1607:A:H8	1.65	0.41
57:SB:85:LYS:HD3	57:SB:85:LYS:HA	1.81	0.41
57:SB:146:ARG:HA	57:SB:146:ARG:HD2	1.87	0.41
57:SB:199:LYS:HB2	57:SB:199:LYS:HE3	1.86	0.41
59:SD:170:THR:HG23	59:SD:187:LYS:HG2	2.02	0.41
62:SG:221:LYS:HB3	62:SG:221:LYS:HE3	1.79	0.41
67:SL:111:VAL:HG12	67:SL:140:PHE:HB2	2.03	0.41
72:SQ:25:CYS:SG	72:SQ:68:ILE:HG12	2.61	0.41
74:SS:121:ARG:HG3	74:SS:131:VAL:HB	2.02	0.41
3:CR:24:LEU:HD21	3:CR:112:ILE:HD13	2.03	0.41
5:L5:124:C:OP1	20:LN:144:ARG:HD2	2.21	0.41
5:L5:691:C:H2'	5:L5:692:A:C8	2.56	0.41
5:L5:1670:G:O2'	5:L5:1854:G:H5'	2.21	0.41
5:L5:2347:A:C4	37:Le:31:ILE:HD11	2.56	0.41
5:L5:3668:C:H5'	8:LA:8:GLN:O	2.21	0.41
5:L5:4452:U:H6	5:L5:4452:U:H2'	1.55	0.41
5:L5:4635:A:H3'	5:L5:4636:U:H4'	2.03	0.41
8:LA:70:LYS:HE3	8:LA:72:ARG:HH12	1.86	0.41
14:LG:43:GLN:HE21	14:LG:43:GLN:HA	1.86	0.41
17:LJ:161:GLU:HG3	17:LJ:164:ARG:NH1	2.36	0.41
25:LS:13:VAL:HG22	25:LS:29:ARG:HB2	2.03	0.41
50:Ls:69:LEU:HD11	50:Ls:76:GLU:HB3	2.03	0.41
51:Lt:92:ARG:HA	51:Lt:92:ARG:HD2	1.76	0.41
54:NM:173:TYR:HE1	54:NM:193:SER:HA	1.86	0.41
54:NM:196:PHE:HB2	54:NM:381:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:NM:204:PRO:HD2	54:NM:370:GLU:HG2	2.02	0.41
55:S2:65:C:C4	62:SG:133:LEU:HD13	2.55	0.41
55:S2:804:U:H5	55:S2:859:G:H1	1.68	0.41
55:S2:1283:C:H4'	55:S2:1287:A:H5'	2.03	0.41
55:S2:1497:G:C6	66:SK:25:LYS:HD2	2.56	0.41
56:SA:143:PRO:HG3	77:SV:32:ILE:HG13	2.02	0.41
58:SC:204:ILE:HB	58:SC:211:LYS:HD3	2.02	0.41
61:SF:165:ASN:HB3	61:SF:167:LYS:H	1.86	0.41
62:SG:41:LEU:HD23	62:SG:41:LEU:HA	1.96	0.41
73:SR:58:MET:HE3	73:SR:58:MET:HB3	1.73	0.41
5:L5:1590:C:H3'	5:L5:1591:U:H4'	2.03	0.40
5:L5:1695:U:H2'	5:L5:1696:C:C6	2.57	0.40
5:L5:2521:G:H4'	39:Lg:26:PRO:HD2	2.02	0.40
5:L5:5024:C:N4	5:L5:5028:G:H21	2.19	0.40
10:LC:137:VAL:HG21	10:LC:150:LEU:HD21	2.03	0.40
16:LI:73:ASN:HB2	16:LI:87:MET:HE1	2.03	0.40
22:LP:117:ILE:HD12	22:LP:148:MET:HE2	2.02	0.40
40:Lh:94:ARG:HE	40:Lh:94:ARG:HB2	1.60	0.40
47:Lo:33:LEU:HA	47:Lo:38:LYS:HG2	2.01	0.40
55:S2:1232:U:H2'	55:S2:1233:G:H8	1.86	0.40
55:S2:1348:G:H1	55:S2:1381:G:N2	2.05	0.40
56:SA:44:ASP:C	73:SR:126:MET:HG2	2.46	0.40
59:SD:72:VAL:HB	66:SK:68:TYR:HD2	1.85	0.40
66:SK:49:MET:HB3	66:SK:49:MET:HE3	1.82	0.40
80:SY:27:VAL:HG21	80:SY:35:VAL:HG21	2.02	0.40
5:L5:25:A:H2'	5:L5:26:C:H6	1.86	0.40
5:L5:2017:A:HO2'	5:L5:2018:C:H6	1.66	0.40
5:L5:2029:A:H2'	5:L5:2030:A:C8	2.57	0.40
5:L5:3899:G:H8	5:L5:3899:G:H5''	1.85	0.40
5:L5:4345:C:H2'	5:L5:4346:U:C6	2.56	0.40
12:LE:128:HIS:C	12:LE:128:HIS:CD2	2.99	0.40
13:LF:86:GLU:HG3	26:LT:136:ARG:HB2	2.03	0.40
14:LG:171:PRO:HB3	14:LG:181:TYR:CE1	2.57	0.40
32:LZ:103:ASP:HA	32:LZ:104:PRO:HD3	1.90	0.40
35:Lc:38:ILE:HD11	35:Lc:46:VAL:HG21	2.03	0.40
36:Ld:81:PRO:HG2	36:Ld:84:ILE:HD11	2.03	0.40
51:Lt:132:ILE:HD13	51:Lt:132:ILE:HA	1.90	0.40
55:S2:1681:U:H2'	55:S2:1682:C:C6	2.56	0.40
55:S2:1797:U:H2'	55:S2:1798:C:C6	2.57	0.40
55:S2:1798:C:H2'	55:S2:1799:G:O4'	2.21	0.40
56:SA:52:LYS:HD3	77:SV:83:PHE:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SA:104:THR:O	56:SA:107:THR:HG23	2.20	0.40
62:SG:1:MET:HE3	62:SG:109:LEU:HB2	2.01	0.40
65:SJ:31:LEU:HD12	65:SJ:31:LEU:HA	1.94	0.40
72:SQ:50:LYS:HA	72:SQ:50:LYS:HD2	1.82	0.40
3:CR:9:ASP:O	3:CR:13:GLU:HG2	2.21	0.40
5:L5:1857:C:H2'	5:L5:1858:A:C8	2.57	0.40
5:L5:4674:C:H2'	5:L5:4675:U:C6	2.57	0.40
6:L7:3:C:H2'	6:L7:4:U:C6	2.56	0.40
31:LY:30:MET:O	31:LY:49:ILE:HG12	2.21	0.40
32:LZ:60:LYS:HE2	32:LZ:60:LYS:HB2	1.79	0.40
43:Lk:70:LYS:HD3	43:Lk:70:LYS:HA	1.82	0.40
44:Ll:16:LYS:HD2	44:Ll:49:LEU:HD22	2.03	0.40
54:Nm:319:THR:H	54:Nm:322:ARG:HB2	1.85	0.40
55:S2:609:U:H2'	55:S2:610:G:H8	1.86	0.40
55:S2:1410:C:H2'	55:S2:1411:G:C8	2.57	0.40
58:SC:183:LYS:HG2	58:SC:197:PRO:HD2	2.03	0.40
65:SJ:119:LEU:HD21	65:SJ:158:ASP:HA	2.03	0.40
74:SS:114:LEU:HD23	74:SS:114:LEU:HA	1.94	0.40
88:Sg:237:ASN:HB3	88:Sg:287:THR:HA	2.03	0.40
5:L5:136:C:N4	40:Lh:79:LYS:HE3	2.37	0.40
5:L5:1751:A:H2'	5:L5:1752:G:C8	2.57	0.40
5:L5:2538:U:H2'	5:L5:2539:C:C6	2.56	0.40
5:L5:3648:A:H1'	5:L5:3785:A:N6	2.37	0.40
17:LJ:94:LEU:HD22	17:LJ:98:ASN:HD22	1.86	0.40
55:S2:1407:U:H2'	55:S2:1408:U:H6	1.87	0.40
64:SI:62:VAL:HA	64:SI:77:ARG:HA	2.03	0.40
71:SP:77:LYS:HE3	71:SP:77:LYS:HB2	1.75	0.40
88:Sg:202:PRO:HG2	88:Sg:243:PRO:HA	2.03	0.40
5:L5:300:A:H2	20:LN:93:LYS:HD3	1.86	0.40
5:L5:4734:A:H1'	5:L5:4735:G:C8	2.56	0.40
9:LB:286:LYS:HE3	9:LB:286:LYS:HB2	1.82	0.40
12:LE:163:VAL:HG11	12:LE:201:ILE:HD11	2.03	0.40
16:LI:208:LYS:HA	16:LI:211:VAL:HG22	2.03	0.40
23:LQ:119:LYS:HE3	23:LQ:121:LEU:HD21	2.04	0.40
26:LT:87:LYS:HA	26:LT:87:LYS:HD2	1.90	0.40
41:Li:25:ARG:H	41:Li:25:ARG:HG2	1.72	0.40
50:Ls:189:ILE:HG22	50:Ls:201:PRO:HG3	2.03	0.40
61:SF:34:SER:HA	84:Sc:55:VAL:HB	2.03	0.40
61:SF:144:LEU:HD23	84:Sc:49:PRO:HG2	2.03	0.40
64:SI:130:THR:HG23	64:SI:132:GLU:H	1.86	0.40
68:SM:122:ASP:HA	68:SM:125:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SS:142:ARG:HB3	74:SS:143:GLY:H	1.62	0.40
85:Sd:33:LYS:HD3	85:Sd:34:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CR	411/437 (94%)	401 (98%)	10 (2%)	0	100	100
4	CZ	52/55 (94%)	42 (81%)	8 (15%)	2 (4%)	2	1
8	LA	246/257 (96%)	232 (94%)	14 (6%)	0	100	100
9	LB	393/403 (98%)	378 (96%)	15 (4%)	0	100	100
10	LC	362/427 (85%)	340 (94%)	20 (6%)	2 (1%)	21	23
11	LD	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	36	42
12	LE	213/288 (74%)	194 (91%)	19 (9%)	0	100	100
13	LF	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
14	LG	225/266 (85%)	214 (95%)	11 (5%)	0	100	100
15	LH	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
16	LI	203/214 (95%)	191 (94%)	11 (5%)	1 (0%)	24	27
17	LJ	167/178 (94%)	159 (95%)	8 (5%)	0	100	100
18	LL	203/211 (96%)	192 (95%)	11 (5%)	0	100	100
19	LM	137/215 (64%)	131 (96%)	6 (4%)	0	100	100
20	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
21	LO	198/203 (98%)	194 (98%)	4 (2%)	0	100	100
22	LP	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
23	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	LR	174/196 (89%)	173 (99%)	1 (1%)	0	100	100
25	LS	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
26	LT	157/160 (98%)	145 (92%)	11 (7%)	1 (1%)	21	23
27	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
28	LV	129/140 (92%)	123 (95%)	6 (5%)	0	100	100
29	LW	111/157 (71%)	103 (93%)	8 (7%)	0	100	100
30	LX	118/156 (76%)	113 (96%)	5 (4%)	0	100	100
31	LY	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
32	LZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
33	La	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	19
34	Lb	73/159 (46%)	72 (99%)	1 (1%)	0	100	100
35	Lc	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
36	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
37	Le	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
38	Lf	107/110 (97%)	98 (92%)	9 (8%)	0	100	100
39	Lg	112/117 (96%)	103 (92%)	9 (8%)	0	100	100
40	Lh	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
41	Li	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
42	Lj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
43	Lk	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
44	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
45	Lm	50/128 (39%)	50 (100%)	0	0	100	100
46	Ln	22/25 (88%)	22 (100%)	0	0	100	100
47	Lo	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
48	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
49	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
50	Ls	210/317 (66%)	204 (97%)	6 (3%)	0	100	100
51	Lt	158/165 (96%)	157 (99%)	1 (1%)	0	100	100
52	NA	65/215 (30%)	60 (92%)	5 (8%)	0	100	100
53	NB	120/162 (74%)	108 (90%)	12 (10%)	0	100	100
54	NM	394/496 (79%)	379 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	SA	214/295 (72%)	204 (95%)	9 (4%)	1 (0%)	24	27
57	SB	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
58	SC	217/293 (74%)	210 (97%)	7 (3%)	0	100	100
59	SD	219/243 (90%)	208 (95%)	11 (5%)	0	100	100
60	SE	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
61	SF	177/204 (87%)	168 (95%)	8 (4%)	1 (1%)	21	23
62	SG	229/249 (92%)	209 (91%)	18 (8%)	2 (1%)	14	14
63	SH	179/194 (92%)	169 (94%)	10 (6%)	0	100	100
64	SI	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
65	SJ	177/194 (91%)	173 (98%)	4 (2%)	0	100	100
66	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
67	SL	140/158 (89%)	132 (94%)	8 (6%)	0	100	100
68	SM	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
69	SN	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
70	SO	132/151 (87%)	121 (92%)	11 (8%)	0	100	100
71	SP	127/145 (88%)	119 (94%)	8 (6%)	0	100	100
72	SQ	140/146 (96%)	134 (96%)	6 (4%)	0	100	100
73	SR	129/135 (96%)	114 (88%)	15 (12%)	0	100	100
74	SS	139/152 (91%)	120 (86%)	19 (14%)	0	100	100
75	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
76	SU	99/119 (83%)	92 (93%)	7 (7%)	0	100	100
77	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
78	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
79	SX	139/143 (97%)	130 (94%)	8 (6%)	1 (1%)	18	19
80	SY	121/133 (91%)	117 (97%)	4 (3%)	0	100	100
81	SZ	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
82	Sa	97/115 (84%)	90 (93%)	7 (7%)	0	100	100
83	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
84	Sc	61/69 (88%)	55 (90%)	6 (10%)	0	100	100
85	Sd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
86	Se	53/133 (40%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	Sf	61/156 (39%)	53 (87%)	8 (13%)	0	100	100
88	Sg	304/317 (96%)	274 (90%)	30 (10%)	0	100	100
All	All	12535/14609 (86%)	11892 (95%)	630 (5%)	13 (0%)	49	57

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CZ	22	PRO
56	SA	196	GLU
10	LC	111	TRP
11	LD	59	ASP
79	SX	10	ALA
10	LC	186	SER
33	La	17	HIS
26	LT	129	LYS
62	SG	33	ALA
62	SG	130	PRO
4	CZ	21	LYS
61	SF	80	GLY
16	LI	15	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	
3	CR	356/375 (95%)	346 (97%)	10 (3%)	38	52
4	CZ	25/49 (51%)	23 (92%)	2 (8%)	11	13
8	LA	190/199 (96%)	184 (97%)	6 (3%)	34	47
9	LB	343/349 (98%)	338 (98%)	5 (2%)	57	73
10	LC	299/348 (86%)	290 (97%)	9 (3%)	36	49
11	LD	241/250 (96%)	238 (99%)	3 (1%)	63	78
12	LE	191/252 (76%)	181 (95%)	10 (5%)	21	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	LF	194/215 (90%)	192 (99%)	2 (1%)	68	81
14	LG	188/223 (84%)	179 (95%)	9 (5%)	23	30
15	LH	167/171 (98%)	164 (98%)	3 (2%)	51	68
16	LI	174/181 (96%)	170 (98%)	4 (2%)	44	59
17	LJ	136/149 (91%)	134 (98%)	2 (2%)	57	73
18	LL	164/177 (93%)	158 (96%)	6 (4%)	30	41
19	LM	114/161 (71%)	109 (96%)	5 (4%)	25	34
20	LN	171/172 (99%)	166 (97%)	5 (3%)	37	51
21	LO	170/174 (98%)	165 (97%)	5 (3%)	37	51
22	LP	132/163 (81%)	126 (96%)	6 (4%)	24	33
23	LQ	161/165 (98%)	159 (99%)	2 (1%)	63	78
24	LR	150/175 (86%)	144 (96%)	6 (4%)	28	38
25	LS	156/157 (99%)	155 (99%)	1 (1%)	78	89
26	LT	135/140 (96%)	131 (97%)	4 (3%)	36	49
27	LU	86/115 (75%)	84 (98%)	2 (2%)	44	59
28	LV	99/107 (92%)	97 (98%)	2 (2%)	48	64
29	LW	61/126 (48%)	59 (97%)	2 (3%)	33	45
30	LX	107/133 (80%)	106 (99%)	1 (1%)	70	84
31	LY	123/135 (91%)	120 (98%)	3 (2%)	43	58
32	LZ	117/118 (99%)	115 (98%)	2 (2%)	53	69
33	La	118/121 (98%)	116 (98%)	2 (2%)	53	69
34	Lb	59/126 (47%)	58 (98%)	1 (2%)	53	69
35	Lc	79/97 (81%)	77 (98%)	2 (2%)	42	56
36	Ld	94/110 (86%)	90 (96%)	4 (4%)	26	35
37	Le	113/121 (93%)	108 (96%)	5 (4%)	25	34
38	Lf	87/89 (98%)	86 (99%)	1 (1%)	65	79
39	Lg	93/100 (93%)	90 (97%)	3 (3%)	34	47
40	Lh	108/110 (98%)	107 (99%)	1 (1%)	70	84
41	Li	81/89 (91%)	76 (94%)	5 (6%)	16	20
42	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	75
43	Lk	57/65 (88%)	52 (91%)	5 (9%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	Ll	47/48 (98%)	46 (98%)	1 (2%)	47	63
45	Lm	47/116 (40%)	45 (96%)	2 (4%)	26	35
46	Ln	23/24 (96%)	23 (100%)	0	100	100
47	Lo	93/94 (99%)	90 (97%)	3 (3%)	34	47
48	Lp	71/75 (95%)	70 (99%)	1 (1%)	59	75
49	Lr	107/121 (88%)	102 (95%)	5 (5%)	23	31
50	Ls	180/258 (70%)	174 (97%)	6 (3%)	33	45
51	Lt	132/137 (96%)	125 (95%)	7 (5%)	20	26
52	NA	60/183 (33%)	58 (97%)	2 (3%)	33	45
53	NB	106/136 (78%)	101 (95%)	5 (5%)	23	31
54	NM	353/443 (80%)	350 (99%)	3 (1%)	73	85
56	SA	170/243 (70%)	163 (96%)	7 (4%)	27	37
57	SB	191/231 (83%)	185 (97%)	6 (3%)	35	48
58	SC	175/225 (78%)	170 (97%)	5 (3%)	37	51
59	SD	148/202 (73%)	144 (97%)	4 (3%)	39	53
60	SE	196/225 (87%)	189 (96%)	7 (4%)	31	42
61	SF	142/170 (84%)	136 (96%)	6 (4%)	26	36
62	SG	138/218 (63%)	136 (99%)	2 (1%)	59	75
63	SH	109/174 (63%)	107 (98%)	2 (2%)	51	68
64	SI	149/180 (83%)	149 (100%)	0	100	100
65	SJ	143/168 (85%)	140 (98%)	3 (2%)	47	63
66	SK	65/136 (48%)	61 (94%)	4 (6%)	16	20
67	SL	121/142 (85%)	117 (97%)	4 (3%)	33	45
68	SM	104/108 (96%)	100 (96%)	4 (4%)	29	40
69	SN	123/131 (94%)	122 (99%)	1 (1%)	73	85
70	SO	95/119 (80%)	94 (99%)	1 (1%)	65	79
71	SP	98/130 (75%)	96 (98%)	2 (2%)	48	64
72	SQ	103/121 (85%)	99 (96%)	4 (4%)	28	39
73	SR	84/122 (69%)	80 (95%)	4 (5%)	23	30
74	SS	112/132 (85%)	109 (97%)	3 (3%)	39	53
75	ST	105/115 (91%)	100 (95%)	5 (5%)	23	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	SU	68/107 (64%)	66 (97%)	2 (3%)	37	51
77	SV	62/67 (92%)	60 (97%)	2 (3%)	34	47
78	SW	110/113 (97%)	108 (98%)	2 (2%)	51	68
79	SX	109/115 (95%)	106 (97%)	3 (3%)	38	52
80	SY	86/115 (75%)	81 (94%)	5 (6%)	18	22
81	SZ	56/103 (54%)	53 (95%)	3 (5%)	20	25
82	Sa	83/98 (85%)	79 (95%)	4 (5%)	23	30
83	Sb	65/76 (86%)	63 (97%)	2 (3%)	35	48
84	Sc	51/62 (82%)	44 (86%)	7 (14%)	3	3
85	Sd	44/49 (90%)	43 (98%)	1 (2%)	44	59
86	Se	39/104 (38%)	39 (100%)	0	100	100
87	Sf	56/140 (40%)	55 (98%)	1 (2%)	51	68
88	Sg	201/275 (73%)	183 (91%)	18 (9%)	9	9
All	All	10232/12438 (82%)	9926 (97%)	306 (3%)	37	49

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CR	22	LYS
3	CR	100	ILE
3	CR	175	ASP
3	CR	270	LEU
3	CR	317	VAL
3	CR	328	ILE
3	CR	330	ARG
3	CR	331	TYR
3	CR	398	GLU
3	CR	409	ILE
4	CZ	35	GLU
4	CZ	47	LEU
8	LA	15	VAL
8	LA	74	GLU
8	LA	102	LEU
8	LA	207	VAL
8	LA	208	GLU
8	LA	246	LEU
9	LB	59	GLU

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Mol	Chain	Res	Type
9	LB	73	VAL
9	LB	74	GLU
9	LB	159	VAL
9	LB	231	VAL
10	LC	1	MET
10	LC	16	GLU
10	LC	56	GLU
10	LC	62	THR
10	LC	229	LEU
10	LC	232	VAL
10	LC	272	SER
10	LC	319	LEU
10	LC	334	THR
11	LD	75	VAL
11	LD	115	MET
11	LD	133	GLU
12	LE	51	VAL
12	LE	104	THR
12	LE	106	VAL
12	LE	107	VAL
12	LE	112	MET
12	LE	118	THR
12	LE	128	HIS
12	LE	174	LEU
12	LE	175	VAL
12	LE	184	VAL
13	LF	63	GLN
13	LF	152	GLU
14	LG	33	GLU
14	LG	35	ARG
14	LG	43	GLN
14	LG	55	VAL
14	LG	89	ARG
14	LG	105	GLU
14	LG	201	THR
14	LG	222	ILE
14	LG	241	VAL
15	LH	16	VAL
15	LH	161	ILE
15	LH	187	VAL
16	LI	31	ILE
16	LI	43	VAL

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Mol	Chain	Res	Type
16	LI	123	GLN
16	LI	142	LEU
17	LJ	73	THR
17	LJ	148	THR
18	LL	64	VAL
18	LL	70	VAL
18	LL	106	SER
18	LL	139	SER
18	LL	143	GLU
18	LL	159	ASN
19	LM	25	VAL
19	LM	48	GLN
19	LM	54	CYS
19	LM	70	GLN
19	LM	135	LEU
20	LN	18	VAL
20	LN	89	VAL
20	LN	142	ILE
20	LN	148	THR
20	LN	182	HIS
21	LO	31	ARG
21	LO	36	VAL
21	LO	49	ARG
21	LO	119	VAL
21	LO	189	ILE
22	LP	2	VAL
22	LP	13	LYS
22	LP	20	SER
22	LP	21	ASN
22	LP	79	THR
22	LP	137	ASN
23	LQ	100	VAL
23	LQ	136	THR
24	LR	29	THR
24	LR	31	GLU
24	LR	41	ILE
24	LR	51	ILE
24	LR	113	LYS
24	LR	162	ARG
25	LS	124	ILE
26	LT	43	LYS
26	LT	72	VAL

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Mol	Chain	Res	Type
26	LT	81	LYS
26	LT	149	GLU
27	LU	75	GLU
27	LU	117	ILE
28	LV	22	VAL
28	LV	96	LEU
29	LW	43	LYS
29	LW	63	GLN
30	LX	148	ASP
31	LY	25	ILE
31	LY	69	LYS
31	LY	111	LEU
32	LZ	26	VAL
32	LZ	100	VAL
33	La	32	ARG
33	La	140	VAL
34	Lb	22	LYS
35	Lc	28	VAL
35	Lc	80	GLU
36	Ld	26	THR
36	Ld	46	LEU
36	Ld	55	LYS
36	Ld	63	ARG
37	Le	57	ASN
37	Le	66	THR
37	Le	89	LEU
37	Le	105	SER
37	Le	117	GLN
38	Lf	67	THR
39	Lg	2	VAL
39	Lg	31	VAL
39	Lg	38	VAL
40	Lh	97	LYS
41	Li	17	VAL
41	Li	18	THR
41	Li	46	GLU
41	Li	58	MET
41	Li	81	ILE
42	Lj	31	LYS
43	Lk	12	LEU
43	Lk	23	VAL
43	Lk	46	VAL

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Mol	Chain	Res	Type
43	Lk	47	ILE
43	Lk	57	LYS
44	Ll	46	ARG
45	Lm	99	CYS
45	Lm	127	VAL
47	Lo	2	VAL
47	Lo	68	LEU
47	Lo	69	ARG
48	Lp	30	GLU
49	Lr	44	ILE
49	Lr	60	VAL
49	Lr	78	VAL
49	Lr	80	THR
49	Lr	124	VAL
50	Ls	28	PHE
50	Ls	35	VAL
50	Ls	53	VAL
50	Ls	54	LEU
50	Ls	55	MET
50	Ls	96	THR
51	Lt	32	ILE
51	Lt	46	ILE
51	Lt	58	ILE
51	Lt	74	VAL
51	Lt	105	THR
51	Lt	115	GLN
51	Lt	125	LEU
52	NA	106	ILE
52	NA	111	VAL
53	NB	53	VAL
53	NB	64	MET
53	NB	71	VAL
53	NB	87	THR
53	NB	103	LEU
54	NM	324	MET
54	NM	439	LEU
54	NM	474	LEU
56	SA	50	ASN
56	SA	104	THR
56	SA	112	ILE
56	SA	130	ASP
56	SA	154	LEU

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Mol	Chain	Res	Type
56	SA	157	VAL
56	SA	197	VAL
57	SB	89	GLU
57	SB	97	LEU
57	SB	98	THR
57	SB	106	THR
57	SB	166	LYS
57	SB	199	LYS
58	SC	73	MET
58	SC	137	VAL
58	SC	260	VAL
58	SC	262	THR
58	SC	270	THR
59	SD	46	THR
59	SD	59	LEU
59	SD	64	ARG
59	SD	84	VAL
60	SE	26	VAL
60	SE	46	ILE
60	SE	111	VAL
60	SE	112	HIS
60	SE	123	LEU
60	SE	189	LEU
60	SE	208	VAL
61	SF	20	PHE
61	SF	111	VAL
61	SF	125	SER
61	SF	126	THR
61	SF	171	GLU
61	SF	202	SER
62	SG	26	THR
62	SG	70	HIS
63	SH	76	GLN
63	SH	172	THR
65	SJ	111	GLN
65	SJ	121	LYS
65	SJ	132	GLN
66	SK	40	VAL
66	SK	43	LEU
66	SK	49	MET
66	SK	58	VAL
67	SL	67	SER

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Mol	Chain	Res	Type
67	SL	119	ASP
67	SL	120	VAL
67	SL	146	THR
68	SM	64	LEU
68	SM	89	VAL
68	SM	103	VAL
68	SM	127	TYR
69	SN	134	VAL
70	SO	97	LEU
71	SP	20	VAL
71	SP	37	TYR
72	SQ	34	VAL
72	SQ	46	THR
72	SQ	105	LYS
72	SQ	120	LEU
73	SR	8	THR
73	SR	73	LEU
73	SR	78	ARG
73	SR	91	LEU
74	SS	45	LEU
74	SS	83	PHE
74	SS	90	VAL
75	ST	37	VAL
75	ST	87	VAL
75	ST	93	SER
75	ST	113	VAL
75	ST	121	ARG
76	SU	66	ARG
76	SU	111	GLU
77	SV	32	ILE
77	SV	83	PHE
78	SW	74	VAL
78	SW	115	GLU
79	SX	7	LEU
79	SX	123	VAL
79	SX	125	VAL
80	SY	19	GLN
80	SY	27	VAL
80	SY	32	LYS
80	SY	74	MET
80	SY	78	SER
81	SZ	58	LEU

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Mol	Chain	Res	Type
81	SZ	110	THR
81	SZ	113	THR
82	Sa	2	THR
82	Sa	67	LEU
82	Sa	87	ARG
82	Sa	96	THR
83	Sb	11	SER
83	Sb	55	LEU
84	Sc	18	LEU
84	Sc	32	VAL
84	Sc	35	MET
84	Sc	45	ASN
84	Sc	50	VAL
84	Sc	57	THR
84	Sc	61	SER
85	Sd	5	GLN
87	Sf	132	MET
88	Sg	14	HIS
88	Sg	18	VAL
88	Sg	38	LYS
88	Sg	62	HIS
88	Sg	69	VAL
88	Sg	131	LEU
88	Sg	135	LEU
88	Sg	141	THR
88	Sg	152	SER
88	Sg	165	ILE
88	Sg	166	VAL
88	Sg	174	VAL
88	Sg	184	LEU
88	Sg	186	THR
88	Sg	200	VAL
88	Sg	241	PHE
88	Sg	288	SER
88	Sg	303	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
3	CR	132	HIS
3	CR	185	GLN
3	CR	401	GLN

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Mol	Chain	Res	Type
8	LA	187	HIS
8	LA	205	ASN
9	LB	203	GLN
9	LB	376	HIS
10	LC	38	ASN
10	LC	43	ASN
10	LC	310	HIS
10	LC	329	ASN
11	LD	111	ASN
11	LD	157	ASN
11	LD	202	GLN
12	LE	128	HIS
15	LH	39	ASN
15	LH	98	HIS
15	LH	156	ASN
15	LH	169	ASN
16	LI	123	GLN
16	LI	147	HIS
17	LJ	65	ASN
17	LJ	168	GLN
20	LN	29	GLN
20	LN	32	GLN
20	LN	37	HIS
20	LN	181	HIS
21	LO	167	HIS
21	LO	180	GLN
22	LP	10	ASN
22	LP	21	ASN
22	LP	75	GLN
22	LP	133	HIS
23	LQ	162	HIS
24	LR	34	ASN
24	LR	40	GLN
24	LR	121	HIS
27	LU	116	GLN
31	LY	14	ASN
31	LY	20	ASN
32	LZ	97	ASN
32	LZ	127	ASN
33	La	67	GLN
34	Lb	6	ASN
35	Lc	19	GLN

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Mol	Chain	Res	Type
35	Lc	40	GLN
36	Ld	79	ASN
36	Ld	121	ASN
38	Lf	21	GLN
38	Lf	55	ASN
38	Lf	56	ASN
39	Lg	3	GLN
40	Lh	20	GLN
40	Lh	65	GLN
41	Li	12	ASN
41	Li	20	ASN
42	Lj	13	ASN
44	Ll	4	HIS
44	Ll	17	GLN
49	Lr	36	ASN
49	Lr	85	ASN
50	Ls	159	GLN
50	Ls	195	ASN
51	Lt	103	ASN
52	NA	87	GLN
52	NA	134	GLN
53	NB	7	ASN
53	NB	8	GLN
53	NB	73	HIS
53	NB	86	ASN
53	NB	93	HIS
54	NM	350	HIS
54	NM	359	GLN
57	SB	75	GLN
57	SB	186	ASN
59	SD	145	GLN
59	SD	179	GLN
59	SD	226	GLN
61	SF	36	GLN
61	SF	65	GLN
62	SG	177	GLN
63	SH	126	HIS
63	SH	165	ASN
64	SI	52	ASN
64	SI	168	GLN
65	SJ	132	GLN
65	SJ	154	GLN

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Mol	Chain	Res	Type
67	SL	11	GLN
67	SL	83	GLN
67	SL	106	HIS
67	SL	141	ASN
69	SN	13	GLN
69	SN	62	GLN
70	SO	38	ASN
72	SQ	24	HIS
72	SQ	48	GLN
72	SQ	86	GLN
75	ST	51	ASN
75	ST	83	GLN
78	SW	56	HIS
79	SX	77	ASN
80	SY	63	HIS
80	SY	89	HIS
82	Sa	86	ASN
83	Sb	29	ASN
83	Sb	51	GLN
84	Sc	7	GLN
88	Sg	117	ASN
88	Sg	237	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CM	11/409 (2%)	2 (18%)	0
2	CP	74/75 (98%)	24 (32%)	2 (2%)
5	L5	3633/5070 (71%)	742 (20%)	21 (0%)
55	S2	1704/1869 (91%)	473 (27%)	21 (1%)
6	L7	119/121 (98%)	16 (13%)	0
7	L8	155/157 (98%)	29 (18%)	2 (1%)
All	All	5696/7701 (73%)	1286 (22%)	46 (0%)

All (1286) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	CM	318	C
1	CM	323	U
2	CP	2	G
2	CP	4	U

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Mol	Chain	Res	Type
2	CP	5	C
2	CP	6	G
2	CP	8	U
2	CP	9	G
2	CP	15	G
2	CP	16	G
2	CP	17	G
2	CP	19	U
2	CP	22	G
2	CP	29	G
2	CP	35	G
2	CP	46	U
2	CP	49	C
2	CP	50	G
2	CP	57	A
2	CP	58	A
2	CP	68	A
2	CP	69	G
2	CP	70	C
2	CP	72	C
2	CP	73	C
2	CP	75	A
5	L5	21	G
5	L5	30	C
5	L5	39	A
5	L5	48	G
5	L5	56	A
5	L5	59	A
5	L5	64	A
5	L5	65	A
5	L5	69	A
5	L5	73	A
5	L5	74	G
5	L5	91	G
5	L5	98	A
5	L5	104	G
5	L5	108	A
5	L5	109	G
5	L5	110	C
5	L5	119	G
5	L5	120	A
5	L5	133	C

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Mol	Chain	Res	Type
5	L5	134	G
5	L5	135	G
5	L5	136	C
5	L5	137	G
5	L5	139	G
5	L5	143	C
5	L5	144	G
5	L5	152	U
5	L5	159	C
5	L5	165	A
5	L5	172	C
5	L5	183	C
5	L5	184	U
5	L5	185	C
5	L5	188	G
5	L5	189	G
5	L5	200	U
5	L5	210	C
5	L5	216	C
5	L5	217	C
5	L5	218	A
5	L5	220	C
5	L5	233	U
5	L5	234	G
5	L5	254	G
5	L5	255	C
5	L5	261	G
5	L5	266	C
5	L5	267	G
5	L5	269	G
5	L5	280	G
5	L5	297	U
5	L5	306	A
5	L5	315	G
5	L5	316	U
5	L5	340	C
5	L5	350	C
5	L5	387	G
5	L5	388	A
5	L5	407	A
5	L5	409	G
5	L5	410	A

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Mol	Chain	Res	Type
5	L5	411	G
5	L5	412	G
5	L5	449	C
5	L5	450	G
5	L5	452	A
5	L5	453	G
5	L5	454	U
5	L5	456	C
5	L5	457	G
5	L5	461	G
5	L5	464	G
5	L5	467	U
5	L5	474	C
5	L5	485	C
5	L5	486	C
5	L5	489	C
5	L5	493	G
5	L5	494	U
5	L5	497	G
5	L5	498	C
5	L5	500	G
5	L5	501	C
5	L5	502	C
5	L5	503	C
5	L5	504	G
5	L5	505	G
5	L5	509	A
5	L5	510	U
5	L5	512	U
5	L5	513	U
5	L5	514	U
5	L5	515	C
5	L5	517	C
5	L5	518	G
5	L5	643	C
5	L5	644	G
5	L5	646	G
5	L5	654	C
5	L5	655	C
5	L5	657	C
5	L5	658	C
5	L5	660	A

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Mol	Chain	Res	Type
5	L5	666	G
5	L5	667	A
5	L5	668	C
5	L5	669	C
5	L5	673	C
5	L5	674	G
5	L5	675	C
5	L5	676	C
5	L5	686	A
5	L5	687	U
5	L5	688	U
5	L5	692	A
5	L5	696	C
5	L5	697	G
5	L5	703	G
5	L5	704	C
5	L5	706	C
5	L5	708	G
5	L5	729	G
5	L5	730	G
5	L5	731	G
5	L5	738	C
5	L5	739	G
5	L5	740	G
5	L5	742	G
5	L5	746	A
5	L5	758	G
5	L5	760	G
5	L5	904	C
5	L5	905	C
5	L5	912	G
5	L5	913	U
5	L5	914	U
5	L5	915	A
5	L5	916	C
5	L5	917	A
5	L5	918	G
5	L5	923	C
5	L5	924	C
5	L5	926	G
5	L5	929	A
5	L5	932	A

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Mol	Chain	Res	Type
5	L5	933	G
5	L5	945	U
5	L5	959	G
5	L5	960	A
5	L5	961	G
5	L5	962	C
5	L5	965	G
5	L5	966	A
5	L5	967	C
5	L5	969	C
5	L5	970	G
5	L5	972	C
5	L5	977	C
5	L5	984	C
5	L5	988	C
5	L5	989	U
5	L5	990	C
5	L5	991	C
5	L5	992	C
5	L5	993	G
5	L5	1069	G
5	L5	1070	G
5	L5	1075	G
5	L5	1083	U
5	L5	1168	G
5	L5	1173	G
5	L5	1178	G
5	L5	1179	U
5	L5	1180	C
5	L5	1181	C
5	L5	1182	C
5	L5	1183	C
5	L5	1184	A
5	L5	1187	G
5	L5	1193	C
5	L5	1196	G
5	L5	1202	C
5	L5	1203	G
5	L5	1205	G
5	L5	1209	U
5	L5	1211	G
5	L5	1214	C

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Mol	Chain	Res	Type
5	L5	1215	C
5	L5	1218	G
5	L5	1235	G
5	L5	1238	A
5	L5	1241	C
5	L5	1253	G
5	L5	1258	G
5	L5	1259	G
5	L5	1260	G
5	L5	1266	G
5	L5	1269	G
5	L5	1270	A
5	L5	1271	G
5	L5	1272	C
5	L5	1273	G
5	L5	1274	A
5	L5	1275	G
5	L5	1277	G
5	L5	1280	C
5	L5	1284	G
5	L5	1285	U
5	L5	1287	G
5	L5	1293	G
5	L5	1294	A
5	L5	1295	C
5	L5	1296	G
5	L5	1301	C
5	L5	1303	A
5	L5	1304	C
5	L5	1312	A
5	L5	1324	A
5	L5	1326	A
5	L5	1337	A
5	L5	1344	C
5	L5	1354	A
5	L5	1358	G
5	L5	1359	G
5	L5	1365	C
5	L5	1366	G
5	L5	1379	C
5	L5	1387	A
5	L5	1393	G

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Mol	Chain	Res	Type
5	L5	1394	G
5	L5	1397	A
5	L5	1398	A
5	L5	1404	G
5	L5	1405	C
5	L5	1408	G
5	L5	1410	U
5	L5	1411	C
5	L5	1420	A
5	L5	1435	G
5	L5	1437	C
5	L5	1439	C
5	L5	1441	C
5	L5	1442	C
5	L5	1443	A
5	L5	1444	G
5	L5	1447	C
5	L5	1454	G
5	L5	1457	G
5	L5	1465	G
5	L5	1480	C
5	L5	1483	C
5	L5	1493	G
5	L5	1494	U
5	L5	1497	A
5	L5	1498	G
5	L5	1502	G
5	L5	1514	U
5	L5	1534	A
5	L5	1547	A
5	L5	1552	G
5	L5	1564	A
5	L5	1566	C
5	L5	1578	U
5	L5	1591	U
5	L5	1596	U
5	L5	1624	G
5	L5	1625	G
5	L5	1631	A
5	L5	1633	G
5	L5	1634	A
5	L5	1638	A

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Mol	Chain	Res	Type
5	L5	1640	C
5	L5	1641	G
5	L5	1642	A
5	L5	1654	G
5	L5	1656	U
5	L5	1661	C
5	L5	1663	C
5	L5	1676	C
5	L5	1677	U
5	L5	1684	A
5	L5	1685	G
5	L5	1691	G
5	L5	1697	G
5	L5	1699	A
5	L5	1700	G
5	L5	1705	G
5	L5	1707	C
5	L5	1734	G
5	L5	1740	C
5	L5	1742	A
5	L5	1750	G
5	L5	1756	U
5	L5	1758	G
5	L5	1760	G
5	L5	1765	A
5	L5	1767	A
5	L5	1787	A
5	L5	1797	G
5	L5	1804	A
5	L5	1810	G
5	L5	1820	C
5	L5	1821	G
5	L5	1822	U
5	L5	1834	U
5	L5	1836	G
5	L5	1837	A
5	L5	1842	G
5	L5	1855	G
5	L5	1869	G
5	L5	1891	A
5	L5	1897	A
5	L5	1912	G

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Mol	Chain	Res	Type
5	L5	1918	U
5	L5	1919	G
5	L5	1920	C
5	L5	1921	C
5	L5	1922	G
5	L5	1931	C
5	L5	1932	A
5	L5	1936	C
5	L5	1940	G
5	L5	1948	G
5	L5	1961	G
5	L5	1962	A
5	L5	1965	G
5	L5	1976	G
5	L5	1980	U
5	L5	1981	G
5	L5	1983	A
5	L5	1984	A
5	L5	1985	G
5	L5	1986	U
5	L5	1987	C
5	L5	1991	A
5	L5	1992	U
5	L5	1997	U
5	L5	2001	G
5	L5	2002	A
5	L5	2004	U
5	L5	2007	G
5	L5	2016	C
5	L5	2017	A
5	L5	2018	C
5	L5	2024	G
5	L5	2025	A
5	L5	2026	A
5	L5	2046	G
5	L5	2048	U
5	L5	2055	G
5	L5	2056	G
5	L5	2069	A
5	L5	2084	C
5	L5	2085	G
5	L5	2089	G

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Mol	Chain	Res	Type
5	L5	2092	G
5	L5	2095	A
5	L5	2098	G
5	L5	2101	C
5	L5	2103	G
5	L5	2106	G
5	L5	2107	C
5	L5	2108	G
5	L5	2116	C
5	L5	2117	G
5	L5	2118	G
5	L5	2119	C
5	L5	2120	G
5	L5	2121	C
5	L5	2122	G
5	L5	2123	C
5	L5	2250	C
5	L5	2252	G
5	L5	2253	A
5	L5	2254	G
5	L5	2255	C
5	L5	2256	C
5	L5	2258	C
5	L5	2269	C
5	L5	2277	C
5	L5	2289	C
5	L5	2300	A
5	L5	2301	G
5	L5	2313	A
5	L5	2316	G
5	L5	2332	A
5	L5	2333	G
5	L5	2348	G
5	L5	2351	C
5	L5	2360	A
5	L5	2395	A
5	L5	2397	G
5	L5	2417	A
5	L5	2421	G
5	L5	2422	C
5	L5	2424	G
5	L5	2425	U

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Mol	Chain	Res	Type
5	L5	2441	C
5	L5	2450	G
5	L5	2453	A
5	L5	2464	C
5	L5	2465	C
5	L5	2475	G
5	L5	2483	G
5	L5	2484	A
5	L5	2487	G
5	L5	2489	C
5	L5	2490	U
5	L5	2491	C
5	L5	2493	G
5	L5	2503	G
5	L5	2504	C
5	L5	2505	C
5	L5	2506	G
5	L5	2513	A
5	L5	2519	U
5	L5	2520	C
5	L5	2537	A
5	L5	2544	G
5	L5	2545	U
5	L5	2546	G
5	L5	2547	G
5	L5	2554	U
5	L5	2555	G
5	L5	2573	A
5	L5	2583	C
5	L5	2587	A
5	L5	2589	C
5	L5	2601	A
5	L5	2611	A
5	L5	2618	G
5	L5	2627	C
5	L5	2638	G
5	L5	2653	C
5	L5	2662	G
5	L5	2669	C
5	L5	2676	A
5	L5	2687	U
5	L5	2694	G

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Mol	Chain	Res	Type
5	L5	2695	A
5	L5	2696	A
5	L5	2703	G
5	L5	2708	U
5	L5	2710	C
5	L5	2711	G
5	L5	2712	G
5	L5	2721	G
5	L5	2724	G
5	L5	2726	G
5	L5	2739	C
5	L5	2742	G
5	L5	2743	A
5	L5	2754	G
5	L5	2761	U
5	L5	2763	U
5	L5	2764	A
5	L5	2769	U
5	L5	2770	C
5	L5	2788	U
5	L5	2789	A
5	L5	2790	U
5	L5	2814	C
5	L5	2815	A
5	L5	2826	U
5	L5	2827	G
5	L5	2838	G
5	L5	2842	G
5	L5	2848	G
5	L5	2855	G
5	L5	2856	C
5	L5	2858	A
5	L5	2867	C
5	L5	2877	G
5	L5	2890	C
5	L5	2892	C
5	L5	2894	A
5	L5	2896	G
5	L5	2897	G
5	L5	2900	U
5	L5	2902	G
5	L5	2903	G

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Mol	Chain	Res	Type
5	L5	2905	C
5	L5	2906	G
5	L5	2907	G
5	L5	2908	U
5	L5	3585	G
5	L5	3588	C
5	L5	3591	C
5	L5	3593	C
5	L5	3594	C
5	L5	3595	U
5	L5	3596	A
5	L5	3597	G
5	L5	3599	A
5	L5	3604	A
5	L5	3605	C
5	L5	3615	G
5	L5	3618	C
5	L5	3626	G
5	L5	3630	A
5	L5	3635	A
5	L5	3644	U
5	L5	3646	A
5	L5	3662	A
5	L5	3664	G
5	L5	3673	C
5	L5	3674	G
5	L5	3685	C
5	L5	3711	A
5	L5	3713	U
5	L5	3727	A
5	L5	3735	G
5	L5	3736	A
5	L5	3748	A
5	L5	3750	G
5	L5	3753	G
5	L5	3761	C
5	L5	3771	C
5	L5	3775	A
5	L5	3776	G
5	L5	3777	G
5	L5	3784	A
5	L5	3785	A

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Mol	Chain	Res	Type
5	L5	3786	U
5	L5	3810	C
5	L5	3814	U
5	L5	3817	A
5	L5	3818	U
5	L5	3819	G
5	L5	3823	G
5	L5	3838	U
5	L5	3839	G
5	L5	3840	U
5	L5	3841	C
5	L5	3867	A
5	L5	3876	A
5	L5	3877	A
5	L5	3878	C
5	L5	3879	G
5	L5	3885	G
5	L5	3897	G
5	L5	3899	G
5	L5	3901	A
5	L5	3905	A
5	L5	3906	A
5	L5	3907	G
5	L5	3908	A
5	L5	3915	U
5	L5	3926	C
5	L5	3930	U
5	L5	3939	G
5	L5	3942	A
5	L5	3943	A
5	L5	3944	G
5	L5	3947	A
5	L5	3949	A
5	L5	4064	C
5	L5	4065	G
5	L5	4076	G
5	L5	4084	G
5	L5	4099	G
5	L5	4102	C
5	L5	4104	G
5	L5	4107	G
5	L5	4113	U

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Mol	Chain	Res	Type
5	L5	4114	C
5	L5	4115	G
5	L5	4116	C
5	L5	4119	C
5	L5	4122	G
5	L5	4128	A
5	L5	4131	G
5	L5	4133	C
5	L5	4135	G
5	L5	4137	C
5	L5	4138	C
5	L5	4140	C
5	L5	4141	G
5	L5	4142	C
5	L5	4143	G
5	L5	4145	C
5	L5	4150	G
5	L5	4154	G
5	L5	4155	C
5	L5	4162	C
5	L5	4163	U
5	L5	4170	A
5	L5	4183	G
5	L5	4184	G
5	L5	4191	G
5	L5	4203	A
5	L5	4222	G
5	L5	4228	G
5	L5	4229	U
5	L5	4233	A
5	L5	4249	G
5	L5	4251	A
5	L5	4254	G
5	L5	4257	A
5	L5	4258	C
5	L5	4268	A
5	L5	4273	A
5	L5	4281	A
5	L5	4290	U
5	L5	4291	G
5	L5	4296	U
5	L5	4304	A

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Mol	Chain	Res	Type
5	L5	4305	G
5	L5	4314	C
5	L5	4319	C
5	L5	4329	G
5	L5	4330	G
5	L5	4332	C
5	L5	4349	C
5	L5	4364	G
5	L5	4373	G
5	L5	4376	A
5	L5	4377	G
5	L5	4378	A
5	L5	4387	C
5	L5	4391	G
5	L5	4394	A
5	L5	4422	A
5	L5	4438	U
5	L5	4444	C
5	L5	4448	G
5	L5	4449	A
5	L5	4452	U
5	L5	4453	C
5	L5	4464	A
5	L5	4466	C
5	L5	4475	G
5	L5	4500	U
5	L5	4512	U
5	L5	4513	A
5	L5	4515	G
5	L5	4519	C
5	L5	4524	G
5	L5	4548	A
5	L5	4549	G
5	L5	4554	G
5	L5	4560	C
5	L5	4567	G
5	L5	4573	G
5	L5	4575	G
5	L5	4590	A
5	L5	4600	G
5	L5	4601	U
5	L5	4608	G

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Mol	Chain	Res	Type
5	L5	4617	G
5	L5	4633	G
5	L5	4634	U
5	L5	4636	U
5	L5	4637	G
5	L5	4638	U
5	L5	4639	G
5	L5	4652	G
5	L5	4656	A
5	L5	4670	C
5	L5	4672	A
5	L5	4677	U
5	L5	4687	A
5	L5	4700	A
5	L5	4708	A
5	L5	4709	U
5	L5	4719	G
5	L5	4720	C
5	L5	4732	G
5	L5	4733	C
5	L5	4734	A
5	L5	4740	G
5	L5	4741	C
5	L5	4742	G
5	L5	4745	G
5	L5	4754	G
5	L5	4757	C
5	L5	4759	C
5	L5	4761	G
5	L5	4765	G
5	L5	4771	C
5	L5	4772	C
5	L5	4773	C
5	L5	4775	C
5	L5	4860	G
5	L5	4868	G
5	L5	4870	G
5	L5	4871	C
5	L5	4875	G
5	L5	4881	U
5	L5	4882	U
5	L5	4883	C

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Mol	Chain	Res	Type
5	L5	4889	G
5	L5	4894	A
5	L5	4895	C
5	L5	4896	G
5	L5	4900	C
5	L5	4901	G
5	L5	4910	G
5	L5	4912	G
5	L5	4914	C
5	L5	4925	U
5	L5	4927	G
5	L5	4928	C
5	L5	4931	G
5	L5	4934	A
5	L5	4937	C
5	L5	4940	C
5	L5	4941	G
5	L5	4943	A
5	L5	4955	A
5	L5	4960	G
5	L5	4963	G
5	L5	4966	A
5	L5	4976	U
5	L5	4979	A
5	L5	4988	U
5	L5	4989	U
5	L5	4990	C
5	L5	4991	U
5	L5	5007	A
5	L5	5009	G
5	L5	5014	A
5	L5	5017	G
5	L5	5022	U
5	L5	5023	C
5	L5	5024	C
5	L5	5025	C
5	L5	5026	U
5	L5	5028	G
5	L5	5029	C
5	L5	5030	U
5	L5	5031	G
5	L5	5034	A

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Mol	Chain	Res	Type
5	L5	5041	G
5	L5	5049	G
5	L5	5050	C
5	L5	5054	C
5	L5	5058	A
5	L5	5061	A
5	L5	5062	G
5	L5	5069	U
6	L7	20	U
6	L7	22	A
6	L7	23	A
6	L7	27	G
6	L7	33	U
6	L7	53	U
6	L7	54	A
6	L7	63	C
6	L7	64	G
6	L7	97	G
6	L7	100	A
6	L7	102	U
6	L7	110	G
6	L7	111	C
6	L7	117	G
6	L7	120	U
7	L8	16	G
7	L8	23	C
7	L8	34	U
7	L8	35	C
7	L8	48	A
7	L8	52	A
7	L8	59	A
7	L8	63	U
7	L8	77	A
7	L8	82	A
7	L8	83	C
7	L8	84	A
7	L8	86	U
7	L8	87	G
7	L8	88	A
7	L8	94	G
7	L8	103	A
7	L8	105	C

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Mol	Chain	Res	Type
7	L8	110	U
7	L8	111	U
7	L8	112	G
7	L8	114	G
7	L8	124	U
7	L8	125	C
7	L8	126	C
7	L8	127	U
7	L8	150	C
7	L8	151	G
7	L8	153	C
55	S2	7	G
55	S2	17	C
55	S2	33	G
55	S2	41	G
55	S2	44	U
55	S2	46	A
55	S2	56	G
55	S2	58	C
55	S2	59	U
55	S2	66	G
55	S2	67	C
55	S2	68	A
55	S2	71	G
55	S2	72	C
55	S2	73	C
55	S2	75	G
55	S2	76	U
55	S2	80	G
55	S2	84	A
55	S2	85	A
55	S2	86	C
55	S2	96	C
55	S2	99	A
55	S2	101	U
55	S2	103	A
55	S2	113	G
55	S2	114	G
55	S2	121	U
55	S2	126	G
55	S2	127	C
55	S2	128	U

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Mol	Chain	Res	Type
55	S2	130	G
55	S2	143	U
55	S2	144	U
55	S2	145	G
55	S2	149	A
55	S2	151	C
55	S2	155	G
55	S2	160	U
55	S2	161	U
55	S2	162	C
55	S2	163	U
55	S2	167	G
55	S2	168	C
55	S2	170	A
55	S2	182	C
55	S2	193	C
55	S2	198	U
55	S2	202	G
55	S2	207	G
55	S2	210	U
55	S2	211	G
55	S2	214	U
55	S2	219	U
55	S2	290	U
55	S2	293	C
55	S2	295	C
55	S2	306	C
55	S2	308	G
55	S2	309	G
55	S2	310	C
55	S2	311	C
55	S2	312	G
55	S2	313	A
55	S2	314	U
55	S2	319	C
55	S2	322	C
55	S2	323	C
55	S2	324	C
55	S2	325	C
55	S2	326	C
55	S2	328	U
55	S2	329	G

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Mol	Chain	Res	Type
55	S2	335	G
55	S2	339	A
55	S2	340	C
55	S2	347	G
55	S2	351	G
55	S2	360	A
55	S2	362	C
55	S2	364	A
55	S2	368	U
55	S2	370	G
55	S2	380	G
55	S2	381	C
55	S2	385	G
55	S2	386	C
55	S2	398	A
55	S2	400	C
55	S2	409	C
55	S2	413	G
55	S2	438	G
55	S2	448	A
55	S2	449	A
55	S2	450	C
55	S2	452	G
55	S2	464	A
55	S2	465	A
55	S2	466	G
55	S2	471	G
55	S2	472	C
55	S2	473	A
55	S2	474	G
55	S2	482	G
55	S2	487	U
55	S2	488	U
55	S2	489	A
55	S2	492	C
55	S2	493	A
55	S2	496	C
55	S2	500	A
55	S2	502	C
55	S2	503	C
55	S2	506	G
55	S2	516	A

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Mol	Chain	Res	Type
55	S2	525	A
55	S2	531	A
55	S2	532	C
55	S2	536	A
55	S2	537	C
55	S2	539	C
55	S2	540	U
55	S2	541	U
55	S2	542	U
55	S2	543	C
55	S2	544	G
55	S2	545	A
55	S2	547	G
55	S2	549	C
55	S2	551	U
55	S2	554	A
55	S2	555	A
55	S2	556	U
55	S2	559	G
55	S2	560	A
55	S2	561	A
55	S2	563	G
55	S2	567	C
55	S2	575	A
55	S2	576	A
55	S2	581	U
55	S2	583	A
55	S2	587	A
55	S2	589	G
55	S2	590	A
55	S2	591	U
55	S2	593	C
55	S2	595	U
55	S2	596	U
55	S2	604	A
55	S2	605	A
55	S2	606	G
55	S2	607	U
55	S2	608	C
55	S2	612	U
55	S2	613	G
55	S2	614	C

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Mol	Chain	Res	Type
55	S2	617	G
55	S2	628	A
55	S2	631	U
55	S2	632	C
55	S2	643	A
55	S2	650	A
55	S2	651	U
55	S2	652	U
55	S2	655	A
55	S2	660	C
55	S2	668	A
55	S2	669	A
55	S2	671	A
55	S2	672	A
55	S2	673	G
55	S2	688	U
55	S2	689	U
55	S2	690	G
55	S2	692	G
55	S2	693	A
55	S2	694	G
55	S2	696	G
55	S2	697	G
55	S2	732	U
55	S2	733	C
55	S2	734	C
55	S2	735	C
55	S2	736	C
55	S2	738	C
55	S2	739	C
55	S2	746	C
55	S2	747	U
55	S2	748	C
55	S2	749	U
55	S2	751	G
55	S2	752	G
55	S2	753	C
55	S2	790	C
55	S2	791	C
55	S2	795	A
55	S2	796	G
55	S2	797	C

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Mol	Chain	Res	Type
55	S2	799	U
55	S2	801	U
55	S2	807	G
55	S2	808	A
55	S2	809	A
55	S2	810	A
55	S2	811	A
55	S2	812	A
55	S2	813	A
55	S2	818	A
55	S2	821	G
55	S2	827	A
55	S2	830	A
55	S2	834	C
55	S2	835	C
55	S2	836	G
55	S2	837	A
55	S2	838	G
55	S2	839	C
55	S2	840	C
55	S2	841	G
55	S2	842	C
55	S2	847	A
55	S2	856	C
55	S2	860	G
55	S2	861	A
55	S2	868	G
55	S2	869	A
55	S2	870	A
55	S2	872	A
55	S2	873	G
55	S2	874	G
55	S2	878	G
55	S2	880	G
55	S2	883	U
55	S2	888	U
55	S2	889	U
55	S2	890	U
55	S2	891	G
55	S2	892	U
55	S2	893	U
55	S2	894	G

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Mol	Chain	Res	Type
55	S2	895	G
55	S2	896	U
55	S2	898	U
55	S2	900	C
55	S2	901	G
55	S2	903	A
55	S2	904	A
55	S2	905	C
55	S2	909	G
55	S2	912	C
55	S2	913	A
55	S2	917	U
55	S2	919	A
55	S2	920	A
55	S2	922	A
55	S2	924	G
55	S2	926	A
55	S2	930	C
55	S2	933	G
55	S2	934	G
55	S2	958	G
55	S2	963	A
55	S2	970	G
55	S2	971	G
55	S2	972	A
55	S2	990	A
55	S2	992	A
55	S2	997	A
55	S2	1001	A
55	S2	1017	U
55	S2	1018	U
55	S2	1019	C
55	S2	1021	U
55	S2	1023	A
55	S2	1027	A
55	S2	1055	A
55	S2	1060	A
55	S2	1061	U
55	S2	1062	A
55	S2	1078	C
55	S2	1083	A
55	S2	1084	A

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Mol	Chain	Res	Type
55	S2	1085	C
55	S2	1090	C
55	S2	1096	G
55	S2	1099	G
55	S2	1100	A
55	S2	1101	U
55	S2	1102	G
55	S2	1105	G
55	S2	1108	G
55	S2	1112	U
55	S2	1114	U
55	S2	1116	C
55	S2	1120	U
55	S2	1121	G
55	S2	1126	G
55	S2	1131	G
55	S2	1133	A
55	S2	1140	G
55	S2	1142	G
55	S2	1143	A
55	S2	1144	A
55	S2	1145	A
55	S2	1146	C
55	S2	1147	C
55	S2	1149	A
55	S2	1153	C
55	S2	1154	U
55	S2	1155	U
55	S2	1157	G
55	S2	1168	G
55	S2	1181	A
55	S2	1183	A
55	S2	1195	A
55	S2	1207	G
55	S2	1212	G
55	S2	1215	C
55	S2	1217	A
55	S2	1221	G
55	S2	1224	G
55	S2	1242	U
55	S2	1243	U
55	S2	1251	A

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Mol	Chain	Res	Type
55	S2	1253	A
55	S2	1256	G
55	S2	1257	G
55	S2	1259	A
55	S2	1260	A
55	S2	1268	C
55	S2	1271	C
55	S2	1272	C
55	S2	1273	C
55	S2	1274	G
55	S2	1275	G
55	S2	1276	A
55	S2	1281	G
55	S2	1282	A
55	S2	1285	G
55	S2	1286	G
55	S2	1289	U
55	S2	1297	U
55	S2	1298	G
55	S2	1299	A
55	S2	1300	U
55	S2	1301	A
55	S2	1302	G
55	S2	1303	C
55	S2	1308	U
55	S2	1313	A
55	S2	1314	U
55	S2	1320	G
55	S2	1321	G
55	S2	1326	U
55	S2	1332	A
55	S2	1342	U
55	S2	1348	G
55	S2	1371	U
55	S2	1372	U
55	S2	1378	A
55	S2	1382	A
55	S2	1384	C
55	S2	1396	A
55	S2	1397	U
55	S2	1402	A
55	S2	1415	C

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Mol	Chain	Res	Type
55	S2	1419	C
55	S2	1420	G
55	S2	1421	A
55	S2	1422	G
55	S2	1423	C
55	S2	1429	G
55	S2	1438	A
55	S2	1449	G
55	S2	1450	G
55	S2	1454	A
55	S2	1462	U
55	S2	1463	U
55	S2	1475	G
55	S2	1477	U
55	S2	1487	A
55	S2	1489	A
55	S2	1490	G
55	S2	1494	U
55	S2	1497	G
55	S2	1498	A
55	S2	1506	A
55	S2	1508	A
55	S2	1510	G
55	S2	1519	U
55	S2	1520	G
55	S2	1521	C
55	S2	1522	A
55	S2	1526	G
55	S2	1527	C
55	S2	1533	A
55	S2	1535	U
55	S2	1546	G
55	S2	1547	C
55	S2	1548	G
55	S2	1553	C
55	S2	1555	U
55	S2	1556	A
55	S2	1563	G
55	S2	1567	G
55	S2	1569	A
55	S2	1570	G
55	S2	1579	A

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Mol	Chain	Res	Type
55	S2	1580	A
55	S2	1585	U
55	S2	1586	U
55	S2	1587	G
55	S2	1588	A
55	S2	1589	A
55	S2	1595	U
55	S2	1597	C
55	S2	1598	G
55	S2	1599	U
55	S2	1601	A
55	S2	1602	U
55	S2	1613	G
55	S2	1614	A
55	S2	1621	U
55	S2	1623	A
55	S2	1624	U
55	S2	1639	G
55	S2	1644	C
55	S2	1648	G
55	S2	1654	G
55	S2	1661	A
55	S2	1663	A
55	S2	1664	A
55	S2	1665	G
55	S2	1671	G
55	S2	1678	A
55	S2	1680	G
55	S2	1694	U
55	S2	1695	A
55	S2	1698	C
55	S2	1719	A
55	S2	1721	U
55	S2	1722	G
55	S2	1743	G
55	S2	1744	G
55	S2	1745	A
55	S2	1748	G
55	S2	1753	C
55	S2	1754	G
55	S2	1755	C
55	S2	1773	C

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Mol	Chain	Res	Type
55	S2	1781	A
55	S2	1782	G
55	S2	1783	C
55	S2	1784	G
55	S2	1786	U
55	S2	1813	A
55	S2	1819	A
55	S2	1824	A
55	S2	1825	A
55	S2	1829	G
55	S2	1835	A
55	S2	1838	U
55	S2	1849	G
55	S2	1850	A
55	S2	1851	A
55	S2	1852	C
55	S2	1860	A
55	S2	1861	G
55	S2	1862	G
55	S2	1863	A
55	S2	1865	C
55	S2	1868	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	CP	3	C
2	CP	21	U
5	L5	42	A
5	L5	406	C
5	L5	504	G
5	L5	914	U
5	L5	955	G
5	L5	1082	C
5	L5	1633	G
5	L5	2117	G
5	L5	2416	G
5	L5	2675	G
5	L5	2760	G
5	L5	2788	U
5	L5	3614	G
5	L5	3673	C

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Continued from previous page...

Mol	Chain	Res	Type
5	L5	3784	A
5	L5	3876	A
5	L5	4305	G
5	L5	4600	G
5	L5	4633	G
5	L5	4699	U
5	L5	4913	G
7	L8	86	U
7	L8	87	G
55	S2	85	A
55	S2	113	G
55	S2	144	U
55	S2	213	G
55	S2	465	A
55	S2	604	A
55	S2	688	U
55	S2	912	C
55	S2	971	G
55	S2	1060	A
55	S2	1120	U
55	S2	1145	A
55	S2	1165	G
55	S2	1273	C
55	S2	1285	G
55	S2	1519	U
55	S2	1585	U
55	S2	1597	C
55	S2	1601	A
55	S2	1664	A
55	S2	1860	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
3	LYO	CR	63	3	7,9,10	0.80	0	7,10,12	1.15	1 (14%)

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
3	LYO	CR	63	3	-	3/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CR	63	LYO	CB-CG-CD	-2.17	107.82	112.42

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CR	63	LYO	N-CA-CB-CG
3	CR	63	LYO	C-CA-CB-CG
3	CR	63	LYO	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 199 ligands modelled in this entry, 199 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

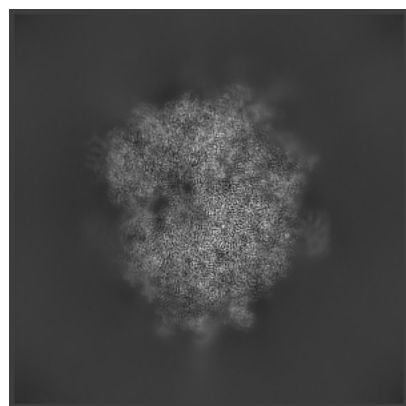
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52581. These allow visual inspection of the internal detail of the map and identification of artifacts.

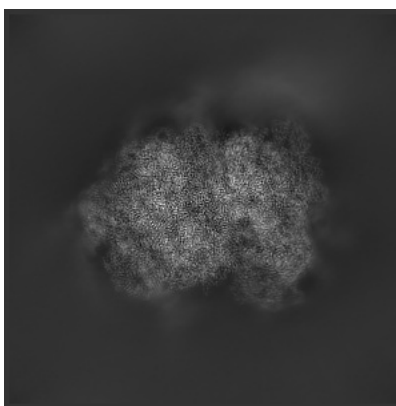
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

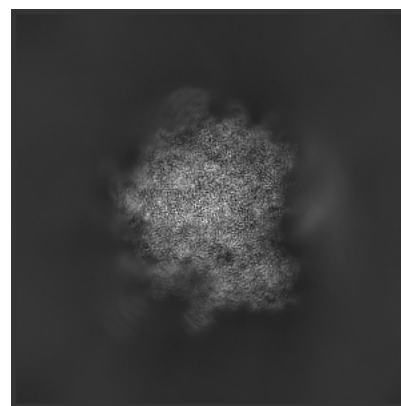
6.1.1 Primary map



X

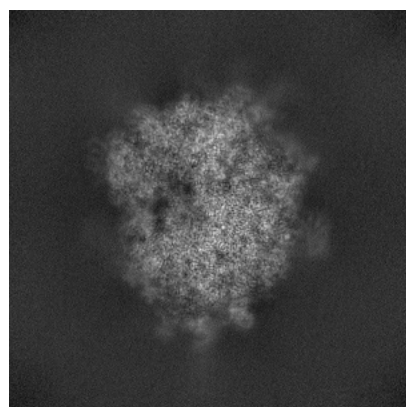


Y

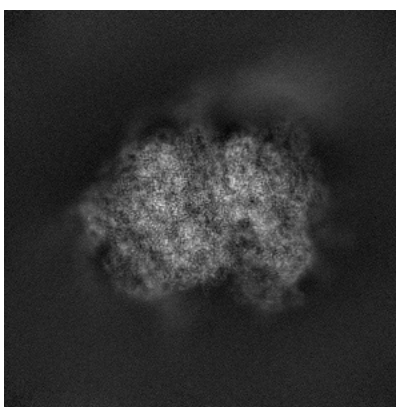


Z

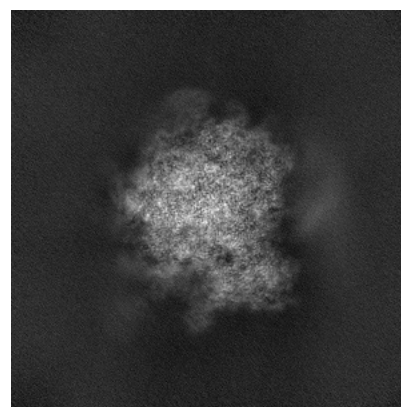
6.1.2 Raw map



X



Y

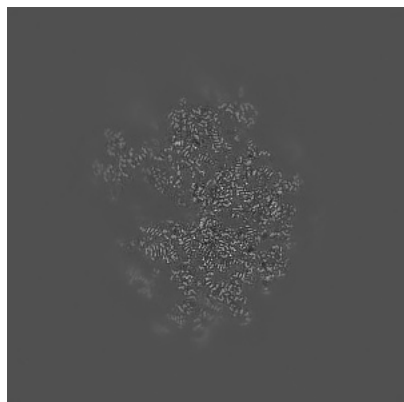


Z

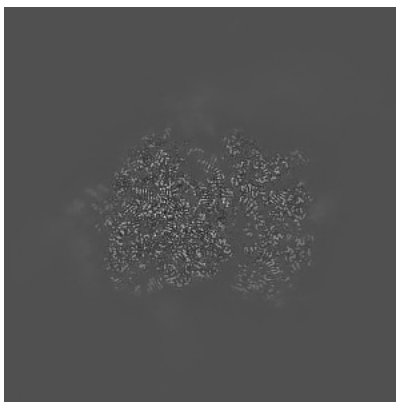
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

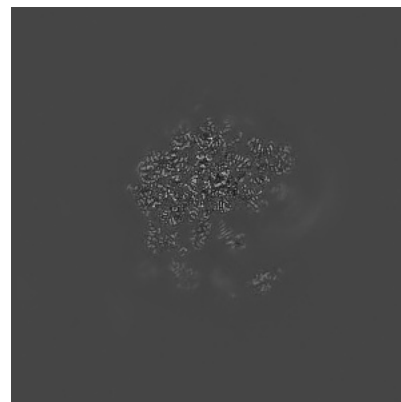
6.2.1 Primary map



X Index: 320

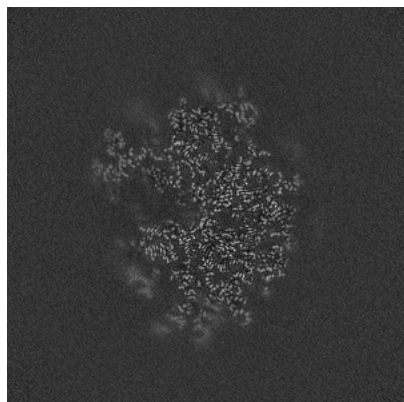


Y Index: 320

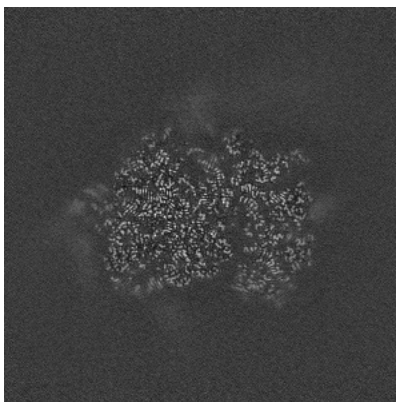


Z Index: 320

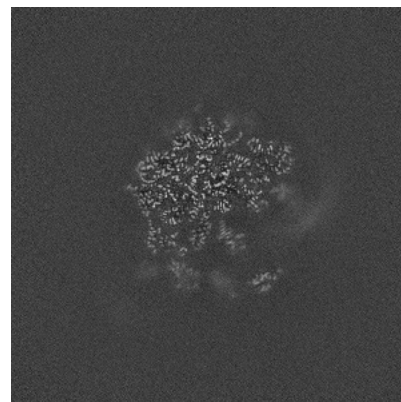
6.2.2 Raw map



X Index: 320



Y Index: 320

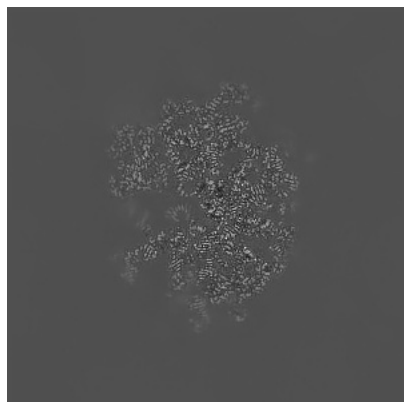


Z Index: 320

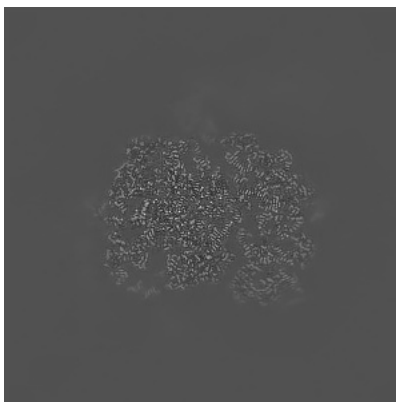
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

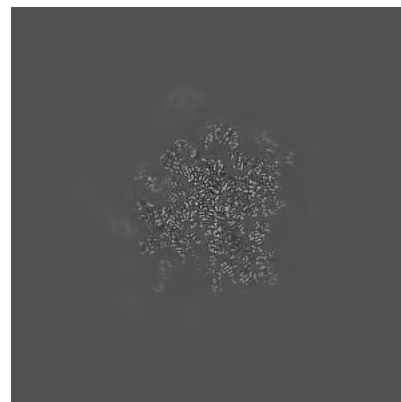
6.3.1 Primary map



X Index: 342

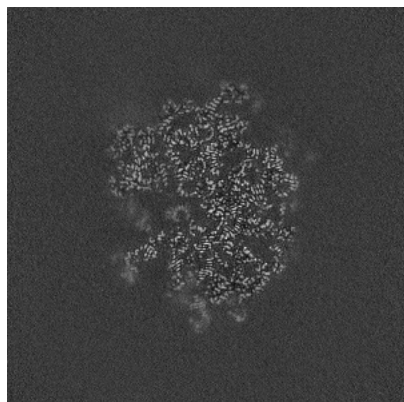


Y Index: 333

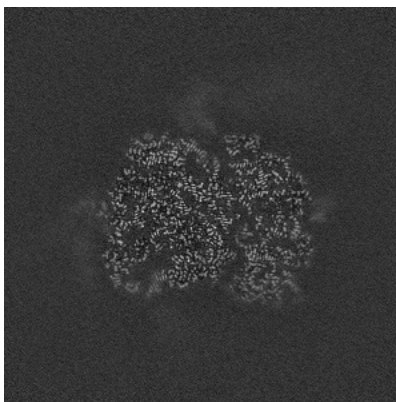


Z Index: 256

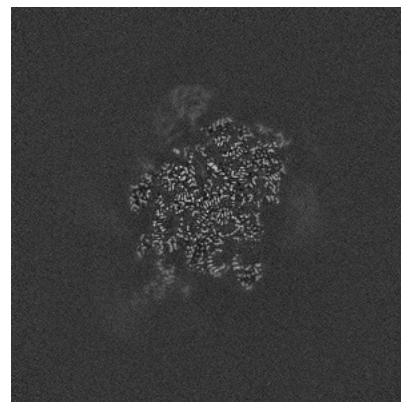
6.3.2 Raw map



X Index: 342



Y Index: 327

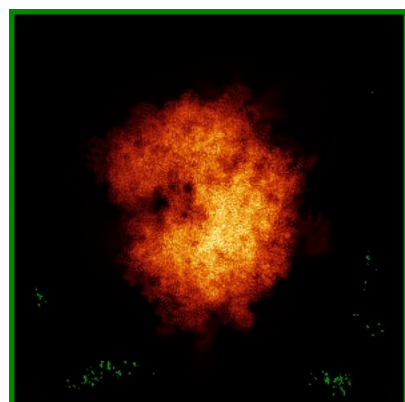


Z Index: 284

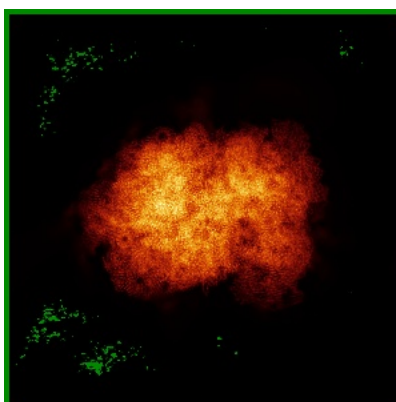
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

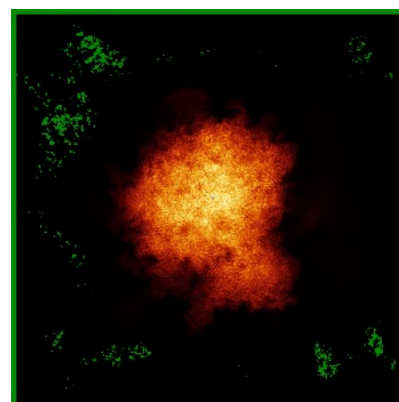
6.4.1 Primary map



X

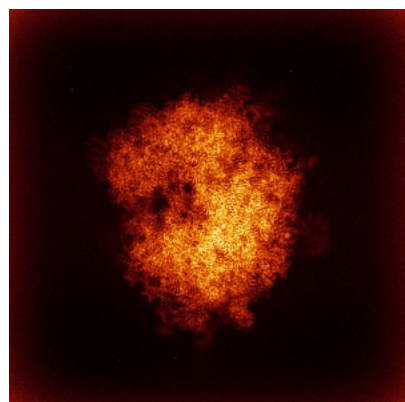


Y

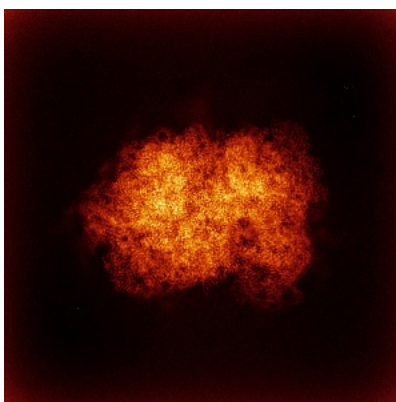


Z

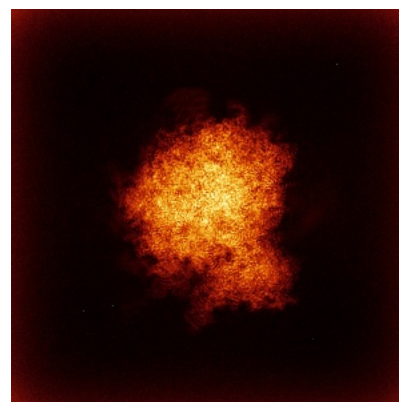
6.4.2 Raw map



X



Y

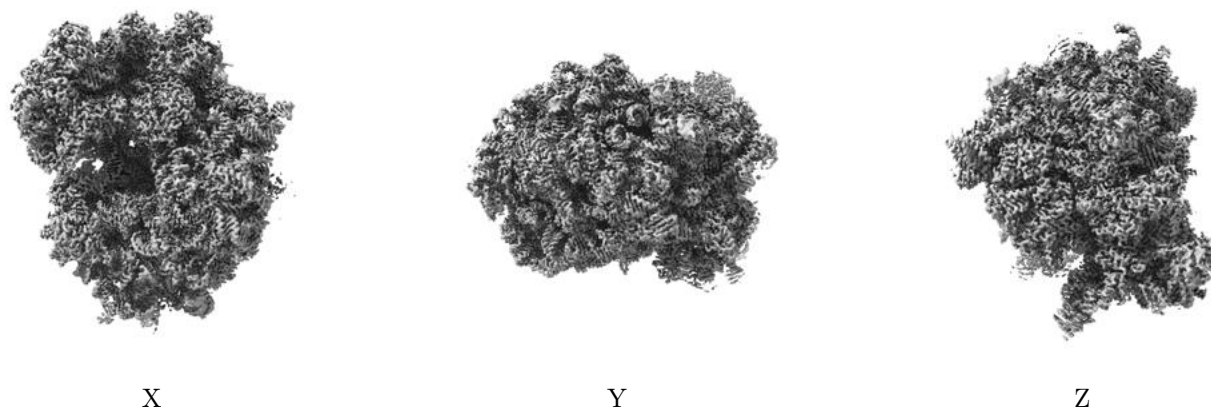


Z

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

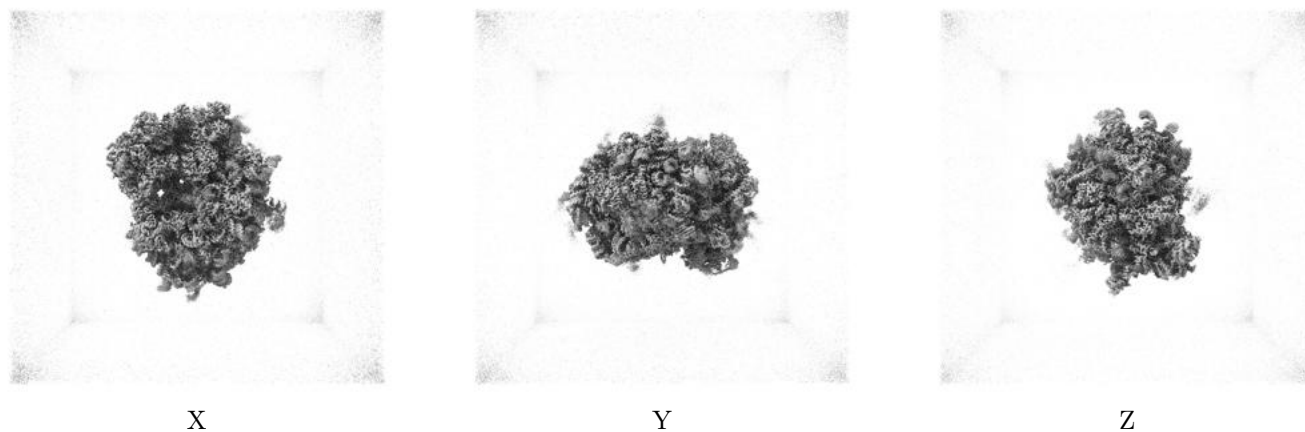
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

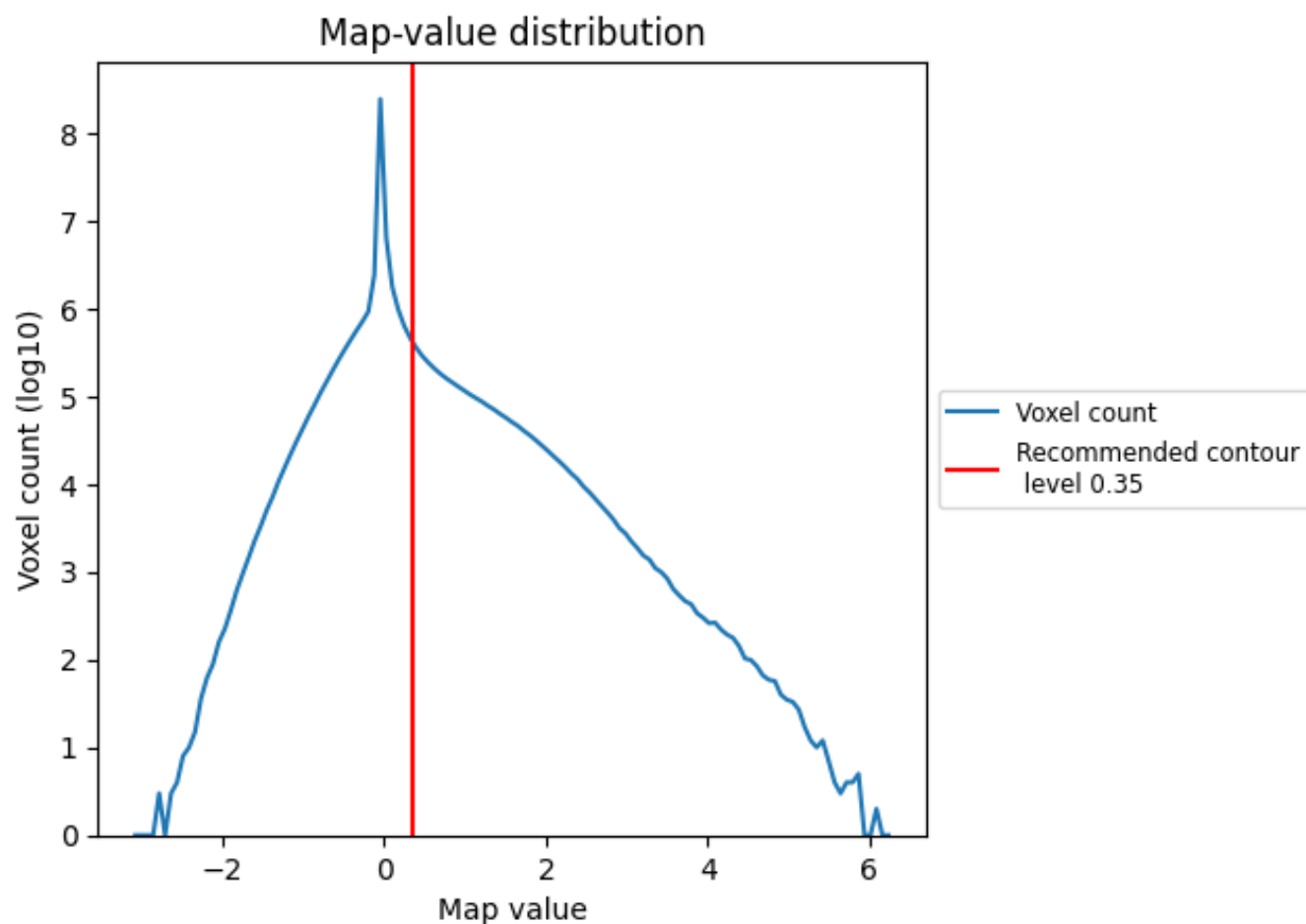
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

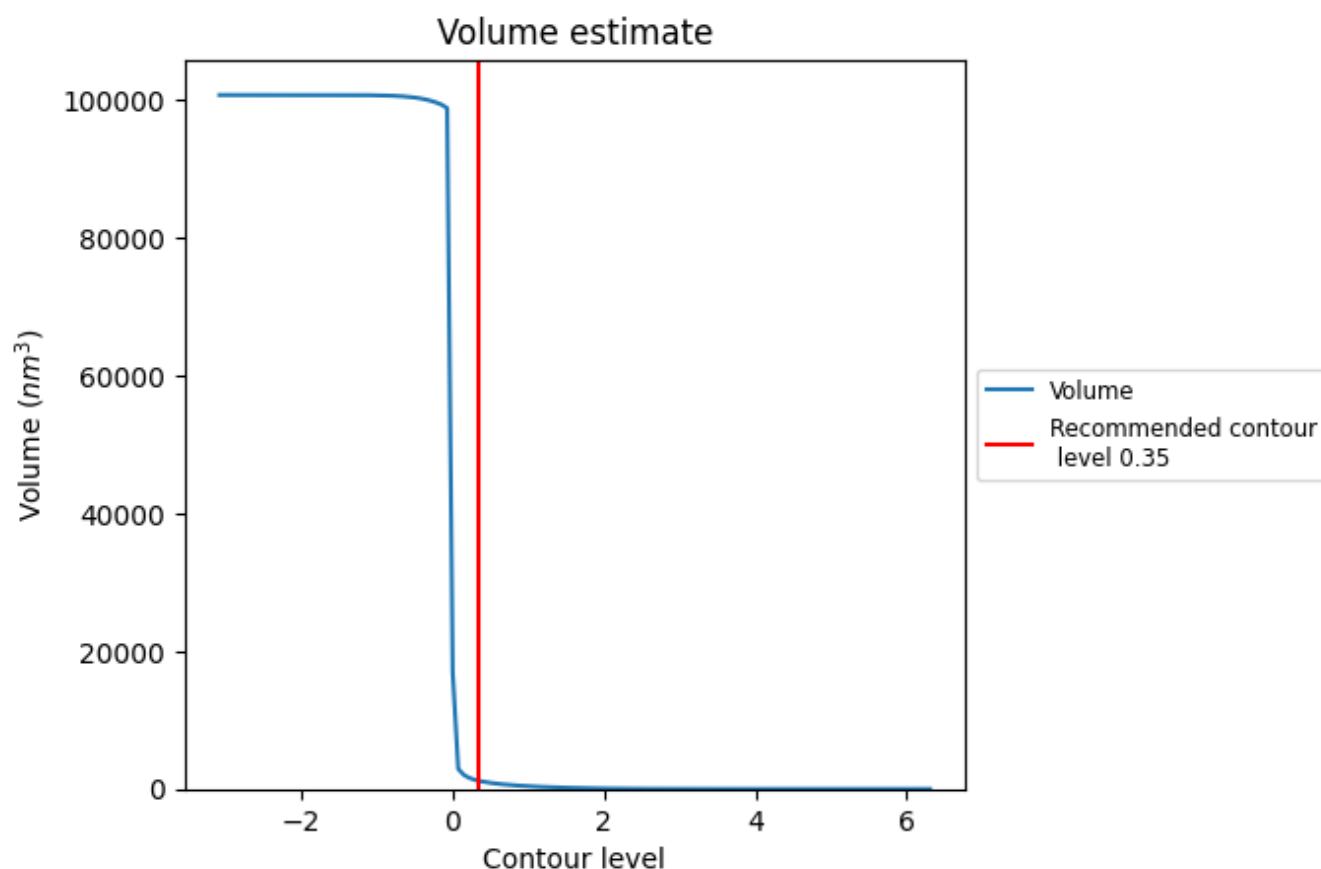
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

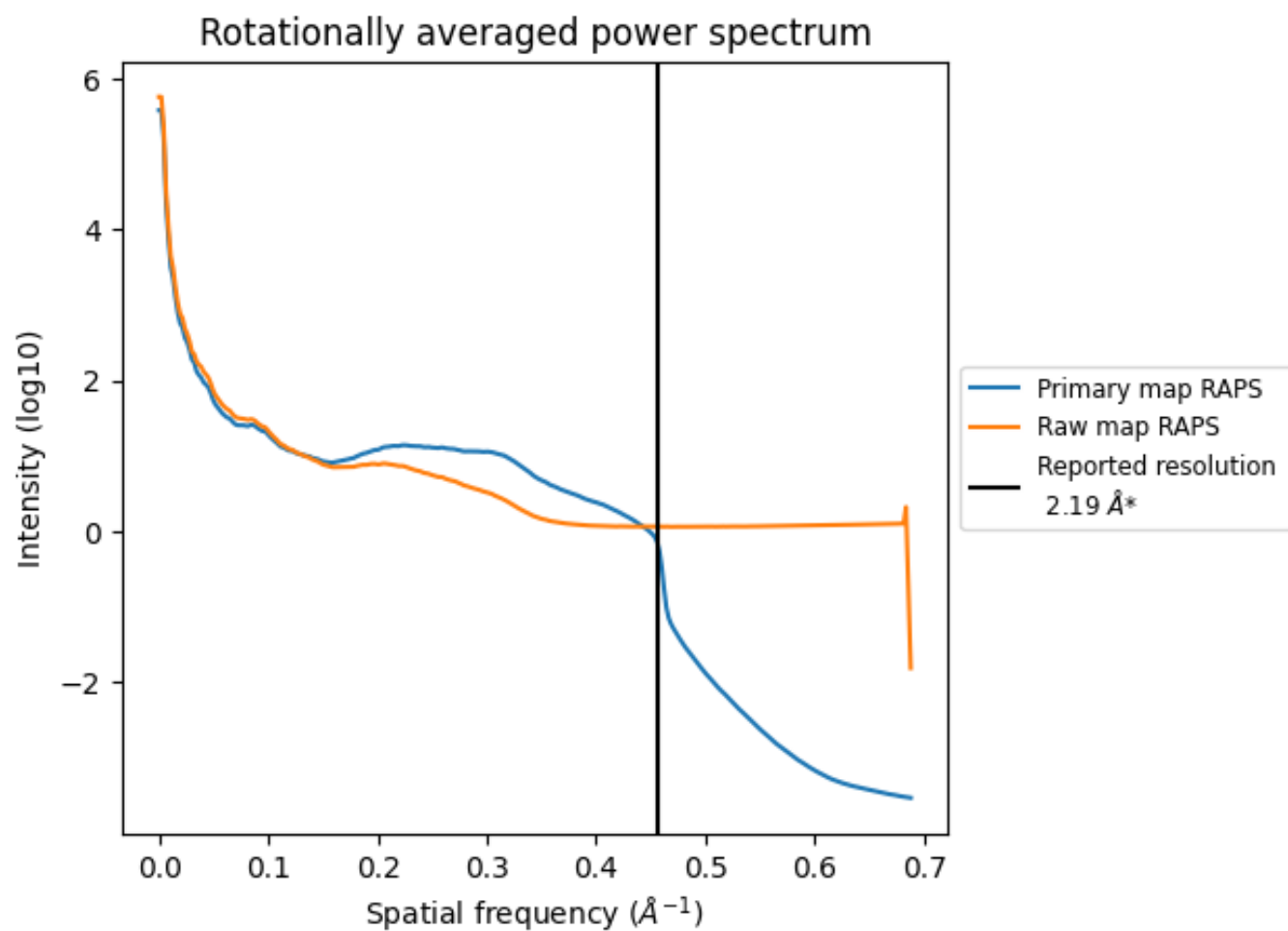
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1179 nm^3 ; this corresponds to an approximate mass of 1065 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 ⓘ

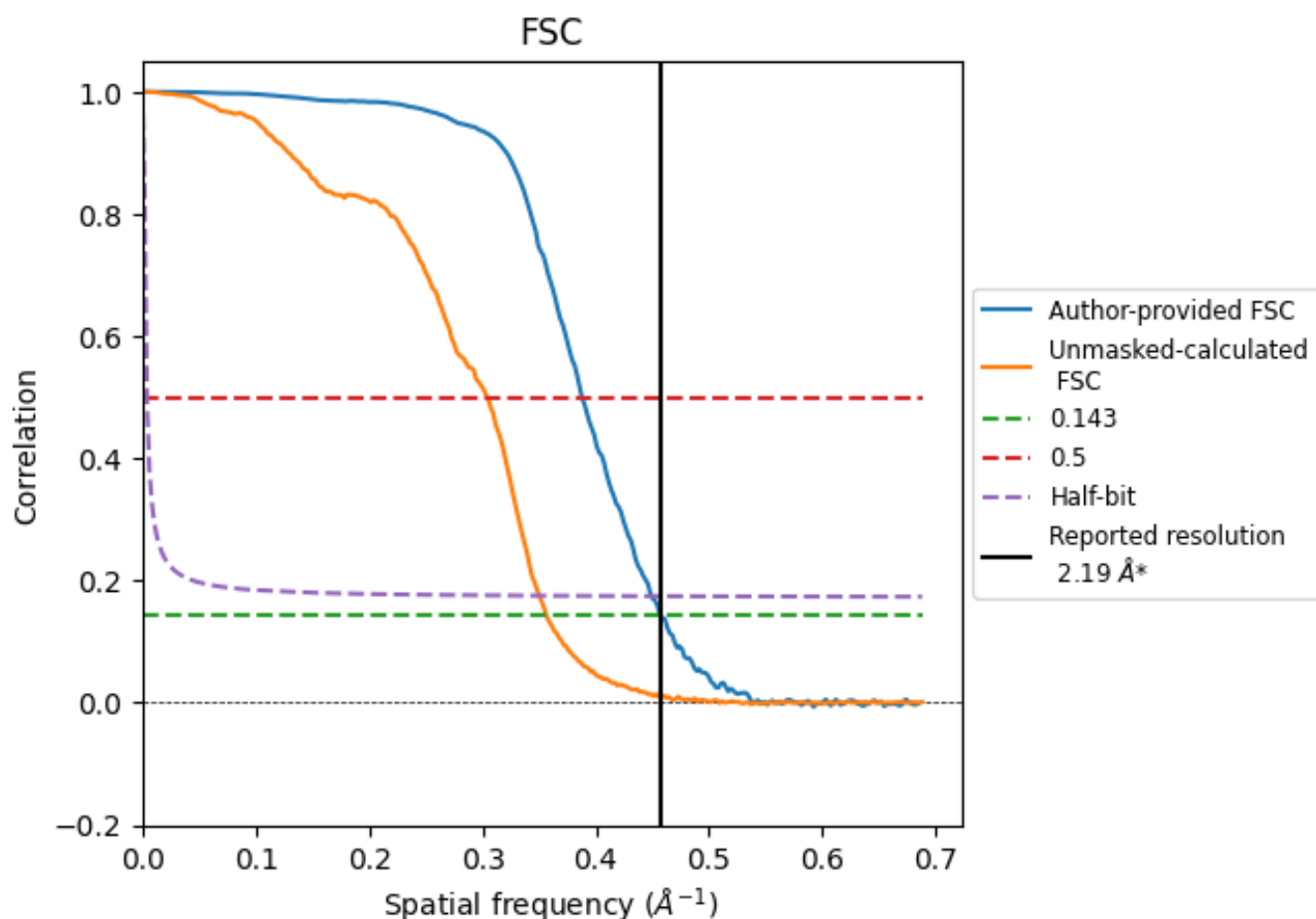


*Reported resolution corresponds to spatial frequency of 0.457 \AA^{-1}

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 0.457 \AA^{-1}

8.2 Resolution estimates [i](#)

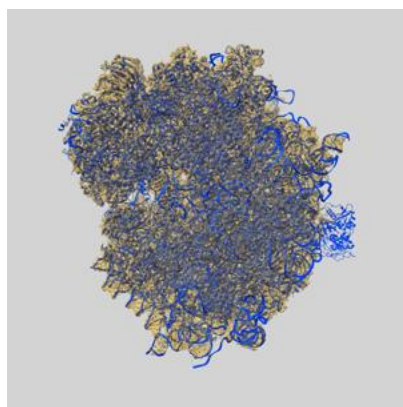
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.58	2.23
Unmasked-calculated*	2.81	3.29	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.81 differs from the reported value 2.19 by more than 10 %

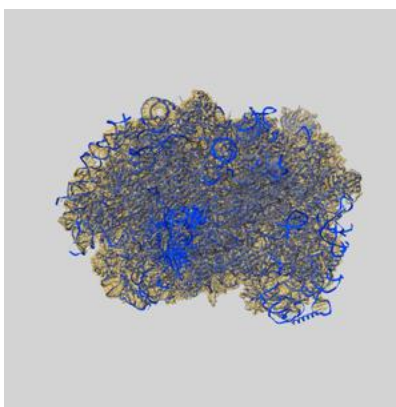
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52581 and PDB model 9I2D. Per-residue inclusion information can be found in section 3 on page 22.

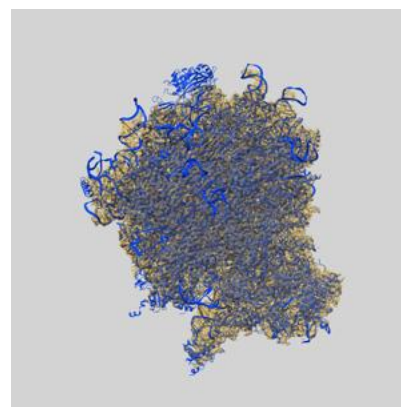
9.1 Map-model overlay [i](#)



X



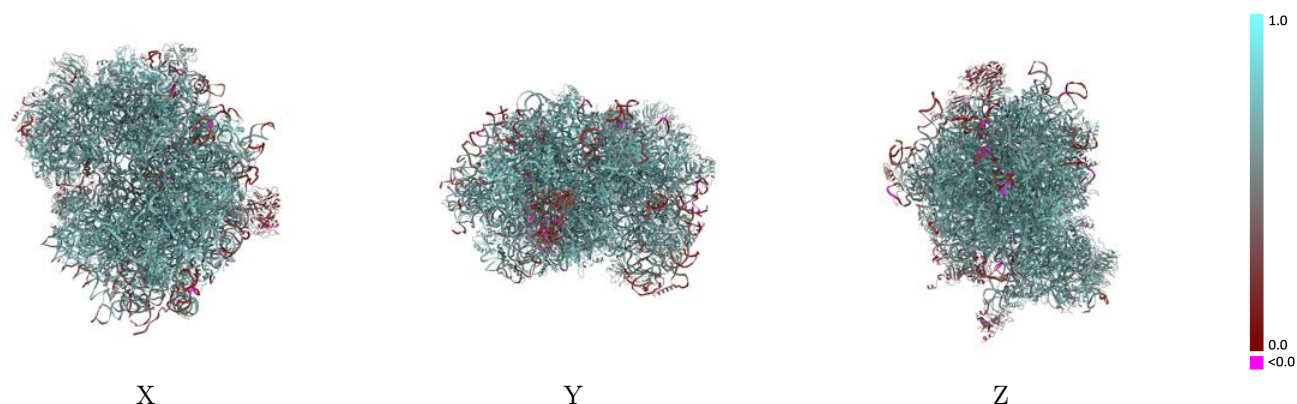
Y



Z

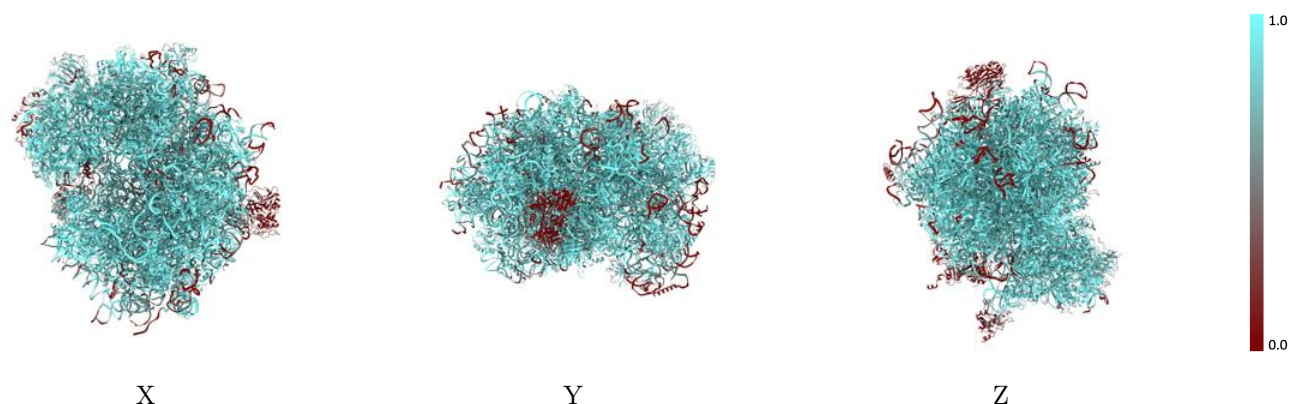
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



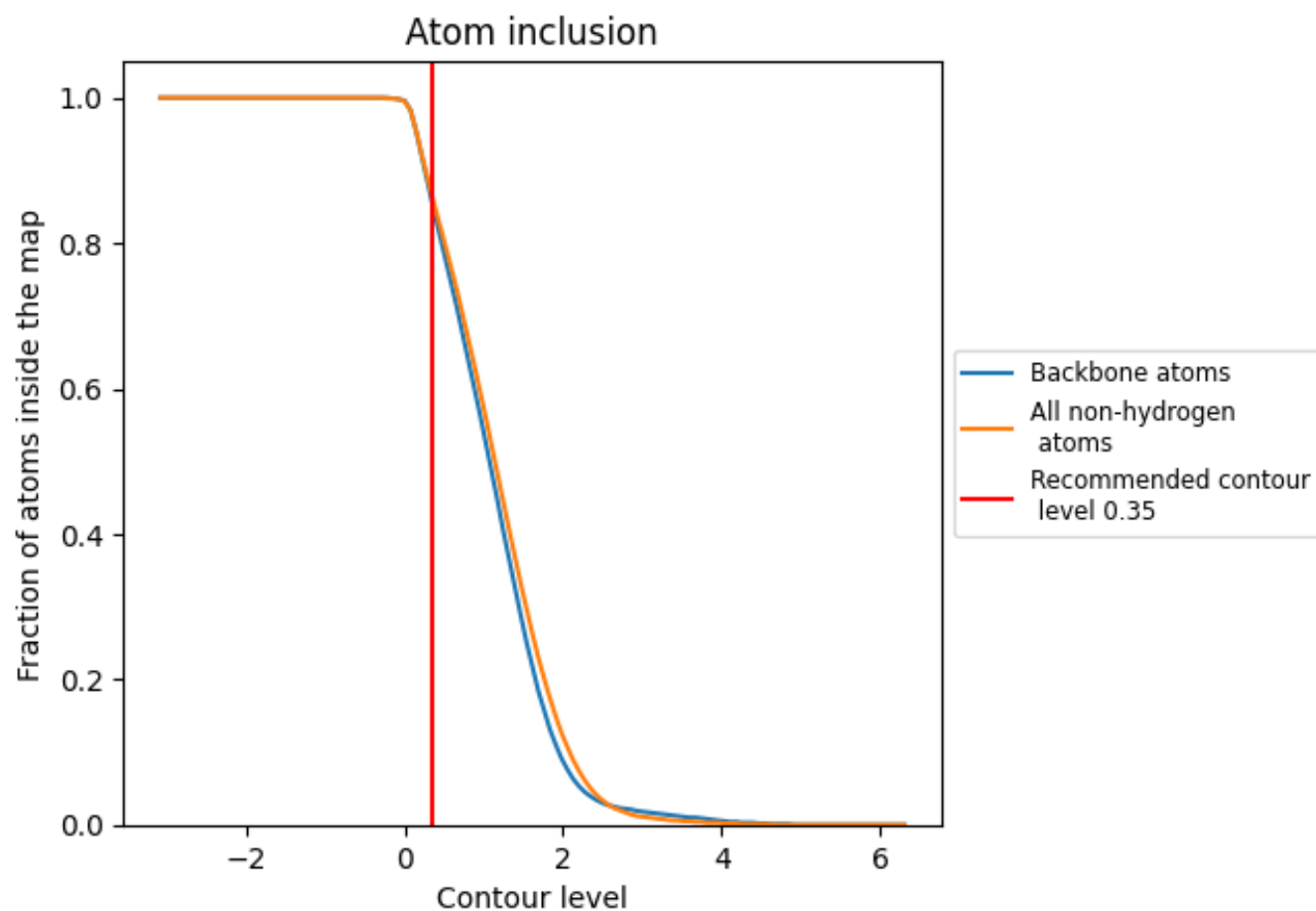
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.6390
CM	 0.8830	 0.6250
CP	 0.8500	 0.6020
CR	 0.6350	 0.5480
CZ	 0.5210	 0.5460
L5	 0.8960	 0.6510
L7	 0.9840	 0.7010
L8	 0.9230	 0.6640
LA	 0.9800	 0.7390
LB	 0.9500	 0.7080
LC	 0.9510	 0.7160
LD	 0.9140	 0.6640
LE	 0.9050	 0.6510
LF	 0.9520	 0.7190
LG	 0.8760	 0.6540
LH	 0.9340	 0.6720
LI	 0.9350	 0.6880
LJ	 0.9030	 0.6430
LL	 0.9210	 0.6800
LM	 0.9330	 0.6890
LN	 0.9910	 0.7450
LO	 0.9590	 0.7240
LP	 0.9530	 0.7220
LQ	 0.9780	 0.7400
LR	 0.9350	 0.7040
LS	 0.9710	 0.7180
LT	 0.9050	 0.6790
LU	 0.8190	 0.6120
LV	 0.9630	 0.7190
LW	 0.6540	 0.5550
LX	 0.9280	 0.7010
LY	 0.9250	 0.6960
LZ	 0.9340	 0.6860
La	 0.9730	 0.7310
Lb	 0.8170	 0.6320



























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Chain	Atom inclusion	Q-score
Lc	 0.9300	 0.6960
Ld	 0.9290	 0.6980
Le	 0.9740	 0.7380
Lf	 0.9760	 0.7300
Lg	 0.9170	 0.6980
Lh	 0.9250	 0.6960
Li	 0.9150	 0.6780
Lj	 0.9850	 0.7320
Lk	 0.8250	 0.6300
Ll	 0.9500	 0.7100
Lm	 0.9470	 0.7060
Ln	 0.9710	 0.7340
Lo	 0.9400	 0.7090
Lp	 0.9540	 0.7360
Lr	 0.9580	 0.7090
Ls	 0.1910	 0.3150
Lt	 0.1680	 0.3930
NA	 0.0000	 0.1250
NB	 0.1440	 0.2580
NM	 0.0630	 0.2430
S2	 0.8760	 0.6210
SA	 0.9360	 0.6750
SB	 0.9020	 0.6700
SC	 0.9480	 0.6870
SD	 0.8560	 0.6280
SE	 0.9230	 0.6420
SF	 0.8910	 0.6380
SG	 0.7760	 0.5630
SH	 0.8430	 0.5920
SI	 0.9060	 0.6560
SJ	 0.9180	 0.6480
SK	 0.8480	 0.5970
SL	 0.9310	 0.6900
SM	 0.2030	 0.2980
SN	 0.9590	 0.7080
SO	 0.9430	 0.6940
SP	 0.8520	 0.6170
SQ	 0.8990	 0.6410
SR	 0.8490	 0.5850
SS	 0.8890	 0.6230
ST	 0.9030	 0.6440
SU	 0.7830	 0.5810

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Chain	Atom inclusion	Q-score
SV	 0.9500	 0.6800
SW	 0.9760	 0.7180
SX	 0.9370	 0.6800
SY	 0.8600	 0.6030
SZ	 0.8520	 0.6040
Sa	 0.9290	 0.6740
Sb	 0.8700	 0.6290
Sc	 0.7710	 0.5530
Sd	 0.9450	 0.6720
Se	 0.7880	 0.6200
Sf	 0.3330	 0.3130
Sg	 0.7410	 0.5690