



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 6ZU5 / pdb_00006zu5
EMDB ID : EMD-11437
Title : Structure of the Paranoosema locustae ribosome in complex with Lso2
Authors : Ehrenbolger, K.; Jespersen, N.; Sharma, H.; Sokolova, Y.Y.; Tokarev, Y.S.;
Vossbrinck, C.R.; Barandun, J.
Deposited on : 2020-07-21
Resolution : 2.90 Å(reported)
Based on initial model : 4V88

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

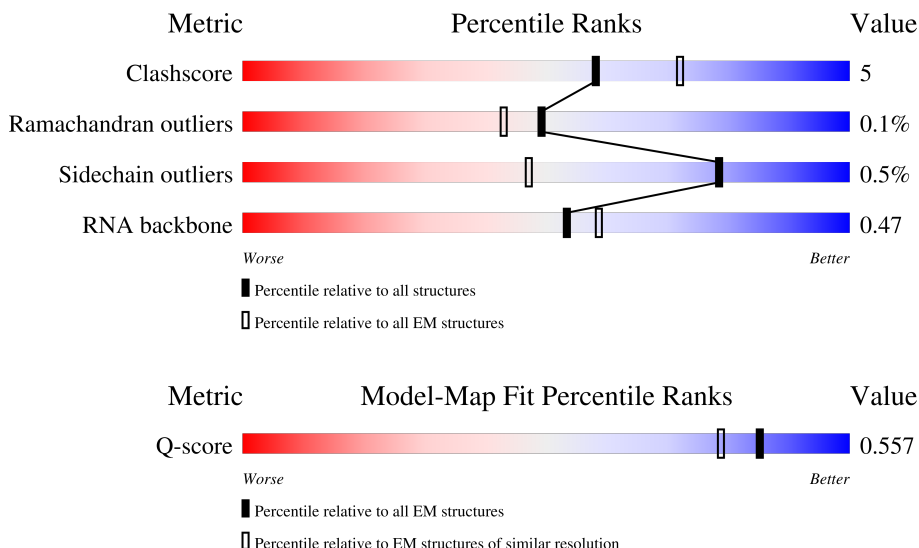
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	L50	2639	
2	L70	119	
3	LA0	247	

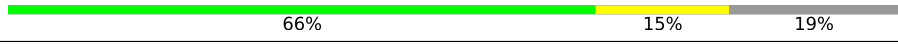
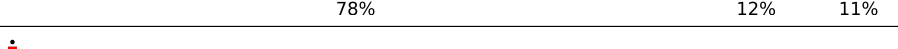
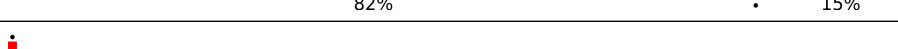
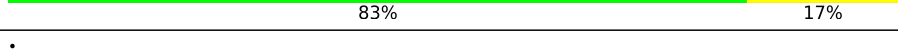
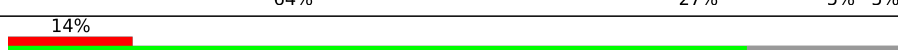
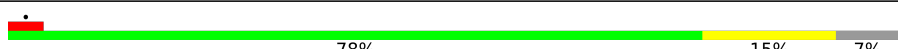
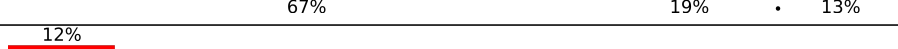
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Mol	Chain	Length	Quality of chain
4	LAA	155	
5	LB0	385	
6	LBB	64	
7	LC0	330	
8	LCC	108	
9	LD0	266	
10	LDD	109	
11	LE0	180	
12	LEE	132	
13	LF0	254	
14	LFF	108	
15	LG0	216	
16	LGG	113	
17	LH0	186	
18	LHH	126	
19	LI0	218	
20	LII	98	
21	LJ0	174	
22	LJJ	95	
23	LL0	166	
24	LLL	51	
25	LM0	108	
26	LMM	132	
27	LN0	204	
28	LNN	77	

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Mol	Chain	Length	Quality of chain
29	LO0	198	
30	LOO	112	
31	LP0	171	
32	LPP	86	
33	LQ0	178	
34	LR0	166	
35	LS0	175	
36	LT0	160	
37	LU0	114	
38	LV0	140	
39	LW0	133	
40	LX0	106	
41	LY0	140	
42	LZ0	127	
43	S60	1400	
44	SA0	242	
45	SAA	104	
46	SB0	230	
47	SBB	86	
48	SC0	255	
49	SCC	65	
50	SD0	217	
51	SDD	63	
52	SE0	267	
53	SEE	60	

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Mol	Chain	Length	Quality of chain
54	SF0	195	
55	SG0	222	
56	SGG	330	
57	SH0	176	
58	SI0	175	
59	SJ0	187	
60	SK0	102	
61	SL0	160	
62	SN0	146	
63	SO0	135	
64	SP0	146	
65	SQ0	145	
66	SR0	123	
67	SS0	161	
68	ST0	141	
69	SU0	111	
70	SV0	66	
71	SW0	127	
72	SX0	140	
73	SY0	133	
74	SZ0	126	

2 Entry composition

There are 77 unique types of molecules in this entry. The entry contains 165175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L50	2455	Total	C	N	O	P	0	0
			52573	23405	9675	17038	2455		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L70	119	Total	C	N	O	P	0	0
			2546	1136	461	830	119		

- Molecule 3 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA0	246	Total	C	N	O	S	0	0
			1862	1159	373	323	7		

- Molecule 4 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LAA	145	Total	C	N	O	S	0	0
			1139	718	229	182	10		

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB0	363	Total	C	N	O	S	0	0
			2887	1835	532	510	10		

- Molecule 6 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LBB	63	Total	C	N	O	S	0	0
			527	322	116	88	1		

- Molecule 7 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC0	325	Total	C	N	O	S	0	0
			2555	1610	466	462	17		

- Molecule 8 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LCC	100	Total	C	N	O	S	0	0
			774	500	136	136	2		

- Molecule 9 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD0	258	Total	C	N	O	S	0	0
			2118	1339	394	376	9		

- Molecule 10 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LDD	103	Total	C	N	O	S	0	0
			854	550	158	142	4		

- Molecule 11 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LE0	179	Total	C	N	O	S	0	0
			1405	897	247	254	7		

- Molecule 12 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LEE	121	Total	C	N	O	S	0	0
			1005	639	203	159	4		

- Molecule 13 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LF0	247	Total	C	N	O	S	0	0
			2050	1299	385	353	13		

- Molecule 14 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LFF	104	Total	C	N	O	S	0	0
			832	528	155	146	3		

- Molecule 15 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG0	202	Total	C	N	O	S	0	0
			1637	1041	300	286	10		

- Molecule 16 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LGG	100	Total	C	N	O	S	0	0
			802	493	171	133	5		

- Molecule 17 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LH0	184	Total	C	N	O	S	0	0
			1455	908	266	269	12		

- Molecule 18 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LHH	120	Total	C	N	O	S	0	0
			1024	641	200	175	8		

- Molecule 19 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LI0	209	Total	C	N	O	S	0	0
			1676	1058	328	281	9		

- Molecule 20 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LII	97	Total	C	N	O	S	0	0
			789	496	158	130	5		

- Molecule 21 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJ0	168	Total	C	N	O	S	0	0
			1336	841	249	239	7		

- Molecule 22 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LJJ	89	Total	C	N	O	S	0	0
			707	425	163	113	6		

- Molecule 23 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LL0	164	Total	C	N	O	S	0	0
			1354	859	256	231	8		

- Molecule 24 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LLL	51	Total	C	N	O	S	0	0
			453	282	103	66	2		

- Molecule 25 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LM0	97	Total	C	N	O	S	0	0
			799	498	144	154	3		

- Molecule 26 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LMM	54	Total	C	N	O	S	0	0
			429	262	90	71	6		

- Molecule 27 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LN0	203	Total	C	N	O	S	0	0
			1654	1027	344	277	6		

- Molecule 28 is a protein called Lso2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LNN	75	Total	C	N	O	S	0	0
			638	394	123	117	4		

- Molecule 29 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LO0	196	Total	C	N	O	S	0	0
			1601	1022	289	281	9		

- Molecule 30 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LOO	91	Total	C	N	O	S	0	0
			756	463	164	124	5		

- Molecule 31 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LP0	153	Total	C	N	O	S	0	0
			1236	785	240	205	6		

- Molecule 32 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LPP	81	Total	C	N	O	S	0	0
			603	380	114	105	4		

- Molecule 33 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LQ0	176	Total	C	N	O	S	0	0
			1388	883	253	248	4		

- Molecule 34 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LR0	161	Total	C	N	O	S	0	0
			1275	797	261	209	8		

- Molecule 35 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LS0	169	Total	C	N	O	S	0	0
			1414	910	250	246	8		

- Molecule 36 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LT0	160	Total	C	N	O	S	0	0
			1311	820	266	218	7		

- Molecule 37 is a protein called eL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	LU0	97	Total	C	N	O	0	0
			481	287	97	97		

- Molecule 38 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LV0	138	Total	C	N	O	S	0	0
			1048	652	208	181	7		

- Molecule 39 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LW0	93	Total	C	N	O	S	0	0
			698	444	130	123	1		

- Molecule 40 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LX0	98	Total	C	N	O	S	0	0
			765	488	138	137	2		

- Molecule 41 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LY0	138	Total	C	N	O	S	0	0
			1138	701	230	197	10		

- Molecule 42 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LZ0	127	Total	C	N	O	S	0	0
			1001	645	177	173	6		

- Molecule 43 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S60	1336	Total	C	N	O	P	0	0
			28876	12841	5457	9242	1336		

- Molecule 44 is a protein called uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	SA0	202	Total	C	N	O	0	0
			1000	596	202	202		

- Molecule 45 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SAA	97	Total	C	N	O	S	0	0
			778	482	157	134	5		

- Molecule 46 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SB0	196	Total	C	N	O	S	0	0
			1580	1003	289	282	6		

- Molecule 47 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SBB	80	Total	C	N	O	S	0	0
			642	404	121	109	8		

- Molecule 48 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SC0	221	Total	C	N	O	S	0	0
			1711	1092	304	308	7		

- Molecule 49 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SCC	55	Total	C	N	O	S	0	0
			419	265	73	77	4		

- Molecule 50 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD0	213	Total	C	N	O	S	0	0
			1690	1077	300	304	9		

- Molecule 51 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SDD	59	Total	C	N	O	S	0	0
			488	308	99	77	4		

- Molecule 52 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE0	257	Total	C	N	O	S	0	0
			2031	1293	357	369	12		

- Molecule 53 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SEE	49	Total	C	N	O	S	0	0
			334	203	72	57	2		

- Molecule 54 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SF0	186	Total	C	N	O	S	0	0
			1447	901	278	258	10		

- Molecule 55 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG0	218	Total	C	N	O	S	0	0
			1760	1112	331	307	10		

- Molecule 56 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SGG	307	Total	C	N	O	S	0	0
			2306	1443	402	443	18		

- Molecule 57 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SH0	156	Total	C	N	O	S	0	0
			1003	614	184	200	5		

- Molecule 58 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SI0	169	Total	C	N	O	S	0	0
			1353	850	252	243	8		

- Molecule 59 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SJ0	164	Total	C	N	O	S	0	0
			1357	855	258	238	6		

- Molecule 60 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SK0	74	Total	C	N	O	S	0	0
			592	385	107	96	4		

- Molecule 61 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SL0	133	Total	C	N	O	S	0	0
			1102	711	199	187	5		

- Molecule 62 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN0	142	Total	C	N	O	S	0	0
			1137	715	221	195	6		

- Molecule 63 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO0	128	Total	C	N	O	S	0	0
			950	583	192	172	3		

- Molecule 64 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP0	112	Total	C	N	O	S	0	0
			896	570	159	160	7		

- Molecule 65 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ0	127	Total	C	N	O	S	0	0
			1012	649	177	181	5		

- Molecule 66 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR0	113	Total	C	N	O	S	0	0
			800	503	155	141	1		

- Molecule 67 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS0	144	Total	C	N	O	S	0	0
			1140	709	223	202	6		

- Molecule 68 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST0	139	Total	C	N	O	S	0	0
			1115	701	213	195	6		

- Molecule 69 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU0	99	Total	C	N	O	S	0	0
			787	498	141	145	3		

- Molecule 70 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV0	63	Total	C	N	O	S	0	0
			462	290	82	88	2		

- Molecule 71 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SW0	127	Total	C	N	O	S	0	0
			1001	633	183	175	10		

- Molecule 72 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX0	138	Total	C	N	O	S	0	0
			1089	691	207	187	4		

- Molecule 73 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY0	123	Total	C	N	O	S	0	0
			964	595	195	168	6		

- Molecule 74 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ0	72	Total	C	N	O	S	0	0
			548	340	104	101	3		

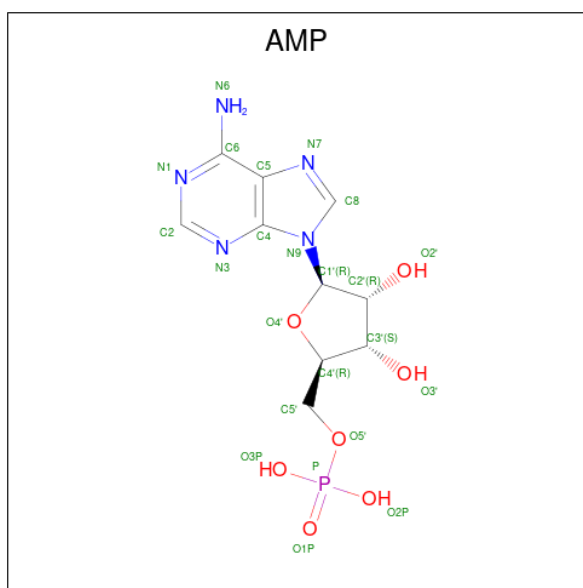
- Molecule 75 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
75	L50	152	Total	Mg	0
			152	152	
75	L70	4	Total	Mg	0
			4	4	
75	LA0	1	Total	Mg	0
			1	1	
75	LJJ	1	Total	Mg	0
			1	1	
75	LV0	1	Total	Mg	0
			1	1	
75	S60	20	Total	Mg	0
			20	20	

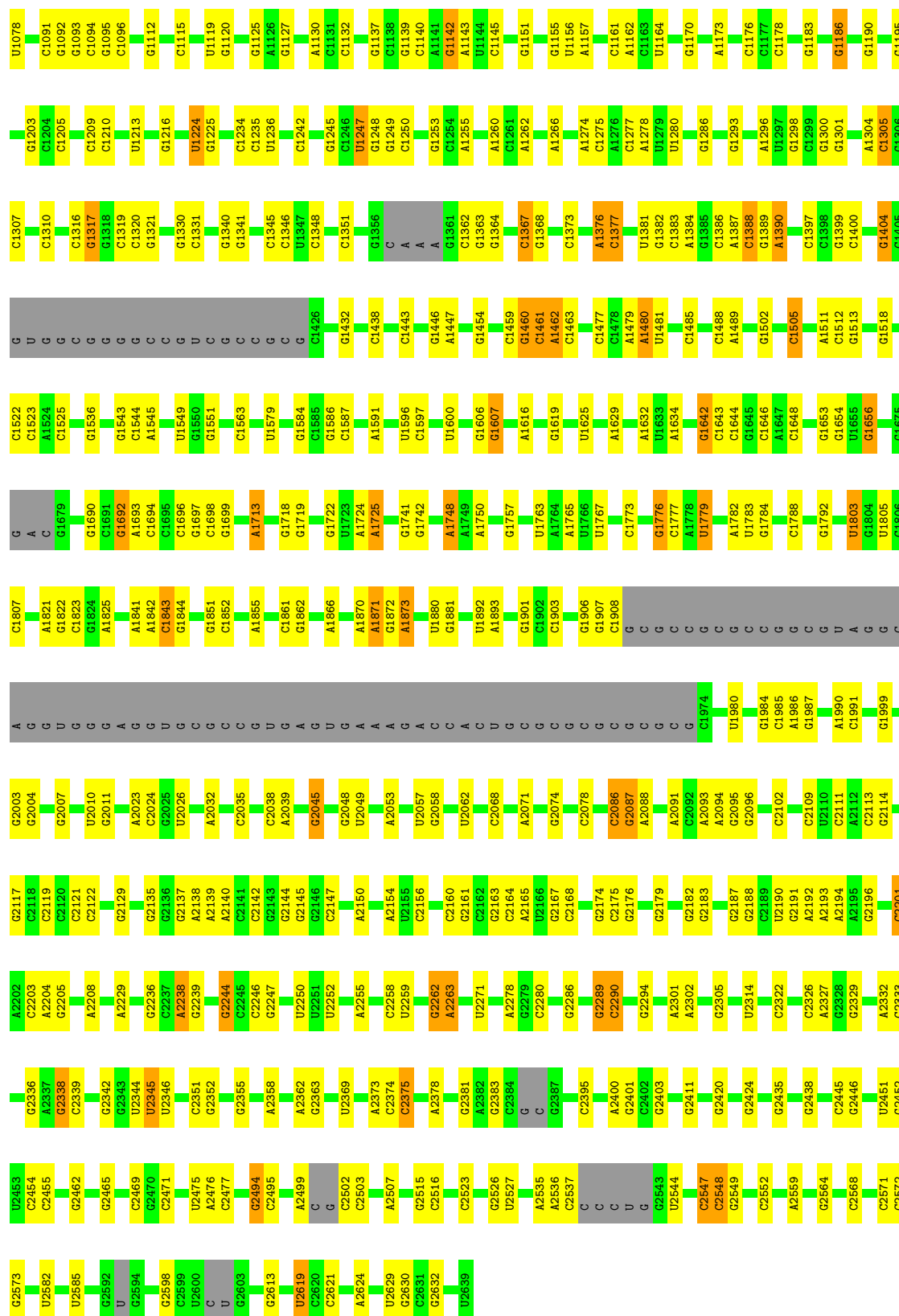
- Molecule 76 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
76	LGG	1	Total	Zn	0
			1	1	
76	LJJ	1	Total	Zn	0
			1	1	
76	LMM	1	Total	Zn	0
			1	1	
76	LOO	1	Total	Zn	0
			1	1	
76	LPP	1	Total	Zn	0
			1	1	
76	SAA	1	Total	Zn	0
			1	1	
76	SBB	1	Total	Zn	0
			1	1	
76	SDD	1	Total	Zn	0
			1	1	

- Molecule 77 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					AltConf
77	LH0	1	Total	C	N	O	P	0
			23	10	5	7	1	



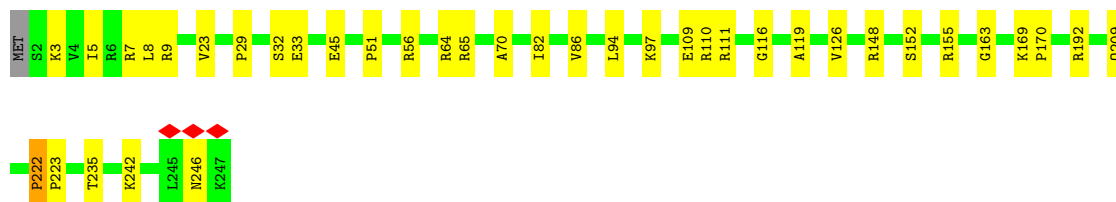
• Molecule 2: 5S rRNA

Chain L70: 75% 20% 5%



• Molecule 3: uL2

Chain LA0: 84% 15%



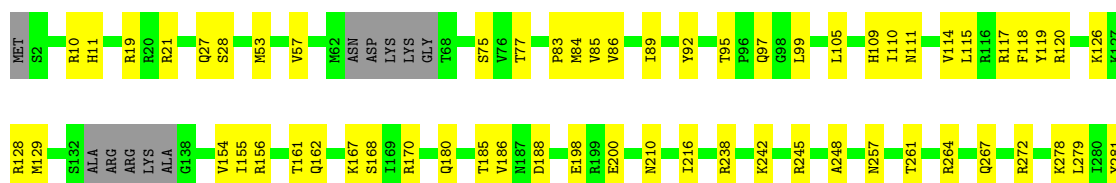
• Molecule 4: uL15

Chain LAA: 76% 17% 6%



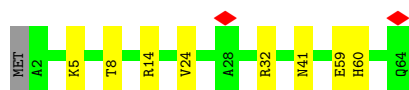
• Molecule 5: uL3

Chain LB0: 74% 21% 6%



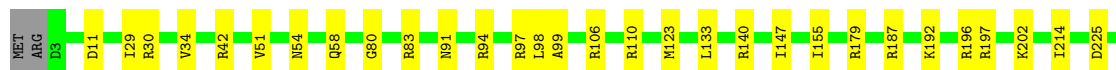
• Molecule 6: eL29

Chain LBB: 86% 12%

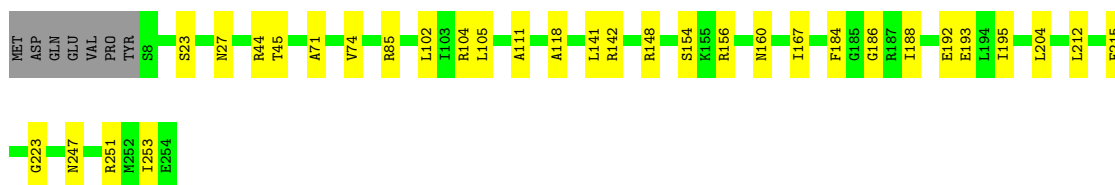


• Molecule 7: uL4

Chain LC0: 87% 12%



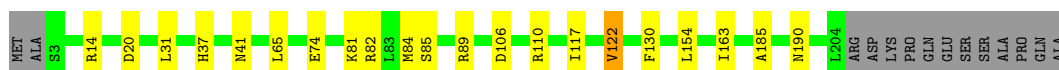
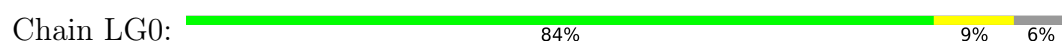




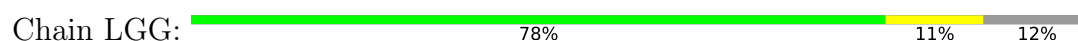
• Molecule 14: eL33



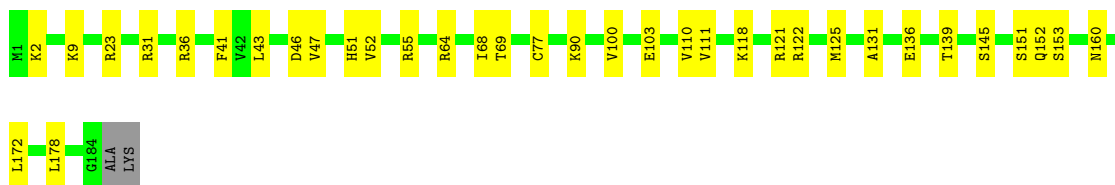
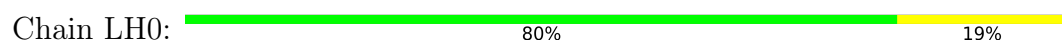
• Molecule 15: eL8



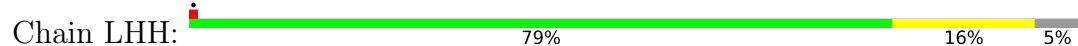
• Molecule 16: eL34



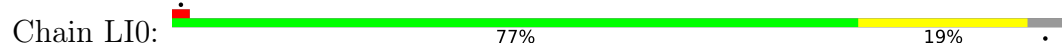
• Molecule 17: uL6

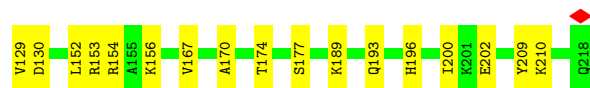


• Molecule 18: uL29



• Molecule 19: uL16





• Molecule 20: eL36

Chain LII: 89% 9% ..



• Molecule 21: uL5

Chain LJ0: 84% 12% .



• Molecule 22: eL37

Chain LJJ: 77% 17% 6%



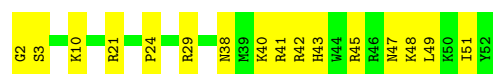
• Molecule 23: eL13

Chain LL0: 86% 13% .



• Molecule 24: eL39

Chain LLL: 69% 31%

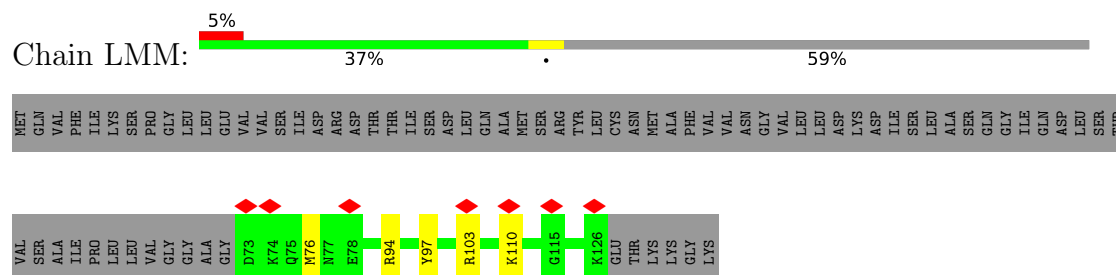


• Molecule 25: eL14

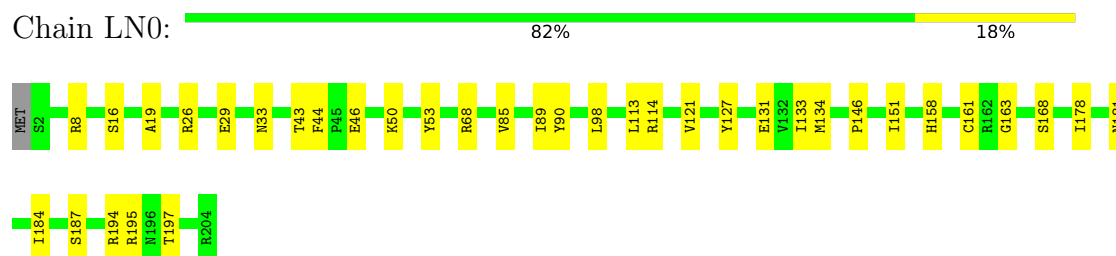
Chain LM0: 71% 19% 10%



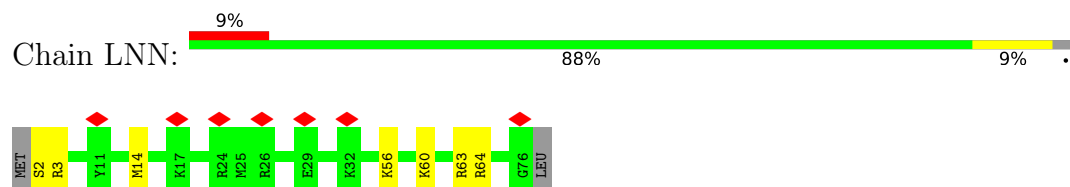
- Molecule 26: eL40



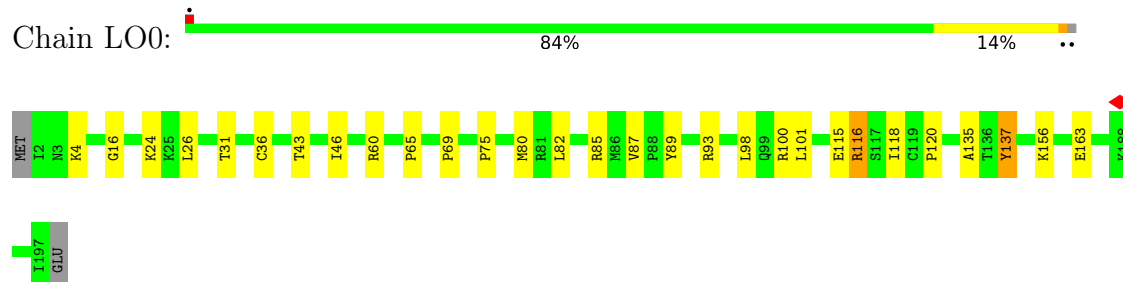
- Molecule 27: eL15



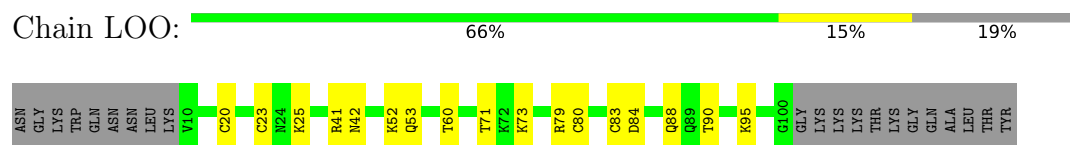
- Molecule 28: Lso2



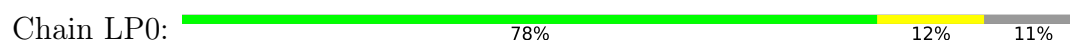
- Molecule 29: uL13

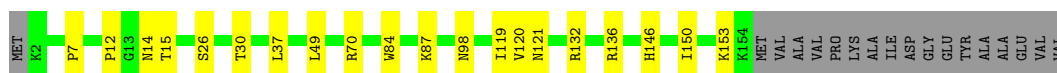


- Molecule 30: eL42

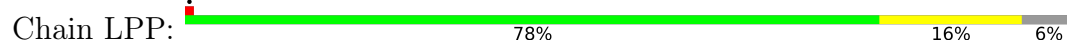


- Molecule 31: uL22

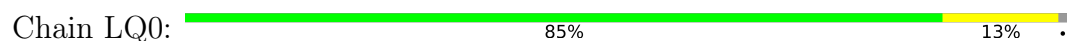




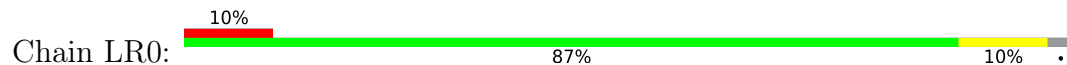
• Molecule 32: eL43



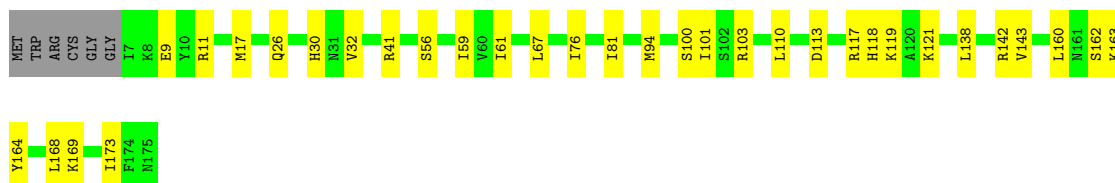
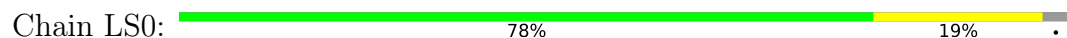
• Molecule 33: eL18



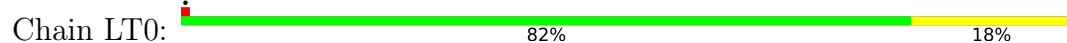
• Molecule 34: eL19



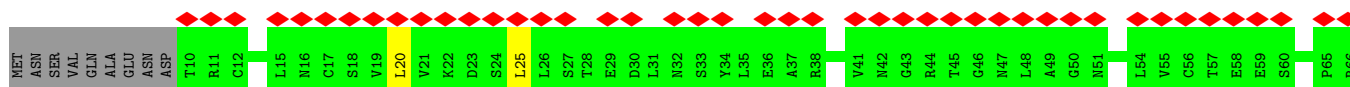
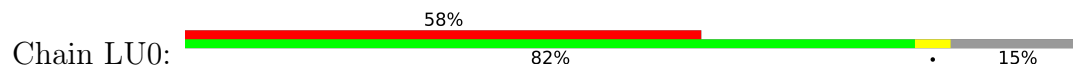
• Molecule 35: eL20

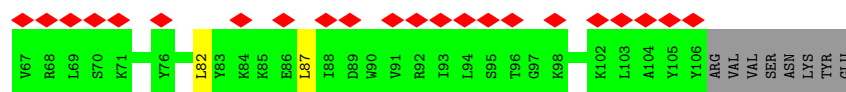


• Molecule 36: eL21

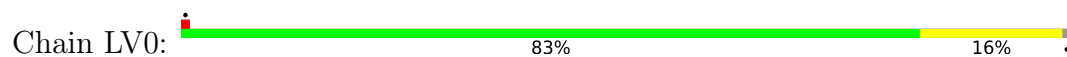


• Molecule 37: eL22

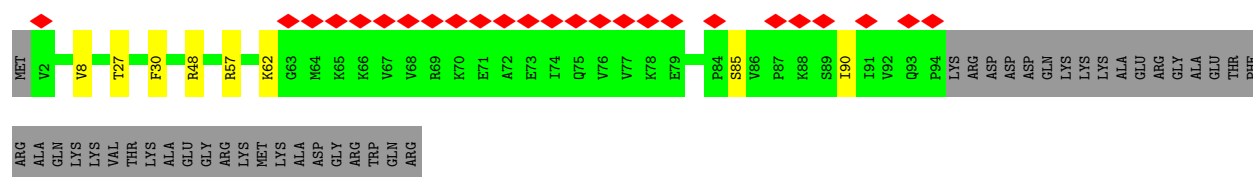




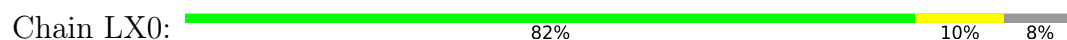
• Molecule 38: uL14



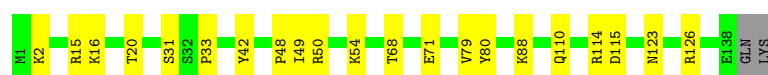
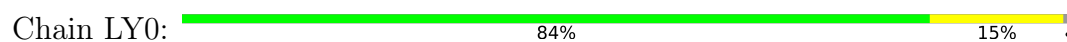
• Molecule 39: eL24



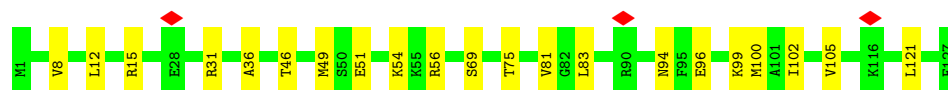
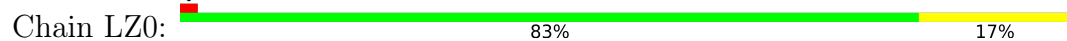
• Molecule 40: uL23



• Molecule 41: uL24

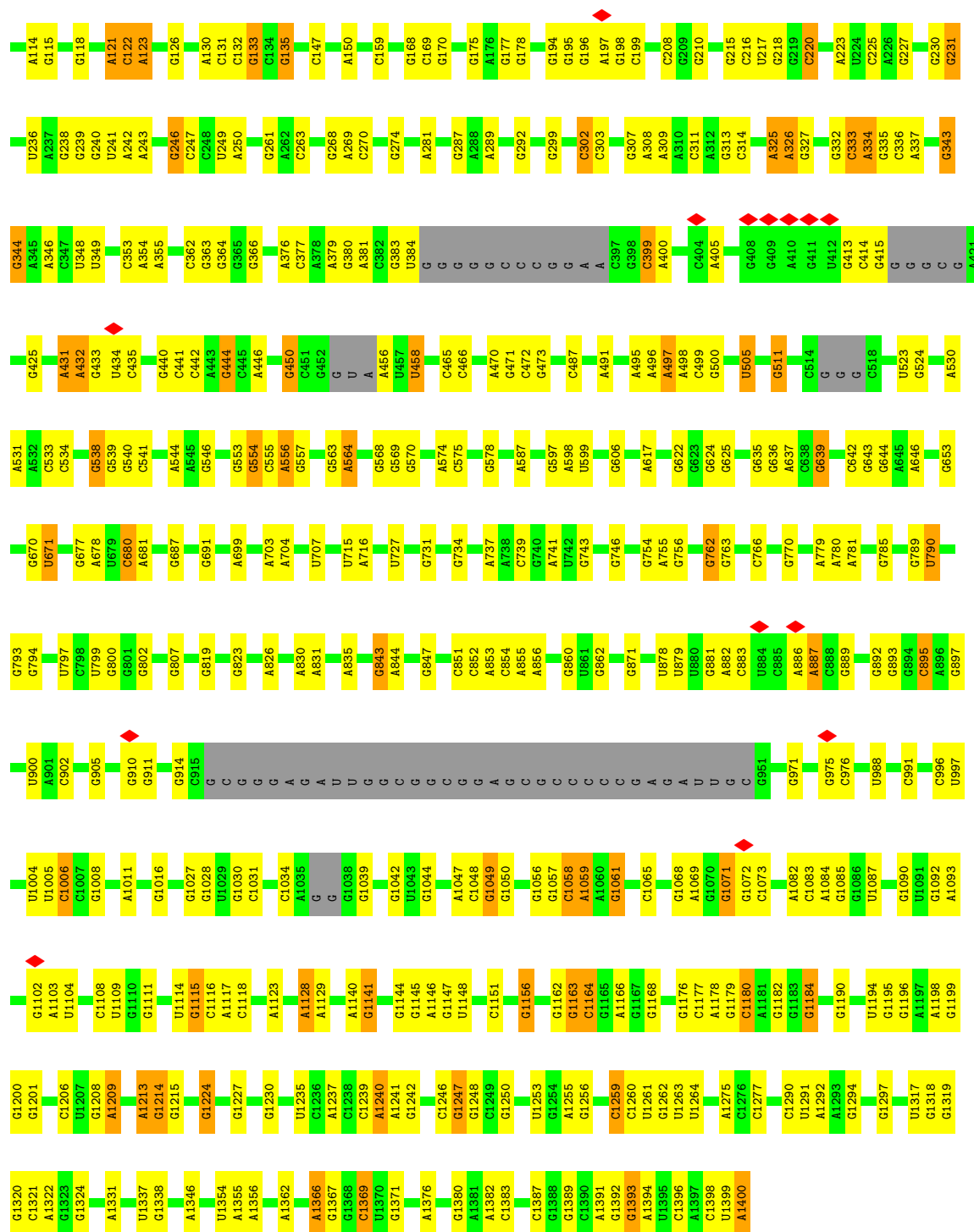


• Molecule 42: eL27

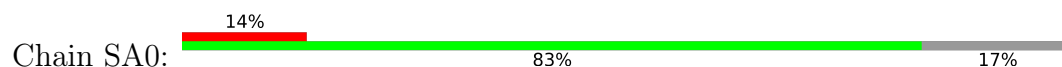


• Molecule 43: 18S rRNA





• Molecule 44: uS2



ILE
GLN
GLU
GLN
LYS
GLU
LYS
ASN
GLU
THR
SER
PHE
GLN
VAL
LYS
ASP
ALA
ALA
PRO
GLU
VAL
PRO
ALA
ALA
GLU
GLN
TRP
ASP
ALA

• Molecule 45: eS26

Chain SAA:  78% 15% 7%

MET P2 K13 K15 K19 C23 S28 K32 D33 K34 K37 L44 L45 D51 R54 I58 Y59 F60 E61 Q72 S76 R85 E90 F98 HIS ALA ARG VAL LYS GLN

• Molecule 46: eS1

Chain SB0:  67% 19% 15%

MET ALA LYS ASP GLN PRO VAL THR LYS SER LEU LYS GLY LEU LYS LYS ALA THR ASP S24 K28 E29 G45 L48 C49 T50 Q52 N53 T54 N57 L58 E59 L63 G72 V90 R96 S100 E101 F102 E106 T109 K112

K118 W119 H120 I123 E124 D128 V129 C130 H136 L137 R138 V139 F140 V141 T142 R148 PRO GLY SER VAL SER R154 T155 C156 V163 V166 V173 E177 K189 I199 L207 P208 T214 A215 R222 R223 R224 PRO GLU VAL ILE ARG ASN

• Molecule 47: eS27

Chain SBB:  6% 70% 23% 7%

MET ALA ILE K4 D5 L6 E12 E13 L14 R15 R20 K21 R22 Q26 F31 R35 C36 S37 S38 C39 D40 R53 T54 C55 P56 S57 C58 V61 E73 G74 D75 I81 K82 R83 LEU VAL GLU

• Molecule 48: uS5

Chain SC0:  67% 19% 13%

MET GLU SER VAL ALA GLY ARG ASN THR GLY PRO LEU PRO ARG LYS GLU ALA VAL ARG PRO VAL PRO ARG GLN ASP LYS E32 T37 D38 L39 G40 I41 L42 V43 N49 L58 I65 K86 R89 R93 A106 S116 K117 E118 T121

A122 V137 R138 L139 G140 F141 E149 K155 S162 M165 R166 K172 G173 S174 R177 V181 P182 A189 G190 V191 K192 D193 T205 K210 A211 T212 C221 V224 P225 E226 F227 W228 P233 N236 P237 L238 S239 R240 Y241 S242 R243 E247 Y248 R249

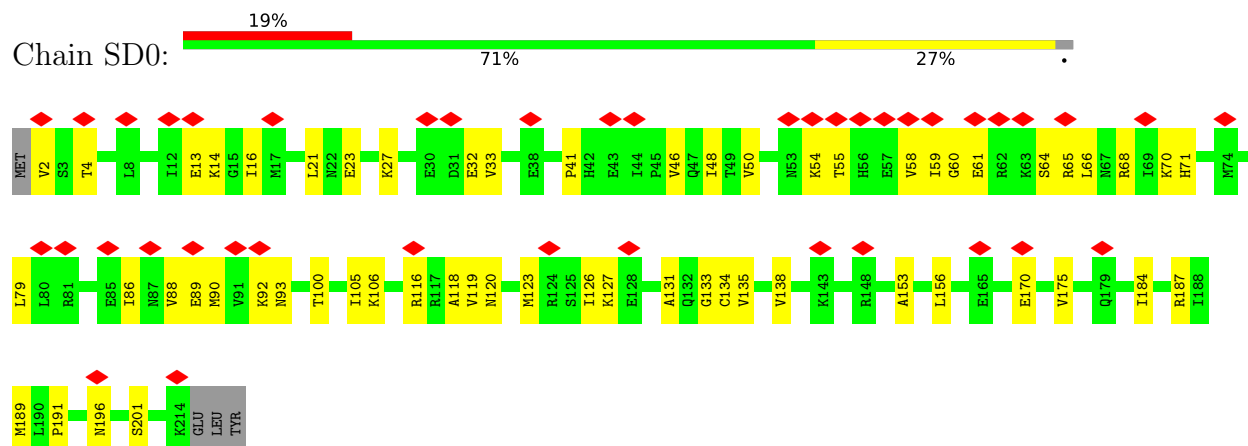
E250 K251 I252 ALA ARG LYS

• Molecule 49: eS28

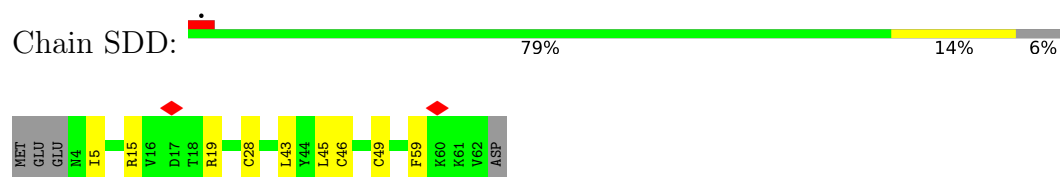
Chain SCC:  12% 65% 18% 15%

MET THR ASP Q4 V5 Q12 K16 T24 Q27 L28 D32 T33 G34 R39 V50 L53 L54 D55 C56 E57 R58 GLU HIS ARG ARG GLY ARG PHE

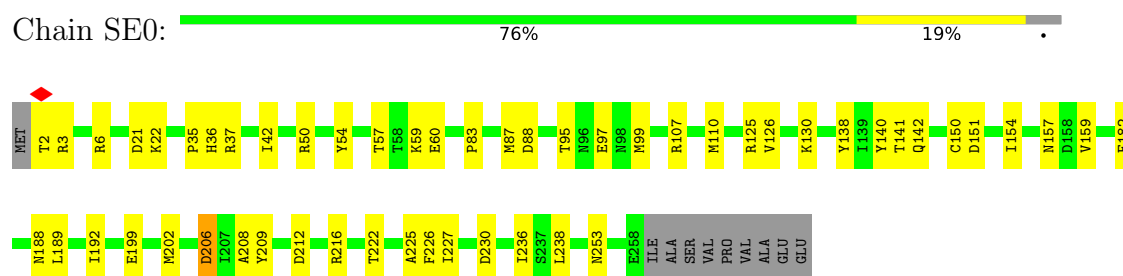
- Molecule 50: uS3



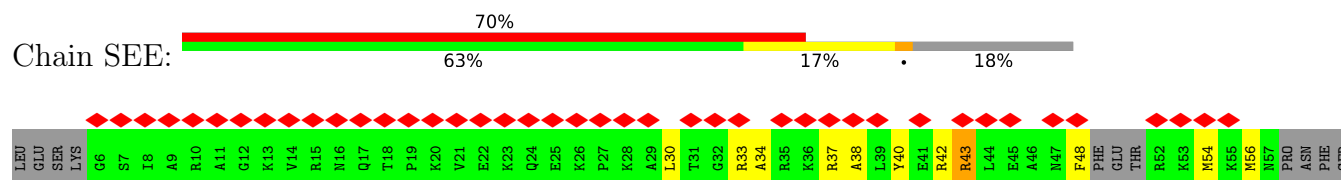
- Molecule 51: uS14



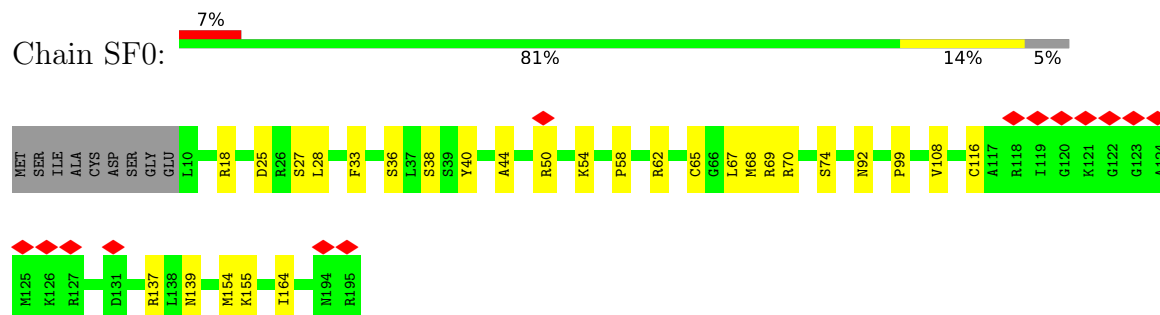
- Molecule 52: eS4



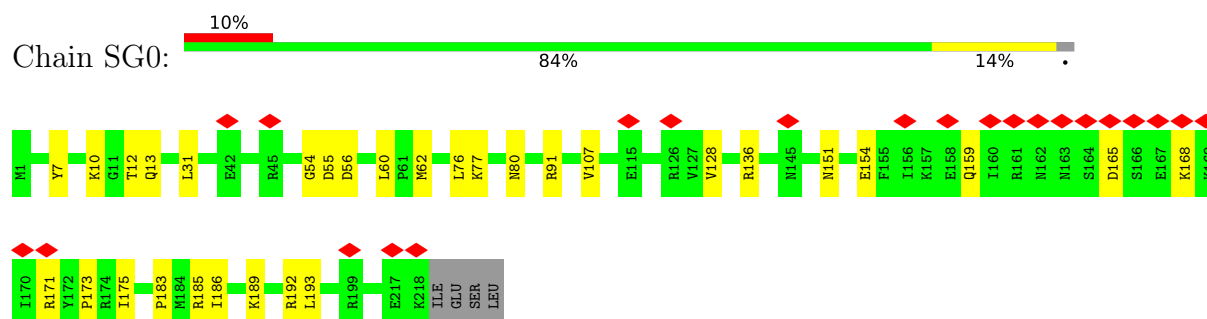
- Molecule 53: eS30



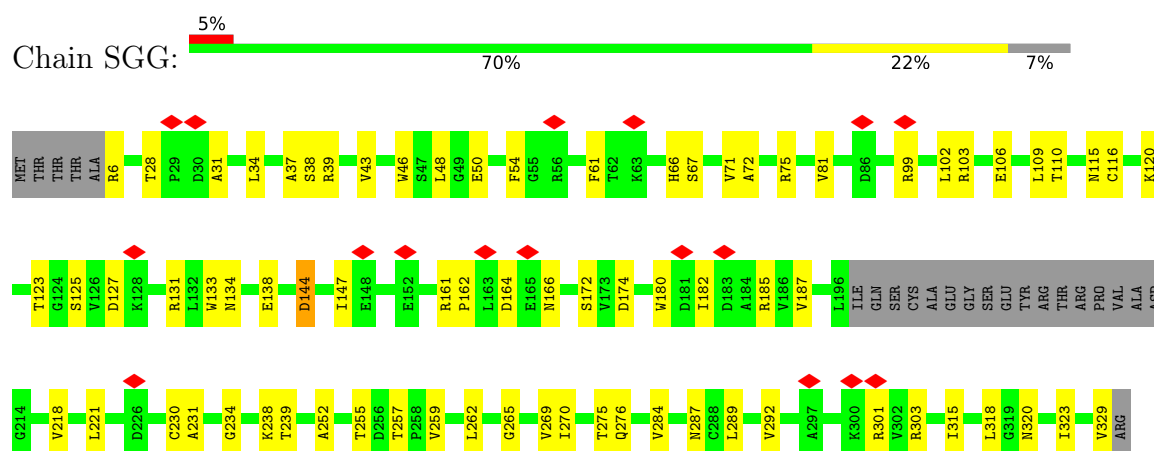
- Molecule 54: uS7



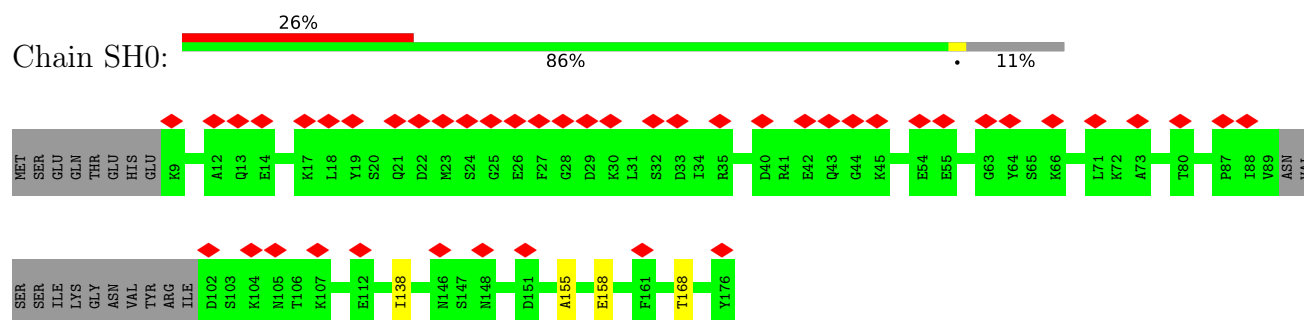
- Molecule 55: eS6



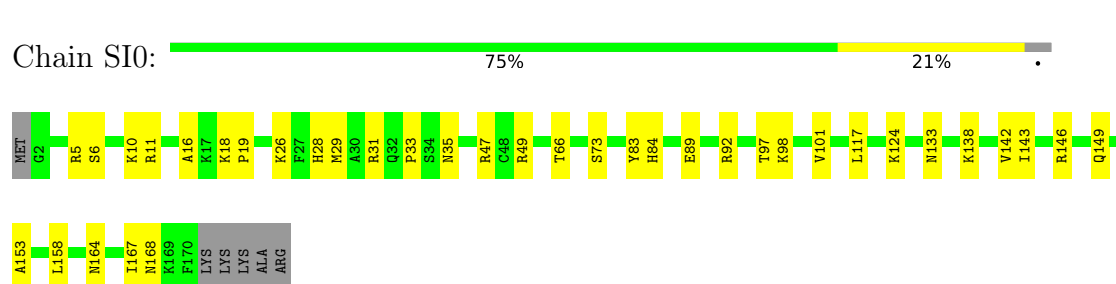
- Molecule 56: RACK1



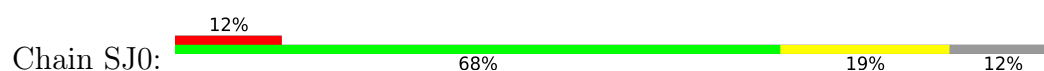
- Molecule 57: eS7

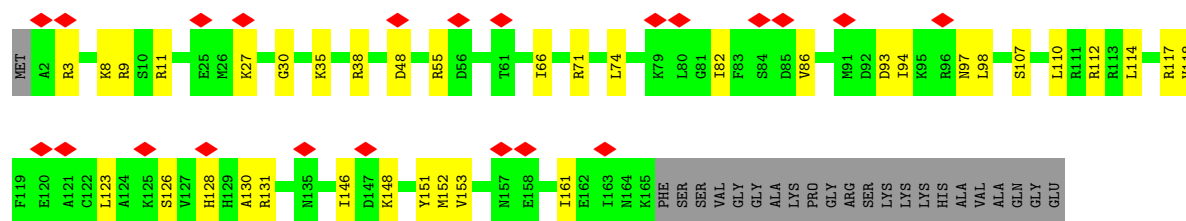


- Molecule 58: eS8

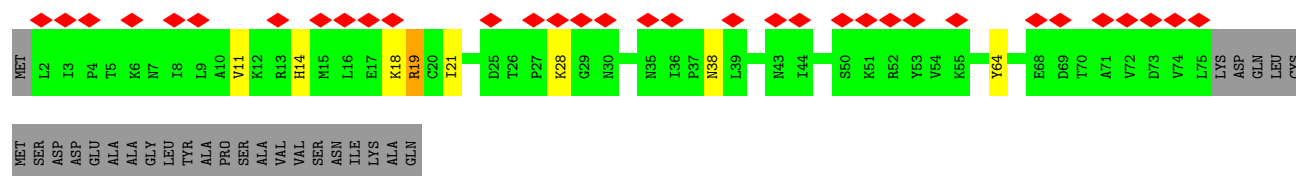


- Molecule 59: uS4

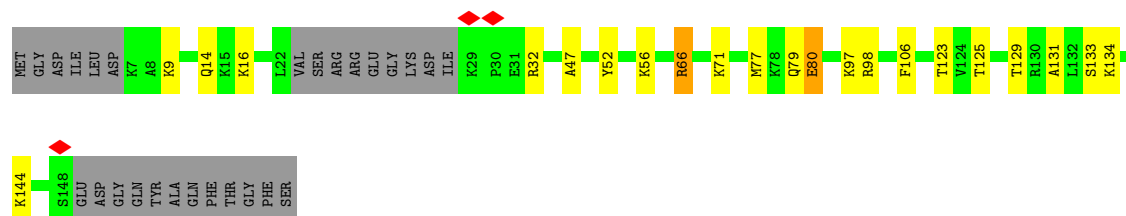




• Molecule 60: eS10



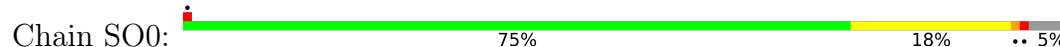
• Molecule 61: uS17



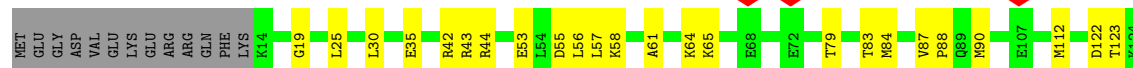
• Molecule 62: uS15

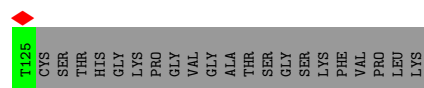


• Molecule 63: uS11



• Molecule 64: uS19





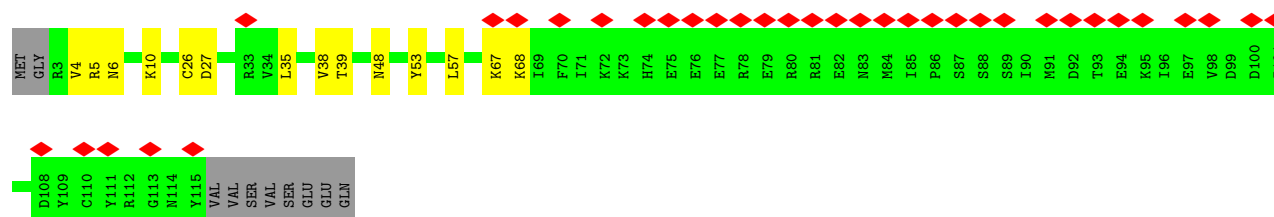
• Molecule 65: uS9

Chain SQ0: 77% 11% 12%



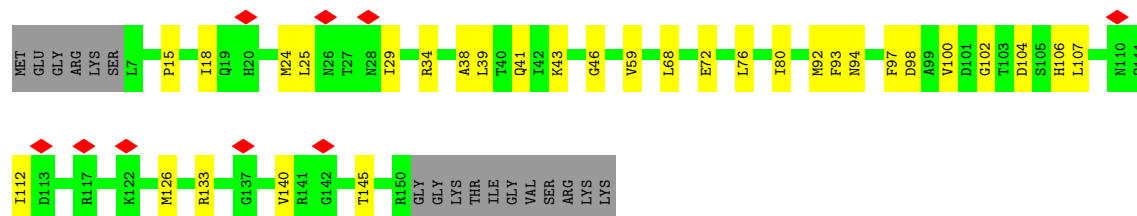
• Molecule 66: eS17

Chain SR0: 28% 80% 11% 8%



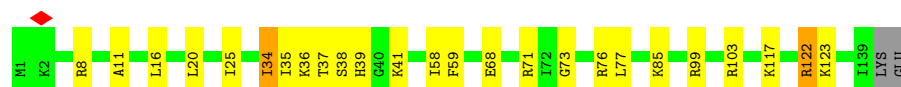
• Molecule 67: uS13

Chain SS0: 6% 70% 19% 11%



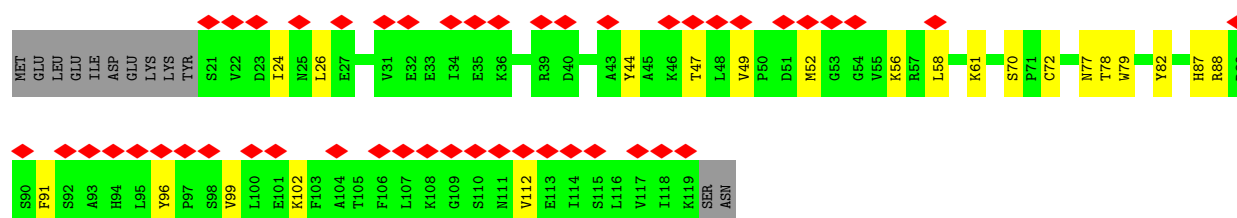
• Molecule 68: eS19

Chain ST0: 81% 16% 2%



• Molecule 69: uS10

Chain SU0: 42% 69% 20% 11%



- Molecule 70: eS21

Chain SV0: 



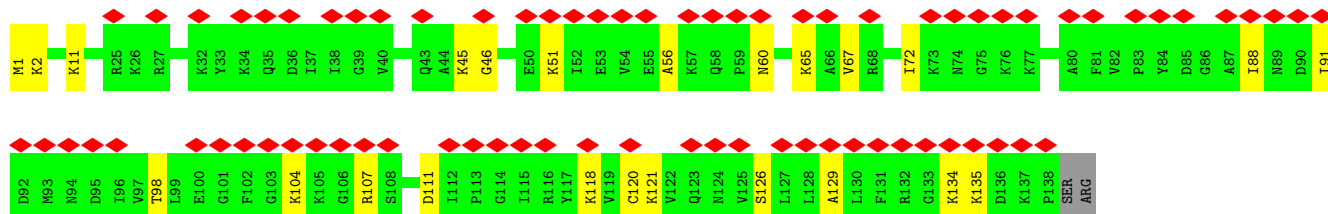
- Molecule 71: uS8

Chain SW0: 



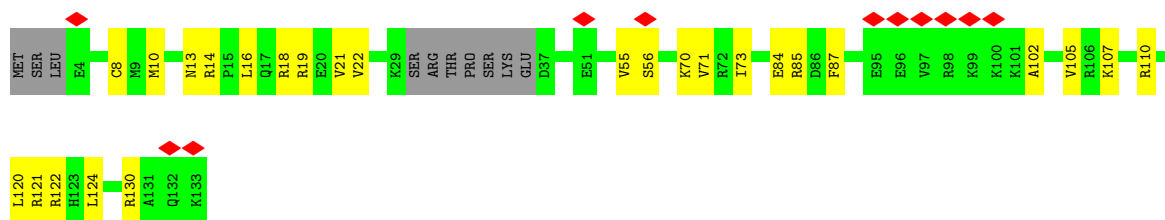
- Molecule 72: uS12

Chain SX0: 

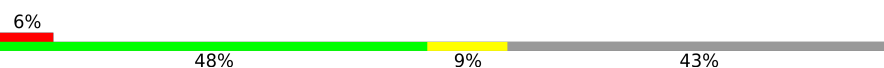


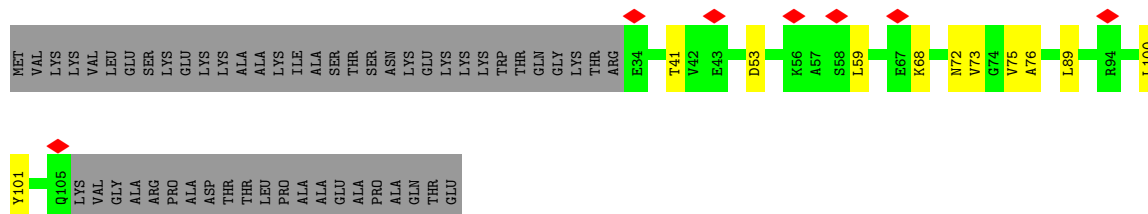
- Molecule 73: eS24

Chain SY0: 



- Molecule 74: eS25

Chain SZ0: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124947	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L50	0.59	0/58781	0.44	1/91678 (0.0%)
2	L70	0.53	0/2848	0.40	0/4439
3	LA0	0.55	1/1896 (0.1%)	0.67	3/2556 (0.1%)
4	LAA	0.57	0/1167	0.63	0/1560
5	LB0	0.53	0/2938	0.60	0/3942
6	LBB	0.47	0/538	0.51	0/715
7	LC0	0.58	0/2602	0.59	0/3503
8	LCC	0.38	0/787	0.57	0/1061
9	LD0	0.45	0/2156	0.57	0/2878
10	LDD	0.47	0/872	0.46	0/1170
11	LE0	0.36	0/1426	0.69	0/1921
12	LEE	0.54	0/1028	0.56	0/1370
13	LF0	0.50	0/2091	0.56	0/2796
14	LFF	0.52	0/849	0.53	0/1140
15	LG0	0.50	0/1664	0.57	0/2236
16	LGG	0.48	0/813	0.60	0/1086
17	LH0	0.40	0/1474	0.60	0/1978
18	LHH	0.51	0/1037	0.57	0/1379
19	LI0	0.48	0/1707	0.53	0/2277
20	LII	0.47	0/802	0.53	0/1069
21	LJ0	0.41	0/1353	0.55	0/1804
22	LJJ	0.58	0/715	0.59	0/939
23	LL0	0.55	0/1382	0.59	0/1850
24	LLL	0.53	0/461	0.56	0/612
25	LM0	0.42	0/806	0.50	0/1081
26	LMM	0.28	0/431	0.52	0/565
27	LN0	0.63	0/1684	0.56	0/2251
28	LNN	0.26	0/642	0.52	0/838
29	LO0	0.51	0/1628	0.51	0/2176
30	LOO	0.53	0/767	0.55	0/1013
31	LP0	0.55	0/1260	0.58	0/1694
32	LPP	0.50	0/613	0.54	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LQ0	0.52	0/1411	0.51	0/1891
34	LR0	0.48	0/1296	0.58	0/1723
35	LS0	0.51	0/1437	0.56	0/1914
36	LT0	0.51	0/1339	0.55	0/1789
37	LU0	0.27	0/480	0.75	0/668
38	LV0	0.52	1/1062 (0.1%)	0.54	0/1430
39	LW0	0.41	0/711	0.60	0/961
40	LX0	0.47	0/777	0.49	0/1047
41	LY0	0.53	0/1149	0.57	0/1516
42	LZ0	0.39	0/1017	0.52	0/1357
43	S60	0.42	0/32357	0.38	0/50521
44	SA0	0.27	0/999	0.57	0/1391
45	SAA	0.43	0/792	0.56	0/1058
46	SB0	0.40	0/1604	0.55	0/2148
47	SBB	0.35	0/651	0.62	0/868
48	SC0	0.38	0/1740	0.59	0/2336
49	SCC	0.34	0/423	0.59	0/569
50	SD0	0.31	0/1715	0.58	0/2297
51	SDD	0.36	0/497	0.67	0/659
52	SE0	0.39	0/2070	0.63	3/2780 (0.1%)
53	SEE	0.25	0/334	0.60	0/444
54	SF0	0.36	0/1463	0.57	0/1956
55	SG0	0.34	0/1783	0.56	0/2370
56	SGG	0.34	0/2343	0.62	0/3172
57	SH0	0.31	0/1014	0.53	0/1383
58	SI0	0.43	0/1376	0.55	0/1834
59	SJ0	0.31	0/1378	0.68	0/1842
60	SK0	0.32	0/605	0.66	0/818
61	SL0	0.45	0/1128	0.66	5/1509 (0.3%)
62	SN0	0.40	0/1160	0.49	0/1564
63	SO0	0.47	0/961	0.68	2/1291 (0.2%)
64	SP0	0.35	0/909	0.57	0/1218
65	SQ0	0.39	0/1030	0.59	0/1386
66	SR0	0.34	0/810	0.65	0/1095
67	SS0	0.35	0/1156	0.57	0/1546
68	ST0	0.39	0/1131	0.57	2/1505 (0.1%)
69	SU0	0.25	0/801	0.52	0/1077
70	SV0	0.33	0/468	0.55	0/637
71	SW0	0.45	0/1015	0.61	2/1358 (0.1%)
72	SX0	0.31	0/1102	0.63	0/1468
73	SY0	0.28	0/970	0.59	0/1287
74	SZ0	0.34	0/552	0.61	0/743
All	All	0.50	2/176234 (0.0%)	0.50	18/256820 (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	LAA	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	LV0	110	GLY	C-N	-5.42	1.22	1.33
3	LA0	222	PRO	CA-C	-5.42	1.48	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	SE0	42	ILE	N-CA-C	-6.01	104.26	109.19
3	LA0	163	GLY	CA-C-N	5.90	132.98	121.41
3	LA0	163	GLY	C-N-CA	5.90	132.98	121.41
61	SL0	79	GLN	CA-C-N	5.66	132.36	121.54
61	SL0	79	GLN	C-N-CA	5.66	132.36	121.54
52	SE0	138	TYR	CA-CB-CG	5.54	123.86	113.90
3	LA0	222	PRO	O-C-N	-5.47	118.58	121.15
71	SW0	54	ARG	CA-C-N	5.26	128.72	120.82
71	SW0	54	ARG	C-N-CA	5.26	128.72	120.82
52	SE0	42	ILE	CB-CA-C	5.24	114.46	109.33
63	SO0	122	ASP	CA-C-N	5.21	131.50	121.54
63	SO0	122	ASP	C-N-CA	5.21	131.50	121.54
61	SL0	131	ALA	CA-C-N	5.18	127.99	120.79
61	SL0	131	ALA	C-N-CA	5.18	127.99	120.79
61	SL0	80	GLU	N-CA-CB	-5.13	101.81	110.49
68	ST0	36	LYS	CA-C-N	5.10	131.28	121.54
68	ST0	36	LYS	C-N-CA	5.10	131.28	121.54
1	L50	434	A	C2'-C3'-O3'	5.02	121.23	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LAA	23	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L50	52573	0	26704	282	0
2	L70	2546	0	1284	13	0
3	LA0	1862	0	1962	27	0
4	LAA	1139	0	1192	22	0
5	LB0	2887	0	3005	56	0
6	LBB	527	0	529	7	0
7	LC0	2555	0	2610	28	0
8	LCC	774	0	815	10	0
9	LD0	2118	0	2171	26	0
10	LDD	854	0	901	5	0
11	LE0	1405	0	1461	19	0
12	LEE	1005	0	1050	7	0
13	LF0	2050	0	2091	24	0
14	LFF	832	0	848	7	0
15	LG0	1637	0	1722	13	0
16	LGG	802	0	848	8	0
17	LH0	1455	0	1490	22	0
18	LHH	1024	0	1102	17	0
19	LI0	1676	0	1747	29	0
20	LII	789	0	859	9	0
21	LJ0	1336	0	1399	12	0
22	LJJ	707	0	749	10	0
23	LL0	1354	0	1421	18	0
24	LLL	453	0	493	13	0
25	LM0	799	0	811	12	0
26	LMM	429	0	471	6	0
27	LN0	1654	0	1713	22	0
28	LNN	638	0	675	6	0
29	LO0	1601	0	1691	21	0
30	LOO	756	0	803	13	0
31	LP0	1236	0	1311	15	0
32	LPP	603	0	626	9	0
33	LQ0	1388	0	1461	16	0
34	LR0	1275	0	1332	15	0
35	LS0	1414	0	1485	24	0
36	LT0	1311	0	1355	25	0
37	LU0	481	0	205	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LV0	1048	0	1123	15	0
39	LW0	698	0	699	6	0
40	LX0	765	0	803	10	0
41	LY0	1138	0	1208	13	0
42	LZ0	1001	0	1062	16	0
43	S60	28876	0	14519	176	0
44	SA0	1000	0	442	0	0
45	SAA	778	0	796	13	0
46	SB0	1580	0	1651	27	0
47	SBB	642	0	684	14	0
48	SC0	1711	0	1804	35	0
49	SCC	419	0	440	7	0
50	SD0	1690	0	1792	38	0
51	SDD	488	0	500	8	0
52	SE0	2031	0	2100	35	0
53	SEE	334	0	290	9	0
54	SF0	1447	0	1526	17	0
55	SG0	1760	0	1875	22	0
56	SGG	2306	0	2268	40	0
57	SH0	1003	0	739	2	0
58	SI0	1353	0	1395	29	0
59	SJ0	1357	0	1411	30	0
60	SK0	592	0	612	5	0
61	SL0	1102	0	1132	16	0
62	SN0	1137	0	1180	14	0
63	SO0	950	0	995	21	0
64	SP0	896	0	958	17	0
65	SQ0	1012	0	1048	10	0
66	SR0	800	0	701	11	0
67	SS0	1140	0	1176	20	0
68	ST0	1115	0	1174	15	0
69	SU0	787	0	807	15	0
70	SV0	462	0	435	7	0
71	SW0	1001	0	1047	17	0
72	SX0	1089	0	1189	16	0
73	SY0	964	0	978	17	0
74	SZ0	548	0	573	6	0
75	L50	152	0	0	0	0
75	L70	4	0	0	0	0
75	LA0	1	0	0	0	0
75	LJJ	1	0	0	0	0
75	LV0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	S60	20	0	0	0	0
76	LGG	1	0	0	0	0
76	LJJ	1	0	0	0	0
76	LMM	1	0	0	0	0
76	LOO	1	0	0	0	0
76	LPP	1	0	0	0	0
76	SAA	1	0	0	0	0
76	SBB	1	0	0	0	0
76	SDD	1	0	0	0	0
77	LH0	23	0	12	1	0
All	All	165175	0	125536	1261	0

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

All (1261) 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)
48:SC0:221:CYS:HG	70:SV0:17:HIS:HD1	1.24	0.83
61:SL0:14:GLN:HE22	61:SL0:32:ARG:HE	1.27	0.82
1:L50:855:C:H42	1:L50:871:C:H42	1.39	0.70
8:LCC:16:PRO:HG3	8:LCC:82:VAL:HB	1.75	0.69
55:SG0:173:PRO:HG2	55:SG0:175:ILE:HD11	1.75	0.69
52:SE0:107:ARG:HG2	52:SE0:189:LEU:HB3	1.75	0.69
18:LHH:32:GLN:HE22	40:LX0:30:GLY:H	1.38	0.68
1:L50:1454:G:H21	16:LGG:79:ASN:HD21	1.40	0.68
61:SL0:32:ARG:NH1	61:SL0:52:TYR:O	2.27	0.68
1:L50:1300:G:N7	42:LZ0:15:ARG:NH1	2.42	0.68
17:LH0:110:VAL:HG12	17:LH0:122:ARG:HG2	1.76	0.68
1:L50:1873:A:N7	1:L50:2263:A:N6	2.43	0.67
56:SGG:34:LEU:HB3	56:SGG:46:TRP:HB2	1.77	0.67
1:L50:1825:A:N3	31:LP0:132:ARG:NH2	2.41	0.67
21:LJ0:90:GLU:HG2	21:LJ0:170:VAL:HB	1.76	0.67
71:SW0:27:VAL:HG22	71:SW0:56:GLY:HA3	1.78	0.66
12:LEE:40:ASN:HD22	12:LEE:43:ARG:H	1.44	0.66
24:LLL:21:ARG:HH12	24:LLL:24:PRO:HG3	1.60	0.66
29:LO0:116:ARG:NH1	29:LO0:163:GLU:OE1	2.28	0.66
23:LL0:45:PRO:HG2	23:LL0:129:ALA:HB1	1.78	0.65
27:LN0:184:ILE:O	27:LN0:194:ARG:NH2	2.30	0.65
1:L50:1137:G:OP2	7:LC0:106:ARG:NH1	2.29	0.65
1:L50:595:C:H42	1:L50:606:A:H61	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:353:U:H5''	23:LL0:99:LYS:HE3	1.78	0.65
3:LA0:8:LEU:HD21	3:LA0:223:PRO:HB2	1.79	0.65
43:S60:1090:G:N2	51:SDD:49:CYS:SG	2.69	0.65
62:SN0:87:ASP:HB3	62:SN0:125:LEU:HD21	1.79	0.64
43:S60:440:G:H22	43:S60:456:A:H5'	1.62	0.64
9:LD0:38:ASP:OD1	36:LT0:69:ARG:NH2	2.30	0.64
43:S60:1156:G:N7	68:ST0:99:ARG:NH2	2.46	0.64
29:LO0:36:CYS:SG	29:LO0:156:LYS:NZ	2.70	0.64
1:L50:2494:G:H21	17:LH0:152:GLN:HE22	1.45	0.64
25:LM0:11:LEU:HD12	25:LM0:57:ASP:HB2	1.80	0.64
68:ST0:117:LYS:HA	68:ST0:122:ARG:HA	1.80	0.64
30:LOO:53:GLN:HE22	30:LOO:60:THR:H	1.44	0.63
1:L50:2549:G:H5''	5:LB0:128:ARG:HD3	1.79	0.63
1:L50:1091:C:OP1	7:LC0:196:ARG:NH1	2.31	0.63
1:L50:2045:G:OP1	19:LI0:24:ARG:NH1	2.32	0.63
71:SW0:2:ASN:ND2	71:SW0:73:CYS:SG	2.72	0.63
1:L50:2455:C:OP2	34:LR0:62:ARG:NH2	2.32	0.63
13:LF0:142:ARG:NH2	13:LF0:192:GLU:OE1	2.32	0.63
1:L50:502:C:OP1	33:LQ0:145:ARG:NH1	2.32	0.62
5:LB0:28:SER:O	5:LB0:272:ARG:NH2	2.31	0.62
33:LQ0:100:VAL:HG22	33:LQ0:120:HIS:HB2	1.81	0.62
1:L50:393:A:H5'	24:LLL:40:LYS:HZ3	1.64	0.62
29:LO0:16:GLY:HA2	29:LO0:82:LEU:HD21	1.82	0.62
18:LHH:58:ARG:NH2	40:LX0:16:THR:O	2.32	0.62
45:SAA:37:LYS:HG2	45:SAA:72:GLN:HG2	1.81	0.62
51:SDD:5:ILE:HD11	64:SP0:30:LEU:HB2	1.81	0.62
1:L50:2229:A:OP1	19:LI0:154:ARG:NH1	2.33	0.62
73:SY0:56:SER:HB2	73:SY0:70:LYS:HG3	1.82	0.62
23:LL0:71:GLY:O	23:LL0:98:ARG:NH1	2.33	0.62
54:SF0:18:ARG:HE	54:SF0:36:SER:HA	1.63	0.62
55:SG0:31:LEU:HD21	55:SG0:62:MET:HE3	1.82	0.62
1:L50:2109:C:HO2'	1:L50:2135:G:HO2'	1.42	0.62
5:LB0:27:GLN:HE21	5:LB0:272:ARG:HE	1.48	0.62
11:LE0:58:VAL:HG12	11:LE0:104:ARG:HA	1.82	0.62
72:SX0:104:LYS:HG3	72:SX0:107:ARG:HB2	1.81	0.62
19:LI0:38:ARG:NH1	19:LI0:83:ASP:O	2.33	0.61
58:SI0:133:ASN:HB3	58:SI0:138:LYS:HB2	1.82	0.61
1:L50:304:G:N7	18:LHH:106:LYS:NZ	2.48	0.61
43:S60:1148:U:H5'	68:ST0:73:GLY:HA3	1.82	0.61
19:LI0:170:ALA:HA	19:LI0:177:SER:HA	1.81	0.61
53:SEE:33:ARG:NH2	59:SJ0:128:HIS:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:397:C:N3	1:L50:569:G:O2'	2.33	0.61
1:L50:1296:A:N6	1:L50:1461:C:O2	2.33	0.61
43:S60:1194:U:OP2	64:SP0:43:ARG:NH2	2.33	0.61
5:LB0:10:ARG:NH1	5:LB0:261:THR:O	2.33	0.61
29:LO0:46:ILE:HG12	29:LO0:135:ALA:HB2	1.82	0.61
1:L50:1155:G:N7	31:LP0:26:SER:OG	2.32	0.61
43:S60:246:G:H3'	61:SL0:134:LYS:HB2	1.83	0.61
5:LB0:92:TYR:HB2	5:LB0:154:VAL:HB	1.83	0.61
21:LJ0:28:GLU:HG3	21:LJ0:32:ARG:HD3	1.83	0.61
60:SK0:28:LYS:O	60:SK0:38:ASN:ND2	2.31	0.61
28:LNN:2:SER:N	43:S60:1369:C:OP1	2.33	0.61
56:SGG:109:LEU:HD21	56:SGG:123:THR:HB	1.83	0.61
1:L50:472:U:OP1	4:LAA:21:ARG:NH2	2.34	0.61
43:S60:1141:G:OP1	65:SQ0:72:ARG:NH1	2.33	0.61
7:LC0:155:ILE:HG13	7:LC0:214:ILE:HG21	1.81	0.60
29:LO0:60:ARG:HA	29:LO0:69:PRO:HD2	1.83	0.60
56:SGG:289:LEU:HD21	56:SGG:292:VAL:HG23	1.83	0.60
5:LB0:10:ARG:NH2	5:LB0:11:HIS:O	2.34	0.60
1:L50:730:C:OP1	33:LQ0:139:ARG:NH1	2.34	0.60
50:SD0:14:LYS:HG2	50:SD0:79:LEU:HD21	1.83	0.60
43:S60:505:U:OP2	43:S60:680:C:N4	2.35	0.60
11:LE0:26:PRO:HB2	11:LE0:30:LEU:HB2	1.84	0.60
13:LF0:45:THR:HG22	13:LF0:192:GLU:HB2	1.83	0.60
1:L50:169:G:H5'	23:LL0:55:VAL:HB	1.82	0.60
58:SI0:84:HIS:NE2	58:SI0:97:THR:OG1	2.31	0.60
29:LO0:26:LEU:O	29:LO0:100:ARG:NH1	2.33	0.60
1:L50:1459:C:OP2	42:LZ0:56:ARG:NH2	2.35	0.60
13:LF0:141:LEU:HD22	13:LF0:195:ILE:HG23	1.84	0.60
64:SP0:44:ARG:NH2	64:SP0:53:GLU:OE2	2.34	0.60
1:L50:1696:C:OP2	30:LOO:41:ARG:NH1	2.34	0.60
23:LL0:18:ARG:HB2	27:LN0:197:THR:HG22	1.84	0.60
1:L50:830:A:H4'	36:LT0:115:ARG:HD3	1.83	0.59
61:SL0:98:ARG:HH12	72:SX0:2:LYS:HA	1.65	0.59
9:LD0:48:ARG:NH2	9:LD0:70:ASP:OD2	2.35	0.59
43:S60:344:G:H5'	72:SX0:45:LYS:HE3	1.83	0.59
11:LE0:62:GLU:OE2	14:LFF:99:LYS:NZ	2.35	0.59
7:LC0:259:GLU:HB3	7:LC0:270:LEU:HD23	1.84	0.59
1:L50:1525:C:OP1	5:LB0:245:ARG:NH2	2.34	0.59
1:L50:1861:C:O2'	5:LB0:264:ARG:NH1	2.33	0.59
29:LO0:26:LEU:HD11	29:LO0:101:LEU:HG	1.84	0.59
1:L50:1692:G:OP1	20:LII:67:ARG:NH1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SGG:230:CYS:SG	56:SGG:231:ALA:N	2.75	0.59
56:SGG:115:ASN:HD22	56:SGG:120:LYS:H	1.50	0.59
56:SGG:37:ALA:HB2	56:SGG:71:VAL:HB	1.85	0.59
56:SGG:180:TRP:HB3	56:SGG:187:VAL:HA	1.85	0.59
1:L50:901:G:OP2	14:LFF:71:ARG:NH2	2.34	0.58
46:SB0:90:VAL:HA	46:SB0:100:SER:HA	1.85	0.58
49:SCC:12:GLN:HB2	49:SCC:27:GLN:HB3	1.85	0.58
50:SD0:64:SER:OG	50:SD0:68:ARG:NH1	2.36	0.58
1:L50:1195:G:O6	24:LLL:2:GLY:N	2.36	0.58
1:L50:1725:A:H62	43:S60:1356:A:H1'	1.67	0.58
1:L50:1368:G:H1	1:L50:1397:C:H42	1.50	0.58
19:LI0:21:ARG:O	19:LI0:24:ARG:NH2	2.36	0.58
19:LI0:38:ARG:NH2	19:LI0:45:GLU:OE1	2.35	0.58
27:LN0:114:ARG:NH1	27:LN0:151:ILE:O	2.36	0.58
1:L50:2564:G:H1'	31:LP0:70:ARG:HD3	1.85	0.58
1:L50:1632:A:OP2	3:LA0:192:ARG:NH1	2.36	0.58
1:L50:814:A:O2'	6:LBB:41:ASN:ND2	2.36	0.58
5:LB0:77:THR:HG21	5:LB0:324:ILE:HG12	1.84	0.58
50:SD0:60:GLY:HA3	50:SD0:65:ARG:HG2	1.84	0.58
63:SO0:63:GLN:HG2	63:SO0:106:ASN:HD21	1.67	0.58
1:L50:1178:C:OP1	34:LR0:8:ARG:NH1	2.36	0.58
52:SE0:35:PRO:HD2	52:SE0:83:PRO:HG2	1.85	0.58
67:SS0:29:ILE:HG22	67:SS0:41:GLN:HB2	1.85	0.58
54:SF0:62:ARG:NH1	54:SF0:139:ASN:OD1	2.37	0.58
56:SGG:125:SER:OG	56:SGG:127:ASP:OD1	2.22	0.58
13:LF0:223:GLY:O	13:LF0:251:ARG:NH2	2.37	0.58
31:LP0:37:LEU:HD21	31:LP0:49:LEU:HD11	1.86	0.58
1:L50:1460:G:N7	42:LZ0:56:ARG:NH1	2.52	0.58
46:SB0:148:ARG:HG2	46:SB0:208:PRO:HG2	1.85	0.58
59:SJ0:146:ILE:HG22	59:SJ0:148:LYS:H	1.69	0.58
1:L50:2255:A:H5''	19:LI0:114:GLY:HA2	1.85	0.57
69:SU0:24:ILE:HB	69:SU0:91:PHE:HB2	1.86	0.57
43:S60:1115:G:OP1	67:SS0:145:THR:N	2.36	0.57
43:S60:1068:G:N2	43:S60:1071:G:OP2	2.36	0.57
1:L50:1699:G:N2	1:L50:1699:G:OP2	2.37	0.57
4:LAA:96:ILE:O	4:LAA:120:ARG:NH2	2.35	0.57
5:LB0:216:ILE:HB	5:LB0:333:ALA:HB3	1.87	0.57
54:SF0:28:LEU:HD12	54:SF0:108:VAL:HG12	1.86	0.57
71:SW0:28:THR:H	71:SW0:31:THR:HG22	1.69	0.57
19:LI0:93:PRO:O	19:LI0:125:ARG:NH1	2.38	0.57
48:SC0:155:LYS:NZ	71:SW0:88:ASP:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD0:58:VAL:HG11	50:SD0:88:VAL:HG21	1.85	0.57
59:SJ0:114:LEU:HA	59:SJ0:117:ARG:HB2	1.86	0.57
7:LC0:133:LEU:HD11	11:LE0:7:LEU:HD23	1.87	0.57
13:LF0:85:ARG:NH2	13:LF0:105:LEU:O	2.37	0.57
43:S60:1008:G:OP1	66:SR0:68:LYS:NZ	2.37	0.57
1:L50:1345:C:O2'	1:L50:1348:C:N4	2.37	0.57
7:LC0:286:VAL:HA	7:LC0:289:LEU:HD23	1.87	0.57
43:S60:263:C:H5''	58:SI0:16:ALA:HB2	1.86	0.57
43:S60:511:G:O2'	71:SW0:55:GLN:NE2	2.37	0.57
58:SI0:89:GLU:OE1	58:SI0:92:ARG:NH1	2.38	0.57
43:S60:1195:G:O6	64:SP0:43:ARG:NH1	2.38	0.57
45:SAA:45:ILE:HD11	63:SO0:113:VAL:HG11	1.87	0.57
43:S60:1253:U:OP2	54:SF0:54:LYS:NZ	2.37	0.57
1:L50:761:G:H5'	19:LI0:40:ARG:HD2	1.86	0.56
24:LLL:10:LYS:NZ	40:LX0:78:ARG:O	2.33	0.56
21:LJ0:109:HIS:HD2	21:LJ0:123:TYR:H	1.53	0.56
49:SCC:50:VAL:HG13	54:SF0:27:SER:HA	1.86	0.56
63:SO0:78:HIS:ND1	63:SO0:111:GLY:O	2.37	0.56
1:L50:141:C:H5''	23:LL0:14:LYS:HG2	1.88	0.56
1:L50:238:A:OP2	18:LHH:108:ARG:NE	2.37	0.56
1:L50:1132:C:H4'	11:LE0:10:LEU:HD13	1.86	0.56
7:LC0:140:ARG:HD3	7:LC0:179:ARG:HD3	1.86	0.56
20:LII:9:ARG:NH1	20:LII:10:VAL:O	2.38	0.56
43:S60:746:G:OP1	62:SN0:2:ALA:N	2.38	0.56
48:SC0:236:ASN:ND2	48:SC0:239:SER:OG	2.38	0.56
52:SE0:125:ARG:NH2	52:SE0:157:ASN:OD1	2.37	0.56
71:SW0:37:LYS:NZ	71:SW0:107:MET:O	2.38	0.56
1:L50:300:A:N6	18:LHH:105:CYS:SG	2.78	0.56
7:LC0:91:ASN:HB3	7:LC0:99:ALA:H	1.70	0.56
36:LT0:121:ARG:HE	36:LT0:123:GLU:HG3	1.70	0.56
48:SC0:106:ALA:HA	48:SC0:190:GLY:HA3	1.88	0.56
1:L50:2629:U:OP1	10:LDD:77:ARG:NH2	2.38	0.56
2:L70:16:C:OP1	21:LJ0:147:ARG:NH1	2.38	0.56
8:LCC:48:ASN:ND2	8:LCC:76:ASN:OD1	2.39	0.56
11:LE0:34:ILE:HD11	12:LEE:7:VAL:HG22	1.87	0.56
13:LF0:148:ARG:NH1	13:LF0:253:ILE:O	2.38	0.56
19:LI0:31:LEU:HD22	19:LI0:65:LEU:HB3	1.87	0.56
45:SAA:32:LYS:O	45:SAA:37:LYS:NZ	2.38	0.56
53:SEE:37:ARG:NH1	59:SJ0:30:GLY:O	2.39	0.56
13:LF0:154:SER:OG	13:LF0:156:ARG:NH1	2.39	0.56
43:S60:43:C:OP2	43:S60:346:A:N6	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S60:121:A:O2'	55:SG0:189:LYS:NZ	2.39	0.56
1:L50:2160:C:O2'	30:LOO:88:GLN:NE2	2.39	0.56
5:LB0:83:PRO:O	5:LB0:162:GLN:NE2	2.38	0.56
9:LD0:48:ARG:NH1	9:LD0:123:ASP:OD2	2.39	0.56
43:S60:132:C:OP1	73:SY0:121:ARG:NH1	2.36	0.56
43:S60:281:A:O2'	61:SL0:97:LYS:NZ	2.38	0.56
52:SE0:87:MET:HE1	52:SE0:236:ILE:HD13	1.88	0.56
5:LB0:278:LYS:NZ	5:LB0:323:GLY:O	2.39	0.56
39:LW0:90:ILE:HG12	55:SG0:159:GLN:HB3	1.88	0.56
56:SGG:38:SER:OG	56:SGG:39:ARG:N	2.36	0.56
69:SU0:49:VAL:HG23	69:SU0:52:MET:HB2	1.86	0.56
3:LA0:97:LYS:HB3	3:LA0:152:SER:HB3	1.88	0.55
5:LB0:92:TYR:HB3	5:LB0:99:LEU:HD22	1.88	0.55
43:S60:10:G:H21	48:SC0:86:LYS:HA	1.71	0.55
43:S60:606:G:H21	63:SO0:36:THR:HG21	1.72	0.55
52:SE0:21:ASP:OD1	52:SE0:21:ASP:N	2.37	0.55
73:SY0:10:MET:HA	73:SY0:21:VAL:HG12	1.88	0.55
4:LAA:125:MET:HB3	4:LAA:147:SER:HB3	1.87	0.55
52:SE0:126:VAL:HA	52:SE0:141:THR:HA	1.87	0.55
9:LD0:83:ARG:NH1	9:LD0:84:TYR:OH	2.38	0.55
13:LF0:167:ILE:HD11	33:LQ0:5:ALA:HB2	1.88	0.55
41:LY0:31:SER:HA	41:LY0:48:PRO:HA	1.87	0.55
43:S60:599:U:H3	43:S60:635:G:H22	1.53	0.55
59:SJ0:66:ILE:HG22	59:SJ0:94:ILE:HD12	1.88	0.55
70:SV0:27:PHE:O	70:SV0:41:LEU:N	2.36	0.55
1:L50:138:U:O2	30:LOO:52:LYS:NZ	2.39	0.55
11:LE0:18:ILE:HD12	12:LEE:73:LEU:HB3	1.88	0.55
1:L50:2344:U:H2'	1:L50:2345:U:H2'	1.89	0.55
1:L50:413:A:H5''	41:LY0:88:LYS:HG2	1.88	0.55
1:L50:1512:C:OP1	34:LR0:21:LYS:NZ	2.39	0.55
43:S60:1129:A:H62	43:S60:1178:A:H62	1.55	0.55
1:L50:1362:C:O2	1:L50:1404:G:N2	2.35	0.55
1:L50:2244:G:H5'	19:LI0:63:GLU:HB3	1.87	0.55
56:SGG:239:THR:HG22	56:SGG:259:VAL:HG11	1.89	0.55
1:L50:580:G:O2'	16:LGG:15:ASN:ND2	2.38	0.55
15:LG0:65:LEU:HD22	15:LG0:154:LEU:HD11	1.89	0.55
33:LQ0:68:ALA:HA	33:LQ0:97:MET:HE1	1.88	0.55
43:S60:1141:G:N2	43:S60:1246:C:O2	2.40	0.55
50:SD0:127:LYS:NZ	50:SD0:134:CYS:SG	2.80	0.55
52:SE0:59:LYS:NZ	73:SY0:84:GLU:O	2.39	0.55
1:L50:1776:G:O2'	1:L50:1779:U:OP2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S60:239:G:OP2	58:SI0:146:ARG:NH1	2.40	0.55
56:SGG:6:ARG:HB3	56:SGG:329:VAL:HB	1.89	0.55
1:L50:331:G:H5'	27:LN0:98:LEU:HG	1.88	0.55
1:L50:1317:G:OP2	3:LA0:65:ARG:NH2	2.40	0.55
8:LCC:99:GLU:OE1	62:SN0:43:LYS:NZ	2.40	0.55
30:LOO:79:ARG:NH1	30:LOO:84:ASP:OD2	2.39	0.55
43:S60:895:C:N4	43:S60:1114:U:O5'	2.40	0.55
49:SCC:5:VAL:HG12	49:SCC:54:LEU:HB3	1.89	0.55
54:SF0:154:MET:HG2	54:SF0:155:LYS:HG3	1.88	0.55
1:L50:869:C:OP2	6:LBB:5:LYS:NZ	2.39	0.54
42:LZ0:81:VAL:HG23	42:LZ0:83:LEU:HD13	1.89	0.54
43:S60:240:G:N7	58:SI0:146:ARG:NH2	2.56	0.54
1:L50:213:G:O2'	15:LG0:89:ARG:NH2	2.40	0.54
5:LB0:185:THR:O	5:LB0:188:ASP:N	2.37	0.54
13:LF0:104:ARG:NH1	13:LF0:212:LEU:O	2.40	0.54
16:LGG:41:VAL:HG12	16:LGG:56:ILE:HD13	1.90	0.54
1:L50:333:G:OP2	27:LN0:68:ARG:NH1	2.37	0.54
1:L50:1047:G:O3'	35:LS0:121:LYS:NZ	2.41	0.54
1:L50:1170:G:N2	1:L50:1173:A:OP2	2.40	0.54
6:LBB:59:GLU:OE1	6:LBB:60:HIS:NE2	2.40	0.54
43:S60:1049:G:N2	43:S60:1050:G:O6	2.36	0.54
46:SB0:59:GLU:HB3	46:SB0:63:LEU:HD23	1.87	0.54
46:SB0:72:GLY:HA3	63:SO0:112:ARG:HH11	1.72	0.54
48:SC0:236:ASN:HD22	70:SV0:24:GLN:HG2	1.72	0.54
50:SD0:65:ARG:HA	50:SD0:68:ARG:HB2	1.89	0.54
1:L50:1851:G:OP2	29:LO0:89:TYR:OH	2.24	0.54
1:L50:2286:G:O2'	26:LMM:97:TYR:O	2.24	0.54
1:L50:2322:C:OP1	38:LV0:43:LYS:NZ	2.41	0.54
8:LCC:84:ASP:HB3	8:LCC:89:ILE:HD11	1.89	0.54
9:LD0:233:HIS:HB2	9:LD0:236:TYR:HE2	1.72	0.54
17:LH0:100:VAL:HG12	17:LH0:111:VAL:HG22	1.90	0.54
43:S60:844:A:O2'	43:S60:1366:A:N7	2.38	0.54
46:SB0:173:VAL:HG11	46:SB0:199:ILE:HG12	1.90	0.54
1:L50:1091:C:O2'	7:LC0:42:ARG:NH2	2.40	0.54
35:LS0:26:GLN:HA	36:LT0:146:ASN:HD21	1.71	0.54
43:S60:26:U:O2'	43:S60:344:G:N2	2.40	0.54
52:SE0:125:ARG:NH1	52:SE0:225:ALA:O	2.40	0.54
1:L50:237:C:H5'	18:LHH:99:MET:HA	1.90	0.54
1:L50:1373:C:OP1	42:LZ0:31:ARG:NH1	2.41	0.54
43:S60:241:U:O2	58:SI0:5:ARG:NH2	2.40	0.54
46:SB0:124:GLU:HG2	46:SB0:142:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SF0:67:LEU:HD21	54:SF0:164:ILE:HD11	1.87	0.54
1:L50:2548:C:OP2	5:LB0:126:LYS:NZ	2.39	0.54
3:LA0:192:ARG:NH2	3:LA0:209:GLN:OE1	2.41	0.54
29:LO0:31:THR:HA	29:LO0:100:ARG:HB3	1.90	0.54
43:S60:1164:C:H5'	68:ST0:76:ARG:HD2	1.89	0.54
48:SC0:141:PHE:O	71:SW0:95:GLN:NE2	2.40	0.54
43:S60:307:G:OP2	58:SI0:47:ARG:NH1	2.35	0.54
43:S60:308:A:OP1	58:SI0:49:ARG:NH1	2.37	0.54
43:S60:544:A:O2'	59:SJ0:9:ARG:NH2	2.39	0.54
1:L50:1305:C:OP2	16:LGG:74:ARG:NH2	2.35	0.54
43:S60:1042:G:OP1	69:SU0:87:HIS:ND1	2.40	0.54
45:SAA:13:LYS:O	45:SAA:15:ARG:NH1	2.41	0.54
46:SB0:130:CYS:SG	46:SB0:136:HIS:ND1	2.75	0.54
1:L50:536:A:N6	1:L50:538:C:O2'	2.40	0.53
5:LB0:115:LEU:HA	5:LB0:118:PHE:HD2	1.72	0.53
58:SI0:164:ASN:HA	58:SI0:167:ILE:HG12	1.90	0.53
43:S60:1065:C:OP2	54:SF0:50:ARG:NH1	2.40	0.53
43:S60:1318:G:O2'	43:S60:1322:A:N6	2.41	0.53
45:SAA:44:LEU:HD21	63:SO0:115:ASP:HB2	1.90	0.53
55:SG0:54:GLY:HA3	55:SG0:62:MET:HE2	1.90	0.53
56:SGG:265:GLY:HA3	56:SGG:270:ILE:HG23	1.90	0.53
1:L50:1477:C:H41	24:LLL:3:SER:HB2	1.73	0.53
41:LY0:123:ASN:OD1	41:LY0:126:ARG:NH2	2.42	0.53
43:S60:1163:G:O6	50:SD0:2:VAL:N	2.41	0.53
47:SBB:31:PHE:HB2	47:SBB:81:ILE:HG21	1.89	0.53
58:SI0:117:LEU:HD11	58:SI0:124:LYS:HD2	1.89	0.53
13:LF0:188:ILE:HD11	13:LF0:204:LEU:HD13	1.91	0.53
17:LH0:46:ASP:OD1	17:LH0:55:ARG:NH2	2.41	0.53
35:LS0:11:ARG:HB2	35:LS0:67:LEU:HD11	1.90	0.53
61:SL0:123:THR:HG23	61:SL0:144:LYS:HB3	1.90	0.53
68:ST0:38:SER:HB3	68:ST0:41:LYS:HG2	1.90	0.53
1:L50:343:G:O6	1:L50:350:C:N4	2.42	0.53
43:S60:42:A:H1'	43:S60:287:G:H1'	1.90	0.53
52:SE0:208:ALA:HB2	52:SE0:222:THR:HG22	1.89	0.53
1:L50:558:C:OP1	7:LC0:97:ARG:NH2	2.39	0.53
13:LF0:188:ILE:HG23	13:LF0:193:GLU:HB3	1.90	0.53
5:LB0:353:ASP:OD1	5:LB0:357:LYS:NZ	2.41	0.53
43:S60:1006:C:O2'	66:SR0:10:LYS:NZ	2.41	0.53
56:SGG:28:THR:OG1	56:SGG:31:ALA:O	2.27	0.53
64:SP0:112:MET:HE2	67:SS0:126:MET:HB2	1.91	0.53
1:L50:611:G:OP2	34:LR0:92:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LAA:142:GLY:O	4:LAA:143:ARG:NH2	2.39	0.53
33:LQ0:88:ASP:O	33:LQ0:111:LYS:NZ	2.41	0.53
46:SB0:140:PHE:O	46:SB0:215:ALA:N	2.40	0.53
49:SCC:55:ASP:OD2	49:SCC:58:ARG:NH2	2.42	0.53
1:L50:1377:C:O2'	1:L50:1390:A:N3	2.40	0.53
1:L50:2183:G:H5''	30:LOO:73:LYS:HD2	1.90	0.53
9:LD0:209:ASP:OD1	9:LD0:209:ASP:N	2.40	0.53
1:L50:2435:G:OP1	5:LB0:19:ARG:NH2	2.41	0.52
2:L70:13:A:OP1	2:L70:109:U:O2'	2.24	0.52
17:LH0:23:ARG:NH1	17:LH0:41:PHE:O	2.42	0.52
18:LHH:80:LEU:O	22:LJJ:87:ARG:NH2	2.39	0.52
29:LO0:120:PRO:HB3	35:LS0:173:ILE:HD13	1.90	0.52
52:SE0:188:ASN:OD1	52:SE0:216:ARG:NH2	2.43	0.52
56:SGG:161:ARG:HB3	56:SGG:164:ASP:HB2	1.91	0.52
58:SI0:83:TYR:HB3	58:SI0:101:VAL:HB	1.91	0.52
1:L50:2167:G:OP1	20:LII:2:ARG:NH1	2.42	0.52
15:LG0:14:ARG:HB3	15:LG0:31:LEU:HD11	1.91	0.52
19:LI0:174:THR:HG22	19:LI0:196:HIS:HA	1.91	0.52
1:L50:936:G:OP2	26:LMM:110:LYS:NZ	2.43	0.52
1:L50:1579:U:OP2	34:LR0:74:ARG:NH2	2.43	0.52
5:LB0:53:MET:HG2	5:LB0:77:THR:HB	1.91	0.52
25:LM0:96:THR:HA	25:LM0:99:GLU:HB2	1.91	0.52
43:S60:444:G:OP2	72:SX0:65:LYS:NZ	2.43	0.52
43:S60:1400:A:N6	46:SB0:154:ARG:O	2.43	0.52
51:SDD:28:CYS:HB2	51:SDD:46:CYS:HB3	1.92	0.52
1:L50:277:G:OP1	41:LY0:15:ARG:NH2	2.39	0.52
1:L50:1186:G:O2'	1:L50:1513:G:N2	2.42	0.52
5:LB0:95:THR:HG22	5:LB0:97:GLN:H	1.75	0.52
23:LL0:103:LYS:NZ	23:LL0:107:ASP:OD2	2.42	0.52
35:LS0:113:ASP:OD1	35:LS0:117:ARG:NH1	2.43	0.52
43:S60:121:A:H1'	43:S60:123:A:H8	1.74	0.52
43:S60:194:G:O6	55:SG0:192:ARG:NH2	2.42	0.52
48:SC0:181:VAL:HG23	48:SC0:182:PRO:HD3	1.92	0.52
50:SD0:131:ALA:HA	50:SD0:191:PRO:HD3	1.91	0.52
5:LB0:167:LYS:O	5:LB0:170:ARG:NH1	2.42	0.52
5:LB0:285:ASN:HB3	5:LB0:288:GLU:HG2	1.91	0.52
28:LNN:60:LYS:HG3	28:LNN:63:ARG:HH21	1.74	0.52
33:LQ0:67:LEU:HD13	33:LQ0:99:ILE:HD13	1.91	0.52
38:LV0:40:ILE:HD11	38:LV0:64:SER:HB3	1.91	0.52
56:SGG:72:ALA:HB3	56:SGG:81:VAL:HB	1.91	0.52
1:L50:37:G:O2'	1:L50:99:A:N1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LOO:53:GLN:NE2	30:LOO:60:THR:OG1	2.42	0.52
59:SJ0:126:SER:O	59:SJ0:130:ALA:N	2.43	0.52
43:S60:533:C:OP1	52:SE0:22:LYS:NZ	2.42	0.52
46:SB0:177:GLU:O	46:SB0:189:LYS:NZ	2.38	0.52
48:SC0:237:PRO:HA	48:SC0:240:ARG:HB3	1.92	0.52
50:SD0:13:GLU:HG3	50:SD0:79:LEU:HD22	1.90	0.52
42:LZ0:99:LYS:HA	42:LZ0:102:ILE:HG22	1.91	0.52
45:SAA:58:ILE:HG13	63:SO0:12:PHE:HZ	1.74	0.52
49:SCC:16:LYS:HD3	49:SCC:24:THR:HB	1.92	0.52
1:L50:874:G:OP2	6:LBB:14:ARG:NH1	2.42	0.52
1:L50:1807:C:O2	38:LV0:21:GLN:NE2	2.38	0.52
1:L50:2502:C:O2'	26:LMM:103:ARG:NH1	2.42	0.52
4:LAA:82:ILE:HB	4:LAA:87:LEU:HD12	1.91	0.52
30:LOO:71:THR:HG22	30:LOO:95:LYS:HG2	1.90	0.52
42:LZ0:8:VAL:HB	42:LZ0:121:LEU:HD12	1.92	0.52
65:SQ0:17:ALA:HB2	65:SQ0:74:GLY:HA3	1.92	0.52
67:SS0:43:LYS:HG2	67:SS0:112:ILE:HD12	1.92	0.52
29:LOO:115:GLU:HG2	35:LS0:168:LEU:HD22	1.90	0.52
1:L50:2305:G:O3'	38:LV0:46:ARG:NH2	2.43	0.51
2:L70:61:U:O3'	9:LD0:255:ARG:NH1	2.43	0.51
48:SC0:162:SER:O	48:SC0:162:SER:OG	2.21	0.51
56:SGG:276:GLN:HA	56:SGG:303:ARG:HG3	1.92	0.51
67:SS0:15:PRO:HB2	67:SS0:18:ILE:HD11	1.93	0.51
69:SU0:26:LEU:HD12	69:SU0:112:VAL:HG11	1.92	0.51
25:LM0:15:ARG:NH1	35:LS0:160:LEU:O	2.41	0.51
5:LB0:84:MET:HG2	5:LB0:161:THR:HA	1.92	0.51
5:LB0:343:ASN:ND2	5:LB0:345:GLU:O	2.44	0.51
18:LHH:3:ILE:O	18:LHH:53:ARG:NH1	2.42	0.51
42:LZ0:46:THR:HG22	42:LZ0:49:MET:HE3	1.92	0.51
43:S60:862:G:N1	43:S60:1215:G:OP2	2.39	0.51
1:L50:930:A:N3	1:L50:2246:C:O2'	2.41	0.51
1:L50:1274:A:H1'	1:L50:1277:C:H41	1.75	0.51
11:LE0:169:MET:HE1	11:LE0:178:LEU:HD11	1.92	0.51
17:LH0:90:LYS:HB2	17:LH0:178:LEU:HG	1.92	0.51
17:LH0:103:GLU:OE1	17:LH0:122:ARG:NH1	2.38	0.51
40:LX0:39:LEU:HD23	40:LX0:43:ASN:HD22	1.74	0.51
43:S60:314:C:O2'	55:SG0:91:ARG:O	2.24	0.51
43:S60:380:G:O2'	43:S60:544:A:N3	2.42	0.51
48:SC0:38:ASP:HA	48:SC0:41:ILE:HD12	1.92	0.51
7:LC0:51:VAL:HG21	7:LC0:98:LEU:HD21	1.91	0.51
17:LH0:121:ARG:NH1	17:LH0:160:ASN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LM0:59:VAL:HG12	25:LM0:61:ILE:HG12	1.92	0.51
27:LN0:181:ASN:O	27:LN0:195:ARG:NH2	2.42	0.51
43:S60:54:A:OP1	73:SY0:110:ARG:NH2	2.39	0.51
43:S60:534:C:O2	43:S60:553:G:N2	2.44	0.51
43:S60:1294:G:O2'	43:S60:1346:A:N6	2.43	0.51
53:SEE:54:MET:HE2	53:SEE:56:MET:HG2	1.92	0.51
64:SP0:44:ARG:HH22	64:SP0:83:THR:HG23	1.76	0.51
29:LO0:75:PRO:HB3	29:LO0:137:TYR:HB3	1.93	0.51
35:LS0:81:ILE:HG21	35:LS0:110:LEU:HD22	1.92	0.51
43:S60:168:G:N7	61:SL0:16:LYS:NZ	2.57	0.51
43:S60:381:A:OP2	59:SJ0:38:ARG:NH2	2.36	0.51
50:SD0:59:ILE:HG22	50:SD0:66:LEU:HD13	1.93	0.51
61:SL0:32:ARG:NH2	61:SL0:47:ALA:O	2.44	0.51
1:L50:1316:C:O3'	3:LA0:56:ARG:NH1	2.43	0.51
1:L50:1634:A:N6	1:L50:1656:G:O2'	2.37	0.51
19:LI0:115:MET:O	19:LI0:118:SER:OG	2.27	0.51
46:SB0:29:GLU:HB2	46:SB0:96:ARG:HH22	1.76	0.51
48:SC0:137:VAL:HG21	48:SC0:189:ALA:HB1	1.92	0.51
13:LF0:44:ARG:NH1	13:LF0:193:GLU:OE2	2.44	0.51
24:LLL:49:LEU:HB3	24:LLL:51:ILE:HG12	1.93	0.51
48:SC0:58:LEU:HG	48:SC0:238:LEU:HD13	1.93	0.51
1:L50:107:G:H1'	1:L50:108:C:H2'	1.93	0.51
36:LT0:43:VAL:H	36:LT0:57:HIS:CD2	2.28	0.51
38:LV0:37:MET:HB3	38:LV0:63:CYS:HB3	1.93	0.51
48:SC0:233:PRO:HG2	70:SV0:42:ILE:HG23	1.93	0.51
55:SG0:12:THR:HG22	55:SG0:128:VAL:HG23	1.92	0.51
56:SGG:166:ASN:HB3	56:SGG:182:ILE:HG22	1.92	0.51
1:L50:1642:G:O2'	3:LA0:148:ARG:NH2	2.44	0.51
38:LV0:23:GLY:HA2	38:LV0:38:GLN:HE21	1.76	0.51
43:S60:94:G:N1	58:SI0:19:PRO:O	2.44	0.51
43:S60:1201:G:H4'	43:S60:1239:C:H4'	1.93	0.51
1:L50:1986:A:OP1	3:LA0:111:ARG:NH1	2.41	0.50
1:L50:2495:C:O3'	17:LH0:151:SER:OG	2.27	0.50
9:LD0:50:VAL:HA	9:LD0:123:ASP:HB3	1.93	0.50
30:LOO:20:CYS:HB3	30:LOO:23:CYS:HB2	1.93	0.50
35:LS0:41:ARG:HG2	35:LS0:61:ILE:HD13	1.92	0.50
43:S60:216:C:H5''	61:SL0:106:PHE:HE2	1.77	0.50
55:SG0:165:ASP:OD1	55:SG0:165:ASP:N	2.43	0.50
72:SX0:46:GLY:HA2	72:SX0:72:ILE:HG13	1.92	0.50
74:SZ0:89:LEU:HD13	74:SZ0:101:TYR:HB3	1.93	0.50
14:LFF:84:GLU:HG3	14:LFF:108:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S60:1128:A:N6	43:S60:1180:C:O2	2.44	0.50
56:SGG:134:ASN:HD21	56:SGG:138:GLU:HB2	1.77	0.50
59:SJ0:74:LEU:HD13	59:SJ0:86:VAL:HG11	1.92	0.50
8:LCC:54:ARG:HD3	8:LCC:71:ILE:HD11	1.93	0.50
13:LF0:74:VAL:HG12	36:LT0:139:VAL:HG22	1.92	0.50
27:LN0:158:HIS:HB3	27:LN0:161:CYS:HB2	1.93	0.50
43:S60:1184:G:N2	43:S60:1209:A:OP2	2.40	0.50
1:L50:130:C:O2'	1:L50:562:A:N1	2.39	0.50
1:L50:377:C:OP2	7:LC0:196:ARG:NH2	2.43	0.50
1:L50:2039:A:OP2	36:LT0:1:MET:N	2.43	0.50
11:LE0:156:ILE:HG21	11:LE0:159:MET:HE2	1.93	0.50
69:SU0:70:SER:OG	69:SU0:72:CYS:SG	2.67	0.50
1:L50:257:G:N1	1:L50:260:C:OP2	2.44	0.50
1:L50:1274:A:OP2	34:LR0:42:ARG:NH2	2.36	0.50
1:L50:2182:G:O2'	30:LOO:90:THR:OG1	2.26	0.50
1:L50:2582:U:H5''	5:LB0:304:MET:HE2	1.93	0.50
47:SBB:5:ASP:HA	71:SW0:21:GLN:HE22	1.76	0.50
52:SE0:151:ASP:HB3	52:SE0:154:ILE:HG13	1.92	0.50
1:L50:633:U:O2'	31:LP0:136:ARG:NH2	2.39	0.50
22:LJJ:27:TYR:HA	22:LJJ:34:CYS:HA	1.93	0.50
39:LW0:57:ARG:NH2	39:LW0:62:LYS:O	2.44	0.50
43:S60:687:G:N1	43:S60:734:G:O2'	2.36	0.50
43:S60:1058:C:O4'	66:SR0:67:LYS:NZ	2.45	0.50
64:SP0:57:LEU:HD23	64:SP0:84:MET:HE1	1.94	0.50
1:L50:664:G:O6	3:LA0:3:LYS:NZ	2.45	0.50
43:S60:241:U:OP1	58:SI0:31:ARG:NH1	2.41	0.50
43:S60:1147:G:H5'	68:ST0:76:ARG:HG3	1.93	0.50
45:SAA:45:ILE:HA	63:SO0:97:GLN:HE22	1.76	0.50
50:SD0:89:GLU:OE1	50:SD0:92:LYS:NZ	2.44	0.50
50:SD0:138:VAL:HG22	50:SD0:184:ILE:HG22	1.93	0.50
59:SJ0:126:SER:O	59:SJ0:126:SER:OG	2.29	0.50
70:SV0:27:PHE:HB2	70:SV0:41:LEU:HB2	1.93	0.50
1:L50:123:C:OP1	27:LN0:187:SER:OG	2.30	0.50
1:L50:2262:G:H5''	1:L50:2263:A:H5''	1.93	0.50
3:LA0:242:LYS:O	3:LA0:246:ASN:ND2	2.45	0.50
18:LHH:40:LYS:HB2	18:LHH:43:GLU:HG3	1.94	0.50
42:LZ0:51:GLU:HG2	42:LZ0:54:LYS:HE2	1.94	0.50
43:S60:538:G:H3'	43:S60:539:G:H8	1.76	0.50
43:S60:835:A:H5''	45:SAA:2:PRO:HB3	1.94	0.50
43:S60:1031:C:O3'	56:SGG:103:ARG:NH1	2.44	0.50
52:SE0:54:TYR:OH	52:SE0:97:GLU:OE2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:1536:G:O2'	1:L50:1803:U:O4	2.27	0.50
3:LA0:86:VAL:HG22	3:LA0:94:LEU:HB3	1.94	0.50
19:LI0:50:VAL:HG12	19:LI0:167:VAL:HG22	1.94	0.50
36:LT0:13:ARG:NH2	36:LT0:54:LYS:O	2.45	0.50
48:SC0:116:SER:HB3	48:SC0:122:ALA:HB2	1.93	0.50
57:SH0:155:ALA:HA	57:SH0:158:GLU:HB2	1.94	0.50
67:SS0:107:LEU:HD23	67:SS0:112:ILE:HA	1.94	0.50
3:LA0:29:PRO:HD2	3:LA0:82:ILE:HG21	1.94	0.49
22:LJJ:21:ARG:NH2	22:LJJ:41:GLU:O	2.31	0.49
46:SB0:45:GLY:HA3	63:SO0:31:LEU:HD22	1.94	0.49
48:SC0:43:VAL:HG21	48:SC0:65:ILE:HG23	1.94	0.49
64:SP0:61:ALA:HA	64:SP0:64:LYS:HD2	1.93	0.49
19:LI0:52:LEU:HB2	19:LI0:152:LEU:HD22	1.94	0.49
54:SF0:25:ASP:OD2	54:SF0:137:ARG:NH1	2.42	0.49
73:SY0:120:LEU:HG	73:SY0:124:LEU:HD23	1.94	0.49
9:LD0:158:GLY:HA2	9:LD0:169:VAL:HG13	1.94	0.49
43:S60:897:G:O2'	51:SDD:15:ARG:NH2	2.45	0.49
50:SD0:68:ARG:HG2	60:SK0:19:ARG:CZ	2.42	0.49
1:L50:336:A:N3	20:LII:82:ARG:NH1	2.61	0.49
1:L50:2271:U:OP1	38:LV0:50:ASN:ND2	2.36	0.49
18:LHH:17:GLU:OE2	18:LHH:58:ARG:NH1	2.45	0.49
43:S60:856:A:N3	43:S60:1253:U:O2'	2.39	0.49
64:SP0:87:VAL:H	64:SP0:90:MET:HE3	1.77	0.49
15:LG0:82:ARG:O	15:LG0:85:SER:OG	2.29	0.49
35:LS0:9:GLU:OE2	35:LS0:103:ARG:NH1	2.46	0.49
41:LY0:42:TYR:OH	41:LY0:110:GLN:NE2	2.46	0.49
1:L50:2138:A:OP1	9:LD0:155:ARG:NE	2.45	0.49
20:LII:25:ARG:HD2	23:LL0:96:MET:HE3	1.95	0.49
47:SBB:14:LEU:O	47:SBB:22:ARG:NE	2.46	0.49
1:L50:391:G:O2'	1:L50:402:G:O6	2.27	0.49
1:L50:1216:G:N7	1:L50:1480:A:O2'	2.40	0.49
1:L50:2057:U:H2'	1:L50:2058:G:C8	2.48	0.49
13:LF0:118:ALA:N	36:LT0:133:GLY:O	2.46	0.49
17:LH0:31:ARG:NH1	17:LH0:145:SER:OG	2.39	0.49
27:LN0:29:GLU:O	27:LN0:33:ASN:ND2	2.45	0.49
43:S60:39:G:H5'	59:SJO:3:ARG:HD3	1.95	0.49
43:S60:131:C:OP2	73:SY0:122:ARG:NH1	2.39	0.49
43:S60:1108:C:OP1	51:SDD:19:ARG:NH1	2.44	0.49
46:SB0:28:LYS:HA	46:SB0:50:THR:HA	1.95	0.49
50:SD0:105:ILE:HG22	50:SD0:118:ALA:HB1	1.95	0.49
1:L50:1382:G:OP1	34:LR0:103:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:1443:C:OP1	3:LA0:169:LYS:NZ	2.45	0.49
1:L50:2355:G:N2	1:L50:2358:A:OP2	2.39	0.49
17:LH0:136:GLU:O	17:LH0:139:THR:OG1	2.30	0.49
1:L50:2424:G:H21	17:LH0:118:LYS:HE2	1.77	0.49
15:LG0:106:ASP:OD2	15:LG0:110:ARG:NH1	2.46	0.49
27:LN0:44:PHE:HE2	27:LN0:121:VAL:HA	1.78	0.49
46:SB0:50:THR:OG1	46:SB0:52:GLN:NE2	2.46	0.49
46:SB0:102:PHE:O	46:SB0:222:ARG:NH2	2.46	0.49
48:SC0:116:SER:OG	48:SC0:117:LYS:N	2.45	0.49
1:L50:1511:A:H5'	34:LR0:56:THR:HB	1.94	0.48
9:LD0:260:LEU:O	19:LI0:210:LYS:NZ	2.39	0.48
28:LNN:3:ARG:O	43:S60:843:G:N2	2.42	0.48
52:SE0:95:THR:HG22	73:SY0:14:ARG:HB3	1.94	0.48
23:LL0:52:ARG:NH1	23:LL0:70:ARG:O	2.46	0.48
56:SGG:221:LEU:HA	56:SGG:262:LEU:HD23	1.94	0.48
36:LT0:125:LEU:HD23	36:LT0:128:LEU:HD21	1.94	0.48
43:S60:491:A:O2'	43:S60:497:A:N1	2.44	0.48
72:SX0:51:LYS:HA	72:SX0:67:VAL:HG12	1.94	0.48
1:L50:483:G:O2'	1:L50:1143:A:OP1	2.30	0.48
1:L50:487:C:H2'	1:L50:488:A:C8	2.49	0.48
38:LV0:45:VAL:HG11	38:LV0:53:PRO:HB3	1.95	0.48
1:L50:344:G:O2'	4:LAA:61:THR:O	2.32	0.48
1:L50:2238:A:OP2	26:LMM:94:ARG:NE	2.47	0.48
11:LE0:59:VAL:HG13	11:LE0:103:LEU:HB3	1.95	0.48
31:LP0:30:THR:HG23	31:LP0:120:VAL:HG11	1.94	0.48
58:SI0:11:ARG:O	61:SL0:134:LYS:NZ	2.46	0.48
1:L50:1183:G:OP1	1:L50:2462:G:O2'	2.28	0.48
1:L50:1822:G:H5'	31:LP0:87:LYS:HB2	1.95	0.48
19:LI0:91:VAL:HG11	19:LI0:129:VAL:HG12	1.94	0.48
43:S60:17:C:O2'	43:S60:830:A:N1	2.43	0.48
43:S60:1389:G:OP2	63:SO0:130:ARG:NH2	2.38	0.48
1:L50:2035:C:O2	36:LT0:59:ARG:NH1	2.47	0.48
58:SI0:143:ILE:HD12	58:SI0:153:ALA:HB1	1.95	0.48
72:SX0:88:ILE:HD12	72:SX0:91:ILE:HD11	1.94	0.48
1:L50:665:C:H3'	3:LA0:9:ARG:HH21	1.79	0.48
1:L50:2096:G:O2'	36:LT0:14:PHE:O	2.30	0.48
23:LL0:86:TYR:O	23:LL0:89:THR:OG1	2.28	0.48
43:S60:274:G:OP1	43:S60:554:G:N2	2.39	0.48
43:S60:337:A:N3	43:S60:349:U:O2'	2.40	0.48
43:S60:871:G:H5'	43:S60:883:C:H42	1.78	0.48
43:S60:1337:U:H2'	43:S60:1338:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:168:G:OP1	23:LL0:102:ASN:ND2	2.41	0.48
1:L50:1112:G:N2	1:L50:1115:C:OP2	2.44	0.48
50:SD0:170:GLU:HB2	50:SD0:187:ARG:HG2	1.95	0.48
52:SE0:253:ASN:HA	59:SJ0:71:ARG:HH12	1.79	0.48
59:SJ0:94:ILE:O	59:SJ0:98:LEU:N	2.42	0.48
67:SS0:18:ILE:HD13	74:SZ0:41:THR:HG22	1.95	0.48
1:L50:163:C:H5''	27:LN0:178:ILE:HG12	1.96	0.48
9:LD0:75:TYR:O	9:LD0:106:ARG:NH1	2.47	0.48
27:LN0:113:LEU:HB2	27:LN0:134:MET:HE2	1.96	0.48
38:LV0:46:ARG:NH1	38:LV0:47:GLY:O	2.47	0.48
43:S60:671:U:O2	62:SN0:48:SER:OG	2.30	0.48
58:SI0:164:ASN:O	58:SI0:168:ASN:ND2	2.47	0.48
5:LB0:285:ASN:HA	5:LB0:316:ASP:HA	1.95	0.47
7:LC0:202:LYS:NZ	7:LC0:225:ASP:OD2	2.45	0.47
13:LF0:184:PHE:O	13:LF0:186:GLY:N	2.47	0.47
21:LJ0:95:SER:OG	21:LJ0:103:GLY:O	2.32	0.47
32:LPP:46:SER:OG	32:LPP:57:CYS:SG	2.71	0.47
33:LQ0:81:VAL:HG12	33:LQ0:83:ALA:H	1.79	0.47
39:LW0:85:SER:OG	55:SG0:171:ARG:O	2.28	0.47
43:S60:121:A:H4'	43:S60:122:C:H5'	1.95	0.47
57:SH0:138:ILE:HA	57:SH0:168:THR:HG23	1.96	0.47
58:SI0:142:VAL:HG13	58:SI0:158:LEU:HD21	1.96	0.47
65:SQ0:115:ASP:HB3	65:SQ0:118:THR:HG23	1.95	0.47
9:LD0:18:LEU:HD21	36:LT0:25:LYS:HG2	1.95	0.47
30:LOO:80:CYS:SG	30:LOO:83:CYS:HB2	2.54	0.47
43:S60:1151:C:OP2	68:ST0:103:ARG:NE	2.39	0.47
56:SGG:106:GLU:OE1	56:SGG:131:ARG:NH2	2.46	0.47
71:SW0:52:ASP:O	71:SW0:54:ARG:NH1	2.47	0.47
73:SY0:55:VAL:HA	73:SY0:71:VAL:HA	1.96	0.47
1:L50:249:A:N1	1:L50:272:A:O2'	2.39	0.47
1:L50:396:G:N2	1:L50:399:A:OP2	2.38	0.47
22:LJJ:13:LYS:O	22:LJJ:14:ARG:NH1	2.40	0.47
34:LR0:116:THR:HG23	34:LR0:119:GLU:H	1.80	0.47
43:S60:1391:A:N7	45:SAA:34:LYS:NZ	2.61	0.47
1:L50:2010:U:H5''	1:L50:2011:G:H5'	1.96	0.47
1:L50:2547:C:O2'	1:L50:2549:G:OP2	2.32	0.47
10:LDD:55:VAL:HG13	10:LDD:71:MET:HE1	1.97	0.47
50:SD0:55:THR:HG23	50:SD0:90:MET:HB3	1.97	0.47
22:LJJ:2:SER:O	22:LJJ:7:SER:OG	2.27	0.47
27:LN0:16:SER:HB2	27:LN0:19:ALA:H	1.80	0.47
63:SO0:83:GLY:H	63:SO0:117:THR:HG22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:1549:U:N3	1:L50:1607:G:OP2	2.43	0.47
5:LB0:110:ILE:HG23	5:LB0:114:VAL:HG13	1.97	0.47
48:SC0:139:LEU:HB2	48:SC0:149:GLU:HG3	1.96	0.47
50:SD0:133:GLY:H	50:SD0:189:MET:HB3	1.80	0.47
56:SGG:301:ARG:HH21	66:SR0:27:ASP:HA	1.80	0.47
59:SJ0:82:ILE:H	59:SJ0:112:ARG:NH2	2.13	0.47
67:SS0:98:ASP:HB3	67:SS0:102:GLY:H	1.78	0.47
1:L50:691:G:N2	1:L50:715:C:OP1	2.48	0.47
5:LB0:83:PRO:HB2	5:LB0:200:GLU:HB3	1.97	0.47
15:LG0:185:ALA:O	15:LG0:190:ASN:ND2	2.48	0.47
18:LHH:1:MET:HE3	18:LHH:4:ARG:HA	1.95	0.47
27:LN0:43:THR:OG1	27:LN0:131:GLU:OE2	2.28	0.47
43:S60:208:C:H5''	52:SE0:37:ARG:HG2	1.97	0.47
1:L50:2119:C:OP1	6:LBB:32:ARG:NH2	2.35	0.47
31:LP0:7:PRO:HD3	31:LP0:119:ILE:HD13	1.96	0.47
43:S60:1056:G:O2'	43:S60:1059:A:N6	2.47	0.47
52:SE0:60:GLU:HB3	73:SY0:16:LEU:HD11	1.96	0.47
54:SF0:44:ALA:O	65:SQ0:124:ARG:NH2	2.46	0.47
1:L50:2338:G:N3	5:LB0:248:ALA:HB1	2.30	0.47
18:LHH:13:VAL:HG11	18:LHH:62:LEU:HD13	1.96	0.47
27:LN0:46:GLU:OE2	27:LN0:50:LYS:NZ	2.35	0.47
29:LO0:80:MET:HE3	29:LO0:98:LEU:HD22	1.96	0.47
43:S60:399:C:H5	43:S60:413:G:H21	1.62	0.47
54:SF0:33:PHE:HB3	54:SF0:58:PRO:HA	1.97	0.47
56:SGG:303:ARG:NH1	66:SR0:26:CYS:SG	2.88	0.47
1:L50:509:A:N1	1:L50:524:G:O2'	2.43	0.47
1:L50:836:G:H1'	13:LF0:102:LEU:HD22	1.97	0.47
1:L50:1330:G:OP2	1:L50:1432:G:N2	2.41	0.47
7:LC0:317:ILE:HD11	13:LF0:148:ARG:HA	1.97	0.47
21:LJ0:10:ARG:NH2	21:LJ0:151:LYS:O	2.43	0.47
46:SB0:123:ILE:HG12	46:SB0:163:VAL:HG13	1.97	0.47
47:SBB:53:ARG:NH1	62:SN0:56:ASP:O	2.48	0.47
1:L50:169:G:O2'	23:LL0:67:ARG:NH2	2.48	0.46
1:L50:309:A:OP2	27:LN0:8:ARG:NH1	2.36	0.46
5:LB0:281:TYR:HB3	5:LB0:349:ILE:HD11	1.96	0.46
11:LE0:161:ARG:O	11:LE0:165:THR:OG1	2.28	0.46
19:LI0:153:ARG:HA	19:LI0:156:LYS:HG2	1.97	0.46
56:SGG:172:SER:OG	56:SGG:174:ASP:OD1	2.29	0.46
64:SP0:55:ASP:HA	64:SP0:58:LYS:HB2	1.97	0.46
73:SY0:8:CYS:HB3	73:SY0:22:VAL:HG23	1.96	0.46
1:L50:52:C:OP2	24:LLL:21:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LHH:28:LEU:HD22	40:LX0:24:ALA:HA	1.97	0.46
72:SX0:98:THR:OG1	72:SX0:120:CYS:SG	2.71	0.46
1:L50:833:A:O2'	36:LT0:130:ARG:O	2.31	0.46
11:LE0:75:GLN:NE2	11:LE0:99:GLU:OE2	2.49	0.46
37:LU0:82:LEU:O	37:LU0:87:LEU:N	2.37	0.46
38:LV0:36:ILE:HD12	38:LV0:67:LYS:HD2	1.96	0.46
43:S60:383:G:OP1	59:SJ0:131:ARG:NE	2.38	0.46
52:SE0:57:THR:HG22	52:SE0:59:LYS:H	1.79	0.46
52:SE0:99:MET:HE3	52:SE0:99:MET:HB2	1.87	0.46
1:L50:481:A:OP2	1:L50:2259:U:O2'	2.28	0.46
43:S60:96:C:OP1	43:S60:292:G:O2'	2.28	0.46
43:S60:639:G:OP1	45:SAA:19:LYS:NZ	2.43	0.46
50:SD0:126:ILE:HG21	50:SD0:134:CYS:HB3	1.96	0.46
59:SJ0:118:VAL:HG13	59:SJ0:123:LEU:HB2	1.96	0.46
68:ST0:39:HIS:O	68:ST0:85:LYS:NZ	2.38	0.46
1:L50:187:C:OP2	1:L50:2156:C:O2'	2.27	0.46
24:LLL:48:LYS:HA	24:LLL:48:LYS:HD3	1.77	0.46
41:LY0:16:LYS:O	41:LY0:20:THR:OG1	2.29	0.46
43:S60:333:C:O2	43:S60:336:C:N4	2.49	0.46
43:S60:854:C:H1'	43:S60:1259:C:H42	1.80	0.46
43:S60:1291:U:H2'	43:S60:1292:A:C8	2.51	0.46
52:SE0:212:ASP:OD1	52:SE0:216:ARG:N	2.48	0.46
63:SO0:24:THR:HG21	63:SO0:58:ALA:HB2	1.96	0.46
13:LF0:71:ALA:HA	36:LT0:142:SER:HA	1.96	0.46
52:SE0:125:ARG:O	52:SE0:142:GLN:N	2.46	0.46
65:SQ0:46:MET:HA	65:SQ0:80:ILE:HG23	1.98	0.46
1:L50:48:C:H1'	1:L50:62:A:H2'	1.98	0.46
1:L50:761:G:H21	19:LI0:193:GLN:HB3	1.79	0.46
5:LB0:279:LEU:HD23	5:LB0:281:TYR:HE1	1.81	0.46
7:LC0:293:ASP:OD2	7:LC0:293:ASP:N	2.47	0.46
28:LNN:56:LYS:HB3	28:LNN:56:LYS:HE2	1.81	0.46
35:LS0:138:LEU:HD13	35:LS0:143:VAL:HG23	1.98	0.46
43:S60:49:C:N4	43:S60:334:A:OP2	2.47	0.46
56:SGG:43:VAL:HG13	56:SGG:61:PHE:HD2	1.81	0.46
56:SGG:318:LEU:HD23	56:SGG:320:ASN:HD21	1.81	0.46
1:L50:22:C:OP1	7:LC0:192:LYS:NZ	2.45	0.46
1:L50:2336:G:O2'	1:L50:2339:C:OP2	2.33	0.46
21:LJ0:93:LYS:HG3	21:LJ0:171:LEU:HB3	1.97	0.46
31:LP0:12:PRO:HA	31:LP0:15:THR:HG22	1.98	0.46
35:LS0:162:SER:OG	35:LS0:163:LYS:N	2.48	0.46
43:S60:53:C:H4'	73:SY0:107:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S60:1387:C:OP1	63:SO0:125:ARG:NH2	2.47	0.46
64:SP0:25:LEU:HG	64:SP0:88:PRO:HG3	1.98	0.46
68:ST0:16:LEU:HD21	68:ST0:59:PHE:HD2	1.81	0.46
69:SU0:96:TYR:HB2	69:SU0:99:VAL:HG23	1.96	0.46
12:LEE:19:ARG:O	12:LEE:22:SER:OG	2.32	0.46
13:LF0:111:ALA:HB3	13:LF0:215:PHE:HB2	1.98	0.46
19:LI0:113:THR:HG22	19:LI0:116:ARG:HB3	1.97	0.46
30:LOO:23:CYS:HB3	30:LOO:25:LYS:HB2	1.98	0.46
43:S60:556:A:N6	71:SW0:77:CYS:SG	2.89	0.46
45:SAA:23:CYS:HB3	45:SAA:28:SER:H	1.81	0.46
69:SU0:99:VAL:HG13	69:SU0:102:LYS:HE2	1.97	0.46
1:L50:183:G:OP1	4:LAA:60:CYS:N	2.47	0.45
1:L50:426:G:O2'	31:LP0:98:ASN:ND2	2.48	0.45
1:L50:879:G:O2'	12:LEE:45:LYS:O	2.32	0.45
1:L50:911:C:OP2	29:LO0:93:ARG:NH2	2.47	0.45
1:L50:921:A:OP1	1:L50:937:C:O2'	2.26	0.45
5:LB0:27:GLN:HE21	5:LB0:272:ARG:NE	2.14	0.45
48:SC0:243:ARG:NH1	48:SC0:247:GLU:OE1	2.49	0.45
68:ST0:35:ILE:HG22	68:ST0:37:THR:H	1.81	0.45
73:SY0:19:ARG:HB2	73:SY0:73:ILE:HB	1.98	0.45
1:L50:1301:G:N2	1:L50:1304:A:OP2	2.40	0.45
1:L50:1644:C:OP2	3:LA0:110:ARG:NH1	2.49	0.45
1:L50:453:C:N4	1:L50:464:G:O6	2.49	0.45
1:L50:909:C:H5''	29:LO0:24:LYS:HD3	1.98	0.45
1:L50:1224:U:OP1	40:LX0:35:LYS:NZ	2.37	0.45
7:LC0:192:LYS:HA	7:LC0:197:ARG:HA	1.98	0.45
15:LG0:81:LYS:HA	15:LG0:84:MET:HG2	1.98	0.45
27:LN0:163:GLY:HA2	27:LN0:168:SER:HB2	1.98	0.45
43:S60:1016:G:H5''	50:SD0:156:LEU:HD12	1.98	0.45
46:SB0:123:ILE:HD13	46:SB0:166:VAL:HG21	1.99	0.45
62:SN0:26:VAL:HG11	62:SN0:60:ILE:HG12	1.97	0.45
1:L50:692:C:OP2	4:LAA:26:ARG:NH2	2.49	0.45
1:L50:891:U:O2'	1:L50:903:A:N3	2.45	0.45
21:LJ0:32:ARG:NE	21:LJ0:120:ILE:O	2.47	0.45
24:LLL:43:HIS:H	24:LLL:47:ASN:HD22	1.63	0.45
43:S60:126:G:O6	55:SG0:136:ARG:NH2	2.50	0.45
48:SC0:139:LEU:HD22	48:SC0:191:VAL:HG12	1.99	0.45
48:SC0:174:SER:N	48:SC0:193:ASP:OD2	2.49	0.45
50:SD0:23:GLU:OE2	50:SD0:27:LYS:NZ	2.45	0.45
50:SD0:196:ASN:HD21	50:SD0:201:SER:HB2	1.82	0.45
52:SE0:230:ASP:OD2	52:SE0:230:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SGG:269:VAL:HG12	56:SGG:284:VAL:HB	1.99	0.45
67:SS0:39:LEU:HD11	67:SS0:80:ILE:HD11	1.99	0.45
69:SU0:44:TYR:O	69:SU0:47:THR:OG1	2.33	0.45
1:L50:1748:A:OP2	1:L50:1773:C:N4	2.49	0.45
1:L50:2113:C:H2'	1:L50:2114:G:H8	1.82	0.45
7:LC0:133:LEU:HD21	11:LE0:7:LEU:HB3	1.98	0.45
25:LM0:32:ASP:OD2	35:LS0:142:ARG:NH1	2.50	0.45
38:LV0:14:ILE:HG13	38:LV0:128:ILE:HD11	1.99	0.45
43:S60:64:A:H3'	43:S60:65:G:H8	1.81	0.45
43:S60:762:G:O2'	47:SBB:15:ARG:NH2	2.48	0.45
1:L50:284:C:OP1	1:L50:285:C:N4	2.49	0.45
1:L50:1077:G:N2	1:L50:1078:U:O4	2.45	0.45
1:L50:1094:C:H4'	11:LE0:9:MET:HE1	1.98	0.45
1:L50:1823:C:OP1	31:LP0:87:LYS:NZ	2.45	0.45
3:LA0:64:ARG:HE	3:LA0:64:ARG:HB3	1.57	0.45
29:LO0:60:ARG:HD2	29:LO0:65:PRO:HB3	1.99	0.45
43:S60:135:G:N2	55:SG0:55:ASP:OD2	2.49	0.45
43:S60:1235:U:H3	43:S60:1240:A:H2	1.65	0.45
48:SC0:239:SER:HA	48:SC0:242:SER:HB2	1.98	0.45
1:L50:628:U:N3	1:L50:2369:U:OP1	2.39	0.45
1:L50:1893:A:N1	3:LA0:222:PRO:HB3	2.31	0.45
1:L50:2454:C:OP2	34:LR0:62:ARG:NH1	2.49	0.45
1:L50:2523:C:OP1	5:LB0:272:ARG:NH1	2.42	0.45
4:LAA:93:ASP:O	4:LAA:120:ARG:NH2	2.44	0.45
5:LB0:89:ILE:HD12	5:LB0:105:LEU:HD23	1.98	0.45
9:LD0:27:ASP:HB3	9:LD0:30:HIS:HB3	1.99	0.45
43:S60:575:C:C4	47:SBB:21:LYS:HG2	2.52	0.45
43:S60:1034:C:H4'	69:SU0:56:LYS:HE2	1.99	0.45
58:SI0:83:TYR:OH	61:SL0:9:LYS:O	2.33	0.45
72:SX0:121:LYS:HA	72:SX0:126:SER:HA	1.98	0.45
1:L50:665:C:H3'	3:LA0:9:ARG:NH2	2.32	0.45
1:L50:2201:C:OP2	1:L50:2346:U:O2'	2.33	0.45
1:L50:2568:C:OP1	5:LB0:117:ARG:NH2	2.40	0.45
7:LC0:29:ILE:HG23	7:LC0:123:MET:HB3	1.98	0.45
35:LS0:94:MET:HE1	35:LS0:118:HIS:CE1	2.52	0.45
43:S60:24:U:OP1	59:SJ0:8:LYS:NZ	2.50	0.45
43:S60:220:C:OP1	72:SX0:11:LYS:NZ	2.50	0.45
43:S60:1247:G:H2'	43:S60:1248:G:H8	1.81	0.45
47:SBB:22:ARG:HH11	47:SBB:26:GLN:HB2	1.81	0.45
56:SGG:66:HIS:CD2	56:SGG:67:SER:H	2.34	0.45
1:L50:1690:G:N2	1:L50:1693:A:OP2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:2094:A:H2'	1:L50:2095:G:C8	2.52	0.45
43:S60:991:C:OP1	48:SC0:93:ARG:NH2	2.49	0.45
46:SB0:109:THR:HA	46:SB0:112:LYS:HG2	1.98	0.45
48:SC0:37:THR:HG23	48:SC0:40:GLY:H	1.82	0.45
48:SC0:118:GLU:O	48:SC0:121:THR:OG1	2.33	0.45
48:SC0:224:VAL:HG23	48:SC0:226:GLU:H	1.81	0.45
55:SG0:76:LEU:HD12	55:SG0:80:ASN:HB3	1.97	0.45
62:SN0:37:ILE:HG23	62:SN0:50:ILE:HG21	1.99	0.45
67:SS0:68:LEU:HD22	67:SS0:72:GLU:HG3	1.98	0.45
72:SX0:56:ALA:HB1	72:SX0:111:ASP:HB2	1.99	0.45
1:L50:2137:G:N2	1:L50:2140:A:OP2	2.46	0.45
19:LI0:59:GLN:HG2	19:LI0:128:ARG:HG2	1.99	0.45
32:LPP:76:GLY:O	32:LPP:80:ASN:ND2	2.50	0.45
38:LV0:5:HIS:O	38:LV0:43:LYS:NZ	2.43	0.45
43:S60:384:U:O4	59:SJ0:35:LYS:NZ	2.50	0.45
47:SBB:54:THR:HG22	47:SBB:61:VAL:HA	1.98	0.45
54:SF0:92:ASN:HB2	54:SF0:99:PRO:HG3	1.98	0.45
1:L50:232:U:C4	15:LG0:122:VAL:HG23	2.51	0.44
1:L50:337:A:OP1	20:LII:86:LYS:NZ	2.49	0.44
2:L70:63:A:N6	19:LI0:202:GLU:OE1	2.49	0.44
6:LBB:5:LYS:HE3	6:LBB:8:THR:HB	1.98	0.44
35:LS0:162:SER:HB3	35:LS0:164:TYR:CZ	2.53	0.44
43:S60:456:A:O2'	43:S60:458:U:OP1	2.35	0.44
46:SB0:54:THR:HG1	46:SB0:57:ASN:H	1.61	0.44
58:SI0:26:LYS:HG2	58:SI0:29:MET:HG2	1.99	0.44
1:L50:480:C:O2	1:L50:1843:C:O2'	2.34	0.44
4:LAA:76:SER:OG	4:LAA:113:GLY:O	2.28	0.44
13:LF0:160:ASN:OD1	13:LF0:160:ASN:N	2.47	0.44
24:LLL:41:ARG:HD2	24:LLL:41:ARG:HA	1.77	0.44
31:LP0:121:ASN:HB2	31:LP0:146:HIS:HB2	1.99	0.44
43:S60:465:C:H5''	53:SEE:42:ARG:HH22	1.81	0.44
46:SB0:128:ASP:OD1	46:SB0:138:ARG:NE	2.49	0.44
47:SBB:6:LEU:HD23	71:SW0:23:LEU:HB2	2.00	0.44
49:SCC:28:LEU:HD12	49:SCC:53:LEU:HD21	1.99	0.44
67:SS0:34:ARG:O	67:SS0:38:ALA:N	2.47	0.44
1:L50:445:C:H2'	1:L50:446:A:C8	2.52	0.44
1:L50:551:U:O2	23:LL0:10:ASN:ND2	2.51	0.44
3:LA0:23:VAL:HG23	3:LA0:45:GLU:HG3	1.99	0.44
13:LF0:247:ASN:O	13:LF0:251:ARG:NH1	2.46	0.44
17:LH0:2:LYS:H	17:LH0:64:ARG:HH12	1.66	0.44
43:S60:94:G:H22	58:SI0:18:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SBB:20:ARG:HH21	62:SN0:13:GLU:H	1.65	0.44
59:SJ0:11:ARG:NH2	59:SJ0:48:ASP:OD2	2.49	0.44
1:L50:2289:G:H5''	1:L50:2290:C:H5'	2.00	0.44
16:LGG:86:GLU:HG3	42:LZ0:12:LEU:HB3	1.99	0.44
32:LPP:33:GLN:HB3	32:LPP:69:PHE:HB3	1.98	0.44
43:S60:49:C:H2'	43:S60:333:C:H41	1.82	0.44
43:S60:241:U:H1'	58:SI0:5:ARG:HD2	1.99	0.44
43:S60:523:U:H2'	43:S60:524:G:H8	1.82	0.44
43:S60:797:U:OP2	72:SX0:1:MET:N	2.49	0.44
52:SE0:199:GLU:OE1	52:SE0:209:TYR:OH	2.28	0.44
55:SG0:56:ASP:HB3	55:SG0:60:LEU:H	1.82	0.44
58:SI0:6:SER:HB3	58:SI0:28:HIS:CD2	2.52	0.44
59:SJ0:152:MET:HE2	59:SJ0:152:MET:HB2	1.87	0.44
61:SL0:77:MET:HE3	61:SL0:77:MET:HB3	1.81	0.44
2:L70:90:A:C5	2:L70:91:C:H1'	2.53	0.44
5:LB0:57:VAL:HB	5:LB0:351:PHE:HB3	2.00	0.44
7:LC0:34:VAL:HG11	7:LC0:243:LEU:HD21	2.00	0.44
9:LD0:37:GLN:HE21	9:LD0:38:ASP:H	1.65	0.44
14:LFF:71:ARG:HG3	14:LFF:80:ALA:HB3	1.98	0.44
19:LI0:61:SER:HA	19:LI0:126:VAL:HG12	1.99	0.44
43:S60:1109:U:OP2	51:SDD:15:ARG:NH2	2.51	0.44
43:S60:1371:G:N7	63:SO0:131:ARG:NH2	2.58	0.44
52:SE0:159:VAL:HG23	52:SE0:227:ILE:HD12	1.99	0.44
42:LZ0:36:ALA:HB1	42:LZ0:105:VAL:HG11	1.99	0.44
43:S60:175:G:H4'	52:SE0:202:MET:HE2	2.00	0.44
43:S60:231:G:O2'	58:SI0:10:LYS:NZ	2.51	0.44
46:SB0:106:GLU:OE2	46:SB0:112:LYS:NZ	2.49	0.44
48:SC0:39:LEU:HD22	48:SC0:65:ILE:HD13	1.99	0.44
55:SG0:183:PRO:HA	55:SG0:186:ILE:HD12	1.99	0.44
56:SGG:110:THR:HG23	56:SGG:125:SER:HA	2.00	0.44
67:SS0:59:VAL:HG21	67:SS0:76:LEU:HD11	1.99	0.44
71:SW0:7:THR:HG23	71:SW0:24:ILE:HD13	1.99	0.44
1:L50:545:C:H5''	7:LC0:110:ARG:HG3	2.00	0.44
1:L50:858:C:O2'	1:L50:2032:A:OP2	2.33	0.44
1:L50:1225:G:O2'	40:LX0:75:ASN:ND2	2.51	0.44
5:LB0:110:ILE:HG22	5:LB0:115:LEU:HD23	2.00	0.44
9:LD0:204:LYS:HB3	9:LD0:206:ILE:HG12	2.00	0.44
50:SD0:50:VAL:HG13	50:SD0:88:VAL:HG23	1.98	0.44
52:SE0:206:ASP:N	52:SE0:206:ASP:OD1	2.50	0.44
56:SGG:144:ASP:OD1	56:SGG:144:ASP:N	2.48	0.44
3:LA0:170:PRO:HG3	32:LPP:25:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LGG:25:THR:OG1	16:LGG:29:ARG:O	2.29	0.44
35:LS0:56:SER:HA	35:LS0:59:ILE:HD12	2.00	0.44
43:S60:366:G:OP1	73:SY0:107:LYS:NZ	2.36	0.44
50:SD0:4:THR:HA	69:SU0:61:LYS:HD3	1.99	0.44
55:SG0:151:ASN:HB3	55:SG0:154:GLU:HB3	1.99	0.44
56:SGG:147:ILE:HD11	56:SGG:185:ARG:HB3	2.00	0.44
74:SZ0:72:ASN:HB3	74:SZ0:75:VAL:HG12	1.99	0.44
74:SZ0:73:VAL:HA	74:SZ0:76:ALA:HB3	1.98	0.44
1:L50:482:C:H2'	1:L50:483:G:C8	2.53	0.44
9:LD0:36:ARG:NH2	36:LT0:93:GLU:OE2	2.51	0.44
21:LJ0:92:LYS:HA	21:LJ0:172:LEU:HB2	1.99	0.44
43:S60:523:U:H4'	71:SW0:119:GLY:HA3	1.99	0.44
43:S60:826:A:N3	43:S60:1290:C:O2'	2.49	0.44
61:SL0:71:LYS:HG2	61:SL0:125:THR:HB	2.00	0.44
74:SZ0:53:ASP:OD1	74:SZ0:68:LYS:NZ	2.50	0.44
1:L50:505:A:H2'	1:L50:506:G:C8	2.53	0.43
1:L50:1130:A:O2'	11:LE0:12:ARG:NH2	2.50	0.43
1:L50:1164:U:H5'	10:LDD:29:PRO:HB3	2.00	0.43
1:L50:1363:G:H2'	1:L50:1364:G:H8	1.83	0.43
15:LG0:130:PHE:HA	20:LII:47:ILE:HD11	2.00	0.43
36:LT0:100:CYS:SG	36:LT0:101:ASN:N	2.91	0.43
41:LY0:54:LYS:HD3	41:LY0:68:THR:HG22	1.98	0.43
48:SC0:174:SER:O	48:SC0:177:ARG:NH1	2.51	0.43
55:SG0:77:LYS:H	55:SG0:80:ASN:ND2	2.15	0.43
1:L50:90:C:OP1	22:LJJ:74:ARG:NH2	2.51	0.43
1:L50:602:A:C5	1:L50:603:C:H1'	2.53	0.43
1:L50:693:U:O2'	1:L50:1871:A:N1	2.47	0.43
1:L50:1713:A:H5''	3:LA0:235:THR:HB	2.00	0.43
1:L50:2438:G:C2	5:LB0:75:SER:HB3	2.53	0.43
2:L70:11:A:N6	9:LD0:14:PHE:O	2.51	0.43
2:L70:119:U:N3	9:LD0:235:ASP:O	2.44	0.43
14:LFF:95:GLU:OE2	29:LO0:4:LYS:NZ	2.40	0.43
34:LR0:4:LEU:HD21	34:LR0:32:LEU:HB3	1.99	0.43
41:LY0:115:ASP:OD1	41:LY0:115:ASP:N	2.51	0.43
43:S60:343:G:N1	43:S60:346:A:OP2	2.40	0.43
46:SB0:48:LEU:HG	63:SO0:35:GLU:HG2	2.00	0.43
53:SEE:33:ARG:HB3	59:SJ0:35:LYS:HA	2.00	0.43
1:L50:930:A:H61	1:L50:1027:G:H2'	1.82	0.43
1:L50:2411:G:O2'	1:L50:2420:G:O6	2.32	0.43
8:LCC:97:ASP:OD1	8:LCC:97:ASP:N	2.44	0.43
18:LHH:99:MET:HB3	27:LN0:146:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LO0:118:ILE:HG23	35:LS0:169:LYS:HG2	2.01	0.43
43:S60:637:A:OP1	43:S60:727:U:O2'	2.30	0.43
43:S60:678:A:OP2	62:SN0:124:ARG:NH2	2.51	0.43
50:SD0:61:GLU:HB2	50:SD0:64:SER:HB3	2.00	0.43
60:SK0:11:VAL:HA	60:SK0:14:HIS:HB3	2.01	0.43
65:SQ0:100:ASP:OD1	65:SQ0:100:ASP:N	2.45	0.43
67:SS0:93:PHE:HA	67:SS0:106:HIS:HD2	1.83	0.43
1:L50:593:C:O2'	1:L50:1383:C:OP1	2.30	0.43
1:L50:1502:G:N1	1:L50:1505:C:OP2	2.30	0.43
1:L50:1893:A:H5'	27:LN0:89:ILE:HG13	2.00	0.43
2:L70:48:G:O2'	9:LD0:197:THR:O	2.30	0.43
4:LAA:77:LYS:NZ	33:LQ0:89:ASN:OD1	2.48	0.43
11:LE0:61:LEU:HD11	11:LE0:103:LEU:HB2	2.01	0.43
24:LLL:42:ARG:HG3	24:LLL:47:ASN:HB2	1.99	0.43
38:LV0:36:ILE:HB	38:LV0:67:LYS:HG2	2.00	0.43
39:LW0:48:ARG:NH1	43:S60:1324:G:O2'	2.45	0.43
42:LZ0:8:VAL:O	42:LZ0:75:THR:OG1	2.30	0.43
43:S60:597:G:H2'	43:S60:598:A:C8	2.54	0.43
43:S60:799:U:H2'	43:S60:800:G:H8	1.83	0.43
50:SD0:71:HIS:CE1	60:SK0:18:LYS:HB2	2.54	0.43
67:SS0:97:PHE:N	67:SS0:104:ASP:OD1	2.49	0.43
72:SX0:129:ALA:O	72:SX0:134:LYS:N	2.50	0.43
1:L50:549:C:H2'	1:L50:550:A:C8	2.53	0.43
3:LA0:119:ALA:HB2	3:LA0:126:VAL:HG23	2.01	0.43
7:LC0:83:ARG:HA	7:LC0:83:ARG:HD2	1.78	0.43
15:LG0:37:HIS:O	15:LG0:41:ASN:ND2	2.49	0.43
25:LM0:84:GLU:HG2	25:LM0:92:ARG:HH22	1.84	0.43
40:LX0:98:LYS:HE2	40:LX0:98:LYS:HB3	1.88	0.43
50:SD0:135:VAL:HG23	50:SD0:153:ALA:HB2	2.01	0.43
68:ST0:71:ARG:HG2	68:ST0:123:LYS:HD3	2.00	0.43
1:L50:39:G:N2	18:LHH:83:ARG:HB2	2.34	0.43
1:L50:1247:U:OP1	27:LN0:127:TYR:OH	2.31	0.43
5:LB0:21:ARG:HE	5:LB0:267:GLN:NE2	2.16	0.43
15:LG0:74:GLU:OE2	15:LG0:82:ARG:NH2	2.51	0.43
33:LQ0:92:LEU:HD23	33:LQ0:92:LEU:HA	1.92	0.43
33:LQ0:170:LYS:NZ	33:LQ0:171:ASN:OD1	2.41	0.43
52:SE0:2:THR:OG1	52:SE0:3:ARG:N	2.49	0.43
53:SEE:43:ARG:HH12	53:SEE:48:PHE:HB2	1.84	0.43
61:SL0:133:SER:OG	61:SL0:134:LYS:N	2.51	0.43
67:SS0:94:ASN:H	67:SS0:106:HIS:CD2	2.37	0.43
71:SW0:15:ASN:ND2	71:SW0:66:LEU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:394:C:O2'	7:LC0:80:GLY:O	2.27	0.43
1:L50:2621:C:H4'	5:LB0:311:GLY:HA2	2.00	0.43
3:LA0:32:SER:OG	3:LA0:33:GLU:OE1	2.36	0.43
4:LAA:86:GLN:NE2	23:LL0:151:VAL:O	2.52	0.43
22:LJJ:66:LEU:HD23	22:LJJ:66:LEU:HA	1.84	0.43
36:LT0:4:ASN:HA	36:LT0:8:ARG:HD2	2.01	0.43
50:SD0:70:LYS:HE2	50:SD0:70:LYS:HB3	1.86	0.43
52:SE0:110:MET:HE3	52:SE0:110:MET:HB2	1.82	0.43
67:SS0:92:MET:HE1	68:ST0:34:ILE:HD12	1.99	0.43
72:SX0:129:ALA:HB1	72:SX0:135:LYS:HB2	2.00	0.43
73:SY0:85:ARG:HD2	73:SY0:87:PHE:HE1	1.84	0.43
74:SZ0:59:LEU:HD11	74:SZ0:100:LEU:HD23	2.00	0.43
1:L50:121:C:O2'	1:L50:366:A:N3	2.43	0.43
1:L50:691:G:H5''	4:LAA:29:PRO:HG3	2.01	0.43
1:L50:2568:C:O2'	5:LB0:170:ARG:O	2.32	0.43
3:LA0:51:PRO:HG2	3:LA0:70:ALA:HB3	2.01	0.43
5:LB0:210:ASN:HB2	5:LB0:343:ASN:HD22	1.83	0.43
9:LD0:186:MET:HG2	9:LD0:194:TYR:HB2	1.99	0.43
13:LF0:23:SER:O	13:LF0:27:ASN:ND2	2.38	0.43
32:LPP:58:LYS:HE2	32:LPP:58:LYS:HB2	1.73	0.43
47:SBB:83:ARG:HB3	62:SN0:24:HIS:CE1	2.54	0.43
50:SD0:105:ILE:HG13	50:SD0:184:ILE:HD12	2.00	0.43
52:SE0:192:ILE:HD13	52:SE0:238:LEU:HD22	2.00	0.43
53:SEE:40:TYR:HE2	59:SJ0:27:LYS:HA	1.83	0.43
59:SJ0:161:ILE:H	59:SJ0:161:ILE:HG13	1.65	0.43
64:SP0:56:LEU:HD13	64:SP0:79:THR:HB	2.00	0.43
67:SS0:24:MET:HG2	67:SS0:25:LEU:HG	2.01	0.43
70:SV0:19:ASP:OD2	70:SV0:22:SER:N	2.50	0.43
1:L50:1388:C:H5'	8:LCC:28:TYR:HB3	2.00	0.43
3:LA0:5:ILE:HD12	3:LA0:7:ARG:HB3	2.00	0.43
4:LAA:132:LYS:HD3	4:LAA:136:MET:HE3	2.01	0.43
23:LL0:14:LYS:HB2	23:LL0:17:ILE:HG12	2.01	0.43
25:LM0:24:TYR:HB3	25:LM0:37:VAL:HB	2.01	0.43
43:S60:1194:U:O2'	43:S60:1237:A:N3	2.48	0.43
56:SGG:66:HIS:CG	56:SGG:67:SER:H	2.37	0.43
62:SN0:102:LEU:HD21	62:SN0:111:ALA:HB3	2.01	0.43
69:SU0:58:LEU:HB2	69:SU0:88:ARG:HB2	2.01	0.43
69:SU0:99:VAL:HA	69:SU0:102:LYS:HG2	2.01	0.43
1:L50:203:A:N1	1:L50:361:U:O2'	2.44	0.43
1:L50:1591:A:O2'	58:SI0:89:GLU:OE1	2.37	0.43
1:L50:1763:U:O2'	1:L50:1765:A:N7	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LH0:36:ARG:NH2	17:LH0:77:CYS:SG	2.92	0.43
36:LT0:91:ARG:HB2	36:LT0:94:HIS:HD2	1.84	0.43
43:S60:564:A:C4	71:SW0:104:SER:HA	2.54	0.43
43:S60:691:G:H4'	43:S60:1376:A:H4'	2.01	0.43
56:SGG:255:THR:HG21	56:SGG:259:VAL:HB	2.00	0.43
63:SO0:87:VAL:HG12	63:SO0:123:ARG:HB2	2.00	0.43
63:SO0:131:ARG:HA	63:SO0:131:ARG:HD2	1.85	0.43
1:L50:159:A:N1	1:L50:203:A:O2'	2.49	0.42
1:L50:575:C:H2'	1:L50:576:G:C8	2.54	0.42
19:LI0:38:ARG:HH11	19:LI0:83:ASP:HB3	1.84	0.42
43:S60:133:G:N2	55:SG0:13:GLN:OE1	2.41	0.42
43:S60:1061:G:H5'	66:SR0:4:VAL:HG22	2.00	0.42
50:SD0:32:GLU:HG2	50:SD0:54:LYS:HD2	2.01	0.42
50:SD0:48:ILE:HB	50:SD0:86:ILE:HG22	2.01	0.42
56:SGG:218:VAL:HA	56:SGG:234:GLY:HA2	2.01	0.42
1:L50:778:G:OP1	28:LNN:64:ARG:NH1	2.52	0.42
38:LV0:120:PRO:HG3	39:LW0:27:THR:HA	2.01	0.42
43:S60:635:G:H2'	43:S60:636:G:C8	2.54	0.42
43:S60:780:A:H2'	43:S60:781:A:C8	2.54	0.42
43:S60:1224:G:N7	65:SQ0:15:LYS:HE2	2.34	0.42
52:SE0:130:LYS:HB3	52:SE0:140:TYR:HE2	1.84	0.42
64:SP0:112:MET:HE3	64:SP0:112:MET:HB2	1.79	0.42
66:SR0:57:LEU:HD23	66:SR0:57:LEU:HA	1.90	0.42
1:L50:138:U:H5''	27:LN0:85:VAL:HB	2.01	0.42
1:L50:325:C:O2	30:LOO:42:ASN:ND2	2.33	0.42
1:L50:494:U:H2'	1:L50:495:G:C8	2.54	0.42
1:L50:548:A:OP2	4:LAA:6:LYS:NZ	2.51	0.42
1:L50:666:G:OP2	3:LA0:9:ARG:NH2	2.43	0.42
1:L50:2139:A:H2'	1:L50:2140:A:C8	2.54	0.42
20:LII:25:ARG:HB2	20:LII:28:LYS:HB2	2.00	0.42
25:LM0:36:ILE:HD11	35:LS0:76:ILE:HG13	2.00	0.42
34:LR0:106:LEU:HD23	34:LR0:106:LEU:HA	1.91	0.42
42:LZ0:31:ARG:HA	42:LZ0:69:SER:HB3	2.00	0.42
43:S60:971:G:H5''	69:SU0:78:THR:HG21	2.01	0.42
46:SB0:120:HIS:CD2	46:SB0:156:CYS:HB2	2.54	0.42
52:SE0:21:ASP:OD1	52:SE0:50:ARG:NH2	2.52	0.42
5:LB0:168:SER:OG	5:LB0:310:TYR:O	2.25	0.42
8:LCC:42:TYR:HB3	8:LCC:94:ILE:HB	2.01	0.42
11:LE0:61:LEU:O	11:LE0:66:THR:OG1	2.36	0.42
14:LFF:88:PRO:HG2	14:LFF:91:LYS:HG2	2.02	0.42
36:LT0:47:ILE:HG13	36:LT0:93:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:LW0:8:VAL:HG21	39:LW0:30:PHE:HB3	2.00	0.42
43:S60:790:U:H1'	48:SC0:166:ARG:HH11	1.83	0.42
43:S60:807:G:O2'	43:S60:823:G:O6	2.25	0.42
43:S60:1224:G:O2'	43:S60:1250:G:O6	2.28	0.42
46:SB0:28:LYS:HB3	46:SB0:48:LEU:HD12	2.00	0.42
50:SD0:106:LYS:HG3	50:SD0:175:VAL:HG22	2.00	0.42
55:SG0:55:ASP:HB2	55:SG0:107:VAL:HG12	2.01	0.42
56:SGG:238:LYS:HZ2	56:SGG:252:ALA:HB1	1.85	0.42
63:SO0:82:ARG:HA	63:SO0:117:THR:HG22	2.01	0.42
73:SY0:102:ALA:HB3	73:SY0:105:VAL:HG23	2.02	0.42
1:L50:628:U:OP2	5:LB0:238:ARG:NH2	2.49	0.42
1:L50:1047:G:O5'	35:LS0:119:LYS:NZ	2.52	0.42
1:L50:2038:C:OP2	36:LT0:8:ARG:NH2	2.52	0.42
4:LAA:96:ILE:HG23	23:LL0:153:THR:HB	2.01	0.42
5:LB0:85:VAL:HG22	5:LB0:200:GLU:HG2	2.01	0.42
5:LB0:119:TYR:CZ	5:LB0:129:MET:HG2	2.55	0.42
41:LY0:71:GLU:HB3	41:LY0:80:TYR:HB2	2.00	0.42
43:S60:431:A:N3	43:S60:466:C:O2'	2.39	0.42
43:S60:882:A:N3	43:S60:887:A:O2'	2.46	0.42
47:SBB:38:SER:OG	47:SBB:58:CYS:SG	2.73	0.42
58:SI0:146:ARG:HE	58:SI0:149:GLN:HG3	1.85	0.42
73:SY0:13:ASN:HB3	73:SY0:18:ARG:HG2	2.01	0.42
1:L50:1367:C:H3'	1:L50:1368:G:C8	2.54	0.42
4:LAA:143:ARG:HG3	23:LL0:163:PHE:HB2	2.01	0.42
22:LJJ:66:LEU:HA	22:LJJ:69:VAL:HG12	2.01	0.42
56:SGG:102:LEU:HB3	56:SGG:133:TRP:CE2	2.55	0.42
65:SQ0:56:ARG:NH2	65:SQ0:110:ASN:O	2.41	0.42
68:ST0:8:ARG:HB3	68:ST0:11:ALA:HB3	2.01	0.42
71:SW0:48:THR:HG23	71:SW0:59:ILE:HB	2.01	0.42
1:L50:506:G:OP1	7:LC0:30:ARG:NH2	2.34	0.42
1:L50:627:C:H4'	1:L50:1545:A:H5'	2.01	0.42
1:L50:697:U:H3'	4:LAA:13:GLY:HA2	2.01	0.42
1:L50:1091:C:H2'	1:L50:1092:G:C8	2.55	0.42
9:LD0:32:TYR:OH	36:LT0:93:GLU:OE2	2.31	0.42
24:LLL:38:ASN:HB3	24:LLL:41:ARG:HG2	2.02	0.42
35:LS0:169:LYS:HE2	35:LS0:169:LYS:HB3	1.84	0.42
43:S60:379:A:H5''	59:SJ0:8:LYS:HE2	2.02	0.42
50:SD0:127:LYS:HD3	50:SD0:127:LYS:HA	1.84	0.42
53:SEE:30:LEU:HD12	53:SEE:34:ALA:HB1	2.01	0.42
1:L50:1253:G:N2	15:LG0:20:ASP:OD2	2.48	0.42
1:L50:1851:G:OP1	29:LO0:85:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LGG:68:SER:OG	16:LGG:69:GLN:OE1	2.35	0.42
50:SD0:41:PRO:HA	50:SD0:46:VAL:HG22	2.02	0.42
1:L50:1368:G:N2	1:L50:1397:C:N3	2.64	0.42
1:L50:2507:A:N1	17:LH0:69:THR:HG21	2.35	0.42
17:LH0:172:LEU:HB2	26:LMM:76:MET:HE1	2.01	0.42
43:S60:74:A:N3	43:S60:130:A:O2'	2.45	0.42
43:S60:425:G:O2'	43:S60:432:A:N1	2.48	0.42
43:S60:881:G:O2'	43:S60:1087:U:OP1	2.31	0.42
48:SC0:172:LYS:O	59:SJ0:55:ARG:NH1	2.51	0.42
55:SG0:7:TYR:HB3	55:SG0:10:LYS:HB2	2.02	0.42
59:SJ0:151:TYR:HD2	59:SJ0:153:VAL:HG12	1.84	0.42
1:L50:2619:U:O4'	10:LDD:20:ARG:NH1	2.52	0.42
5:LB0:109:HIS:HE1	5:LB0:111:ASN:HB3	1.83	0.42
16:LGG:76:TYR:HB2	16:LGG:85:LEU:HD13	2.02	0.42
21:LJ0:50:ALA:HB1	21:LJ0:59:ILE:HD12	2.01	0.42
32:LPP:42:CYS:HB3	32:LPP:60:CYS:SG	2.59	0.42
33:LQ0:163:PRO:HD3	33:LQ0:175:ARG:HG2	2.02	0.42
43:S60:1111:G:O2'	64:SP0:123:THR:OG1	2.33	0.42
56:SGG:315:ILE:HD11	56:SGG:323:ILE:HG22	2.02	0.42
59:SJ0:82:ILE:HG13	59:SJ0:117:ARG:HH11	1.84	0.42
1:L50:1042:U:OP2	29:LO0:43:THR:OG1	2.33	0.41
1:L50:2026:U:HO2'	1:L50:2150:A:HO2'	1.62	0.41
18:LHH:62:LEU:HD23	40:LX0:15:VAL:HG13	2.02	0.41
18:LHH:85:THR:HG22	18:LHH:87:ALA:H	1.85	0.41
19:LI0:54:SER:OG	19:LI0:130:ASP:O	2.35	0.41
31:LP0:7:PRO:HG2	31:LP0:150:ILE:HD12	2.02	0.41
43:S60:1393:G:N2	45:SAA:76:SER:OG	2.47	0.41
56:SGG:75:ARG:NH1	56:SGG:116:CYS:SG	2.93	0.41
60:SK0:21:ILE:HG22	60:SK0:64:TYR:HA	2.02	0.41
66:SR0:35:LEU:O	66:SR0:39:THR:OG1	2.35	0.41
69:SU0:77:ASN:HB2	69:SU0:79:TRP:HE1	1.85	0.41
1:L50:170:G:H3'	23:LL0:70:ARG:HD2	2.02	0.41
1:L50:1156:U:H2'	1:L50:1157:A:H8	1.85	0.41
1:L50:2086:C:H4'	1:L50:2087:G:H5''	2.02	0.41
2:L70:29:C:O2'	2:L70:50:A:N1	2.48	0.41
2:L70:83:G:O2'	2:L70:85:G:OP1	2.37	0.41
5:LB0:155:ILE:HD13	5:LB0:155:ILE:HA	1.91	0.41
11:LE0:86:PRO:HG2	11:LE0:89:ILE:HD12	2.02	0.41
22:LJJ:28:HIS:HB3	22:LJJ:31:LYS:HB2	2.02	0.41
38:LV0:35:LYS:HA	38:LV0:35:LYS:HD2	1.86	0.41
42:LZ0:46:THR:H	42:LZ0:49:MET:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S60:1123:A:O2'	43:S60:1242:G:OP1	2.38	0.41
50:SD0:33:VAL:HG11	50:SD0:100:THR:HG23	2.02	0.41
50:SD0:120:ASN:HA	50:SD0:123:MET:HG2	2.02	0.41
51:SDD:43:LEU:HB3	51:SDD:45:LEU:HD23	2.02	0.41
52:SE0:150:CYS:HB3	52:SE0:154:ILE:HD12	2.02	0.41
55:SG0:193:LEU:HD23	55:SG0:193:LEU:HA	1.93	0.41
59:SJ0:82:ILE:HG13	59:SJ0:117:ARG:NH1	2.35	0.41
59:SJ0:107:SER:HA	59:SJ0:110:LEU:HD12	2.01	0.41
63:SO0:10:LEU:H	63:SO0:10:LEU:HG	1.48	0.41
65:SQ0:27:ASP:O	65:SQ0:64:ASN:ND2	2.51	0.41
1:L50:35:C:O2	22:LJJ:70:ARG:NH1	2.47	0.41
1:L50:1462:A:H1'	1:L50:1463:C:H5	1.86	0.41
17:LH0:43:LEU:N	77:LH0:500:AMP:O2'	2.53	0.41
32:LPP:38:GLU:HA	32:LPP:45:THR:HA	2.02	0.41
43:S60:26:U:H2'	43:S60:27:G:C8	2.55	0.41
43:S60:325:A:H3'	43:S60:326:A:H8	1.85	0.41
45:SAA:51:ASP:HA	45:SAA:54:ARG:HD2	2.02	0.41
46:SB0:141:VAL:HA	46:SB0:214:THR:HA	2.02	0.41
55:SG0:168:LYS:HD3	55:SG0:168:LYS:HA	1.78	0.41
68:ST0:20:LEU:HD22	68:ST0:25:ILE:HD11	2.02	0.41
1:L50:286:C:H5'	41:LY0:33:PRO:HD3	2.03	0.41
1:L50:821:U:H4'	9:LD0:42:HIS:CD2	2.55	0.41
1:L50:830:A:O2'	1:L50:832:A:N1	2.52	0.41
1:L50:1060:C:O2'	13:LF0:148:ARG:NH2	2.39	0.41
1:L50:1119:U:H2'	1:L50:1120:G:H8	1.85	0.41
1:L50:1363:G:H2'	1:L50:1364:G:C8	2.55	0.41
1:L50:2475:U:H2'	1:L50:2476:A:C8	2.54	0.41
17:LH0:125:MET:HE3	17:LH0:131:ALA:HB2	2.02	0.41
34:LR0:114:HIS:HE1	34:LR0:143:GLU:HG3	1.84	0.41
35:LS0:100:SER:OG	35:LS0:101:ILE:N	2.53	0.41
41:LY0:49:ILE:HD13	41:LY0:79:VAL:HG11	2.02	0.41
65:SQ0:24:MET:HE2	65:SQ0:24:MET:HB3	1.93	0.41
68:ST0:58:ILE:HG23	68:ST0:77:LEU:HD21	2.02	0.41
9:LD0:28:TYR:HA	9:LD0:31:ARG:HB3	2.01	0.41
31:LP0:14:ASN:HB3	31:LP0:153:LYS:HG2	2.02	0.41
35:LS0:26:GLN:NE2	36:LT0:147:THR:O	2.52	0.41
43:S60:292:G:OP1	52:SE0:6:ARG:NH2	2.53	0.41
48:SC0:236:ASN:HB3	70:SV0:24:GLN:HE21	1.85	0.41
50:SD0:21:LEU:HD23	50:SD0:21:LEU:HA	1.91	0.41
64:SP0:19:GLY:N	67:SS0:100:VAL:O	2.40	0.41
64:SP0:122:ASP:N	64:SP0:122:ASP:OD1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L50:627:C:H3'	1:L50:628:U:H4'	2.02	0.41
8:LCC:34:LEU:HD22	8:LCC:95:LEU:HD11	2.02	0.41
14:LFF:53:VAL:HG23	14:LFF:66:ARG:HG2	2.03	0.41
36:LT0:43:VAL:H	36:LT0:57:HIS:HD2	1.68	0.41
43:S60:1227:G:N3	54:SF0:74:SER:OG	2.48	0.41
47:SBB:35:ARG:HE	47:SBB:35:ARG:HB3	1.67	0.41
53:SEE:30:LEU:HD11	53:SEE:38:ALA:HB2	2.03	0.41
63:SO0:79:VAL:HG11	63:SO0:100:LEU:HD12	2.01	0.41
1:L50:404:A:OP1	7:LC0:94:ARG:NH1	2.47	0.41
1:L50:2373:A:O2'	1:L50:2375:C:OP1	2.34	0.41
5:LB0:353:ASP:HA	5:LB0:364:GLN:HE22	1.84	0.41
20:LII:17:LEU:HD23	20:LII:17:LEU:HA	1.89	0.41
25:LM0:5:PHE:H	25:LM0:10:ARG:NH1	2.19	0.41
33:LQ0:22:ARG:H	33:LQ0:22:ARG:HG2	1.70	0.41
35:LS0:30:HIS:CD2	35:LS0:32:VAL:HG22	2.56	0.41
43:S60:642:C:H5''	46:SB0:118:LYS:HG3	2.03	0.41
43:S60:1048:C:OP1	66:SR0:48:ASN:ND2	2.40	0.41
43:S60:1213:A:H4'	43:S60:1214:G:H5'	2.01	0.41
47:SBB:20:ARG:NH2	62:SN0:13:GLU:H	2.18	0.41
66:SR0:5:ARG:HH21	66:SR0:53:TYR:HD1	1.69	0.41
17:LH0:47:VAL:HA	17:LH0:52:VAL:HA	2.03	0.41
21:LJ0:14:ILE:HD13	21:LJ0:77:ARG:HG2	2.03	0.41
24:LLL:43:HIS:CD2	24:LLL:45:ARG:H	2.39	0.41
43:S60:236:U:OP2	61:SL0:56:LYS:NZ	2.49	0.41
43:S60:302:C:H2'	43:S60:303:C:C6	2.55	0.41
43:S60:450:G:O6	72:SX0:60:ASN:ND2	2.54	0.41
46:SB0:207:LEU:HD23	46:SB0:207:LEU:HA	1.92	0.41
48:SC0:165:MET:HG2	48:SC0:212:THR:HA	2.02	0.41
71:SW0:50:ILE:N	71:SW0:57:LYS:O	2.53	0.41
1:L50:555:A:OP1	4:LAA:27:LYS:NZ	2.44	0.41
1:L50:891:U:H2'	1:L50:892:C:O4'	2.20	0.41
1:L50:1376:A:N1	1:L50:1386:C:O2'	2.47	0.41
1:L50:2160:C:H2'	1:L50:2161:G:C8	2.55	0.41
1:L50:2239:G:OP1	26:LMM:97:TYR:OH	2.36	0.41
1:L50:2339:C:OP1	5:LB0:242:LYS:NZ	2.51	0.41
1:L50:2471:C:H5''	5:LB0:359:GLY:HA2	2.02	0.41
2:L70:46:C:OP1	9:LD0:134:ARG:N	2.46	0.41
2:L70:71:U:H2'	2:L70:72:G:O4'	2.20	0.41
3:LA0:109:GLU:HG2	3:LA0:116:GLY:N	2.35	0.41
10:LDD:8:ALA:N	10:LDD:107:TYR:O	2.53	0.41
19:LI0:52:LEU:HD11	19:LI0:156:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LPP:48:LYS:HE3	32:LPP:48:LYS:HB3	1.95	0.41
33:LQ0:23:ASN:HB3	33:LQ0:26:LEU:HB3	2.02	0.41
37:LU0:20:LEU:O	37:LU0:25:LEU:N	2.42	0.41
43:S60:62:G:O2'	43:S60:74:A:N6	2.53	0.41
43:S60:472:C:H2'	43:S60:473:G:H8	1.86	0.41
48:SC0:225:PRO:HA	48:SC0:228:TRP:CD1	2.55	0.41
50:SD0:116:ARG:HA	50:SD0:119:VAL:HG12	2.03	0.41
52:SE0:182:PHE:N	52:SE0:226:PHE:O	2.40	0.41
58:SI0:66:THR:HG22	58:SI0:73:SER:HB3	2.03	0.41
67:SS0:133:ARG:HD3	67:SS0:140:VAL:HG23	2.03	0.41
1:L50:2203:C:H2'	1:L50:2204:A:C8	2.56	0.41
8:LCC:36:GLN:NE2	42:LZ0:69:SER:O	2.47	0.41
19:LI0:200:ILE:HD13	19:LI0:200:ILE:HA	1.88	0.41
25:LM0:17:LEU:HA	25:LM0:20:ARG:HG2	2.03	0.41
28:LNN:14:MET:HE3	28:LNN:14:MET:HB3	1.82	0.41
41:LY0:50:ARG:HD2	41:LY0:114:ARG:HD2	2.03	0.41
43:S60:217:U:H2'	43:S60:218:G:C8	2.57	0.41
43:S60:988:U:O3'	48:SC0:210:LYS:NZ	2.52	0.41
43:S60:1206:C:H5''	67:SS0:46:GLY:H	1.86	0.41
49:SCC:33:THR:OG1	49:SCC:34:GLY:N	2.54	0.41
51:SDD:59:PHE:HB3	69:SU0:82:TYR:HB3	2.03	0.41
54:SF0:38:SER:OG	54:SF0:40:TYR:O	2.29	0.41
54:SF0:67:LEU:O	54:SF0:69:ARG:N	2.54	0.41
59:SJ0:93:ASP:O	59:SJ0:97:ASN:ND2	2.34	0.41
1:L50:333:G:OP1	1:L50:1901:G:O2'	2.38	0.40
1:L50:1092:G:OP2	7:LC0:187:ARG:NH1	2.37	0.40
1:L50:1551:G:O2'	34:LR0:82:LYS:O	2.32	0.40
1:L50:1821:A:H5''	31:LP0:84:TRP:O	2.21	0.40
1:L50:1892:U:H2'	1:L50:1893:A:C8	2.57	0.40
1:L50:2378:A:O2'	5:LB0:257:ASN:HB3	2.21	0.40
1:L50:2469:C:O2'	1:L50:2585:U:OP1	2.32	0.40
4:LAA:77:LYS:O	4:LAA:80:SER:OG	2.36	0.40
5:LB0:291:LYS:HB2	5:LB0:298:LEU:HD23	2.03	0.40
9:LD0:63:LEU:HB3	9:LD0:72:SER:HA	2.03	0.40
12:LEE:19:ARG:HG3	12:LEE:33:ARG:H	1.85	0.40
13:LF0:44:ARG:HD2	13:LF0:44:ARG:HA	1.84	0.40
42:LZ0:96:GLU:O	42:LZ0:100:MET:N	2.52	0.40
43:S60:249:U:H2'	43:S60:250:A:C8	2.56	0.40
43:S60:1006:C:H5'	66:SR0:6:ASN:HA	2.03	0.40
1:L50:386:C:O2	1:L50:390:A:O2'	2.30	0.40
1:L50:2057:U:OP1	1:L50:2142:C:O2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LAA:118:LEU:HG	33:LQ0:92:LEU:HD12	2.03	0.40
7:LC0:237:LEU:HA	7:LC0:237:LEU:HD13	1.86	0.40
19:LI0:12:CYS:HA	19:LI0:59:GLN:HE21	1.86	0.40
19:LI0:189:LYS:NZ	19:LI0:209:TYR:OH	2.54	0.40
25:LM0:21:ASN:OD1	25:LM0:21:ASN:N	2.55	0.40
25:LM0:65:MET:HE2	25:LM0:69:GLU:HB3	2.03	0.40
41:LY0:2:LYS:HE3	41:LY0:2:LYS:HB3	1.90	0.40
52:SE0:36:HIS:NE2	52:SE0:88:ASP:OD2	2.54	0.40
54:SF0:65:CYS:HA	54:SF0:68:MET:HE2	2.02	0.40
56:SGG:50:GLU:O	56:SGG:54:PHE:N	2.52	0.40
61:SL0:66:ARG:NH1	61:SL0:129:THR:O	2.54	0.40
64:SP0:35:GLU:HA	64:SP0:42:ARG:HD3	2.03	0.40
1:L50:162:C:OP2	1:L50:341:G:N2	2.46	0.40
5:LB0:86:VAL:O	5:LB0:198:GLU:N	2.54	0.40
5:LB0:156:ARG:HG2	5:LB0:180:GLN:HA	2.03	0.40
7:LC0:54:ASN:HB3	7:LC0:58:GLN:HE21	1.87	0.40
12:LEE:119:LEU:HD23	12:LEE:119:LEU:HA	1.94	0.40
33:LQ0:8:SER:O	33:LQ0:10:LYS:N	2.51	0.40
43:S60:104:A:N3	43:S60:243:A:O2'	2.49	0.40
50:SD0:13:GLU:HA	50:SD0:16:ILE:HG22	2.02	0.40
54:SF0:70:ARG:HD2	54:SF0:70:ARG:HA	1.79	0.40
56:SGG:257:THR:OG1	56:SGG:275:THR:OG1	2.25	0.40
62:SN0:2:ALA:HB2	62:SN0:9:ARG:HH11	1.87	0.40
1:L50:1140:C:O2'	1:L50:1142:G:OP2	2.38	0.40
1:L50:1381:U:OP1	34:LR0:100:ARG:NE	2.49	0.40
1:L50:1654:G:O2'	1:L50:1783:U:OP2	2.32	0.40
1:L50:2351:C:H2'	1:L50:2352:G:C8	2.57	0.40
1:L50:2499:A:H5'	17:LH0:68:ILE:HD12	2.03	0.40
1:L50:2552:C:P	5:LB0:120:ARG:HG2	2.62	0.40
2:L70:44:C:OP2	21:LJ0:137:ARG:NH2	2.55	0.40
4:LAA:96:ILE:HD13	4:LAA:96:ILE:HA	1.98	0.40
17:LH0:9:LYS:HD2	17:LH0:51:HIS:CE1	2.56	0.40
17:LH0:125:MET:SD	17:LH0:153:SER:HB3	2.61	0.40
27:LN0:53:TYR:HB2	27:LN0:133:ILE:HD13	2.04	0.40
40:LX0:99:ILE:HD13	40:LX0:99:ILE:HA	1.87	0.40
43:S60:578:G:H5'	62:SN0:4:MET:HE3	2.03	0.40
43:S60:790:U:O3'	48:SC0:166:ARG:NH1	2.54	0.40
58:SI0:33:PRO:O	58:SI0:35:ASN:ND2	2.54	0.40
72:SX0:1:MET:HE3	72:SX0:1:MET:HB2	1.85	0.40
1:L50:2451:U:H2'	1:L50:2452:G:C8	2.56	0.40
6:LBB:24:VAL:HG11	36:LT0:85:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LE0:65:PHE:HB3	11:LE0:68:ARG:HG3	2.02	0.40
15:LG0:117:ILE:HB	15:LG0:163:ILE:HB	2.03	0.40
29:LO0:87:VAL:HG21	29:LO0:98:LEU:HG	2.03	0.40
32:LPP:47:VAL:HA	32:LPP:57:CYS:HA	2.03	0.40
35:LS0:17:MET:HE2	35:LS0:17:MET:HB2	1.83	0.40
43:S60:238:G:H5''	58:SI0:98:LYS:HB3	2.03	0.40
43:S60:354:A:H2'	43:S60:355:A:H8	1.87	0.40
63:SO0:82:ARG:HG2	63:SO0:83:GLY:O	2.22	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	LA0	244/247 (99%)	234 (96%)	10 (4%)	0	100	100
4	LAA	143/155 (92%)	133 (93%)	9 (6%)	1 (1%)	18	48
5	LB0	357/385 (93%)	348 (98%)	8 (2%)	1 (0%)	36	65
6	LBB	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
7	LC0	323/330 (98%)	313 (97%)	9 (3%)	1 (0%)	36	65
8	LCC	98/108 (91%)	96 (98%)	2 (2%)	0	100	100
9	LD0	256/266 (96%)	249 (97%)	7 (3%)	0	100	100
10	LDD	101/109 (93%)	100 (99%)	1 (1%)	0	100	100
11	LE0	177/180 (98%)	159 (90%)	18 (10%)	0	100	100
12	LEE	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
13	LF0	245/254 (96%)	238 (97%)	7 (3%)	0	100	100
14	LFF	102/108 (94%)	102 (100%)	0	0	100	100
15	LG0	200/216 (93%)	198 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LGG	98/113 (87%)	95 (97%)	3 (3%)	0	100	100
17	LH0	182/186 (98%)	177 (97%)	5 (3%)	0	100	100
18	LHH	118/126 (94%)	113 (96%)	5 (4%)	0	100	100
19	LI0	205/218 (94%)	202 (98%)	3 (2%)	0	100	100
20	LII	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
21	LJ0	166/174 (95%)	162 (98%)	4 (2%)	0	100	100
22	LJJ	87/95 (92%)	85 (98%)	2 (2%)	0	100	100
23	LL0	162/166 (98%)	154 (95%)	8 (5%)	0	100	100
24	LLL	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
25	LM0	93/108 (86%)	92 (99%)	1 (1%)	0	100	100
26	LMM	52/132 (39%)	51 (98%)	1 (2%)	0	100	100
27	LN0	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
28	LNN	73/77 (95%)	73 (100%)	0	0	100	100
29	LO0	194/198 (98%)	193 (100%)	1 (0%)	0	100	100
30	LOO	89/112 (80%)	85 (96%)	4 (4%)	0	100	100
31	LP0	151/171 (88%)	147 (97%)	4 (3%)	0	100	100
32	LPP	79/86 (92%)	75 (95%)	4 (5%)	0	100	100
33	LQ0	174/178 (98%)	170 (98%)	4 (2%)	0	100	100
34	LR0	159/166 (96%)	156 (98%)	3 (2%)	0	100	100
35	LS0	167/175 (95%)	165 (99%)	2 (1%)	0	100	100
36	LT0	158/160 (99%)	151 (96%)	7 (4%)	0	100	100
37	LU0	95/114 (83%)	89 (94%)	6 (6%)	0	100	100
38	LV0	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
39	LW0	91/133 (68%)	86 (94%)	5 (6%)	0	100	100
40	LX0	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
41	LY0	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
42	LZ0	125/127 (98%)	124 (99%)	1 (1%)	0	100	100
44	SA0	200/242 (83%)	191 (96%)	9 (4%)	0	100	100
45	SAA	95/104 (91%)	95 (100%)	0	0	100	100
46	SB0	192/230 (84%)	187 (97%)	5 (3%)	0	100	100
47	SBB	78/86 (91%)	75 (96%)	2 (3%)	1 (1%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	SC0	219/255 (86%)	203 (93%)	16 (7%)	0	100	100
49	SCC	53/65 (82%)	51 (96%)	2 (4%)	0	100	100
50	SD0	211/217 (97%)	201 (95%)	10 (5%)	0	100	100
51	SDD	57/63 (90%)	55 (96%)	2 (4%)	0	100	100
52	SE0	255/267 (96%)	242 (95%)	13 (5%)	0	100	100
53	SEE	45/60 (75%)	42 (93%)	3 (7%)	0	100	100
54	SF0	184/195 (94%)	174 (95%)	10 (5%)	0	100	100
55	SG0	216/222 (97%)	210 (97%)	6 (3%)	0	100	100
56	SGG	303/330 (92%)	284 (94%)	17 (6%)	2 (1%)	18	48
57	SH0	152/176 (86%)	147 (97%)	5 (3%)	0	100	100
58	SI0	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
59	SJ0	162/187 (87%)	151 (93%)	11 (7%)	0	100	100
60	SK0	72/102 (71%)	68 (94%)	4 (6%)	0	100	100
61	SL0	129/160 (81%)	122 (95%)	6 (5%)	1 (1%)	16	44
62	SN0	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
63	SO0	126/135 (93%)	123 (98%)	2 (2%)	1 (1%)	16	44
64	SP0	110/146 (75%)	107 (97%)	3 (3%)	0	100	100
65	SQ0	125/145 (86%)	116 (93%)	9 (7%)	0	100	100
66	SR0	111/123 (90%)	108 (97%)	3 (3%)	0	100	100
67	SS0	142/161 (88%)	139 (98%)	3 (2%)	0	100	100
68	ST0	137/141 (97%)	133 (97%)	4 (3%)	0	100	100
69	SU0	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
70	SV0	61/66 (92%)	60 (98%)	1 (2%)	0	100	100
71	SW0	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
72	SX0	136/140 (97%)	128 (94%)	8 (6%)	0	100	100
73	SY0	119/133 (90%)	114 (96%)	5 (4%)	0	100	100
74	SZ0	70/126 (56%)	68 (97%)	2 (3%)	0	100	100
All	All	10146/11144 (91%)	9789 (96%)	349 (3%)	8 (0%)	49	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	LAA	24	LYS

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Mol	Chain	Res	Type
63	SO0	123	ARG
56	SGG	287	ASN
5	LB0	186	VAL
61	SL0	80	GLU
7	LC0	147	ILE
47	SBB	56	PRO
56	SGG	162	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	LA0	199/200 (100%)	198 (100%)	1 (0%)	81	93
4	LAA	122/131 (93%)	122 (100%)	0	100	100
5	LB0	316/335 (94%)	316 (100%)	0	100	100
6	LBB	54/55 (98%)	54 (100%)	0	100	100
7	LC0	275/280 (98%)	274 (100%)	1 (0%)	84	94
8	LCC	82/88 (93%)	82 (100%)	0	100	100
9	LD0	223/231 (96%)	221 (99%)	2 (1%)	70	90
10	LDD	94/99 (95%)	94 (100%)	0	100	100
11	LE0	156/164 (95%)	156 (100%)	0	100	100
12	LEE	105/115 (91%)	105 (100%)	0	100	100
13	LF0	213/220 (97%)	213 (100%)	0	100	100
14	LFF	90/94 (96%)	90 (100%)	0	100	100
15	LG0	180/191 (94%)	179 (99%)	1 (1%)	78	93
16	LGG	86/96 (90%)	86 (100%)	0	100	100
17	LH0	163/164 (99%)	163 (100%)	0	100	100
18	LHH	114/120 (95%)	114 (100%)	0	100	100
19	LI0	174/180 (97%)	174 (100%)	0	100	100
20	LII	84/85 (99%)	83 (99%)	1 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	LJ0	145/151 (96%)	145 (100%)	0	100	100
22	LJJ	73/79 (92%)	72 (99%)	1 (1%)	59	85
23	LL0	146/148 (99%)	146 (100%)	0	100	100
24	LLL	48/48 (100%)	47 (98%)	1 (2%)	47	77
25	LM0	92/101 (91%)	92 (100%)	0	100	100
26	LMM	46/112 (41%)	46 (100%)	0	100	100
27	LN0	170/171 (99%)	168 (99%)	2 (1%)	63	86
28	LNN	65/67 (97%)	65 (100%)	0	100	100
29	LO0	174/176 (99%)	172 (99%)	2 (1%)	65	88
30	LOO	83/100 (83%)	83 (100%)	0	100	100
31	LP0	134/147 (91%)	134 (100%)	0	100	100
32	LPP	61/65 (94%)	61 (100%)	0	100	100
33	LQ0	148/150 (99%)	148 (100%)	0	100	100
34	LR0	126/142 (89%)	126 (100%)	0	100	100
35	LS0	157/161 (98%)	157 (100%)	0	100	100
36	LT0	139/139 (100%)	139 (100%)	0	100	100
38	LV0	114/116 (98%)	113 (99%)	1 (1%)	70	90
39	LW0	72/114 (63%)	72 (100%)	0	100	100
40	LX0	80/88 (91%)	80 (100%)	0	100	100
41	LY0	123/125 (98%)	123 (100%)	0	100	100
42	LZ0	106/106 (100%)	105 (99%)	1 (1%)	70	90
45	SAA	83/89 (93%)	83 (100%)	0	100	100
46	SB0	174/204 (85%)	174 (100%)	0	100	100
47	SBB	72/77 (94%)	70 (97%)	2 (3%)	38	72
48	SC0	185/214 (86%)	182 (98%)	3 (2%)	55	83
49	SCC	47/56 (84%)	46 (98%)	1 (2%)	47	77
50	SD0	191/195 (98%)	190 (100%)	1 (0%)	81	93
51	SDD	50/54 (93%)	50 (100%)	0	100	100
52	SE0	227/235 (97%)	226 (100%)	1 (0%)	84	94
53	SEE	21/51 (41%)	20 (95%)	1 (5%)	23	55
54	SF0	157/164 (96%)	156 (99%)	1 (1%)	78	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	SG0	189/198 (96%)	188 (100%)	1 (0%)	81	93
56	SGG	247/266 (93%)	244 (99%)	3 (1%)	63	86
57	SH0	67/160 (42%)	67 (100%)	0	100	100
58	SI0	150/155 (97%)	150 (100%)	0	100	100
59	SJ0	149/165 (90%)	149 (100%)	0	100	100
60	SK0	64/92 (70%)	63 (98%)	1 (2%)	55	83
61	SL0	119/142 (84%)	118 (99%)	1 (1%)	73	90
62	SN0	122/125 (98%)	122 (100%)	0	100	100
63	SO0	96/103 (93%)	92 (96%)	4 (4%)	26	60
64	SP0	102/130 (78%)	101 (99%)	1 (1%)	68	89
65	SQ0	109/122 (89%)	108 (99%)	1 (1%)	70	90
66	SR0	64/116 (55%)	63 (98%)	1 (2%)	55	83
67	SS0	121/134 (90%)	121 (100%)	0	100	100
68	ST0	118/120 (98%)	115 (98%)	3 (2%)	42	74
69	SU0	88/100 (88%)	88 (100%)	0	100	100
70	SV0	46/59 (78%)	46 (100%)	0	100	100
71	SW0	110/110 (100%)	109 (99%)	1 (1%)	70	90
72	SX0	116/118 (98%)	115 (99%)	1 (1%)	70	90
73	SY0	96/125 (77%)	95 (99%)	1 (1%)	68	89
74	SZ0	60/103 (58%)	60 (100%)	0	100	100
All	All	8472/9336 (91%)	8429 (100%)	43 (0%)	78	93

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LA0	155	ARG
7	LC0	11	ASP
9	LD0	30	HIS
9	LD0	103	VAL
15	LG0	122	VAL
20	LII	82	ARG
22	LJJ	53	ARG
24	LLL	29	ARG
27	LN0	26	ARG
27	LN0	90	TYR

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Mol	Chain	Res	Type
29	LO0	116	ARG
29	LO0	137	TYR
38	LV0	48	ARG
42	LZ0	94	ASN
47	SBB	36	CYS
47	SBB	82	LYS
48	SC0	181	VAL
48	SC0	205	THR
48	SC0	243	ARG
49	SCC	50	VAL
50	SD0	93	ASN
52	SE0	206	ASP
53	SEE	43	ARG
54	SF0	116	CYS
55	SG0	185	ARG
56	SGG	48	LEU
56	SGG	99	ARG
56	SGG	144	ASP
60	SK0	19	ARG
61	SL0	66	ARG
63	SO0	10	LEU
63	SO0	24	THR
63	SO0	123	ARG
63	SO0	134	ARG
64	SP0	65	LYS
65	SQ0	60	LYS
66	SR0	38	VAL
68	ST0	34	ILE
68	ST0	68	GLU
68	ST0	122	ARG
71	SW0	48	THR
72	SX0	118	LYS
73	SY0	130	ARG

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L50	2443/2639 (92%)	457 (18%)	19 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L70	118/119 (99%)	17 (14%)	1 (0%)
43	S60	1329/1400 (94%)	281 (21%)	15 (1%)
All	All	3890/4158 (93%)	755 (19%)	35 (0%)

All (755) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L50	35	C
1	L50	36	C
1	L50	49	G
1	L50	50	G
1	L50	55	A
1	L50	60	A
1	L50	63	G
1	L50	65	C
1	L50	76	U
1	L50	79	G
1	L50	84	G
1	L50	97	C
1	L50	99	A
1	L50	100	C
1	L50	101	A
1	L50	107	G
1	L50	108	C
1	L50	110	G
1	L50	112	C
1	L50	122	C
1	L50	134	A
1	L50	137	A
1	L50	143	C
1	L50	151	C
1	L50	153	G
1	L50	154	A
1	L50	159	A
1	L50	160	A
1	L50	167	A
1	L50	169	G
1	L50	171	A
1	L50	183	G
1	L50	186	G
1	L50	190	G
1	L50	193	A

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Mol	Chain	Res	Type
1	L50	196	A
1	L50	203	A
1	L50	204	G
1	L50	205	C
1	L50	207	C
1	L50	210	A
1	L50	213	G
1	L50	214	C
1	L50	215	A
1	L50	222	A
1	L50	223	U
1	L50	224	C
1	L50	225	G
1	L50	232	U
1	L50	237	C
1	L50	238	A
1	L50	239	G
1	L50	240	C
1	L50	245	C
1	L50	246	G
1	L50	261	A
1	L50	271	C
1	L50	272	A
1	L50	274	A
1	L50	279	G
1	L50	280	A
1	L50	282	A
1	L50	292	C
1	L50	294	G
1	L50	296	G
1	L50	298	G
1	L50	301	G
1	L50	304	G
1	L50	305	A
1	L50	307	C
1	L50	308	G
1	L50	309	A
1	L50	310	G
1	L50	311	U
1	L50	324	U
1	L50	325	C
1	L50	326	A

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Mol	Chain	Res	Type
1	L50	327	U
1	L50	336	A
1	L50	338	G
1	L50	339	C
1	L50	343	G
1	L50	346	G
1	L50	362	A
1	L50	375	G
1	L50	378	C
1	L50	387	A
1	L50	388	C
1	L50	390	A
1	L50	397	C
1	L50	410	A
1	L50	412	G
1	L50	417	G
1	L50	428	C
1	L50	429	G
1	L50	435	A
1	L50	436	G
1	L50	438	G
1	L50	453	C
1	L50	454	G
1	L50	461	U
1	L50	462	G
1	L50	467	C
1	L50	468	C
1	L50	472	U
1	L50	481	A
1	L50	492	A
1	L50	509	A
1	L50	513	C
1	L50	517	C
1	L50	518	C
1	L50	520	C
1	L50	521	G
1	L50	526	A
1	L50	527	G
1	L50	533	G
1	L50	537	U
1	L50	539	G
1	L50	540	A

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Mol	Chain	Res	Type
1	L50	553	C
1	L50	560	A
1	L50	571	A
1	L50	584	A
1	L50	600	A
1	L50	615	C
1	L50	618	C
1	L50	624	G
1	L50	628	U
1	L50	633	U
1	L50	651	C
1	L50	661	G
1	L50	662	C
1	L50	668	A
1	L50	670	G
1	L50	671	A
1	L50	674	A
1	L50	675	A
1	L50	677	C
1	L50	678	G
1	L50	679	A
1	L50	686	U
1	L50	691	G
1	L50	698	C
1	L50	703	C
1	L50	713	C
1	L50	714	G
1	L50	732	C
1	L50	733	G
1	L50	734	C
1	L50	752	C
1	L50	753	A
1	L50	787	C
1	L50	789	A
1	L50	791	C
1	L50	793	G
1	L50	798	G
1	L50	799	C
1	L50	805	G
1	L50	806	G
1	L50	815	G
1	L50	820	G

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Mol	Chain	Res	Type
1	L50	832	A
1	L50	833	A
1	L50	838	G
1	L50	851	G
1	L50	858	C
1	L50	863	A
1	L50	865	G
1	L50	878	U
1	L50	879	G
1	L50	883	A
1	L50	884	C
1	L50	885	A
1	L50	886	C
1	L50	887	A
1	L50	888	A
1	L50	893	G
1	L50	912	C
1	L50	913	A
1	L50	915	C
1	L50	916	U
1	L50	917	G
1	L50	919	G
1	L50	924	C
1	L50	925	A
1	L50	927	A
1	L50	928	C
1	L50	933	G
1	L50	935	C
1	L50	939	G
1	L50	1032	U
1	L50	1034	G
1	L50	1035	A
1	L50	1036	C
1	L50	1040	G
1	L50	1044	A
1	L50	1045	G
1	L50	1056	A
1	L50	1069	A
1	L50	1070	C
1	L50	1071	A
1	L50	1072	G
1	L50	1077	G

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Mol	Chain	Res	Type
1	L50	1093	G
1	L50	1095	G
1	L50	1096	C
1	L50	1125	G
1	L50	1127	G
1	L50	1139	G
1	L50	1142	G
1	L50	1145	C
1	L50	1151	G
1	L50	1161	C
1	L50	1162	A
1	L50	1176	C
1	L50	1186	G
1	L50	1190	G
1	L50	1203	G
1	L50	1205	C
1	L50	1209	C
1	L50	1210	C
1	L50	1213	U
1	L50	1224	U
1	L50	1234	C
1	L50	1235	C
1	L50	1236	U
1	L50	1242	C
1	L50	1245	G
1	L50	1247	U
1	L50	1248	G
1	L50	1249	G
1	L50	1250	C
1	L50	1255	A
1	L50	1260	A
1	L50	1262	A
1	L50	1266	A
1	L50	1275	C
1	L50	1278	A
1	L50	1280	U
1	L50	1286	G
1	L50	1293	G
1	L50	1298	G
1	L50	1305	C
1	L50	1307	C
1	L50	1310	C

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Mol	Chain	Res	Type
1	L50	1317	G
1	L50	1319	C
1	L50	1320	C
1	L50	1321	G
1	L50	1331	C
1	L50	1340	G
1	L50	1341	G
1	L50	1346	C
1	L50	1351	C
1	L50	1367	C
1	L50	1376	A
1	L50	1377	C
1	L50	1384	A
1	L50	1387	A
1	L50	1388	C
1	L50	1389	G
1	L50	1390	A
1	L50	1399	G
1	L50	1400	C
1	L50	1404	G
1	L50	1438	C
1	L50	1446	G
1	L50	1447	A
1	L50	1460	G
1	L50	1461	C
1	L50	1462	A
1	L50	1479	A
1	L50	1480	A
1	L50	1481	U
1	L50	1485	C
1	L50	1488	C
1	L50	1489	A
1	L50	1505	C
1	L50	1518	G
1	L50	1522	C
1	L50	1523	C
1	L50	1543	G
1	L50	1544	C
1	L50	1563	C
1	L50	1584	G
1	L50	1586	G
1	L50	1587	C

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Mol	Chain	Res	Type
1	L50	1596	U
1	L50	1597	C
1	L50	1600	U
1	L50	1606	G
1	L50	1607	G
1	L50	1616	A
1	L50	1619	G
1	L50	1625	U
1	L50	1629	A
1	L50	1643	C
1	L50	1646	C
1	L50	1648	C
1	L50	1653	G
1	L50	1656	G
1	L50	1692	G
1	L50	1694	C
1	L50	1697	G
1	L50	1698	C
1	L50	1713	A
1	L50	1718	G
1	L50	1719	G
1	L50	1722	G
1	L50	1724	A
1	L50	1725	A
1	L50	1741	G
1	L50	1742	G
1	L50	1748	A
1	L50	1750	A
1	L50	1757	G
1	L50	1767	U
1	L50	1776	G
1	L50	1777	C
1	L50	1779	U
1	L50	1782	A
1	L50	1784	G
1	L50	1788	C
1	L50	1792	G
1	L50	1803	U
1	L50	1805	U
1	L50	1841	A
1	L50	1842	A
1	L50	1843	C

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Mol	Chain	Res	Type
1	L50	1844	G
1	L50	1852	C
1	L50	1855	A
1	L50	1862	G
1	L50	1866	A
1	L50	1870	A
1	L50	1871	A
1	L50	1872	G
1	L50	1873	A
1	L50	1880	U
1	L50	1881	G
1	L50	1906	G
1	L50	1907	G
1	L50	1908	C
1	L50	1980	U
1	L50	1984	G
1	L50	1985	C
1	L50	1987	G
1	L50	1990	A
1	L50	1991	C
1	L50	1999	G
1	L50	2003	G
1	L50	2004	G
1	L50	2007	G
1	L50	2023	A
1	L50	2024	C
1	L50	2045	G
1	L50	2048	G
1	L50	2049	U
1	L50	2053	A
1	L50	2062	U
1	L50	2068	C
1	L50	2071	A
1	L50	2074	G
1	L50	2078	C
1	L50	2086	C
1	L50	2087	G
1	L50	2088	A
1	L50	2091	A
1	L50	2093	A
1	L50	2102	C
1	L50	2111	C

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Mol	Chain	Res	Type
1	L50	2117	G
1	L50	2122	C
1	L50	2129	G
1	L50	2144	G
1	L50	2145	G
1	L50	2147	C
1	L50	2154	A
1	L50	2163	G
1	L50	2164	C
1	L50	2165	A
1	L50	2168	C
1	L50	2174	G
1	L50	2175	C
1	L50	2176	G
1	L50	2179	G
1	L50	2187	G
1	L50	2188	G
1	L50	2190	U
1	L50	2191	G
1	L50	2192	A
1	L50	2193	A
1	L50	2194	A
1	L50	2196	G
1	L50	2201	C
1	L50	2205	G
1	L50	2208	A
1	L50	2236	G
1	L50	2238	A
1	L50	2244	G
1	L50	2247	G
1	L50	2250	U
1	L50	2252	U
1	L50	2258	C
1	L50	2262	G
1	L50	2263	A
1	L50	2278	A
1	L50	2280	C
1	L50	2289	G
1	L50	2290	C
1	L50	2294	G
1	L50	2301	A
1	L50	2302	A

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Mol	Chain	Res	Type
1	L50	2314	U
1	L50	2326	C
1	L50	2327	A
1	L50	2329	G
1	L50	2332	A
1	L50	2333	C
1	L50	2338	G
1	L50	2342	G
1	L50	2345	U
1	L50	2362	A
1	L50	2363	G
1	L50	2374	C
1	L50	2375	C
1	L50	2381	G
1	L50	2383	G
1	L50	2395	C
1	L50	2400	A
1	L50	2401	G
1	L50	2403	G
1	L50	2445	C
1	L50	2446	G
1	L50	2465	G
1	L50	2477	C
1	L50	2494	G
1	L50	2503	C
1	L50	2515	G
1	L50	2516	C
1	L50	2527	U
1	L50	2535	A
1	L50	2536	A
1	L50	2537	C
1	L50	2544	U
1	L50	2547	C
1	L50	2548	C
1	L50	2559	A
1	L50	2571	C
1	L50	2572	C
1	L50	2573	G
1	L50	2598	G
1	L50	2613	G
1	L50	2619	U
1	L50	2624	A

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Mol	Chain	Res	Type
1	L50	2630	G
1	L50	2632	G
2	L70	7	G
2	L70	13	A
2	L70	22	A
2	L70	27	A
2	L70	33	A
2	L70	50	A
2	L70	53	U
2	L70	54	A
2	L70	64	G
2	L70	72	G
2	L70	74	A
2	L70	89	G
2	L70	91	C
2	L70	100	A
2	L70	101	A
2	L70	109	U
2	L70	110	A
43	S60	4	C
43	S60	26	U
43	S60	33	G
43	S60	41	G
43	S60	42	A
43	S60	46	A
43	S60	56	G
43	S60	59	A
43	S60	60	G
43	S60	64	A
43	S60	71	C
43	S60	73	G
43	S60	84	G
43	S60	93	G
43	S60	94	G
43	S60	95	A
43	S60	100	G
43	S60	103	A
43	S60	104	A
43	S60	105	U
43	S60	114	A
43	S60	115	G
43	S60	118	G

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Mol	Chain	Res	Type
43	S60	121	A
43	S60	122	C
43	S60	123	A
43	S60	133	G
43	S60	135	G
43	S60	147	C
43	S60	150	A
43	S60	159	C
43	S60	169	C
43	S60	170	G
43	S60	177	G
43	S60	178	G
43	S60	195	G
43	S60	196	G
43	S60	197	A
43	S60	198	G
43	S60	199	C
43	S60	210	G
43	S60	215	G
43	S60	220	C
43	S60	223	A
43	S60	225	C
43	S60	227	G
43	S60	230	G
43	S60	231	G
43	S60	242	A
43	S60	246	G
43	S60	247	C
43	S60	261	G
43	S60	268	G
43	S60	269	A
43	S60	270	C
43	S60	289	A
43	S60	299	G
43	S60	302	C
43	S60	309	A
43	S60	311	C
43	S60	313	G
43	S60	325	A
43	S60	326	A
43	S60	327	G
43	S60	332	G

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Mol	Chain	Res	Type
43	S60	333	C
43	S60	334	A
43	S60	335	G
43	S60	343	G
43	S60	344	G
43	S60	348	U
43	S60	353	C
43	S60	362	C
43	S60	363	G
43	S60	364	G
43	S60	376	A
43	S60	377	C
43	S60	399	C
43	S60	400	A
43	S60	405	A
43	S60	414	C
43	S60	415	G
43	S60	431	A
43	S60	432	A
43	S60	433	G
43	S60	434	U
43	S60	435	C
43	S60	441	C
43	S60	442	C
43	S60	444	G
43	S60	446	A
43	S60	450	G
43	S60	458	U
43	S60	470	A
43	S60	471	G
43	S60	487	C
43	S60	495	A
43	S60	496	A
43	S60	497	A
43	S60	498	A
43	S60	499	C
43	S60	500	G
43	S60	505	U
43	S60	511	G
43	S60	530	A
43	S60	531	A
43	S60	538	G

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Mol	Chain	Res	Type
43	S60	540	G
43	S60	541	C
43	S60	546	G
43	S60	554	G
43	S60	555	C
43	S60	556	A
43	S60	557	G
43	S60	563	G
43	S60	564	A
43	S60	568	G
43	S60	569	G
43	S60	570	G
43	S60	574	A
43	S60	587	A
43	S60	617	A
43	S60	622	G
43	S60	624	G
43	S60	625	G
43	S60	639	G
43	S60	643	G
43	S60	644	G
43	S60	646	A
43	S60	653	G
43	S60	670	G
43	S60	671	U
43	S60	677	G
43	S60	680	C
43	S60	681	A
43	S60	699	A
43	S60	703	A
43	S60	704	A
43	S60	707	U
43	S60	715	U
43	S60	716	A
43	S60	731	G
43	S60	737	A
43	S60	739	C
43	S60	741	A
43	S60	743	G
43	S60	754	G
43	S60	755	A
43	S60	756	G

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Mol	Chain	Res	Type
43	S60	762	G
43	S60	763	G
43	S60	766	C
43	S60	770	G
43	S60	779	A
43	S60	785	G
43	S60	789	G
43	S60	790	U
43	S60	793	G
43	S60	794	G
43	S60	802	G
43	S60	819	G
43	S60	831	A
43	S60	843	G
43	S60	847	G
43	S60	851	C
43	S60	852	C
43	S60	853	A
43	S60	855	A
43	S60	860	G
43	S60	878	U
43	S60	879	U
43	S60	886	A
43	S60	887	A
43	S60	889	G
43	S60	892	G
43	S60	893	G
43	S60	895	C
43	S60	900	U
43	S60	902	C
43	S60	905	G
43	S60	910	G
43	S60	911	G
43	S60	914	G
43	S60	975	G
43	S60	976	C
43	S60	996	C
43	S60	997	U
43	S60	1004	U
43	S60	1005	U
43	S60	1006	C
43	S60	1011	A

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Mol	Chain	Res	Type
43	S60	1027	G
43	S60	1028	G
43	S60	1030	G
43	S60	1039	G
43	S60	1044	G
43	S60	1047	A
43	S60	1049	G
43	S60	1058	C
43	S60	1059	A
43	S60	1061	G
43	S60	1069	A
43	S60	1071	G
43	S60	1072	G
43	S60	1073	C
43	S60	1082	A
43	S60	1083	C
43	S60	1084	A
43	S60	1085	G
43	S60	1092	G
43	S60	1093	A
43	S60	1102	G
43	S60	1103	A
43	S60	1104	U
43	S60	1115	G
43	S60	1116	C
43	S60	1117	A
43	S60	1118	C
43	S60	1128	A
43	S60	1140	A
43	S60	1141	G
43	S60	1144	G
43	S60	1145	G
43	S60	1146	A
43	S60	1156	G
43	S60	1162	G
43	S60	1163	G
43	S60	1164	C
43	S60	1166	A
43	S60	1168	G
43	S60	1176	G
43	S60	1177	C
43	S60	1179	G

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Mol	Chain	Res	Type
43	S60	1180	C
43	S60	1182	G
43	S60	1184	G
43	S60	1190	G
43	S60	1196	G
43	S60	1198	A
43	S60	1199	G
43	S60	1200	G
43	S60	1208	G
43	S60	1209	A
43	S60	1213	A
43	S60	1214	G
43	S60	1224	G
43	S60	1230	G
43	S60	1240	A
43	S60	1241	A
43	S60	1247	G
43	S60	1255	A
43	S60	1256	G
43	S60	1259	C
43	S60	1260	C
43	S60	1261	U
43	S60	1262	G
43	S60	1264	U
43	S60	1275	A
43	S60	1277	C
43	S60	1297	G
43	S60	1317	U
43	S60	1319	G
43	S60	1320	G
43	S60	1321	C
43	S60	1331	A
43	S60	1354	U
43	S60	1355	A
43	S60	1362	A
43	S60	1366	A
43	S60	1367	G
43	S60	1369	C
43	S60	1380	G
43	S60	1382	A
43	S60	1383	C
43	S60	1392	G

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Mol	Chain	Res	Type
43	S60	1393	G
43	S60	1394	A
43	S60	1396	C
43	S60	1398	C
43	S60	1399	U
43	S60	1400	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L50	96	C
1	L50	245	C
1	L50	323	G
1	L50	434	A
1	L50	623	C
1	L50	670	G
1	L50	837	C
1	L50	1234	C
1	L50	1248	G
1	L50	1399	G
1	L50	1642	G
1	L50	1841	A
1	L50	1903	C
1	L50	2121	C
1	L50	2164	C
1	L50	2192	A
1	L50	2289	G
1	L50	2445	C
1	L50	2526	G
2	L70	71	U
43	S60	70	G
43	S60	72	G
43	S60	103	A
43	S60	195	G
43	S60	197	A
43	S60	326	A
43	S60	431	A
43	S60	530	A
43	S60	762	G
43	S60	1057	G
43	S60	1115	G
43	S60	1162	G

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Mol	Chain	Res	Type
43	S60	1208	G
43	S60	1213	A
43	S60	1263	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 187 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
77	AMP	LH0	500	-	25,25,25	1.37	5 (20%)	37,38,38	1.90	10 (27%)

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
77	AMP	LH0	500	-	-	3/10/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	LH0	500	AMP	C5-C4	4.05	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	LH0	500	AMP	C5-N7	-2.52	1.34	1.39
77	LH0	500	AMP	C5-C6	2.45	1.47	1.41
77	LH0	500	AMP	C4-N9	-2.37	1.32	1.37
77	LH0	500	AMP	C8-N7	2.08	1.35	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	LH0	500	AMP	C5-C4-N3	-5.46	119.20	126.72
77	LH0	500	AMP	N3-C4-N9	4.33	134.53	127.17
77	LH0	500	AMP	C2-N3-C4	3.69	120.84	111.83
77	LH0	500	AMP	N3-C2-N1	-3.46	123.34	128.58
77	LH0	500	AMP	C4-C5-N7	-3.39	106.71	110.58
77	LH0	500	AMP	C4-N9-C8	3.00	108.89	105.74
77	LH0	500	AMP	C5-N7-C8	2.47	107.34	103.45
77	LH0	500	AMP	N9-C8-N7	-2.22	110.79	113.94
77	LH0	500	AMP	C6-C5-N7	2.21	136.35	132.09
77	LH0	500	AMP	O3P-P-O2P	2.14	115.84	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
77	LH0	500	AMP	C5'-O5'-P-O1P
77	LH0	500	AMP	C5'-O5'-P-O2P
77	LH0	500	AMP	C5'-O5'-P-O3P

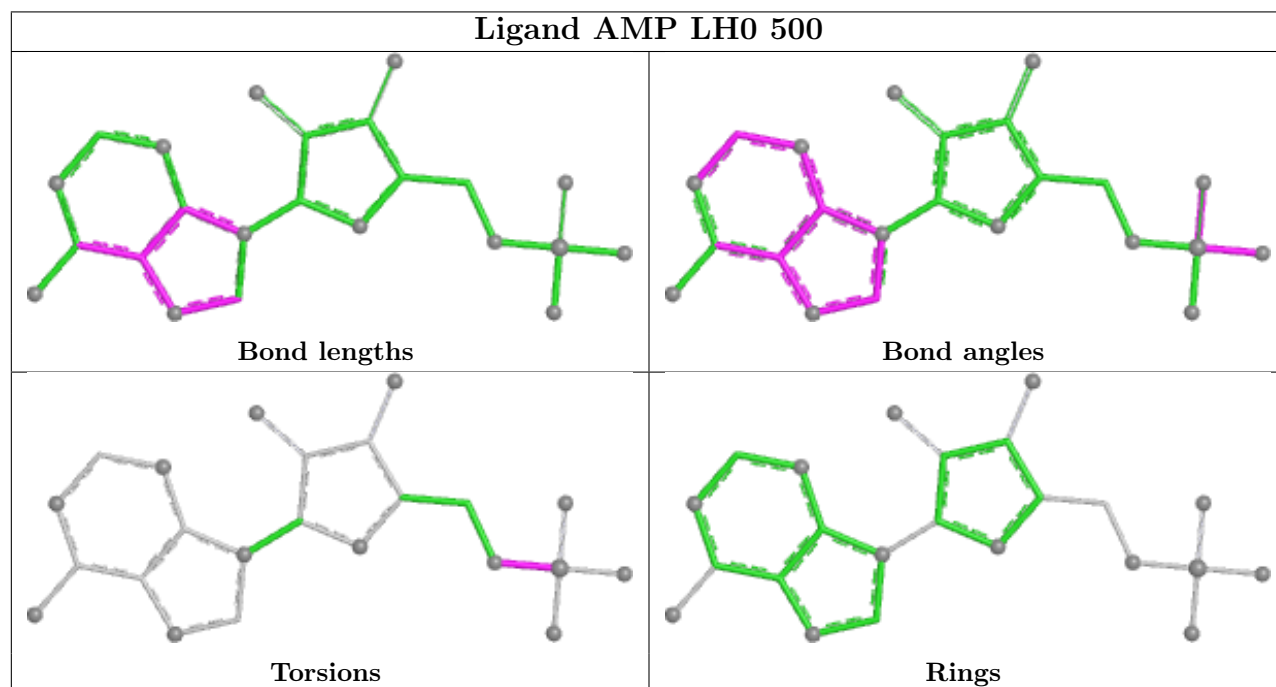
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	LH0	500	AMP	1	0

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

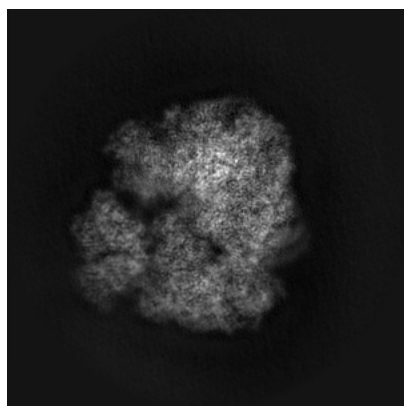
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11437. These allow visual inspection of the internal detail of the map and identification of artifacts.

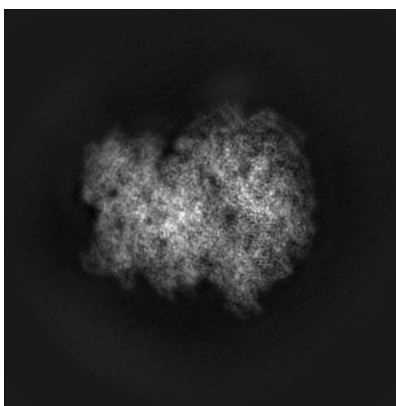
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

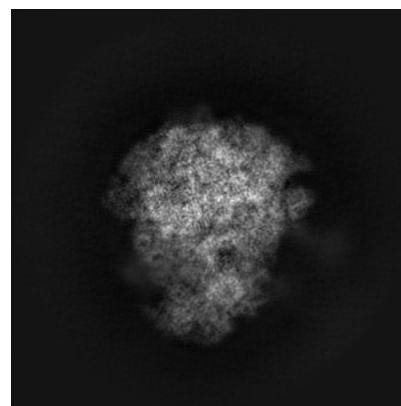
6.1.1 Primary map



X

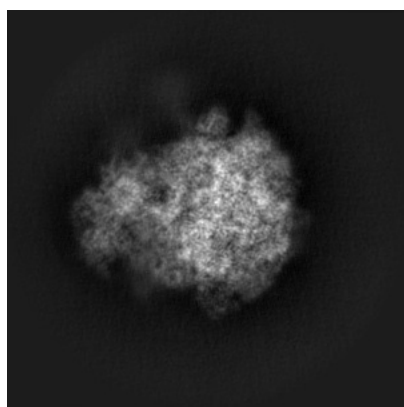


Y

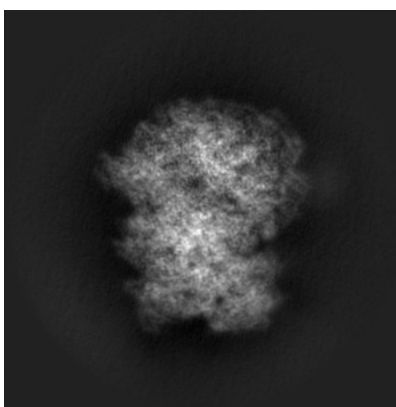


Z

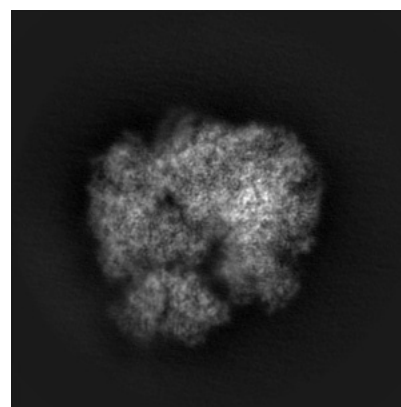
6.1.2 Raw map



X



Y

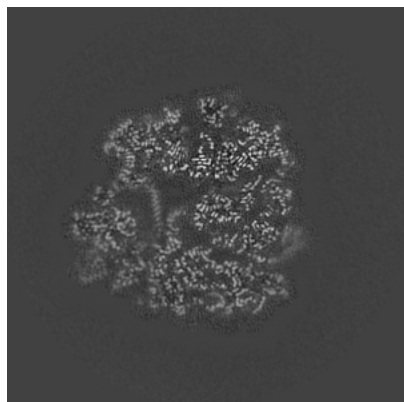


Z

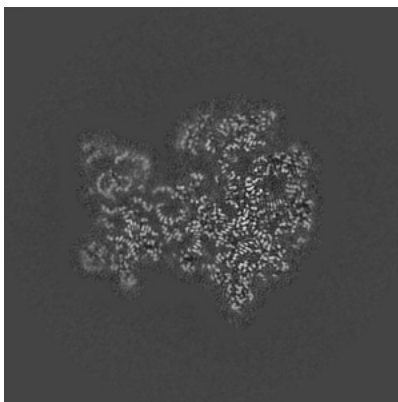
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

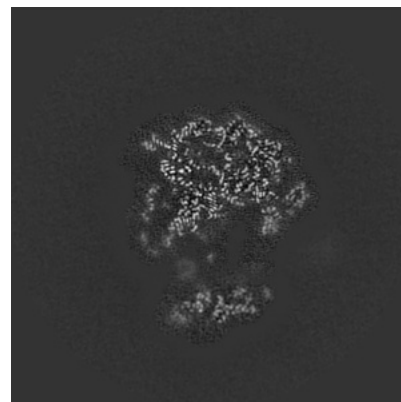
6.2.1 Primary map



X Index: 200

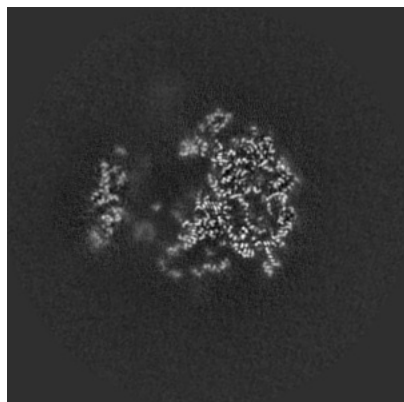


Y Index: 200

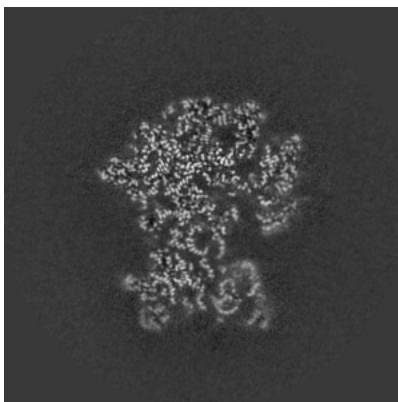


Z Index: 200

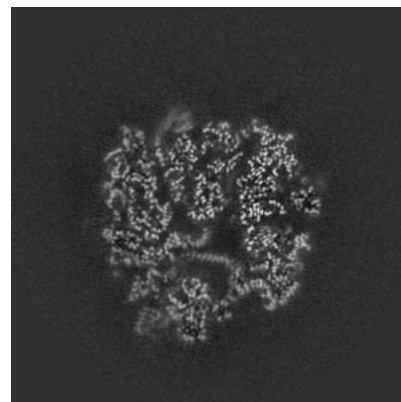
6.2.2 Raw map



X Index: 200



Y Index: 200

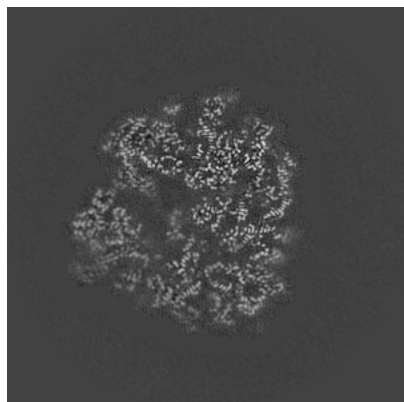


Z Index: 200

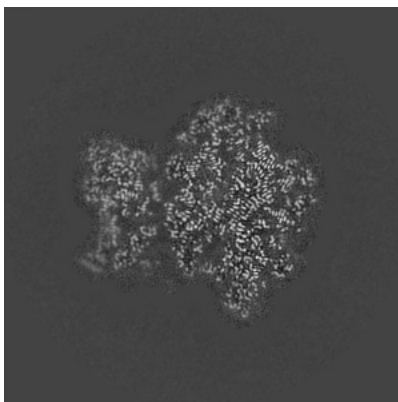
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

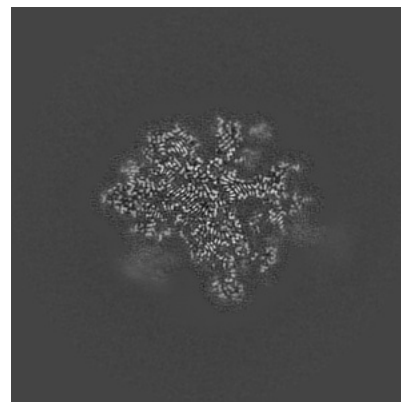
6.3.1 Primary map



X Index: 205

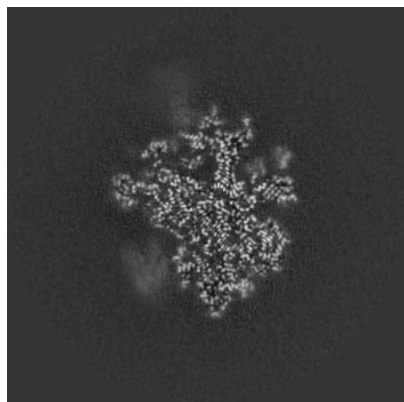


Y Index: 211

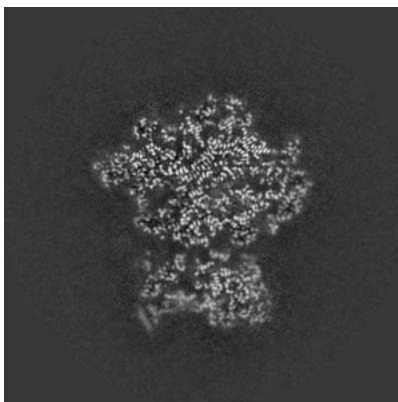


Z Index: 238

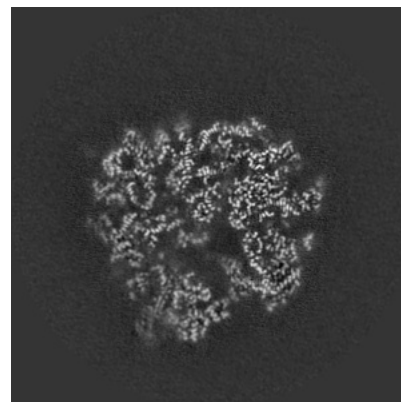
6.3.2 Raw map



X Index: 238



Y Index: 211

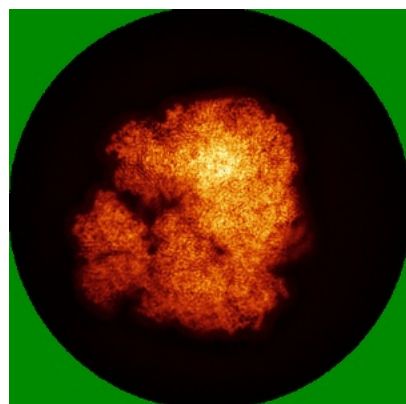


Z Index: 205

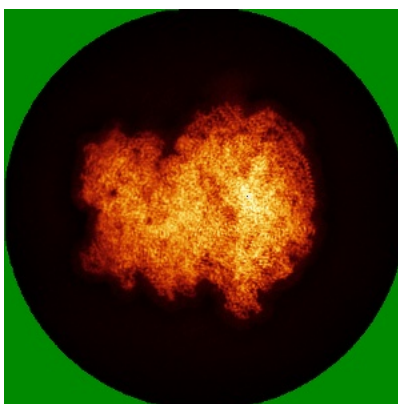
The images above show the largest variance slices of the map in three orthogonal directions.

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

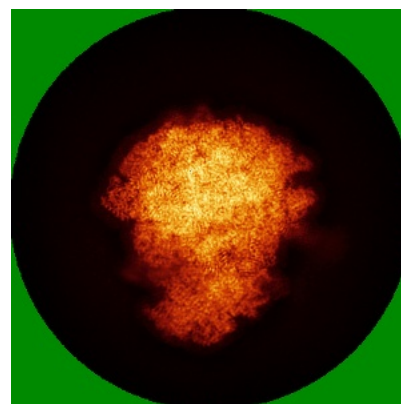
6.4.1 Primary map



X

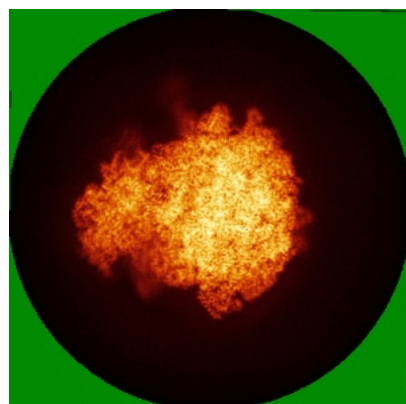


Y

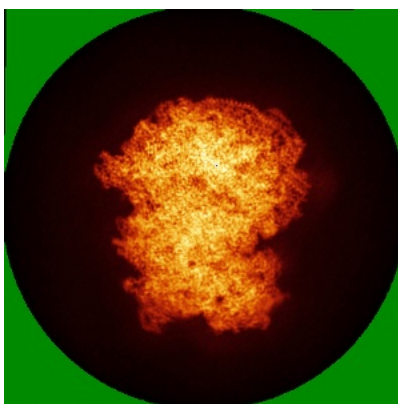


Z

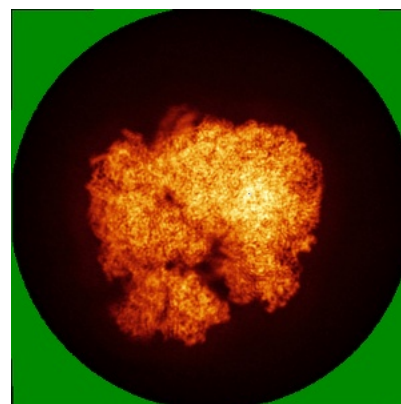
6.4.2 Raw map



X



Y

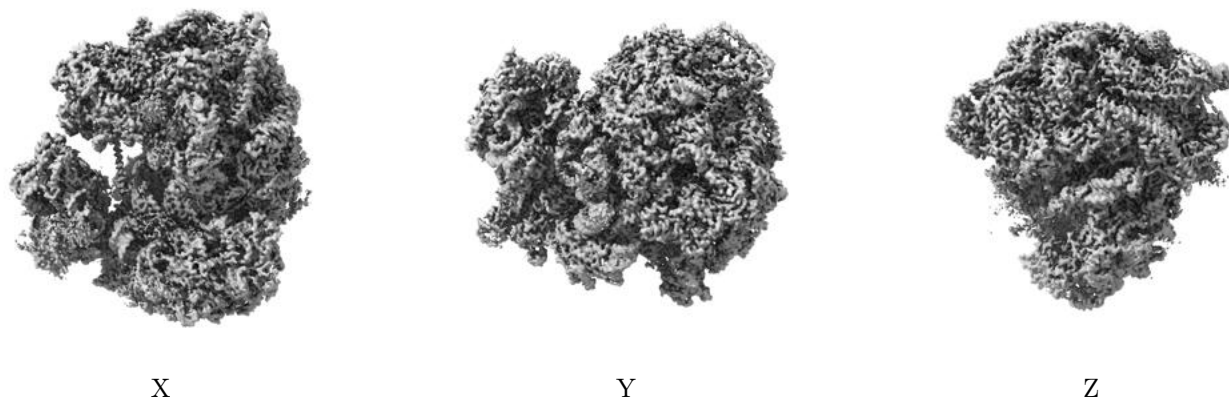


Z

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

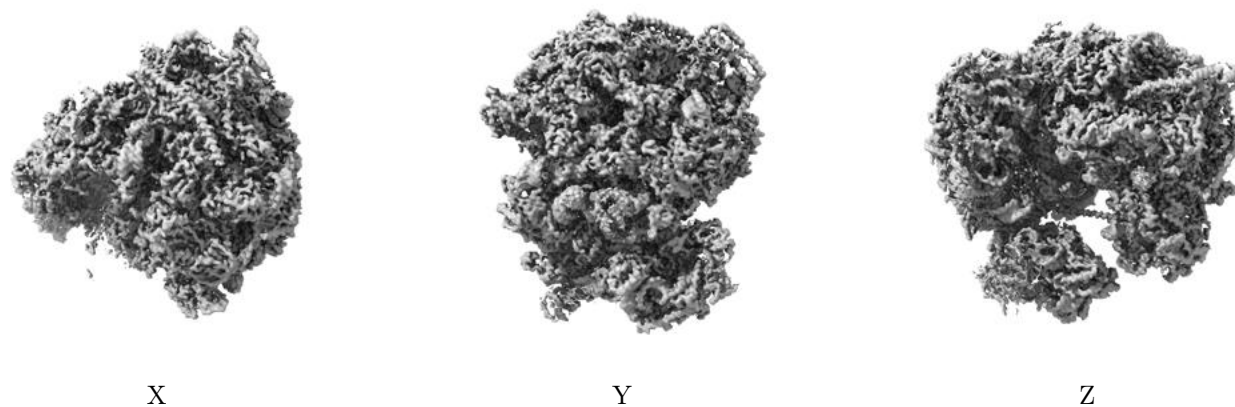
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

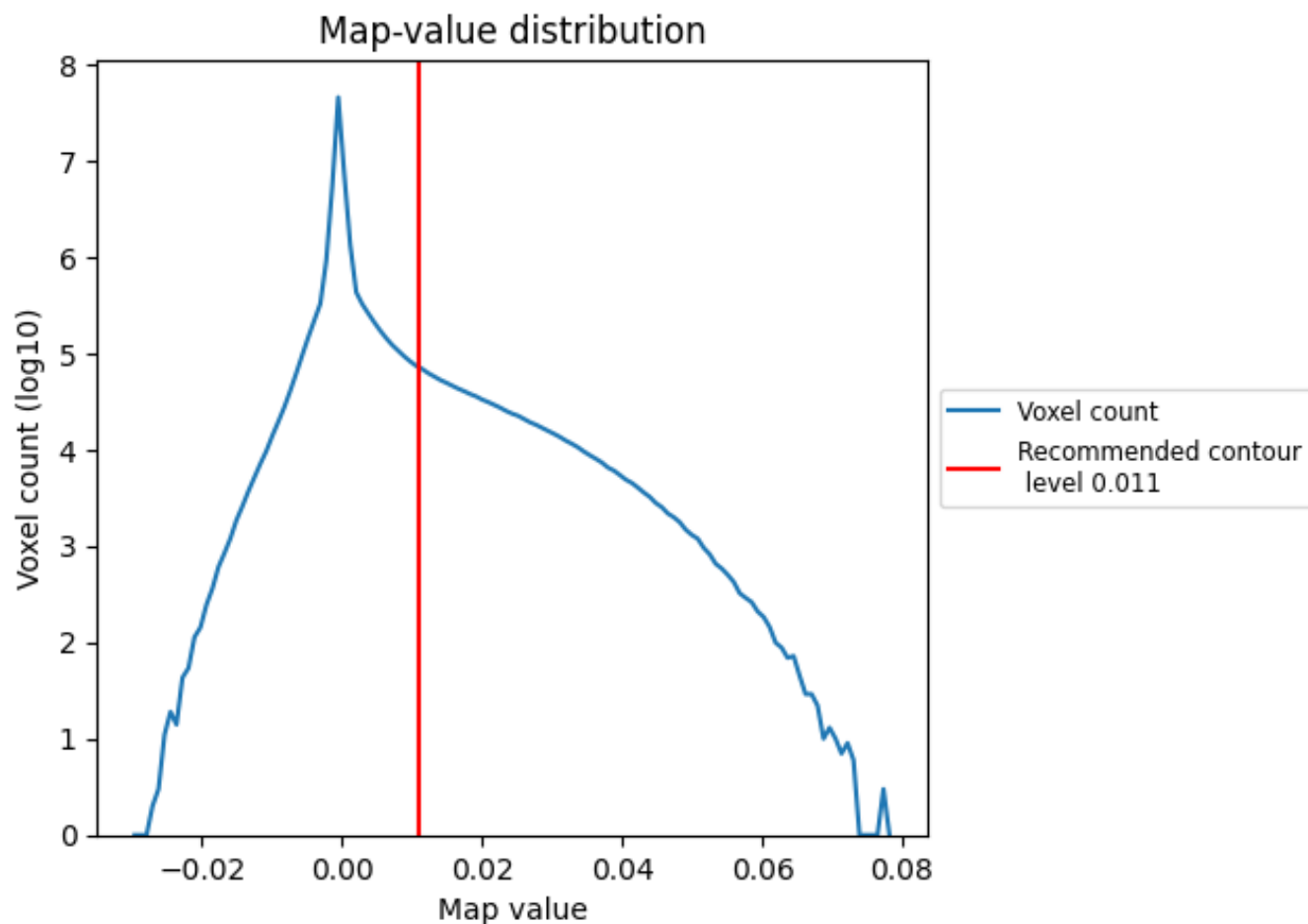
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

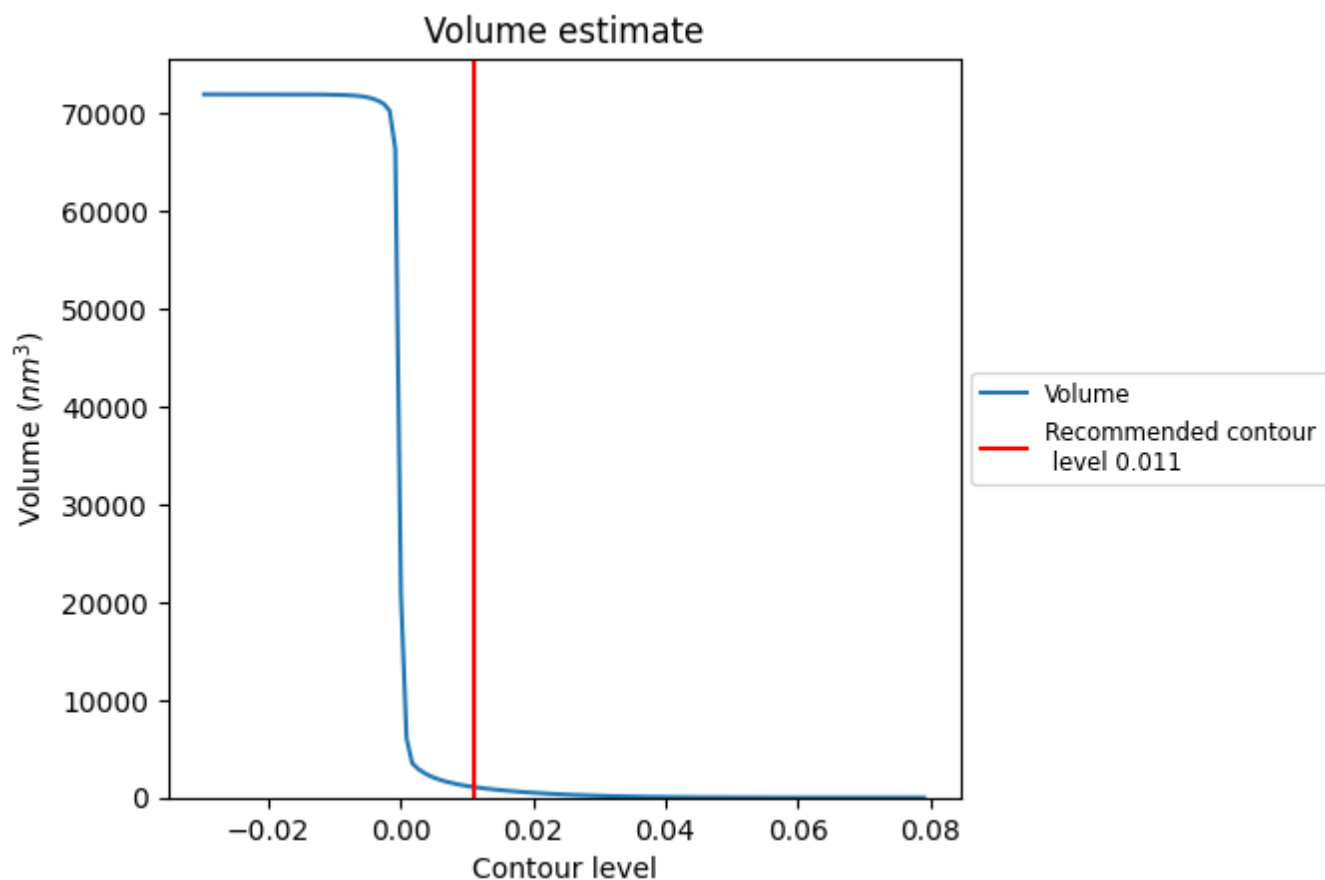
This section contains the results of statistical analysis of the map.

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.

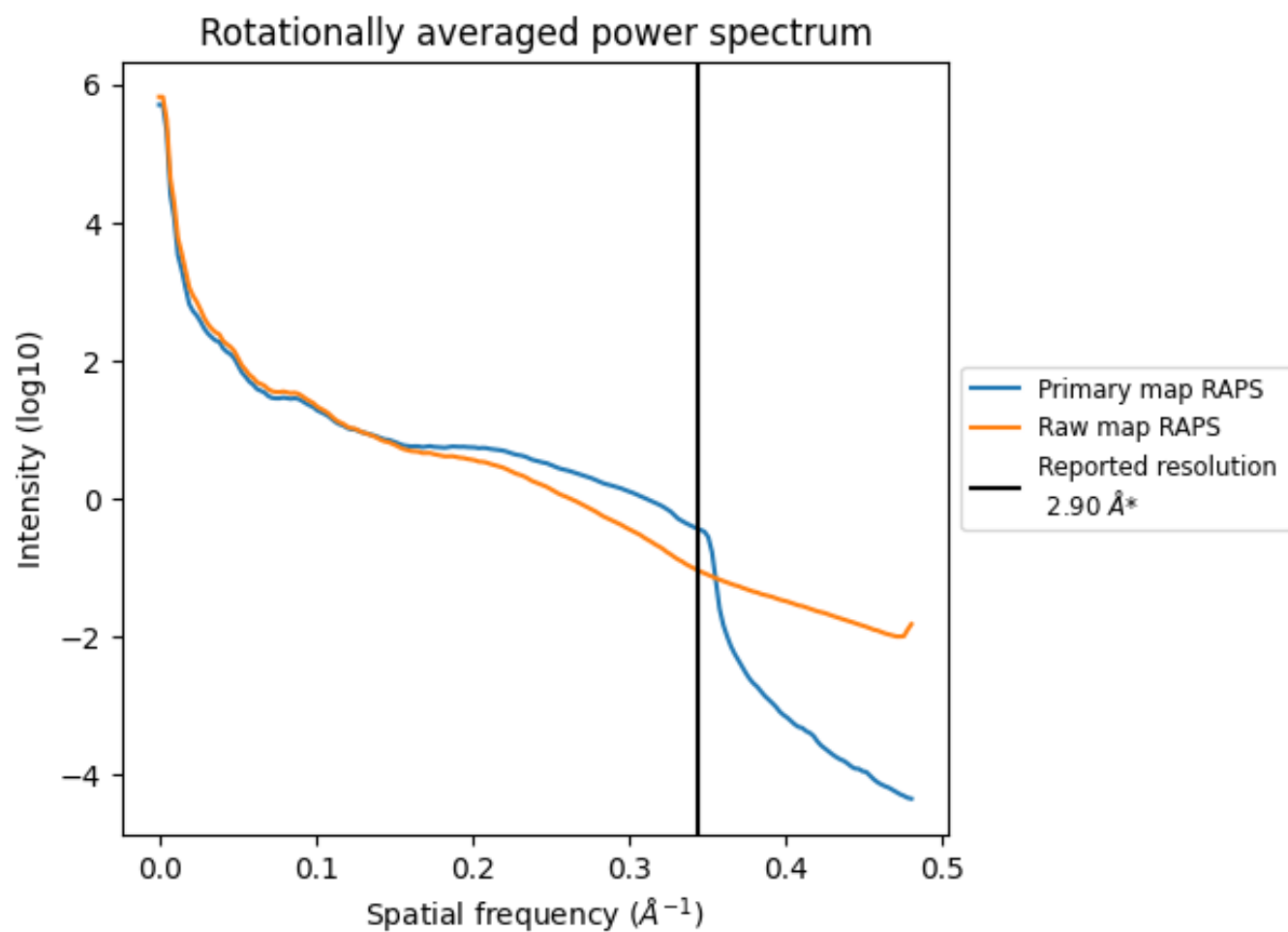
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1089 nm³; this corresponds to an approximate mass of 984 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

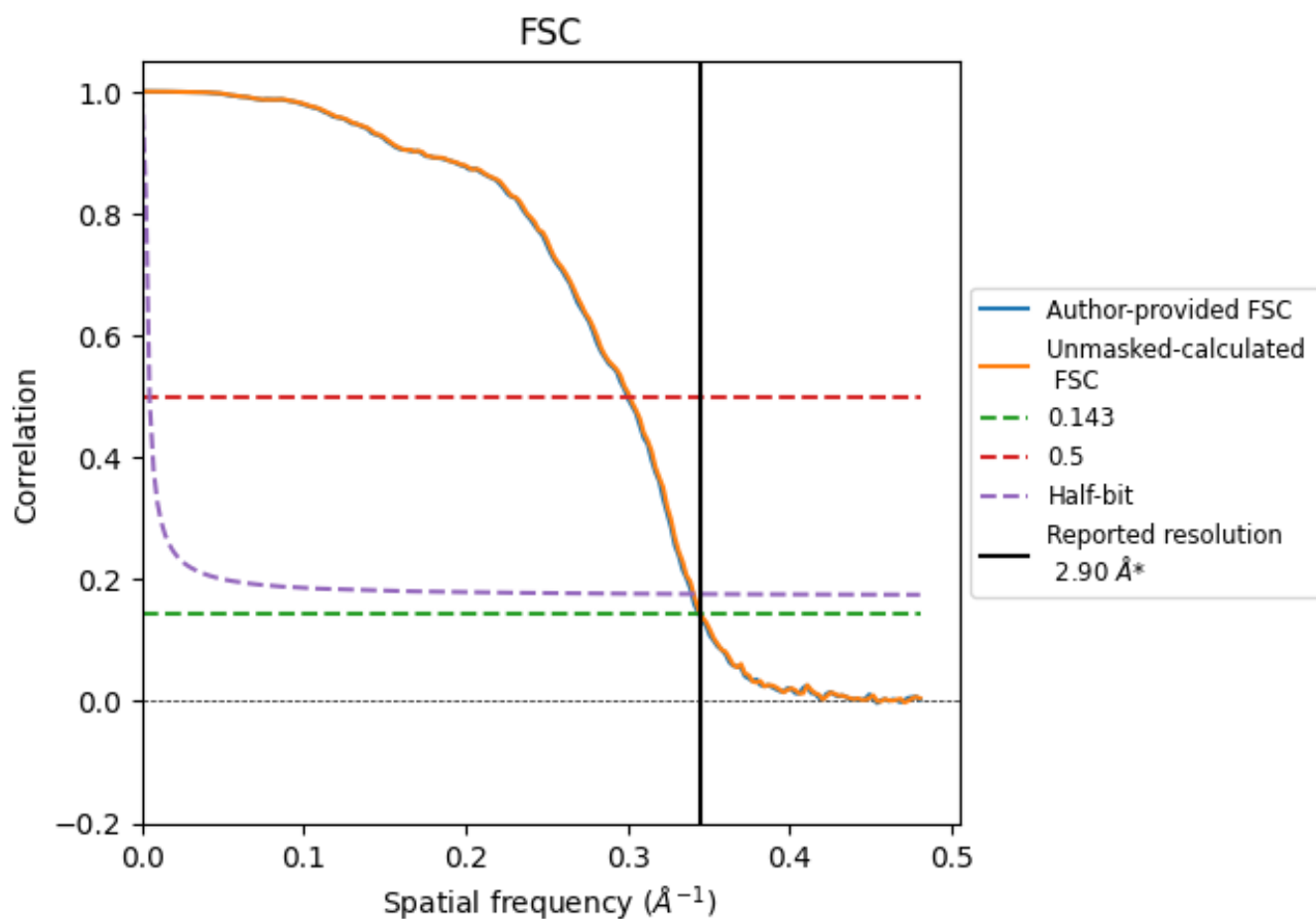


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

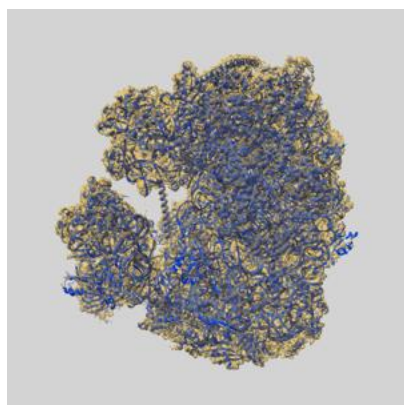
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.34	2.94
Unmasked-calculated*	2.90	3.32	2.93

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

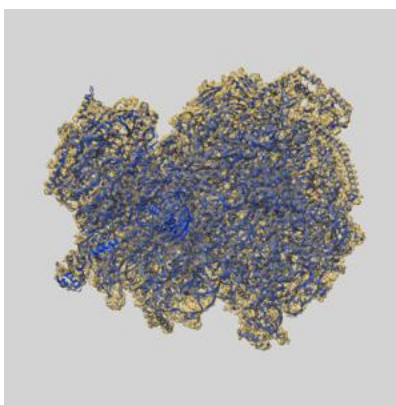
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11437 and PDB model 6ZU5. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

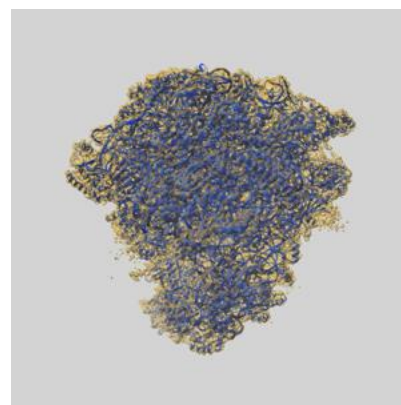
9.1 Map-model overlay [i](#)



X



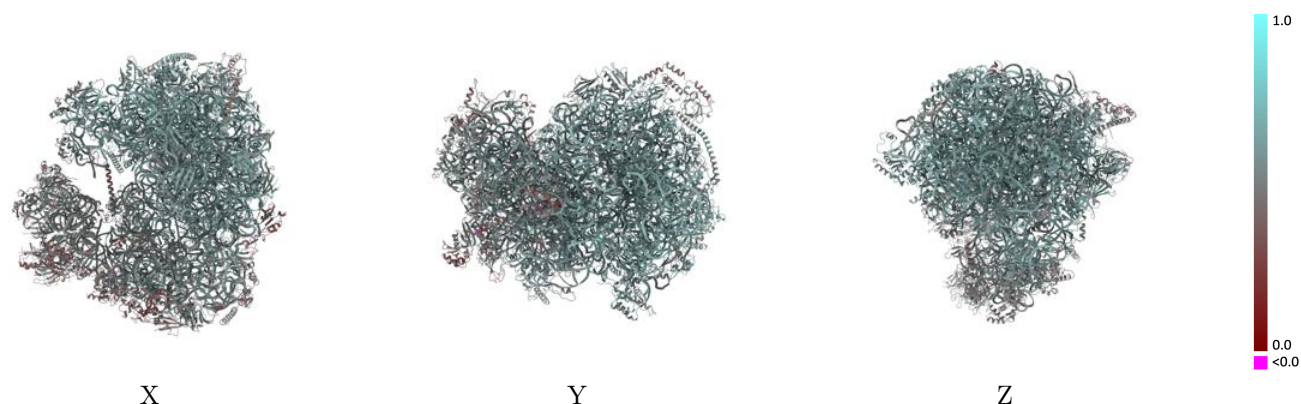
Y



Z

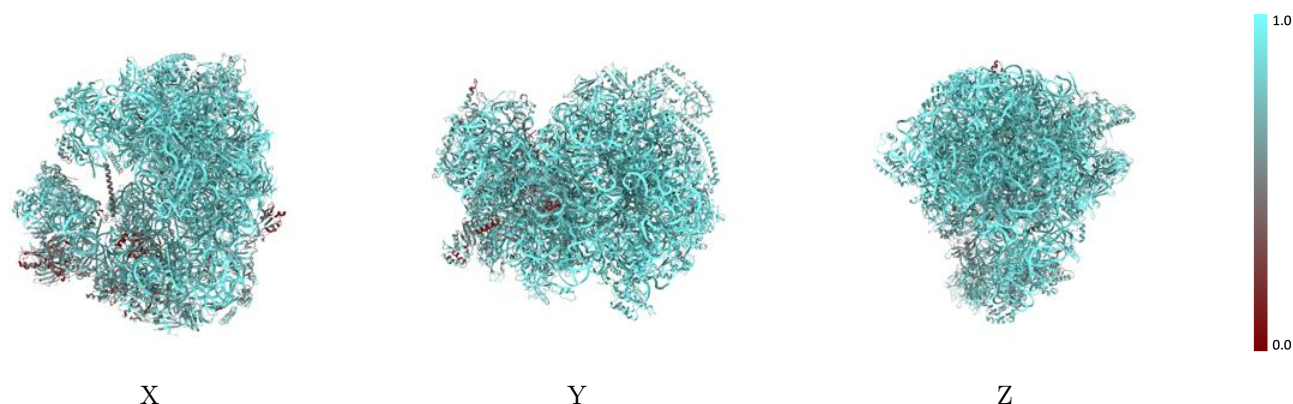
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



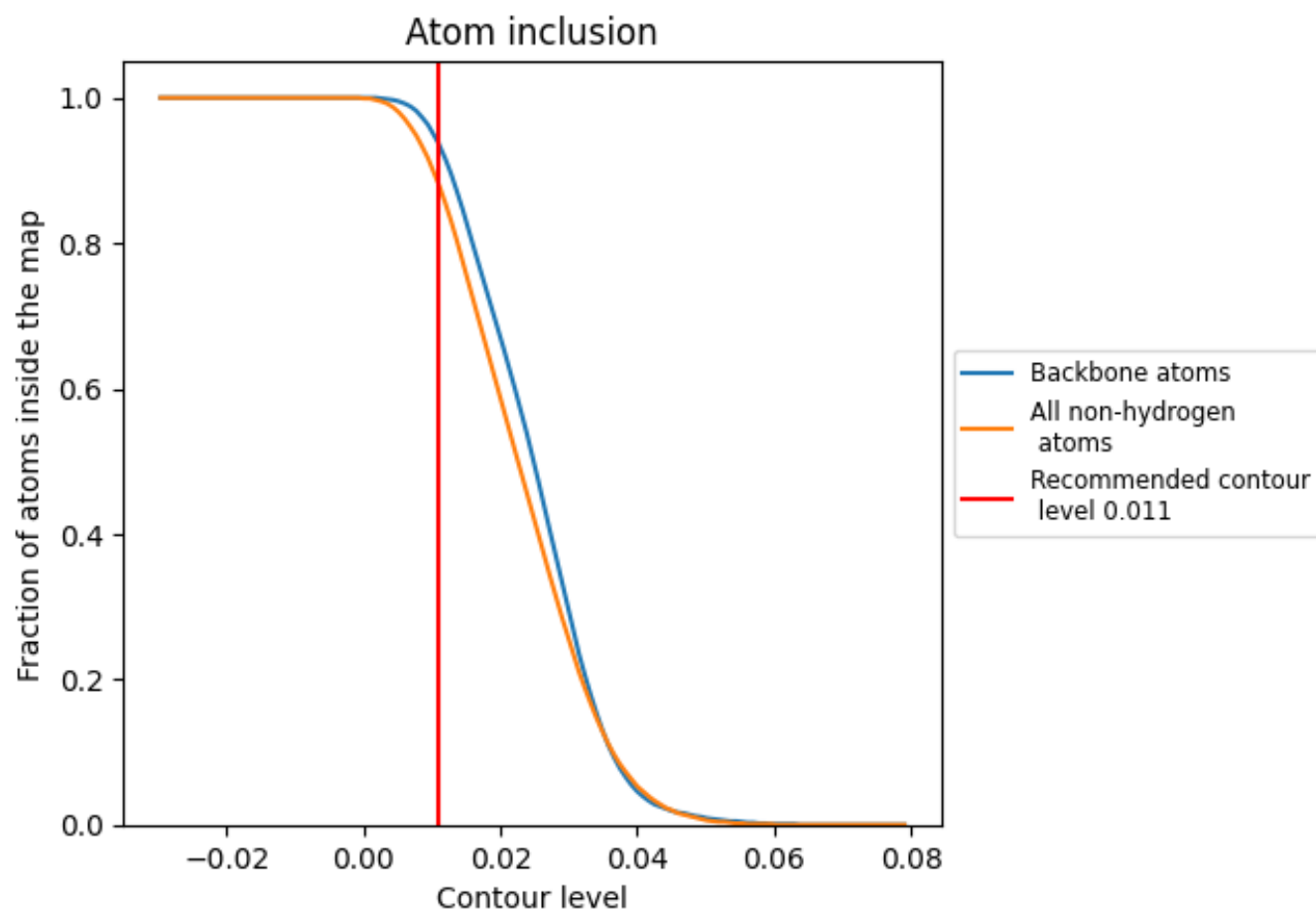
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.5570
L50	 0.9820	 0.6020
L70	 0.9940	 0.5920
LA0	 0.8740	 0.5960
LAA	 0.9300	 0.6080
LB0	 0.8830	 0.5870
LBB	 0.8610	 0.5620
LC0	 0.9120	 0.5980
LCC	 0.7920	 0.5310
LD0	 0.8590	 0.5490
LDD	 0.8760	 0.5780
LE0	 0.7040	 0.4980
LEE	 0.9130	 0.5990
LF0	 0.8990	 0.5860
LFF	 0.9040	 0.6000
LG0	 0.8890	 0.5730
LGG	 0.8870	 0.5850
LH0	 0.8190	 0.5320
LHH	 0.9190	 0.5870
LI0	 0.8800	 0.5790
LII	 0.8940	 0.5850
LJ0	 0.7850	 0.5240
LJJ	 0.9360	 0.6150
LL0	 0.9190	 0.5930
LLL	 0.8920	 0.5930
LM0	 0.8240	 0.5370
LMM	 0.6260	 0.5160
LN0	 0.9650	 0.6300
LNN	 0.6240	 0.4660
LO0	 0.8720	 0.5740
LOO	 0.9070	 0.6090
LP0	 0.9250	 0.6050
LPP	 0.8630	 0.5950
LQ0	 0.8980	 0.5950
LR0	 0.8330	 0.5600



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Chain	Atom inclusion	Q-score
LS0	 0.8820	 0.5880
LT0	 0.9040	 0.5950
LU0	 0.2990	 0.2930
LV0	 0.8640	 0.5880
LW0	 0.6540	 0.5110
LX0	 0.9240	 0.5920
LY0	 0.9120	 0.5890
LZ0	 0.8300	 0.5270
S60	 0.9290	 0.5300
SA0	 0.6830	 0.4300
SAA	 0.7670	 0.5460
SB0	 0.7920	 0.5260
SBB	 0.7480	 0.4800
SC0	 0.7270	 0.4970
SCC	 0.6120	 0.4590
SD0	 0.5480	 0.4510
SDD	 0.7530	 0.5080
SE0	 0.7910	 0.5230
SEE	 0.2180	 0.3980
SF0	 0.7050	 0.4860
SG0	 0.6900	 0.4890
SGG	 0.6590	 0.4500
SH0	 0.5880	 0.4350
SI0	 0.8200	 0.5400
SJ0	 0.6320	 0.4350
SK0	 0.4280	 0.3860
SL0	 0.8360	 0.5690
SN0	 0.7960	 0.5470
SO0	 0.8170	 0.5410
SP0	 0.7380	 0.4740
SQ0	 0.7570	 0.5060
SR0	 0.6010	 0.4380
SS0	 0.7160	 0.4820
ST0	 0.7870	 0.4890
SU0	 0.3960	 0.4400
SV0	 0.6090	 0.4350
SW0	 0.8140	 0.5410
SX0	 0.4100	 0.4860
SY0	 0.6840	 0.4640
SZ0	 0.6960	 0.4530