



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:02 PM UTC

PDB ID : 8K2D / pdb_00008k2d
EMDB ID : EMD-36839
Title : Cryo-EM structure of the yeast 80S ribosome with tigecycline, eEF2, Stm1 and eIF5A
Authors : Buschauer, R.; Beckmann, R.; Cheng, J.
Deposited on : 2023-07-12
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

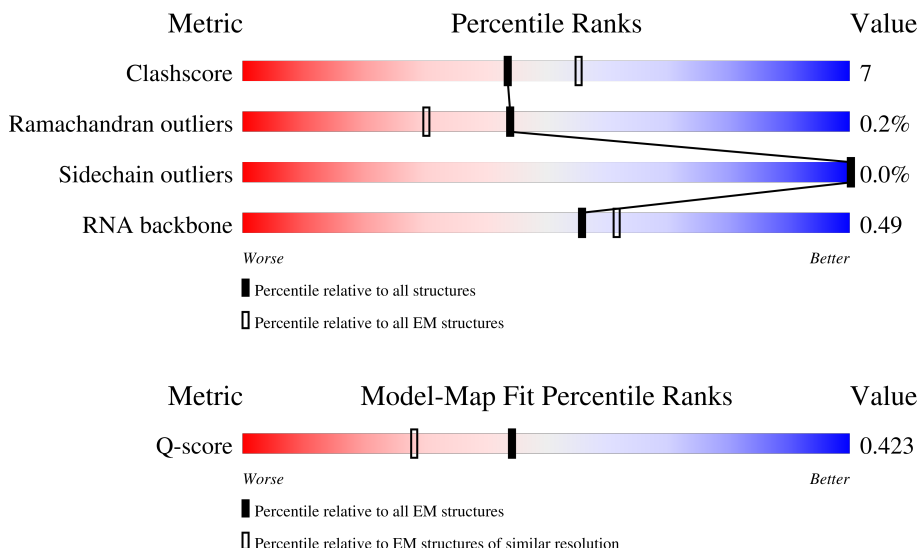
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



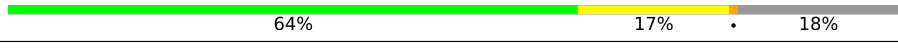
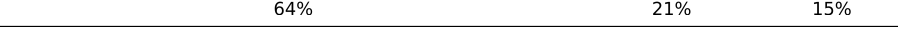
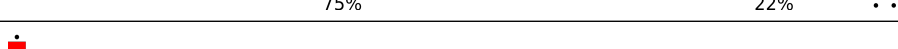
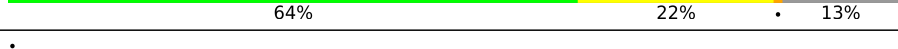
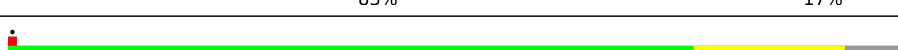
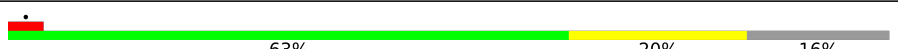
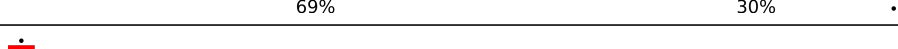
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	C2	1800	
2	C1	3396	
3	C4	121	

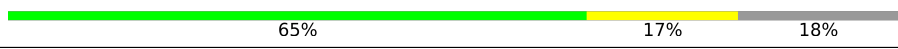
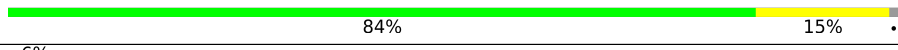
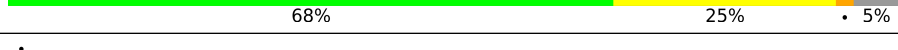
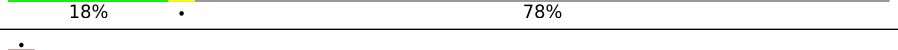
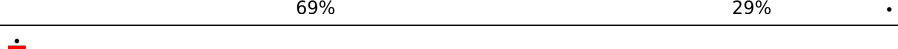
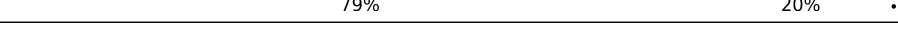
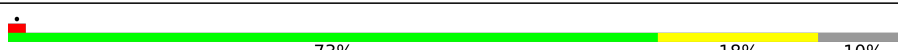
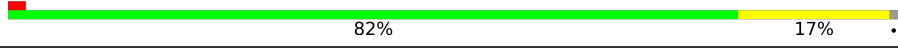
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Mol	Chain	Length	Quality of chain
4	C3	158	
5	SA	252	
6	SB	255	
7	SC	254	
8	SD	240	
9	SE	261	
10	SF	225	
11	SG	236	
12	SH	190	
13	SI	200	
14	SJ	197	
15	SK	105	
16	SL	156	
17	SM	143	
18	SN	151	
19	SO	137	
20	SP	142	
21	SQ	143	
22	SR	136	
23	SS	146	
24	ST	144	
25	SU	121	
26	SV	87	
27	SW	130	
28	SX	145	

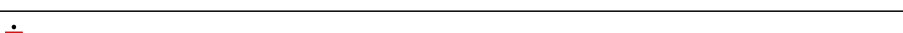
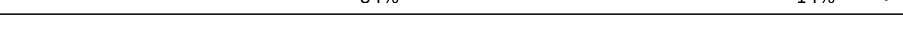
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Mol	Chain	Length	Quality of chain
29	SY	135	
30	SZ	108	
31	Sa	119	
32	Sb	82	
33	Sc	67	
34	Sd	56	
35	Se	63	
36	Sf	152	
37	Sg	319	
38	LA	254	
39	LB	387	
40	LC	362	
41	LD	297	
42	LE	176	
43	LF	244	
44	LG	256	
45	LH	191	
46	LI	221	
47	LJ	174	
48	LK	165	
49	LL	199	
50	LM	138	
51	LN	204	
52	LO	199	
53	LP	184	

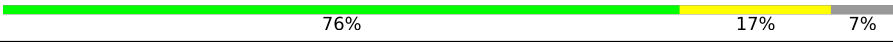
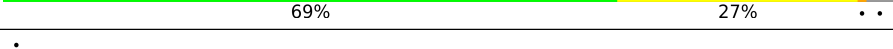
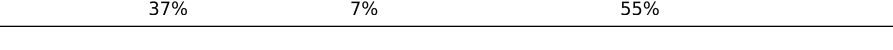
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Mol	Chain	Length	Quality of chain
54	LQ	186	
55	LR	189	
56	LS	172	
57	LT	160	
58	LU	121	
59	LV	137	
60	LW	155	
61	LX	142	
62	LY	127	
63	LZ	136	
64	La	149	
65	Lb	59	
66	Lc	105	
67	Ld	113	
68	Le	130	
69	Lf	107	
70	Lg	121	
71	Lh	120	
72	Li	100	
73	Lj	88	
74	Lk	78	
75	Ll	51	
76	Lm	128	
77	Ln	25	
78	Lo	106	

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Mol	Chain	Length	Quality of chain
79	Lp	92	
80	CE	157	
81	L1	217	
82	P0	312	
83	CD	842	
84	CS	273	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 210169 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	1700	Total	C	N	O	P	0	0
			36234	16201	6426	11907	1700		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	3188	Total	C	N	O	P	0	0
			68200	30463	12307	22242	3188		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C4	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 5 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SA	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 6 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SB	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 9 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 11 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	SH	185	Total	C	N	O	0	0
			1486	954	266	266		

- Molecule 13 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 14 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 15 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SK	92	Total	C	N	O	S	0	0
			741	478	121	140	2		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SL	146	Total	C	N	O	S	0	0
			1168	747	221	197	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SP	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

- Molecule 21 is a protein called Small ribosomal subunit protein uS9A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	SQ	141	Total	C	N	O		
			1105	708	203	194	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SR	115	Total	C	N	O	S		
			896	557	172	165	2	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SS	145	Total	C	N	O	S		
			1192	743	237	210	2	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein eS19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	ST	143	Total	C	N	O	S		
			1112	694	208	208	2	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SU	101	Total	C	N	O	S		
			805	512	145	147	1	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SV	87	Total	C	N	O	S		
			684	420	125	137	2	0	0

- Molecule 27 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SW	129	Total	C	N	O	S		
			1021	650	188	180	3	0	0

- Molecule 28 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 29 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 30 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SZ	69	Total	C	N	O		0	0
			558	357	103	98			

- Molecule 31 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sa	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 32 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 33 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 34 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 35 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 36 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	33	Total	C	N	O	S	0	0
			248	153	46	45	4		

- Molecule 37 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sg	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

- Molecule 38 is a protein called Large ribosomal subunit protein uL2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 40 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 42 is a protein called Large ribosomal subunit protein eL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 43 is a protein called Large ribosomal subunit protein uL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 44 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 45 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LI	209	Total	C	N	O	S	0	0
			1696	1077	321	293	5		

- Molecule 47 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called Large ribosomal subunit protein uL11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LK	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL13A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	LL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 50 is a protein called Large ribosomal subunit protein eL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 51 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LO	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	LP	175	Total	C	N	O	0	0
			1378	856	273	249		

- Molecule 54 is a protein called Large ribosomal subunit protein eL18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called Large ribosomal subunit protein eL19A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	LR	174	Total	C	N	O	0	0
			1365	843	286	236		

- Molecule 56 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 57 is a protein called Large ribosomal subunit protein eL21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL22A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 59 is a protein called Large ribosomal subunit protein uL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LV	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 60 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 61 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 62 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LY	124	Total	C	N	O		0	0
			976	614	190	172			

- Molecule 63 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	LZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 64 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	La	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Lb	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 67 is a protein called Large ribosomal subunit protein eL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ld	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 68 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Le	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 69 is a protein called Large ribosomal subunit protein eL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Lf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called Large ribosomal subunit protein eL34A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called Large ribosomal subunit protein uL29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 72 is a protein called Large ribosomal subunit protein eL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Li	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lj	82	Total	C	N	O	S	0	0
			650	396	142	107	5		

- Molecule 74 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 75 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ll	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called Ubiquitin-ribosomal protein eL40A fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 77 is a protein called Large ribosomal subunit protein eL41A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ln	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 78 is a protein called Large ribosomal subunit protein eL42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 79 is a protein called Large ribosomal subunit protein eL43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lp	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	CE	146	Total	C	N	O	S	0	0
			1097	686	184	218	9		

- Molecule 81 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	L1	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 82 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	P0	203	Total	C	N	O	S	0	0
			1571	1006	272	289	4		

- Molecule 83 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CD	816	Total	C	N	O	S	0	0
			6348	4042	1079	1197	30		

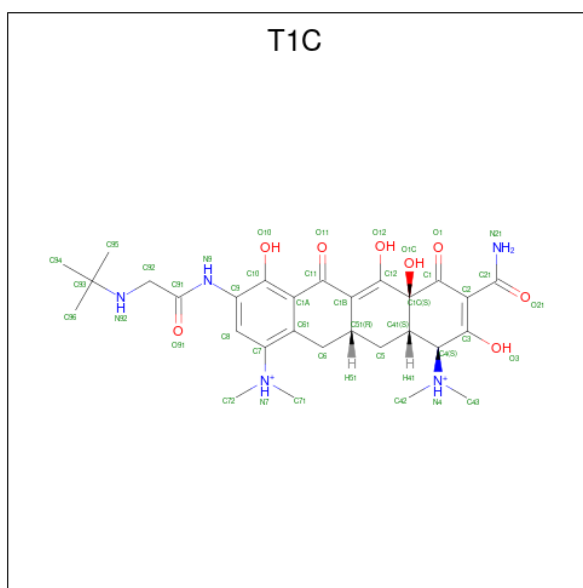
- Molecule 84 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	CS	122	Total	C	N	O	0	0
			919	541	184	194		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	C2	1	Total	Zn	0
			1	1	
85	SM	1	Total	Zn	0
			1	1	
85	Sa	1	Total	Zn	0
			1	1	
85	Sb	1	Total	Zn	0
			1	1	
85	Lg	1	Total	Zn	0
			1	1	
85	Lj	1	Total	Zn	0
			1	1	
85	Lm	1	Total	Zn	0
			1	1	
85	Lo	1	Total	Zn	0
			1	1	
85	Lp	1	Total	Zn	0
			1	1	

- Molecule 86 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈).

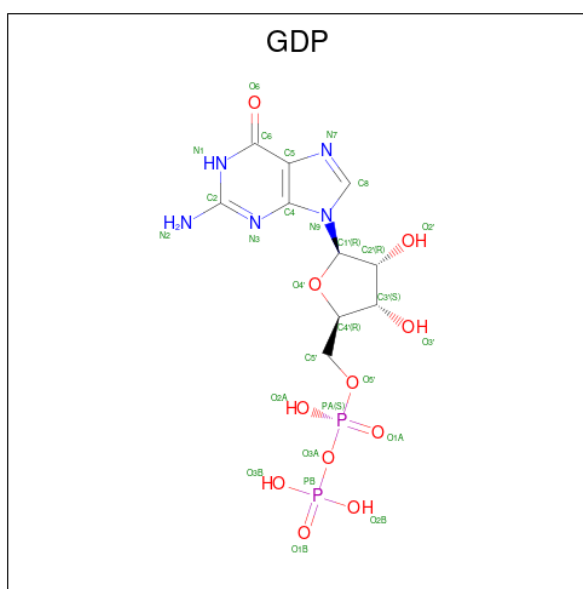


Mol	Chain	Residues	Atoms				AltConf
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	

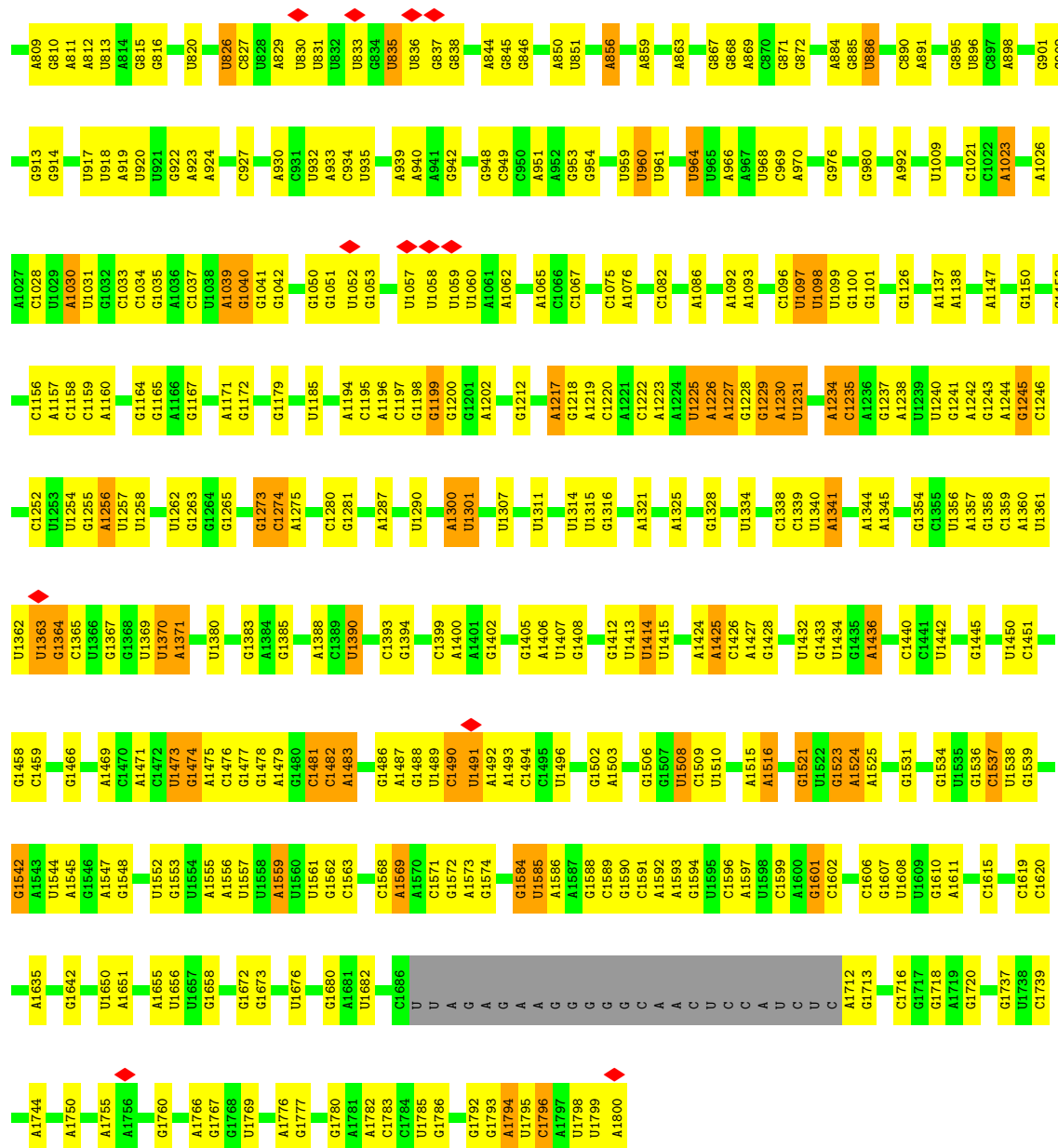
- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	C1	2	Total	Mg	0
			2	2	
87	C3	1	Total	Mg	0
			1	1	
87	CD	1	Total	Mg	0
			1	1	

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

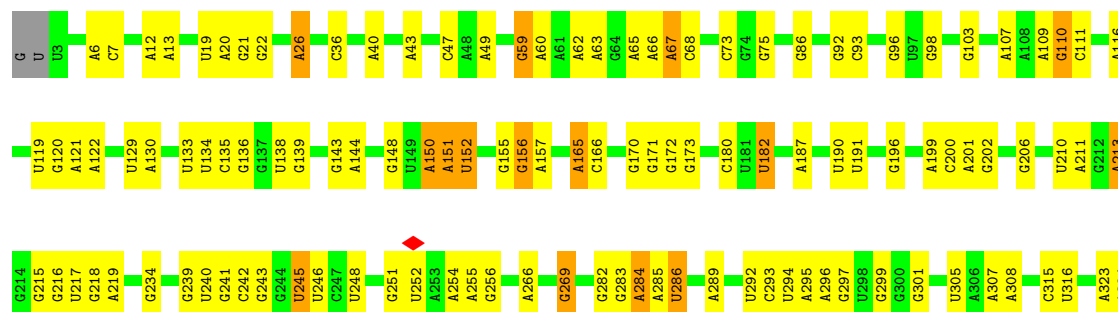


Mol	Chain	Residues	Atoms					AltConf
88	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	



• Molecule 2: 23S rRNA

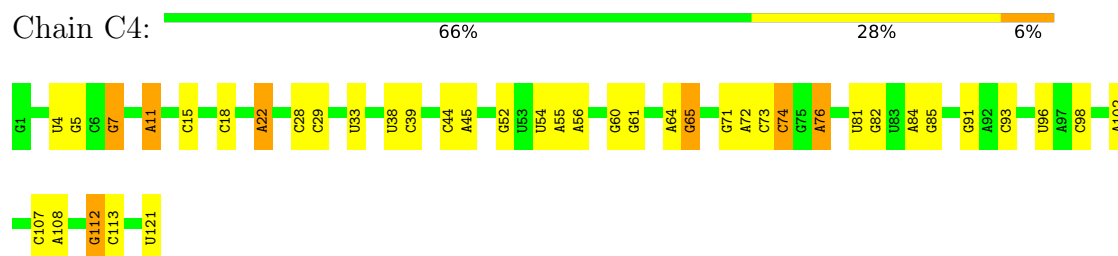
Chain C1: 62% 28% 6%



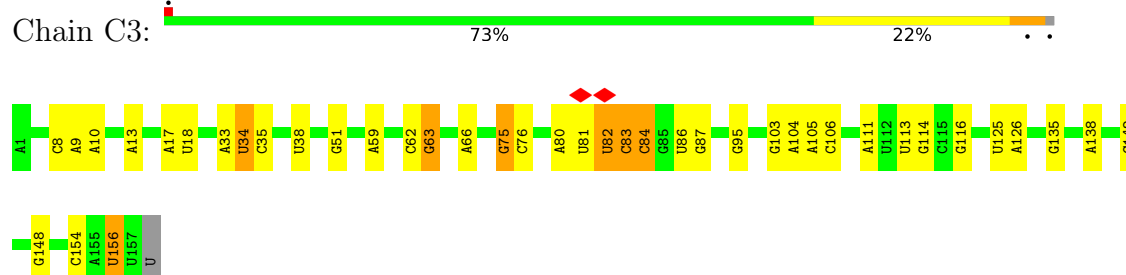


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A3320	G3242	C3043	U2923	G2796	A2697	A2488	A2401	A2232	C2114	G	U	A1893
C3321	A3243	G3044	U2923	G2800	G2698	C2489	A2402	A2232	A2120	C	G	U1894
A3322	A3244	G3045	A2933	A2801	G2700	C2490	G2403	A2244	G2121	U	A	A1895
C3323	A3245	A3046	U2935	A2802	G2700	U2493	A2404	G2249	G2122	U	C	U1899
C3324	G3246	A3049	U2936	A2803	A2703	A2494	C2407	G2256	U2129	G	U	G1906
A3335	G3247	U3050	G2937	A2806	A2704	U2498	U2408	C2257	A2131	U	U	C1907
U3341	U3251	G3053	G2938	C2810	A2705	U2498	U2411	U2260	U2137	G	U	A1909
A3342	A3252	U3056	G2939	G2814	A2706	A2502	G2412	U2260	G2130	U	U	A1910
G3343	G3253	G3059	A2940	G2815	A2707	C2507	A2413	C2267	U2140	U	G	U1911
A3344	U3259	U3068	C2941	G2816	A2708	U2508	G2414	U2268	U2141	C	U	A1912
G3345	G3263	A3069	G2942	A2817	U2719	U2508	A2419	U2269	A2142	U	G	A1913
U3351	A3268	A3070	G2943	U2818	U2720	A2511	U2433	A2271	A2144	U	G	U1925
U3352	U3269	G3075	C2947	G2823	U2721	U2515	U2437	G2272	U2154	U	U	G1940
G3353	A3274	U3078	U2948	G2824	U2722	G2522	A2438	U2273	G2155	U	U	G1953
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U3355	G3276	A3086	G2950	A2836	U2724	A2524	G2442	C2287	G2160	C	U	U
G3356	U3277	U3090	U2953	A2844	U2725	G2525	A2443	G2288	G2161	U	U	U
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A3359	U3280	C3092	U2981	C2849	G2648	U2539	G2448	U2294	G2171	U	G	U
U3362	U3281	A3093	A2982	C2852	U2652	C2539	G2451	G2307	G2176	U	G	U
G3363	U3282	A3094	C2983	A2853	U2652	C2540	G2452	C2308	U2176	U	G	U
U3368	U3283	U3107	U2987	C2857	A2656	U2541	U2453	U2310	U2176	C	U	U
G3369	G3284	G3109	A2988	U2861	G2753	U2542	U2455	A2313	G2185	U	U	U
A3375	C3285	A3114	G2989	C2867	G2662	U2543	A2456	U2314	U2193	U	U	U
U3376	U3286	U3117	U2996	U2871	G2663	U2544	G2457	G2315	G2194	U	U	U
C3378	G3287	C3119	G2997	A2872	C2666	A2547	A2458	U2334	U2205	U	U	U
C3379	G3288	U3119	G2998	G2875	G2669	C2548	U2460	U2335	G2206	U	U	U
G3386	G3289	A3122	A3011	U2875	A2671	U2552	G2463	U2344	A2093	C	A	U
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G3395	G3291	A3130	G3015	A2887	A2673	A2554	G2465	A2207	G2095	U	G	U
U3396	U3292	U3131	A3016	U2888	G2674	G2555	G2466	A2208	G2096	U	G	U
U3399	U3293	U3132	A3017	C2889	A2675	G2556	G2467	U2209	U2097	U	C	U
U3400	U3294	C3137	C3017	U2896	G2677	A2557	G2468	A2213	C2098	C	A	U
G3408	C3308	A3142	A3021	A2896	A2678	C2560	U2470	A2214	C2101	U	U	U
G3409	G3309	A3143	G3022	A2897	U2683	C2562	U2471	U2217	U2102	U	G	U
A3310	A3310	C3143	G3028	G2898	U2688	G2563	U2472	G2375	U2103	U	G	U
U3313	U3313	G3149	G3028	C2899	U2688	G2563	C2473	G2385	A2104	U	U	U
A3314	U3314	U3231	A3032	G2908	G2690	C2568	G2477	U2388	G2105	U	G	U
G3315	G3315	U3152	U3037	U2761	A2691	A2569	U2481	A2223	A2106	U	U	U
A3316	A3316	U3153	U3037	U2761	A2691	A2570	G2481	A2224	A2107	U	A	U
U3317	C3323	C	U3037	U2761	U2571	C2572	A2485	U2225	G2110	U	G	U
G3318	G3324	U	U3041	G2786	C2572	G2574	A2486	A2228	U2112	U	C	U

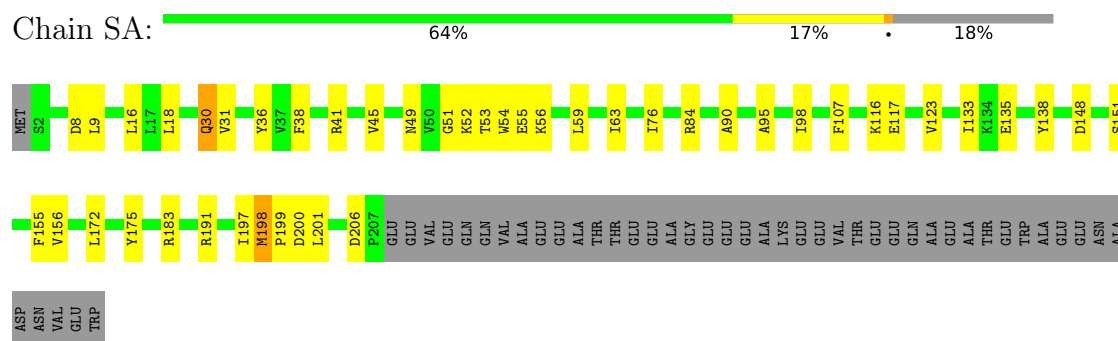
- Molecule 3: 5S rRNA



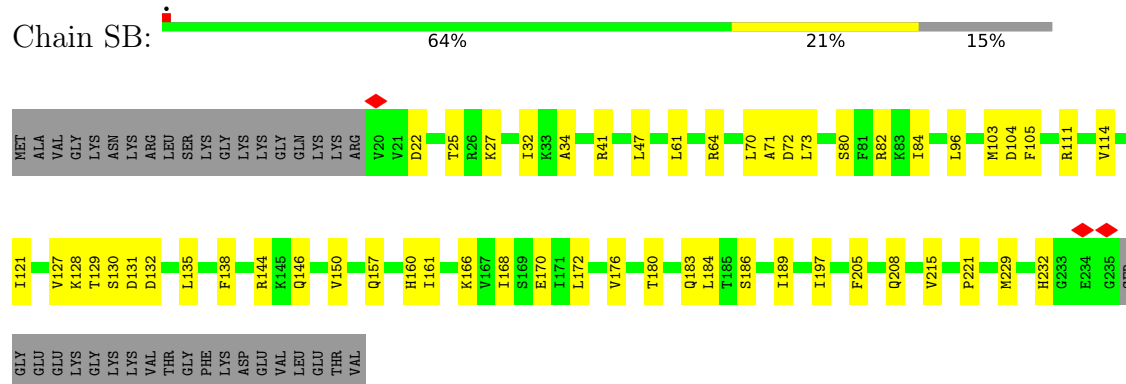
- Molecule 4: 5.8S rRNA



- Molecule 5: Small ribosomal subunit protein uS2A

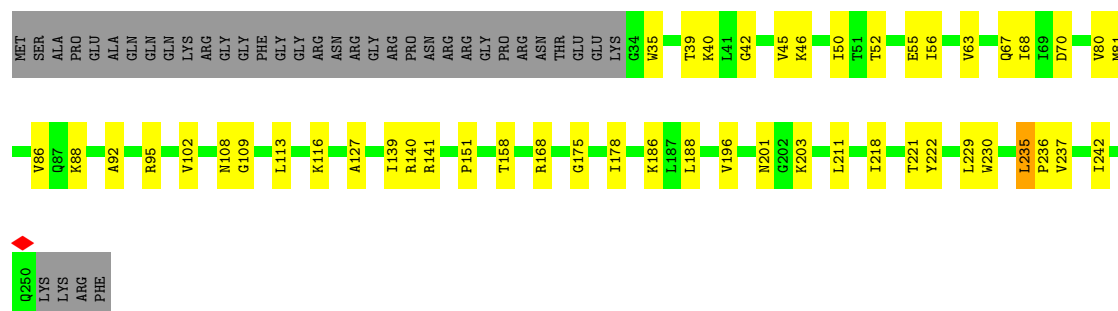


- Molecule 6: 40S ribosomal protein S1-A



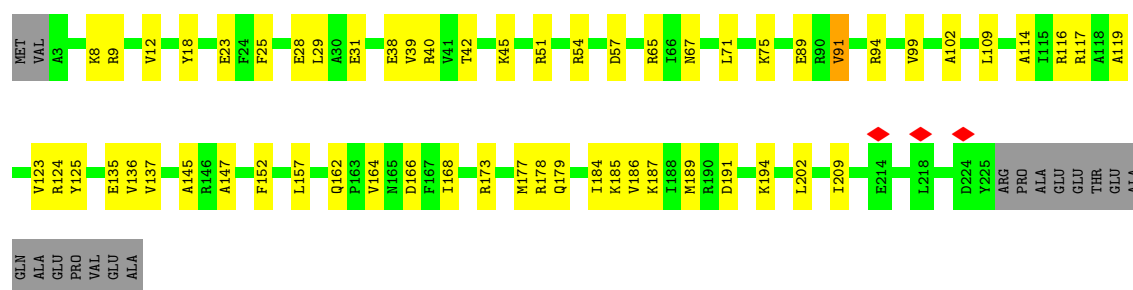
- Molecule 7: 40S ribosomal protein S2





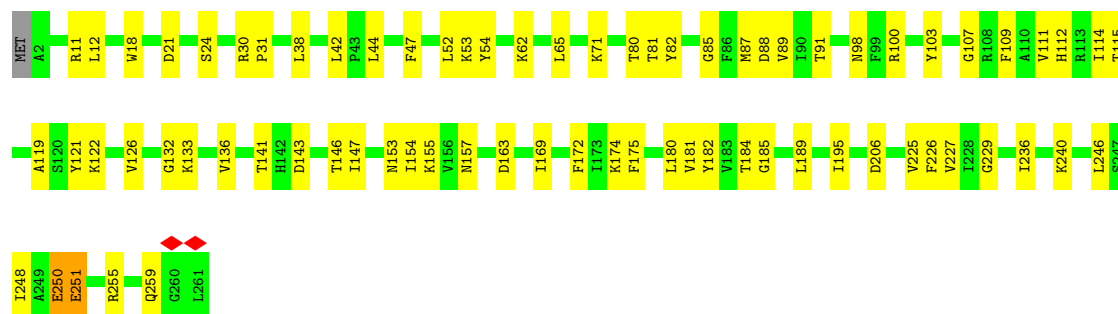
- Molecule 8: Small ribosomal subunit protein uS3

Chain SD: 69% 24% 7%



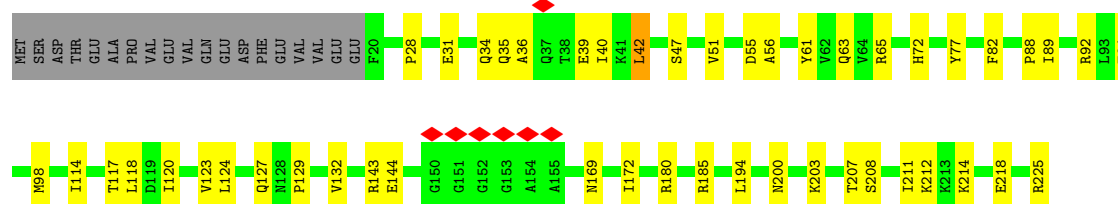
- Molecule 9: 40S ribosomal protein S4-A

Chain SE: 71% 28% 1%

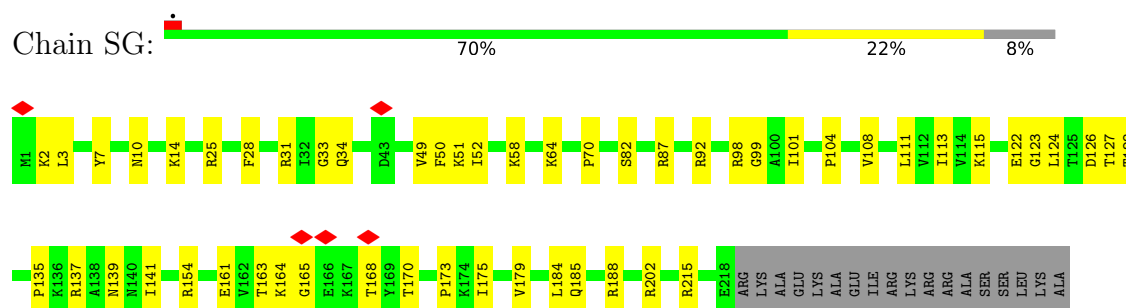


- Molecule 10: Small ribosomal subunit protein uS7

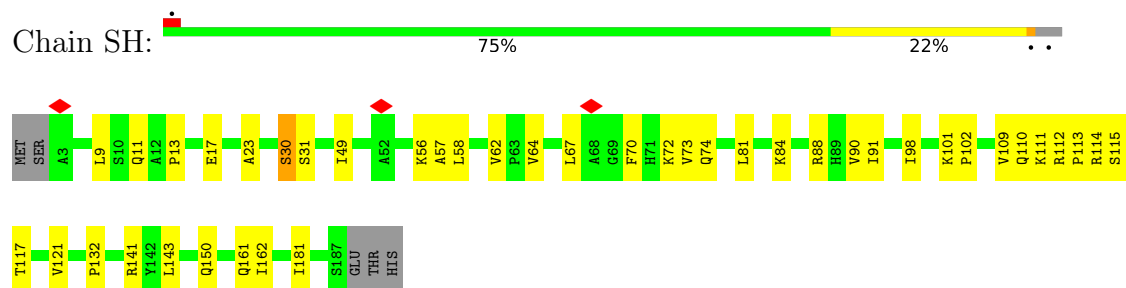
Chain SF: 70% 21% 8%



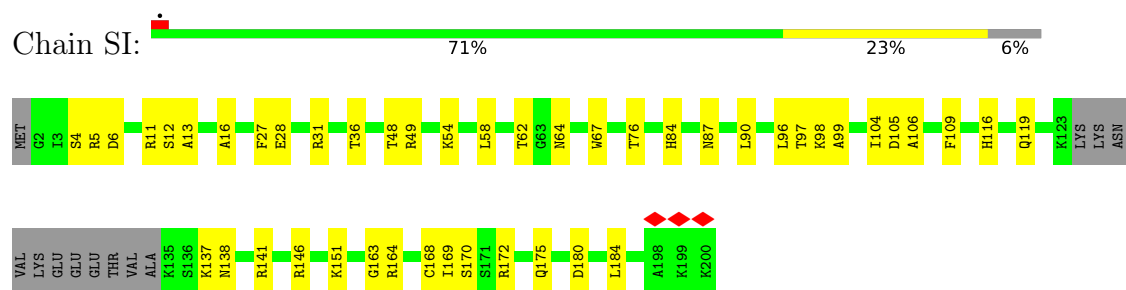
- Molecule 11: 40S ribosomal protein S6-A



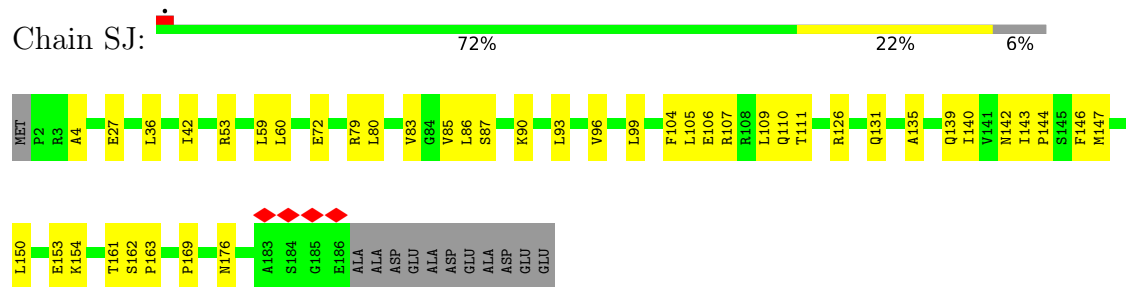
- Molecule 12: 40S ribosomal protein S7-A



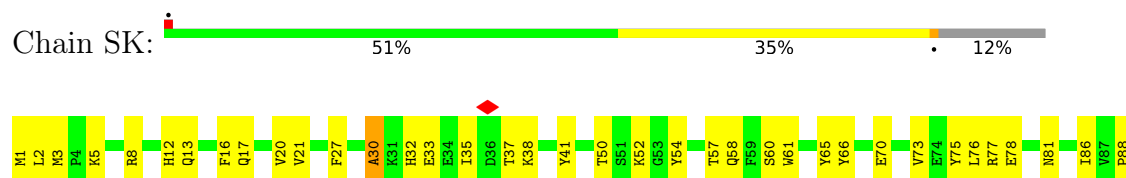
- Molecule 13: 40S ribosomal protein S8-A



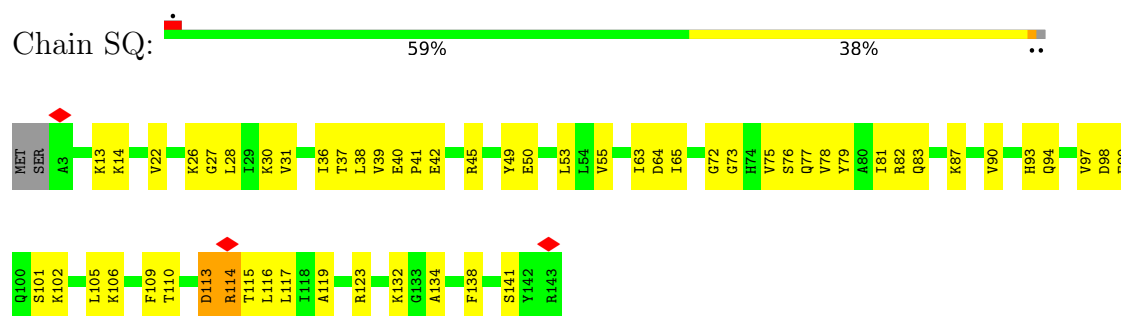
- Molecule 14: 40S ribosomal protein S9-A



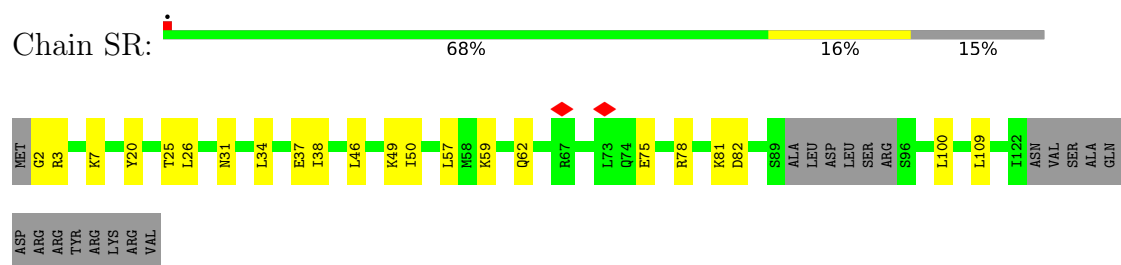
- Molecule 15: Small ribosomal subunit protein eS10A



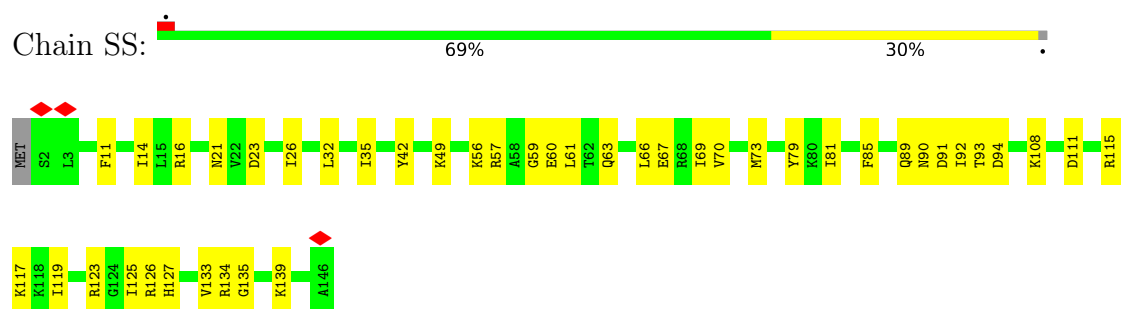
- Molecule 21: Small ribosomal subunit protein uS9A



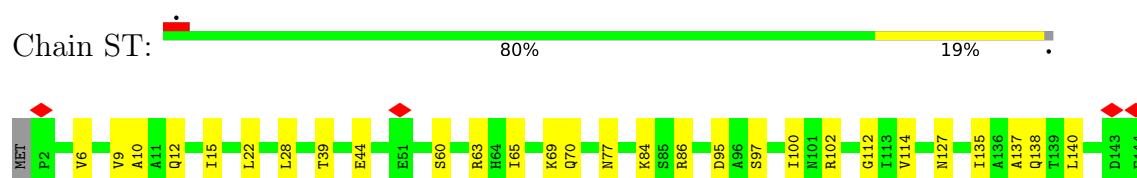
- Molecule 22: Small ribosomal subunit protein eS17A



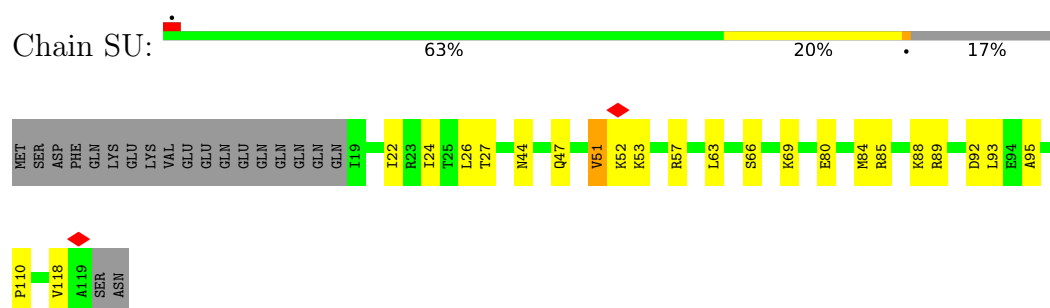
- Molecule 23: Small ribosomal subunit protein uS13A



- Molecule 24: Small ribosomal subunit protein eS19A



- Molecule 25: Small ribosomal subunit protein uS10



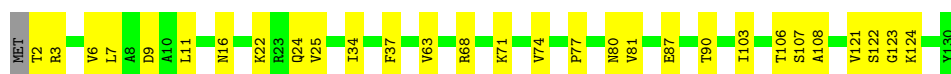
- Molecule 26: Small ribosomal subunit protein eS21A

Chain SV:  76% 24%



- Molecule 27: 40S ribosomal protein S22-A

Chain SW:  77% 22%



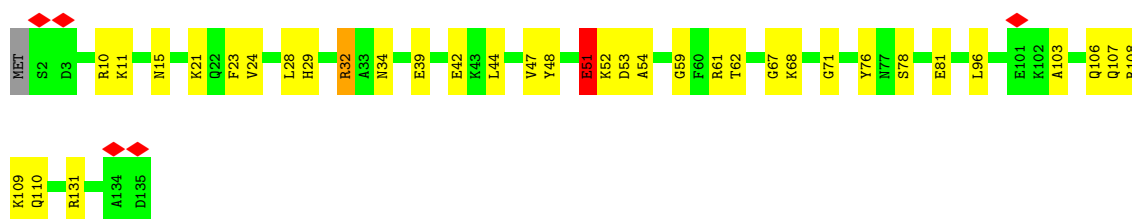
- Molecule 28: 40S ribosomal protein S23-A

Chain SX:  83% 17%



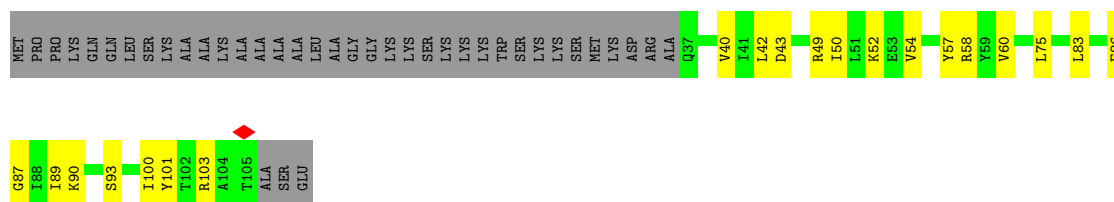
- Molecule 29: 40S ribosomal protein S24-A

Chain SY:  73% 25% ...



- Molecule 30: Small ribosomal subunit protein eS25A

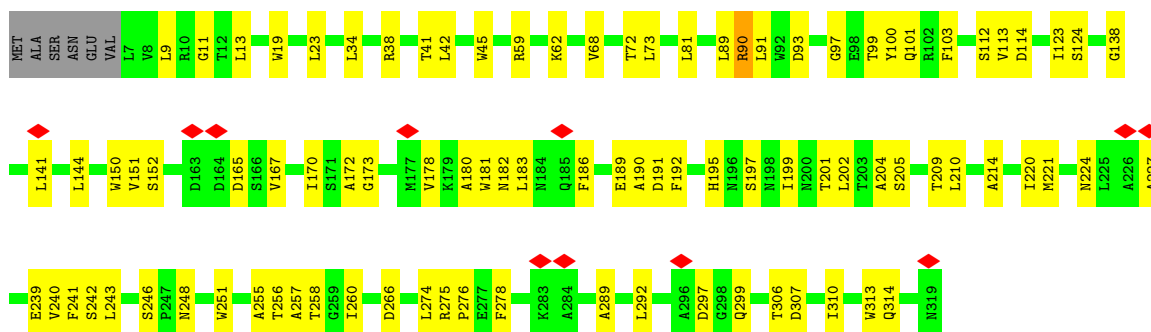
Chain SZ:  45% 19% 36%



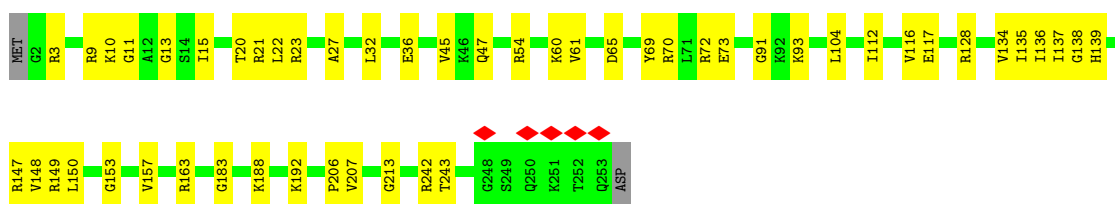
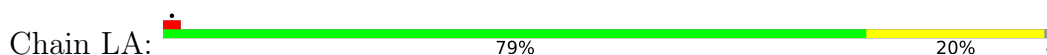
- Molecule 31: Small ribosomal subunit protein eS26B

Chain Sa:  65% 17% 18%

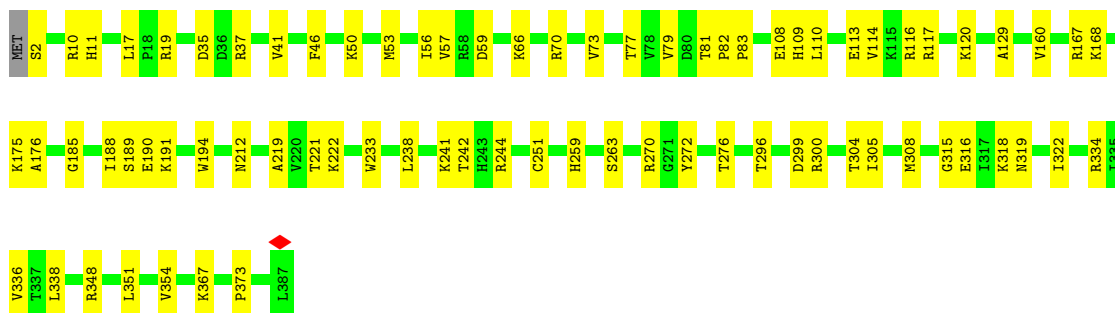
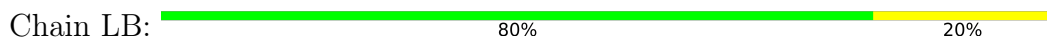




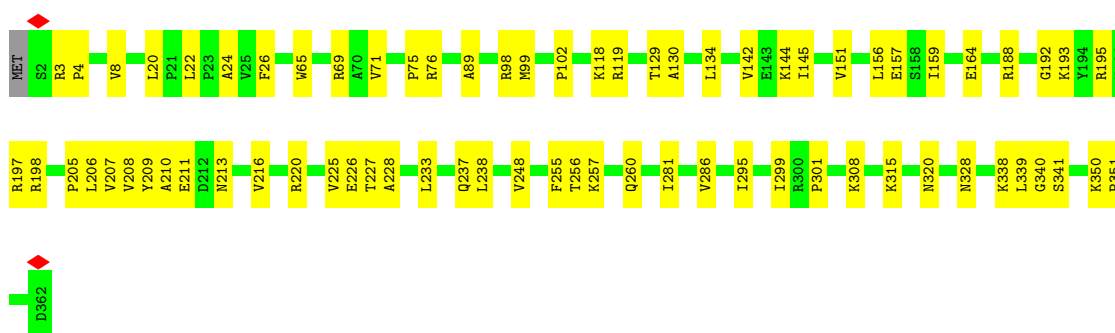
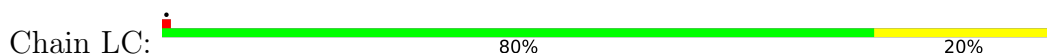
- Molecule 38: Large ribosomal subunit protein uL2A



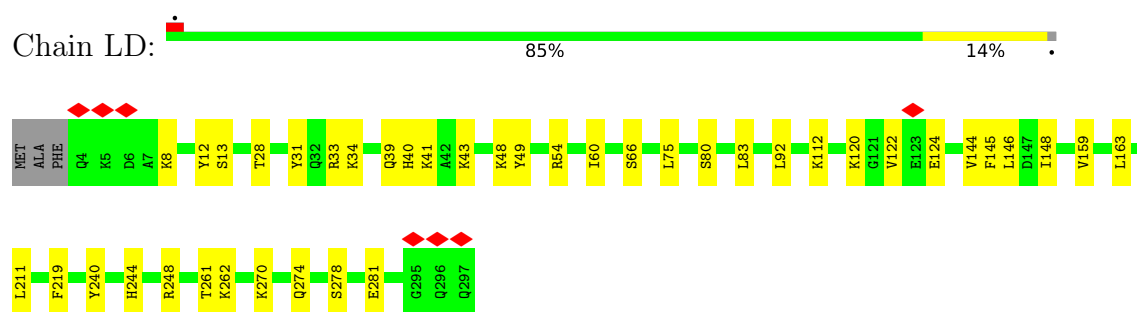
- Molecule 39: Large ribosomal subunit protein uL3



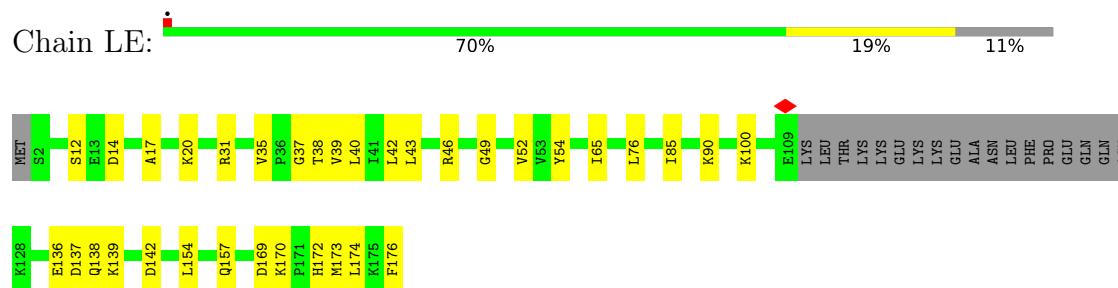
- Molecule 40: Large ribosomal subunit protein uL4A



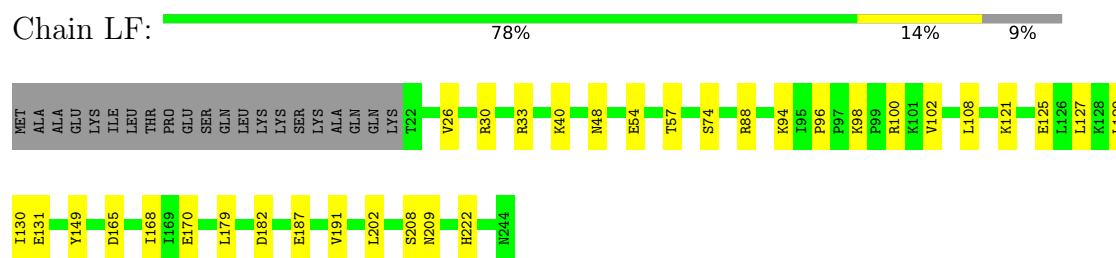
- Molecule 41: Large ribosomal subunit protein uL18



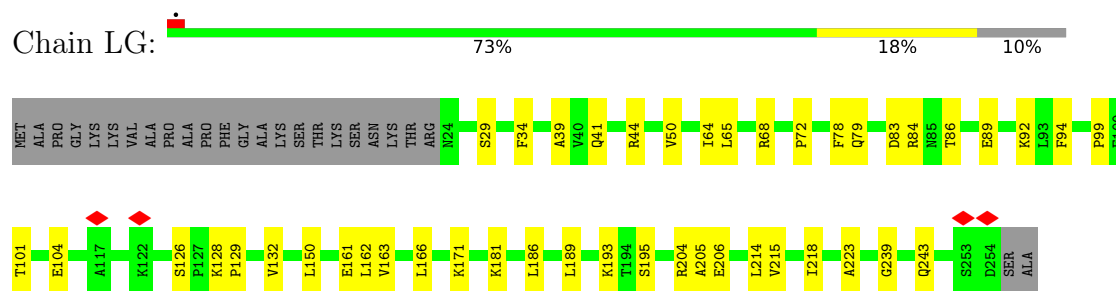
- Molecule 42: Large ribosomal subunit protein eL6A



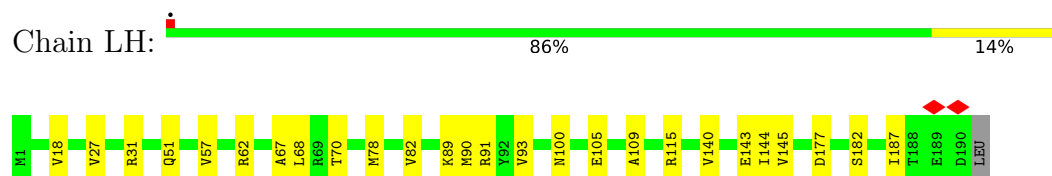
- Molecule 43: Large ribosomal subunit protein uL30A



- Molecule 44: Large ribosomal subunit protein eL8A

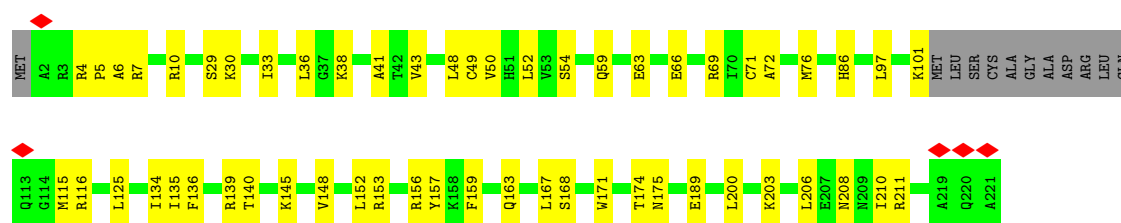


- Molecule 45: Large ribosomal subunit protein uL6A



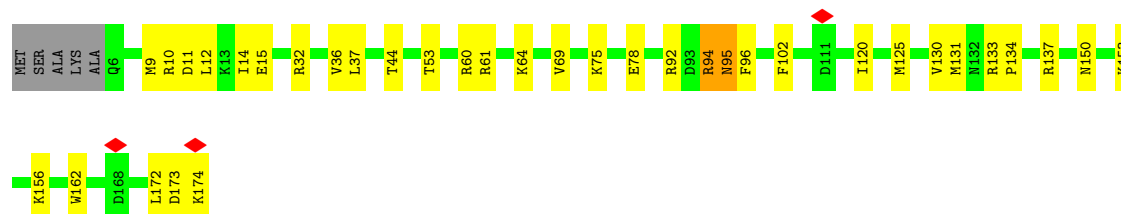
- Molecule 46: Large ribosomal subunit protein uL16

Chain LI: 



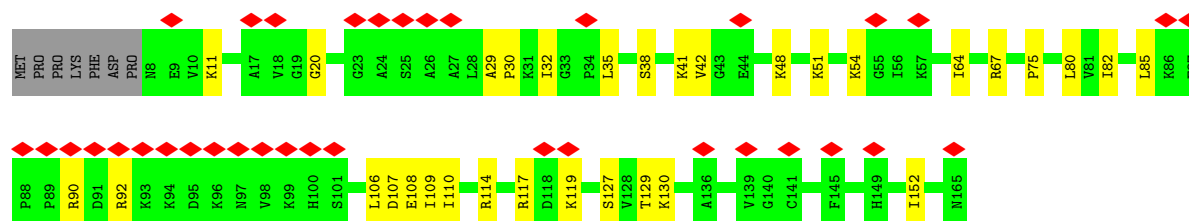
- Molecule 47: Large ribosomal subunit protein uL5A

Chain LJ: 



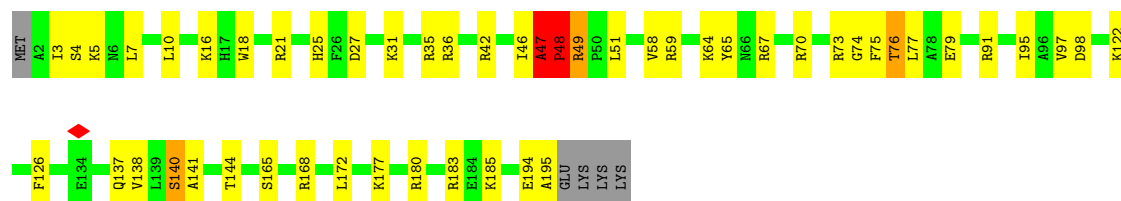
- Molecule 48: Large ribosomal subunit protein uL11A

Chain LK: 



- Molecule 49: Large ribosomal subunit protein eL13A

Chain LL: 

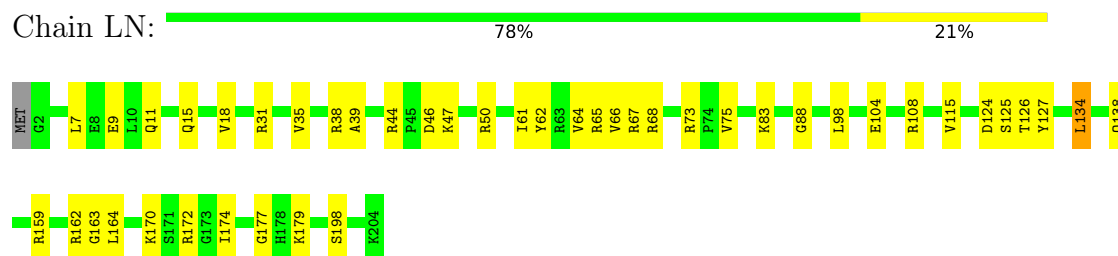


- Molecule 50: Large ribosomal subunit protein eL14A

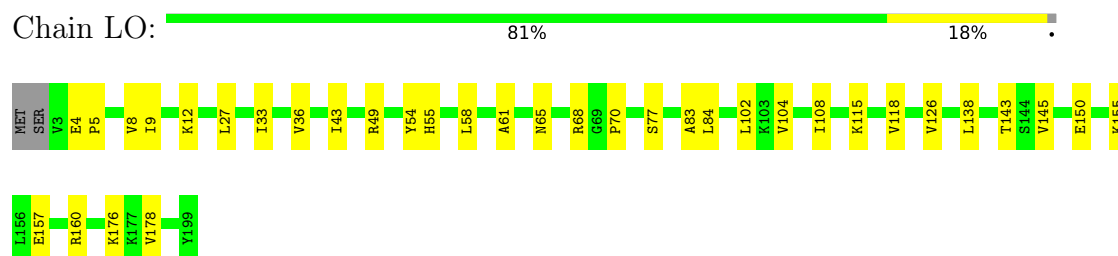
Chain LM: 



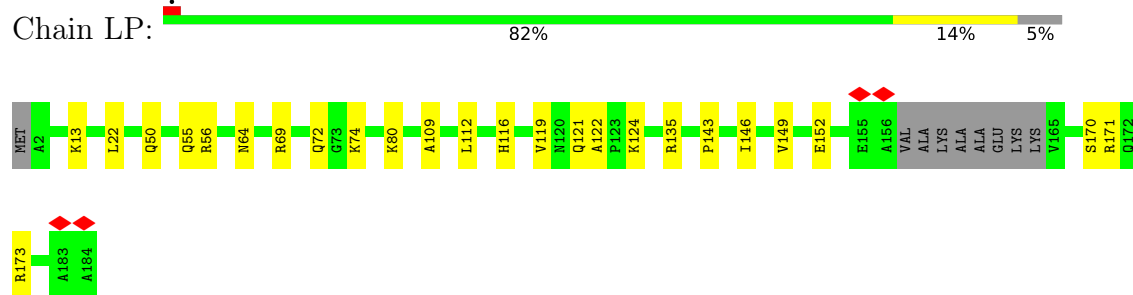
- Molecule 51: Large ribosomal subunit protein eL15A



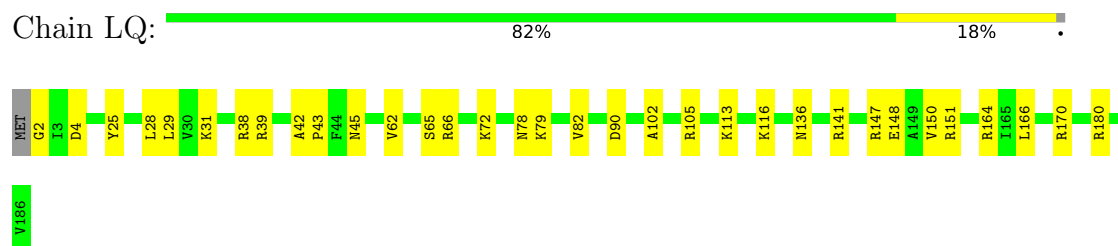
- Molecule 52: Large ribosomal subunit protein uL13A



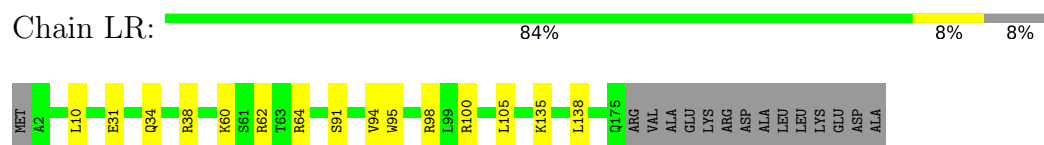
- Molecule 53: Large ribosomal subunit protein uL22A



- Molecule 54: Large ribosomal subunit protein eL18A

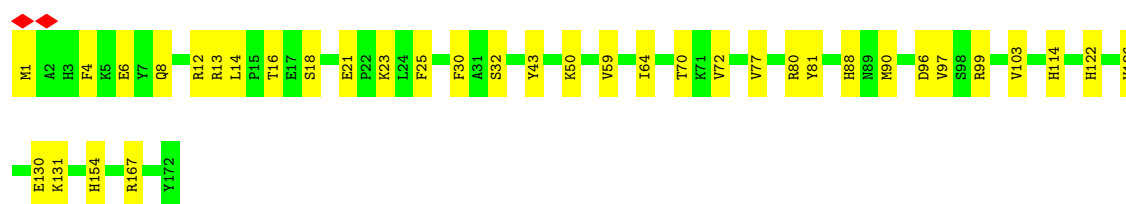


- Molecule 55: Large ribosomal subunit protein eL19A



- Molecule 56: Large ribosomal subunit protein eL20A

Chain LS:  79% 21%



- Molecule 57: Large ribosomal subunit protein eL21A

Chain LT:  74% 24% ..



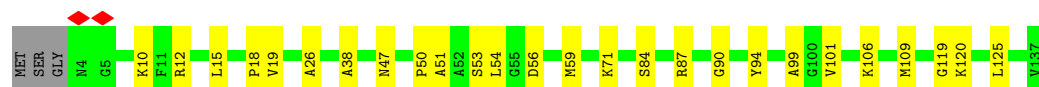
- Molecule 58: Large ribosomal subunit protein eL22A

Chain LU:  69% 12% 19%



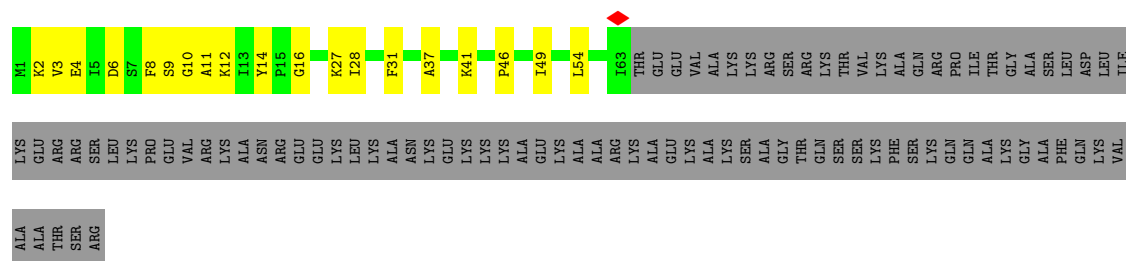
- Molecule 59: Large ribosomal subunit protein uL14A

Chain LV:  79% 19% .



- Molecule 60: Large ribosomal subunit protein eL24A

Chain LW:  28% 12% 59%



- Molecule 61: Large ribosomal subunit protein uL23

Chain LX:  75% 9% 15%



- Molecule 62: Large ribosomal subunit protein uL24A

Chain LY: 85% 13% .



- Molecule 63: Large ribosomal subunit protein eL27A

Chain LZ: 75% 24% ..



- Molecule 64: Large ribosomal subunit protein uL15

Chain La: 77% 21% ..



- Molecule 65: Large ribosomal subunit protein eL29

Chain Lb: 83% 14% ..



- Molecule 66: Large ribosomal subunit protein eL30

Chain Lc: 80% 15% 5%



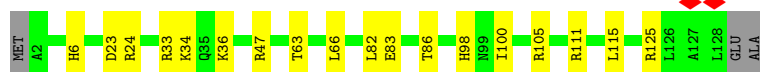
- Molecule 67: Large ribosomal subunit protein eL31A

Chain Ld: 6% 75% 21% .



- Molecule 68: Large ribosomal subunit protein eL32

Chain Le:  84% 14%



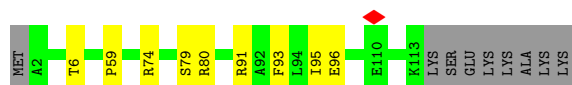
- Molecule 69: Large ribosomal subunit protein eL33A

Chain Lf:  66% 33%



- Molecule 70: Large ribosomal subunit protein eL34A

Chain Lg:  85% 7% 7%



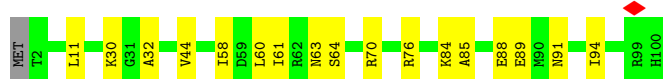
- Molecule 71: Large ribosomal subunit protein uL29A

Chain Lh:  84% 15%



- Molecule 72: Large ribosomal subunit protein eL36A

Chain Li:  82% 17%



- Molecule 73: Large ribosomal subunit protein eL37A

Chain Lj:  76% 17% 7%



- Molecule 74: Large ribosomal subunit protein eL38

Chain Lk:  71% 28%



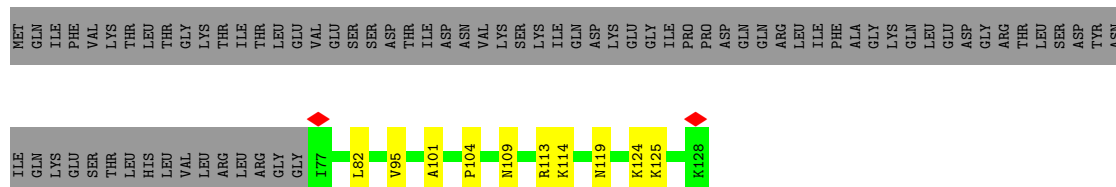
- Molecule 75: Large ribosomal subunit protein eL39

Chain Ll:  78% 20%

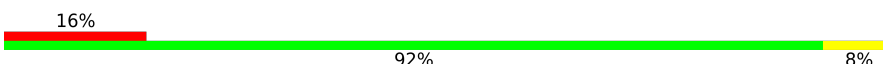


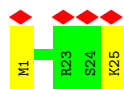
- Molecule 76: Ubiquitin-ribosomal protein eL40A fusion protein

Chain Lm:  33% 8% 59%



- Molecule 77: Large ribosomal subunit protein eL41A

Chain Ln:  16% 92% 8%



- Molecule 78: Large ribosomal subunit protein eL42A

Chain Lo:  81% 18%



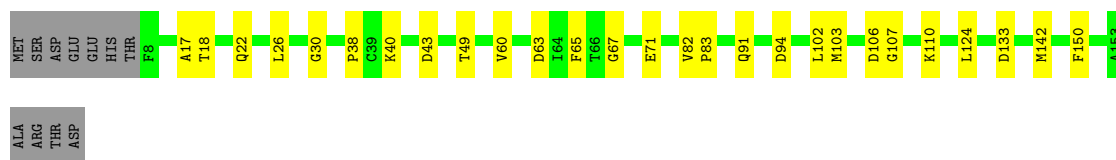
- Molecule 79: Large ribosomal subunit protein eL43A

Chain Lp:  78% 21%



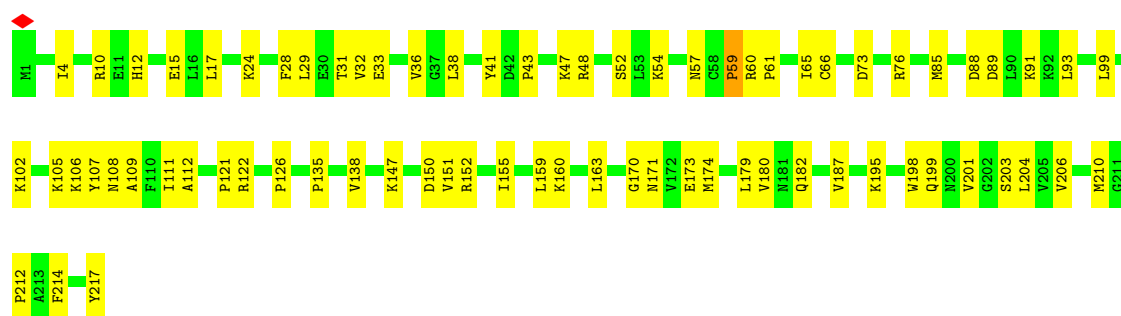
- Molecule 80: Eukaryotic translation initiation factor 5A-1

Chain CE:  76% 17% 7%



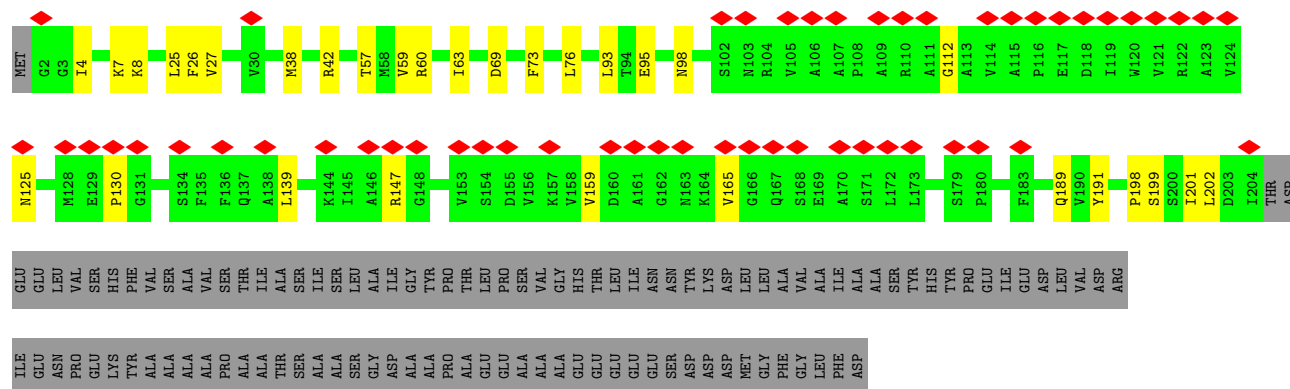
- Molecule 81: Large ribosomal subunit protein uL1A

Chain L1:  66% 33%



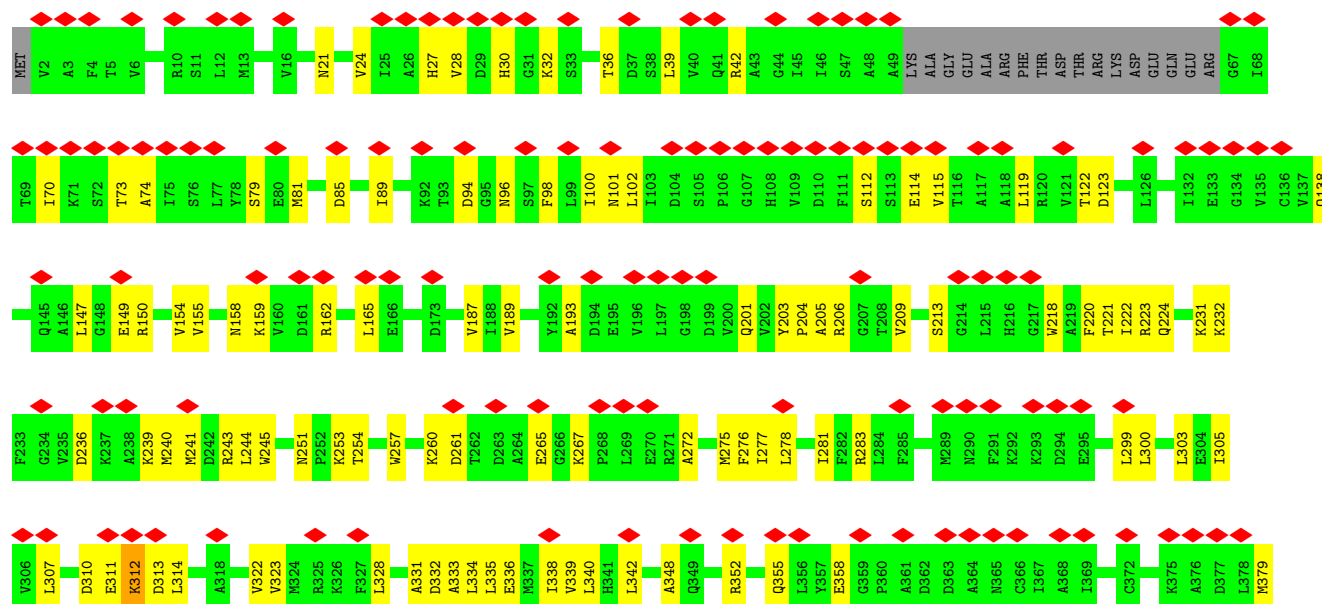
- Molecule 82: Large ribosomal subunit protein uL10

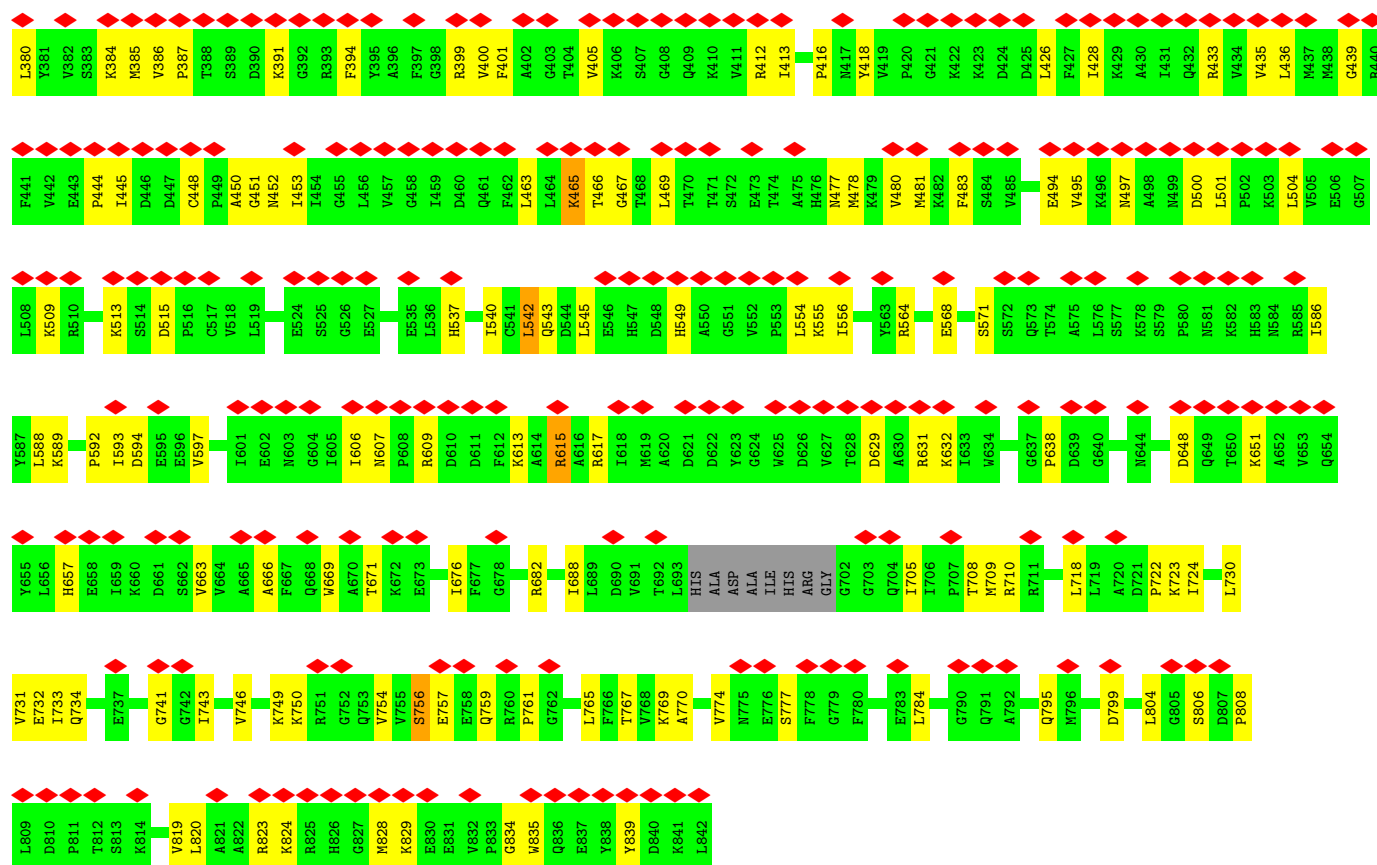
Chain P0:  17% 55% 10% 35%



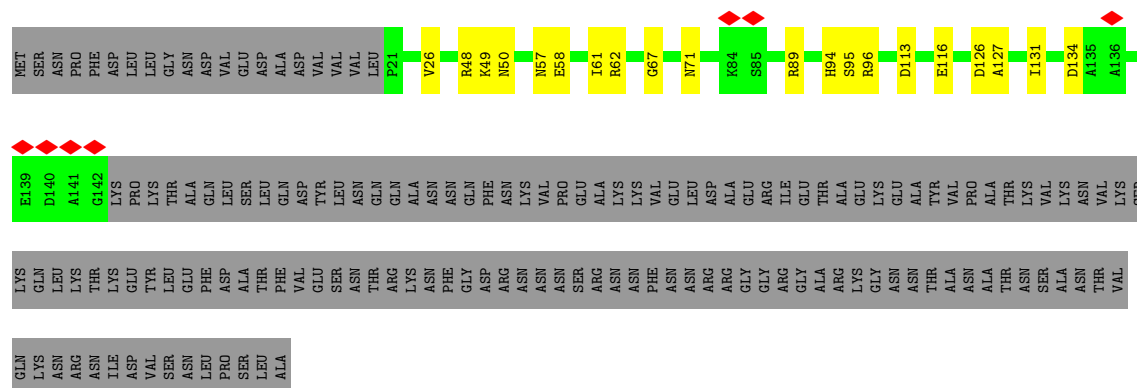
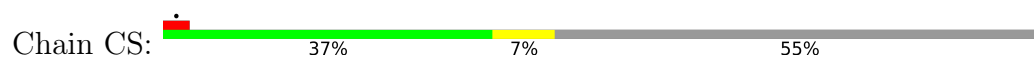
- Molecule 83: Elongation factor 2

Chain CD:  43% 69% 27%





• Molecule 84: Suppressor protein STM1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.447	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	406.56, 406.56, 406.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.847, 0.847, 0.847	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T1C, 5CT, MG, ZN, GDP

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	C2	0.23	0/40528	0.36	0/63141
2	C1	0.33	0/76341	0.37	1/119019 (0.0%)
3	C4	0.25	0/2883	0.30	0/4491
4	C3	0.31	0/3724	0.35	0/5798
5	SA	0.29	0/1623	0.69	1/2222 (0.0%)
6	SB	0.31	0/1748	0.67	0/2352
7	SC	0.32	0/1665	0.63	0/2263
8	SD	0.31	0/1759	0.73	2/2368 (0.1%)
9	SE	0.29	0/2109	0.67	3/2839 (0.1%)
10	SF	0.28	0/1629	0.64	0/2202
11	SG	0.23	0/1779	0.53	0/2379
12	SH	0.30	0/1511	0.68	2/2036 (0.1%)
13	SI	0.29	0/1514	0.57	0/2021
14	SJ	0.31	0/1519	0.66	1/2035 (0.0%)
15	SK	0.38	0/757	0.83	0/1022
16	SL	0.26	0/1194	0.47	0/1610
17	SM	0.34	0/898	0.86	0/1220
18	SN	0.30	0/1215	0.65	1/1638 (0.1%)
19	SO	0.27	0/960	0.56	0/1290
20	SP	0.27	0/959	0.69	0/1288
21	SQ	0.30	0/1125	0.71	2/1510 (0.1%)
22	SR	0.34	0/904	0.78	1/1210 (0.1%)
23	SS	0.32	0/1211	0.76	0/1628
24	ST	0.24	0/1130	0.53	0/1517
25	SU	0.30	0/815	0.72	0/1102
26	SV	0.30	0/693	0.71	0/935
27	SW	0.28	0/1038	0.56	0/1395
28	SX	0.28	0/1139	0.56	0/1518
29	SY	0.28	0/1087	0.82	3/1449 (0.2%)
30	SZ	0.32	0/566	0.74	2/761 (0.3%)
31	Sa	0.28	0/782	0.54	0/1047
32	Sb	0.22	0/620	0.69	0/838

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sc	0.30	0/499	0.75	0/670
34	Sd	0.25	0/452	0.55	0/600
35	Se	0.40	0/483	0.71	1/643 (0.2%)
36	Sf	0.23	0/253	0.64	0/340
37	Sg	0.25	0/2456	0.71	0/3343
38	LA	0.39	0/1946	0.69	2/2614 (0.1%)
39	LB	0.33	0/3146	0.54	0/4228
40	LC	0.33	0/2800	0.59	0/3790
41	LD	0.26	0/2408	0.55	0/3248
42	LE	0.29	0/1269	0.57	0/1705
43	LF	0.31	0/1828	0.59	0/2461
44	LG	0.32	0/1795	0.66	0/2429
45	LH	0.33	0/1531	0.63	0/2062
46	LI	0.30	0/1732	0.57	1/2323 (0.0%)
47	LJ	0.27	0/1374	0.69	0/1842
48	LK	0.22	0/1210	0.51	0/1627
49	LL	0.32	0/1573	0.73	3/2113 (0.1%)
50	LM	0.30	0/1074	0.53	0/1446
51	LN	0.39	1/1757 (0.1%)	0.52	0/2354
52	LO	0.37	0/1585	0.57	0/2128
53	LP	0.30	0/1400	0.48	0/1882
54	LQ	0.28	0/1465	0.50	0/1965
55	LR	0.31	0/1382	0.53	0/1849
56	LS	0.33	0/1481	0.57	0/1990
57	LT	0.31	0/1300	0.58	0/1743
58	LU	0.27	0/794	0.57	0/1076
59	LV	0.32	0/1008	0.56	0/1356
60	LW	0.32	0/533	0.60	0/707
61	LX	0.37	0/974	0.65	0/1314
62	LY	0.25	0/987	0.48	0/1318
63	LZ	0.33	0/1118	0.69	1/1497 (0.1%)
64	La	0.35	0/1204	0.69	2/1612 (0.1%)
65	Lb	0.29	0/473	0.69	0/629
66	Lc	0.24	0/775	0.52	0/1040
67	Ld	0.30	0/897	0.53	0/1205
68	Le	0.37	0/1041	0.67	0/1394
69	Lf	0.36	0/868	0.55	0/1168
70	Lg	0.30	0/890	0.47	0/1189
71	Lh	0.31	0/974	0.58	0/1297
72	Li	0.29	0/777	0.55	0/1033
73	Lj	0.37	0/665	0.48	0/882
74	Lk	0.25	0/614	0.55	0/822
75	Ll	0.39	0/443	0.64	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Lm	0.27	0/423	0.54	0/562
77	Ln	0.25	0/234	0.45	0/300
78	Lo	0.29	0/860	0.49	0/1136
79	Lp	0.33	0/701	0.68	0/934
80	CE	0.34	0/1097	0.74	0/1476
81	L1	0.35	0/1745	0.75	0/2342
82	P0	0.23	0/1598	0.58	0/2161
83	CD	0.33	0/6469	0.73	8/8760 (0.1%)
84	CS	0.31	0/929	0.60	1/1245 (0.1%)
All	All	0.30	1/224715 (0.0%)	0.49	38/328582 (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
5	SA	0	1
10	SF	0	1
12	SH	0	3
16	SL	0	1
17	SM	0	1
21	SQ	0	2
23	SS	0	2
25	SU	0	1
29	SY	0	1
32	Sb	0	1
35	Se	0	1
37	Sg	0	1
38	LA	0	1
40	LC	0	1
47	LJ	0	1
49	LL	0	2
57	LT	0	1
64	La	0	1
65	Lb	0	1
72	Li	0	1
79	Lp	0	1
83	CD	0	2
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	LN	134	LEU	CG-CD2	-5.04	1.35	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CD	606	ILE	CA-C-N	9.07	133.90	121.20
83	CD	606	ILE	C-N-CA	9.07	133.90	121.20
64	La	47	LYS	CA-C-N	8.76	138.27	121.54
64	La	47	LYS	C-N-CA	8.76	138.27	121.54
49	LL	140	SER	CA-C-N	7.56	135.97	121.54
49	LL	140	SER	C-N-CA	7.56	135.97	121.54
35	Se	56	MET	CG-SD-CE	-7.04	85.41	100.90
38	LA	139	HIS	CA-C-N	-6.92	114.49	122.52
38	LA	139	HIS	C-N-CA	-6.92	114.49	122.52
63	LZ	103	GLN	CA-CB-CG	6.73	127.55	114.10
29	SY	48	TYR	CA-C-N	6.60	134.15	121.54
29	SY	48	TYR	C-N-CA	6.60	134.15	121.54
83	CD	312	LYS	CA-CB-CG	6.58	127.26	114.10
83	CD	615	ARG	CB-CG-CD	-6.42	96.53	111.30
14	SJ	142	ASN	N-CA-C	-6.15	106.42	114.04
49	LL	48	PRO	N-CA-C	6.13	125.09	112.47
21	SQ	114	ARG	CA-C-N	5.93	132.86	121.54
21	SQ	114	ARG	C-N-CA	5.93	132.86	121.54
9	SE	251	GLU	N-CA-CB	5.73	119.17	110.28
84	CS	89	ARG	N-CA-C	-5.65	107.03	114.04
12	SH	30	SER	CA-C-N	5.57	131.72	121.70
12	SH	30	SER	C-N-CA	5.57	131.72	121.70
22	SR	38	ILE	N-CA-C	-5.40	107.04	112.17
5	SA	198	MET	CA-CB-CG	5.28	124.65	114.10
18	SN	35	GLU	N-CA-CB	5.27	119.14	110.39
9	SE	250	GLU	CA-C-N	-5.26	112.31	120.31
9	SE	250	GLU	C-N-CA	-5.26	112.31	120.31
83	CD	240	MET	CG-SD-CE	5.24	112.42	100.90
46	LI	66	GLU	CA-CB-CG	5.18	124.45	114.10
83	CD	149	GLU	CA-C-N	5.16	129.88	122.35
83	CD	149	GLU	C-N-CA	5.16	129.88	122.35
2	C1	2772	C	P-O3'-C3'	5.13	127.90	120.20
8	SD	147	ALA	CA-C-N	5.12	132.73	123.27
8	SD	147	ALA	C-N-CA	5.12	132.73	123.27
30	SZ	43	ASP	CA-C-N	5.09	131.27	121.54
30	SZ	43	ASP	C-N-CA	5.09	131.27	121.54
29	SY	51	GLU	CA-CB-CG	5.06	124.23	114.10
83	CD	542	LEU	CB-CG-CD2	-5.04	95.59	110.70

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	CD	750	LYS	Peptide
83	CD	756	SER	Peptide
38	LA	13	GLY	Peptide
40	LC	144	LYS	Peptide
47	LJ	94	ARG	Peptide
49	LL	47	ALA	Peptide
49	LL	49	ARG	Peptide
57	LT	102	ARG	Sidechain
64	La	17	ALA	Peptide
65	Lb	21	ILE	Peptide
72	Li	64	SER	Peptide
79	Lp	51	ALA	Peptide
5	SA	206	ASP	Peptide
10	SF	42	LEU	Peptide
12	SH	111	LYS	Peptide
12	SH	30	SER	Peptide
12	SH	31	SER	Peptide
16	SL	120	GLY	Peptide
17	SM	128	ALA	Peptide
21	SQ	113	ASP	Peptide
21	SQ	40	GLU	Peptide
23	SS	60	GLU	Peptide
23	SS	90	ASN	Peptide
25	SU	51	VAL	Peptide
29	SY	51	GLU	Peptide
32	Sb	75	GLU	Peptide
35	Se	44	PHE	Peptide
37	Sg	90	ARG	Sidechain

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	C2	36234	0	18231	331	0
2	C1	68200	0	34275	476	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C4	2579	0	1304	24	0
4	C3	3333	0	1685	23	0
5	SA	1583	0	1578	31	0
6	SB	1722	0	1793	39	0
7	SC	1635	0	1723	36	0
8	SD	1734	0	1817	43	0
9	SE	2068	0	2154	55	0
10	SF	1609	0	1675	37	0
11	SG	1755	0	1846	37	0
12	SH	1486	0	1576	27	0
13	SI	1489	0	1525	35	0
14	SJ	1494	0	1573	28	0
15	SK	741	0	691	22	0
16	SL	1168	0	1233	16	0
17	SM	890	0	887	22	0
18	SN	1192	0	1255	18	0
19	SO	949	0	985	16	0
20	SP	939	0	968	23	0
21	SQ	1105	0	1166	44	0
22	SR	896	0	902	17	0
23	SS	1192	0	1222	31	0
24	ST	1112	0	1124	20	0
25	SU	805	0	874	18	0
26	SV	684	0	672	19	0
27	SW	1021	0	1060	22	0
28	SX	1121	0	1196	19	0
29	SY	1073	0	1132	32	0
30	SZ	558	0	598	13	0
31	Sa	769	0	814	17	0
32	Sb	610	0	633	7	0
33	Sc	497	0	535	11	0
34	Sd	442	0	432	5	0
35	Se	475	0	525	15	0
36	Sf	248	0	237	4	0
37	Sg	2403	0	2350	65	0
38	LA	1912	0	1976	40	0
39	LB	3075	0	3142	50	0
40	LC	2748	0	2859	48	0
41	LD	2359	0	2311	29	0
42	LE	1248	0	1339	27	0
43	LF	1791	0	1869	24	0
44	LG	1763	0	1819	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	LH	1510	0	1576	17	0
46	LI	1696	0	1731	39	0
47	LJ	1353	0	1383	30	0
48	LK	1196	0	1257	19	0
49	LL	1548	0	1613	44	0
50	LM	1059	0	1154	16	0
51	LN	1720	0	1779	39	0
52	LO	1555	0	1659	24	0
53	LP	1378	0	1404	16	0
54	LQ	1441	0	1543	30	0
55	LR	1365	0	1414	12	0
56	LS	1445	0	1487	26	0
57	LT	1276	0	1323	36	0
58	LU	778	0	791	10	0
59	LV	993	0	1040	19	0
60	LW	521	0	551	13	0
61	LX	959	0	1023	8	0
62	LY	976	0	1064	12	0
63	LZ	1092	0	1155	22	0
64	La	1173	0	1215	22	0
65	Lb	462	0	491	5	0
66	Lc	767	0	816	9	0
67	Ld	883	0	918	20	0
68	Le	1020	0	1090	13	0
69	Lf	850	0	880	27	0
70	Lg	880	0	942	8	0
71	Lh	965	0	1067	16	0
72	Li	770	0	846	14	0
73	Lj	650	0	650	10	0
74	Lk	608	0	671	15	0
75	Ll	436	0	475	7	0
76	Lm	417	0	455	9	0
77	Ln	233	0	284	2	0
78	Lo	847	0	915	14	0
79	Lp	694	0	734	13	0
80	CE	1097	0	1078	22	0
81	L1	1718	0	1811	51	0
82	P0	1571	0	1614	21	0
83	CD	6348	0	6422	159	0
84	CS	919	0	913	17	0
85	C2	1	0	0	0	0
85	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Lj	1	0	0	0	0
85	Lm	1	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	1	0	0	0	0
85	SM	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sb	1	0	0	0	0
86	C1	252	0	228	4	0
87	C1	2	0	0	0	0
87	C3	1	0	0	0	0
87	CD	1	0	0	0	0
88	CD	28	0	12	0	0
All	All	210169	0	159035	2365	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 7.

All (2365) 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)
60:LW:4:GLU:O	60:LW:12:LYS:HA	1.36	1.22
47:LJ:92:ARG:O	47:LJ:95:ASN:HB2	1.42	1.20
79:Lp:53:GLY:HA2	79:Lp:66:GLY:O	1.55	1.07
2:C1:3165:A:N6	2:C1:3285:C:H42	1.54	1.04
1:C2:1588:G:H1	1:C2:1608:U:H3	1.02	1.01
2:C1:3165:A:H61	2:C1:3285:C:N4	1.57	0.99
1:C2:699:U:H3	1:C2:739:G:H1	0.98	0.97
1:C2:486:G:H1	1:C2:501:U:H3	0.98	0.96
63:LZ:121:ARG:O	63:LZ:125:GLY:HA2	1.64	0.96
83:CD:607:ASN:HB3	83:CD:615:ARG:HH22	1.35	0.91
8:SD:25:PHE:O	8:SD:29:LEU:HB3	1.72	0.90
25:SU:99:ILE:HG13	25:SU:102:ARG:HE	1.39	0.87
29:SY:29:HIS:O	29:SY:67:GLY:HA2	1.74	0.86
35:Se:55:ARG:HE	35:Se:56:MET:H	1.23	0.86
1:C2:826:U:H3	1:C2:846:G:H1	0.87	0.85
83:CD:494:GLU:HB2	83:CD:555:LYS:HE3	1.55	0.85
2:C1:3162:C:N4	2:C1:3163:A:N6	2.25	0.84
17:SM:93:ASP:O	17:SM:97:LEU:HB2	1.79	0.83
2:C1:3165:A:H61	2:C1:3285:C:H42	0.83	0.82
2:C1:2940:A:N7	39:LB:2:SER:N	2.26	0.82
78:Lo:63:LYS:HD3	78:Lo:87:ARG:HH12	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:385:MET:HE3	83:CD:394:PHE:HB2	1.63	0.80
1:C2:895:G:H1	1:C2:917:U:H3	1.33	0.77
37:Sg:89:LEU:HB2	37:Sg:103:PHE:HB2	1.66	0.76
7:SC:81:MET:HE1	7:SC:186:LYS:HB3	1.67	0.76
1:C2:1067:C:H5''	6:SB:150:VAL:HG12	1.68	0.76
9:SE:31:PRO:HG2	9:SE:38:LEU:HG	1.67	0.76
39:LB:57:VAL:HG22	39:LB:73:VAL:HG12	1.69	0.74
25:SU:24:ILE:HD13	25:SU:93:LEU:HD23	1.68	0.74
81:L1:31:THR:HG21	81:L1:60:ARG:HG2	1.69	0.74
2:C1:3162:C:N4	2:C1:3163:A:H62	1.83	0.74
52:LO:27:LEU:HD21	52:LO:102:LEU:HB2	1.70	0.73
21:SQ:27:GLY:HA2	21:SQ:63:ILE:O	1.88	0.73
63:LZ:106:GLN:HA	63:LZ:109:GLU:HG3	1.71	0.73
37:Sg:260:ILE:HB	37:Sg:274:LEU:HB3	1.70	0.72
2:C1:3165:A:N1	2:C1:3285:C:N3	2.38	0.72
12:SH:150:GLN:HB3	12:SH:181:ILE:HG22	1.70	0.72
18:SN:4:MET:SD	18:SN:124:ARG:NH2	2.63	0.72
46:LI:33:ILE:HD12	46:LI:36:LEU:HD21	1.71	0.72
83:CD:348:ALA:O	83:CD:352:ARG:HB2	1.88	0.71
42:LE:43:LEU:HD11	42:LE:85:ILE:HG13	1.73	0.71
1:C2:127:G:N7	11:SG:202:ARG:NH2	2.39	0.71
13:SI:62:THR:HA	13:SI:76:THR:O	1.89	0.71
1:C2:1610:G:H4'	10:SF:98:MET:HE1	1.72	0.71
55:LR:105:LEU:HD23	55:LR:138:LEU:HD23	1.73	0.70
2:C1:1481:A:O2'	2:C1:1858:A:N3	2.22	0.70
59:LV:10:LYS:NZ	59:LV:56:ASP:OD1	2.24	0.70
2:C1:182:U:H3	2:C1:234:G:H1	1.39	0.70
83:CD:504:LEU:HD12	83:CD:554:LEU:HD22	1.74	0.70
47:LJ:94:ARG:O	47:LJ:96:PHE:N	2.24	0.70
83:CD:542:LEU:HD21	83:CD:556:ILE:HD12	1.74	0.70
38:LA:21:ARG:HE	38:LA:22:LEU:HG	1.56	0.70
42:LE:35:VAL:HG21	42:LE:90:LYS:HE3	1.74	0.69
13:SI:64:ASN:O	13:SI:180:ASP:HA	1.91	0.69
81:L1:210:MET:HG2	81:L1:212:PRO:HD2	1.74	0.69
1:C2:1339:C:O2'	1:C2:1341:A:N7	2.26	0.69
37:Sg:180:ALA:HB3	37:Sg:190:ALA:HB3	1.75	0.69
83:CD:743:ILE:HG12	83:CD:784:LEU:HD11	1.73	0.69
1:C2:144:U:H5	11:SG:137:ARG:HH22	1.40	0.69
80:CE:124:LEU:HD12	80:CE:150:PHE:HB3	1.74	0.69
76:Lm:95:VAL:HA	76:Lm:101:ALA:O	1.93	0.69
2:C1:911:C:H42	38:LA:3:ARG:HH11	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LH:105:GLU:OE2	45:LH:109:ALA:N	2.26	0.69
83:CD:159:LYS:HE3	83:CD:162:ARG:HD3	1.75	0.68
2:C1:1201:C:H42	2:C1:2857:C:H5"	1.58	0.68
4:C3:154:C:H5"	44:LG:181:LYS:HD3	1.74	0.68
20:SP:32:ASP:OD1	20:SP:35:LYS:NZ	2.26	0.68
20:SP:111:MET:HG2	23:SS:119:ILE:HB	1.74	0.68
6:SB:160:HIS:HB3	6:SB:205:PHE:HE2	1.59	0.68
49:LL:27:ASP:O	49:LL:31:LYS:HB2	1.92	0.68
83:CD:607:ASN:O	83:CD:615:ARG:NH1	2.26	0.68
2:C1:2728:G:N7	57:LT:87:LYS:NZ	2.42	0.68
3:C4:76:A:N3	56:LS:50:LYS:NZ	2.41	0.68
8:SD:116:ARG:NH1	84:CS:116:GLU:OE2	2.27	0.68
59:LV:87:ARG:HH22	59:LV:120:LYS:HB3	1.59	0.67
30:SZ:83:LEU:O	30:SZ:87:GLY:HA2	1.94	0.67
1:C2:209:U:H2'	1:C2:210:A:H8	1.59	0.67
2:C1:727:G:OP2	2:C1:742:G:N2	2.27	0.67
46:LI:30:LYS:HG3	46:LI:63:GLU:HB3	1.74	0.67
2:C1:363:G:OP2	73:Lj:56:ARG:NH2	2.27	0.67
2:C1:939:U:OP2	64:La:26:ARG:NH2	2.27	0.67
2:C1:1474:A:O2'	67:Ld:57:GLN:NE2	2.28	0.67
2:C1:1639:C:OP2	70:Lg:74:ARG:NH2	2.27	0.67
17:SM:63:VAL:HG21	17:SM:66:VAL:HG13	1.75	0.67
9:SE:100:ARG:HB3	9:SE:112:HIS:HB3	1.77	0.67
46:LI:29:SER:HB3	46:LI:125:LEU:HD12	1.76	0.67
49:LL:16:LYS:O	49:LL:21:ARG:NH2	2.27	0.67
37:Sg:19:TRP:H	37:Sg:38:ARG:HB2	1.59	0.67
51:LN:68:ARG:HB3	51:LN:126:THR:O	1.95	0.67
63:LZ:13:VAL:O	63:LZ:20:GLY:N	2.28	0.67
2:C1:992:A:H5"	57:LT:43:LYS:HD2	1.77	0.66
44:LG:163:VAL:HA	44:LG:166:LEU:HD13	1.77	0.66
66:Lc:17:VAL:HG11	66:Lc:92:ILE:HD12	1.77	0.66
6:SB:61:LEU:HD12	6:SB:96:LEU:HD13	1.76	0.66
63:LZ:101:PHE:O	63:LZ:106:GLN:NE2	2.27	0.66
1:C2:868:G:H1	1:C2:960:U:H3	1.39	0.66
29:SY:53:ASP:HB2	29:SY:96:LEU:HD21	1.76	0.66
1:C2:637:C:O2	12:SH:114:ARG:NH1	2.29	0.66
19:SO:20:TYR:HB3	19:SO:27:PHE:HB2	1.78	0.66
44:LG:128:LYS:HD3	44:LG:129:PRO:HD2	1.77	0.66
49:LL:180:ARG:HD3	72:Li:11:LEU:HD11	1.76	0.66
8:SD:75:LYS:NZ	15:SK:20:VAL:O	2.28	0.66
37:Sg:240:VAL:HA	37:Sg:256:THR:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:196:G:O6	13:SI:137:LYS:NZ	2.24	0.66
2:C1:1256:G:H4'	48:LK:127:SER:HB2	1.78	0.66
28:SX:93:LEU:HD21	35:Se:8:LEU:HD23	1.78	0.66
14:SJ:93:LEU:HA	14:SJ:96:VAL:HG12	1.78	0.65
1:C2:223:U:H3	1:C2:838:G:H1	1.44	0.65
73:Lj:21:ARG:NH2	73:Lj:41:ALA:O	2.25	0.65
1:C2:187:G:H3'	13:SI:138:ASN:HD21	1.61	0.65
1:C2:298:C:H5'	9:SE:38:LEU:HD13	1.78	0.65
63:LZ:42:LEU:HD22	63:LZ:101:PHE:HE2	1.61	0.65
83:CD:253:LYS:HD2	83:CD:254:THR:HG23	1.77	0.65
2:C1:2948:C:OP1	39:LB:244:ARG:NH2	2.30	0.65
17:SM:28:LEU:HA	17:SM:31:VAL:HG22	1.79	0.65
2:C1:3042:U:OP2	2:C1:3092:C:N4	2.29	0.65
5:SA:30:GLN:NE2	5:SA:151:SER:O	2.29	0.65
29:SY:61:ARG:NH1	29:SY:62:THR:O	2.30	0.65
83:CD:734:GLN:HB3	83:CD:765:LEU:HD11	1.78	0.65
51:LN:66:VAL:HG21	51:LN:98:LEU:HB3	1.78	0.65
1:C2:126:A:H62	1:C2:291:G:H21	1.43	0.64
10:SF:92:ARG:NH2	10:SF:169:ASN:OD1	2.30	0.64
49:LL:126:PHE:HD2	71:Lh:115:LYS:HG3	1.60	0.64
1:C2:1034:C:HO2'	27:SW:2:THR:N	1.94	0.64
2:C1:804:C:OP1	40:LC:98:ARG:NH2	2.30	0.64
49:LL:42:ARG:O	49:LL:46:ILE:HB	1.97	0.64
1:C2:1553:G:H1	20:SP:40:ARG:HH22	1.45	0.64
1:C2:1555:A:N6	34:Sd:14:TYR:OH	2.30	0.64
1:C2:1559:A:H5''	23:SS:135:GLY:HA3	1.80	0.64
8:SD:51:ARG:HG3	8:SD:89:GLU:HB3	1.80	0.64
30:SZ:60:VAL:HB	30:SZ:101:TYR:HB2	1.79	0.64
1:C2:104:A:OP2	1:C2:308:C:N4	2.27	0.64
1:C2:1542:G:N2	1:C2:1569:A:OP2	2.31	0.64
17:SM:29:LYS:HZ1	17:SM:100:TRP:CD1	2.16	0.64
68:Le:83:GLU:HA	68:Le:86:THR:HG23	1.80	0.64
48:LK:29:ALA:HB1	83:CD:761:PRO:HG3	1.80	0.64
50:LM:55:ARG:NH1	56:LS:70:THR:O	2.30	0.64
5:SA:198:MET:HE1	5:SA:200:ASP:HB2	1.79	0.64
19:SO:80:HIS:HA	19:SO:113:GLY:O	1.98	0.64
23:SS:67:GLU:HA	23:SS:70:VAL:HG12	1.79	0.64
46:LI:174:THR:OG1	46:LI:175:ASN:N	2.29	0.64
24:ST:22:LEU:HD12	24:ST:28:LEU:HD21	1.78	0.63
1:C2:1442:U:H5''	83:CD:651:LYS:HE2	1.79	0.63
7:SC:39:THR:HG23	7:SC:42:GLY:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1594:G:OP2	1:C2:1596:C:N4	2.30	0.63
47:LJ:94:ARG:C	47:LJ:96:PHE:H	2.07	0.63
1:C2:1235:C:H4'	36:Sf:147:VAL:HG22	1.81	0.63
2:C1:1149:G:OP2	69:Lf:21:ARG:NH2	2.30	0.63
6:SB:168:ILE:HG12	6:SB:197:ILE:HD11	1.81	0.63
44:LG:204:ARG:HG2	44:LG:205:ALA:H	1.64	0.63
52:LO:65:ASN:HB3	52:LO:68:ARG:HG2	1.79	0.63
1:C2:325:G:H4'	16:SL:83:THR:HG21	1.80	0.63
2:C1:813:G:O2'	73:Lj:45:ARG:NH2	2.29	0.63
40:LC:20:LEU:HD12	40:LC:255:PHE:HD2	1.62	0.63
1:C2:332:U:O2'	13:SI:5:ARG:NH1	2.32	0.63
82:P0:112:GLY:N	82:P0:165:VAL:O	2.31	0.63
2:C1:1807:G:OP1	63:LZ:133:LYS:NZ	2.30	0.63
2:C1:3192:U:H3	2:C1:3200:G:H1	1.46	0.63
7:SC:35:TRP:O	7:SC:46:LYS:NZ	2.29	0.63
17:SM:59:LEU:HB3	17:SM:123:VAL:HB	1.81	0.63
37:Sg:59:ARG:HH22	37:Sg:97:GLY:HA3	1.64	0.63
39:LB:10:ARG:NH2	39:LB:263:SER:O	2.32	0.63
59:LV:10:LYS:HD3	59:LV:125:LEU:HD11	1.80	0.63
68:Le:111:ARG:HE	68:Le:115:LEU:HD13	1.63	0.63
1:C2:1556:A:H8	20:SP:40:ARG:HH21	1.46	0.62
38:LA:3:ARG:HB2	38:LA:207:VAL:HG22	1.81	0.62
82:P0:198:PRO:HD2	82:P0:201:ILE:HD12	1.81	0.62
83:CD:189:VAL:O	83:CD:193:ALA:HB2	1.99	0.62
2:C1:2294:U:OP2	59:LV:71:LYS:NZ	2.23	0.62
7:SC:237:VAL:HG23	7:SC:242:ILE:HD11	1.81	0.62
10:SF:118:LEU:HD22	10:SF:129:PRO:HB2	1.81	0.62
7:SC:63:VAL:HG13	7:SC:68:ILE:HD11	1.82	0.62
12:SH:132:PRO:HB2	12:SH:161:GLN:HE21	1.65	0.62
2:C1:1769:G:O2'	58:LU:99:LYS:NZ	2.33	0.62
3:C4:22:A:H61	41:LD:270:LYS:HE2	1.65	0.62
11:SG:70:PRO:HA	11:SG:99:GLY:HA3	1.82	0.62
37:Sg:299:GLN:HB3	37:Sg:314:GLN:HE22	1.64	0.62
2:C1:3343:G:H21	2:C1:3362:A:H2	1.47	0.62
8:SD:117:ARG:NH1	84:CS:126:ASP:OD2	2.29	0.62
39:LB:10:ARG:NH1	39:LB:11:HIS:O	2.32	0.62
8:SD:178:ARG:NH1	8:SD:179:GLN:OE1	2.31	0.62
9:SE:88:ASP:O	9:SE:100:ARG:HA	2.00	0.62
42:LE:37:GLY:HA2	42:LE:54:TYR:O	1.99	0.62
23:SS:16:ARG:NH2	23:SS:21:ASN:OD1	2.32	0.62
28:SX:130:VAL:HG23	28:SX:131:SER:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:LV:101:VAL:HG21	59:LV:109:MET:HE3	1.80	0.62
1:C2:334:G:O6	13:SI:5:ARG:NH2	2.33	0.62
39:LB:316:GLU:HG3	39:LB:318:LYS:HD3	1.80	0.62
45:LH:18:VAL:HG12	45:LH:27:VAL:HG13	1.80	0.62
58:LU:22:PRO:HB2	58:LU:28:PHE:HB2	1.82	0.62
2:C1:1757:A:OP1	58:LU:94:ARG:NH2	2.32	0.61
4:C3:156:U:OP2	44:LG:84:ARG:NH2	2.33	0.61
40:LC:256:THR:O	40:LC:260:GLN:NE2	2.32	0.61
1:C2:1474:G:H2'	1:C2:1475:A:H8	1.65	0.61
45:LH:31:ARG:HH12	45:LH:187:ILE:HD12	1.65	0.61
3:C4:107:C:OP2	46:LI:203:LYS:NZ	2.32	0.61
1:C2:1242:A:OP1	20:SP:59:LYS:NZ	2.33	0.61
2:C1:1241:U:H5''	48:LK:92:ARG:HH22	1.64	0.61
8:SD:51:ARG:HB3	8:SD:91:VAL:HG22	1.82	0.61
29:SY:11:LYS:HB2	29:SY:24:VAL:HG22	1.80	0.61
45:LH:93:VAL:HG23	45:LH:177:ASP:HA	1.82	0.61
67:Ld:77:ARG:HD2	67:Ld:89:LEU:HD13	1.82	0.61
83:CD:338:ILE:HA	83:CD:342:LEU:HD12	1.81	0.61
6:SB:229:MET:O	6:SB:232:HIS:C	2.44	0.61
12:SH:11:GLN:HG3	12:SH:13:PRO:HD2	1.82	0.61
15:SK:21:VAL:HB	15:SK:66:TYR:HB2	1.80	0.61
78:Lo:67:LYS:HG3	78:Lo:87:ARG:HE	1.63	0.61
1:C2:1229:G:N2	1:C2:1256:A:C8	2.68	0.61
37:Sg:172:ALA:HB1	37:Sg:199:ILE:HD12	1.83	0.61
51:LN:159:ARG:HB2	51:LN:164:LEU:HB2	1.81	0.61
81:L1:38:LEU:HB2	81:L1:163:LEU:HD22	1.83	0.61
81:L1:138:VAL:HG22	81:L1:147:LYS:HG2	1.82	0.61
2:C1:2193:U:H5''	2:C1:2194:G:H5'	1.83	0.61
20:SP:85:ILE:HG22	20:SP:112:LEU:HD23	1.83	0.61
11:SG:25:ARG:HE	11:SG:28:PHE:HD2	1.49	0.61
14:SJ:110:GLN:OE1	14:SJ:126:ARG:NE	2.32	0.61
63:LZ:97:SER:N	63:LZ:100:THR:OG1	2.34	0.61
28:SX:144:ARG:O	83:CD:509:LYS:NZ	2.32	0.61
83:CD:224:GLN:NE2	83:CD:336:GLU:OE2	2.31	0.61
1:C2:330:G:OP2	13:SI:172:ARG:NH1	2.34	0.60
1:C2:1262:U:H5''	83:CD:617:ARG:NH1	2.16	0.60
32:Sb:38:PRO:HD3	32:Sb:77:THR:HG22	1.83	0.60
54:LQ:62:VAL:HG23	54:LQ:66:ARG:HD2	1.83	0.60
83:CD:155:VAL:HB	83:CD:209:VAL:HG22	1.83	0.60
5:SA:41:ARG:HH21	5:SA:45:VAL:HG21	1.66	0.60
1:C2:65:A:H2	1:C2:84:A:H62	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:1671:C:OP1	55:LR:60:LYS:NZ	2.33	0.60
5:SA:175:TYR:OH	5:SA:197:ILE:O	2.19	0.60
40:LC:8:VAL:HG22	40:LC:151:VAL:HG11	1.82	0.60
51:LN:73:ARG:HG2	51:LN:75:VAL:HG23	1.83	0.60
21:SQ:109:PHE:O	21:SQ:113:ASP:HB3	2.01	0.60
38:LA:150:LEU:O	38:LA:153:GLY:N	2.31	0.60
40:LC:71:VAL:HB	40:LC:76:ARG:HH21	1.65	0.60
2:C1:687:U:OP2	49:LL:36:ARG:NH1	2.34	0.60
5:SA:36:TYR:OH	5:SA:56:LYS:NZ	2.34	0.60
1:C2:1050:G:OP1	32:Sb:70:LYS:NZ	2.35	0.60
12:SH:161:GLN:HG2	12:SH:162:ILE:HG23	1.84	0.60
29:SY:32:ARG:NH2	29:SY:34:ASN:OD1	2.35	0.60
39:LB:238:LEU:HB3	39:LB:242:THR:HG21	1.82	0.60
52:LO:157:GLU:OE1	52:LO:160:ARG:NH1	2.34	0.60
1:C2:1601:G:OP1	24:ST:86:ARG:NH2	2.35	0.60
2:C1:215:G:OP1	62:LY:12:ARG:NH1	2.34	0.60
2:C1:3163:A:N1	2:C1:3288:G:C6	2.70	0.60
5:SA:56:LYS:HD3	26:SV:82:VAL:HG21	1.82	0.60
27:SW:80:ASN:OD1	27:SW:124:LYS:NZ	2.28	0.60
2:C1:1390:A:N6	2:C1:1418:A:O2'	2.34	0.60
2:C1:3269:U:H3'	42:LE:46:ARG:HH12	1.65	0.60
4:C3:103:G:OP2	4:C3:105:A:O2'	2.20	0.60
49:LL:3:ILE:HD13	64:La:45:MET:HE3	1.84	0.60
81:L1:111:ILE:HD11	81:L1:151:VAL:HG21	1.82	0.60
83:CD:272:ALA:HA	83:CD:275:MET:HG2	1.83	0.60
2:C1:1603:A:H61	61:LX:71:THR:HG21	1.66	0.60
14:SJ:86:LEU:HG	14:SJ:90:LYS:HB3	1.83	0.60
53:LP:22:LEU:HD12	53:LP:146:ILE:HD12	1.84	0.60
8:SD:209:ILE:O	22:SR:20:TYR:OH	2.20	0.60
48:LK:32:ILE:HD13	48:LK:42:VAL:HG21	1.83	0.60
81:L1:73:ASP:OD1	81:L1:76:ARG:NH2	2.35	0.60
83:CD:30:HIS:O	83:CD:158:ASN:ND2	2.33	0.60
83:CD:835:TRP:O	83:CD:839:TYR:HB2	2.01	0.60
1:C2:513:U:H1'	14:SJ:131:GLN:OE1	2.01	0.59
2:C1:1722:U:OP1	55:LR:100:ARG:NH1	2.35	0.59
27:SW:81:VAL:O	27:SW:122:SER:OG	2.19	0.59
1:C2:762:A:OP1	14:SJ:79:ARG:NH2	2.35	0.59
2:C1:1235:U:H4'	2:C1:1236:G:H5'	1.85	0.59
2:C1:3068:U:OP2	55:LR:62:ARG:NH2	2.34	0.59
49:LL:48:PRO:HG2	71:Lh:115:LYS:HZ1	1.67	0.59
80:CE:94:ASP:HB3	81:L1:126:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:756:SER:OG	83:CD:757:GLU:N	2.30	0.59
1:C2:1537:C:H5'	1:C2:1572:G:H22	1.67	0.59
2:C1:781:G:OP1	54:LQ:151:ARG:NH1	2.35	0.59
2:C1:3149:G:O2'	39:LB:129:ALA:O	2.20	0.59
4:C3:142:C:OP1	51:LN:38:ARG:NH1	2.35	0.59
23:SS:126:ARG:HG2	23:SS:133:VAL:HA	1.84	0.59
83:CD:638:PRO:HG3	83:CD:671:THR:HG22	1.84	0.59
1:C2:1785:U:OP1	19:SO:136:ARG:NH2	2.33	0.59
2:C1:103:G:OP1	49:LL:70:ARG:NH1	2.35	0.59
13:SI:168:CYS:HB2	13:SI:184:LEU:HD11	1.83	0.59
2:C1:1953:G:N2	2:C1:2093:A:N7	2.50	0.59
8:SD:135:GLU:HG3	8:SD:187:LYS:HB3	1.85	0.59
17:SM:133:LEU:HD12	17:SM:137:MET:HE1	1.83	0.59
68:Le:98:HIS:O	68:Le:125:ARG:NH2	2.35	0.59
81:L1:43:PRO:HB3	81:L1:159:LEU:HD21	1.84	0.59
1:C2:1263:G:OP1	83:CD:617:ARG:NH2	2.35	0.59
1:C2:1488:G:H3'	1:C2:1515:A:H61	1.67	0.59
11:SG:14:LYS:HD2	11:SG:123:GLY:HA3	1.84	0.59
62:LY:32:SER:HA	62:LY:49:PRO:HA	1.84	0.59
2:C1:439:C:O2'	2:C1:494:G:N2	2.35	0.59
51:LN:31:ARG:NH1	51:LN:124:ASP:OD2	2.36	0.59
81:L1:4:ILE:HD11	81:L1:217:TYR:HB2	1.83	0.59
1:C2:1563:C:OP1	24:ST:84:LYS:NZ	2.35	0.59
40:LC:207:VAL:O	40:LC:227:THR:HA	2.02	0.59
1:C2:29:U:H2'	1:C2:30:G:H8	1.68	0.59
4:C3:63:G:O2'	71:Lh:49:LYS:NZ	2.35	0.59
37:Sg:113:VAL:HA	37:Sg:123:ILE:O	2.03	0.59
81:L1:65:ILE:HG13	81:L1:109:ALA:HB3	1.85	0.59
8:SD:99:VAL:HG23	8:SD:173:ARG:HH22	1.67	0.59
23:SS:11:PHE:HD1	23:SS:59:GLY:HA3	1.68	0.59
24:ST:137:ALA:O	24:ST:140:LEU:N	2.36	0.59
46:LI:208:ASN:HA	46:LI:211:ARG:HG2	1.85	0.59
49:LL:25:HIS:HE2	51:LN:198:SER:HG	1.49	0.59
78:Lo:47:GLN:HE22	78:Lo:54:THR:H	1.51	0.59
83:CD:732:GLU:HB2	83:CD:795:GLN:HB2	1.85	0.59
2:C1:1813:A:N7	2:C1:1814:A:N6	2.50	0.58
6:SB:127:VAL:HG21	6:SB:176:VAL:HG21	1.85	0.58
8:SD:71:LEU:HB3	15:SK:20:VAL:HG21	1.84	0.58
51:LN:35:VAL:HA	51:LN:65:ARG:HE	1.68	0.58
83:CD:412:ARG:HD3	83:CD:426:LEU:HD11	1.85	0.58
83:CD:588:LEU:HB3	83:CD:688:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:1047:A:N3	2:C1:2633:U:O2'	2.35	0.58
2:C1:3324:C:OP1	67:Ld:19:ARG:NH1	2.37	0.58
9:SE:42:LEU:HB2	9:SE:109:PHE:CD2	2.38	0.58
11:SG:98:ARG:NH1	11:SG:101:ILE:O	2.35	0.58
80:CE:83:PRO:HB3	80:CE:142:MET:HE2	1.85	0.58
83:CD:669:TRP:HB3	83:CD:710:ARG:HH12	1.68	0.58
1:C2:1263:G:H5'	83:CD:613:LYS:HE3	1.84	0.58
21:SQ:94:GLN:HA	21:SQ:102:LYS:HD2	1.85	0.58
41:LD:122:VAL:HG12	41:LD:124:GLU:H	1.67	0.58
2:C1:292:U:OP2	51:LN:68:ARG:NH2	2.37	0.58
67:Ld:6:ASP:O	67:Ld:77:ARG:NH1	2.37	0.58
1:C2:1287:A:N1	1:C2:1328:G:O2'	2.35	0.58
1:C2:1481:C:OP1	24:ST:63:ARG:NH2	2.37	0.58
2:C1:2967:A:H5''	38:LA:213:GLY:HA3	1.85	0.58
2:C1:3090:U:OP1	39:LB:270:ARG:NH2	2.34	0.58
37:Sg:91:LEU:HB3	37:Sg:101:GLN:HG3	1.85	0.58
37:Sg:209:THR:HG23	37:Sg:210:LEU:HD12	1.86	0.58
70:Lg:79:SER:OG	70:Lg:80:ARG:NH1	2.35	0.58
80:CE:43:ASP:HB3	80:CE:60:VAL:HB	1.86	0.58
2:C1:3045:G:OP1	39:LB:19:ARG:NH2	2.37	0.58
1:C2:159:U:O2	11:SG:87:ARG:NH1	2.37	0.58
11:SG:163:THR:HG22	11:SG:168:THR:HG22	1.84	0.58
52:LO:143:THR:HG21	52:LO:150:GLU:HB2	1.85	0.58
80:CE:133:ASP:OD1	80:CE:133:ASP:N	2.33	0.58
2:C1:1793:C:OP2	79:Lp:49:ARG:NH2	2.36	0.58
2:C1:1814:A:H4'	2:C1:1815:U:H5'	1.85	0.58
39:LB:113:GLU:HB2	39:LB:176:ALA:HB2	1.86	0.58
83:CD:79:SER:HB3	83:CD:98:PHE:HB2	1.86	0.58
83:CD:265:GLU:OE1	83:CD:267:LYS:HG2	2.04	0.58
83:CD:705:ILE:O	83:CD:708:THR:OG1	2.19	0.58
3:C4:15:C:O2'	41:LD:8:LYS:NZ	2.35	0.58
9:SE:122:LYS:NZ	9:SE:143:ASP:OD2	2.36	0.58
10:SF:200:ASN:O	10:SF:203:LYS:O	2.22	0.58
37:Sg:34:LEU:HG	37:Sg:73:LEU:HD11	1.85	0.58
48:LK:35:LEU:O	48:LK:67:ARG:NH1	2.36	0.58
56:LS:8:GLN:HB3	56:LS:64:ILE:HD11	1.85	0.58
79:Lp:49:ARG:HH21	79:Lp:52:ALA:HB2	1.68	0.58
1:C2:1572:G:O2'	10:SF:185:ARG:NH1	2.37	0.58
2:C1:825:U:OP2	38:LA:21:ARG:NH1	2.37	0.58
4:C3:38:U:O2'	71:Lh:83:LYS:NZ	2.31	0.58
27:SW:11:LEU:HD11	27:SW:37:PHE:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LS:96:ASP:OD1	56:LS:97:VAL:N	2.37	0.58
1:C2:190:C:N4	13:SI:137:LYS:HE2	2.19	0.57
1:C2:435:C:H5''	28:SX:50:LYS:HE2	1.86	0.57
1:C2:612:U:OP2	28:SX:5:LYS:NZ	2.36	0.57
2:C1:351:A:N6	75:Ll:37:TYR:O	2.37	0.57
2:C1:2557:A:OP1	38:LA:69:TYR:OH	2.20	0.57
2:C1:3315:G:OP1	39:LB:116:ARG:NH2	2.37	0.57
30:SZ:49:ARG:O	30:SZ:52:LYS:N	2.37	0.57
65:Lb:8:THR:HG22	65:Lb:10:HIS:H	1.68	0.57
79:Lp:52:ALA:HB1	79:Lp:68:ALA:HA	1.84	0.57
81:L1:171:ASN:H	81:L1:174:MET:HE2	1.69	0.57
2:C1:1096:U:H5''	57:LT:116:ARG:HH22	1.68	0.57
37:Sg:9:LEU:HD23	37:Sg:11:GLY:H	1.68	0.57
51:LN:66:VAL:O	51:LN:127:TYR:HA	2.03	0.57
67:Ld:55:LEU:HB2	67:Ld:95:PRO:HD3	1.85	0.57
74:Lk:24:THR:HG22	74:Lk:76:ASN:HB3	1.86	0.57
1:C2:123:G:H21	9:SE:146:THR:HG21	1.69	0.57
2:C1:2953:U:H2'	2:C1:2954:U:H2'	1.85	0.57
33:Sc:64:ARG:HH21	33:Sc:65:ARG:HE	1.51	0.57
37:Sg:183:LEU:HB2	37:Sg:186:PHE:HE1	1.68	0.57
83:CD:213:SER:OG	83:CD:218:TRP:NE1	2.37	0.57
2:C1:737:G:H5'	86:C1:3406:T1C:H432	1.86	0.57
2:C1:2703:A:N6	41:LD:28:THR:O	2.38	0.57
83:CD:119:LEU:HA	83:CD:122:THR:HG22	1.87	0.57
1:C2:1656:U:O2'	2:C1:2292:U:O2'	2.23	0.57
6:SB:160:HIS:HB3	6:SB:205:PHE:CE2	2.40	0.57
13:SI:99:ALA:N	13:SI:169:ILE:O	2.36	0.57
60:LW:6:ASP:HB3	60:LW:10:GLY:H	1.70	0.57
9:SE:255:ARG:HG3	9:SE:259:GLN:HE22	1.69	0.57
17:SM:93:ASP:OD1	17:SM:96:GLN:NE2	2.37	0.57
27:SW:3:ARG:NH1	27:SW:9:ASP:OD2	2.37	0.57
36:Sf:121:CYS:HB3	36:Sf:130:VAL:HG21	1.85	0.57
43:LF:127:LEU:HA	43:LF:130:ILE:HG22	1.86	0.57
57:LT:118:GLU:O	57:LT:121:ALA:N	2.37	0.57
7:SC:139:ILE:HG13	7:SC:218:ILE:HG23	1.87	0.57
32:Sb:20:LYS:HA	32:Sb:29:ARG:HH21	1.69	0.57
33:Sc:10:ALA:O	33:Sc:53:ILE:HA	2.04	0.57
2:C1:297:G:OP2	2:C1:297:G:N2	2.30	0.57
8:SD:28:GLU:HG3	15:SK:58:GLN:HG2	1.87	0.57
10:SF:94:THR:HG22	10:SF:114:ILE:HG13	1.87	0.57
15:SK:8:ARG:O	15:SK:12:HIS:ND1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:307:LEU:HD21	83:CD:323:VAL:HG12	1.86	0.57
83:CD:718:LEU:HG	83:CD:834:GLY:HA2	1.87	0.57
1:C2:126:A:H62	1:C2:291:G:N2	2.02	0.57
83:CD:100:ILE:HG21	83:CD:338:ILE:HD12	1.87	0.57
1:C2:1226:A:O2'	1:C2:1256:A:N1	2.37	0.57
21:SQ:49:TYR:HB3	21:SQ:53:LEU:HD23	1.86	0.57
25:SU:22:ILE:HG22	25:SU:118:VAL:HA	1.87	0.57
81:L1:10:ARG:HE	81:L1:180:VAL:HG21	1.67	0.57
2:C1:508:U:H3	2:C1:583:G:H1	1.53	0.56
14:SJ:150:LEU:O	14:SJ:154:LYS:NZ	2.33	0.56
23:SS:63:GLN:O	23:SS:66:LEU:N	2.38	0.56
45:LH:100:ASN:HB3	45:LH:115:ARG:HG3	1.87	0.56
1:C2:337:G:N2	1:C2:340:U:OP2	2.37	0.56
1:C2:1225:U:H3'	1:C2:1226:A:H8	1.70	0.56
2:C1:728:G:H5''	54:LQ:43:PRO:HB2	1.87	0.56
2:C1:3162:C:C4	2:C1:3163:A:N6	2.71	0.56
12:SH:9:LEU:HD22	12:SH:17:GLU:HG2	1.86	0.56
15:SK:5:LYS:HA	15:SK:8:ARG:HD3	1.86	0.56
29:SY:106:GLN:HG3	29:SY:110:GLN:HE22	1.70	0.56
46:LI:38:LYS:HG2	46:LI:41:ALA:HB2	1.87	0.56
72:Li:70:ARG:HD3	72:Li:84:LYS:HG2	1.87	0.56
74:Lk:26:LYS:NZ	74:Lk:28:ASN:OD1	2.37	0.56
1:C2:521:A:H1'	29:SY:34:ASN:HD22	1.70	0.56
2:C1:1057:A:H5'	43:LF:98:LYS:HE2	1.86	0.56
25:SU:69:LYS:HD3	25:SU:80:GLU:HB3	1.87	0.56
26:SV:15:ARG:NH1	26:SV:33:GLN:OE1	2.39	0.56
29:SY:10:ARG:HB2	29:SY:24:VAL:HG23	1.87	0.56
46:LI:52:LEU:HB2	46:LI:152:LEU:HD13	1.88	0.56
59:LV:15:LEU:HD23	59:LV:53:SER:HB3	1.87	0.56
63:LZ:99:GLU:O	63:LZ:106:GLN:NE2	2.38	0.56
79:Lp:50:GLY:O	79:Lp:54:ILE:HB	2.05	0.56
83:CD:114:GLU:OE2	83:CD:384:LYS:NZ	2.38	0.56
83:CD:155:VAL:O	83:CD:209:VAL:HA	2.06	0.56
83:CD:629:ASP:O	83:CD:632:LYS:N	2.38	0.56
1:C2:1591:C:H2'	1:C2:1592:A:H8	1.71	0.56
14:SJ:87:SER:HB3	14:SJ:90:LYS:HB2	1.87	0.56
20:SP:64:LYS:NZ	20:SP:90:ILE:O	2.38	0.56
29:SY:10:ARG:O	29:SY:11:LYS:C	2.48	0.56
44:LG:65:LEU:O	44:LG:68:ARG:C	2.49	0.56
54:LQ:78:ASN:O	54:LQ:136:ASN:ND2	2.39	0.56
1:C2:227:U:H2'	1:C2:228:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1316:G:OP1	22:SR:7:LYS:HG2	2.06	0.56
2:C1:2786:G:N2	64:La:58:MET:SD	2.76	0.56
20:SP:96:ILE:HG12	20:SP:116:LEU:HB3	1.87	0.56
23:SS:69:ILE:HG22	23:SS:73:MET:HE1	1.86	0.56
18:SN:39:LYS:HA	18:SN:42:ARG:HH21	1.70	0.56
1:C2:1534:G:OP1	23:SS:57:ARG:NH2	2.39	0.56
4:C3:82:U:H1'	4:C3:83:C:H2'	1.88	0.56
2:C1:3041:U:OP1	59:LV:12:ARG:NH1	2.38	0.56
9:SE:87:MET:HE1	9:SE:236:ILE:HD12	1.88	0.56
11:SG:3:LEU:HD21	11:SG:111:LEU:HD12	1.87	0.56
11:SG:64:LYS:NZ	11:SG:82:SER:O	2.38	0.56
34:Sd:36:LEU:HB3	34:Sd:38:ILE:HG12	1.86	0.56
40:LC:206:LEU:HB3	40:LC:248:VAL:HG22	1.88	0.56
42:LE:12:SER:OG	42:LE:14:ASP:OD1	2.23	0.56
1:C2:1383:G:OP1	25:SU:89:ARG:NH2	2.38	0.56
11:SG:154:ARG:NH1	11:SG:154:ARG:O	2.39	0.56
17:SM:66:VAL:HG11	17:SM:71:ILE:HD11	1.88	0.56
37:Sg:246:SER:HB3	37:Sg:251:TRP:HB2	1.87	0.56
63:LZ:88:ASP:HB3	63:LZ:121:ARG:HH12	1.71	0.56
83:CD:123:ASP:OD1	83:CD:352:ARG:NH2	2.37	0.56
83:CD:333:ALA:O	83:CD:336:GLU:HG2	2.06	0.56
2:C1:1412:G:OP1	68:Le:105:ARG:NH2	2.39	0.56
14:SJ:163:PRO:HB3	14:SJ:169:PRO:HA	1.88	0.56
16:SL:124:THR:HB	16:SL:141:LYS:HB3	1.88	0.56
21:SQ:39:VAL:HG22	21:SQ:41:PRO:HD3	1.87	0.56
12:SH:73:VAL:HG23	12:SH:74:GLN:H	1.71	0.55
44:LG:94:PHE:HB3	44:LG:189:LEU:HD11	1.86	0.55
54:LQ:170:ARG:NH1	64:La:56:VAL:O	2.37	0.55
1:C2:539:G:H1'	1:C2:540:G:H21	1.71	0.55
6:SB:27:LYS:HD3	6:SB:47:LEU:HD13	1.88	0.55
49:LL:141:ALA:HA	49:LL:144:THR:HB	1.87	0.55
78:Lo:73:GLU:HG2	78:Lo:80:ARG:HG2	1.87	0.55
81:L1:198:TRP:HA	81:L1:201:VAL:HG22	1.89	0.55
83:CD:283:ARG:HH11	83:CD:299:LEU:HG	1.70	0.55
2:C1:431:U:OP1	69:Lf:65:ARG:NH1	2.39	0.55
2:C1:824:C:H5''	38:LA:21:ARG:HG3	1.89	0.55
2:C1:3358:U:H2'	2:C1:3359:A:H8	1.70	0.55
18:SN:62:GLN:HB2	18:SN:65:VAL:HG12	1.88	0.55
43:LF:102:VAL:HG12	43:LF:130:ILE:HD12	1.88	0.55
50:LM:23:ILE:O	50:LM:30:GLY:N	2.38	0.55
63:LZ:98:THR:HA	63:LZ:101:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Lf:52:VAL:HG22	69:Lf:66:VAL:HG12	1.88	0.55
1:C2:884:A:H2'	1:C2:885:G:C8	2.42	0.55
1:C2:1474:G:H2'	1:C2:1475:A:C8	2.41	0.55
27:SW:106:THR:HG22	27:SW:108:ALA:H	1.71	0.55
46:LI:43:VAL:O	46:LI:171:TRP:NE1	2.40	0.55
46:LI:54:SER:HB2	46:LI:135:ILE:HD11	1.88	0.55
69:Lf:13:HIS:O	69:Lf:95:GLY:N	2.38	0.55
1:C2:354:C:H5''	13:SI:16:ALA:HB2	1.89	0.55
1:C2:434:G:N1	1:C2:437:A:OP2	2.37	0.55
2:C1:912:G:OP2	38:LA:9:ARG:NH2	2.40	0.55
2:C1:2572:C:O2'	2:C1:2573:G:O4'	2.23	0.55
9:SE:246:LEU:HD12	9:SE:250:GLU:HG3	1.89	0.55
53:LP:109:ALA:HA	53:LP:112:LEU:HG	1.88	0.55
82:P0:73:PHE:HA	82:P0:76:LEU:HB2	1.89	0.55
2:C1:3016:A:H2'	2:C1:3017:A:H8	1.71	0.55
21:SQ:13:LYS:HG3	21:SQ:14:LYS:H	1.71	0.55
46:LI:59:GLN:HE22	46:LI:97:LEU:HD21	1.72	0.55
1:C2:1390:U:OP2	22:SR:49:LYS:NZ	2.40	0.55
2:C1:3379:C:H4'	39:LB:315:GLY:HA2	1.87	0.55
3:C4:28:C:OP1	47:LJ:137:ARG:NH1	2.33	0.55
6:SB:144:ARG:HD3	6:SB:208:GLN:HB3	1.88	0.55
1:C2:17:C:O2'	1:C2:1137:A:N1	2.40	0.55
2:C1:3308:C:O2'	53:LP:69:ARG:O	2.23	0.55
7:SC:113:LEU:HD11	7:SC:211:LEU:HB3	1.89	0.55
41:LD:240:TYR:O	41:LD:244:HIS:ND1	2.40	0.55
53:LP:170:SER:HA	53:LP:173:ARG:HE	1.72	0.55
81:L1:29:LEU:HD11	81:L1:171:ASN:HB3	1.88	0.55
1:C2:1273:G:H4'	1:C2:1274:C:H5'	1.89	0.55
1:C2:1365:C:O3'	21:SQ:30:LYS:NZ	2.40	0.55
2:C1:943:U:H3'	64:La:13:GLY:HA2	1.89	0.55
2:C1:3070:A:OP1	55:LR:62:ARG:NH1	2.38	0.55
10:SF:77:TYR:OH	21:SQ:114:ARG:NH1	2.40	0.55
37:Sg:178:VAL:HB	37:Sg:192:PHE:HB2	1.87	0.55
42:LE:42:LEU:O	42:LE:49:GLY:N	2.40	0.55
53:LP:122:ALA:HB3	53:LP:143:PRO:HB2	1.89	0.55
74:Lk:12:LEU:HB3	74:Lk:16:ARG:HH12	1.71	0.55
1:C2:1231:U:H3	1:C2:1254:U:H3	1.54	0.55
2:C1:2880:U:OP1	59:LV:47:ASN:ND2	2.40	0.55
6:SB:71:ALA:HB2	6:SB:80:SER:HA	1.89	0.55
23:SS:92:ILE:HG23	23:SS:93:THR:HG22	1.88	0.55
47:LJ:36:VAL:HG22	47:LJ:120:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:209:U:H2'	1:C2:210:A:C8	2.41	0.54
1:C2:333:A:N7	13:SI:49:ARG:HD3	2.22	0.54
11:SG:50:PHE:CE1	11:SG:113:ILE:HG12	2.42	0.54
26:SV:9:VAL:HG12	26:SV:10:GLU:H	1.72	0.54
55:LR:31:GLU:HA	55:LR:34:GLN:HB2	1.88	0.54
59:LV:54:LEU:HD21	59:LV:119:GLY:HA3	1.89	0.54
1:C2:930:A:N3	6:SB:111:ARG:NH1	2.55	0.54
9:SE:153:ASN:O	9:SE:174:LYS:NZ	2.29	0.54
55:LR:105:LEU:HD13	55:LR:135:LYS:HZ2	1.71	0.54
64:La:17:ALA:O	64:La:19:LYS:N	2.40	0.54
2:C1:361:A:OP1	73:Lj:24:ARG:NH1	2.39	0.54
44:LG:171:LYS:NZ	44:LG:223:ALA:O	2.40	0.54
49:LL:91:ARG:NH1	49:LL:97:VAL:O	2.40	0.54
60:LW:4:GLU:O	60:LW:12:LYS:CA	2.31	0.54
83:CD:147:LEU:O	83:CD:150:ARG:NH1	2.41	0.54
1:C2:333:A:H2'	1:C2:334:G:C8	2.42	0.54
2:C1:294:U:OP2	51:LN:15:GLN:NE2	2.40	0.54
8:SD:57:ASP:O	8:SD:65:ARG:NH2	2.41	0.54
23:SS:49:LYS:NZ	23:SS:81:ILE:HG13	2.21	0.54
59:LV:15:LEU:HD13	59:LV:51:ALA:HB3	1.89	0.54
62:LY:35:LEU:HD23	62:LY:39:LEU:HB3	1.88	0.54
1:C2:231:U:O2	1:C2:234:G:O6	2.25	0.54
2:C1:3310:A:OP1	53:LP:74:LYS:NZ	2.40	0.54
40:LC:193:LYS:HA	40:LC:198:ARG:HA	1.90	0.54
45:LH:57:VAL:HG22	45:LH:68:LEU:HD22	1.89	0.54
1:C2:895:G:H21	19:SO:38:THR:HG21	1.71	0.54
1:C2:1098:U:OP1	7:SC:168:ARG:NE	2.38	0.54
1:C2:1380:U:O2'	1:C2:1516:A:N1	2.34	0.54
2:C1:216:G:OP1	62:LY:16:ARG:NH1	2.39	0.54
2:C1:2514:U:OP1	44:LG:68:ARG:NE	2.40	0.54
2:C1:2573:G:H2'	2:C1:2574:G:C8	2.42	0.54
11:SG:161:GLU:HA	11:SG:170:THR:HA	1.88	0.54
37:Sg:167:VAL:HB	37:Sg:183:LEU:HD21	1.89	0.54
42:LE:172:HIS:HD2	42:LE:173:MET:HE2	1.72	0.54
56:LS:130:GLU:HG2	56:LS:131:LYS:HG2	1.87	0.54
64:La:44:ASN:O	64:La:47:LYS:O	2.25	0.54
83:CD:81:MET:O	83:CD:96:ASN:ND2	2.38	0.54
83:CD:385:MET:HG3	83:CD:394:PHE:HD2	1.72	0.54
83:CD:545:LEU:HA	83:CD:549:HIS:HB2	1.90	0.54
2:C1:3276:G:O6	53:LP:171:ARG:NH2	2.40	0.54
44:LG:132:VAL:HG11	44:LG:189:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:204:PRO:HG3	83:CD:209:VAL:HB	1.89	0.54
10:SF:61:TYR:OH	33:Sc:52:ASP:OD2	2.26	0.54
29:SY:29:HIS:O	29:SY:67:GLY:CA	2.53	0.54
80:CE:133:ASP:OD2	81:L1:122:ARG:NE	2.38	0.54
83:CD:81:MET:HE2	83:CD:85:ASP:HB3	1.90	0.54
1:C2:428:A:N3	1:C2:440:U:O2'	2.36	0.54
2:C1:63:A:H5''	51:LN:174:ILE:HG21	1.90	0.54
4:C3:75:G:H2'	4:C3:76:C:C6	2.42	0.54
35:Se:55:ARG:HE	35:Se:56:MET:N	2.01	0.54
49:LL:47:ALA:O	49:LL:49:ARG:N	2.40	0.54
51:LN:115:VAL:HA	51:LN:134:LEU:HD23	1.90	0.54
83:CD:754:VAL:HA	83:CD:770:ALA:HA	1.90	0.54
2:C1:1480:G:O2'	2:C1:1871:U:O4	2.21	0.54
2:C1:2617:U:O2'	46:LI:116:ARG:NH2	2.41	0.54
10:SF:117:THR:HG21	10:SF:194:LEU:HD23	1.90	0.54
10:SF:143:ARG:NH2	33:Sc:55:VAL:HG22	2.22	0.54
14:SJ:107:ARG:NH1	14:SJ:153:GLU:OE2	2.40	0.54
14:SJ:161:THR:HG22	14:SJ:162:SER:H	1.73	0.54
47:LJ:32:ARG:HG2	47:LJ:120:ILE:HA	1.89	0.54
56:LS:13:ARG:NH1	56:LS:50:LYS:O	2.41	0.54
83:CD:74:ALA:HB1	83:CD:101:ASN:OD1	2.08	0.54
1:C2:953:G:H2'	1:C2:954:G:H8	1.73	0.53
4:C3:75:G:OP2	62:LY:74:TYR:OH	2.24	0.53
12:SH:70:PHE:O	12:SH:74:GLN:HB2	2.07	0.53
14:SJ:135:ALA:HA	14:SJ:140:ILE:HA	1.88	0.53
51:LN:68:ARG:CB	51:LN:126:THR:O	2.57	0.53
2:C1:515:C:H2'	2:C1:516:A:H8	1.73	0.53
2:C1:2768:U:H2'	2:C1:2769:A:H8	1.72	0.53
22:SR:26:LEU:HD21	22:SR:62:GLN:NE2	2.24	0.53
38:LA:138:GLY:HA3	38:LA:147:ARG:HB2	1.91	0.53
80:CE:63:ASP:O	80:CE:67:GLY:N	2.41	0.53
37:Sg:103:PHE:HE1	37:Sg:138:GLY:HA2	1.73	0.53
39:LB:168:LYS:O	39:LB:319:ASN:ND2	2.39	0.53
40:LC:208:VAL:HG12	40:LC:228:ALA:HB3	1.90	0.53
47:LJ:96:PHE:O	47:LJ:156:LYS:NZ	2.36	0.53
63:LZ:121:ARG:O	63:LZ:125:GLY:CA	2.49	0.53
83:CD:497:ASN:HB3	83:CD:500:ASP:HB2	1.89	0.53
1:C2:871:G:H2'	1:C2:872:G:C8	2.44	0.53
2:C1:1024:G:O6	2:C1:1027:A:N7	2.41	0.53
10:SF:89:ILE:HD12	10:SF:92:ARG:HD3	1.91	0.53
12:SH:56:LYS:HB2	12:SH:88:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SI:84:HIS:HE2	13:SI:97:THR:HG1	1.51	0.53
37:Sg:201:THR:HB	37:Sg:243:LEU:HD23	1.90	0.53
81:L1:41:TYR:OH	81:L1:195:LYS:N	2.37	0.53
83:CD:497:ASN:ND2	83:CD:500:ASP:OD2	2.41	0.53
1:C2:318:U:H4'	13:SI:11:ARG:HE	1.73	0.53
2:C1:26:A:N3	2:C1:328:U:O2'	2.40	0.53
2:C1:110:G:OP2	49:LL:73:ARG:NH2	2.42	0.53
2:C1:585:A:OP1	69:Lf:70:LYS:NZ	2.32	0.53
2:C1:608:A:OP1	40:LC:315:LYS:NZ	2.39	0.53
2:C1:2896:A:OP1	76:Lm:124:LYS:NZ	2.38	0.53
11:SG:135:PRO:HG2	11:SG:141:ILE:HD13	1.90	0.53
29:SY:11:LYS:O	29:SY:23:PHE:HA	2.08	0.53
29:SY:78:SER:OG	29:SY:81:GLU:OE2	2.26	0.53
41:LD:211:LEU:HB3	41:LD:219:PHE:HB2	1.91	0.53
53:LP:50:GLN:OE1	53:LP:56:ARG:NH2	2.40	0.53
1:C2:5:U:H2'	1:C2:6:G:H8	1.73	0.53
1:C2:1179:G:O6	23:SS:139:LYS:NZ	2.40	0.53
2:C1:2307:G:O2'	2:C1:2310:U:OP2	2.26	0.53
11:SG:31:ARG:HB3	11:SG:101:ILE:HD13	1.91	0.53
33:Sc:15:VAL:HG12	33:Sc:28:VAL:HG12	1.89	0.53
38:LA:32:LEU:HD21	38:LA:163:ARG:HD3	1.91	0.53
43:LF:48:ASN:ND2	43:LF:182:ASP:OD2	2.36	0.53
49:LL:140:SER:OG	49:LL:141:ALA:N	2.42	0.53
67:Ld:14:ILE:HD13	67:Ld:36:ILE:HD13	1.91	0.53
74:Lk:58:ASP:HB3	74:Lk:61:LYS:HG2	1.90	0.53
2:C1:1684:U:OP1	58:LU:86:LYS:NZ	2.39	0.53
2:C1:2433:U:H1'	51:LN:125:SER:HB2	1.91	0.53
10:SF:51:VAL:O	10:SF:65:ARG:NH2	2.42	0.53
26:SV:3:ASN:HD21	26:SV:7:GLN:HB3	1.73	0.53
40:LC:281:ILE:HG22	54:LQ:25:TYR:HD2	1.74	0.53
63:LZ:46:ILE:HG12	63:LZ:68:ILE:HD11	1.90	0.53
81:L1:32:VAL:N	81:L1:170:GLY:O	2.37	0.53
83:CD:73:THR:HB	83:CD:439:GLY:HA2	1.90	0.53
1:C2:868:G:H2'	1:C2:869:A:H8	1.74	0.53
2:C1:1672:U:OP1	55:LR:64:ARG:NH1	2.41	0.53
3:C4:98:C:O2'	43:LF:131:GLU:OE1	2.25	0.53
4:C3:66:A:OP1	71:Lh:10:ARG:NH2	2.41	0.53
6:SB:132:ASP:HB3	6:SB:221:PRO:HB3	1.89	0.53
9:SE:185:GLY:H	9:SE:189:LEU:HD13	1.72	0.53
21:SQ:42:GLU:OE1	21:SQ:45:ARG:NH2	2.42	0.53
37:Sg:42:LEU:HD11	37:Sg:68:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LS:81:TYR:CE1	56:LS:90:MET:HE3	2.44	0.53
2:C1:47:C:H5''	49:LL:16:LYS:HG2	1.90	0.53
2:C1:664:U:H2'	2:C1:665:A:C8	2.44	0.53
2:C1:1355:A:O2'	54:LQ:31:LYS:NZ	2.42	0.53
2:C1:2722:U:O2'	57:LT:88:ARG:O	2.24	0.53
2:C1:3092:C:O2'	2:C1:3094:A:OP2	2.21	0.53
44:LG:89:GLU:HA	44:LG:92:LYS:HE2	1.89	0.53
48:LK:82:ILE:HA	48:LK:85:LEU:HD12	1.91	0.53
1:C2:555:A:N3	1:C2:590:C:O2'	2.34	0.53
1:C2:1356:U:H2'	1:C2:1357:A:H8	1.73	0.53
2:C1:681:U:O2	2:C1:696:C:N4	2.31	0.53
2:C1:1477:A:OP1	2:C1:3075:G:O2'	2.23	0.53
37:Sg:183:LEU:HB2	37:Sg:186:PHE:CE1	2.44	0.53
41:LD:278:SER:OG	41:LD:281:GLU:OE1	2.22	0.53
50:LM:135:LEU:HD11	52:LO:178:VAL:HA	1.90	0.53
64:La:80:THR:HA	64:La:87:ARG:NH1	2.24	0.53
73:Lj:59:THR:OG1	73:Lj:64:MET:SD	2.67	0.53
78:Lo:68:VAL:HG23	78:Lo:85:LEU:HB2	1.90	0.53
81:L1:88:ASP:HA	81:L1:91:LYS:HE2	1.90	0.53
1:C2:153:G:H2'	1:C2:154:G:H8	1.73	0.52
1:C2:1199:G:N2	34:Sd:30:LEU:O	2.32	0.52
2:C1:1547:G:OP1	51:LN:108:ARG:NH2	2.40	0.52
9:SE:44:LEU:HD23	9:SE:82:TYR:HB3	1.90	0.52
41:LD:39:GLN:HE21	41:LD:43:LYS:HD2	1.74	0.52
59:LV:18:PRO:HA	59:LV:51:ALA:HA	1.91	0.52
74:Lk:5:ILE:HD11	74:Lk:11:PHE:HD2	1.74	0.52
1:C2:826:U:O4	1:C2:846:G:O6	2.27	0.52
1:C2:1656:U:HO2'	2:C1:2292:U:HO2'	1.51	0.52
2:C1:284:A:H5''	2:C1:285:A:H5'	1.91	0.52
2:C1:340:C:OP2	40:LC:195:ARG:NH1	2.34	0.52
2:C1:860:G:OP1	79:Lp:17:ARG:NH2	2.42	0.52
27:SW:11:LEU:HD12	27:SW:74:VAL:HB	1.89	0.52
33:Sc:8:THR:O	33:Sc:55:VAL:HA	2.09	0.52
48:LK:114:ARG:HA	48:LK:117:ARG:HG2	1.90	0.52
81:L1:102:LYS:O	81:L1:106:LYS:HB2	2.10	0.52
83:CD:335:LEU:O	83:CD:339:VAL:HG12	2.09	0.52
1:C2:444:C:OP2	29:SY:108:ARG:NH1	2.42	0.52
5:SA:148:ASP:H	5:SA:151:SER:HB3	1.73	0.52
47:LJ:53:THR:HG22	47:LJ:61:ARG:H	1.75	0.52
52:LO:84:LEU:HD22	52:LO:102:LEU:HD22	1.91	0.52
81:L1:89:ASP:O	81:L1:93:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1171:A:H2'	1:C2:1172:G:H8	1.74	0.52
29:SY:44:LEU:HA	29:SY:47:VAL:HG12	1.92	0.52
29:SY:103:ALA:O	29:SY:108:ARG:NH2	2.41	0.52
52:LO:126:VAL:O	56:LS:154:HIS:NE2	2.39	0.52
2:C1:1147:G:OP1	68:Le:47:ARG:NH1	2.43	0.52
2:C1:1192:C:OP1	76:Lm:113:ARG:NH2	2.43	0.52
11:SG:58:LYS:NZ	11:SG:104:PRO:O	2.42	0.52
24:ST:6:VAL:HA	24:ST:9:VAL:HG12	1.90	0.52
41:LD:75:LEU:O	41:LD:112:LYS:NZ	2.38	0.52
56:LS:1:MET:N	56:LS:32:SER:OG	2.40	0.52
79:Lp:20:SER:O	79:Lp:24:ARG:HG3	2.09	0.52
1:C2:332:U:OP2	13:SI:175:GLN:NE2	2.38	0.52
1:C2:1482:C:O2'	21:SQ:72:GLY:O	2.26	0.52
2:C1:1258:U:H1'	82:P0:38:MET:HE1	1.91	0.52
5:SA:55:GLU:HB2	26:SV:79:LEU:HD22	1.90	0.52
6:SB:135:LEU:HD11	6:SB:215:VAL:HB	1.91	0.52
20:SP:43:ARG:HH22	20:SP:47:ARG:HH11	1.57	0.52
42:LE:52:VAL:HG21	42:LE:65:ILE:HG23	1.92	0.52
52:LO:61:ALA:HA	52:LO:70:PRO:HD2	1.90	0.52
60:LW:27:LYS:NZ	60:LW:28:ILE:O	2.42	0.52
83:CD:515:ASP:OD2	83:CD:537:HIS:NE2	2.43	0.52
1:C2:1610:G:OP1	10:SF:72:HIS:NE2	2.42	0.52
2:C1:937:G:N2	2:C1:961:C:OP1	2.42	0.52
24:ST:69:LYS:HG2	24:ST:70:GLN:HG2	1.92	0.52
39:LB:41:VAL:HG12	39:LB:185:GLY:HA3	1.92	0.52
1:C2:1548:G:H1'	23:SS:89:GLN:NE2	2.25	0.52
2:C1:152:U:OP1	71:Lh:106:LYS:NZ	2.36	0.52
7:SC:235:LEU:HD12	7:SC:236:PRO:HD2	1.92	0.52
21:SQ:27:GLY:CA	21:SQ:63:ILE:O	2.57	0.52
54:LQ:82:VAL:HG22	54:LQ:102:ALA:HB3	1.91	0.52
63:LZ:33:SER:OG	63:LZ:35:SER:O	2.27	0.52
69:Lf:35:VAL:HG13	69:Lf:40:ASP:HB2	1.90	0.52
83:CD:819:VAL:O	83:CD:823:ARG:HG2	2.09	0.52
1:C2:1041:G:H2'	1:C2:1042:G:C8	2.45	0.52
1:C2:1171:A:H2'	1:C2:1172:G:C8	2.45	0.52
1:C2:1676:U:H5''	13:SI:58:LEU:HD21	1.92	0.52
2:C1:1747:G:H21	74:Lk:2:ALA:HB1	1.75	0.52
2:C1:2218:G:H2'	2:C1:2219:A:H8	1.75	0.52
39:LB:222:LYS:O	39:LB:272:TYR:N	2.40	0.52
54:LQ:38:ARG:HE	54:LQ:39:ARG:HG3	1.75	0.52
63:LZ:26:VAL:HG11	63:LZ:96:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ld:23:VAL:O	67:Ld:28:ARG:NH1	2.43	0.52
74:Lk:46:ARG:HH11	74:Lk:51:LEU:HB2	1.75	0.52
1:C2:844:A:H2'	1:C2:845:G:H8	1.75	0.52
2:C1:75:G:H5''	49:LL:58:VAL:HG13	1.92	0.52
2:C1:879:U:O2'	53:LP:135:ARG:NH1	2.43	0.52
2:C1:2374:C:N4	2:C1:2941:A:O4'	2.43	0.52
2:C1:2806:U:OP1	80:CE:49:THR:OG1	2.28	0.52
8:SD:136:VAL:HG12	8:SD:186:VAL:HG22	1.91	0.52
45:LH:91:ARG:HG2	45:LH:182:SER:HB2	1.91	0.52
73:Lj:31:LYS:HB3	73:Lj:33:THR:HG22	1.91	0.52
1:C2:1358:G:H2'	1:C2:1359:C:C6	2.45	0.51
1:C2:1642:G:H5'	77:Ln:1:MET:HB2	1.92	0.51
2:C1:297:G:O2'	72:Li:32:ALA:O	2.26	0.51
2:C1:1024:G:N2	2:C1:1026:A:OP2	2.43	0.51
9:SE:11:ARG:NH1	9:SE:21:ASP:OD1	2.40	0.51
27:SW:22:LYS:HD3	32:Sb:3:LEU:HA	1.92	0.51
1:C2:1473:U:O4	10:SF:180:ARG:NE	2.42	0.51
2:C1:119:U:H4'	2:C1:120:G:H3'	1.91	0.51
2:C1:718:G:OP2	2:C1:718:G:N2	2.41	0.51
21:SQ:115:THR:O	21:SQ:117:LEU:N	2.41	0.51
44:LG:41:GLN:OE1	44:LG:44:ARG:NH1	2.43	0.51
51:LN:39:ALA:O	51:LN:61:ILE:HB	2.11	0.51
51:LN:62:TYR:CE2	51:LN:134:LEU:HD12	2.45	0.51
67:Ld:44:MET:HG2	67:Ld:77:ARG:HH21	1.74	0.51
69:Lf:19:SER:OG	69:Lf:20:LYS:N	2.44	0.51
81:L1:93:LEU:HD11	81:L1:99:LEU:HB3	1.92	0.51
82:P0:73:PHE:HD1	82:P0:76:LEU:HD12	1.75	0.51
1:C2:1561:U:H2'	1:C2:1562:G:H8	1.76	0.51
2:C1:681:U:O4	40:LC:118:LYS:NZ	2.31	0.51
2:C1:3163:A:N6	2:C1:3288:G:O6	2.43	0.51
8:SD:31:GLU:O	8:SD:54:ARG:NH2	2.39	0.51
9:SE:71:LYS:HB2	9:SE:91:THR:HB	1.92	0.51
42:LE:136:GLU:HA	42:LE:139:LYS:HE2	1.92	0.51
49:LL:122:LYS:HG3	71:Lh:118:ILE:HG23	1.92	0.51
83:CD:201:GLN:O	83:CD:206:ARG:NH1	2.43	0.51
83:CD:663:VAL:HA	83:CD:709:MET:SD	2.51	0.51
83:CD:666:ALA:HB3	83:CD:709:MET:SD	2.50	0.51
1:C2:244:A:OP1	9:SE:155:LYS:NZ	2.43	0.51
2:C1:2736:A:OP1	57:LT:92:ARG:NH2	2.43	0.51
2:C1:3231:U:H2'	2:C1:3232:G:H8	1.75	0.51
7:SC:45:VAL:HG11	7:SC:68:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:54:TYR:O	29:SY:15:ASN:ND2	2.44	0.51
14:SJ:106:GLU:HA	14:SJ:111:THR:HG21	1.91	0.51
45:LH:51:GLN:OE1	45:LH:51:GLN:N	2.44	0.51
49:LL:74:GLY:HA3	49:LL:98:ASP:HB2	1.93	0.51
54:LQ:113:LYS:HG3	54:LQ:116:LYS:HE3	1.93	0.51
62:LY:55:GLU:HG3	62:LY:108:LYS:HE3	1.92	0.51
66:Lc:23:TYR:OH	66:Lc:83:LYS:NZ	2.43	0.51
1:C2:250:C:H2'	1:C2:251:A:H8	1.75	0.51
1:C2:1217:A:H2	15:SK:27:PHE:HB3	1.76	0.51
10:SF:72:HIS:ND1	21:SQ:79:TYR:OH	2.39	0.51
63:LZ:18:TYR:HA	63:LZ:21:LYS:HD2	1.92	0.51
1:C2:85:A:N3	1:C2:148:A:O2'	2.40	0.51
7:SC:158:THR:HG21	7:SC:221:THR:HA	1.92	0.51
20:SP:17:TYR:HB3	20:SP:20:VAL:HG23	1.93	0.51
21:SQ:13:LYS:HG2	21:SQ:76:SER:HA	1.92	0.51
23:SS:127:HIS:CD2	23:SS:133:VAL:HG11	2.45	0.51
52:LO:54:TYR:CD2	52:LO:145:VAL:HG21	2.45	0.51
83:CD:412:ARG:HG2	83:CD:428:ILE:HG13	1.92	0.51
1:C2:786:C:OP1	9:SE:240:LYS:NZ	2.43	0.51
9:SE:126:VAL:O	9:SE:157:ASN:HA	2.11	0.51
18:SN:33:VAL:HG21	18:SN:66:ILE:HD12	1.91	0.51
19:SO:84:ARG:HB3	19:SO:118:VAL:HG23	1.93	0.51
37:Sg:112:SER:O	37:Sg:124:SER:HA	2.10	0.51
44:LG:186:LEU:HB3	44:LG:195:SER:HB2	1.93	0.51
50:LM:18:GLY:HA2	50:LM:72:LEU:HD12	1.92	0.51
57:LT:39:ILE:HG12	57:LT:63:VAL:HG22	1.92	0.51
83:CD:307:LEU:HD13	83:CD:312:LYS:HA	1.93	0.51
1:C2:844:A:H2'	1:C2:845:G:C8	2.46	0.51
1:C2:1502:G:O6	24:ST:102:ARG:NH2	2.39	0.51
2:C1:595:G:OP1	43:LF:33:ARG:NH2	2.43	0.51
2:C1:1061:A:O2'	57:LT:102:ARG:NH2	2.43	0.51
2:C1:2662:G:H2'	2:C1:2663:G:H8	1.76	0.51
17:SM:130:THR:OG1	17:SM:131:ASP:N	2.44	0.51
35:Se:17:GLN:HB3	83:CD:609:ARG:HD2	1.92	0.51
72:Li:60:LEU:O	72:Li:63:ASN:C	2.54	0.51
79:Lp:46:THR:OG1	79:Lp:57:CYS:SG	2.64	0.51
1:C2:566:C:O2'	35:Se:10:ARG:NH2	2.43	0.51
1:C2:1414:U:H5''	22:SR:3:ARG:HD3	1.92	0.51
2:C1:293:C:O3'	72:Li:76:ARG:NH2	2.43	0.51
2:C1:640:U:OP1	64:La:21:ARG:NH1	2.39	0.51
2:C1:1613:A:OP1	74:Lk:2:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SA:84:ARG:NH1	5:SA:201:LEU:O	2.44	0.51
9:SE:153:ASN:OD1	11:SG:215:ARG:NH1	2.38	0.51
12:SH:101:LYS:HD2	12:SH:102:PRO:HD2	1.93	0.51
38:LA:136:ILE:HD13	38:LA:148:VAL:HG12	1.93	0.51
1:C2:1405:G:H2'	1:C2:1406:A:H8	1.75	0.51
5:SA:107:PHE:HB2	5:SA:135:GLU:HG2	1.92	0.51
13:SI:98:LYS:NZ	13:SI:170:SER:O	2.39	0.51
15:SK:50:THR:HG21	15:SK:57:THR:HB	1.92	0.51
16:SL:109:VAL:HG12	16:SL:137:PHE:HB2	1.92	0.51
19:SO:128:LYS:HE2	31:Sa:27:SER:HB3	1.93	0.51
23:SS:70:VAL:HA	23:SS:73:MET:HE2	1.93	0.51
39:LB:110:LEU:HD12	39:LB:114:VAL:HG11	1.93	0.51
44:LG:34:PHE:H	44:LG:39:ALA:HB3	1.76	0.51
44:LG:239:GLY:O	44:LG:243:GLN:HB2	2.11	0.51
56:LS:23:LYS:HA	57:LT:146:ASN:HD21	1.74	0.51
68:Le:34:LYS:O	68:Le:36:LYS:NZ	2.40	0.51
69:Lf:15:SER:OG	69:Lf:16:TYR:N	2.44	0.51
1:C2:140:A:H1'	11:SG:179:VAL:HG11	1.93	0.50
1:C2:1065:A:N3	6:SB:146:GLN:NE2	2.59	0.50
2:C1:394:G:N1	2:C1:397:A:OP2	2.44	0.50
2:C1:792:G:H5''	64:La:2:PRO:HD2	1.92	0.50
2:C1:978:G:H4'	2:C1:979:U:H5''	1.92	0.50
2:C1:1177:G:N7	69:Lf:20:LYS:NZ	2.58	0.50
2:C1:3303:G:O2'	2:C1:3305:A:N6	2.43	0.50
6:SB:229:MET:O	6:SB:232:HIS:O	2.29	0.50
39:LB:221:THR:O	39:LB:334:ARG:NH1	2.44	0.50
41:LD:80:SER:HA	41:LD:83:LEU:HD23	1.92	0.50
41:LD:148:ILE:HG22	41:LD:159:VAL:HG21	1.93	0.50
43:LF:165:ASP:HB3	43:LF:168:ILE:HG12	1.92	0.50
1:C2:1195:C:N4	21:SQ:141:SER:OG	2.44	0.50
1:C2:1591:C:H2'	1:C2:1592:A:C8	2.46	0.50
9:SE:85:GLY:N	9:SE:88:ASP:OD2	2.44	0.50
12:SH:113:PRO:HG2	12:SH:116:ARG:HD2	1.93	0.50
20:SP:75:PRO:HA	20:SP:93:VAL:HG13	1.94	0.50
83:CD:241:MET:HA	83:CD:244:LEU:HB2	1.93	0.50
83:CD:676:ILE:HD11	83:CD:722:PRO:HB2	1.92	0.50
1:C2:16:G:O6	7:SC:203:LYS:NZ	2.44	0.50
1:C2:1370:U:H4'	1:C2:1371:A:H4'	1.93	0.50
2:C1:2228:A:O5'	81:L1:199:GLN:NE2	2.40	0.50
6:SB:70:LEU:HD12	6:SB:73:LEU:HB2	1.93	0.50
8:SD:102:ALA:HB1	8:SD:173:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SM:61:VAL:HB	17:SM:121:VAL:HB	1.92	0.50
66:Lc:40:LYS:HB3	66:Lc:101:LEU:HD11	1.94	0.50
83:CD:756:SER:H	83:CD:769:LYS:HG3	1.76	0.50
2:C1:2536:A:H62	2:C1:2540:A:H62	1.59	0.50
13:SI:96:LEU:HD11	13:SI:169:ILE:HG13	1.93	0.50
23:SS:94:ASP:OD1	23:SS:94:ASP:N	2.45	0.50
58:LU:32:SER:OG	58:LU:83:TYR:OH	2.27	0.50
80:CE:22:GLN:O	80:CE:26:LEU:HG	2.11	0.50
83:CD:613:LYS:O	83:CD:617:ARG:HG2	2.12	0.50
1:C2:5:U:H2'	1:C2:6:G:C8	2.47	0.50
1:C2:699:U:O4	1:C2:739:G:O6	2.30	0.50
2:C1:286:U:O2'	51:LN:179:LYS:O	2.29	0.50
16:SL:57:LYS:HD2	16:SL:131:ILE:HG23	1.92	0.50
17:SM:43:ARG:HH22	17:SM:120:VAL:H	1.59	0.50
21:SQ:90:VAL:HG21	21:SQ:106:LYS:HD3	1.94	0.50
27:SW:37:PHE:HE1	27:SW:103:ILE:HG13	1.77	0.50
59:LV:87:ARG:O	59:LV:90:GLY:N	2.33	0.50
67:Ld:44:MET:HB3	67:Ld:77:ARG:HE	1.74	0.50
78:Lo:2:VAL:N	78:Lo:90:HIS:O	2.44	0.50
83:CD:607:ASN:C	83:CD:615:ARG:HH12	2.17	0.50
1:C2:1393:C:H2'	1:C2:1394:G:H8	1.76	0.50
2:C1:173:G:H1	2:C1:245:U:H3	1.60	0.50
2:C1:3162:C:H42	2:C1:3163:A:N6	2.06	0.50
27:SW:37:PHE:CE1	27:SW:103:ILE:HG13	2.47	0.50
40:LC:216:VAL:O	40:LC:220:ARG:HB3	2.11	0.50
40:LC:295:ILE:O	40:LC:299:ILE:HG12	2.11	0.50
57:LT:42:ILE:O	57:LT:59:GLY:N	2.45	0.50
75:Ll:26:TRP:HA	75:Ll:29:LEU:HG	1.94	0.50
81:L1:66:CYS:HB2	81:L1:107:TYR:CD2	2.47	0.50
1:C2:647:G:H22	1:C2:687:G:H1	1.60	0.50
3:C4:7:G:OP1	41:LD:33:ARG:NH1	2.45	0.50
8:SD:67:ASN:ND2	15:SK:92:ILE:O	2.45	0.50
11:SG:34:GLN:O	11:SG:51:LYS:HA	2.12	0.50
35:Se:31:LYS:HA	35:Se:35:TYR:HB2	1.94	0.50
37:Sg:201:THR:OG1	37:Sg:241:PHE:O	2.29	0.50
39:LB:348:ARG:HA	39:LB:351:LEU:HB2	1.93	0.50
72:Li:60:LEU:O	72:Li:63:ASN:O	2.30	0.50
82:P0:95:GLU:HA	82:P0:98:ASN:HB2	1.93	0.50
2:C1:656:A:H2'	2:C1:657:A:C8	2.46	0.50
2:C1:1124:U:O2'	2:C1:2635:A:OP1	2.29	0.50
2:C1:1560:G:H2'	2:C1:1561:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:3050:U:O2'	60:LW:16:GLY:O	2.30	0.50
2:C1:3289:G:H2'	2:C1:3290:G:H8	1.76	0.50
5:SA:156:VAL:O	26:SV:65:SER:OG	2.29	0.50
8:SD:136:VAL:HG23	8:SD:152:PHE:HD2	1.76	0.50
9:SE:42:LEU:HB2	9:SE:109:PHE:CE2	2.47	0.50
13:SI:36:THR:OG1	13:SI:96:LEU:O	2.25	0.50
21:SQ:31:VAL:HG13	21:SQ:36:ILE:HG22	1.93	0.50
37:Sg:151:VAL:HA	37:Sg:173:GLY:HA2	1.94	0.50
46:LI:189:GLU:HB2	46:LI:200:LEU:HB3	1.94	0.50
75:Ll:27:ILE:O	75:Ll:33:ASN:ND2	2.45	0.50
83:CD:495:VAL:HG11	83:CD:501:LEU:HA	1.94	0.50
1:C2:1097:U:O4	7:SC:201:ASN:ND2	2.45	0.50
2:C1:765:C:O2	49:LL:183:ARG:NH2	2.44	0.50
2:C1:831:G:O2'	2:C1:1864:A:N3	2.41	0.50
2:C1:1024:G:O6	2:C1:1027:A:C5	2.65	0.50
2:C1:1786:G:H2'	2:C1:1787:A:C8	2.47	0.50
5:SA:123:VAL:HG11	5:SA:133:ILE:HD11	1.94	0.50
10:SF:127:GLN:NE2	10:SF:132:VAL:HB	2.27	0.50
53:LP:121:GLN:OE1	53:LP:124:LYS:NZ	2.45	0.50
78:Lo:28:TYR:HB3	78:Lo:69:VAL:HG13	1.94	0.50
83:CD:358:GLU:H	83:CD:478:MET:HA	1.76	0.50
83:CD:450:ALA:O	83:CD:452:ASN:ND2	2.45	0.50
2:C1:2688:U:OP1	41:LD:12:TYR:OH	2.30	0.49
10:SF:42:LEU:HD22	10:SF:47:SER:HA	1.94	0.49
25:SU:63:LEU:HB2	25:SU:84:MET:HB3	1.94	0.49
39:LB:66:LYS:O	39:LB:70:ARG:NH2	2.44	0.49
74:Lk:14:LEU:HD11	74:Lk:52:TYR:CG	2.47	0.49
81:L1:85:MET:HE1	81:L1:89:ASP:OD2	2.12	0.49
2:C1:1699:A:O2'	74:Lk:3:ARG:NH1	2.46	0.49
24:ST:135:ILE:HG23	24:ST:138:GLN:HE21	1.77	0.49
39:LB:219:ALA:HB2	39:LB:336:VAL:HG23	1.93	0.49
40:LC:3:ARG:HH12	40:LC:24:ALA:HB2	1.77	0.49
47:LJ:64:LYS:HZ1	84:CS:26:VAL:HG22	1.77	0.49
48:LK:11:LYS:HG3	48:LK:64:ILE:HB	1.94	0.49
49:LL:4:SER:O	64:La:44:ASN:ND2	2.45	0.49
56:LS:77:VAL:HG12	56:LS:126:VAL:HG23	1.93	0.49
1:C2:153:G:OP2	29:SY:131:ARG:NH1	2.44	0.49
1:C2:781:U:H6	1:C2:782:U:H3	1.58	0.49
1:C2:800:U:H2'	1:C2:801:G:H8	1.78	0.49
2:C1:1054:A:H5''	2:C1:2637:A:H61	1.77	0.49
2:C1:1280:C:H2'	2:C1:1281:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:1333:C:OP1	54:LQ:2:GLY:N	2.45	0.49
5:SA:117:GLU:HG3	7:SC:40:LYS:HE2	1.95	0.49
9:SE:21:ASP:OD1	9:SE:21:ASP:N	2.45	0.49
32:Sb:34:ASP:HB2	32:Sb:43:ILE:HD11	1.94	0.49
41:LD:41:LYS:NZ	57:LT:32:LYS:O	2.46	0.49
41:LD:120:LYS:O	41:LD:248:ARG:NH1	2.45	0.49
44:LG:78:PHE:O	44:LG:79:GLN:HG3	2.12	0.49
2:C1:201:A:H2'	2:C1:202:G:H8	1.78	0.49
2:C1:917:A:H62	38:LA:3:ARG:HH12	1.59	0.49
2:C1:1382:G:OP2	40:LC:188:ARG:NH1	2.45	0.49
8:SD:9:ARG:HA	8:SD:12:VAL:HG12	1.95	0.49
29:SY:59:GLY:O	29:SY:71:GLY:HA2	2.12	0.49
46:LI:153:ARG:NH2	46:LI:157:TYR:OH	2.45	0.49
52:LO:4:GLU:OE2	52:LO:5:PRO:HD2	2.12	0.49
1:C2:273:G:H1	1:C2:283:U:H3	1.60	0.49
1:C2:1263:G:OP1	83:CD:631:ARG:NH1	2.46	0.49
1:C2:1794:A:H1'	31:Sa:79:ILE:HD13	1.95	0.49
2:C1:1940:G:O2'	2:C1:3362:A:O2'	2.27	0.49
2:C1:2218:G:H2'	2:C1:2219:A:C8	2.48	0.49
2:C1:2507:C:H2'	2:C1:2508:U:C6	2.48	0.49
14:SJ:59:LEU:HD21	14:SJ:72:GLU:HG3	1.94	0.49
27:SW:25:VAL:HG22	27:SW:63:VAL:HB	1.94	0.49
43:LF:187:GLU:O	43:LF:191:VAL:HA	2.13	0.49
49:LL:165:SER:OG	64:La:135:GLU:OE2	2.30	0.49
56:LS:16:THR:HG23	56:LS:18:SER:H	1.76	0.49
59:LV:38:ALA:HB3	59:LV:59:MET:HB2	1.94	0.49
83:CD:399:ARG:HA	83:CD:453:ILE:HA	1.95	0.49
1:C2:260:U:H5'	1:C2:261:U:H5''	1.95	0.49
1:C2:1229:G:C2	1:C2:1256:A:N7	2.81	0.49
1:C2:1363:U:H3'	1:C2:1364:G:H8	1.78	0.49
11:SG:7:TYR:HB2	11:SG:113:ILE:HD12	1.94	0.49
17:SM:98:GLY:O	17:SM:101:ALA:C	2.55	0.49
37:Sg:170:ILE:HD11	37:Sg:204:ALA:HB2	1.94	0.49
44:LG:161:GLU:OE1	51:LN:11:GLN:NE2	2.45	0.49
54:LQ:148:GLU:HA	54:LQ:151:ARG:HG2	1.94	0.49
57:LT:73:GLY:HA2	57:LT:89:LEU:O	2.12	0.49
2:C1:217:U:O2	62:LY:103:LYS:NZ	2.41	0.49
2:C1:1280:C:H2'	2:C1:1281:G:C8	2.48	0.49
2:C1:1785:U:H2'	2:C1:1786:G:C8	2.47	0.49
8:SD:109:LEU:HD12	8:SD:184:ILE:HD11	1.93	0.49
11:SG:33:GLY:N	11:SG:52:ILE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SH:23:ALA:HB2	12:SH:84:LYS:HE2	1.94	0.49
12:SH:62:VAL:HG12	12:SH:64:VAL:H	1.76	0.49
15:SK:2:LEU:O	15:SK:8:ARG:NH2	2.46	0.49
15:SK:16:PHE:CE2	15:SK:76:LEU:HG	2.48	0.49
21:SQ:77:GLN:O	21:SQ:81:ILE:HG12	2.11	0.49
43:LF:88:ARG:HB2	43:LF:108:LEU:HB3	1.94	0.49
50:LM:13:ARG:HH11	50:LM:67:PRO:HD3	1.77	0.49
57:LT:91:LEU:HD12	57:LT:96:ILE:HD11	1.95	0.49
81:L1:59:PRO:HA	81:L1:170:GLY:HA2	1.94	0.49
81:L1:66:CYS:HB2	81:L1:107:TYR:HD2	1.78	0.49
1:C2:1035:G:OP1	18:SN:2:GLY:N	2.46	0.49
1:C2:1524:A:H2'	1:C2:1525:A:C8	2.48	0.49
2:C1:1579:C:H2'	2:C1:1580:A:C8	2.48	0.49
9:SE:107:GLY:HA2	9:SE:189:LEU:HG	1.95	0.49
28:SX:95:PHE:O	28:SX:142:LYS:NZ	2.45	0.49
40:LC:210:ALA:HB1	40:LC:257:LYS:HE2	1.93	0.49
44:LG:99:PRO:HG3	44:LG:132:VAL:HG22	1.94	0.49
51:LN:73:ARG:NH2	51:LN:88:GLY:O	2.45	0.49
71:Lh:101:THR:HG23	71:Lh:104:GLN:H	1.78	0.49
1:C2:1030:A:OP2	31:Sa:8:ASN:ND2	2.42	0.49
1:C2:1237:G:H2'	1:C2:1238:A:H8	1.78	0.49
2:C1:1019:G:H22	2:C1:1033:U:H3	1.59	0.49
2:C1:1404:G:N2	2:C1:1407:A:OP2	2.36	0.49
2:C1:2137:U:OP2	2:C1:2142:A:N6	2.34	0.49
2:C1:2960:C:H2'	2:C1:2961:G:C8	2.48	0.49
5:SA:84:ARG:NH2	22:SR:82:ASP:O	2.45	0.49
13:SI:48:THR:HG21	13:SI:54:LYS:HD3	1.95	0.49
14:SJ:96:VAL:HA	14:SJ:99:LEU:HD23	1.95	0.49
21:SQ:14:LYS:O	21:SQ:123:ARG:NH1	2.46	0.49
38:LA:206:PRO:HD3	38:LA:213:GLY:HA2	1.95	0.49
42:LE:14:ASP:OD1	42:LE:14:ASP:N	2.45	0.49
66:Lc:16:LEU:HB3	66:Lc:98:SER:HB2	1.94	0.49
1:C2:159:U:H1'	11:SG:87:ARG:HH12	1.77	0.49
1:C2:1039:A:O2'	1:C2:1040:G:O5'	2.30	0.49
1:C2:1222:C:H2'	1:C2:1223:A:H8	1.78	0.49
1:C2:1488:G:O2'	1:C2:1494:C:O2	2.23	0.49
2:C1:196:G:N1	2:C1:199:A:OP2	2.45	0.49
2:C1:2662:G:H2'	2:C1:2663:G:C8	2.47	0.49
2:C1:3175:U:OP1	69:Lf:10:LYS:NZ	2.35	0.49
4:C3:51:G:O6	75:Ll:30:ARG:NH2	2.41	0.49
16:SL:102:LYS:O	28:SX:13:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:LL:48:PRO:HB3	49:LL:137:GLN:HB2	1.94	0.49
58:LU:18:ASP:HB2	58:LU:104:ARG:HG2	1.94	0.49
69:Lf:42:GLN:HA	69:Lf:45:LEU:HG	1.95	0.49
83:CD:730:LEU:HB2	83:CD:799:ASP:HB2	1.95	0.49
1:C2:190:C:H1'	1:C2:191:C:H5'	1.95	0.48
2:C1:1239:C:OP1	48:LK:90:ARG:NH1	2.35	0.48
2:C1:1514:G:H1'	75:Ll:44:TRP:HZ2	1.77	0.48
2:C1:3252:G:H2'	2:C1:3253:G:C8	2.48	0.48
9:SE:181:VAL:HG21	9:SE:195:ILE:HD11	1.95	0.48
23:SS:116:LEU:HA	23:SS:119:ILE:HG12	1.95	0.48
24:ST:97:SER:HB3	24:ST:100:ILE:HG12	1.95	0.48
37:Sg:258:THR:HG22	37:Sg:275:ARG:NH1	2.28	0.48
38:LA:45:VAL:HB	38:LA:61:VAL:HG22	1.94	0.48
41:LD:34:LYS:HA	57:LT:27:LEU:HD11	1.93	0.48
47:LJ:75:LYS:HA	47:LJ:78:GLU:HG3	1.95	0.48
47:LJ:150:ASN:OD1	47:LJ:153:LYS:NZ	2.39	0.48
48:LK:48:LYS:HA	48:LK:51:LYS:HE2	1.94	0.48
64:La:71:PRO:HB2	64:La:109:TYR:HD1	1.78	0.48
1:C2:1301:U:H5'	7:SC:88:LYS:HD2	1.94	0.48
1:C2:1466:G:O2'	1:C2:1602:C:OP1	2.31	0.48
1:C2:1552:U:OP2	20:SP:43:ARG:NH2	2.46	0.48
2:C1:2724:U:OP2	2:C1:2726:C:N4	2.46	0.48
2:C1:2836:C:H5	2:C1:2852:C:H42	1.60	0.48
4:C3:8:C:H2'	4:C3:9:A:C8	2.48	0.48
28:SX:53:VAL:HA	28:SX:74:VAL:HG12	1.95	0.48
28:SX:59:ILE:HD12	28:SX:118:PRO:HD2	1.94	0.48
32:Sb:40:CYS:SG	32:Sb:41:LEU:N	2.75	0.48
38:LA:70:ARG:HH21	38:LA:72:ARG:HD3	1.78	0.48
44:LG:162:LEU:HD23	51:LN:7:LEU:HD21	1.94	0.48
69:Lf:38:PRO:HB3	69:Lf:74:THR:HG21	1.95	0.48
1:C2:591:A:H2'	1:C2:592:A:C8	2.49	0.48
1:C2:1156:C:H2'	1:C2:1157:A:C8	2.49	0.48
2:C1:1194:G:H2'	2:C1:1195:A:C8	2.47	0.48
2:C1:3178:A:H2'	52:LO:115:LYS:HD2	1.94	0.48
24:ST:112:GLY:O	24:ST:127:ASN:ND2	2.46	0.48
37:Sg:258:THR:HG22	37:Sg:275:ARG:HH12	1.78	0.48
39:LB:212:ASN:HD21	39:LB:354:VAL:H	1.60	0.48
40:LC:328:ASN:ND2	43:LF:149:TYR:OH	2.46	0.48
49:LL:75:PHE:CD2	49:LL:95:ILE:HG23	2.48	0.48
53:LP:55:GLN:O	53:LP:72:GLN:NE2	2.45	0.48
64:La:94:ALA:HB2	64:La:121:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ld:16:LEU:HA	67:Ld:19:ARG:HB2	1.94	0.48
1:C2:431:C:H4'	83:CD:391:LYS:HB2	1.94	0.48
1:C2:531:C:O2	29:SY:62:THR:OG1	2.31	0.48
1:C2:1311:U:O3'	22:SR:2:GLY:N	2.46	0.48
1:C2:1597:A:C8	34:Sd:14:TYR:HD2	2.31	0.48
2:C1:2675:C:O3'	84:CS:62:ARG:NH2	2.47	0.48
2:C1:3016:A:H2'	2:C1:3017:A:C8	2.48	0.48
39:LB:35:ASP:OD2	39:LB:37:ARG:NH1	2.46	0.48
46:LI:76:MET:HE1	46:LI:148:VAL:HA	1.96	0.48
61:LX:135:ILE:O	61:LX:139:ILE:HD12	2.14	0.48
1:C2:480:G:H1	1:C2:508:U:H3	1.61	0.48
2:C1:7:C:H5''	44:LG:193:LYS:HG2	1.95	0.48
2:C1:1555:U:H3	2:C1:1557:A:H62	1.61	0.48
2:C1:2736:A:H5''	57:LT:92:ARG:HE	1.77	0.48
39:LB:189:SER:OG	39:LB:190:GLU:OE1	2.30	0.48
51:LN:35:VAL:O	51:LN:64:VAL:HA	2.13	0.48
57:LT:28:SER:O	57:LT:32:LYS:HG3	2.14	0.48
1:C2:1040:G:H5'	5:SA:31:VAL:HG11	1.94	0.48
2:C1:266:A:N6	72:Li:30:LYS:HA	2.28	0.48
2:C1:1463:U:H3	2:C1:1467:A:H62	1.61	0.48
2:C1:2542:U:H3	2:C1:2544:U:H5	1.61	0.48
3:C4:107:C:H2'	3:C4:108:A:H8	1.77	0.48
8:SD:164:VAL:HG22	8:SD:168:ILE:HD12	1.95	0.48
11:SG:185:GLN:OE1	11:SG:188:ARG:NH2	2.47	0.48
21:SQ:55:VAL:HG22	21:SQ:105:LEU:HD12	1.95	0.48
22:SR:46:LEU:O	22:SR:50:ILE:HG12	2.14	0.48
37:Sg:13:LEU:HB3	37:Sg:45:TRP:CZ3	2.48	0.48
38:LA:60:LYS:HD2	38:LA:73:GLU:HG2	1.96	0.48
48:LK:30:PRO:HG3	83:CD:759:GLN:HE21	1.78	0.48
56:LS:72:VAL:HA	56:LS:97:VAL:HA	1.96	0.48
67:Ld:24:SER:HB2	67:Ld:27:LYS:HE2	1.95	0.48
81:L1:187:VAL:HG22	81:L1:204:LEU:HD11	1.95	0.48
83:CD:564:ARG:HG2	83:CD:682:ARG:HB2	1.95	0.48
83:CD:586:ILE:HG23	83:CD:688:ILE:HD11	1.94	0.48
1:C2:472:U:O2'	1:C2:769:A:N3	2.43	0.48
1:C2:1561:U:H4'	1:C2:1599:C:H4'	1.95	0.48
2:C1:296:A:N3	2:C1:299:G:O2'	2.46	0.48
2:C1:1027:A:O2'	2:C1:1029:G:OP1	2.32	0.48
2:C1:1420:C:OP2	40:LC:193:LYS:NZ	2.45	0.48
2:C1:2943:G:N2	39:LB:251:CYS:SG	2.86	0.48
6:SB:176:VAL:HA	6:SB:184:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SD:135:GLU:OE1	8:SD:137:VAL:HG23	2.14	0.48
14:SJ:27:GLU:HG3	14:SJ:42:ILE:HG21	1.95	0.48
21:SQ:26:LYS:HE2	21:SQ:28:LEU:HD23	1.96	0.48
21:SQ:93:HIS:HA	21:SQ:97:VAL:HG22	1.96	0.48
26:SV:1:MET:HE2	26:SV:10:GLU:HG2	1.95	0.48
37:Sg:152:SER:N	37:Sg:172:ALA:O	2.46	0.48
40:LC:338:LYS:HE3	40:LC:338:LYS:HB3	1.66	0.48
49:LL:10:LEU:HD23	54:LQ:166:LEU:HD11	1.96	0.48
49:LL:138:VAL:HG22	49:LL:140:SER:H	1.78	0.48
64:La:75:LEU:HD11	64:La:134:ALA:HA	1.94	0.48
83:CD:36:THR:HG22	83:CD:102:LEU:HD21	1.96	0.48
5:SA:18:LEU:HB3	22:SR:100:LEU:HD11	1.95	0.48
8:SD:42:THR:OG1	8:SD:45:LYS:O	2.32	0.48
9:SE:147:ILE:HG21	9:SE:169:ILE:HG12	1.95	0.48
28:SX:70:LYS:HB3	28:SX:93:LEU:HD22	1.96	0.48
48:LK:20:GLY:HA3	48:LK:54:LYS:HG3	1.95	0.48
53:LP:116:HIS:HB3	53:LP:149:VAL:HG22	1.94	0.48
83:CD:27:HIS:CD2	83:CD:138:GLN:HB2	2.49	0.48
83:CD:154:VAL:HB	83:CD:342:LEU:HD11	1.94	0.48
84:CS:67:GLY:O	84:CS:71:ASN:ND2	2.47	0.48
1:C2:1405:G:H2'	1:C2:1406:A:C8	2.49	0.48
6:SB:183:GLN:HA	6:SB:186:SER:HB2	1.96	0.48
37:Sg:19:TRP:HB2	37:Sg:38:ARG:HG3	1.95	0.48
82:P0:130:PRO:HD2	83:CD:187:VAL:HG12	1.96	0.48
83:CD:276:PHE:HB2	83:CD:277:ILE:HD12	1.94	0.48
83:CD:311:GLU:HB3	83:CD:322:VAL:HG21	1.95	0.48
1:C2:1357:A:H2'	1:C2:1358:G:C8	2.48	0.48
1:C2:1592:A:H2'	1:C2:1593:A:H8	1.78	0.48
2:C1:1682:U:O4	58:LU:90:ARG:NH1	2.47	0.48
6:SB:34:ALA:O	6:SB:41:ARG:NH1	2.46	0.48
7:SC:50:ILE:HG21	7:SC:56:ILE:HD11	1.96	0.48
7:SC:67:GLN:HA	7:SC:70:ASP:HB3	1.96	0.48
9:SE:103:TYR:O	9:SE:182:TYR:OH	2.32	0.48
12:SH:64:VAL:HG23	12:SH:67:LEU:HD23	1.95	0.48
15:SK:35:ILE:HG22	15:SK:37:THR:H	1.78	0.48
17:SM:64:SER:HB3	17:SM:92:ALA:HA	1.95	0.48
21:SQ:98:ASP:O	21:SQ:101:SER:OG	2.23	0.48
41:LD:80:SER:OG	41:LD:92:LEU:O	2.27	0.48
2:C1:1329:U:OP1	69:Lf:17:GLN:NE2	2.46	0.47
2:C1:1799:A:H2'	2:C1:1800:A:C8	2.48	0.47
2:C1:1899:G:O2'	2:C1:2334:U:O4	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:2163:C:H1'	38:LA:11:GLY:HA3	1.96	0.47
2:C1:3163:A:C6	2:C1:3288:G:C6	3.02	0.47
2:C1:3268:A:OP1	42:LE:46:ARG:NH2	2.47	0.47
21:SQ:99:GLU:HA	21:SQ:102:LYS:HG2	1.96	0.47
37:Sg:255:ALA:HB1	37:Sg:289:ALA:HB1	1.95	0.47
40:LC:350:LYS:HD3	40:LC:351:PRO:HD2	1.96	0.47
43:LF:74:SER:OG	57:LT:141:VAL:O	2.19	0.47
46:LI:206:LEU:O	46:LI:210:ILE:HG12	2.14	0.47
60:LW:6:ASP:OD2	60:LW:9:SER:N	2.31	0.47
72:Li:58:ILE:HA	72:Li:61:ILE:HG12	1.95	0.47
83:CD:804:LEU:HD23	83:CD:806:SER:H	1.78	0.47
1:C2:78:A:H1'	11:SG:175:ILE:HD13	1.96	0.47
1:C2:460:A:H3'	1:C2:461:G:H8	1.79	0.47
8:SD:124:ARG:HH11	84:CS:127:ALA:HB3	1.78	0.47
10:SF:31:GLU:OE2	10:SF:35:GLN:NE2	2.40	0.47
21:SQ:132:LYS:HG3	21:SQ:138:PHE:HE1	1.79	0.47
46:LI:48:LEU:HD11	46:LI:167:LEU:HD12	1.95	0.47
82:P0:57:THR:HG22	82:P0:60:ARG:HH22	1.79	0.47
1:C2:1672:G:H2'	1:C2:1673:G:C8	2.50	0.47
2:C1:528:U:H2'	2:C1:529:A:C8	2.49	0.47
2:C1:1481:A:N6	2:C1:1872:C:O2	2.47	0.47
2:C1:2418:G:H22	80:CE:71:GLU:HG2	1.79	0.47
2:C1:2446:U:H2'	2:C1:2447:A:C8	2.50	0.47
2:C1:2769:A:H5''	78:Lo:80:ARG:HD3	1.96	0.47
8:SD:8:LYS:HG3	25:SU:63:LEU:HD11	1.95	0.47
19:SO:81:VAL:HG11	19:SO:102:LEU:HD13	1.95	0.47
24:ST:77:ASN:HB3	24:ST:95:ASP:HB3	1.96	0.47
2:C1:242:C:H2'	2:C1:243:G:H8	1.78	0.47
2:C1:1017:C:OP1	84:CS:48:ARG:NH2	2.47	0.47
2:C1:1661:G:H2'	2:C1:1662:G:C8	2.49	0.47
8:SD:38:GLU:HB2	8:SD:51:ARG:HH22	1.79	0.47
28:SX:107:PHE:CE2	28:SX:114:LYS:HG3	2.49	0.47
43:LF:121:LYS:O	43:LF:125:GLU:HG3	2.14	0.47
64:La:126:LYS:HD2	64:La:148:ILE:HD12	1.97	0.47
80:CE:63:ASP:O	80:CE:67:GLY:CA	2.62	0.47
83:CD:231:LYS:HE2	83:CD:232:LYS:HE2	1.97	0.47
83:CD:509:LYS:HE3	83:CD:513:LYS:HE2	1.96	0.47
1:C2:1275:A:O2'	8:SD:145:ALA:O	2.25	0.47
1:C2:1650:U:H2'	1:C2:1651:A:C8	2.50	0.47
1:C2:1682:U:O4	1:C2:1720:G:N2	2.48	0.47
2:C1:2700:G:H5''	57:LT:17:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28: SX:116: ASP: OD1	28: SX:116: ASP: N	2.46	0.47
30: SZ:83: LEU: O	30: SZ:86: GLU: O	2.33	0.47
37: Sg:209: THR: OG1	37: Sg:224: ASN: OD1	2.33	0.47
57: LT:136: ARG: HH11	57: LT:139: ARG: HH22	1.63	0.47
81: L1:61: PRO: O	81: L1:152: ARG: NH2	2.48	0.47
1: C2:405: C: O2'	11: SG:92: ARG: O	2.32	0.47
1: C2:1585: U: H2'	1: C2:1586: A: H8	1.80	0.47
2: C1:799: G: O2'	49: LL:18: TRP: NE1	2.47	0.47
2: C1:874: U: OP2	39: LB:241: LYS: NZ	2.47	0.47
2: C1:957: C: H1'	64: La:43: ILE: HD11	1.96	0.47
2: C1:1019: G: H1	2: C1:1033: U: H3	1.63	0.47
2: C1:3037: U: O3'	39: LB:348: ARG: NH2	2.48	0.47
11: SG:113: ILE: HD11	11: SG:124: LEU: HD13	1.97	0.47
37: Sg:195: HIS: ND1	37: Sg:197: SER: O	2.47	0.47
55: LR:10: LEU: HD22	55: LR:38: ARG: HG3	1.95	0.47
68: Le:100: ILE: O	68: Le:105: ARG: NH1	2.47	0.47
83: CD:24: VAL: HG11	83: CD:32: LYS: HD3	1.96	0.47
1: C2:486: G: N2	1: C2:501: U: O2	2.39	0.47
1: C2:890: C: H2'	1: C2:891: A: H8	1.80	0.47
1: C2:1099: U: OP1	27: SW:71: LYS: NZ	2.47	0.47
2: C1:531: G: H2'	2: C1:532: A: C8	2.50	0.47
2: C1:1233: G: H2'	2: C1:1234: G: C8	2.49	0.47
2: C1:1597: C: H5'	2: C1:1696: A: H1'	1.95	0.47
2: C1:2176: U: OP1	38: LA:54: ARG: NH2	2.48	0.47
2: C1:2467: G: H4'	81: L1:28: PHE: HE2	1.80	0.47
2: C1:3028: G: H5''	83: CD:28: VAL: HG11	1.97	0.47
3: C4:84: A: H2'	3: C4:85: G: C8	2.50	0.47
6: SB:72: ASP: OD1	19: SO:114: ARG: NH2	2.47	0.47
7: SC:52: THR: HG23	7: SC:55: GLU: H	1.80	0.47
9: SE:89: VAL: HG22	9: SE:100: ARG: HE	1.79	0.47
19: SO:84: ARG: HD2	19: SO:118: VAL: HG23	1.97	0.47
23: SS:108: LYS: HA	23: SS:111: ASP: HB2	1.96	0.47
29: SY:59: GLY: O	29: SY:71: GLY: CA	2.63	0.47
38: LA:117: GLU: OE2	38: LA:163: ARG: NH2	2.44	0.47
40: LC:4: PRO: HD2	40: LC:22: LEU: HD23	1.97	0.47
40: LC:157: GLU: HG2	40: LC:209: TYR: HB2	1.95	0.47
42: LE:31: ARG: HH11	69: Lf:107: ILE: H	1.62	0.47
46: LI:134: ILE: HD11	57: LT:160: ILE: HG12	1.96	0.47
49: LL:49: ARG: HH12	71: Lh:113: GLN: NE2	2.13	0.47
71: Lh:115: LYS: HD2	71: Lh:116: TYR: N	2.29	0.47
82: P0:199: SER: HA	82: P0:202: LEU: HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:379:MET:SD	83:CD:401:PHE:HB2	2.55	0.47
83:CD:400:VAL:O	83:CD:451:GLY:N	2.48	0.47
83:CD:465:LYS:HG2	83:CD:466:THR:HG23	1.97	0.47
83:CD:733:ILE:O	83:CD:767:THR:HA	2.15	0.47
1:C2:531:C:H1'	29:SY:61:ARG:HH12	1.79	0.47
1:C2:689:G:H2'	1:C2:690:G:H8	1.79	0.47
1:C2:1476:C:H5''	24:ST:44:GLU:OE2	2.15	0.47
2:C1:138:U:H2'	2:C1:139:G:H8	1.80	0.47
3:C4:60:G:H2'	3:C4:61:G:H8	1.79	0.47
4:C3:135:G:H5''	61:LX:49:LYS:HD2	1.97	0.47
7:SC:109:GLY:HA2	7:SC:139:ILE:HG22	1.96	0.47
13:SI:163:GLY:O	13:SI:164:ARG:NH1	2.48	0.47
20:SP:40:ARG:HD2	20:SP:40:ARG:HA	1.75	0.47
55:LR:91:SER:HA	55:LR:94:VAL:HG12	1.97	0.47
57:LT:12:ARG:O	57:LT:16:GLN:HG3	2.14	0.47
69:Lf:16:TYR:OH	69:Lf:89:LEU:O	2.32	0.47
79:Lp:46:THR:O	79:Lp:57:CYS:HA	2.15	0.47
1:C2:923:A:H2'	1:C2:924:A:C8	2.50	0.47
1:C2:1592:A:H2'	1:C2:1593:A:C8	2.49	0.47
2:C1:2988:C:OP1	52:LO:65:ASN:ND2	2.48	0.47
2:C1:3119:U:H4'	76:Lm:104:PRO:HG2	1.96	0.47
3:C4:11:A:N6	41:LD:13:SER:O	2.43	0.47
10:SF:39:GLU:HG3	10:SF:40:ILE:HD12	1.97	0.47
26:SV:74:GLN:NE2	26:SV:82:VAL:H	2.12	0.47
29:SY:54:ALA:HB1	29:SY:76:TYR:HB2	1.96	0.47
31:Sa:10:ARG:HD2	31:Sa:34:LYS:HA	1.96	0.47
36:Sf:121:CYS:SG	36:Sf:122:SER:N	2.88	0.47
38:LA:27:ALA:HB3	38:LA:128:ARG:HH12	1.79	0.47
38:LA:47:GLN:HG2	38:LA:60:LYS:HB3	1.97	0.47
46:LI:86:HIS:HB3	46:LI:139:ARG:HG2	1.97	0.47
56:LS:6:GLU:CD	56:LS:99:ARG:HH12	2.22	0.47
59:LV:10:LYS:HB2	59:LV:125:LEU:HD21	1.97	0.47
74:Lk:12:LEU:O	74:Lk:15:THR:OG1	2.31	0.47
80:CE:38:PRO:HG3	80:CE:142:MET:HE3	1.96	0.47
83:CD:332:ASP:OD1	83:CD:333:ALA:N	2.47	0.47
83:CD:380:LEU:HB3	83:CD:469:LEU:HB3	1.97	0.47
2:C1:1270:A:H5'	83:CD:741:GLY:HA2	1.96	0.47
2:C1:2160:G:H2'	2:C1:2161:G:H8	1.79	0.47
2:C1:2357:A:H2'	2:C1:2358:A:C8	2.49	0.47
6:SB:121:ILE:HD12	6:SB:161:ILE:HG23	1.97	0.47
20:SP:24:LYS:O	20:SP:28:MET:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SQ:50:GLU:OE1	21:SQ:82:ARG:NH1	2.38	0.47
22:SR:37:GLU:OE1	37:Sg:150:TRP:NE1	2.46	0.47
37:Sg:41:THR:HG22	37:Sg:62:LYS:HG2	1.96	0.47
43:LF:102:VAL:HG21	43:LF:129:LEU:HD22	1.97	0.47
62:LY:74:TYR:CE2	62:LY:77:LYS:HG2	2.50	0.47
82:P0:27:VAL:HB	82:P0:189:GLN:HB2	1.97	0.47
83:CD:746:VAL:HG21	83:CD:784:LEU:HA	1.97	0.47
2:C1:2771:U:O2'	2:C1:2772:C:O4'	2.32	0.46
6:SB:104:ASP:OD1	6:SB:105:PHE:N	2.48	0.46
11:SG:49:VAL:HB	11:SG:115:LYS:HB3	1.97	0.46
11:SG:161:GLU:HG3	11:SG:170:THR:HB	1.97	0.46
13:SI:12:SER:OG	13:SI:13:ALA:N	2.48	0.46
14:SJ:60:LEU:HD23	14:SJ:60:LEU:HA	1.77	0.46
33:Sc:16:LEU:N	33:Sc:27:GLN:O	2.38	0.46
44:LG:65:LEU:O	44:LG:68:ARG:O	2.33	0.46
48:LK:110:ILE:HD13	48:LK:129:THR:HG21	1.98	0.46
1:C2:107:C:H2'	1:C2:108:A:H8	1.79	0.46
1:C2:1037:C:O2	27:SW:16:ASN:ND2	2.48	0.46
1:C2:1075:C:O2'	31:Sa:13:LYS:O	2.33	0.46
2:C1:655:C:H2'	2:C1:656:A:H8	1.81	0.46
3:C4:112:G:H2'	3:C4:113:C:C6	2.50	0.46
4:C3:75:G:H2'	4:C3:76:C:H6	1.80	0.46
6:SB:128:LYS:HE2	6:SB:132:ASP:HA	1.97	0.46
15:SK:32:HIS:CD2	15:SK:33:GLU:H	2.33	0.46
20:SP:25:LEU:HA	20:SP:28:MET:SD	2.55	0.46
22:SR:75:GLU:HA	22:SR:78:ARG:HG2	1.97	0.46
23:SS:14:ILE:HG22	23:SS:23:ASP:HA	1.96	0.46
40:LC:226:GLU:OE2	40:LC:237:GLN:HG2	2.15	0.46
46:LI:72:ALA:O	46:LI:76:MET:HG2	2.14	0.46
60:LW:46:PRO:HB2	60:LW:54:LEU:HD12	1.96	0.46
68:Le:6:HIS:ND1	68:Le:6:HIS:O	2.48	0.46
82:P0:25:LEU:HB2	82:P0:191:TYR:HB3	1.97	0.46
83:CD:774:VAL:HA	83:CD:777:SER:HB3	1.96	0.46
1:C2:1234:A:OP2	1:C2:1245:G:O2'	2.33	0.46
2:C1:627:U:H2'	2:C1:628:A:C8	2.50	0.46
2:C1:1794:G:O2'	2:C1:1796:G:N2	2.48	0.46
6:SB:131:ASP:OD2	6:SB:180:THR:OG1	2.31	0.46
8:SD:40:ARG:HG2	25:SU:110:PRO:HB3	1.97	0.46
8:SD:94:ARG:NH1	8:SD:125:TYR:OH	2.49	0.46
11:SG:2:LYS:HB3	11:SG:108:VAL:HG22	1.97	0.46
13:SI:119:GLN:OE1	13:SI:119:GLN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SK:77:ARG:NH2	15:SK:86:ILE:O	2.48	0.46
25:SU:99:ILE:HG13	25:SU:102:ARG:NE	2.19	0.46
40:LC:65:TRP:HB3	40:LC:69:ARG:HD3	1.97	0.46
49:LL:46:ILE:HD13	49:LL:51:LEU:HA	1.98	0.46
83:CD:435:VAL:HA	83:CD:444:PRO:HA	1.97	0.46
1:C2:1280:C:H2'	1:C2:1281:G:H8	1.80	0.46
1:C2:1490:C:H4'	1:C2:1491:U:H5'	1.97	0.46
2:C1:93:C:OP2	2:C1:2764:C:O2'	2.28	0.46
2:C1:1740:U:H4'	2:C1:1741:A:H5'	1.98	0.46
2:C1:3011:A:N1	2:C1:3043:C:O2'	2.48	0.46
2:C1:3322:A:H2'	2:C1:3323:A:C8	2.50	0.46
5:SA:59:LEU:O	5:SA:63:ILE:HG12	2.15	0.46
8:SD:162:GLN:O	8:SD:166:ASP:HB2	2.15	0.46
13:SI:4:SER:OG	13:SI:6:ASP:OD2	2.33	0.46
13:SI:151:LYS:HD2	13:SI:151:LYS:HA	1.79	0.46
40:LC:26:PHE:CD1	40:LC:130:ALA:HB2	2.50	0.46
62:LY:89:LYS:O	62:LY:92:GLY:N	2.43	0.46
68:Le:63:THR:HA	68:Le:66:LEU:HD12	1.97	0.46
83:CD:433:ARG:HE	83:CD:444:PRO:HB3	1.79	0.46
1:C2:329:G:H5''	13:SI:98:LYS:HB3	1.97	0.46
1:C2:1153:G:P	31:Sa:82:ARG:HH12	2.38	0.46
2:C1:944:C:H4'	68:Le:33:ARG:HE	1.80	0.46
2:C1:1696:A:H2'	2:C1:1697:A:C8	2.51	0.46
2:C1:3015:G:H2'	2:C1:3016:A:H8	1.81	0.46
7:SC:175:GLY:O	14:SJ:53:ARG:NH1	2.49	0.46
13:SI:84:HIS:NE2	13:SI:97:THR:OG1	2.29	0.46
15:SK:60:SER:HB3	15:SK:65:TYR:HE1	1.80	0.46
27:SW:87:GLU:HA	27:SW:90:THR:HG22	1.96	0.46
31:Sa:36:ILE:H	31:Sa:36:ILE:HD12	1.81	0.46
38:LA:147:ARG:HG3	38:LA:157:VAL:HG12	1.97	0.46
45:LH:140:VAL:HG13	45:LH:143:GLU:OE2	2.15	0.46
47:LJ:37:LEU:HD13	47:LJ:69:VAL:HG23	1.97	0.46
56:LS:81:TYR:HE1	56:LS:88:HIS:HB2	1.79	0.46
1:C2:67:A:N6	1:C2:83:G:O2'	2.48	0.46
1:C2:511:A:OP2	14:SJ:176:ASN:ND2	2.45	0.46
1:C2:964:U:OP1	18:SN:128:TYR:OH	2.34	0.46
2:C1:1260:A:H2'	2:C1:1261:G:C4	2.50	0.46
2:C1:1717:U:H2'	2:C1:1718:G:C8	2.51	0.46
2:C1:1895:A:O2'	2:C1:3053:G:H4'	2.16	0.46
14:SJ:147:MET:HE3	14:SJ:147:MET:HB3	1.83	0.46
30:SZ:83:LEU:HG	30:SZ:89:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:LB:50:LYS:HA	39:LB:79:VAL:HG12	1.98	0.46
40:LC:192:GLY:HA2	40:LC:195:ARG:HB2	1.97	0.46
67:Ld:20:LEU:HD11	67:Ld:32:ALA:HB2	1.97	0.46
1:C2:468:A:N1	1:C2:594:A:O2'	2.46	0.46
2:C1:1659:U:H2'	2:C1:1660:C:C6	2.51	0.46
6:SB:121:ILE:HD11	6:SB:161:ILE:HD12	1.96	0.46
8:SD:137:VAL:HB	8:SD:185:LYS:HB3	1.97	0.46
18:SN:87:ASP:OD1	18:SN:88:LEU:N	2.49	0.46
25:SU:95:ALA:HB1	25:SU:99:ILE:HG23	1.98	0.46
37:Sg:214:ALA:HB3	37:Sg:243:LEU:HD21	1.98	0.46
49:LL:177:LYS:HE2	72:Li:11:LEU:HA	1.97	0.46
56:LS:12:ARG:NH1	56:LS:21:GLU:OE1	2.49	0.46
78:Lo:83:LEU:HD23	78:Lo:83:LEU:HA	1.84	0.46
80:CE:106:ASP:OD1	80:CE:107:GLY:N	2.49	0.46
1:C2:1227:A:H62	17:SM:103:LEU:HB3	1.81	0.46
2:C1:36:C:OP2	51:LN:83:LYS:NZ	2.49	0.46
2:C1:567:G:H2'	2:C1:568:G:C8	2.51	0.46
2:C1:1055:A:N3	3:C4:81:U:O2'	2.48	0.46
2:C1:1802:C:O2'	70:Lg:59:PRO:O	2.33	0.46
2:C1:2631:U:OP1	2:C1:2757:U:O2'	2.34	0.46
3:C4:44:C:H2'	3:C4:45:A:H8	1.81	0.46
4:C3:9:A:H2'	4:C3:10:A:C8	2.50	0.46
6:SB:70:LEU:HD21	6:SB:189:ILE:HG23	1.96	0.46
13:SI:87:ASN:HB3	13:SI:90:LEU:HD13	1.96	0.46
23:SS:26:ILE:C	23:SS:57:ARG:HG2	2.41	0.46
43:LF:54:GLU:HA	43:LF:57:THR:HG22	1.98	0.46
59:LV:84:SER:HA	59:LV:94:TYR:HB3	1.98	0.46
63:LZ:23:VAL:HB	63:LZ:43:VAL:HB	1.98	0.46
63:LZ:83:THR:HG22	70:Lg:93:PHE:CZ	2.51	0.46
71:Lh:70:TYR:O	71:Lh:76:GLN:NE2	2.49	0.46
71:Lh:102:GLU:HG2	71:Lh:103:LYS:N	2.31	0.46
1:C2:534:A:H3'	1:C2:535:A:H8	1.80	0.46
1:C2:575:C:N4	28:SX:65:ASN:OD1	2.40	0.46
1:C2:802:G:H21	27:SW:107:SER:HB3	1.80	0.46
1:C2:953:G:H2'	1:C2:954:G:C8	2.49	0.46
2:C1:655:C:H2'	2:C1:656:A:C8	2.50	0.46
5:SA:9:LEU:HD11	5:SA:51:GLY:HA2	1.98	0.46
5:SA:183:ARG:NH2	5:SA:191:ARG:O	2.49	0.46
6:SB:111:ARG:HA	6:SB:114:VAL:HG12	1.97	0.46
13:SI:31:ARG:HH12	13:SI:48:THR:HG22	1.81	0.46
15:SK:13:GLN:O	15:SK:17:GLN:OE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:ST:44:GLU:N	24:ST:44:GLU:OE1	2.48	0.46
25:SU:51:VAL:HG23	25:SU:52:LYS:H	1.80	0.46
37:Sg:13:LEU:HB3	37:Sg:45:TRP:HZ3	1.81	0.46
37:Sg:172:ALA:HB2	37:Sg:202:LEU:HD23	1.97	0.46
52:LO:43:ILE:HD11	52:LO:138:LEU:HD13	1.97	0.46
75:Ll:28:ARG:HB3	75:Ll:28:ARG:NH1	2.30	0.46
1:C2:351:C:H5	1:C2:631:G:H5'	1.81	0.46
1:C2:1241:G:OP2	20:SP:77:ARG:NH2	2.49	0.46
2:C1:120:G:N2	44:LG:126:SER:O	2.47	0.46
2:C1:3291:G:H2'	2:C1:3292:A:C8	2.52	0.46
14:SJ:143:ILE:HA	14:SJ:144:PRO:HD3	1.83	0.46
40:LC:338:LYS:O	40:LC:340:GLY:N	2.49	0.46
45:LH:89:LYS:HG2	45:LH:145:VAL:HG22	1.98	0.46
47:LJ:60:ARG:HH22	78:Lo:104:LEU:C	2.23	0.46
81:L1:108:ASN:OD1	81:L1:109:ALA:N	2.49	0.46
1:C2:922:G:H2'	1:C2:923:A:C8	2.51	0.45
1:C2:1588:G:O6	1:C2:1608:U:O4	2.33	0.45
2:C1:406:G:OP1	2:C1:1415:U:O2'	2.33	0.45
2:C1:1222:G:O2'	2:C1:1286:A:N6	2.49	0.45
2:C1:2185:G:O2'	2:C1:2314:U:OP2	2.31	0.45
2:C1:3242:G:H5'	2:C1:3245:A:H8	1.82	0.45
9:SE:163:ASP:OD1	9:SE:163:ASP:N	2.48	0.45
9:SE:181:VAL:HG22	9:SE:227:VAL:HA	1.97	0.45
10:SF:208:SER:HB3	10:SF:211:ILE:HG12	1.98	0.45
12:SH:114:ARG:HA	12:SH:117:THR:HG23	1.98	0.45
37:Sg:307:ASP:OD1	37:Sg:307:ASP:N	2.49	0.45
39:LB:53:MET:HG2	39:LB:77:THR:HG22	1.98	0.45
41:LD:48:LYS:HG2	41:LD:145:PHE:HE2	1.80	0.45
48:LK:75:PRO:HD2	48:LK:119:LYS:HZ2	1.81	0.45
83:CD:21:ASN:O	83:CD:122:THR:OG1	2.31	0.45
1:C2:158:U:O2'	1:C2:160:C:OP2	2.33	0.45
1:C2:927:C:O2'	19:SO:124:ASP:OD2	2.34	0.45
2:C1:213:A:OP1	62:LY:2:ALA:N	2.49	0.45
2:C1:1221:A:H1'	82:P0:8:LYS:NZ	2.31	0.45
2:C1:1662:G:H22	2:C1:1787:A:H2	1.64	0.45
7:SC:178:ILE:HG12	7:SC:196:VAL:HG22	1.98	0.45
8:SD:54:ARG:HB3	8:SD:57:ASP:HB2	1.99	0.45
10:SF:63:GLN:HB3	10:SF:88:PRO:HA	1.98	0.45
18:SN:67:THR:HG21	18:SN:74:ILE:HD11	1.98	0.45
39:LB:296:THR:HG23	39:LB:299:ASP:H	1.81	0.45
42:LE:37:GLY:CA	42:LE:54:TYR:O	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:LN:46:ASP:OD2	51:LN:50:ARG:NH2	2.48	0.45
65:Lb:39:PHE:HA	65:Lb:42:ASN:HB3	1.98	0.45
66:Lc:30:THR:HG23	66:Lc:91:SER:HB2	1.98	0.45
83:CD:436:LEU:HG	83:CD:445:ILE:HB	1.98	0.45
1:C2:205:U:H2'	1:C2:206:A:H8	1.81	0.45
2:C1:316:U:O2'	72:Li:30:LYS:NZ	2.36	0.45
8:SD:189:MET:HE1	8:SD:202:LEU:HD21	1.98	0.45
10:SF:214:LYS:O	10:SF:218:GLU:HG2	2.15	0.45
11:SG:10:ASN:HD22	11:SG:128:THR:HG22	1.80	0.45
42:LE:100:LYS:NZ	42:LE:137:ASP:OD2	2.47	0.45
45:LH:90:MET:O	45:LH:143:GLU:HA	2.15	0.45
49:LL:18:TRP:O	49:LL:21:ARG:N	2.50	0.45
52:LO:36:VAL:HB	52:LO:108:ILE:HG12	1.99	0.45
56:LS:59:VAL:HG21	57:LT:141:VAL:HG21	1.98	0.45
69:Lf:12:LYS:HA	69:Lf:96:ALA:O	2.17	0.45
80:CE:38:PRO:HG2	80:CE:65:PHE:HE2	1.80	0.45
1:C2:588:U:O2'	35:Se:57:ASN:OD1	2.25	0.45
1:C2:800:U:H2'	1:C2:801:G:C8	2.51	0.45
2:C1:675:C:OP2	54:LQ:105:ARG:NH2	2.47	0.45
2:C1:685:G:OP2	49:LL:35:ARG:NH1	2.49	0.45
2:C1:744:A:H1'	54:LQ:141:ARG:HH11	1.81	0.45
2:C1:1798:A:H2'	2:C1:1799:A:C8	2.51	0.45
2:C1:1799:A:H2'	2:C1:1800:A:H8	1.82	0.45
10:SF:31:GLU:HA	10:SF:34:GLN:HB2	1.99	0.45
18:SN:25:TRP:HB2	32:Sb:82:LYS:NZ	2.32	0.45
38:LA:60:LYS:HD2	38:LA:73:GLU:CG	2.47	0.45
40:LC:211:GLU:OE2	40:LC:213:ASN:ND2	2.49	0.45
47:LJ:10:ARG:O	47:LJ:133:ARG:NH1	2.43	0.45
47:LJ:11:ASP:N	47:LJ:11:ASP:OD1	2.47	0.45
74:Lk:2:ALA:N	74:Lk:51:LEU:O	2.49	0.45
83:CD:158:ASN:OD1	83:CD:159:LYS:N	2.48	0.45
1:C2:29:U:H2'	1:C2:30:G:C8	2.49	0.45
1:C2:1354:G:O6	1:C2:1369:U:O2	2.35	0.45
2:C1:2719:U:H5'	54:LQ:180:ARG:NH2	2.31	0.45
2:C1:3251:U:H2'	2:C1:3252:G:C8	2.52	0.45
8:SD:191:ASP:OD1	8:SD:191:ASP:N	2.46	0.45
9:SE:133:LYS:O	9:SE:136:VAL:HG12	2.16	0.45
10:SF:207:THR:O	10:SF:212:LYS:NZ	2.50	0.45
13:SI:105:ASP:OD1	13:SI:106:ALA:N	2.50	0.45
20:SP:25:LEU:HD12	20:SP:87:PRO:HG3	1.98	0.45
29:SY:106:GLN:O	29:SY:110:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LH:93:VAL:HG12	76:Lm:82:LEU:HD13	1.99	0.45
47:LJ:92:ARG:HG2	47:LJ:172:LEU:HD22	1.97	0.45
49:LL:25:HIS:NE2	51:LN:198:SER:OG	2.40	0.45
50:LM:46:ILE:O	50:LM:55:ARG:HA	2.16	0.45
2:C1:75:G:O3'	49:LL:70:ARG:NH2	2.50	0.45
2:C1:2471:U:OP1	81:L1:24:LYS:NZ	2.45	0.45
2:C1:2761:G:O2'	2:C1:2795:U:O4	2.31	0.45
6:SB:166:LYS:O	6:SB:170:GLU:HG2	2.17	0.45
8:SD:177:MET:HE2	8:SD:177:MET:HB3	1.64	0.45
26:SV:74:GLN:OE1	26:SV:83:TRP:HB3	2.17	0.45
29:SY:28:LEU:HG	29:SY:68:LYS:HG2	1.99	0.45
29:SY:51:GLU:O	29:SY:53:ASP:N	2.50	0.45
37:Sg:81:LEU:HD22	37:Sg:91:LEU:HD13	1.99	0.45
37:Sg:255:ALA:HB2	37:Sg:292:LEU:HG	1.99	0.45
41:LD:40:HIS:CD2	57:LT:69:LYS:HG3	2.52	0.45
51:LN:163:GLY:O	51:LN:172:ARG:NH1	2.43	0.45
80:CE:18:THR:HA	80:CE:82:VAL:O	2.16	0.45
83:CD:571:SER:HB3	83:CD:589:LYS:HD2	1.98	0.45
1:C2:115:G:C8	16:SL:129:ARG:HG3	2.52	0.45
1:C2:482:U:H2'	1:C2:483:A:C8	2.52	0.45
1:C2:590:C:H5''	35:Se:43:ARG:HH22	1.82	0.45
1:C2:1478:G:OP1	24:ST:39:THR:OG1	2.25	0.45
1:C2:1572:G:HO2'	10:SF:185:ARG:NH1	2.13	0.45
2:C1:900:G:H1'	2:C1:1589:A:N6	2.32	0.45
2:C1:1063:G:H22	57:LT:108:ARG:HH12	1.65	0.45
2:C1:1257:C:H2'	2:C1:1258:U:C6	2.52	0.45
2:C1:2213:A:H2'	2:C1:2214:A:C8	2.51	0.45
9:SE:47:PHE:HE1	9:SE:111:VAL:HG12	1.82	0.45
11:SG:123:GLY:O	11:SG:127:THR:OG1	2.32	0.45
38:LA:112:ILE:HG22	38:LA:135:ILE:HG12	1.98	0.45
45:LH:67:ALA:HA	45:LH:70:THR:HG22	1.98	0.45
46:LI:52:LEU:HB3	46:LI:136:PHE:HB2	1.99	0.45
52:LO:55:HIS:HD1	52:LO:58:LEU:HD12	1.82	0.45
80:CE:63:ASP:O	80:CE:67:GLY:HA2	2.17	0.45
1:C2:1274:C:N4	84:CS:94:HIS:O	2.40	0.45
1:C2:1712:A:H3'	1:C2:1713:G:H8	1.82	0.45
86:C1:3401:T1C:H433	86:C1:3401:T1C:H41	1.77	0.45
5:SA:155:PHE:O	26:SV:60:ARG:NH2	2.49	0.45
17:SM:43:ARG:NH2	17:SM:120:VAL:H	2.13	0.45
31:Sa:11:ASN:OD1	31:Sa:11:ASN:N	2.49	0.45
37:Sg:214:ALA:HB2	37:Sg:220:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:LA:36:GLU:OE2	38:LA:163:ARG:NH1	2.50	0.45
51:LN:9:GLU:HB2	72:LI:44:VAL:HG21	1.98	0.45
56:LS:30:PHE:CZ	56:LS:103:VAL:HG21	2.52	0.45
61:LX:59:SER:HB3	61:LX:102:LEU:HD13	1.99	0.45
83:CD:89:ILE:HG12	83:CD:340:LEU:HA	1.98	0.45
1:C2:142:G:P	11:SG:139:ASN:HD21	2.39	0.45
1:C2:1164:G:H2'	1:C2:1165:G:H8	1.82	0.45
2:C1:144:A:OP1	44:LG:193:LYS:NZ	2.50	0.45
2:C1:2344:U:H2'	2:C1:2345:A:C8	2.52	0.45
86:C1:3401:T1C:H941	86:C1:3401:T1C:H921	1.82	0.45
6:SB:32:ILE:HG13	6:SB:96:LEU:HD21	1.99	0.45
7:SC:188:LEU:HD13	7:SC:196:VAL:HG21	1.99	0.45
10:SF:72:HIS:CE1	21:SQ:79:TYR:HH	2.31	0.45
17:SM:93:ASP:OD1	17:SM:93:ASP:N	2.44	0.45
27:SW:122:SER:OG	27:SW:123:GLY:N	2.49	0.45
38:LA:137:ILE:HD13	38:LA:149:ARG:HB2	1.98	0.45
44:LG:78:PHE:CZ	44:LG:163:VAL:HG12	2.52	0.45
50:LM:15:VAL:HG12	50:LM:65:LEU:HD21	1.99	0.45
83:CD:310:ASP:O	83:CD:313:ASP:N	2.50	0.45
1:C2:1586:A:OP1	21:SQ:134:ALA:N	2.50	0.45
2:C1:67:A:O2'	2:C1:315:C:O2	2.32	0.45
2:C1:719:U:O2'	54:LQ:72:LYS:NZ	2.50	0.45
2:C1:1063:G:OP2	2:C1:1063:G:N2	2.50	0.45
2:C1:1203:A:H2'	2:C1:1204:A:C8	2.52	0.45
10:SF:82:PHE:HZ	33:Sc:47:PRO:HB2	1.82	0.45
12:SH:102:PRO:HD3	12:SH:112:ARG:HE	1.82	0.45
23:SS:49:LYS:NZ	23:SS:79:TYR:O	2.37	0.45
26:SV:32:VAL:HG22	26:SV:60:ARG:HD2	1.99	0.45
37:Sg:221:MET:N	37:Sg:221:MET:SD	2.90	0.45
39:LB:160:VAL:HG11	39:LB:194:TRP:HZ3	1.81	0.45
41:LD:54:ARG:NH1	41:LD:148:ILE:O	2.50	0.45
46:LI:5:PRO:HB2	46:LI:7:ARG:HG2	1.99	0.45
46:LI:159:PHE:HB2	46:LI:163:GLN:HE21	1.82	0.45
79:Lp:45:LYS:HE2	79:Lp:45:LYS:HB2	1.73	0.45
80:CE:17:ALA:O	80:CE:83:PRO:HA	2.17	0.45
80:CE:30:GLY:O	80:CE:40:LYS:HA	2.17	0.45
81:L1:212:PRO:HB3	81:L1:214:PHE:CE1	2.52	0.45
83:CD:413:ILE:O	83:CD:426:LEU:HA	2.17	0.45
1:C2:247:A:O2'	16:SL:37:ASN:O	2.33	0.44
1:C2:1584:G:N2	1:C2:1611:A:OP2	2.34	0.44
1:C2:1606:C:H2'	1:C2:1607:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:1257:C:H4'	82:P0:42:ARG:HH12	1.80	0.44
2:C1:1712:G:OP2	66:Lc:32:LYS:NZ	2.41	0.44
2:C1:2548:C:OP1	38:LA:93:LYS:NZ	2.44	0.44
2:C1:2768:U:H2'	2:C1:2769:A:C8	2.52	0.44
21:SQ:83:GLN:HE22	21:SQ:119:ALA:HA	1.82	0.44
25:SU:27:THR:HB	25:SU:88:LYS:HG3	1.98	0.44
42:LE:170:LYS:HB3	42:LE:172:HIS:CE1	2.52	0.44
43:LF:131:GLU:OE2	43:LF:222:HIS:NE2	2.47	0.44
46:LI:50:VAL:HG22	46:LI:167:LEU:HD13	1.99	0.44
54:LQ:42:ALA:HB1	54:LQ:45:ASN:HB2	1.99	0.44
1:C2:329:G:H2'	1:C2:330:G:H8	1.82	0.44
2:C1:515:C:O2'	40:LC:341:SER:O	2.26	0.44
2:C1:3162:C:H2'	2:C1:3163:A:C8	2.53	0.44
2:C1:3214:U:C4	50:LM:121:MET:HG3	2.52	0.44
10:SF:143:ARG:HH22	33:Sc:56:LEU:N	2.15	0.44
14:SJ:85:VAL:HG11	14:SJ:104:PHE:HE1	1.82	0.44
20:SP:83:MET:HB2	20:SP:116:LEU:HD13	1.98	0.44
37:Sg:195:HIS:HD1	37:Sg:197:SER:H	1.65	0.44
60:LW:37:ALA:O	60:LW:41:LYS:HG2	2.16	0.44
83:CD:418:TYR:O	83:CD:477:ASN:ND2	2.50	0.44
83:CD:568:GLU:H	83:CD:723:LYS:HZ1	1.65	0.44
1:C2:153:G:H2'	1:C2:154:G:C8	2.51	0.44
1:C2:1198:G:OP1	1:C2:1199:G:O2'	2.30	0.44
2:C1:1084:A:H2'	2:C1:1085:A:C8	2.52	0.44
2:C1:1108:U:H2'	2:C1:1109:U:C6	2.53	0.44
2:C1:1621:A:H2'	2:C1:1622:U:C6	2.52	0.44
2:C1:2129:U:H2'	2:C1:2130:G:C8	2.52	0.44
2:C1:3107:U:OP1	76:Lm:114:LYS:NZ	2.50	0.44
2:C1:3184:A:N3	2:C1:3187:A:O2'	2.50	0.44
3:C4:44:C:OP2	47:LJ:137:ARG:NH2	2.43	0.44
15:SK:1:MET:HE3	15:SK:41:TYR:HA	1.98	0.44
21:SQ:38:LEU:HD11	24:ST:10:ALA:HB2	1.99	0.44
21:SQ:105:LEU:HD13	21:SQ:105:LEU:HA	1.85	0.44
31:Sa:64:LEU:HD12	31:Sa:64:LEU:HA	1.83	0.44
37:Sg:19:TRP:CD1	37:Sg:306:THR:HA	2.52	0.44
37:Sg:90:ARG:NH2	37:Sg:99:THR:HB	2.32	0.44
46:LI:153:ARG:HA	46:LI:156:ARG:HG2	1.99	0.44
56:LS:1:MET:H2	56:LS:4:PHE:HE1	1.65	0.44
63:LZ:101:PHE:HD1	63:LZ:101:PHE:HA	1.70	0.44
83:CD:820:LEU:HG	83:CD:824:LYS:HE2	1.99	0.44
1:C2:340:U:H2'	1:C2:341:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:477:A:C5	1:C2:538:A:H2	2.34	0.44
1:C2:1655:A:H5''	77:Ln:25:LYS:HD2	1.99	0.44
2:C1:2373:A:N3	2:C1:2824:G:O2'	2.42	0.44
2:C1:2469:G:H4'	81:L1:28:PHE:CD1	2.52	0.44
2:C1:2779:A:O2'	49:LL:180:ARG:NH2	2.48	0.44
7:SC:186:LYS:HD2	7:SC:186:LYS:HA	1.81	0.44
9:SE:12:LEU:HD11	14:SJ:4:ALA:HB2	2.00	0.44
43:LF:170:GLU:HG2	43:LF:179:LEU:HB2	2.00	0.44
83:CD:260:LYS:NZ	83:CD:261:ASP:OD1	2.40	0.44
1:C2:235:G:H2'	1:C2:236:A:C8	2.51	0.44
1:C2:1274:C:H5	84:CS:95:SER:HA	1.82	0.44
1:C2:1290:U:OP1	7:SC:95:ARG:NH2	2.45	0.44
1:C2:1795:U:OP2	31:Sa:4:LYS:NZ	2.47	0.44
1:C2:1796:C:O2'	31:Sa:95:ARG:NH1	2.51	0.44
2:C1:3152:U:OP2	2:C1:3395:G:N1	2.34	0.44
3:C4:39:C:O2'	47:LJ:44:THR:O	2.34	0.44
4:C3:8:C:H2'	4:C3:9:A:H8	1.82	0.44
5:SA:38:PHE:CG	22:SR:109:LEU:HD13	2.52	0.44
10:SF:28:PRO:HG2	21:SQ:37:THR:HG21	1.99	0.44
39:LB:46:PHE:CE2	39:LB:81:THR:HG23	2.53	0.44
42:LE:138:GLN:O	42:LE:142:ASP:HB2	2.17	0.44
43:LF:100:ARG:NH2	54:LQ:4:ASP:OD1	2.43	0.44
60:LW:12:LYS:HZ3	60:LW:14:TYR:HE1	1.65	0.44
83:CD:239:LYS:O	83:CD:243:ARG:NE	2.48	0.44
1:C2:78:A:O2'	11:SG:173:PRO:O	2.33	0.44
1:C2:589:C:OP1	35:Se:42:ARG:NH1	2.50	0.44
2:C1:594:U:OP2	2:C1:609:G:N1	2.40	0.44
2:C1:2781:U:H4'	49:LL:185:LYS:HG3	1.99	0.44
2:C1:3218:A:O2'	2:C1:3278:C:N3	2.45	0.44
6:SB:172:LEU:O	6:SB:176:VAL:HG22	2.18	0.44
11:SG:164:LYS:HG3	11:SG:165:GLY:H	1.83	0.44
12:SH:109:VAL:HG23	12:SH:110:GLN:HG2	1.99	0.44
29:SY:107:GLN:OE1	29:SY:107:GLN:N	2.47	0.44
33:Sc:28:VAL:HG11	33:Sc:48:VAL:HG11	2.00	0.44
37:Sg:299:GLN:HB3	37:Sg:314:GLN:NE2	2.30	0.44
43:LF:202:LEU:HD23	43:LF:202:LEU:HA	1.89	0.44
63:LZ:63:ALA:HA	63:LZ:66:THR:HG22	2.00	0.44
64:La:100:PRO:HG2	64:La:123:VAL:HG23	1.99	0.44
83:CD:223:ARG:HH21	83:CD:241:MET:HE3	1.82	0.44
1:C2:579:A:H5'	8:SD:178:ARG:NH2	2.33	0.44
1:C2:1477:G:H2'	1:C2:1478:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:19:U:H4'	51:LN:138:GLN:HG3	1.99	0.44
2:C1:73:C:N3	49:LL:59:ARG:NH1	2.66	0.44
2:C1:339:C:OP1	2:C1:1380:G:O2'	2.35	0.44
2:C1:1427:U:OP2	64:La:4:ARG:NH1	2.41	0.44
2:C1:1466:G:N2	2:C1:1510:G:H5''	2.32	0.44
2:C1:2898:G:N7	76:Lm:125:LYS:NZ	2.65	0.44
2:C1:3137:C:H5''	39:LB:276:THR:HG21	1.99	0.44
7:SC:141:ARG:O	26:SV:1:MET:HE1	2.17	0.44
9:SE:180:LEU:N	9:SE:229:GLY:O	2.50	0.44
21:SQ:28:LEU:O	21:SQ:64:ASP:HA	2.17	0.44
28:SX:136:TRP:HE3	28:SX:137:LYS:HG3	1.82	0.44
35:Se:39:LEU:HD12	35:Se:43:ARG:HE	1.82	0.44
38:LA:65:ASP:OD2	38:LA:70:ARG:NH2	2.51	0.44
39:LB:108:GLU:HG3	39:LB:109:HIS:ND1	2.33	0.44
42:LE:169:ASP:HB3	42:LE:174:LEU:HD11	2.00	0.44
51:LN:67:ARG:HA	51:LN:67:ARG:HD2	1.86	0.44
59:LV:106:LYS:HA	59:LV:106:LYS:HD2	1.85	0.44
65:Lb:36:ASP:O	65:Lb:40:ARG:HB2	2.17	0.44
66:Lc:10:ILE:O	66:Lc:14:LEU:HG	2.17	0.44
81:L1:48:ARG:NH1	81:L1:160:LYS:O	2.48	0.44
83:CD:342:LEU:HA	83:CD:342:LEU:HD23	1.71	0.44
83:CD:648:ASP:HA	83:CD:688:ILE:HG22	2.00	0.44
2:C1:242:C:H2'	2:C1:243:G:C8	2.52	0.44
2:C1:585:A:H4'	69:Lf:72:THR:HG23	2.00	0.44
8:SD:23:GLU:HG2	15:SK:61:TRP:CD1	2.52	0.44
9:SE:154:ILE:HA	9:SE:174:LYS:NZ	2.33	0.44
21:SQ:114:ARG:HD3	21:SQ:114:ARG:HA	1.74	0.44
23:SS:32:LEU:HA	23:SS:35:ILE:HD12	2.00	0.44
53:LP:13:LYS:HE3	53:LP:152:GLU:HG3	2.00	0.44
54:LQ:25:TYR:HA	54:LQ:28:LEU:HD12	2.00	0.44
59:LV:19:VAL:HG23	59:LV:50:PRO:O	2.17	0.44
81:L1:99:LEU:HA	81:L1:102:LYS:HE2	1.98	0.44
1:C2:231:U:H2'	1:C2:232:U:H2'	1.99	0.44
1:C2:610:G:O2'	1:C2:613:G:O2'	2.25	0.44
1:C2:1164:G:H2'	1:C2:1165:G:C8	2.53	0.44
2:C1:673:U:H2'	2:C1:674:G:C8	2.53	0.44
2:C1:2526:C:H2'	2:C1:2527:G:C8	2.52	0.44
2:C1:3268:A:H5''	42:LE:46:ARG:CZ	2.48	0.44
9:SE:30:ARG:O	9:SE:81:THR:OG1	2.35	0.44
15:SK:52:LYS:HD2	15:SK:52:LYS:HA	1.75	0.44
19:SO:111:ARG:HB3	31:Sa:58:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SQ:87:LYS:HB2	21:SQ:87:LYS:HE3	1.83	0.44
23:SS:11:PHE:CD1	23:SS:59:GLY:HA3	2.52	0.44
27:SW:24:GLN:HA	27:SW:63:VAL:O	2.18	0.44
46:LI:140:THR:HG21	46:LI:148:VAL:HG21	2.00	0.44
49:LL:76:THR:O	49:LL:79:GLU:N	2.51	0.44
81:L1:112:ALA:HB2	81:L1:135:PRO:HB2	2.00	0.44
83:CD:261:ASP:OD1	83:CD:261:ASP:N	2.51	0.44
83:CD:311:GLU:HA	83:CD:314:LEU:HD13	1.99	0.44
1:C2:587:C:H5''	35:Se:26:LYS:NZ	2.33	0.43
1:C2:590:C:H2'	1:C2:591:A:C8	2.52	0.43
1:C2:960:U:O5'	18:SN:55:ARG:NH1	2.51	0.43
2:C1:255:A:H2'	2:C1:256:G:C8	2.52	0.43
2:C1:1743:G:H2'	2:C1:1744:G:H8	1.82	0.43
2:C1:2560:C:N4	2:C1:2575:G:OP2	2.50	0.43
2:C1:3000:A:H5''	39:LB:120:LYS:HE2	1.99	0.43
9:SE:132:GLY:N	9:SE:136:VAL:O	2.44	0.43
37:Sg:182:ASN:N	37:Sg:189:GLU:OE1	2.49	0.43
40:LC:159:ILE:HD12	40:LC:164:GLU:HG3	1.99	0.43
40:LC:315:LYS:HB3	40:LC:320:ASN:HD22	1.83	0.43
42:LE:31:ARG:NH1	69:Lf:107:ILE:H	2.16	0.43
46:LI:49:CYS:HB3	46:LI:168:SER:HB3	2.00	0.43
52:LO:12:LYS:O	56:LS:167:ARG:NH2	2.44	0.43
55:LR:105:LEU:HD22	55:LR:135:LYS:HG3	1.99	0.43
78:Lo:97:LYS:O	78:Lo:99:GLN:NE2	2.51	0.43
81:L1:52:SER:HA	81:L1:155:ILE:O	2.18	0.43
81:L1:65:ILE:HA	81:L1:109:ALA:O	2.18	0.43
83:CD:70:ILE:HG13	83:CD:540:ILE:HD11	1.99	0.43
1:C2:885:G:H5'	6:SB:138:PHE:CZ	2.53	0.43
2:C1:107:A:O2'	2:C1:324:A:N3	2.46	0.43
2:C1:2217:U:H2'	2:C1:2218:G:H8	1.83	0.43
6:SB:111:ARG:HB2	31:Sa:68:TYR:CD2	2.53	0.43
8:SD:157:LEU:HD23	8:SD:189:MET:HB2	2.00	0.43
19:SO:15:GLY:HA3	19:SO:76:ILE:HD11	1.99	0.43
38:LA:242:ARG:NH2	38:LA:243:THR:O	2.51	0.43
44:LG:206:GLU:H	44:LG:206:GLU:CD	2.26	0.43
49:LL:194:GLU:HA	49:LL:195:ALA:HA	1.55	0.43
52:LO:77:SER:HB2	52:LO:104:VAL:HG12	1.99	0.43
60:LW:8:PHE:HZ	60:LW:49:ILE:HG13	1.82	0.43
61:LX:97:LYS:O	61:LX:101:GLU:HG2	2.19	0.43
83:CD:112:SER:HA	83:CD:115:VAL:HB	2.00	0.43
1:C2:585:A:H2'	1:C2:586:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:585:A:H2'	1:C2:586:G:H8	1.83	0.43
1:C2:1553:G:O6	20:SP:43:ARG:NH1	2.50	0.43
2:C1:121:A:N6	44:LG:126:SER:OG	2.48	0.43
2:C1:1675:G:H2'	2:C1:1676:A:H8	1.83	0.43
2:C1:2270:A:H2'	2:C1:2271:A:C8	2.54	0.43
2:C1:3015:G:H2'	2:C1:3016:A:C8	2.53	0.43
6:SB:64:ARG:HE	6:SB:64:ARG:HB2	1.64	0.43
14:SJ:36:LEU:HD21	14:SJ:105:LEU:HD11	2.00	0.43
15:SK:75:TYR:O	15:SK:78:GLU:HG3	2.18	0.43
16:SL:125:VAL:HG12	16:SL:139:VAL:HA	1.99	0.43
22:SR:26:LEU:HD22	22:SR:59:LYS:HE2	1.99	0.43
37:Sg:276:PRO:HB2	37:Sg:278:PHE:HE1	1.83	0.43
41:LD:49:TYR:HB3	41:LD:144:VAL:HG12	1.99	0.43
43:LF:208:SER:OG	43:LF:209:ASN:N	2.51	0.43
50:LM:60:LEU:HA	50:LM:63:VAL:HG22	1.99	0.43
69:Lf:9:VAL:HG23	69:Lf:100:ILE:HB	2.00	0.43
82:P0:59:VAL:O	82:P0:63:ILE:HG12	2.19	0.43
83:CD:221:THR:OG1	83:CD:336:GLU:OE2	2.35	0.43
84:CS:113:ASP:OD1	84:CS:113:ASP:N	2.51	0.43
1:C2:174:U:H3	1:C2:266:A:H62	1.66	0.43
1:C2:1237:G:H2'	1:C2:1238:A:C8	2.53	0.43
2:C1:1128:U:O4'	46:LI:4:ARG:NH2	2.51	0.43
2:C1:1176:C:H2'	2:C1:1177:G:N2	2.33	0.43
2:C1:2563:G:O2'	44:LG:29:SER:OG	2.34	0.43
2:C1:2697:A:H2'	2:C1:2698:G:C8	2.53	0.43
9:SE:206:ASP:OD1	9:SE:206:ASP:N	2.51	0.43
12:SH:49:ILE:HB	12:SH:57:ALA:HB3	2.01	0.43
16:SL:24:LYS:HB2	16:SL:24:LYS:HE2	1.63	0.43
28:SX:61:SER:HB3	28:SX:116:ASP:HB2	2.01	0.43
30:SZ:57:TYR:O	30:SZ:103:ARG:NH1	2.51	0.43
53:LP:119:VAL:HG12	53:LP:146:ILE:HG23	2.01	0.43
67:Ld:27:LYS:HE3	67:Ld:27:LYS:HB2	1.75	0.43
79:Lp:84:ARG:HG3	79:Lp:87:ARG:HH12	1.84	0.43
83:CD:463:LEU:HD11	83:CD:467:GLY:HA3	2.00	0.43
1:C2:52:U:H2'	1:C2:53:G:C8	2.53	0.43
1:C2:867:G:H1	1:C2:961:U:H3	1.67	0.43
1:C2:1300:A:H5'	7:SC:86:VAL:HG21	2.00	0.43
2:C1:1666:G:H2'	2:C1:1667:A:C8	2.53	0.43
2:C1:2373:A:O2'	2:C1:2823:G:N2	2.47	0.43
2:C1:2493:U:H2'	2:C1:2494:A:C8	2.53	0.43
18:SN:33:VAL:HG13	18:SN:54:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SQ:37:THR:O	21:SQ:45:ARG:NH1	2.51	0.43
38:LA:10:LYS:HE2	38:LA:10:LYS:HB2	1.86	0.43
41:LD:49:TYR:CE1	41:LD:66:SER:HB3	2.54	0.43
44:LG:150:LEU:HD13	44:LG:215:VAL:HG12	2.01	0.43
73:Lj:58:THR:O	73:Lj:61:THR:OG1	2.29	0.43
83:CD:387:PRO:HA	83:CD:394:PHE:CD1	2.54	0.43
1:C2:252:U:H2'	1:C2:253:A:H8	1.83	0.43
1:C2:269:G:H2'	1:C2:270:C:H6	1.83	0.43
1:C2:546:U:H2'	1:C2:547:U:C6	2.53	0.43
1:C2:856:A:N6	12:SH:115:SER:O	2.43	0.43
1:C2:1547:A:OP2	23:SS:123:ARG:NH2	2.51	0.43
2:C1:1421:G:H2'	2:C1:1422:G:H8	1.83	0.43
7:SC:140:ARG:HB3	7:SC:221:THR:HG22	2.01	0.43
13:SI:67:TRP:CZ2	13:SI:109:PHE:HB3	2.54	0.43
21:SQ:73:GLY:O	21:SQ:77:GLN:HG2	2.17	0.43
37:Sg:93:ASP:HB3	37:Sg:100:TYR:CE2	2.54	0.43
37:Sg:165:ASP:N	37:Sg:165:ASP:OD1	2.41	0.43
40:LC:299:ILE:HG23	54:LQ:39:ARG:HB3	1.99	0.43
47:LJ:14:ILE:HD13	47:LJ:131:MET:HG2	2.01	0.43
83:CD:594:ASP:HB3	83:CD:597:VAL:HG22	2.00	0.43
1:C2:628:G:OP1	18:SN:120:SER:OG	2.36	0.43
1:C2:895:G:N2	1:C2:917:U:O2	2.33	0.43
2:C1:2345:A:OP1	67:Ld:24:SER:OG	2.34	0.43
2:C1:2828:G:OP2	46:LI:7:ARG:NH2	2.51	0.43
2:C1:3287:U:H3'	2:C1:3288:G:H8	1.84	0.43
3:C4:18:C:OP2	47:LJ:150:ASN:ND2	2.45	0.43
5:SA:76:ILE:HD13	5:SA:98:ILE:HB	2.00	0.43
7:SC:222:TYR:OH	26:SV:12:TYR:O	2.37	0.43
16:SL:94:ILE:HD11	16:SL:101:GLU:CD	2.44	0.43
41:LD:261:THR:OG1	41:LD:262:LYS:N	2.51	0.43
42:LE:38:THR:OG1	42:LE:39:VAL:N	2.51	0.43
61:LX:76:VAL:HG13	61:LX:132:ALA:HB1	2.01	0.43
71:Lh:115:LYS:HD2	71:Lh:116:TYR:H	1.83	0.43
81:L1:57:ASN:HB3	81:L1:182:GLN:NE2	2.33	0.43
84:CS:58:GLU:HA	84:CS:61:ILE:HG22	2.01	0.43
1:C2:86:A:H2'	1:C2:87:C:H6	1.84	0.43
1:C2:115:G:N2	1:C2:334:G:H21	2.17	0.43
1:C2:531:C:H1'	29:SY:61:ARG:NH1	2.33	0.43
1:C2:809:A:H2'	1:C2:810:G:C8	2.53	0.43
2:C1:307:A:H2'	2:C1:308:A:C8	2.54	0.43
2:C1:2618:G:H5'	46:LI:116:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:2981:U:OP2	39:LB:244:ARG:NH1	2.52	0.43
2:C1:2987:A:O2'	39:LB:259:HIS:HB3	2.19	0.43
9:SE:182:TYR:N	9:SE:226:PHE:O	2.51	0.43
10:SF:89:ILE:HD11	10:SF:172:ILE:HD11	2.00	0.43
30:SZ:93:SER:H	30:SZ:100:ILE:HG13	1.84	0.43
37:Sg:45:TRP:CH2	37:Sg:310:ILE:HD12	2.53	0.43
37:Sg:205:SER:HB3	37:Sg:210:LEU:HB2	2.00	0.43
40:LC:75:PRO:HB2	40:LC:89:ALA:HB3	2.00	0.43
40:LC:308:LYS:HE3	40:LC:308:LYS:HB3	1.78	0.43
43:LF:121:LYS:HB2	57:LT:133:ALA:HB3	2.00	0.43
46:LI:36:LEU:HD11	46:LI:69:ARG:HH11	1.84	0.43
48:LK:106:LEU:HA	48:LK:109:ILE:HG12	2.01	0.43
50:LM:21:VAL:HG21	50:LM:35:ILE:HG13	2.01	0.43
50:LM:128:ARG:HA	50:LM:131:VAL:HG12	2.01	0.43
67:Ld:61:LYS:HB2	67:Ld:61:LYS:HE3	1.87	0.43
83:CD:251:ASN:HD21	83:CD:253:LYS:HE3	1.83	0.43
84:CS:49:LYS:NZ	84:CS:50:ASN:H	2.17	0.43
1:C2:53:G:O2'	29:SY:106:GLN:NE2	2.52	0.43
1:C2:107:C:H2'	1:C2:108:A:C8	2.53	0.43
1:C2:976:G:N1	1:C2:1023:A:O2'	2.38	0.43
1:C2:980:G:H4'	1:C2:1776:A:H4'	2.00	0.43
1:C2:1334:U:O3'	25:SU:85:ARG:NH2	2.51	0.43
2:C1:370:U:H4'	2:C1:404:G:H5'	2.00	0.43
2:C1:2097:U:H2'	2:C1:2098:C:C6	2.54	0.43
2:C1:3358:U:H2'	2:C1:3359:A:C8	2.52	0.43
9:SE:175:PHE:HE1	9:SE:225:VAL:HG11	1.84	0.43
36:Sf:130:VAL:HG22	36:Sf:143:LYS:HB3	2.01	0.43
37:Sg:239:GLU:HB3	37:Sg:257:ALA:HB2	2.00	0.43
40:LC:142:VAL:HA	40:LC:145:ILE:HG13	2.00	0.43
42:LE:154:LEU:HD12	42:LE:157:GLN:NE2	2.33	0.43
44:LG:72:PRO:HG2	51:LN:18:VAL:HA	2.01	0.43
45:LH:78:MET:HE3	45:LH:78:MET:HB2	1.69	0.43
46:LI:135:ILE:HG22	46:LI:136:PHE:CD1	2.54	0.43
47:LJ:125:MET:HE2	47:LJ:125:MET:HB3	1.86	0.43
48:LK:130:LYS:HG2	48:LK:152:ILE:HG23	2.00	0.43
59:LV:53:SER:N	59:LV:56:ASP:OD2	2.37	0.43
73:Lj:39:TYR:CD1	73:Lj:40:PRO:HA	2.54	0.43
83:CD:823:ARG:NH2	83:CD:829:LYS:HG2	2.34	0.43
1:C2:859:A:C5	18:SN:73:ARG:HD3	2.53	0.43
2:C1:59:G:H2'	4:C3:33:A:H2'	2.01	0.43
2:C1:904:A:H2	38:LA:15:ILE:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:1340:G:H2'	2:C1:1341:U:C6	2.53	0.43
2:C1:1454:A:N6	2:C1:1879:A:O2'	2.52	0.43
2:C1:2526:C:H2'	2:C1:2527:G:H8	1.84	0.43
7:SC:230:TRP:CD2	27:SW:68:ARG:HD3	2.54	0.43
10:SF:127:GLN:HE22	10:SF:132:VAL:HB	1.82	0.43
12:SH:58:LEU:HB2	12:SH:90:VAL:HA	2.01	0.43
17:SM:31:VAL:HA	17:SM:34:THR:HG22	2.00	0.43
17:SM:42:ALA:HB3	17:SM:122:VAL:HB	2.01	0.43
18:SN:54:LEU:HD12	18:SN:58:HIS:HB2	2.00	0.43
22:SR:34:LEU:HD12	37:Sg:150:TRP:CH2	2.53	0.43
37:Sg:274:LEU:HD21	37:Sg:313:TRP:CE2	2.54	0.43
60:LW:6:ASP:OD1	60:LW:31:PHE:HA	2.18	0.43
82:P0:159:VAL:HG11	82:P0:165:VAL:HG22	2.00	0.43
83:CD:21:ASN:OD1	83:CD:123:ASP:HB2	2.19	0.43
83:CD:94:ASP:OD1	83:CD:94:ASP:N	2.45	0.43
83:CD:823:ARG:HE	83:CD:828:MET:HB2	1.84	0.43
83:CD:823:ARG:HH21	83:CD:828:MET:HB3	1.84	0.43
84:CS:131:ILE:HD12	84:CS:131:ILE:HA	1.91	0.43
1:C2:1226:A:O2'	1:C2:1230:A:O4'	2.37	0.42
2:C1:671:U:H2'	2:C1:672:A:C8	2.54	0.42
2:C1:874:U:N3	2:C1:2978:U:OP1	2.36	0.42
2:C1:2457:G:O2'	2:C1:2481:G:N2	2.52	0.42
2:C1:2696:A:N7	2:C1:2758:A:N6	2.67	0.42
2:C1:3319:U:H3	39:LB:167:ARG:HH21	1.66	0.42
5:SA:8:ASP:O	5:SA:54:TRP:NE1	2.51	0.42
9:SE:248:ILE:HA	9:SE:251:GLU:OE1	2.19	0.42
10:SF:120:ILE:HA	10:SF:123:VAL:HG12	1.99	0.42
10:SF:144:GLU:HG2	10:SF:225:ARG:HH22	1.84	0.42
12:SH:98:ILE:HG12	12:SH:121:VAL:HG11	2.01	0.42
30:SZ:90:LYS:NZ	30:SZ:103:ARG:O	2.45	0.42
39:LB:56:ILE:O	39:LB:73:VAL:HA	2.19	0.42
39:LB:59:ASP:OD1	39:LB:59:ASP:N	2.49	0.42
43:LF:40:LYS:HB3	43:LF:40:LYS:HE3	1.88	0.42
48:LK:38:SER:HB2	48:LK:41:LYS:HG2	2.01	0.42
48:LK:107:ASP:OD1	48:LK:108:GLU:N	2.52	0.42
65:Lb:16:ALA:HB1	65:Lb:21:ILE:HD11	2.01	0.42
69:Lf:56:SER:O	69:Lf:63:LYS:NZ	2.41	0.42
71:Lh:43:LYS:HA	71:Lh:46:THR:HG22	2.00	0.42
1:C2:307:G:OP1	16:SL:103:ARG:NH1	2.45	0.42
1:C2:782:U:H1'	29:SY:21:LYS:HE3	2.00	0.42
1:C2:902:G:OP2	19:SO:24:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:2464:U:H2'	2:C1:2465:G:C8	2.54	0.42
2:C1:2468:A:N1	2:C1:2477:G:O2'	2.48	0.42
2:C1:2507:C:H2'	2:C1:2508:U:H6	1.84	0.42
2:C1:3386:G:H5'	67:Ld:10:ARG:HH22	1.83	0.42
4:C3:84:C:O3'	62:LY:113:LYS:NZ	2.52	0.42
5:SA:90:ALA:HA	5:SA:95:ALA:HB3	2.01	0.42
5:SA:198:MET:HA	5:SA:199:PRO:HD3	1.95	0.42
9:SE:115:THR:O	9:SE:119:ALA:HB2	2.19	0.42
17:SM:129:GLU:H	17:SM:133:LEU:HD21	1.84	0.42
25:SU:44:ASN:HA	25:SU:47:GLN:OE1	2.18	0.42
33:Sc:16:LEU:HD23	33:Sc:16:LEU:HA	1.87	0.42
38:LA:20:THR:HA	38:LA:23:ARG:HG3	2.00	0.42
39:LB:79:VAL:HG21	39:LB:338:LEU:HD11	2.01	0.42
46:LI:101:LYS:HE2	46:LI:101:LYS:HB3	1.81	0.42
46:LI:115:MET:HE3	46:LI:115:MET:HB3	1.89	0.42
47:LJ:131:MET:HE3	47:LJ:131:MET:HB2	1.71	0.42
52:LO:9:ILE:HD13	52:LO:33:ILE:HG23	2.01	0.42
68:Le:23:ASP:OD1	68:Le:24:ARG:N	2.53	0.42
83:CD:165:LEU:HD23	83:CD:165:LEU:HA	1.89	0.42
83:CD:540:ILE:HA	83:CD:543:GLN:HG2	2.01	0.42
83:CD:615:ARG:HD3	83:CD:615:ARG:HA	1.50	0.42
1:C2:968:U:OP1	1:C2:1033:C:O2'	2.37	0.42
1:C2:1525:A:N3	1:C2:1589:C:O2'	2.46	0.42
2:C1:616:G:H2'	2:C1:617:G:C8	2.53	0.42
2:C1:640:U:H2'	2:C1:641:C:C6	2.54	0.42
2:C1:1395:G:O2'	4:C3:18:U:O2	2.37	0.42
2:C1:1635:G:N2	2:C1:1638:A:OP2	2.37	0.42
2:C1:1846:C:OP1	2:C1:1849:C:N4	2.40	0.42
2:C1:2244:A:H5''	38:LA:243:THR:HB	2.00	0.42
2:C1:3021:A:H61	2:C1:3032:A:H5''	1.84	0.42
6:SB:70:LEU:HD22	6:SB:82:ARG:HD2	2.02	0.42
9:SE:172:PHE:CD1	9:SE:174:LYS:HE3	2.53	0.42
17:SM:59:LEU:HA	17:SM:87:PRO:HB2	2.01	0.42
23:SS:117:LYS:HB2	23:SS:117:LYS:HE3	1.71	0.42
26:SV:55:LEU:HD13	26:SV:65:SER:HB2	2.01	0.42
40:LC:134:LEU:HD23	40:LC:134:LEU:HA	1.80	0.42
47:LJ:64:LYS:NZ	84:CS:26:VAL:HG22	2.33	0.42
61:LX:115:ARG:HD3	61:LX:121:LYS:HB2	2.01	0.42
81:L1:47:LYS:HB3	81:L1:47:LYS:HE3	1.74	0.42
1:C2:939:A:H2'	1:C2:940:A:C8	2.55	0.42
2:C1:671:U:H2'	2:C1:672:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:3121:U:H1'	2:C1:3122:A:H5''	2.02	0.42
9:SE:103:TYR:HE2	9:SE:184:THR:HG23	1.85	0.42
18:SN:88:LEU:O	18:SN:92:ILE:HG12	2.20	0.42
18:SN:114:ARG:HA	18:SN:114:ARG:HD3	1.87	0.42
20:SP:60:LEU:HD12	20:SP:60:LEU:HA	1.85	0.42
46:LI:135:ILE:HG22	46:LI:136:PHE:HD1	1.84	0.42
69:Lf:60:ARG:HD3	69:Lf:60:ARG:HA	1.86	0.42
74:Lk:62:ALA:O	74:Lk:66:ILE:HG13	2.19	0.42
1:C2:1521:G:O2'	1:C2:1523:G:OP2	2.30	0.42
2:C1:411:U:H2'	2:C1:412:G:H8	1.84	0.42
2:C1:571:U:H2'	2:C1:572:A:H8	1.84	0.42
2:C1:2442:G:H2'	2:C1:2443:A:H8	1.85	0.42
2:C1:3199:G:H2'	2:C1:3200:G:H8	1.85	0.42
3:C4:81:U:H2'	3:C4:82:G:H8	1.85	0.42
19:SO:18:ARG:HA	19:SO:82:LYS:O	2.19	0.42
27:SW:7:LEU:HD11	27:SW:37:PHE:HD2	1.83	0.42
30:SZ:42:LEU:HD23	30:SZ:75:LEU:HD11	2.02	0.42
31:Sa:47:ALA:HA	31:Sa:50:VAL:HG13	2.02	0.42
38:LA:60:LYS:HA	38:LA:60:LYS:HD3	1.89	0.42
82:P0:26:PHE:HZ	82:P0:93:LEU:HB3	1.84	0.42
83:CD:352:ARG:HG2	83:CD:355:GLN:HE22	1.85	0.42
1:C2:250:C:H2'	1:C2:251:A:C8	2.52	0.42
1:C2:835:U:H2'	1:C2:836:U:C6	2.54	0.42
1:C2:1434:U:O2'	1:C2:1436:A:OP1	2.28	0.42
1:C2:1776:A:H2'	1:C2:1777:G:C8	2.54	0.42
2:C1:269:G:OP2	51:LN:44:ARG:NH1	2.53	0.42
2:C1:335:G:OP2	62:LY:14:LYS:NZ	2.33	0.42
2:C1:929:A:O2'	73:Lj:49:TRP:O	2.37	0.42
2:C1:1497:C:H2'	2:C1:1498:A:C8	2.54	0.42
2:C1:1909:A:H2'	2:C1:1910:A:C8	2.55	0.42
2:C1:2705:A:OP1	41:LD:31:TYR:OH	2.22	0.42
3:C4:64:A:H5'	3:C4:65:G:H5''	2.01	0.42
3:C4:72:A:O2'	3:C4:74:C:OP1	2.28	0.42
5:SA:49:ASN:HB3	5:SA:52:LYS:HB2	2.01	0.42
8:SD:114:ALA:HB3	8:SD:117:ARG:HB2	2.01	0.42
10:SF:129:PRO:HA	10:SF:132:VAL:HG12	2.00	0.42
18:SN:24:ALA:O	18:SN:27:LYS:NZ	2.52	0.42
37:Sg:248:ASN:ND2	37:Sg:297:ASP:O	2.53	0.42
38:LA:116:VAL:HG11	38:LA:134:VAL:HG11	2.02	0.42
54:LQ:65:SER:OG	54:LQ:90:ASP:OD2	2.37	0.42
64:La:85:ASP:OD1	64:La:86:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Le:82:LEU:HD23	68:Le:82:LEU:HA	1.86	0.42
80:CE:102:LEU:HA	80:CE:102:LEU:HD23	1.80	0.42
83:CD:416:PRO:HB3	83:CD:480:VAL:HG11	2.01	0.42
2:C1:515:C:H2'	2:C1:516:A:C8	2.53	0.42
2:C1:597:G:H2'	2:C1:598:A:H8	1.84	0.42
2:C1:1666:G:H2'	2:C1:1667:A:H8	1.85	0.42
2:C1:2547:A:H2'	2:C1:2548:C:O4'	2.19	0.42
4:C3:34:U:H5'	73:Lj:78:PHE:HE2	1.84	0.42
6:SB:22:ASP:OD2	6:SB:25:THR:OG1	2.24	0.42
9:SE:154:ILE:HA	9:SE:174:LYS:HZ1	1.83	0.42
12:SH:81:LEU:HD13	12:SH:90:VAL:HG21	2.02	0.42
57:LT:69:LYS:NZ	57:LT:70:SER:OG	2.52	0.42
64:La:74:ASN:HB3	64:La:115:LYS:HB3	2.01	0.42
80:CE:91:GLN:HB3	80:CE:103:MET:HB3	2.02	0.42
81:L1:17:LEU:HD11	81:L1:179:LEU:HD12	2.01	0.42
1:C2:191:C:O2'	1:C2:192:U:O5'	2.33	0.42
1:C2:836:U:H2'	1:C2:837:G:C8	2.54	0.42
2:C1:1157:G:O2'	2:C1:1169:A:N3	2.47	0.42
2:C1:2540:A:H2'	2:C1:2541:U:H2'	2.01	0.42
2:C1:3275:U:H5'	69:Lf:68:TRP:HZ2	1.85	0.42
2:C1:3287:U:O4	2:C1:3288:G:O6	2.38	0.42
5:SA:49:ASN:O	5:SA:53:THR:HG23	2.19	0.42
14:SJ:126:ARG:HD3	35:Se:33:ARG:HE	1.84	0.42
24:ST:12:GLN:O	24:ST:15:ILE:HG22	2.19	0.42
27:SW:106:THR:HG21	27:SW:121:VAL:HG13	2.02	0.42
37:Sg:224:ASN:ND2	37:Sg:227:ALA:H	2.18	0.42
38:LA:104:LEU:HD22	38:LA:136:ILE:HD11	2.01	0.42
39:LB:300:ARG:HA	39:LB:300:ARG:HD2	1.87	0.42
60:LW:2:LYS:HD3	60:LW:3:VAL:H	1.85	0.42
69:Lf:14:LEU:HD11	69:Lf:31:LYS:HB2	2.02	0.42
81:L1:12:HIS:HA	81:L1:15:GLU:HG2	2.02	0.42
81:L1:212:PRO:HB3	81:L1:214:PHE:HE1	1.83	0.42
83:CD:205:ALA:HB2	83:CD:245:TRP:CD1	2.55	0.42
1:C2:231:U:C2	1:C2:234:G:O6	2.73	0.42
1:C2:885:G:H5'	6:SB:138:PHE:HZ	1.85	0.42
2:C1:532:A:H2'	2:C1:533:A:C8	2.55	0.42
2:C1:896:A:H5'	38:LA:183:GLY:HA2	2.02	0.42
2:C1:2094:C:H2'	2:C1:2095:G:H8	1.84	0.42
21:SQ:38:LEU:HD12	21:SQ:38:LEU:HA	1.85	0.42
35:Se:20:LYS:HA	35:Se:20:LYS:HD3	1.89	0.42
39:LB:304:THR:OG1	39:LB:305:ILE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LC:205:PRO:O	40:LC:225:VAL:HA	2.20	0.42
42:LE:40:LEU:HD11	42:LE:54:TYR:HB2	2.02	0.42
54:LQ:38:ARG:NE	54:LQ:39:ARG:HG3	2.35	0.42
63:LZ:97:SER:O	63:LZ:101:PHE:N	2.53	0.42
67:Ld:112:ASP:N	67:Ld:112:ASP:OD1	2.52	0.42
81:L1:36:VAL:HG12	81:L1:204:LEU:HD12	2.02	0.42
83:CD:222:ILE:HD12	83:CD:241:MET:HB2	2.01	0.42
83:CD:379:MET:HA	83:CD:469:LEU:O	2.20	0.42
83:CD:746:VAL:HA	83:CD:749:LYS:HG2	2.01	0.42
1:C2:918:U:H2'	1:C2:919:A:C8	2.55	0.42
1:C2:1450:U:H2'	1:C2:1451:C:C6	2.55	0.42
1:C2:1483:A:H2	1:C2:1607:G:H1'	1.84	0.42
1:C2:1487:A:H2'	1:C2:1488:G:C8	2.55	0.42
2:C1:592:A:O2'	42:LE:20:LYS:NZ	2.52	0.42
2:C1:1104:G:H2'	2:C1:1105:A:H8	1.84	0.42
2:C1:1827:C:H2'	2:C1:1828:A:C8	2.54	0.42
3:C4:107:C:H2'	3:C4:108:A:C8	2.54	0.42
13:SI:27:PHE:CD1	13:SI:28:GLU:HG2	2.55	0.42
13:SI:76:THR:HG21	13:SI:104:ILE:HD12	2.01	0.42
16:SL:109:VAL:HG11	16:SL:125:VAL:HG11	2.01	0.42
23:SS:42:TYR:HA	23:SS:85:PHE:HE2	1.85	0.42
47:LJ:95:ASN:O	47:LJ:102:PHE:HB2	2.20	0.42
47:LJ:172:LEU:HG	47:LJ:173:ASP:H	1.84	0.42
49:LL:168:ARG:HD3	49:LL:172:LEU:HG	2.01	0.42
50:LM:47:ASP:OD2	50:LM:78:THR:HG22	2.20	0.42
54:LQ:147:ARG:HB3	54:LQ:150:VAL:HG23	2.02	0.42
58:LU:19:VAL:HG12	58:LU:105:LEU:HD22	2.00	0.42
58:LU:56:VAL:HG22	58:LU:65:VAL:HG22	2.02	0.42
78:Lo:46:LYS:HE2	78:Lo:54:THR:HB	2.01	0.42
81:L1:36:VAL:HA	81:L1:203:SER:O	2.20	0.42
83:CD:568:GLU:HA	83:CD:592:PRO:HG3	2.02	0.42
1:C2:482:U:H2'	1:C2:483:A:H8	1.84	0.41
1:C2:639:U:H2'	12:SH:101:LYS:HB2	2.02	0.41
1:C2:1225:U:H3'	1:C2:1226:A:C8	2.54	0.41
1:C2:1280:C:H2'	1:C2:1281:G:C8	2.54	0.41
1:C2:1407:U:H2'	1:C2:1408:G:C8	2.55	0.41
1:C2:1440:C:H4'	83:CD:657:HIS:NE2	2.36	0.41
2:C1:407:A:C2	4:C3:17:A:H1'	2.56	0.41
2:C1:696:C:OP2	40:LC:119:ARG:NH2	2.52	0.41
2:C1:1546:A:O2'	51:LN:104:GLU:OE2	2.31	0.41
3:C4:71:G:H2'	3:C4:72:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SD:94:ARG:NH2	84:CS:134:ASP:OD1	2.41	0.41
15:SK:70:GLU:O	15:SK:73:VAL:N	2.51	0.41
21:SQ:75:VAL:HA	21:SQ:78:VAL:HG12	2.02	0.41
22:SR:57:LEU:HD23	22:SR:57:LEU:HA	1.91	0.41
37:Sg:242:SER:HB3	37:Sg:255:ALA:HB3	2.02	0.41
47:LJ:92:ARG:O	47:LJ:95:ASN:CB	2.36	0.41
52:LO:155:LYS:HB2	52:LO:155:LYS:HE2	1.77	0.41
67:Ld:80:ASN:ND2	67:Ld:88:PRO:HA	2.35	0.41
74:Lk:12:LEU:HB3	74:Lk:16:ARG:NH1	2.35	0.41
80:CE:38:PRO:HG2	80:CE:65:PHE:CE2	2.55	0.41
82:P0:69:ASP:OD1	82:P0:69:ASP:N	2.52	0.41
82:P0:139:LEU:HD23	82:P0:139:LEU:HA	1.91	0.41
83:CD:123:ASP:OD2	83:CD:399:ARG:NH2	2.53	0.41
83:CD:220:PHE:HB3	83:CD:328:LEU:HD13	2.02	0.41
1:C2:538:A:O4'	1:C2:543:C:N4	2.53	0.41
1:C2:773:C:O2'	1:C2:787:G:N2	2.53	0.41
1:C2:885:G:H2'	1:C2:886:U:C6	2.55	0.41
1:C2:1432:U:H4'	1:C2:1433:G:H5''	2.01	0.41
1:C2:1508:U:H2'	1:C2:1509:C:C6	2.56	0.41
2:C1:62:A:OP1	51:LN:162:ARG:NH2	2.54	0.41
2:C1:129:U:H2'	2:C1:130:A:C8	2.55	0.41
2:C1:542:G:H1	2:C1:549:U:H3	1.67	0.41
2:C1:662:U:H2'	2:C1:663:C:C6	2.55	0.41
2:C1:1119:C:H2'	2:C1:1120:A:H8	1.85	0.41
5:SA:135:GLU:HA	5:SA:138:TYR:HD2	1.85	0.41
7:SC:108:ASN:OD1	7:SC:108:ASN:N	2.53	0.41
7:SC:140:ARG:HH21	7:SC:229:LEU:HD13	1.85	0.41
9:SE:18:TRP:HH2	9:SE:31:PRO:HD3	1.85	0.41
9:SE:62:LYS:HD2	9:SE:80:THR:HG21	2.01	0.41
12:SH:64:VAL:HA	12:SH:67:LEU:HD23	2.02	0.41
12:SH:141:ARG:HH21	12:SH:143:LEU:HD11	1.84	0.41
23:SS:115:ARG:O	23:SS:119:ILE:HG23	2.20	0.41
24:ST:135:ILE:HA	24:ST:138:GLN:HG3	2.02	0.41
25:SU:57:ARG:HH11	25:SU:89:ARG:NH1	2.17	0.41
26:SV:38:LYS:HD2	26:SV:49:GLU:HG3	2.02	0.41
39:LB:82:PRO:HA	39:LB:83:PRO:HD3	1.95	0.41
40:LC:281:ILE:HD12	54:LQ:29:LEU:HG	2.02	0.41
41:LD:34:LYS:HE2	57:LT:30:TYR:CZ	2.55	0.41
46:LI:6:ALA:O	46:LI:10:ARG:HB2	2.20	0.41
46:LI:145:LYS:HB2	46:LI:145:LYS:HE3	1.87	0.41
49:LL:64:LYS:O	49:LL:67:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CD:203:TYR:HB3	83:CD:205:ALA:H	1.84	0.41
2:C1:68:C:O3'	51:LN:177:GLY:HA2	2.21	0.41
2:C1:668:G:O2'	54:LQ:164:ARG:NH1	2.53	0.41
2:C1:1063:G:C6	57:LT:109:VAL:HG23	2.55	0.41
2:C1:1246:G:H1'	2:C1:1264:G:H2'	2.02	0.41
2:C1:1269:U:N3	2:C1:1272:C:OP2	2.47	0.41
2:C1:1643:A:H2'	2:C1:1644:C:C2	2.56	0.41
2:C1:1831:U:O2'	4:C3:114:G:OP1	2.29	0.41
2:C1:2669:G:H2'	2:C1:2670:G:H8	1.85	0.41
2:C1:2742:C:H2'	2:C1:2743:A:H8	1.85	0.41
6:SB:157:GLN:O	6:SB:161:ILE:HG12	2.20	0.41
9:SE:141:THR:OG1	9:SE:143:ASP:OD1	2.30	0.41
11:SG:184:LEU:O	11:SG:188:ARG:HG2	2.20	0.41
13:SI:137:LYS:O	13:SI:141:ARG:HG3	2.20	0.41
14:SJ:139:GLN:OE1	14:SJ:140:ILE:N	2.53	0.41
21:SQ:28:LEU:HG	21:SQ:64:ASP:OD1	2.20	0.41
31:Sa:93:LYS:HE3	31:Sa:93:LYS:HB3	1.88	0.41
34:Sd:33:LYS:O	34:Sd:36:LEU:HD13	2.20	0.41
35:Se:55:ARG:HH21	35:Se:56:MET:HB3	1.86	0.41
37:Sg:72:THR:HG21	37:Sg:114:ASP:HA	2.02	0.41
37:Sg:191:ASP:OD1	37:Sg:191:ASP:N	2.52	0.41
38:LA:188:LYS:O	38:LA:192:LYS:HG2	2.20	0.41
47:LJ:9:MET:HE2	47:LJ:134:PRO:HB2	2.02	0.41
47:LJ:174:LYS:HA	47:LJ:174:LYS:HD3	1.78	0.41
53:LP:64:ASN:O	53:LP:80:LYS:NZ	2.38	0.41
56:LS:23:LYS:HD3	57:LT:146:ASN:HD21	1.86	0.41
56:LS:90:MET:HE1	56:LS:114:HIS:CD2	2.55	0.41
71:Lh:30:GLU:OE2	71:Lh:34:GLN:NE2	2.50	0.41
83:CD:85:ASP:O	83:CD:89:ILE:HG13	2.20	0.41
1:C2:31:C:O2'	1:C2:547:U:OP1	2.38	0.41
1:C2:486:G:H2'	1:C2:487:G:C8	2.54	0.41
1:C2:742:U:O2'	1:C2:744:U:OP2	2.22	0.41
1:C2:1425:A:H4'	7:SC:92:ALA:HB1	2.01	0.41
2:C1:631:U:H2'	2:C1:632:G:C8	2.55	0.41
2:C1:1460:A:H2'	2:C1:1461:A:C8	2.55	0.41
2:C1:2486:A:OP2	81:L1:105:LYS:NZ	2.35	0.41
2:C1:2916:U:H2'	2:C1:2917:G:H8	1.85	0.41
6:SB:84:ILE:HD13	6:SB:103:MET:HG2	2.03	0.41
8:SD:18:TYR:HD1	8:SD:39:VAL:HG23	1.85	0.41
12:SH:91:ILE:HD12	12:SH:91:ILE:HA	1.95	0.41
19:SO:125:SER:OG	19:SO:126:THR:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SV:14:PRO:HB2	26:SV:23:ILE:HD12	2.02	0.41
30:SZ:93:SER:HB2	30:SZ:100:ILE:HD11	2.03	0.41
31:Sa:38:ARG:HA	31:Sa:38:ARG:HD3	1.69	0.41
37:Sg:23:LEU:HD21	37:Sg:310:ILE:HD13	2.03	0.41
39:LB:117:ARG:HA	39:LB:175:LYS:HG3	2.02	0.41
41:LD:146:LEU:HD22	41:LD:163:LEU:HD13	2.03	0.41
45:LH:27:VAL:HG12	45:LH:82:VAL:HG11	2.01	0.41
50:LM:113:THR:OG1	50:LM:114:ASP:N	2.54	0.41
63:LZ:17:ARG:H	70:Lg:74:ARG:HG3	1.85	0.41
63:LZ:53:VAL:HG12	63:LZ:65:ARG:HD3	2.03	0.41
79:Lp:76:ALA:O	79:Lp:80:ARG:HG3	2.19	0.41
83:CD:278:LEU:HD23	83:CD:281:ILE:HD12	2.01	0.41
83:CD:331:ALA:O	83:CD:335:LEU:HB3	2.20	0.41
83:CD:405:VAL:HG12	83:CD:448:CYS:HB3	2.01	0.41
1:C2:625:C:H2'	1:C2:626:U:C6	2.56	0.41
1:C2:948:G:H2'	1:C2:949:C:C6	2.54	0.41
1:C2:1101:G:OP1	28:SX:3:LYS:NZ	2.47	0.41
2:C1:12:A:H2'	2:C1:13:A:C8	2.55	0.41
2:C1:2407:C:H2'	2:C1:2408:U:H6	1.84	0.41
2:C1:3163:A:C6	2:C1:3288:G:N1	2.89	0.41
5:SA:16:LEU:HB3	5:SA:172:LEU:HD21	2.01	0.41
8:SD:194:LYS:HA	8:SD:194:LYS:HD3	1.87	0.41
10:SF:124:LEU:O	30:SZ:58:ARG:NH1	2.54	0.41
15:SK:30:ALA:HA	15:SK:38:LYS:HD2	2.03	0.41
25:SU:26:LEU:HD21	25:SU:89:ARG:HB2	2.02	0.41
26:SV:74:GLN:NE2	26:SV:83:TRP:H	2.19	0.41
27:SW:6:VAL:HG22	27:SW:34:ILE:HD11	2.02	0.41
28:SX:109:ARG:HD3	28:SX:114:LYS:HB3	2.03	0.41
28:SX:142:LYS:O	28:SX:144:ARG:NH1	2.54	0.41
31:Sa:12:LYS:HE3	31:Sa:16:GLY:H	1.84	0.41
44:LG:161:GLU:OE2	51:LN:11:GLN:HG2	2.21	0.41
46:LI:163:GLN:OE1	46:LI:163:GLN:N	2.53	0.41
59:LV:26:ALA:HB2	59:LV:99:ALA:HB1	2.02	0.41
68:Le:111:ARG:HD2	68:Le:111:ARG:HA	1.75	0.41
69:Lf:57:LYS:HE2	69:Lf:65:ARG:HH22	1.86	0.41
70:Lg:91:ARG:O	70:Lg:95:ILE:HG12	2.21	0.41
78:Lo:67:LYS:CG	78:Lo:87:ARG:HE	2.31	0.41
80:CE:91:GLN:NE2	81:L1:121:PRO:HG2	2.36	0.41
83:CD:731:VAL:HA	83:CD:795:GLN:O	2.21	0.41
1:C2:368:U:O2'	1:C2:603:U:O2'	2.28	0.41
1:C2:1195:C:N4	21:SQ:141:SER:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:1479:A:H5''	24:ST:60:SER:OG	2.19	0.41
1:C2:1619:C:H2'	1:C2:1620:C:H6	1.84	0.41
2:C1:669:U:H1'	2:C1:1110:U:H4'	2.01	0.41
2:C1:1155:C:OP2	43:LF:94:LYS:NZ	2.52	0.41
2:C1:1193:A:OP2	52:LO:49:ARG:NH2	2.54	0.41
2:C1:2106:A:H2'	2:C1:2107:A:C8	2.55	0.41
2:C1:2727:A:OP2	2:C1:2728:G:N2	2.48	0.41
2:C1:2815:G:N2	2:C1:2818:U:O2	2.49	0.41
2:C1:3192:U:OP1	52:LO:176:LYS:NZ	2.53	0.41
2:C1:3227:A:O2'	50:LM:133:LYS:NZ	2.51	0.41
2:C1:3357:U:H2'	2:C1:3358:U:C6	2.55	0.41
13:SI:116:HIS:CE1	13:SI:146:ARG:HD3	2.55	0.41
21:SQ:87:LYS:HA	21:SQ:90:VAL:HG12	2.02	0.41
22:SR:78:ARG:HA	22:SR:81:LYS:HG2	2.02	0.41
37:Sg:141:LEU:HD23	37:Sg:141:LEU:HA	1.89	0.41
39:LB:17:LEU:HD21	39:LB:233:TRP:HH2	1.86	0.41
39:LB:79:VAL:HG23	39:LB:322:ILE:HB	2.02	0.41
44:LG:64:ILE:HG23	44:LG:68:ARG:NH1	2.35	0.41
75:LI:41:ARG:HD2	75:LI:41:ARG:HA	1.92	0.41
83:CD:39:LEU:HD21	83:CD:334:LEU:HD12	2.01	0.41
83:CD:236:ASP:OD1	83:CD:236:ASP:N	2.51	0.41
1:C2:555:A:H2'	1:C2:556:A:C8	2.56	0.41
1:C2:826:U:H2'	1:C2:827:C:C6	2.56	0.41
1:C2:1545:A:H3'	23:SS:134:ARG:HH12	1.85	0.41
3:C4:96:U:OP1	56:LS:43:TYR:OH	2.32	0.41
11:SG:122:GLU:HA	11:SG:126:ASP:HB2	2.02	0.41
16:SL:85:VAL:HA	16:SL:108:PRO:HA	2.02	0.41
22:SR:25:THR:O	22:SR:31:ASN:ND2	2.40	0.41
37:Sg:144:LEU:HD12	37:Sg:181:TRP:CZ3	2.56	0.41
42:LE:172:HIS:CD2	42:LE:173:MET:HE2	2.54	0.41
47:LJ:12:LEU:HD12	47:LJ:162:TRP:CG	2.56	0.41
48:LK:80:LEU:HD23	48:LK:80:LEU:HA	1.95	0.41
57:LT:43:LYS:HG3	57:LT:58:GLN:HE22	1.86	0.41
57:LT:106:LEU:HA	57:LT:109:VAL:HG12	2.03	0.41
78:Lo:72:LEU:O	78:Lo:80:ARG:HA	2.20	0.41
81:L1:33:GLU:O	81:L1:206:VAL:HA	2.20	0.41
2:C1:20:A:H2'	2:C1:21:G:C8	2.55	0.41
2:C1:949:C:O2'	2:C1:971:G:OP1	2.33	0.41
2:C1:985:U:H2'	2:C1:986:U:H6	1.86	0.41
2:C1:1192:C:H41	2:C1:1301:A:H1'	1.86	0.41
2:C1:1913:A:N3	2:C1:2120:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:2344:U:H2'	2:C1:2345:A:H8	1.85	0.41
2:C1:2555:G:N1	70:Lg:96:GLU:OE2	2.53	0.41
6:SB:129:THR:OG1	6:SB:130:SER:N	2.52	0.41
7:SC:116:LYS:HG2	7:SC:127:ALA:HB3	2.02	0.41
9:SE:65:LEU:HD23	9:SE:65:LEU:HA	1.89	0.41
14:SJ:109:LEU:HB2	14:SJ:146:PHE:HB3	2.03	0.41
17:SM:50:LYS:HA	17:SM:50:LYS:HD2	1.85	0.41
18:SN:62:GLN:O	18:SN:66:ILE:HG12	2.21	0.41
23:SS:125:ILE:HD11	84:CS:57:ASN:OD1	2.20	0.41
38:LA:36:GLU:HG3	38:LA:91:GLY:HA2	2.02	0.41
40:LC:99:MET:HE2	40:LC:102:PRO:HA	2.01	0.41
40:LC:156:LEU:HA	40:LC:159:ILE:HG12	2.02	0.41
43:LF:26:VAL:O	43:LF:30:ARG:HG2	2.20	0.41
43:LF:96:PRO:O	43:LF:100:ARG:HG3	2.20	0.41
47:LJ:15:GLU:HB3	47:LJ:130:VAL:HG23	2.03	0.41
64:La:73:LEU:HD13	64:La:109:TYR:CE2	2.56	0.41
66:Lc:78:GLY:HA2	66:Lc:81:VAL:HG12	2.02	0.41
83:CD:283:ARG:HH22	83:CD:303:LEU:HD21	1.86	0.41
1:C2:17:C:H2'	1:C2:18:C:C6	2.56	0.41
1:C2:417:A:H5'	1:C2:418:G:C8	2.55	0.41
1:C2:513:U:H2'	1:C2:514:G:C8	2.55	0.41
1:C2:895:G:H2'	1:C2:896:U:C6	2.56	0.41
2:C1:86:G:O2'	2:C1:98:G:O6	2.33	0.41
2:C1:155:G:H5''	2:C1:156:G:C8	2.56	0.41
2:C1:269:G:OP1	51:LN:47:LYS:HE3	2.21	0.41
2:C1:729:C:O2'	54:LQ:79:LYS:NZ	2.32	0.41
2:C1:1910:A:H2'	2:C1:1911:A:C8	2.56	0.41
2:C1:2413:A:H2'	2:C1:2414:G:H8	1.85	0.41
2:C1:2486:A:O2'	2:C1:2487:U:O4'	2.37	0.41
2:C1:2611:U:H2'	2:C1:2612:U:C6	2.56	0.41
2:C1:2908:G:H4'	76:Lm:114:LYS:HE3	2.03	0.41
2:C1:3114:A:O2'	45:LH:62:ARG:NH2	2.54	0.41
2:C1:3178:A:C2	52:LO:115:LYS:HG3	2.56	0.41
7:SC:80:VAL:HG23	7:SC:102:VAL:HG12	2.03	0.41
9:SE:115:THR:O	9:SE:119:ALA:CB	2.68	0.41
9:SE:121:TYR:HA	9:SE:163:ASP:HA	2.02	0.41
10:SF:55:ASP:OD1	10:SF:56:ALA:N	2.54	0.41
19:SO:21:ALA:HB1	19:SO:95:GLY:H	1.86	0.41
20:SP:72:LYS:HA	20:SP:73:PRO:HD3	1.94	0.41
25:SU:53:LYS:HE3	25:SU:92:ASP:H	1.84	0.41
29:SY:39:GLU:HA	29:SY:42:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Se:30:PRO:HB2	35:Se:34:ALA:HB1	2.03	0.41
37:Sg:266:ASP:OD1	37:Sg:266:ASP:N	2.53	0.41
41:LD:60:ILE:HB	41:LD:80:SER:HB2	2.03	0.41
42:LE:65:ILE:O	42:LE:76:LEU:HA	2.20	0.41
52:LO:8:VAL:O	52:LO:118:VAL:HG12	2.21	0.41
55:LR:95:TRP:HE3	55:LR:98:ARG:HH21	1.69	0.41
66:Lc:99:ASP:OD1	66:Lc:99:ASP:N	2.49	0.41
72:Li:85:ALA:O	72:Li:88:GLU:HG3	2.21	0.41
72:Li:91:ASN:HA	72:Li:94:ILE:HG22	2.02	0.41
76:Lm:109:ASN:ND2	76:Lm:119:ASN:HB3	2.35	0.41
81:L1:54:LYS:HD3	81:L1:150:ASP:OD1	2.21	0.41
83:CD:42:ARG:HH21	83:CD:331:ALA:HA	1.85	0.41
83:CD:205:ALA:C	83:CD:241:MET:HE1	2.45	0.41
83:CD:257:TRP:CD1	83:CD:257:TRP:H	2.38	0.41
1:C2:459:G:OP1	29:SY:109:LYS:NZ	2.48	0.41
2:C1:1460:A:H2'	2:C1:1461:A:H8	1.86	0.41
2:C1:2597:U:O2	51:LN:125:SER:OG	2.34	0.41
2:C1:3252:G:H2'	2:C1:3253:G:H8	1.86	0.41
4:C3:13:A:O2'	53:LP:121:GLN:O	2.37	0.41
7:SC:81:MET:HG3	7:SC:211:LEU:HD11	2.03	0.41
9:SE:98:ASN:HB2	9:SE:114:ILE:HG13	2.02	0.41
12:SH:72:LYS:HD3	12:SH:72:LYS:HA	1.95	0.41
17:SM:71:ILE:O	17:SM:75:VAL:HG12	2.20	0.41
40:LC:286:VAL:HG11	54:LQ:31:LYS:HD2	2.02	0.41
40:LC:301:PRO:O	54:LQ:39:ARG:NH2	2.54	0.41
44:LG:83:ASP:HB3	44:LG:86:THR:HG22	2.03	0.41
67:Ld:51:LEU:HB3	67:Ld:55:LEU:HD23	2.02	0.41
1:C2:1785:U:H2'	1:C2:1786:G:H8	1.86	0.40
2:C1:68:C:OP2	2:C1:301:G:N2	2.48	0.40
2:C1:753:C:H2'	2:C1:754:G:H8	1.85	0.40
2:C1:1104:G:H2'	2:C1:1105:A:C8	2.56	0.40
2:C1:1129:A:H2'	2:C1:1130:A:C8	2.55	0.40
2:C1:1249:G:H2'	2:C1:1250:G:C8	2.56	0.40
2:C1:2451:G:H2'	2:C1:2452:G:C8	2.56	0.40
5:SA:183:ARG:O	26:SV:44:ARG:NH2	2.54	0.40
7:SC:151:PRO:HG2	26:SV:9:VAL:HG11	2.03	0.40
9:SE:21:ASP:OD2	9:SE:24:SER:OG	2.33	0.40
21:SQ:22:VAL:HG22	21:SQ:65:ILE:HG22	2.03	0.40
39:LB:308:MET:HE3	39:LB:373:PRO:HD3	2.04	0.40
44:LG:101:THR:HG22	44:LG:104:GLU:HG2	2.04	0.40
44:LG:214:LEU:O	44:LG:218:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LS:25:PHE:HE1	57:LT:149:GLN:HE21	1.69	0.40
74:Lk:60:GLY:HA2	74:Lk:63:LYS:NZ	2.36	0.40
81:L1:173:GLU:OE1	81:L1:173:GLU:N	2.51	0.40
82:P0:4:ILE:HG23	82:P0:7:LYS:HE3	2.03	0.40
1:C2:235:G:H2'	1:C2:236:A:H8	1.86	0.40
1:C2:919:A:H2'	1:C2:920:U:C6	2.57	0.40
2:C1:528:U:H2'	2:C1:529:A:H8	1.86	0.40
2:C1:980:A:H5'	86:C1:3406:T1C:H9	1.86	0.40
2:C1:2442:G:H2'	2:C1:2443:A:C8	2.56	0.40
20:SP:31:GLU:HA	20:SP:34:VAL:HG22	2.03	0.40
23:SS:56:LYS:HZ2	23:SS:61:LEU:HG	1.86	0.40
40:LC:188:ARG:NE	40:LC:197:ARG:O	2.43	0.40
56:LS:80:ARG:HG2	56:LS:122:HIS:HB2	2.03	0.40
57:LT:17:ARG:HA	57:LT:17:ARG:HD2	1.90	0.40
60:LW:6:ASP:HB3	60:LW:11:ALA:H	1.87	0.40
72:Li:85:ALA:O	72:Li:89:GLU:HG3	2.21	0.40
83:CD:386:VAL:HA	83:CD:387:PRO:HD3	1.88	0.40
83:CD:593:ILE:HD13	83:CD:593:ILE:HG21	1.91	0.40
1:C2:1222:C:H2'	1:C2:1223:A:C8	2.56	0.40
1:C2:1393:C:H2'	1:C2:1394:G:C8	2.54	0.40
2:C1:1312:C:O2'	52:LO:83:ALA:O	2.39	0.40
2:C1:2103:U:H2'	2:C1:2104:A:C8	2.56	0.40
2:C1:3204:C:H2'	2:C1:3205:G:C8	2.56	0.40
3:C4:4:U:H2'	3:C4:5:G:C8	2.56	0.40
5:SA:116:LYS:HA	5:SA:116:LYS:HD3	1.91	0.40
14:SJ:80:LEU:HA	14:SJ:83:VAL:HG12	2.04	0.40
21:SQ:110:THR:HA	21:SQ:113:ASP:HB3	2.03	0.40
24:ST:65:ILE:HG21	24:ST:114:VAL:HG12	2.03	0.40
29:SY:44:LEU:HA	29:SY:44:LEU:HD23	1.86	0.40
40:LC:233:LEU:HD12	40:LC:238:LEU:HD21	2.02	0.40
46:LI:71:CYS:SG	46:LI:72:ALA:N	2.94	0.40
49:LL:5:LYS:O	49:LL:7:LEU:N	2.54	0.40
50:LM:123:LEU:HD23	50:LM:123:LEU:HA	1.85	0.40
54:LQ:90:ASP:O	54:LQ:113:LYS:NZ	2.49	0.40
57:LT:8:ARG:NH1	57:LT:52:MET:HE1	2.35	0.40
57:LT:17:ARG:NH1	57:LT:47:SER:HB3	2.36	0.40
67:Ld:80:ASN:ND2	67:Ld:87:ASN:O	2.50	0.40
69:Lf:20:LYS:HD2	69:Lf:21:ARG:NH2	2.37	0.40
1:C2:304:U:H5''	16:SL:136:ARG:HD3	2.03	0.40
1:C2:696:C:H4'	1:C2:697:C:H6	1.86	0.40
1:C2:1274:C:H5	84:CS:96:ARG:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:150:A:H2'	2:C1:151:A:H5'	2.03	0.40
2:C1:591:G:O2'	42:LE:17:ALA:O	2.33	0.40
2:C1:792:G:H2'	2:C1:793:C:C6	2.57	0.40
2:C1:1486:G:H21	70:Lg:6:THR:HG22	1.86	0.40
2:C1:1729:A:N6	79:Lp:42:CYS:HA	2.37	0.40
2:C1:2219:A:H2'	2:C1:2220:A:C8	2.56	0.40
2:C1:3086:A:OP1	39:LB:367:LYS:NZ	2.55	0.40
2:C1:3295:A:H2'	2:C1:3296:A:C8	2.57	0.40
8:SD:119:ALA:O	8:SD:123:VAL:HG23	2.21	0.40
9:SE:52:LEU:HD23	9:SE:52:LEU:HA	1.98	0.40
9:SE:53:LYS:HE2	9:SE:53:LYS:HB2	1.95	0.40
25:SU:66:SER:HA	25:SU:80:GLU:O	2.22	0.40
27:SW:77:PRO:HD3	28:SX:7:ARG:HG3	2.03	0.40
39:LB:188:ILE:HD13	39:LB:191:LYS:HD2	2.04	0.40
41:LD:39:GLN:NE2	41:LD:43:LYS:HD2	2.36	0.40
44:LG:50:VAL:HG21	61:LX:27:ARG:HD2	2.03	0.40
57:LT:57:TYR:CG	57:LT:89:LEU:HD21	2.56	0.40
82:P0:76:LEU:HD23	82:P0:76:LEU:HA	1.89	0.40
83:CD:724:ILE:HD11	83:CD:808:PRO:HB3	2.04	0.40
1:C2:284:G:N7	11:SG:188:ARG:NH1	2.70	0.40
1:C2:540:G:H1'	1:C2:542:A:C8	2.57	0.40
2:C1:165:A:H2'	2:C1:166:C:C6	2.57	0.40
2:C1:289:A:OP2	51:LN:170:LYS:NZ	2.54	0.40
2:C1:632:G:H21	69:Lf:23:ASN:HD21	1.68	0.40
2:C1:1259:A:H2'	2:C1:1260:A:C8	2.57	0.40
2:C1:1534:A:H2'	2:C1:1535:A:C8	2.57	0.40
2:C1:1561:G:H2'	2:C1:1562:C:C6	2.56	0.40
2:C1:2154:U:H2'	2:C1:2155:G:C8	2.56	0.40
2:C1:2397:A:H5'	2:C1:2398:A:H5''	2.02	0.40
10:SF:36:ALA:O	10:SF:39:GLU:HG2	2.22	0.40
14:SJ:99:LEU:HA	14:SJ:99:LEU:HD13	1.90	0.40
16:SL:16:GLN:HA	16:SL:17:PRO:HD3	1.98	0.40
16:SL:26:LYS:HB3	16:SL:26:LYS:HE3	1.94	0.40
20:SP:59:LYS:HE2	20:SP:59:LYS:HB3	1.91	0.40
23:SS:57:ARG:CZ	30:SZ:40:VAL:HG21	2.51	0.40
30:SZ:50:ILE:O	30:SZ:54:VAL:HG23	2.22	0.40
40:LC:129:THR:HG21	40:LC:248:VAL:HB	2.04	0.40
42:LE:176:PHE:O	50:LM:113:THR:OG1	2.32	0.40
45:LH:90:MET:HB2	45:LH:144:ILE:HG23	2.03	0.40
49:LL:48:PRO:CG	71:Lh:115:LYS:HZ1	2.33	0.40
49:LL:64:LYS:HD2	49:LL:65:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:LS:14:LEU:HD23	56:LS:14:LEU:HA	1.92	0.40
58:LU:79:LEU:HD23	58:LU:79:LEU:HA	1.87	0.40
65:Lb:52:LYS:HD3	65:Lb:52:LYS:HA	1.84	0.40
69:Lf:67:MET:HE2	69:Lf:67:MET:HB3	1.93	0.40
81:L1:179:LEU:HA	81:L1:179:LEU:HD23	1.78	0.40
82:P0:125:ASN:HD21	82:P0:147:ARG:NH2	2.20	0.40
83:CD:300:LEU:HG	83:CD:305:ILE:HB	2.03	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	
5	SA	204/252 (81%)	175 (86%)	28 (14%)	1 (0%)	24	59
6	SB	214/255 (84%)	196 (92%)	18 (8%)	0	100	100
7	SC	215/254 (85%)	201 (94%)	13 (6%)	1 (0%)	24	59
8	SD	221/240 (92%)	195 (88%)	25 (11%)	1 (0%)	24	59
9	SE	258/261 (99%)	234 (91%)	24 (9%)	0	100	100
10	SF	204/225 (91%)	176 (86%)	28 (14%)	0	100	100
11	SG	216/236 (92%)	202 (94%)	14 (6%)	0	100	100
12	SH	183/190 (96%)	161 (88%)	22 (12%)	0	100	100
13	SI	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
14	SJ	183/197 (93%)	168 (92%)	15 (8%)	0	100	100
15	SK	90/105 (86%)	76 (84%)	9 (10%)	5 (6%)	1	11
16	SL	144/156 (92%)	134 (93%)	10 (7%)	0	100	100
17	SM	122/143 (85%)	85 (70%)	36 (30%)	1 (1%)	16	50
18	SN	148/151 (98%)	138 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	SO	126/137 (92%)	106 (84%)	20 (16%)	0	100	100
20	SP	117/142 (82%)	105 (90%)	11 (9%)	1 (1%)	14	47
21	SQ	139/143 (97%)	123 (88%)	15 (11%)	1 (1%)	18	52
22	SR	111/136 (82%)	102 (92%)	9 (8%)	0	100	100
23	SS	143/146 (98%)	127 (89%)	15 (10%)	1 (1%)	18	52
24	ST	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
25	SU	99/121 (82%)	94 (95%)	5 (5%)	0	100	100
26	SV	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
27	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
28	SX	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
29	SY	132/135 (98%)	117 (89%)	13 (10%)	2 (2%)	8	37
30	SZ	67/108 (62%)	65 (97%)	2 (3%)	0	100	100
31	Sa	95/119 (80%)	81 (85%)	14 (15%)	0	100	100
32	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
33	Sc	61/67 (91%)	54 (88%)	7 (12%)	0	100	100
34	Sd	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
35	Se	58/63 (92%)	50 (86%)	8 (14%)	0	100	100
36	Sf	31/152 (20%)	27 (87%)	4 (13%)	0	100	100
37	Sg	311/319 (98%)	277 (89%)	34 (11%)	0	100	100
38	LA	250/254 (98%)	225 (90%)	25 (10%)	0	100	100
39	LB	384/387 (99%)	366 (95%)	18 (5%)	0	100	100
40	LC	359/362 (99%)	325 (90%)	33 (9%)	1 (0%)	36	68
41	LD	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
42	LE	153/176 (87%)	140 (92%)	13 (8%)	0	100	100
43	LF	221/244 (91%)	218 (99%)	3 (1%)	0	100	100
44	LG	229/256 (90%)	206 (90%)	23 (10%)	0	100	100
45	LH	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
46	LI	205/221 (93%)	196 (96%)	9 (4%)	0	100	100
47	LJ	167/174 (96%)	141 (84%)	25 (15%)	1 (1%)	21	56
48	LK	156/165 (94%)	152 (97%)	4 (3%)	0	100	100
49	LL	192/199 (96%)	171 (89%)	17 (9%)	4 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	LM	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
51	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
52	LO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
53	LP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
54	LQ	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
55	LR	172/189 (91%)	169 (98%)	3 (2%)	0	100	100
56	LS	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
57	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
58	LU	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
59	LV	132/137 (96%)	127 (96%)	5 (4%)	0	100	100
60	LW	61/155 (39%)	59 (97%)	2 (3%)	0	100	100
61	LX	118/142 (83%)	107 (91%)	11 (9%)	0	100	100
62	LY	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
63	LZ	133/136 (98%)	118 (89%)	12 (9%)	3 (2%)	5	29
64	La	146/149 (98%)	124 (85%)	20 (14%)	2 (1%)	9	39
65	Lb	56/59 (95%)	46 (82%)	10 (18%)	0	100	100
66	Lc	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
67	Ld	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
68	Le	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
69	Lf	104/107 (97%)	97 (93%)	7 (7%)	0	100	100
70	Lg	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
71	Lh	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
72	Li	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
73	Lj	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
74	Lk	75/78 (96%)	70 (93%)	4 (5%)	1 (1%)	9	40
75	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
76	Lm	50/128 (39%)	50 (100%)	0	0	100	100
77	Ln	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
78	Lo	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
79	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
80	CE	143/157 (91%)	130 (91%)	12 (8%)	1 (1%)	18	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	L1	215/217 (99%)	190 (88%)	24 (11%)	1 (0%)	24	59
82	P0	201/312 (64%)	194 (96%)	7 (4%)	0	100	100
83	CD	810/842 (96%)	749 (92%)	58 (7%)	3 (0%)	30	62
84	CS	120/273 (44%)	113 (94%)	7 (6%)	0	100	100
All	All	12460/13846 (90%)	11502 (92%)	927 (7%)	31 (0%)	44	73

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	SK	81	ASN
29	SY	32	ARG
47	LJ	95	ASN
49	LL	48	PRO
80	CE	110	LYS
15	SK	88	PRO
20	SP	126	VAL
21	SQ	116	LEU
29	SY	52	LYS
40	LC	339	LEU
49	LL	76	THR
64	La	48	TYR
83	CD	483	PHE
15	SK	54	TYR
49	LL	77	LEU
63	LZ	101	PHE
83	CD	465	LYS
7	SC	235	LEU
49	LL	47	ALA
81	L1	59	PRO
8	SD	91	VAL
17	SM	130	THR
23	SS	91	ASP
74	Lk	17	ARG
5	SA	30	GLN
15	SK	3	MET
15	SK	30	ALA
63	LZ	102	GLU
83	CD	481	MET
63	LZ	104	PRO
64	La	18	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SA	165/210 (79%)	165 (100%)	0	100	100
6	SB	192/224 (86%)	192 (100%)	0	100	100
7	SC	176/205 (86%)	176 (100%)	0	100	100
8	SD	182/195 (93%)	182 (100%)	0	100	100
9	SE	221/222 (100%)	221 (100%)	0	100	100
10	SF	173/191 (91%)	173 (100%)	0	100	100
11	SG	187/201 (93%)	187 (100%)	0	100	100
12	SH	165/170 (97%)	165 (100%)	0	100	100
13	SI	150/161 (93%)	150 (100%)	0	100	100
14	SJ	158/166 (95%)	158 (100%)	0	100	100
15	SK	73/98 (74%)	73 (100%)	0	100	100
16	SL	129/137 (94%)	129 (100%)	0	100	100
17	SM	88/119 (74%)	88 (100%)	0	100	100
18	SN	127/128 (99%)	127 (100%)	0	100	100
19	SO	97/105 (92%)	97 (100%)	0	100	100
20	SP	98/118 (83%)	98 (100%)	0	100	100
21	SQ	117/119 (98%)	117 (100%)	0	100	100
22	SR	92/124 (74%)	92 (100%)	0	100	100
23	SS	128/129 (99%)	128 (100%)	0	100	100
24	ST	115/116 (99%)	115 (100%)	0	100	100
25	SU	94/114 (82%)	94 (100%)	0	100	100
26	SV	74/74 (100%)	74 (100%)	0	100	100
27	SW	110/111 (99%)	110 (100%)	0	100	100
28	SX	119/120 (99%)	119 (100%)	0	100	100
29	SY	112/113 (99%)	112 (100%)	0	100	100
30	SZ	61/89 (68%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Sa	83/100 (83%)	83 (100%)	0	100	100
32	Sb	70/71 (99%)	70 (100%)	0	100	100
33	Sc	56/60 (93%)	56 (100%)	0	100	100
34	Sd	47/49 (96%)	47 (100%)	0	100	100
35	Se	51/54 (94%)	51 (100%)	0	100	100
36	Sf	27/135 (20%)	27 (100%)	0	100	100
37	Sg	255/262 (97%)	255 (100%)	0	100	100
38	LA	192/196 (98%)	192 (100%)	0	100	100
39	LB	318/323 (98%)	318 (100%)	0	100	100
40	LC	288/289 (100%)	288 (100%)	0	100	100
41	LD	243/245 (99%)	242 (100%)	1 (0%)	84	86
42	LE	135/153 (88%)	135 (100%)	0	100	100
43	LF	187/205 (91%)	187 (100%)	0	100	100
44	LG	177/208 (85%)	177 (100%)	0	100	100
45	LH	170/171 (99%)	170 (100%)	0	100	100
46	LI	177/187 (95%)	177 (100%)	0	100	100
47	LJ	147/150 (98%)	147 (100%)	0	100	100
48	LK	129/136 (95%)	129 (100%)	0	100	100
49	LL	154/159 (97%)	154 (100%)	0	100	100
50	LM	108/109 (99%)	108 (100%)	0	100	100
51	LN	175/176 (99%)	175 (100%)	0	100	100
52	LO	160/162 (99%)	160 (100%)	0	100	100
53	LP	139/146 (95%)	139 (100%)	0	100	100
54	LQ	150/151 (99%)	150 (100%)	0	100	100
55	LR	133/154 (86%)	133 (100%)	0	100	100
56	LS	156/156 (100%)	156 (100%)	0	100	100
57	LT	136/137 (99%)	136 (100%)	0	100	100
58	LU	85/107 (79%)	85 (100%)	0	100	100
59	LV	103/105 (98%)	103 (100%)	0	100	100
60	LW	55/129 (43%)	55 (100%)	0	100	100
61	LX	104/118 (88%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LY	107/110 (97%)	107 (100%)	0	100	100
63	LZ	115/116 (99%)	115 (100%)	0	100	100
64	La	118/119 (99%)	118 (100%)	0	100	100
65	Lb	46/47 (98%)	46 (100%)	0	100	100
66	Lc	84/88 (96%)	84 (100%)	0	100	100
67	Ld	94/97 (97%)	94 (100%)	0	100	100
68	Le	109/111 (98%)	109 (100%)	0	100	100
69	Lf	90/91 (99%)	90 (100%)	0	100	100
70	Lg	95/103 (92%)	95 (100%)	0	100	100
71	Lh	103/105 (98%)	103 (100%)	0	100	100
72	Li	80/82 (98%)	80 (100%)	0	100	100
73	Lj	67/71 (94%)	67 (100%)	0	100	100
74	Lk	67/69 (97%)	67 (100%)	0	100	100
75	Ll	45/46 (98%)	44 (98%)	1 (2%)	45	71
76	Lm	47/116 (40%)	47 (100%)	0	100	100
77	Ln	23/23 (100%)	23 (100%)	0	100	100
78	Lo	90/91 (99%)	90 (100%)	0	100	100
79	Lp	71/72 (99%)	71 (100%)	0	100	100
80	CE	116/132 (88%)	116 (100%)	0	100	100
81	L1	198/198 (100%)	198 (100%)	0	100	100
82	P0	171/254 (67%)	171 (100%)	0	100	100
83	CD	695/715 (97%)	695 (100%)	0	100	100
84	CS	97/228 (42%)	97 (100%)	0	100	100
All	All	10541/11646 (90%)	10539 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	LD	274	GLN
75	Ll	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
5	SA	32	HIS
6	SB	40	ASN
6	SB	199	ASN
6	SB	208	GLN
6	SB	209	ASN
6	SB	220	GLN
8	SD	74	GLN
8	SD	162	GLN
9	SE	8	HIS
9	SE	57	ASN
10	SF	63	GLN
10	SF	127	GLN
10	SF	131	GLN
12	SH	11	GLN
12	SH	122	HIS
15	SK	28	ASN
17	SM	84	ASN
19	SO	24	ASN
21	SQ	103	ASN
23	SS	71	GLN
24	ST	64	HIS
24	ST	138	GLN
25	SU	87	HIS
26	SV	35	ASN
28	SX	10	ASN
28	SX	28	ASN
28	SX	75	GLN
29	SY	106	GLN
29	SY	110	GLN
31	Sa	94	ASN
33	Sc	27	GLN
34	Sd	48	ASN
35	Se	51	ASN
38	LA	38	HIS
39	LB	121	ASN
39	LB	224	HIS
39	LB	243	HIS
40	LC	160	GLN
40	LC	304	GLN
40	LC	316	ASN
41	LD	63	GLN
41	LD	274	GLN
43	LF	37	ASN

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Mol	Chain	Res	Type
43	LF	48	ASN
43	LF	64	GLN
44	LG	243	GLN
45	LH	96	HIS
45	LH	163	GLN
46	LI	23	ASN
46	LI	73	ASN
47	LJ	101	ASN
49	LL	99	HIS
49	LL	129	ASN
49	LL	149	GLN
51	LN	86	ASN
52	LO	31	GLN
53	LP	133	HIS
54	LQ	5	HIS
56	LS	108	GLN
56	LS	157	GLN
57	LT	66	ASN
57	LT	134	GLN
59	LV	24	ASN
60	LW	42	GLN
62	LY	120	GLN
63	LZ	29	HIS
63	LZ	127	ASN
64	La	11	HIS
67	Ld	57	GLN
68	Le	26	HIS
68	Le	52	GLN
69	Lf	24	ASN
71	Lh	104	GLN
73	Lj	20	ASN
75	Li	4	GLN
75	Li	33	ASN
78	Lo	47	GLN
80	CE	22	GLN
80	CE	125	GLN
81	L1	12	HIS
82	P0	125	ASN
83	CD	176	GLN
83	CD	216	HIS
83	CD	290	ASN
83	CD	409	GLN

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Mol	Chain	Res	Type
83	CD	432	GLN
83	CD	654	GLN
83	CD	725	GLN
83	CD	753	GLN
83	CD	759	GLN
83	CD	786	GLN
83	CD	795	GLN
84	CS	107	ASN
84	CS	124	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1693/1800 (94%)	389 (22%)	20 (1%)
2	C1	3182/3396 (93%)	605 (19%)	29 (0%)
3	C4	120/121 (99%)	19 (15%)	0
4	C3	156/158 (98%)	24 (15%)	1 (0%)
All	All	5151/5475 (94%)	1037 (20%)	50 (0%)

All (1037) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	4	C
1	C2	17	C
1	C2	25	C
1	C2	26	A
1	C2	27	U
1	C2	34	G
1	C2	42	G
1	C2	43	A
1	C2	45	U
1	C2	46	A
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	66	U
1	C2	67	A
1	C2	68	A
1	C2	71	A
1	C2	72	A

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Mol	Chain	Res	Type
1	C2	77	U
1	C2	78	A
1	C2	79	C
1	C2	104	A
1	C2	114	C
1	C2	115	G
1	C2	123	G
1	C2	127	G
1	C2	128	U
1	C2	132	U
1	C2	137	U
1	C2	140	A
1	C2	141	U
1	C2	144	U
1	C2	153	G
1	C2	158	U
1	C2	166	C
1	C2	168	A
1	C2	178	U
1	C2	179	A
1	C2	185	U
1	C2	188	A
1	C2	189	C
1	C2	190	C
1	C2	191	C
1	C2	192	U
1	C2	193	U
1	C2	194	U
1	C2	195	G
1	C2	196	G
1	C2	197	A
1	C2	198	A
1	C2	220	A
1	C2	229	U
1	C2	230	C
1	C2	233	C
1	C2	235	G
1	C2	238	U
1	C2	239	C
1	C2	240	U
1	C2	241	U
1	C2	246	G

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Mol	Chain	Res	Type
1	C2	250	C
1	C2	257	A
1	C2	265	A
1	C2	266	A
1	C2	271	A
1	C2	272	U
1	C2	273	G
1	C2	275	C
1	C2	276	C
1	C2	277	U
1	C2	278	U
1	C2	280	U
1	C2	287	G
1	C2	299	A
1	C2	308	C
1	C2	309	C
1	C2	314	C
1	C2	316	A
1	C2	319	U
1	C2	322	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	352	A
1	C2	359	A
1	C2	360	A
1	C2	361	C
1	C2	369	A
1	C2	387	A
1	C2	390	G
1	C2	400	A
1	C2	402	C
1	C2	404	G
1	C2	416	A
1	C2	417	A
1	C2	418	G
1	C2	422	G
1	C2	423	G
1	C2	424	C
1	C2	425	A
1	C2	426	G
1	C2	431	C

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Mol	Chain	Res	Type
1	C2	434	G
1	C2	439	U
1	C2	444	C
1	C2	448	C
1	C2	452	A
1	C2	454	U
1	C2	464	A
1	C2	469	C
1	C2	475	A
1	C2	477	A
1	C2	486	G
1	C2	488	G
1	C2	500	C
1	C2	501	U
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	512	A
1	C2	514	G
1	C2	515	A
1	C2	519	C
1	C2	527	A
1	C2	532	U
1	C2	533	U
1	C2	534	A
1	C2	538	A
1	C2	539	G
1	C2	540	G
1	C2	542	A
1	C2	548	G
1	C2	549	G
1	C2	551	G
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	558	U
1	C2	559	C
1	C2	561	G
1	C2	565	C
1	C2	574	G
1	C2	577	G

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Mol	Chain	Res	Type
1	C2	578	U
1	C2	579	A
1	C2	580	A
1	C2	583	C
1	C2	594	A
1	C2	595	G
1	C2	606	A
1	C2	611	U
1	C2	619	A
1	C2	620	A
1	C2	623	A
1	C2	624	G
1	C2	629	U
1	C2	634	G
1	C2	635	A
1	C2	639	U
1	C2	640	U
1	C2	648	G
1	C2	691	C
1	C2	696	C
1	C2	698	U
1	C2	738	G
1	C2	742	U
1	C2	743	U
1	C2	751	G
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	757	A
1	C2	765	G
1	C2	766	U
1	C2	774	A
1	C2	775	G
1	C2	779	U
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	788	A
1	C2	789	A
1	C2	793	A
1	C2	794	U
1	C2	795	U

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Mol	Chain	Res	Type
1	C2	803	A
1	C2	811	A
1	C2	812	A
1	C2	813	U
1	C2	815	G
1	C2	816	G
1	C2	820	U
1	C2	826	U
1	C2	829	A
1	C2	830	U
1	C2	831	U
1	C2	833	U
1	C2	835	U
1	C2	850	A
1	C2	851	U
1	C2	856	A
1	C2	863	A
1	C2	886	U
1	C2	898	A
1	C2	901	G
1	C2	913	G
1	C2	914	G
1	C2	932	U
1	C2	933	A
1	C2	934	C
1	C2	935	U
1	C2	942	G
1	C2	951	A
1	C2	959	U
1	C2	960	U
1	C2	964	U
1	C2	966	A
1	C2	969	C
1	C2	970	A
1	C2	992	A
1	C2	1009	U
1	C2	1021	C
1	C2	1023	A
1	C2	1026	A
1	C2	1028	C
1	C2	1030	A
1	C2	1031	U

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Mol	Chain	Res	Type
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1057	U
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1062	A
1	C2	1076	A
1	C2	1082	C
1	C2	1086	A
1	C2	1092	A
1	C2	1093	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1126	G
1	C2	1138	A
1	C2	1147	A
1	C2	1150	G
1	C2	1158	C
1	C2	1159	C
1	C2	1160	A
1	C2	1167	G
1	C2	1185	U
1	C2	1194	A
1	C2	1196	A
1	C2	1197	C
1	C2	1199	G
1	C2	1200	G
1	C2	1202	A
1	C2	1212	G
1	C2	1217	A
1	C2	1218	G
1	C2	1219	A
1	C2	1220	C
1	C2	1225	U
1	C2	1226	A
1	C2	1228	G
1	C2	1229	G

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Mol	Chain	Res	Type
1	C2	1230	A
1	C2	1231	U
1	C2	1234	A
1	C2	1235	C
1	C2	1240	U
1	C2	1243	G
1	C2	1244	A
1	C2	1245	G
1	C2	1246	C
1	C2	1252	C
1	C2	1255	G
1	C2	1256	A
1	C2	1257	U
1	C2	1258	U
1	C2	1265	G
1	C2	1273	G
1	C2	1274	C
1	C2	1300	A
1	C2	1301	U
1	C2	1307	U
1	C2	1314	U
1	C2	1315	U
1	C2	1321	A
1	C2	1325	A
1	C2	1338	C
1	C2	1340	U
1	C2	1341	A
1	C2	1344	A
1	C2	1345	A
1	C2	1360	A
1	C2	1361	U
1	C2	1362	U
1	C2	1363	U
1	C2	1364	G
1	C2	1367	G
1	C2	1370	U
1	C2	1371	A
1	C2	1385	G
1	C2	1388	A
1	C2	1390	U
1	C2	1399	C
1	C2	1400	A

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Mol	Chain	Res	Type
1	C2	1402	G
1	C2	1412	G
1	C2	1413	U
1	C2	1414	U
1	C2	1415	U
1	C2	1424	A
1	C2	1425	A
1	C2	1426	C
1	C2	1427	A
1	C2	1428	G
1	C2	1436	A
1	C2	1445	G
1	C2	1459	C
1	C2	1469	A
1	C2	1471	A
1	C2	1473	U
1	C2	1474	G
1	C2	1481	C
1	C2	1482	C
1	C2	1483	A
1	C2	1486	G
1	C2	1489	U
1	C2	1490	C
1	C2	1491	U
1	C2	1492	A
1	C2	1493	A
1	C2	1496	U
1	C2	1503	A
1	C2	1506	G
1	C2	1508	U
1	C2	1510	U
1	C2	1516	A
1	C2	1521	G
1	C2	1523	G
1	C2	1524	A
1	C2	1531	G
1	C2	1536	G
1	C2	1537	C
1	C2	1539	G
1	C2	1542	G
1	C2	1544	U
1	C2	1557	U

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Mol	Chain	Res	Type
1	C2	1559	A
1	C2	1569	A
1	C2	1571	C
1	C2	1573	A
1	C2	1574	G
1	C2	1584	G
1	C2	1585	U
1	C2	1590	G
1	C2	1601	G
1	C2	1615	C
1	C2	1635	A
1	C2	1658	G
1	C2	1680	G
1	C2	1716	C
1	C2	1718	G
1	C2	1737	G
1	C2	1739	C
1	C2	1744	A
1	C2	1750	A
1	C2	1755	A
1	C2	1760	G
1	C2	1766	A
1	C2	1767	G
1	C2	1769	U
1	C2	1780	G
1	C2	1782	A
1	C2	1783	C
1	C2	1792	G
1	C2	1793	G
1	C2	1794	A
1	C2	1796	C
1	C2	1798	U
1	C2	1799	U
1	C2	1800	A
2	C1	6	A
2	C1	22	G
2	C1	26	A
2	C1	40	A
2	C1	43	A
2	C1	49	A
2	C1	59	G
2	C1	60	A

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Mol	Chain	Res	Type
2	C1	65	A
2	C1	66	A
2	C1	67	A
2	C1	92	G
2	C1	96	G
2	C1	109	A
2	C1	110	G
2	C1	111	C
2	C1	116	A
2	C1	122	A
2	C1	133	U
2	C1	134	U
2	C1	135	C
2	C1	136	G
2	C1	143	G
2	C1	148	G
2	C1	150	A
2	C1	151	A
2	C1	152	U
2	C1	156	G
2	C1	157	A
2	C1	165	A
2	C1	171	G
2	C1	172	G
2	C1	180	C
2	C1	182	U
2	C1	187	A
2	C1	190	U
2	C1	191	U
2	C1	200	C
2	C1	206	G
2	C1	210	U
2	C1	211	A
2	C1	213	A
2	C1	218	G
2	C1	219	A
2	C1	239	G
2	C1	240	U
2	C1	241	G
2	C1	245	U
2	C1	246	U
2	C1	248	U

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Mol	Chain	Res	Type
2	C1	251	G
2	C1	252	U
2	C1	254	A
2	C1	269	G
2	C1	283	G
2	C1	284	A
2	C1	286	U
2	C1	295	A
2	C1	305	U
2	C1	323	A
2	C1	329	U
2	C1	339	C
2	C1	350	C
2	C1	352	A
2	C1	376	G
2	C1	398	A
2	C1	399	A
2	C1	401	U
2	C1	402	A
2	C1	403	C
2	C1	421	G
2	C1	422	A
2	C1	438	A
2	C1	521	A
2	C1	523	A
2	C1	535	G
2	C1	544	C
2	C1	545	U
2	C1	546	C
2	C1	548	G
2	C1	550	A
2	C1	555	U
2	C1	557	A
2	C1	558	U
2	C1	559	A
2	C1	578	A
2	C1	579	G
2	C1	585	A
2	C1	597	G
2	C1	603	A
2	C1	604	G
2	C1	608	A

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Mol	Chain	Res	Type
2	C1	609	G
2	C1	611	A
2	C1	620	U
2	C1	621	A
2	C1	622	A
2	C1	636	C
2	C1	649	A
2	C1	667	C
2	C1	677	A
2	C1	681	U
2	C1	690	A
2	C1	691	A
2	C1	705	A
2	C1	712	G
2	C1	715	A
2	C1	716	A
2	C1	719	U
2	C1	725	G
2	C1	727	G
2	C1	765	C
2	C1	766	U
2	C1	767	U
2	C1	771	A
2	C1	774	G
2	C1	776	U
2	C1	777	U
2	C1	780	A
2	C1	781	G
2	C1	785	G
2	C1	786	A
2	C1	801	A
2	C1	806	A
2	C1	817	A
2	C1	826	G
2	C1	830	A
2	C1	832	G
2	C1	849	C
2	C1	857	G
2	C1	861	C
2	C1	874	U
2	C1	879	U
2	C1	880	G

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Mol	Chain	Res	Type
2	C1	890	C
2	C1	896	A
2	C1	907	G
2	C1	908	G
2	C1	914	A
2	C1	915	A
2	C1	916	G
2	C1	923	C
2	C1	924	G
2	C1	932	U
2	C1	937	G
2	C1	944	C
2	C1	959	C
2	C1	960	U
2	C1	961	C
2	C1	979	U
2	C1	980	A
2	C1	981	U
2	C1	984	G
2	C1	991	G
2	C1	1002	A
2	C1	1010	G
2	C1	1015	U
2	C1	1016	C
2	C1	1017	C
2	C1	1024	G
2	C1	1025	A
2	C1	1026	A
2	C1	1027	A
2	C1	1028	U
2	C1	1029	G
2	C1	1030	A
2	C1	1032	C
2	C1	1035	G
2	C1	1041	U
2	C1	1047	A
2	C1	1049	C
2	C1	1063	G
2	C1	1064	A
2	C1	1065	A
2	C1	1072	G
2	C1	1081	U

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Mol	Chain	Res	Type
2	C1	1082	U
2	C1	1087	G
2	C1	1093	A
2	C1	1094	U
2	C1	1096	U
2	C1	1097	G
2	C1	1098	A
2	C1	1103	A
2	C1	1104	G
2	C1	1117	G
2	C1	1131	G
2	C1	1143	A
2	C1	1144	U
2	C1	1145	G
2	C1	1153	A
2	C1	1155	C
2	C1	1159	A
2	C1	1177	G
2	C1	1178	G
2	C1	1180	A
2	C1	1181	U
2	C1	1191	U
2	C1	1192	C
2	C1	1196	C
2	C1	1200	A
2	C1	1201	C
2	C1	1207	G
2	C1	1208	U
2	C1	1217	A
2	C1	1219	C
2	C1	1220	U
2	C1	1221	A
2	C1	1222	G
2	C1	1223	A
2	C1	1230	G
2	C1	1232	C
2	C1	1235	U
2	C1	1236	G
2	C1	1239	C
2	C1	1241	U
2	C1	1243	G
2	C1	1245	A

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Mol	Chain	Res	Type
2	C1	1246	G
2	C1	1254	C
2	C1	1256	G
2	C1	1258	U
2	C1	1259	A
2	C1	1263	A
2	C1	1265	U
2	C1	1281	G
2	C1	1285	G
2	C1	1286	A
2	C1	1287	A
2	C1	1289	G
2	C1	1295	G
2	C1	1301	A
2	C1	1305	U
2	C1	1307	G
2	C1	1308	A
2	C1	1309	U
2	C1	1313	G
2	C1	1330	A
2	C1	1345	G
2	C1	1348	U
2	C1	1354	G
2	C1	1357	G
2	C1	1380	G
2	C1	1386	A
2	C1	1392	G
2	C1	1399	A
2	C1	1400	G
2	C1	1417	G
2	C1	1418	A
2	C1	1419	A
2	C1	1434	G
2	C1	1437	C
2	C1	1446	A
2	C1	1450	G
2	C1	1455	U
2	C1	1469	C
2	C1	1482	A
2	C1	1483	G
2	C1	1484	U
2	C1	1487	G

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Mol	Chain	Res	Type
2	C1	1488	G
2	C1	1508	C
2	C1	1522	U
2	C1	1523	U
2	C1	1536	G
2	C1	1539	A
2	C1	1546	A
2	C1	1554	U
2	C1	1555	U
2	C1	1560	G
2	C1	1574	C
2	C1	1575	A
2	C1	1576	G
2	C1	1577	G
2	C1	1578	C
2	C1	1581	C
2	C1	1583	A
2	C1	1587	A
2	C1	1589	A
2	C1	1593	A
2	C1	1605	A
2	C1	1619	A
2	C1	1620	U
2	C1	1629	U
2	C1	1639	C
2	C1	1642	A
2	C1	1643	A
2	C1	1644	C
2	C1	1645	U
2	C1	1646	G
2	C1	1657	C
2	C1	1658	G
2	C1	1683	A
2	C1	1696	A
2	C1	1716	U
2	C1	1717	U
2	C1	1724	U
2	C1	1736	G
2	C1	1741	A
2	C1	1750	A
2	C1	1751	G
2	C1	1760	A

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Mol	Chain	Res	Type
2	C1	1762	C
2	C1	1765	U
2	C1	1770	G
2	C1	1775	G
2	C1	1778	G
2	C1	1780	G
2	C1	1794	G
2	C1	1797	A
2	C1	1808	G
2	C1	1812	G
2	C1	1814	A
2	C1	1816	A
2	C1	1817	G
2	C1	1818	U
2	C1	1821	U
2	C1	1839	A
2	C1	1841	A
2	C1	1842	A
2	C1	1846	C
2	C1	1849	C
2	C1	1858	A
2	C1	1866	C
2	C1	1867	A
2	C1	1878	G
2	C1	1879	A
2	C1	1880	U
2	C1	1886	A
2	C1	1893	A
2	C1	1906	G
2	C1	1907	C
2	C1	1925	U
2	C1	2101	C
2	C1	2102	U
2	C1	2110	G
2	C1	2111	G
2	C1	2113	A
2	C1	2114	C
2	C1	2121	G
2	C1	2122	G
2	C1	2131	A
2	C1	2140	U
2	C1	2144	A

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Mol	Chain	Res	Type
2	C1	2158	A
2	C1	2169	G
2	C1	2171	G
2	C1	2175	U
2	C1	2176	U
2	C1	2205	U
2	C1	2206	G
2	C1	2208	A
2	C1	2209	U
2	C1	2223	A
2	C1	2225	U
2	C1	2229	A
2	C1	2232	A
2	C1	2244	A
2	C1	2249	G
2	C1	2256	A
2	C1	2257	C
2	C1	2260	U
2	C1	2267	C
2	C1	2268	U
2	C1	2269	U
2	C1	2272	G
2	C1	2273	G
2	C1	2274	U
2	C1	2281	A
2	C1	2287	C
2	C1	2288	G
2	C1	2307	G
2	C1	2308	C
2	C1	2310	U
2	C1	2313	A
2	C1	2315	G
2	C1	2334	U
2	C1	2335	G
2	C1	2373	A
2	C1	2374	C
2	C1	2375	G
2	C1	2385	G
2	C1	2388	U
2	C1	2394	G
2	C1	2397	A
2	C1	2401	A

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Mol	Chain	Res	Type
2	C1	2402	A
2	C1	2403	G
2	C1	2404	A
2	C1	2411	U
2	C1	2418	G
2	C1	2419	A
2	C1	2437	G
2	C1	2439	A
2	C1	2446	U
2	C1	2448	G
2	C1	2453	U
2	C1	2455	U
2	C1	2456	A
2	C1	2458	A
2	C1	2460	U
2	C1	2463	G
2	C1	2468	A
2	C1	2469	G
2	C1	2473	C
2	C1	2485	A
2	C1	2488	A
2	C1	2490	C
2	C1	2498	U
2	C1	2502	A
2	C1	2511	A
2	C1	2514	U
2	C1	2515	A
2	C1	2522	G
2	C1	2523	A
2	C1	2524	A
2	C1	2526	C
2	C1	2536	A
2	C1	2538	U
2	C1	2539	C
2	C1	2540	A
2	C1	2541	U
2	C1	2542	U
2	C1	2543	U
2	C1	2544	U
2	C1	2547	A
2	C1	2549	G
2	C1	2552	C

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Mol	Chain	Res	Type
2	C1	2554	A
2	C1	2568	C
2	C1	2569	A
2	C1	2570	U
2	C1	2571	U
2	C1	2572	C
2	C1	2573	G
2	C1	2585	G
2	C1	2593	A
2	C1	2594	C
2	C1	2606	G
2	C1	2607	G
2	C1	2614	G
2	C1	2626	A
2	C1	2635	A
2	C1	2648	G
2	C1	2652	U
2	C1	2656	A
2	C1	2663	G
2	C1	2666	C
2	C1	2672	G
2	C1	2674	A
2	C1	2677	G
2	C1	2678	A
2	C1	2683	U
2	C1	2688	U
2	C1	2689	A
2	C1	2691	A
2	C1	2694	A
2	C1	2696	A
2	C1	2704	A
2	C1	2705	A
2	C1	2708	C
2	C1	2714	G
2	C1	2719	U
2	C1	2727	A
2	C1	2728	G
2	C1	2729	U
2	C1	2737	C
2	C1	2746	A
2	C1	2752	U
2	C1	2753	G

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Mol	Chain	Res	Type
2	C1	2755	C
2	C1	2772	C
2	C1	2773	C
2	C1	2777	G
2	C1	2778	G
2	C1	2796	G
2	C1	2800	G
2	C1	2801	A
2	C1	2803	A
2	C1	2810	C
2	C1	2814	G
2	C1	2817	A
2	C1	2818	U
2	C1	2844	C
2	C1	2845	A
2	C1	2849	C
2	C1	2853	A
2	C1	2861	U
2	C1	2867	C
2	C1	2871	G
2	C1	2872	A
2	C1	2875	U
2	C1	2887	A
2	C1	2888	U
2	C1	2889	C
2	C1	2898	G
2	C1	2899	C
2	C1	2911	A
2	C1	2923	U
2	C1	2933	A
2	C1	2935	U
2	C1	2936	A
2	C1	2938	G
2	C1	2941	A
2	C1	2942	C
2	C1	2947	G
2	C1	2948	C
2	C1	2954	U
2	C1	2983	C
2	C1	2990	G
2	C1	2996	U
2	C1	2997	G

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Mol	Chain	Res	Type
2	C1	3011	A
2	C1	3012	A
2	C1	3021	A
2	C1	3022	G
2	C1	3048	A
2	C1	3056	U
2	C1	3059	G
2	C1	3078	U
2	C1	3079	U
2	C1	3086	A
2	C1	3092	C
2	C1	3109	G
2	C1	3117	C
2	C1	3122	A
2	C1	3129	A
2	C1	3130	A
2	C1	3131	U
2	C1	3142	A
2	C1	3143	C
2	C1	3153	U
2	C1	3158	G
2	C1	3159	C
2	C1	3165	A
2	C1	3170	A
2	C1	3172	A
2	C1	3173	G
2	C1	3174	A
2	C1	3176	G
2	C1	3178	A
2	C1	3179	U
2	C1	3181	C
2	C1	3186	A
2	C1	3187	A
2	C1	3196	U
2	C1	3206	C
2	C1	3207	U
2	C1	3210	A
2	C1	3217	C
2	C1	3218	A
2	C1	3219	G
2	C1	3224	G
2	C1	3227	A

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Mol	Chain	Res	Type
2	C1	3229	G
2	C1	3234	A
2	C1	3235	C
2	C1	3238	G
2	C1	3243	A
2	C1	3244	A
2	C1	3245	A
2	C1	3247	G
2	C1	3259	U
2	C1	3263	G
2	C1	3269	U
2	C1	3270	U
2	C1	3273	A
2	C1	3275	U
2	C1	3276	G
2	C1	3279	A
2	C1	3280	U
2	C1	3281	U
2	C1	3283	U
2	C1	3287	U
2	C1	3288	G
2	C1	3289	G
2	C1	3290	G
2	C1	3294	A
2	C1	3303	G
2	C1	3304	U
2	C1	3313	U
2	C1	3316	A
2	C1	3317	U
2	C1	3318	G
2	C1	3319	U
2	C1	3320	A
2	C1	3335	A
2	C1	3341	U
2	C1	3342	A
2	C1	3345	G
2	C1	3351	U
2	C1	3352	U
2	C1	3355	U
2	C1	3356	G
2	C1	3357	U
2	C1	3358	U

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Mol	Chain	Res	Type
2	C1	3362	A
2	C1	3363	U
2	C1	3368	U
2	C1	3369	G
2	C1	3375	A
2	C1	3378	C
2	C1	3386	G
2	C1	3389	U
2	C1	3396	U
3	C4	7	G
3	C4	11	A
3	C4	22	A
3	C4	29	C
3	C4	33	U
3	C4	38	U
3	C4	52	G
3	C4	54	U
3	C4	55	A
3	C4	56	A
3	C4	65	G
3	C4	73	C
3	C4	74	C
3	C4	76	A
3	C4	91	G
3	C4	93	C
3	C4	102	A
3	C4	112	G
3	C4	121	U
4	C3	34	U
4	C3	35	C
4	C3	59	A
4	C3	62	C
4	C3	63	G
4	C3	75	G
4	C3	80	A
4	C3	81	U
4	C3	82	U
4	C3	83	C
4	C3	84	C
4	C3	86	U
4	C3	87	G
4	C3	95	G

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Mol	Chain	Res	Type
4	C3	104	A
4	C3	106	C
4	C3	111	A
4	C3	113	U
4	C3	116	G
4	C3	125	U
4	C3	126	A
4	C3	138	A
4	C3	148	G
4	C3	156	U

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	103	A
1	C2	187	G
1	C2	272	U
1	C2	417	A
1	C2	422	G
1	C2	555	A
1	C2	558	U
1	C2	755	A
1	C2	1051	G
1	C2	1058	U
1	C2	1097	U
1	C2	1196	A
1	C2	1227	A
1	C2	1255	G
1	C2	1344	A
1	C2	1458	G
1	C2	1481	C
1	C2	1538	U
1	C2	1568	C
1	C2	1573	A
2	C1	65	A
2	C1	151	A
2	C1	170	G
2	C1	282	G
2	C1	715	A
2	C1	1062	A
2	C1	1064	A
2	C1	1081	U

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Mol	Chain	Res	Type
2	C1	1216	C
2	C1	1307	G
2	C1	1493	G
2	C1	1645	U
2	C1	1716	U
2	C1	1815	U
2	C1	1816	A
2	C1	1841	A
2	C1	2101	C
2	C1	2112	U
2	C1	2662	G
2	C1	2772	C
2	C1	3078	U
2	C1	3121	U
2	C1	3158	G
2	C1	3228	C
2	C1	3269	U
2	C1	3289	G
2	C1	3317	U
2	C1	3356	G
2	C1	3357	U
4	C3	80	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
80	5CT	CE	51	80	13,14,15	0.77	0	8,15,17	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	5CT	CE	51	80	-	7/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	CE	51	5CT	C1-C2-C3-C4
80	CE	51	5CT	O1-C2-C3-C4
80	CE	51	5CT	C-CA-CB-CG
80	CE	51	5CT	O-C-CA-CB
80	CE	51	5CT	CG-CD-CE-NZ
80	CE	51	5CT	CE-CD-CG-CB
80	CE	51	5CT	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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
86	T1C	C1	3401	-	45,45,45	1.14	4 (8%)	56,72,72	1.44	9 (16%)
86	T1C	C1	3403	-	45,45,45	1.12	3 (6%)	56,72,72	0.98	2 (3%)
86	T1C	C1	3404	87	45,45,45	1.16	4 (8%)	56,72,72	1.05	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	T1C	C1	3402	-	45,45,45	1.17	4 (8%)	56,72,72	1.14	4 (7%)
88	GDP	CD	902	87	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
86	T1C	C1	3406	87	45,45,45	1.14	4 (8%)	56,72,72	1.14	5 (8%)
86	T1C	C1	3405	-	45,45,45	1.17	4 (8%)	56,72,72	1.44	7 (12%)

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
86	T1C	C1	3401	-	-	11/22/80/80	0/4/4/4
86	T1C	C1	3403	-	-	9/22/80/80	0/4/4/4
86	T1C	C1	3404	87	-	13/22/80/80	0/4/4/4
86	T1C	C1	3402	-	-	13/22/80/80	0/4/4/4
88	GDP	CD	902	87	-	3/16/32/32	0/3/3/3
86	T1C	C1	3406	87	-	13/22/80/80	0/4/4/4
86	T1C	C1	3405	-	-	14/22/80/80	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	C1	3402	T1C	C21-N21	5.07	1.48	1.33
86	C1	3401	T1C	C21-N21	5.05	1.48	1.33
86	C1	3405	T1C	C21-N21	5.02	1.47	1.33
86	C1	3403	T1C	C21-N21	5.01	1.47	1.33
86	C1	3406	T1C	C21-N21	5.00	1.47	1.33
86	C1	3404	T1C	C21-N21	5.00	1.47	1.33
88	CD	902	GDP	C5-C4	3.14	1.47	1.38
86	C1	3405	T1C	C4-N4	2.59	1.52	1.47
86	C1	3404	T1C	C4-N4	2.52	1.52	1.47
86	C1	3402	T1C	C4-N4	2.50	1.52	1.47
88	CD	902	GDP	C6-N1	-2.47	1.34	1.38
86	C1	3406	T1C	O11-C11	2.25	1.28	1.23
86	C1	3401	T1C	O11-C11	2.25	1.28	1.23
86	C1	3402	T1C	O11-C11	2.24	1.27	1.23
86	C1	3405	T1C	O11-C11	2.24	1.27	1.23
86	C1	3404	T1C	O11-C11	2.22	1.27	1.23
86	C1	3403	T1C	C7-N7	2.22	1.48	1.42
86	C1	3401	T1C	C7-N7	2.17	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	C1	3403	T1C	O11-C11	2.17	1.27	1.23
86	C1	3401	T1C	C4-N4	2.14	1.51	1.47
86	C1	3404	T1C	C7-N7	2.13	1.48	1.42
86	C1	3402	T1C	C7-N7	2.13	1.48	1.42
86	C1	3406	T1C	C7-N7	2.08	1.48	1.42
86	C1	3405	T1C	C7-N7	2.04	1.47	1.42
88	CD	902	GDP	C5-N7	-2.04	1.35	1.39
86	C1	3406	T1C	C4-N4	2.01	1.51	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	CD	902	GDP	C5-C4-N3	-6.23	118.47	128.39
88	CD	902	GDP	C2-N3-C4	5.12	121.12	112.30
86	C1	3405	T1C	C1-C1C-C12	4.92	115.64	109.88
88	CD	902	GDP	N9-C4-N3	4.67	135.29	125.95
86	C1	3401	T1C	C11-C1B-C12	4.63	122.47	118.80
86	C1	3402	T1C	C1C-C1-C2	4.41	122.75	115.75
86	C1	3401	T1C	C1C-C1-C2	4.21	122.43	115.75
86	C1	3405	T1C	C11-C1B-C12	4.12	122.06	118.80
86	C1	3401	T1C	C1C-C41-C4	3.87	116.93	111.64
86	C1	3403	T1C	C11-C1B-C12	3.66	121.70	118.80
86	C1	3405	T1C	C61-C7-N7	3.49	123.04	118.87
86	C1	3406	T1C	C11-C1B-C12	3.47	121.55	118.80
86	C1	3406	T1C	O1C-C1C-C12	-3.31	104.84	110.14
86	C1	3406	T1C	C1-C1C-C12	3.27	113.72	109.88
88	CD	902	GDP	C6-C5-N7	3.17	136.06	130.29
86	C1	3405	T1C	O1C-C1C-C12	-3.13	105.14	110.14
86	C1	3403	T1C	C5-C41-C4	-3.03	109.36	113.73
86	C1	3402	T1C	C11-C1B-C12	3.01	121.18	118.80
86	C1	3401	T1C	C61-C6-C51	2.96	117.04	113.12
86	C1	3404	T1C	C11-C1B-C12	2.95	121.13	118.80
86	C1	3405	T1C	C1C-C41-C4	2.94	115.65	111.64
86	C1	3405	T1C	C8-C7-N7	-2.92	116.35	120.89
86	C1	3406	T1C	C1C-C41-C4	2.70	115.33	111.64
86	C1	3406	T1C	C5-C41-C4	-2.70	109.83	113.73
86	C1	3401	T1C	O1C-C1C-C12	-2.67	105.87	110.14
86	C1	3404	T1C	C1C-C1-C2	2.64	119.95	115.75
86	C1	3401	T1C	C5-C51-C1B	-2.62	104.59	110.28
86	C1	3401	T1C	C51-C5-C41	-2.61	105.93	110.38
86	C1	3404	T1C	O1C-C1C-C12	-2.58	106.01	110.14
86	C1	3401	T1C	C1-C1C-C12	2.56	112.89	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	CD	902	GDP	C4-C5-N7	-2.47	106.75	110.67
86	C1	3404	T1C	C1-C1C-C12	2.46	112.76	109.88
86	C1	3404	T1C	C1C-C41-C4	2.41	114.94	111.64
86	C1	3402	T1C	C61-C6-C51	2.37	116.26	113.12
86	C1	3402	T1C	O1C-C1C-C12	-2.36	106.37	110.14
88	CD	902	GDP	C3'-C2'-C1'	2.29	105.80	101.46
88	CD	902	GDP	O6-C6-C5	-2.29	120.50	126.53
86	C1	3401	T1C	C72-N7-C71	-2.05	109.58	116.18
86	C1	3405	T1C	C72-N7-C71	-2.02	109.69	116.18

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	C1	3401	T1C	C94-C93-N92-C92
86	C1	3401	T1C	C95-C93-N92-C92
86	C1	3401	T1C	C96-C93-N92-C92
86	C1	3401	T1C	C41-C4-N4-C43
86	C1	3401	T1C	C1-C2-C21-O21
86	C1	3401	T1C	C1-C2-C21-N21
86	C1	3402	T1C	C92-C91-N9-C9
86	C1	3402	T1C	C1-C2-C21-O21
86	C1	3402	T1C	C1-C2-C21-N21
86	C1	3403	T1C	C92-C91-N9-C9
86	C1	3403	T1C	O91-C91-N9-C9
86	C1	3403	T1C	C1-C2-C21-O21
86	C1	3403	T1C	C1-C2-C21-N21
86	C1	3404	T1C	C91-C92-N92-C93
86	C1	3404	T1C	C92-C91-N9-C9
86	C1	3404	T1C	C1-C2-C21-O21
86	C1	3404	T1C	C1-C2-C21-N21
86	C1	3405	T1C	C94-C93-N92-C92
86	C1	3405	T1C	C95-C93-N92-C92
86	C1	3405	T1C	C92-C91-N9-C9
86	C1	3405	T1C	C3-C4-N4-C43
86	C1	3405	T1C	C1-C2-C21-O21
86	C1	3405	T1C	C1-C2-C21-N21
86	C1	3406	T1C	C92-C91-N9-C9
86	C1	3406	T1C	C41-C4-N4-C42
86	C1	3406	T1C	C1-C2-C21-O21
86	C1	3406	T1C	C1-C2-C21-N21
86	C1	3404	T1C	O91-C91-N9-C9

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Mol	Chain	Res	Type	Atoms
86	C1	3406	T1C	O91-C91-N9-C9
86	C1	3402	T1C	O91-C91-N9-C9
86	C1	3405	T1C	C96-C93-N92-C92
86	C1	3405	T1C	O91-C91-N9-C9
86	C1	3404	T1C	C10-C9-N9-C91
88	CD	902	GDP	C3'-C4'-C5'-O5'
86	C1	3401	T1C	C10-C9-N9-C91
86	C1	3406	T1C	N9-C91-C92-N92
86	C1	3406	T1C	O91-C91-C92-N92
86	C1	3404	T1C	O91-C91-C92-N92
86	C1	3404	T1C	C8-C9-N9-C91
86	C1	3401	T1C	C8-C9-N9-C91
88	CD	902	GDP	O4'-C4'-C5'-O5'
86	C1	3403	T1C	N9-C91-C92-N92
86	C1	3404	T1C	N9-C91-C92-N92
86	C1	3402	T1C	N9-C91-C92-N92
86	C1	3402	T1C	O91-C91-C92-N92
86	C1	3403	T1C	O91-C91-C92-N92
86	C1	3401	T1C	C3-C2-C21-N21
86	C1	3404	T1C	C3-C2-C21-N21
86	C1	3405	T1C	C41-C4-N4-C43
86	C1	3405	T1C	C41-C4-N4-C42
86	C1	3405	T1C	C3-C4-N4-C42
86	C1	3406	T1C	C3-C4-N4-C43
86	C1	3406	T1C	C3-C2-C21-N21
86	C1	3401	T1C	C3-C2-C21-O21
86	C1	3402	T1C	C3-C2-C21-O21
86	C1	3404	T1C	C3-C2-C21-O21
86	C1	3406	T1C	C3-C2-C21-O21
86	C1	3405	T1C	O91-C91-C92-N92
86	C1	3405	T1C	N9-C91-C92-N92
86	C1	3401	T1C	C91-C92-N92-C93
86	C1	3402	T1C	C91-C92-N92-C93
86	C1	3403	T1C	C91-C92-N92-C93
86	C1	3405	T1C	C91-C92-N92-C93
86	C1	3406	T1C	C91-C92-N92-C93
88	CD	902	GDP	C5'-O5'-PA-O3A
86	C1	3402	T1C	C95-C93-N92-C92
86	C1	3402	T1C	C96-C93-N92-C92
86	C1	3406	T1C	C61-C7-N7-C72
86	C1	3402	T1C	C61-C7-N7-C71
86	C1	3402	T1C	C61-C7-N7-C72

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Mol	Chain	Res	Type	Atoms
86	C1	3406	T1C	C61-C7-N7-C71
86	C1	3402	T1C	C3-C2-C21-N21
86	C1	3403	T1C	C3-C2-C21-N21
86	C1	3404	T1C	C41-C4-N4-C43
86	C1	3404	T1C	C41-C4-N4-C42
86	C1	3403	T1C	C3-C2-C21-O21

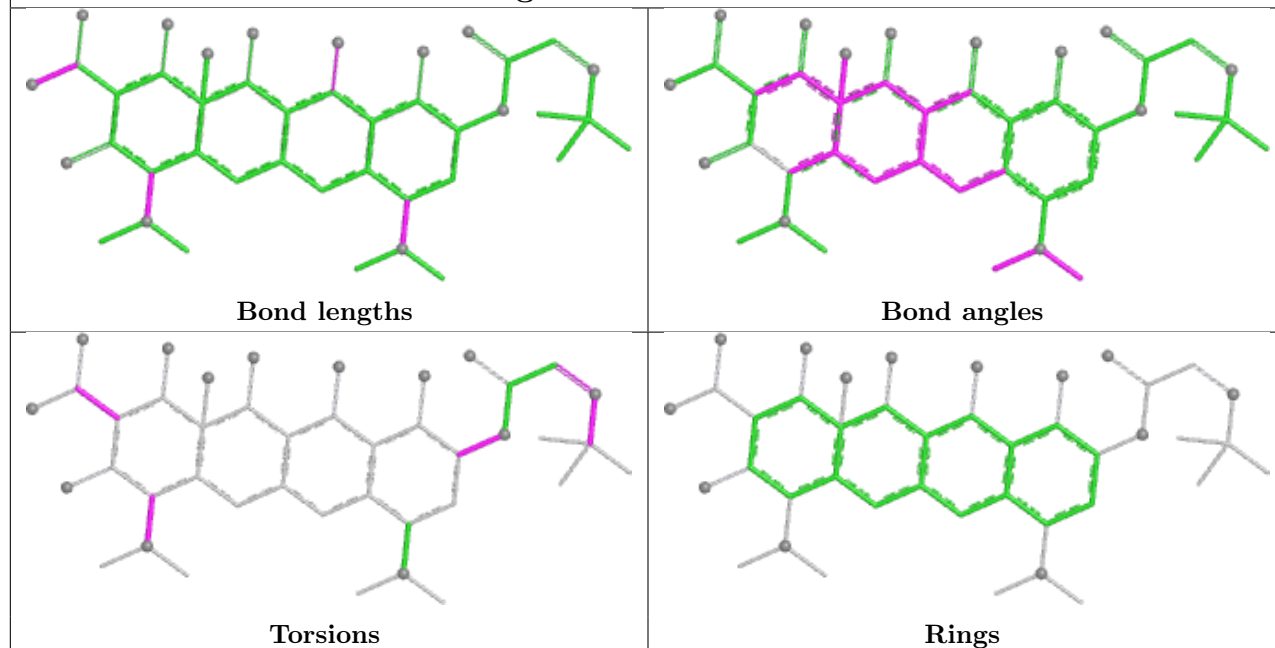
There are no ring outliers.

2 monomers are involved in 4 short contacts:

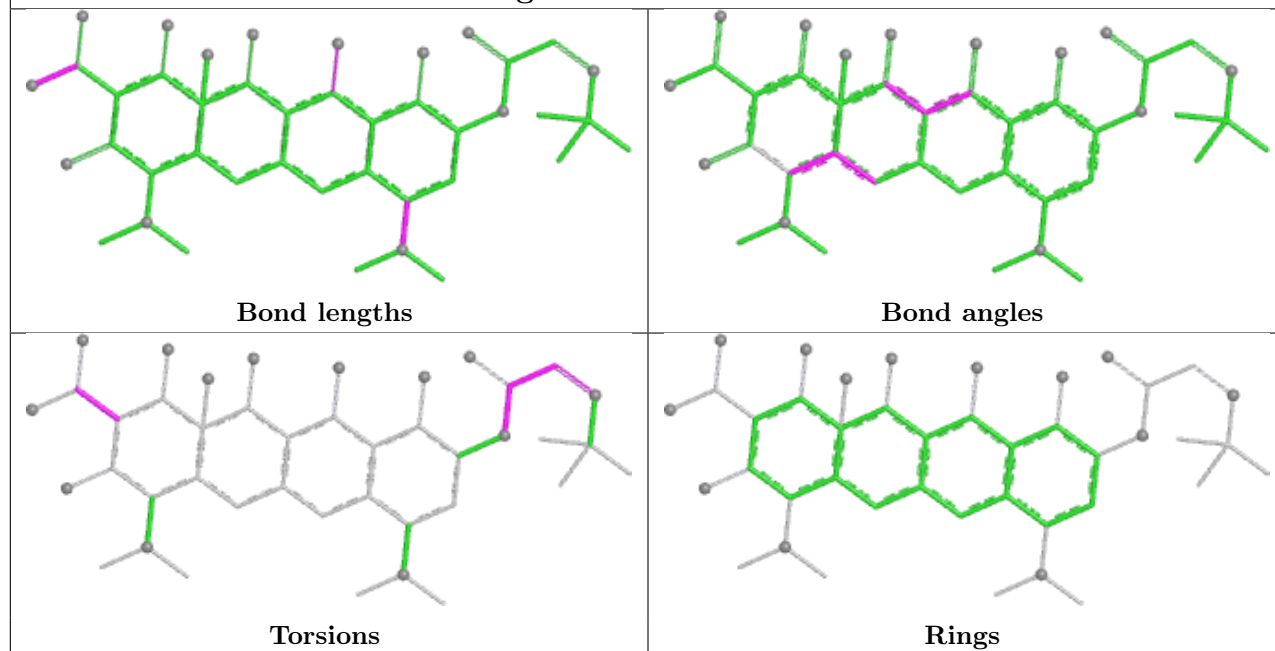
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	C1	3401	T1C	2	0
86	C1	3406	T1C	2	0

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.

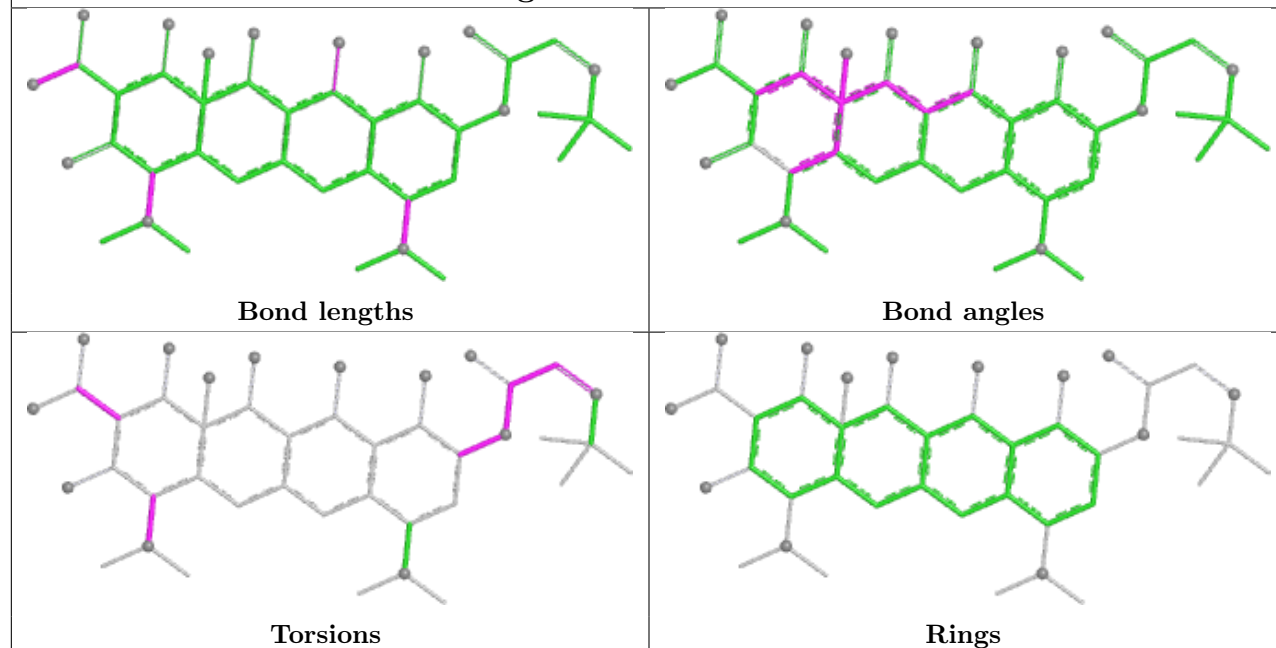
Ligand T1C C1 3401



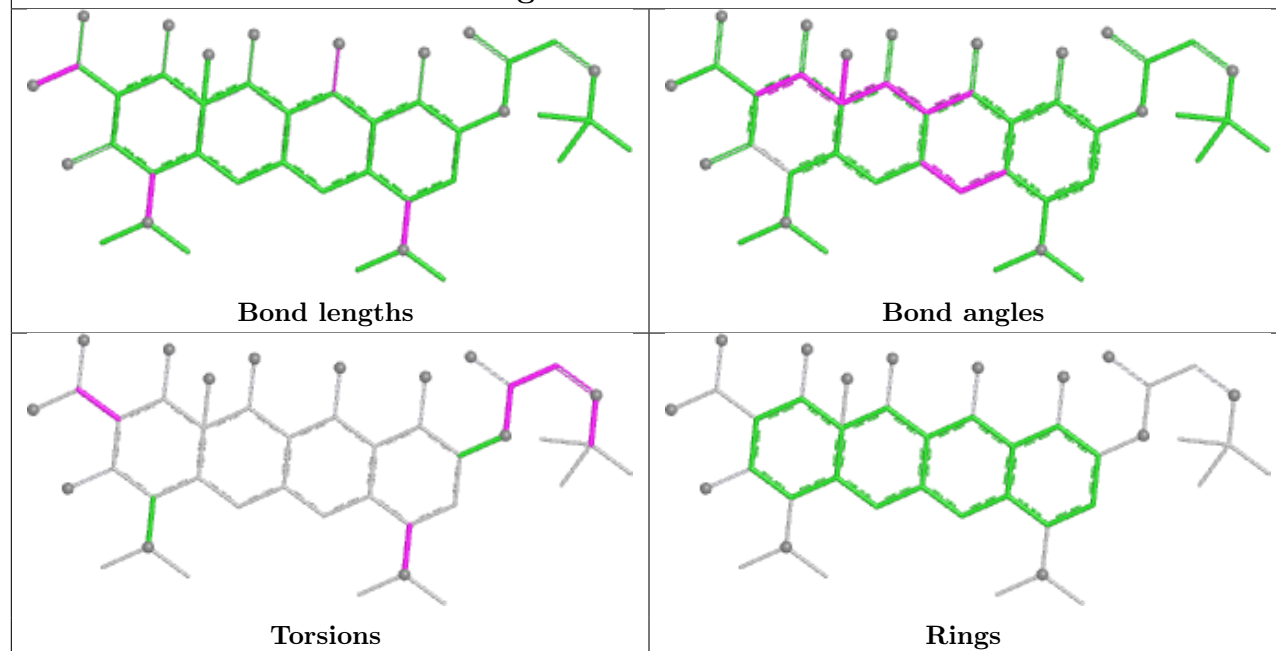
Ligand T1C C1 3403

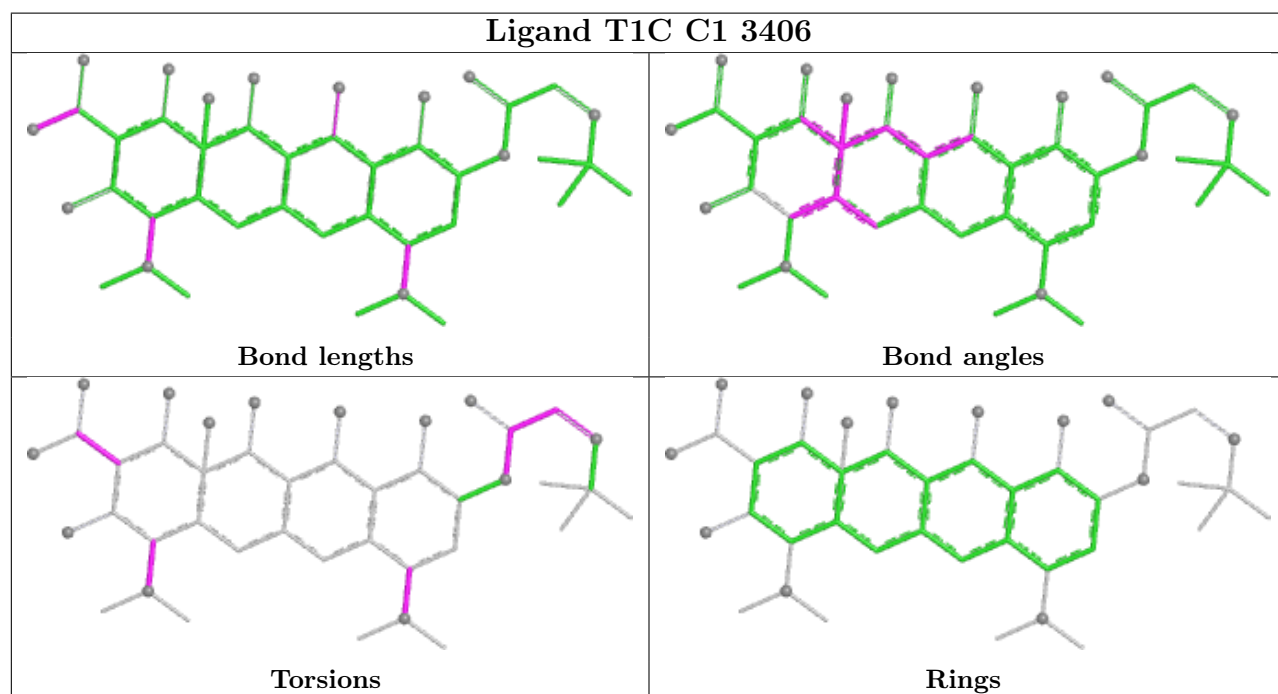
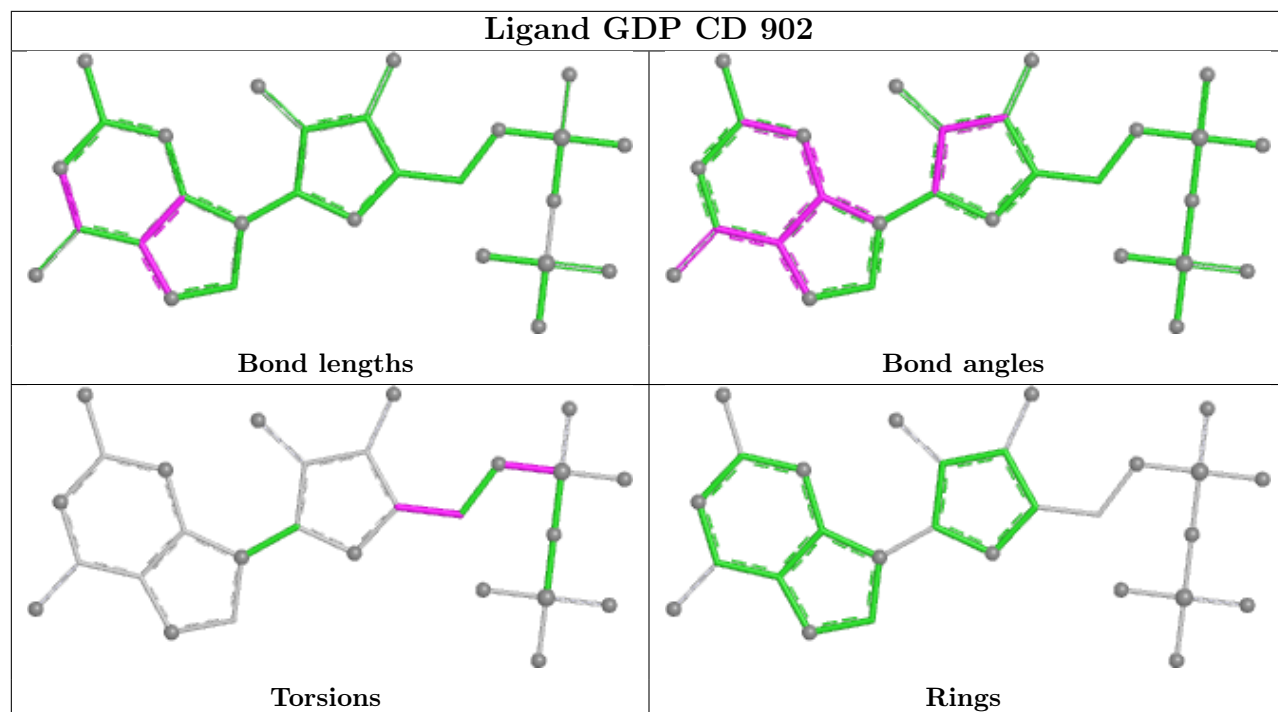


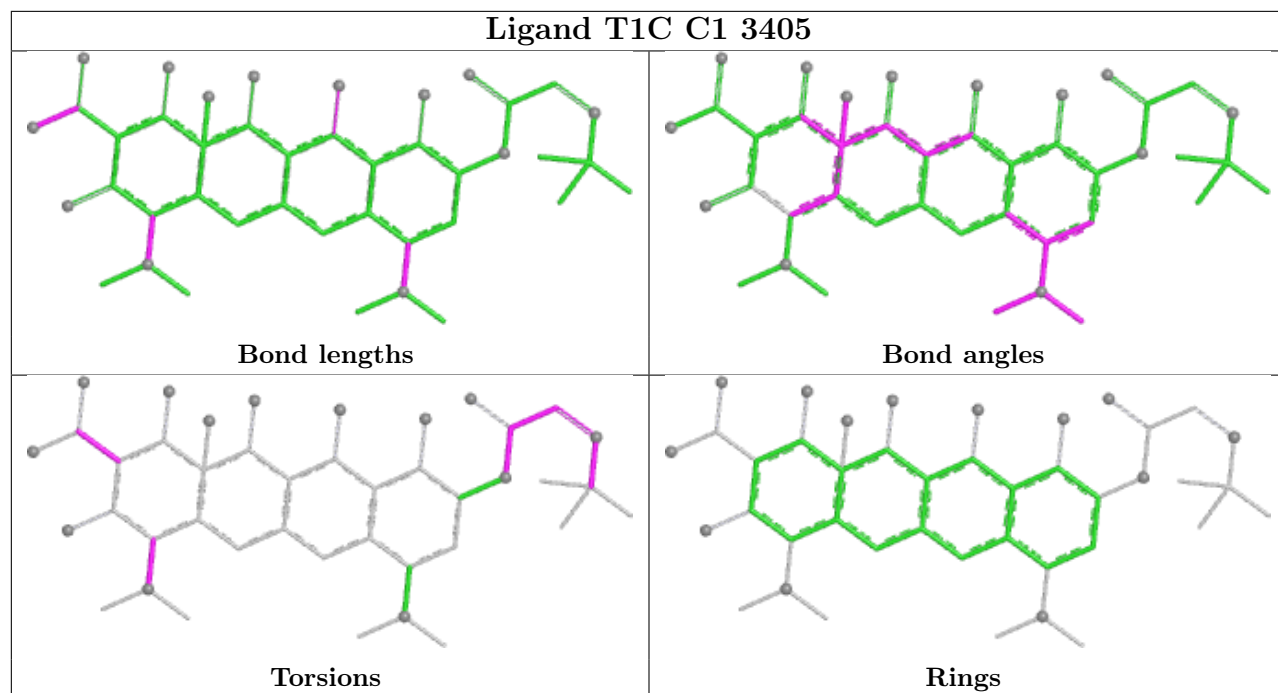
Ligand T1C C1 3404



Ligand T1C C1 3402







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.

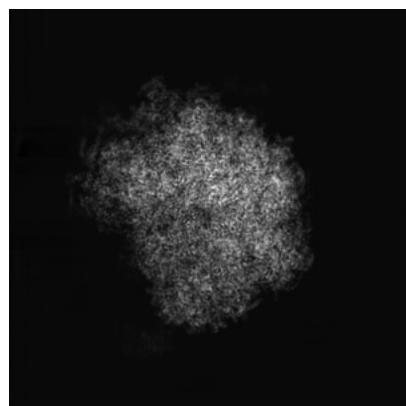
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36839. These allow visual inspection of the internal detail of the map and identification of artifacts.

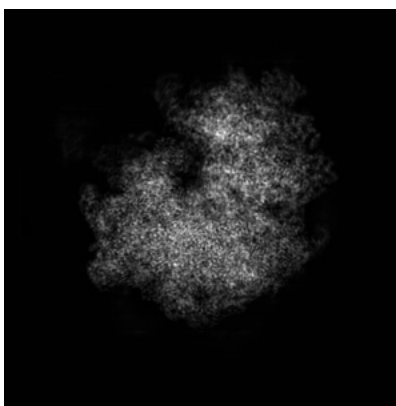
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

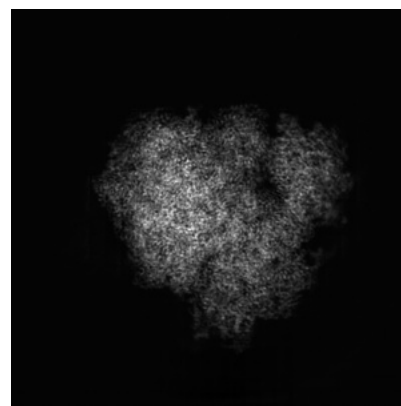
6.1.1 Primary map



X

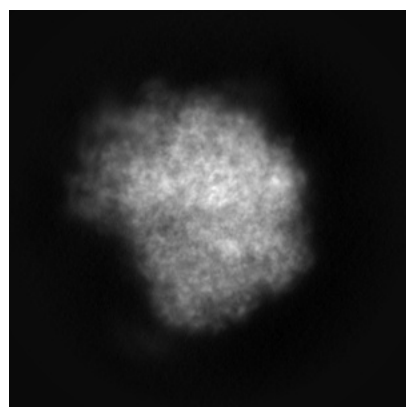


Y

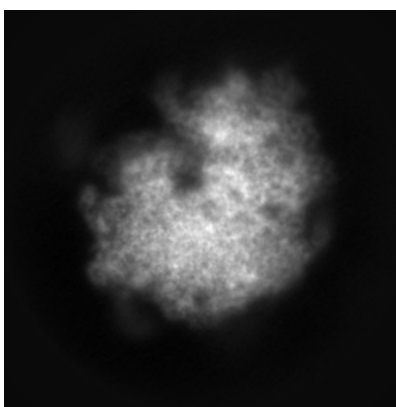


Z

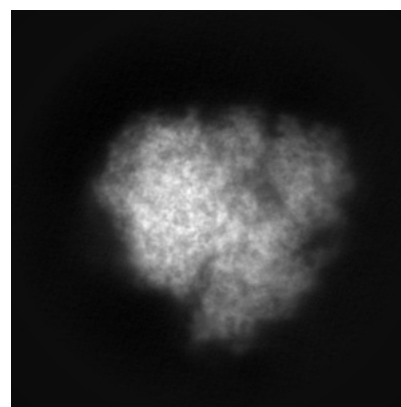
6.1.2 Raw map



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: 240

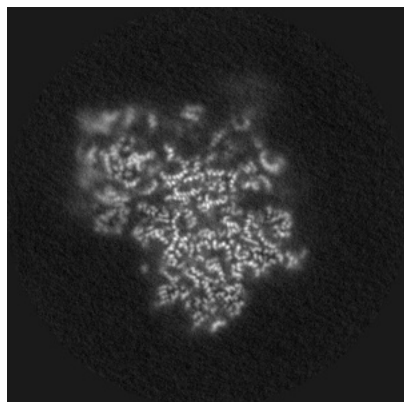


Y Index: 240

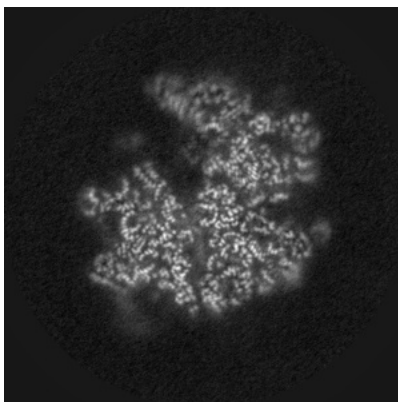


Z Index: 240

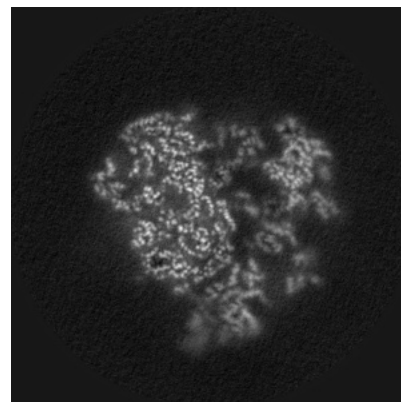
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

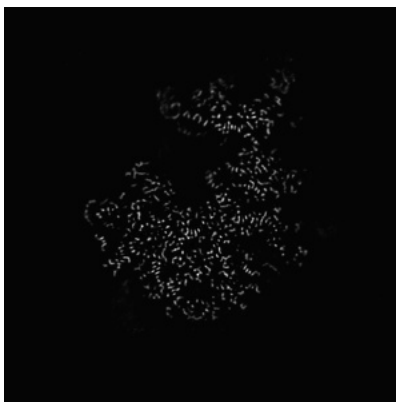
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 215

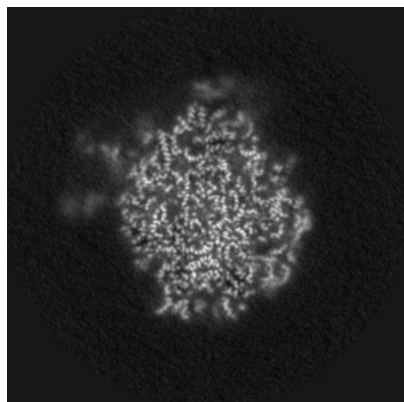


Y Index: 257

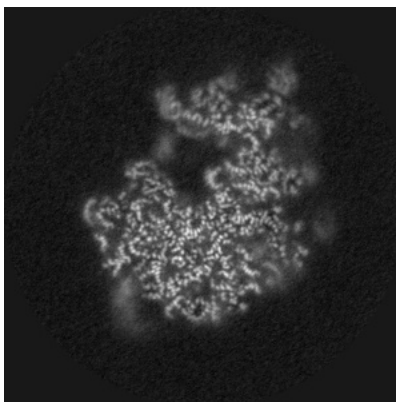


Z Index: 273

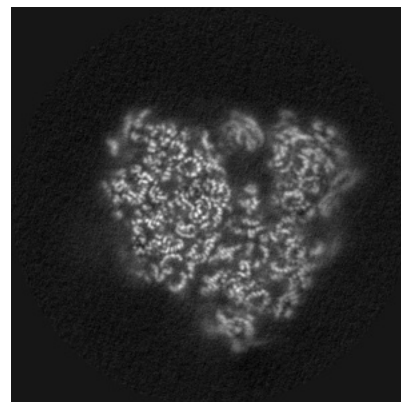
6.3.2 Raw map



X Index: 214



Y Index: 257

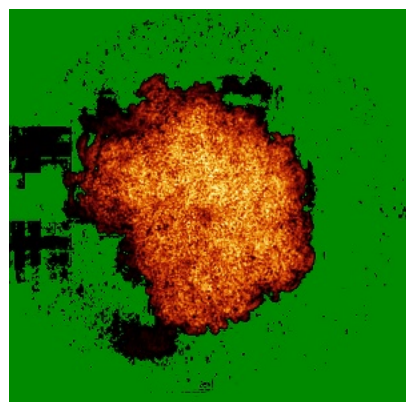


Z Index: 268

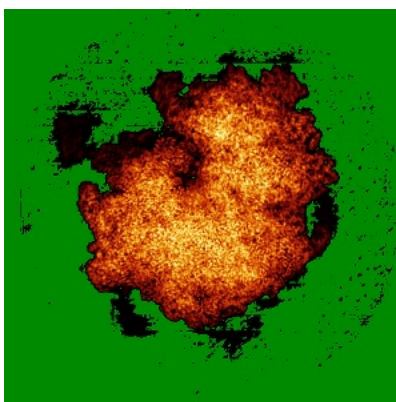
The images above show the largest variance slices of the map in three orthogonal directions.

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

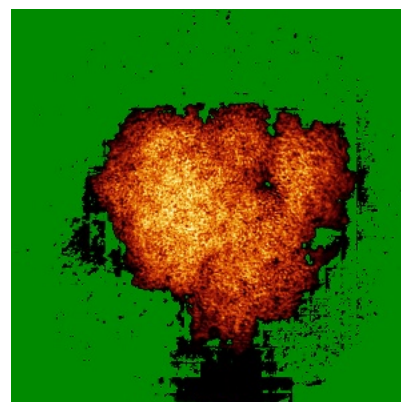
6.4.1 Primary map



X

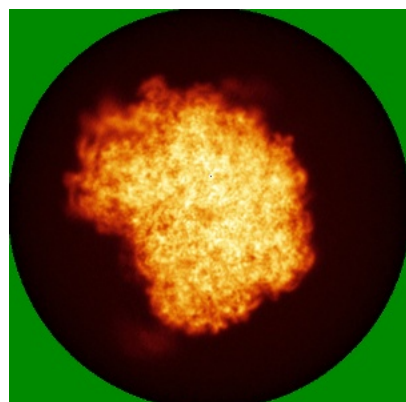


Y

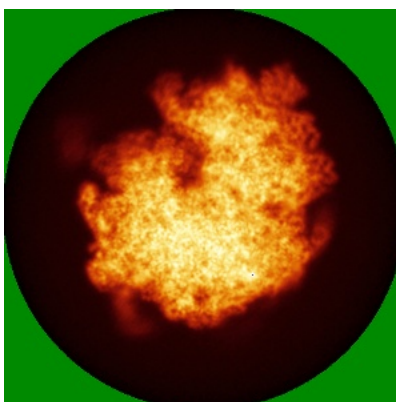


Z

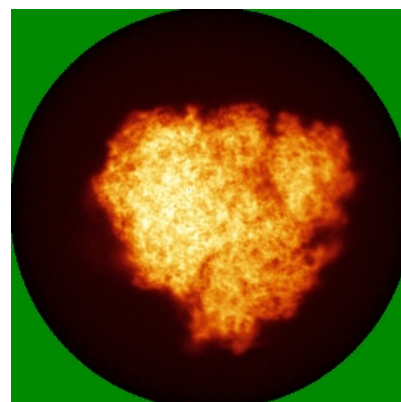
6.4.2 Raw map



X



Y

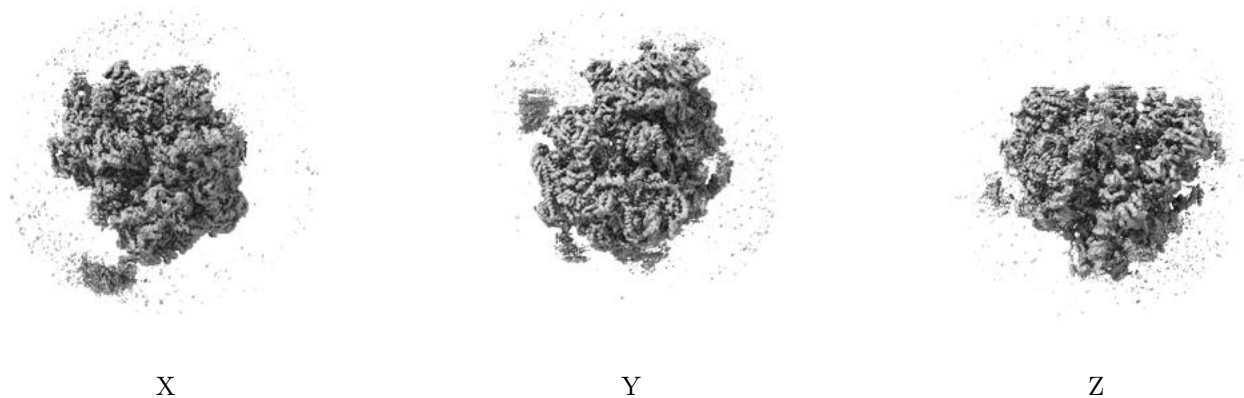


Z

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.

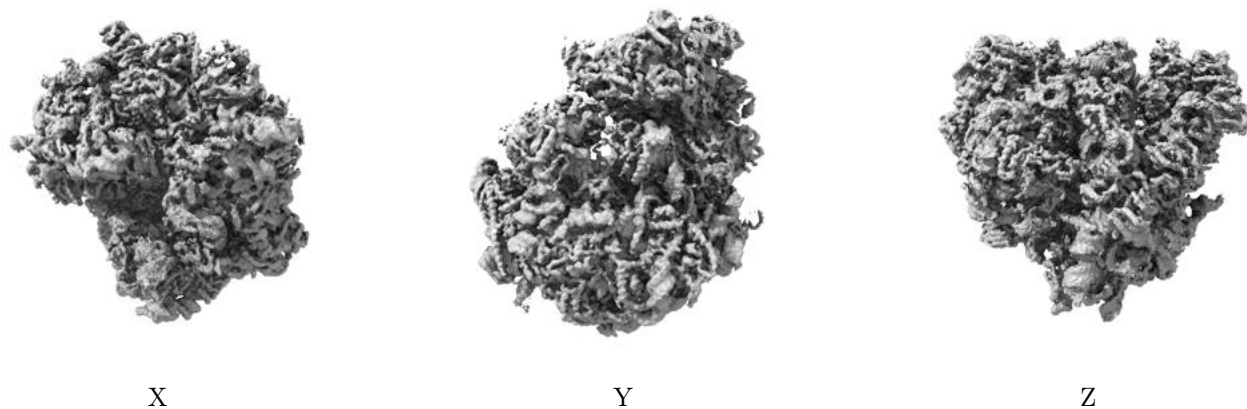
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

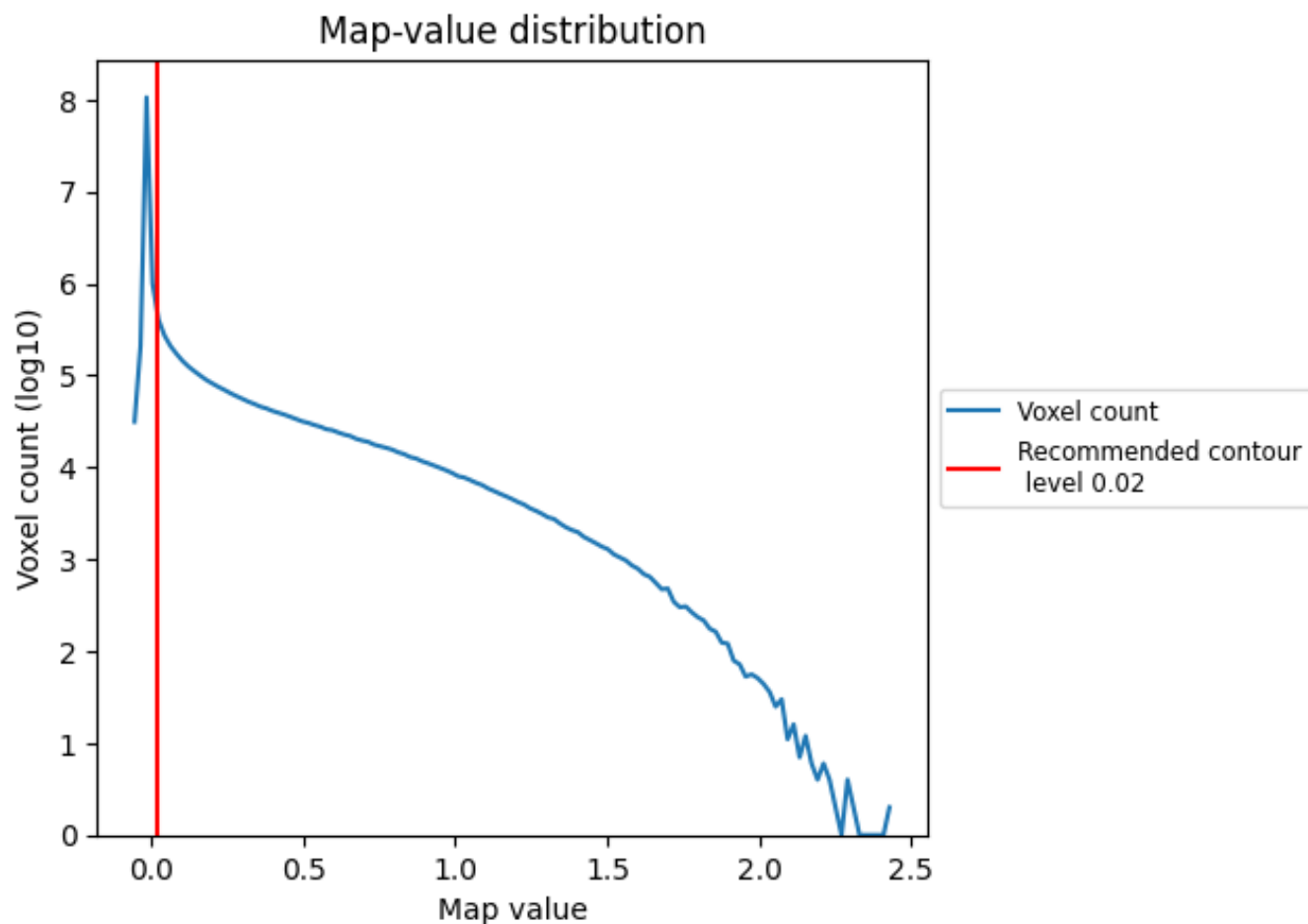
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

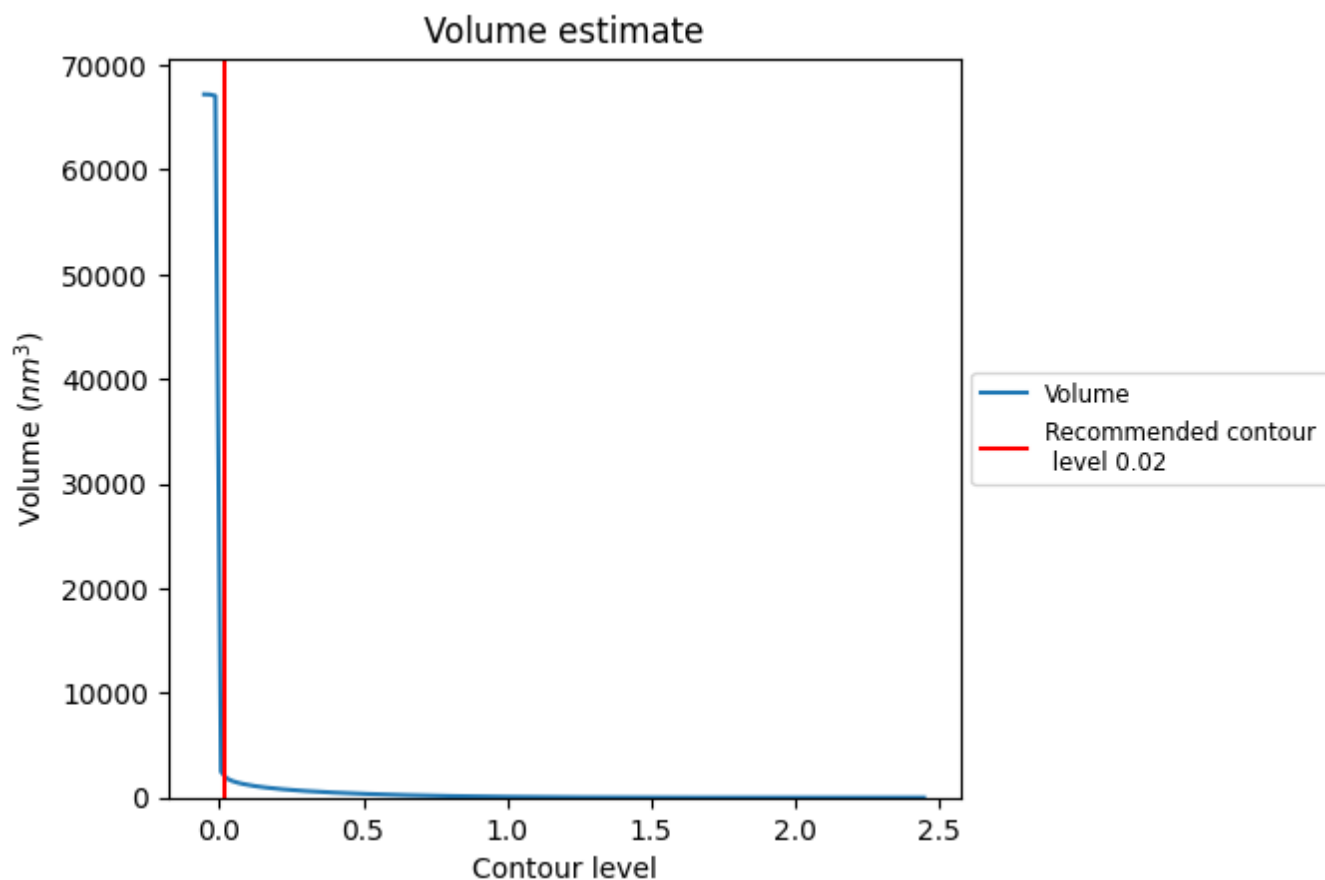
This section contains the results of statistical analysis of the map.

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.

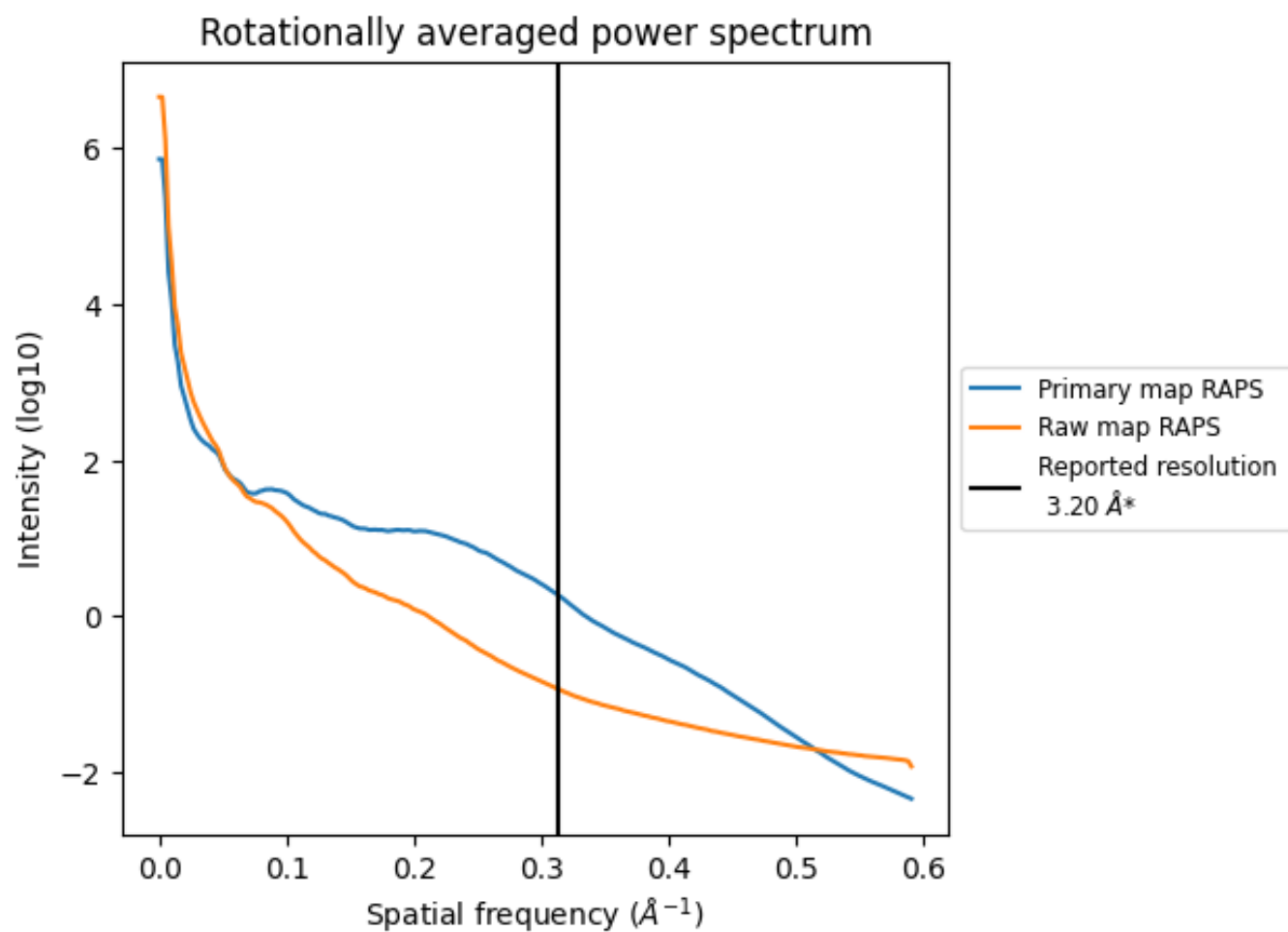
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2009 nm³; this corresponds to an approximate mass of 1814 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 ⓘ

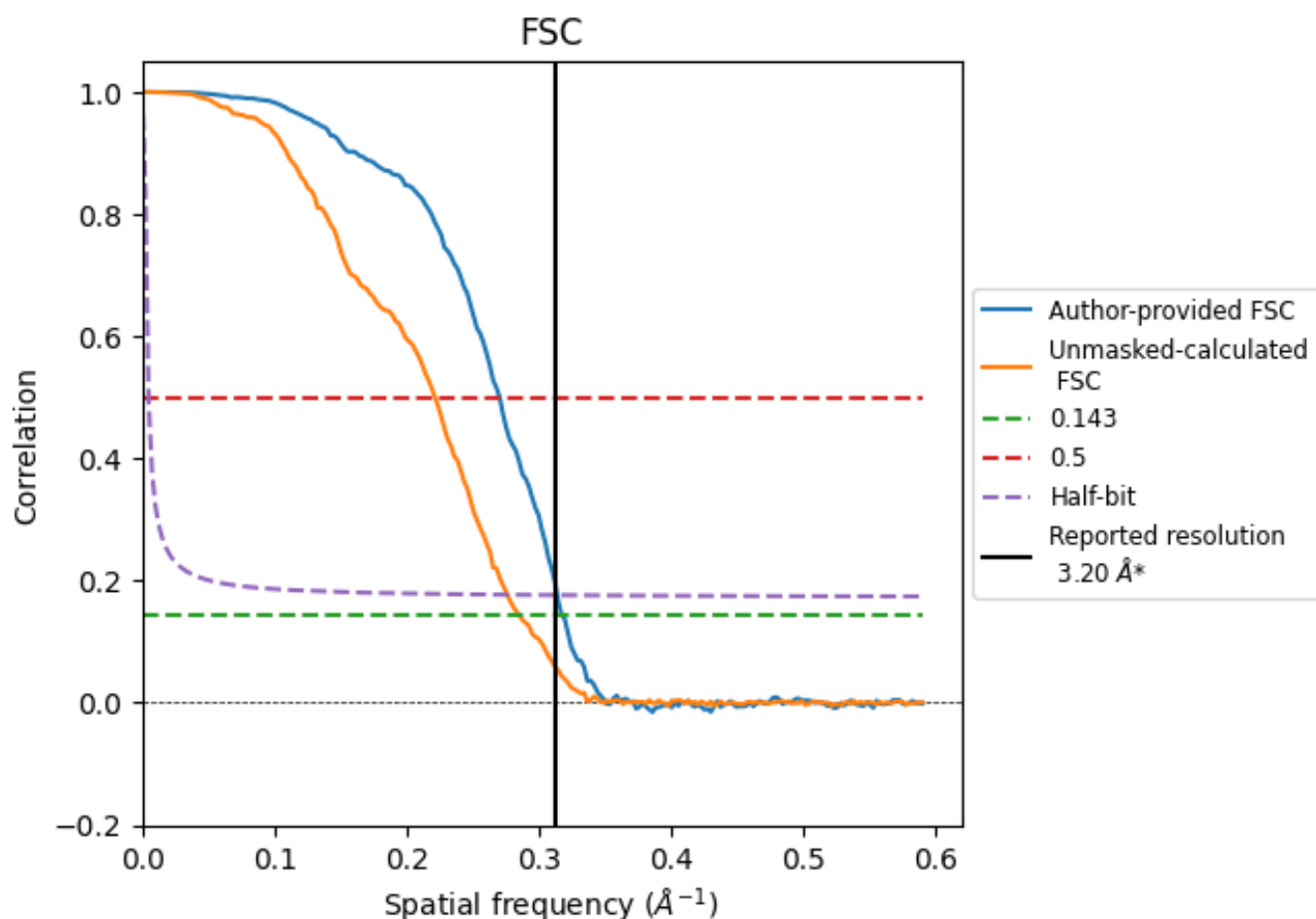


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

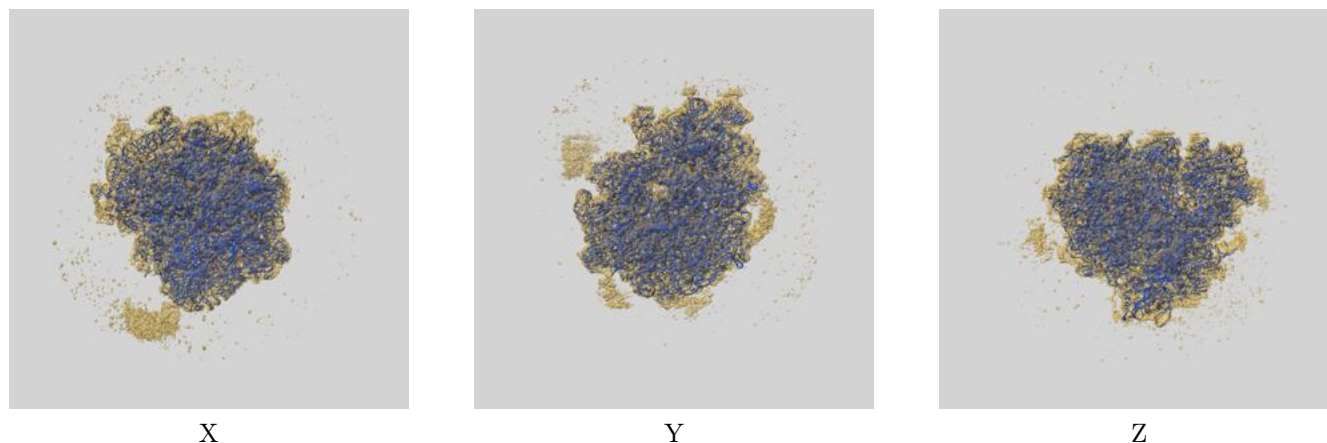
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.70	3.18
Unmasked-calculated*	3.50	4.51	3.62

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

9 Map-model fit [i](#)

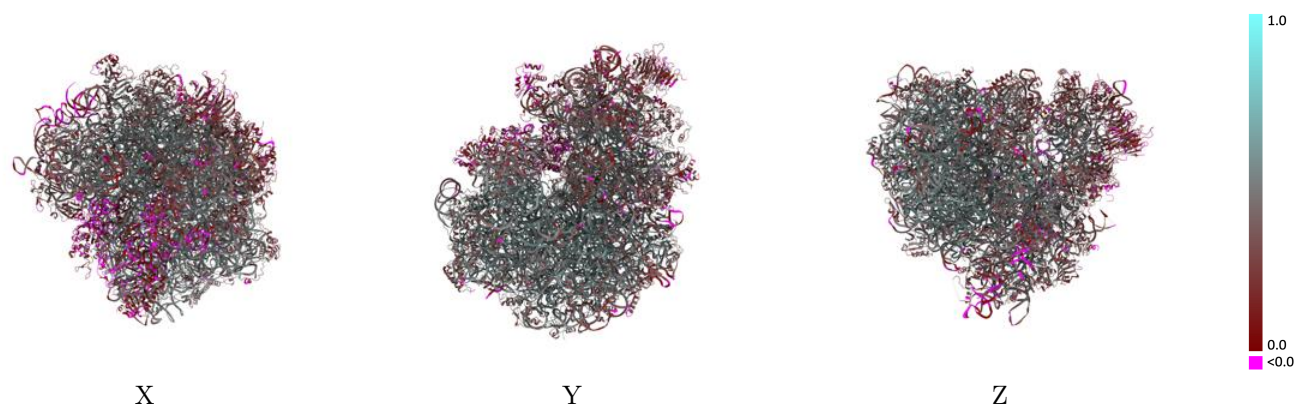
This section contains information regarding the fit between EMDB map EMD-36839 and PDB model 8K2D. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



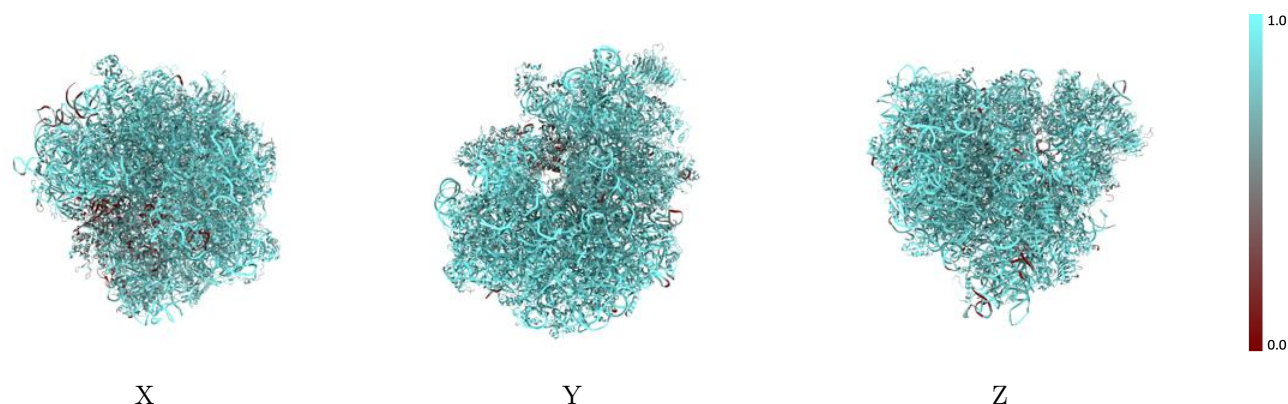
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



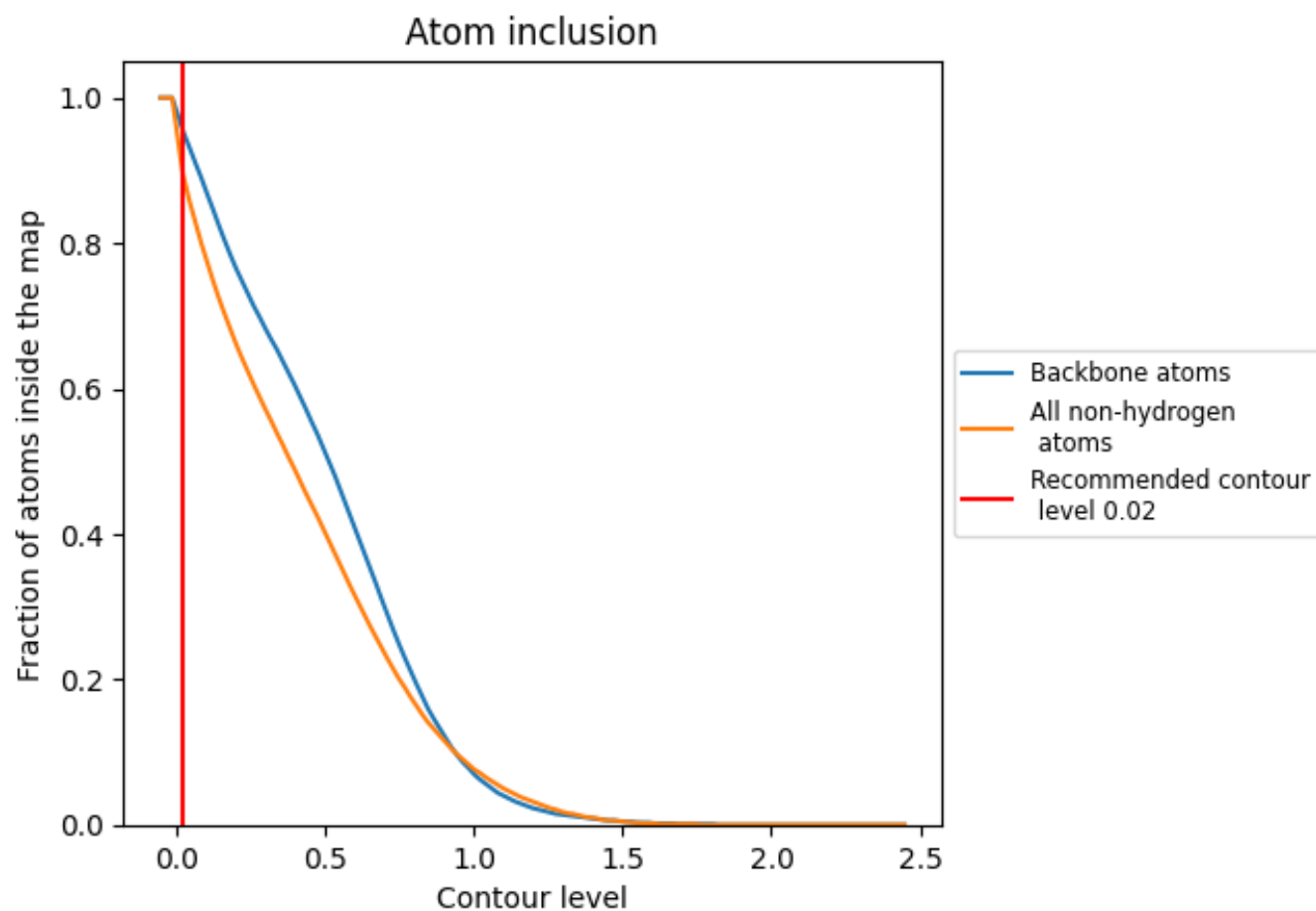
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.4230
C1	 0.9620	 0.5020
C2	 0.9420	 0.4350
C3	 0.9710	 0.5150
C4	 0.9860	 0.5090
CD	 0.4440	 0.0840
CE	 0.8360	 0.3830
CS	 0.7520	 0.2870
L1	 0.8120	 0.3130
LA	 0.9230	 0.4870
LB	 0.9210	 0.4770
LC	 0.9180	 0.4430
LD	 0.8600	 0.3730
LE	 0.8800	 0.4040
LF	 0.9230	 0.4680
LG	 0.8900	 0.3810
LH	 0.8950	 0.4250
LI	 0.8790	 0.4210
LJ	 0.8710	 0.3800
LK	 0.5530	 0.0950
LL	 0.8960	 0.4120
LM	 0.9060	 0.4350
LN	 0.9420	 0.5080
LO	 0.9290	 0.4850
LP	 0.9130	 0.4790
LQ	 0.9180	 0.4610
LR	 0.9230	 0.4750
LS	 0.9190	 0.4660
LT	 0.9040	 0.4640
LU	 0.8670	 0.3870
LV	 0.9040	 0.4670
LW	 0.9010	 0.4500
LX	 0.8910	 0.4410
LY	 0.8850	 0.4330
LZ	 0.8970	 0.4020



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Chain	Atom inclusion	Q-score
La	 0.9290	 0.4640
Lb	 0.8580	 0.4070
Lc	 0.8600	 0.4080
Ld	 0.8540	 0.4350
Le	 0.9000	 0.4730
Lf	 0.9430	 0.5020
Lg	 0.9100	 0.4730
Lh	 0.8680	 0.4160
Li	 0.8590	 0.3880
Lj	 0.9540	 0.5330
Lk	 0.8590	 0.3490
Ll	 0.9160	 0.4700
Lm	 0.8810	 0.4510
Ln	 0.6840	 0.3370
Lo	 0.8720	 0.4510
Lp	 0.9060	 0.4630
P0	 0.5980	 0.1070
SA	 0.9010	 0.3580
SB	 0.8390	 0.3260
SC	 0.8940	 0.4070
SD	 0.8300	 0.3090
SE	 0.8760	 0.3740
SF	 0.8050	 0.2530
SG	 0.7980	 0.2840
SH	 0.8310	 0.2840
SI	 0.8710	 0.3860
SJ	 0.8450	 0.3470
SK	 0.8350	 0.2590
SL	 0.8710	 0.4210
SM	 0.6440	 0.0520
SN	 0.8800	 0.3890
SO	 0.8720	 0.3790
SP	 0.8410	 0.2920
SQ	 0.8480	 0.2960
SR	 0.8280	 0.2760
SS	 0.8530	 0.2990
ST	 0.8320	 0.2860
SU	 0.8430	 0.2770
SV	 0.8780	 0.3650
SW	 0.9220	 0.4620
SX	 0.8850	 0.4200
SY	 0.8000	 0.3060

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Chain	Atom inclusion	Q-score
SZ	 0.8080	 0.2260
Sa	 0.9040	 0.4240
Sb	 0.8990	 0.3820
Sc	 0.7900	 0.2750
Sd	 0.9050	 0.4130
Se	 0.7230	 0.2750
Sf	 0.6430	 0.0470
Sg	 0.8050	 0.1970