



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:42 AM UTC

PDB ID : 8XT0 / pdb_00008xt0
EMDB ID : EMD-38632
Title : Cryo-EM structure of the human 55S mitoribosome with 5um Tigecycline
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2024-01-10
Resolution : 3.20 Å(reported)
Based on initial model : 7A5I

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:

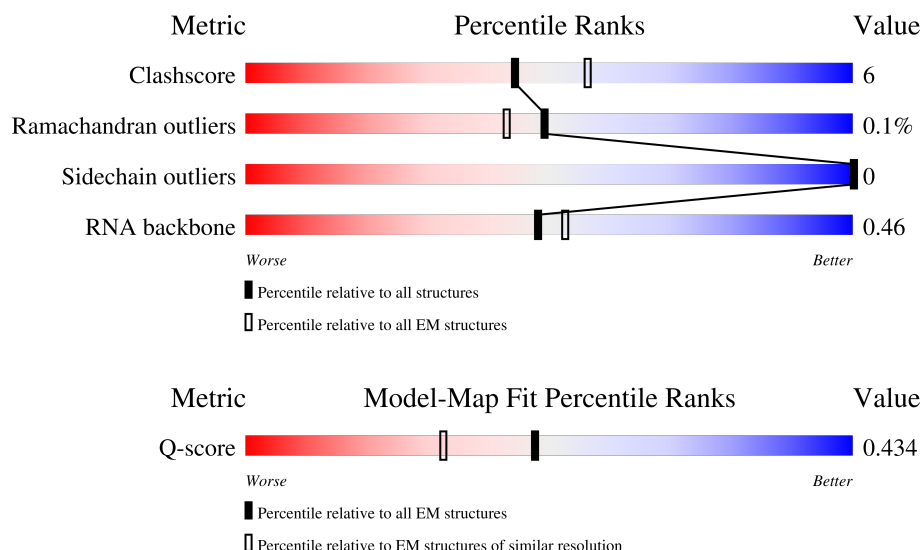
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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.



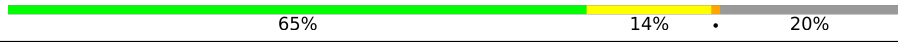
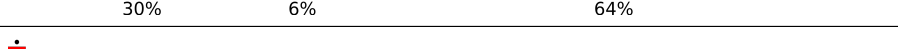
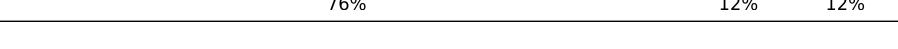
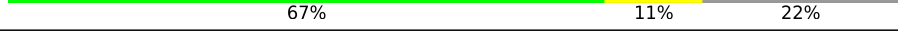
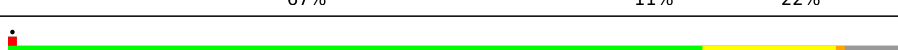
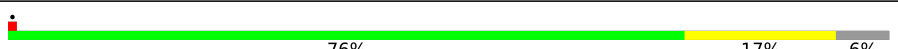
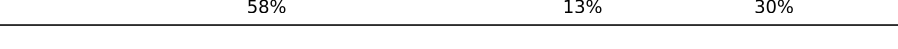
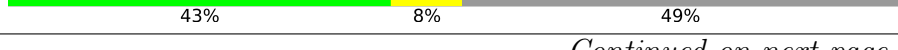
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	L1	1559	
2	L2	69	
3	LB	305	

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Mol	Chain	Length	Quality of chain
4	LC	348	
5	LD	311	
6	LI	267	
7	LJ	261	
8	LK	192	
9	LM	178	
10	LN	145	
11	LO	296	
12	LP	251	
13	LQ	175	
14	LR	179	
15	LS	292	
16	LT	149	
17	LU	205	
18	LV	212	
19	LW	153	
20	LX	216	
21	La	148	
22	Lb	256	
23	Lu	250	
24	Ld	161	
25	Lf	188	
26	Lg	65	
27	Lh	92	
28	Li	188	

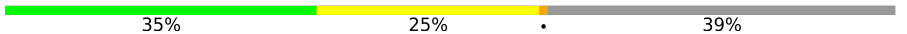
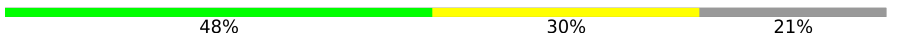
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Mol	Chain	Length	Quality of chain
29	Lj	103	
30	Lk	423	
31	Ll	380	
32	Lm	338	
33	Ln	206	
34	Lo	137	
35	Lp	142	
36	Lq	215	
37	Lr	332	
38	Ls	306	
39	Lt	279	
40	Lv	212	
41	Lw	166	
42	Lx	158	
43	Ly	128	
44	Lz	123	
45	L3	112	
46	L4	138	
47	L5	128	
48	L6	102	
49	L7	206	
50	L8	222	
51	SR	196	
52	Sf	439	
53	SB	296	

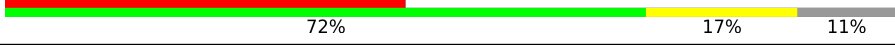
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Mol	Chain	Length	Quality of chain
54	SZ	167	
55	SE	430	
56	SF	125	
57	SG	242	
58	SI	396	
59	SJ	201	
60	SK	194	
61	SL	138	
62	SN	128	
63	SO	257	
64	SP	137	
65	SQ	130	
66	SS	258	
67	ST	142	
68	SW	87	
69	SX	360	
70	SY	190	
71	Sa	173	
72	Sb	205	
73	Sc	414	
74	Sd	187	
75	Se	398	
76	Sg	395	
77	Si	106	
78	Sj	218	

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Mol	Chain	Length	Quality of chain
79	Sk	323	
80	Sm	118	
81	Sn	199	
82	So	689	
83	S1	954	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 165243 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 16s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1500	Total	C	N	O	P	0	0
			31847	14290	5750	10307	1500		

- Molecule 2 is a RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	237	Total	C	N	O	S	0	0
			1851	1151	375	316	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LC	304	Total	C	N	O	S	0	0
			2393	1538	415	429	11		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LD	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LI	95	Total	C	N	O		0	0
			784	498	152	134			

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LJ	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LK	175	Total	C	N	O	S	0	0
			1323	841	237	243	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LM	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LN	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LO	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LP	221	Total	C	N	O	S	0	0
			1779	1138	325	306	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LQ	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LR	146	Total	C	N	O	S	0	0
			1189	743	226	215	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LS	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LT	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LU	160	Total	C	N	O	S	0	0
			1284	829	226	225	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LV	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LW	143	Total	C	N	O	S	0	0
			1188	752	224	208	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LX	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	La	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Lb	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Lu	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ld	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Lf	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Lg	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Lh	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Li	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lj	38	Total	C	N	O	S	0	0
			341	217	72	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lk	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ll	354	Total	C	N	O	S	0	0
			2947	1881	525	532	9		

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lm	293	Total	C	N	O	S	0	0
			2382	1525	404	435	18		

- Molecule 33 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ln	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lo	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 35 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lp	97	Total	C	N	O	S	0	0
			815	514	147	149	5		

- Molecule 36 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lq	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lr	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ls	214	Total	C	N	O	S	0	0
			1754	1117	304	320	13		

- Molecule 39 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lt	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lv	131	Total	C	N	O	S	0	0
			1035	661	169	201	4		

- Molecule 41 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lw	132	Total	C	N	O	S	0	0
			1097	710	191	194	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lx	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 43 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ly	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lz	92	Total	C	N	O	S	0	0
			732	454	142	134	2		

- Molecule 45 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L3	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 46 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L4	83	Total	C	N	O	S	0	0
			703	446	124	130	3		

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L5	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L6	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L7	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L8	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SR	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Sf	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SB	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 54 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SZ	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 55 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SE	320	Total	C	N	O	S	0	0
			2540	1600	473	455	12		

- Molecule 56 is a protein called Small ribosomal subunit protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SF	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 57 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SG	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 58 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SI	304	Total	C	N	O	S	0	0
			2501	1591	444	452	14		

- Molecule 59 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SJ	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 60 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SK	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 61 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SL	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 63 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 64 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 65 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 66 is a protein called Small ribosomal subunit protein mS40.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 67 is a protein called Small ribosomal subunit protein bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 68 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SW	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SW	50	ARG	CYS	variant	UNP P82921

- Molecule 69 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	295	Total	C	N	O	S	0	0
			2405	1530	413	454	8		

- Molecule 70 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SY	126	Total	C	N	O	S	0	0
			1042	673	183	185	1		

- Molecule 71 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Sa	162	Total	C	N	O	S	0	0
			1330	850	231	238	11		

- Molecule 72 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sb	173	Total	C	N	O	S	0	0
			1454	894	294	262	4		

- Molecule 73 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sc	385	Total	C	N	O	S	0	0
			3116	1980	522	603	11		

- Molecule 74 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sd	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 75 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Se	350	Total	C	N	O	S	0	0
			2836	1813	497	515	11		

- Molecule 76 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sg	108	Total	C	N	O	S	0	0
			903	587	145	169	2		

- Molecule 77 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Si	86	Total	C	N	O	S	0	0
			731	467	131	129	4		

- Molecule 78 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sj	201	Total	C	N	O	S	0	0
			1680	1062	321	292	5		

- Molecule 79 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sk	256	Total	C	N	O	S	0	0
			2068	1317	349	392	10		

- Molecule 80 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sm	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 81 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sn	69	Total	C	N	O	S	0	0
			610	393	130	86	1		

- Molecule 82 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	So	616	Total	C	N	O	S	0	0
			4981	3177	849	928	27		

- Molecule 83 is a RNA chain called 12s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	S1	928	Total	C	N	O	P	0	0
			19716	8840	3560	6388	928		

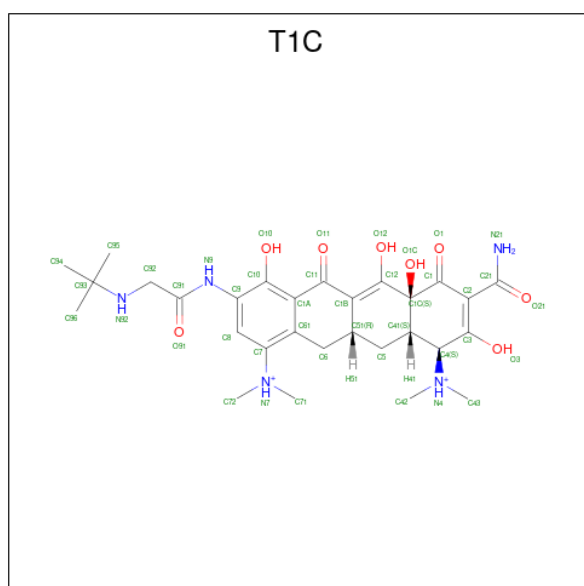
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	873	A	U	conflict	GB 587653923

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	L1	106	Total	Mg	0
			106	106	
84	LB	3	Total	Mg	0
			3	3	
84	LP	1	Total	Mg	0
			1	1	
84	Lw	1	Total	Mg	0
			1	1	
84	L6	1	Total	Mg	0
			1	1	
84	S1	33	Total	Mg	0
			33	33	

- Molecule 85 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).

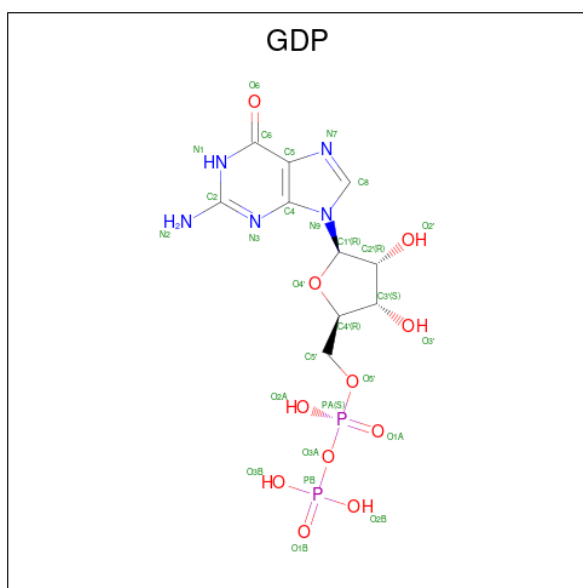


Mol	Chain	Residues	Atoms				AltConf
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	S1	1	Total	C	N	O	0
			42	29	5	8	

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

Mol	Chain	Residues	Atoms		AltConf
86	Lf	1	Total	Zn	0
			1	1	
86	Lj	1	Total	Zn	0
			1	1	
86	SR	1	Total	Zn	0
			1	1	
86	SB	1	Total	Zn	0
			1	1	
86	SS	1	Total	Zn	0
			1	1	
86	ST	1	Total	Zn	0
			1	1	
86	Sa	1	Total	Zn	0
			1	1	

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

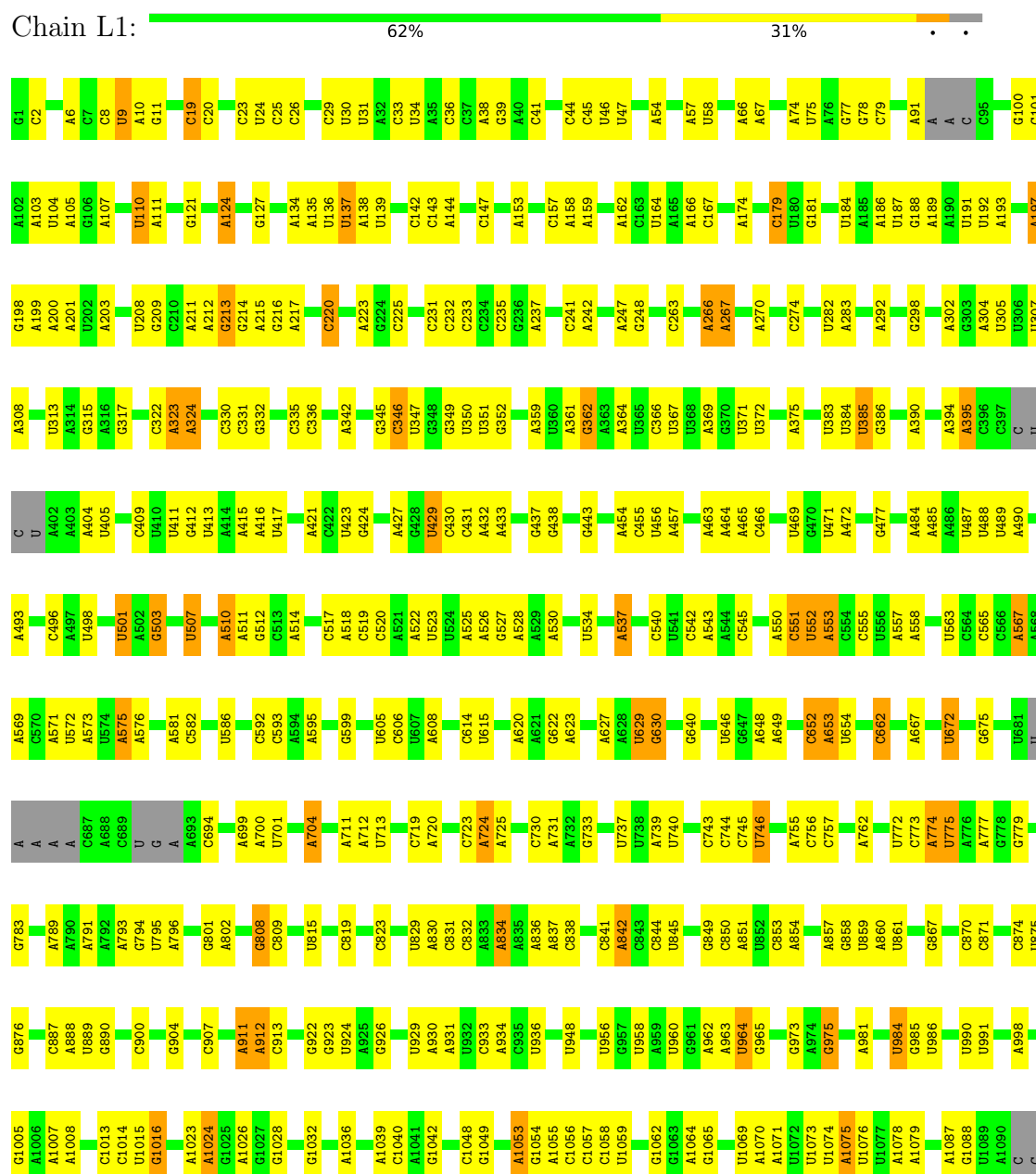


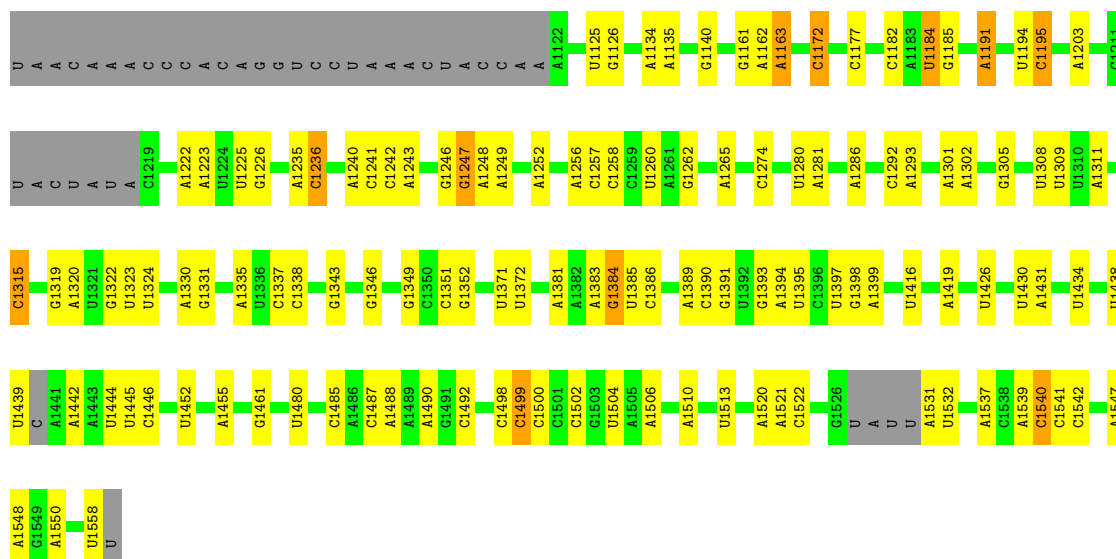
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	Se	1	28	10	5	11	2	0

3 Residue-property plots

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

• Molecule 1: 16s rRNA





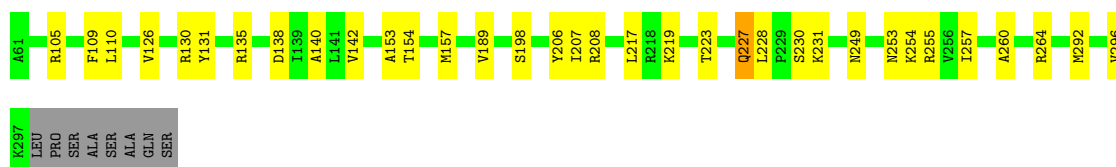
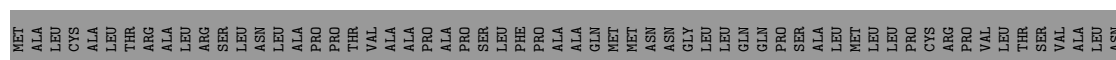
- Molecule 2: Val tRNA

Chain L2: 36% 43% 19%



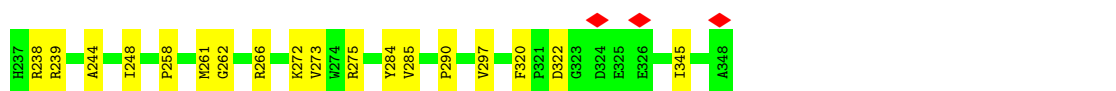
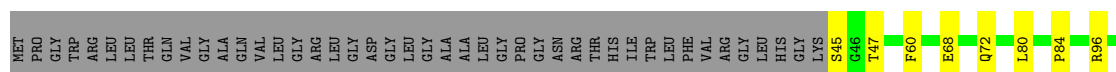
- Molecule 3: Large ribosomal subunit protein uL2m

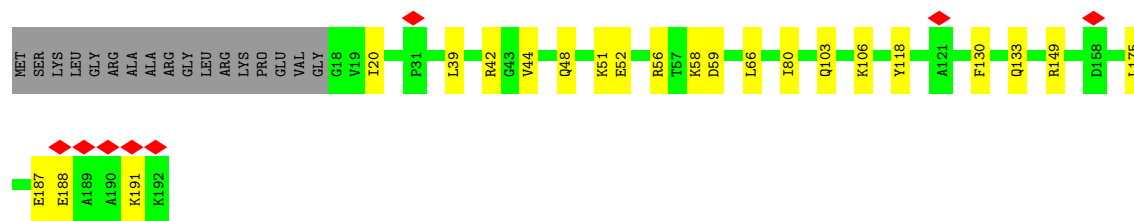
Chain LB: 67% 11% 22%



- Molecule 4: Large ribosomal subunit protein uL3m

Chain LC: 69% 18% 13%





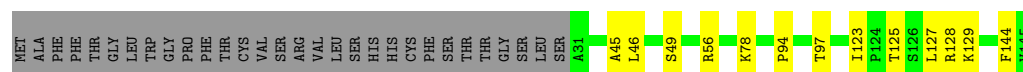
- Molecule 9: Large ribosomal subunit protein uL13m

Chain LM: 89% 11%



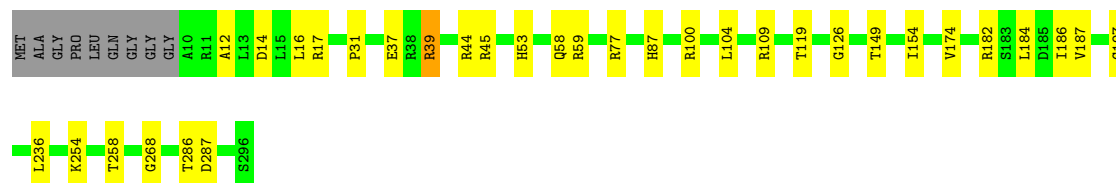
- Molecule 10: Large ribosomal subunit protein uL14m

Chain LN: 70% 9% 21%



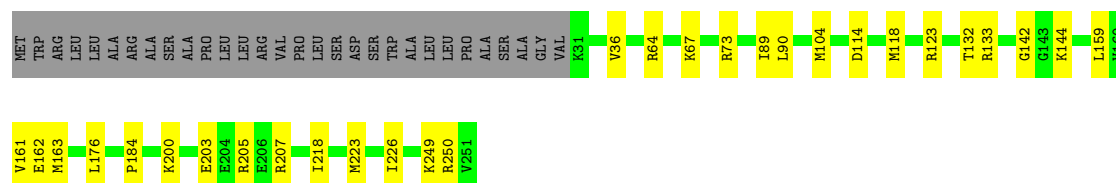
- Molecule 11: Large ribosomal subunit protein uL15m

Chain LO: 86% 11%



- Molecule 12: Large ribosomal subunit protein uL16m

Chain LP: 76% 12% 12%



- Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ: 75% 12% 13%

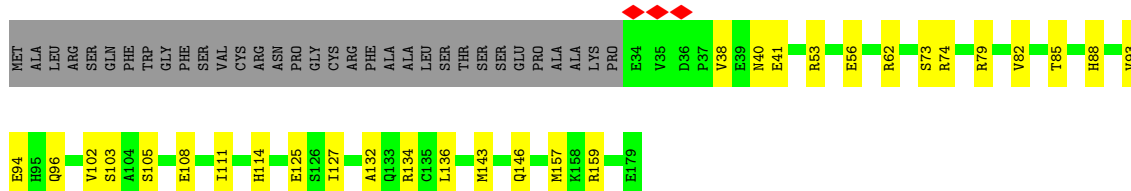


GLY
ILE

- Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain LR:

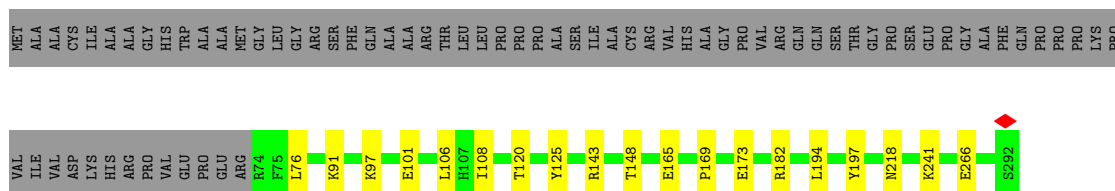
65% 17% 18%



- Molecule 15: Large ribosomal subunit protein bL19m

Chain LS:

68% 7% 25%



- Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:

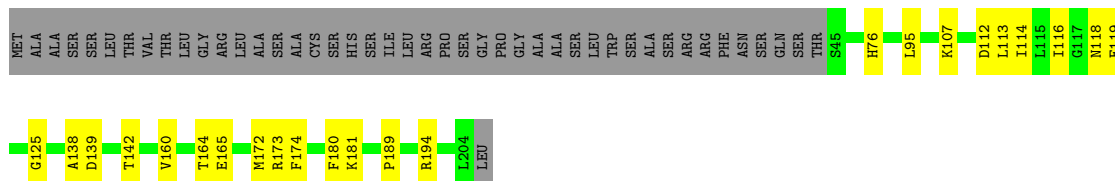
85% 9% 6%



- Molecule 17: Large ribosomal subunit protein bL21m

Chain LU:

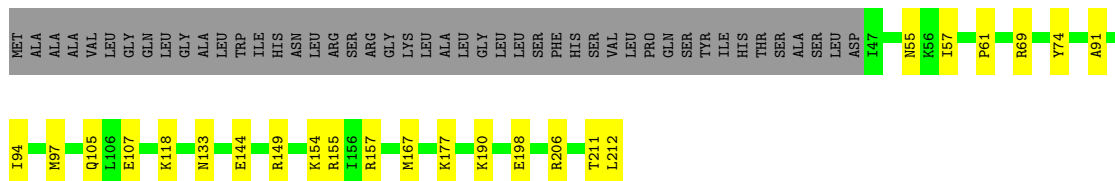
67% 11% 22%



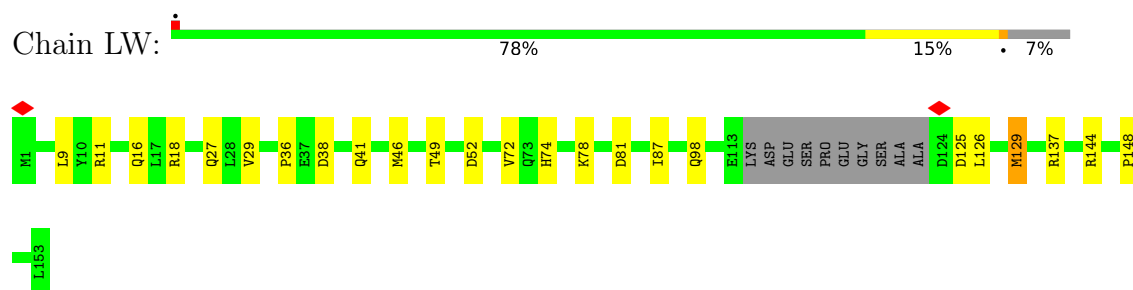
- Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain LV:

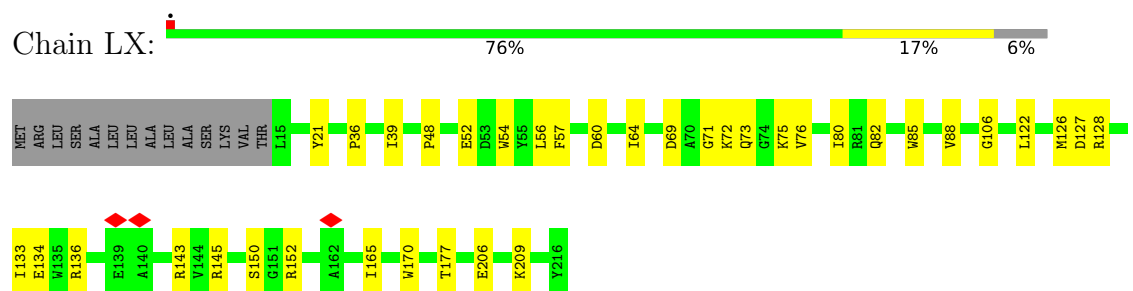
67% 11% 22%



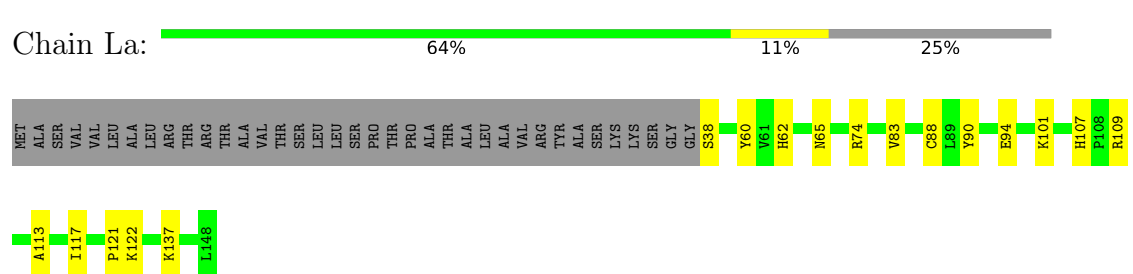
- Molecule 19: Large ribosomal subunit protein uL23m



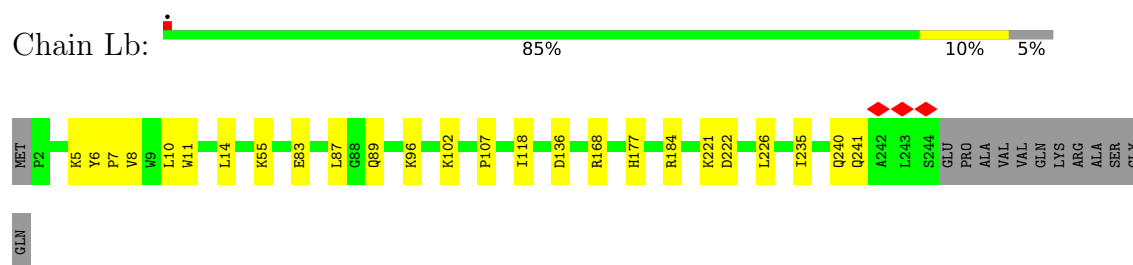
- Molecule 20: Large ribosomal subunit protein uL24m



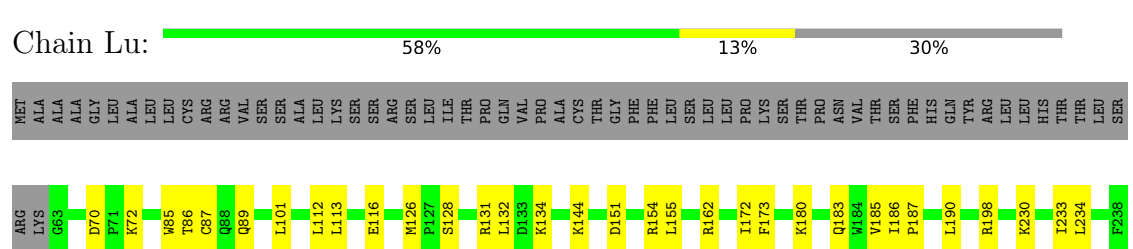
- Molecule 21: Large ribosomal subunit protein bL27m



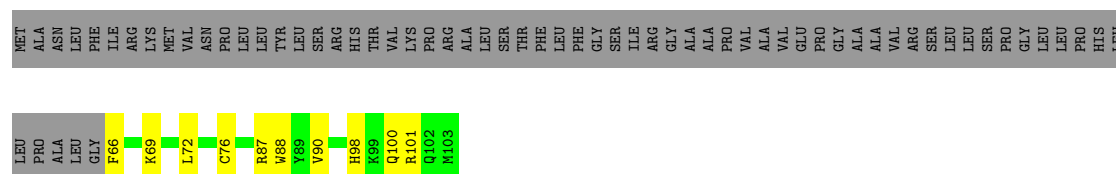
- Molecule 22: Large ribosomal subunit protein bL28m



- Molecule 23: Large ribosomal subunit protein uL29m

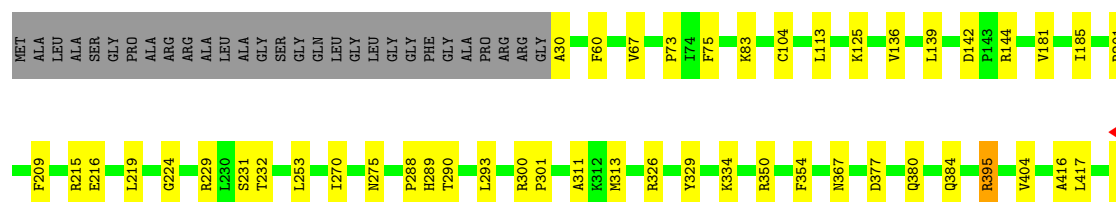


Chain Lj:  27% 10% 63%



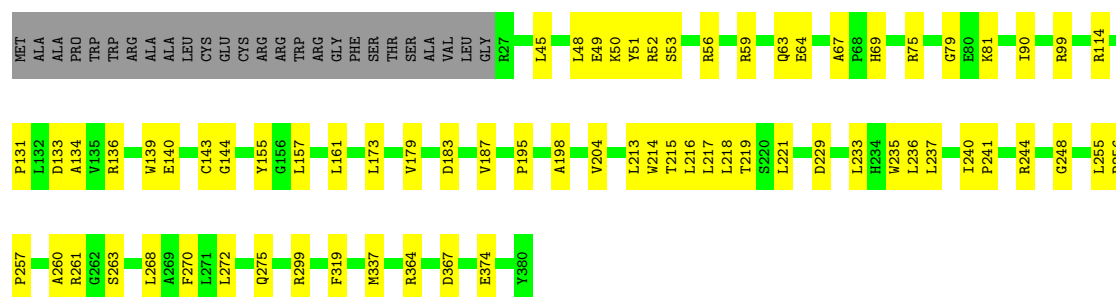
- Molecule 30: Large ribosomal subunit protein mL37

Chain Lk:  82% 11% 7%



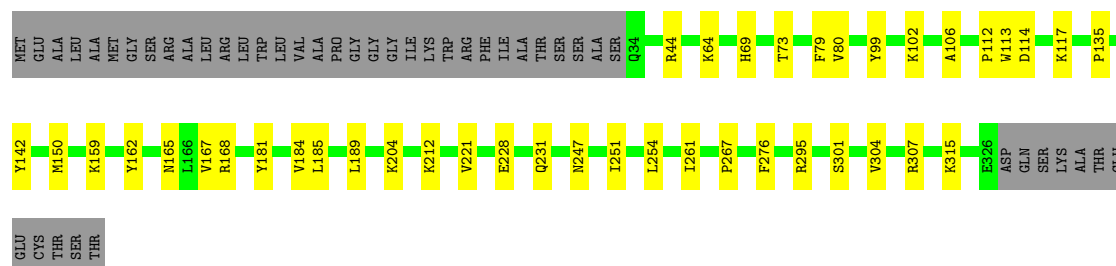
- Molecule 31: Large ribosomal subunit protein mL38

Chain Ll:  75% 18% 7%



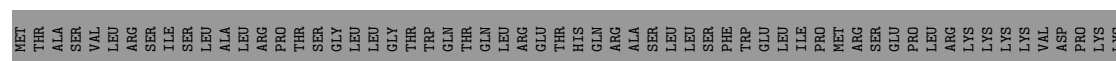
- Molecule 32: Large ribosomal subunit protein mL39

Chain Lm:  75% 12% 13%

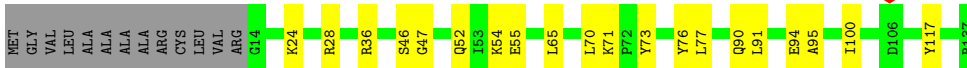
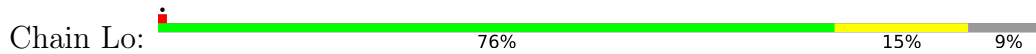


- Molecule 33: Large ribosomal subunit protein mL40

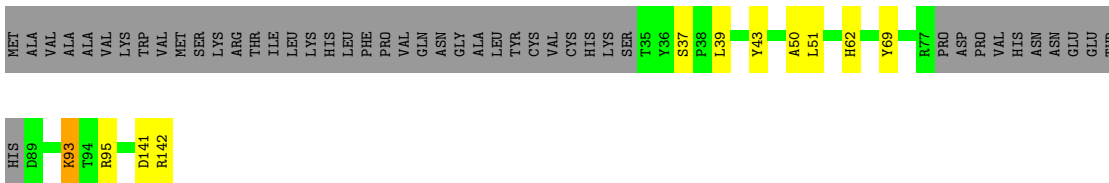
Chain Ln:  36% 11% 52%



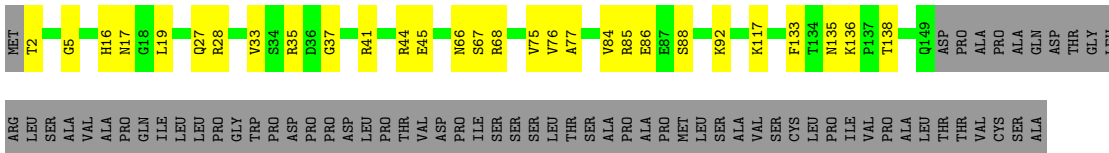
- Molecule 34: Large ribosomal subunit protein mL41



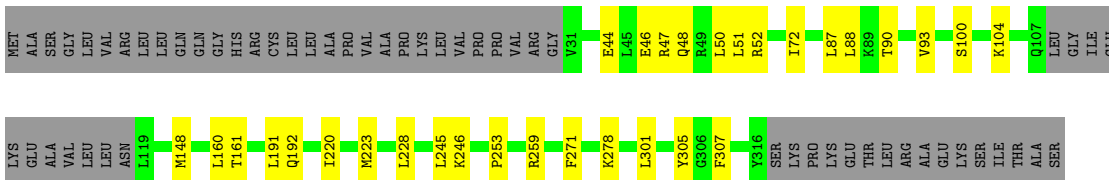
- Molecule 35: Large ribosomal subunit protein mL42



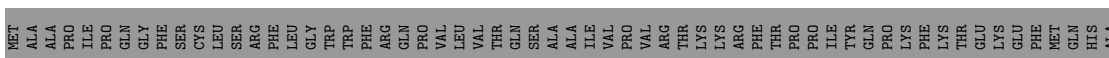
- Molecule 36: Large ribosomal subunit protein mL43

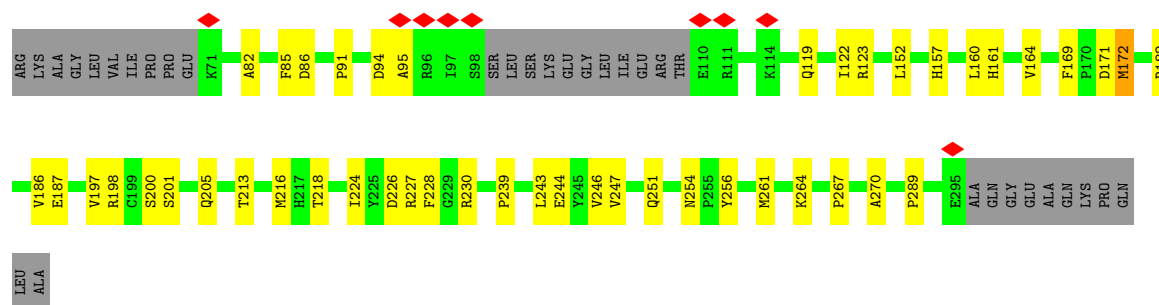


- Molecule 37: Large ribosomal subunit protein mL44

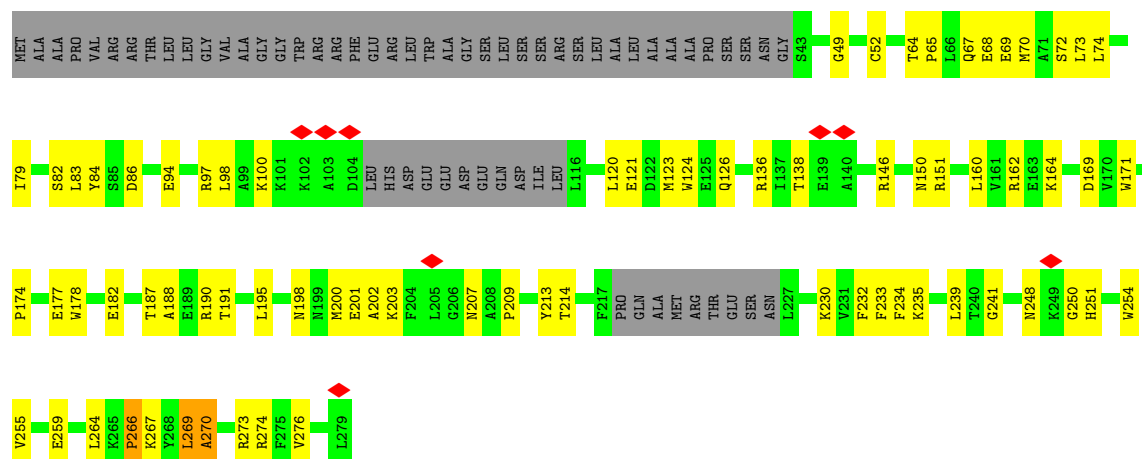


- Molecule 38: Large ribosomal subunit protein mL45

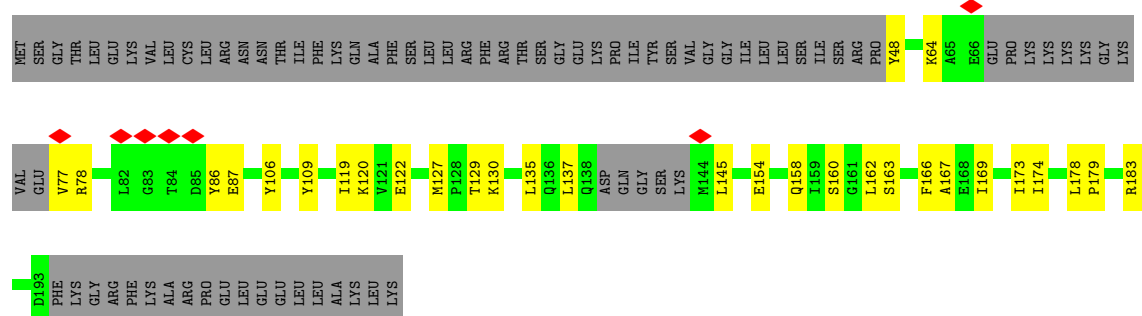




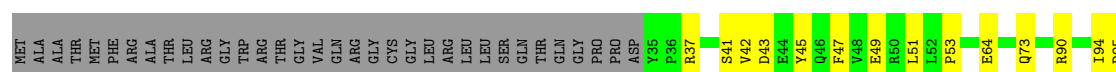
- Molecule 39: Large ribosomal subunit protein mL46



- Molecule 40: Large ribosomal subunit protein mL48

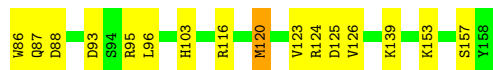
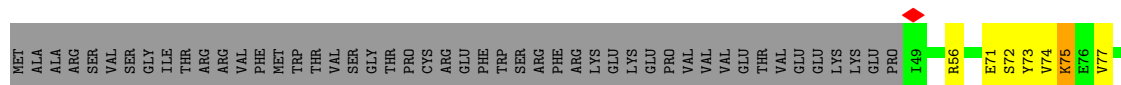


- Molecule 41: Large ribosomal subunit protein mL49

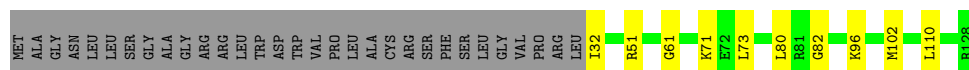




- Molecule 42: Large ribosomal subunit protein mL50



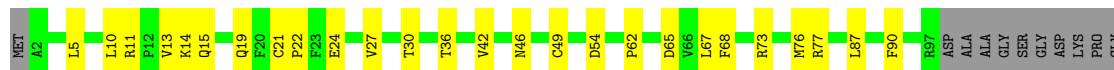
- Molecule 43: Large ribosomal subunit protein mL51



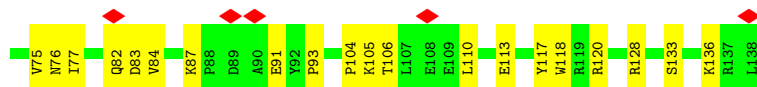
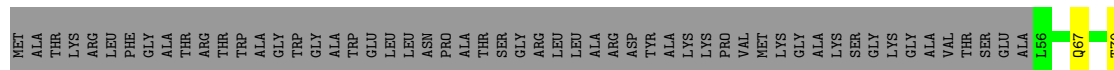
- Molecule 44: 39S ribosomal protein L52, mitochondrial



- Molecule 45: Large ribosomal subunit protein mL53

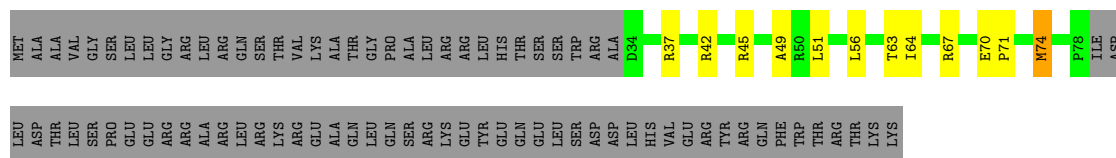


- Molecule 46: Large ribosomal subunit protein mL54



- Molecule 47: Large ribosomal subunit protein mL55

Chain L5:  26% 9% 65%



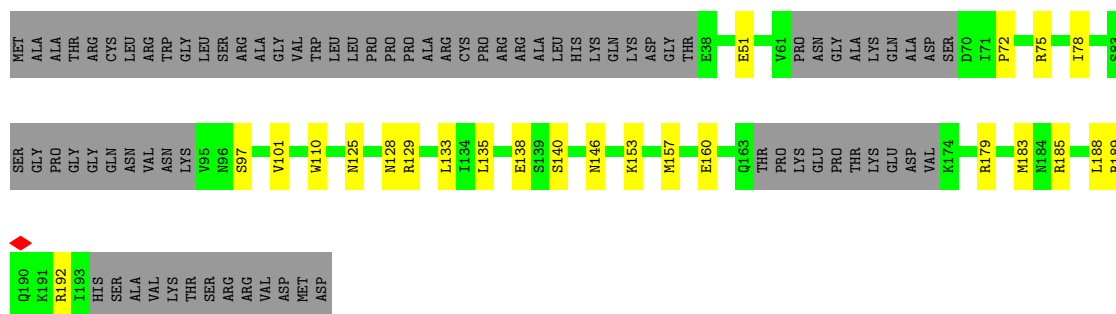
- Molecule 48: Large ribosomal subunit protein mL63

Chain L6:  74% 19% 8%



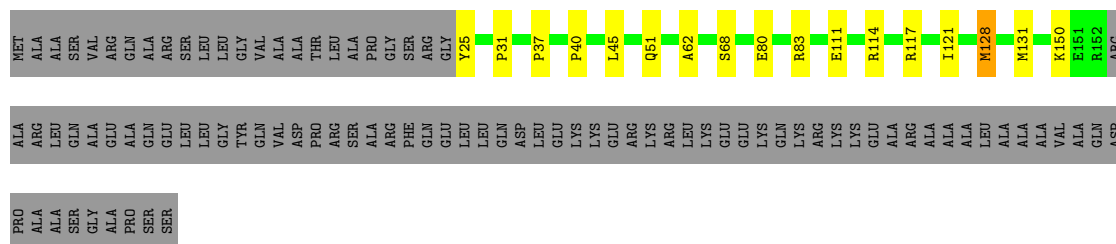
- Molecule 49: Large ribosomal subunit protein mL62

Chain L7:  50% 12% 38%



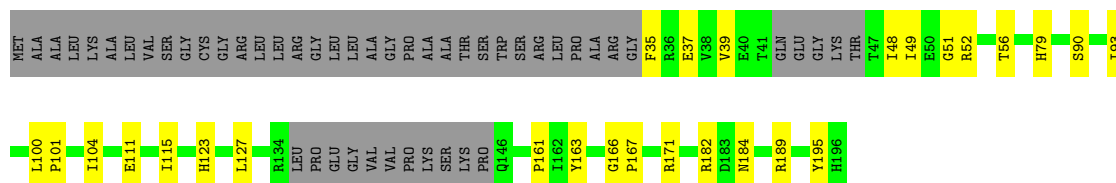
- Molecule 50: Large ribosomal subunit protein mL64

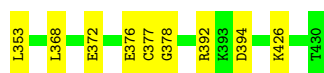
Chain L8:  50% 7% 42%



- Molecule 51: Large ribosomal subunit protein mL66

Chain SR:  61% 14% 26%





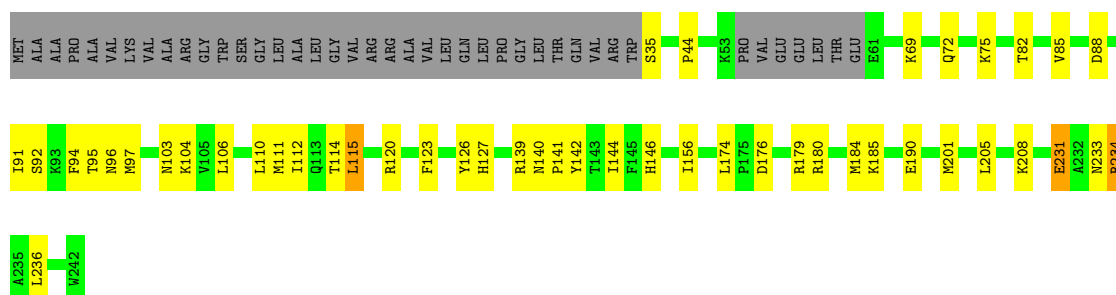
- Molecule 56: Small ribosomal subunit protein bS6m

Chain SF: 76% 22% .



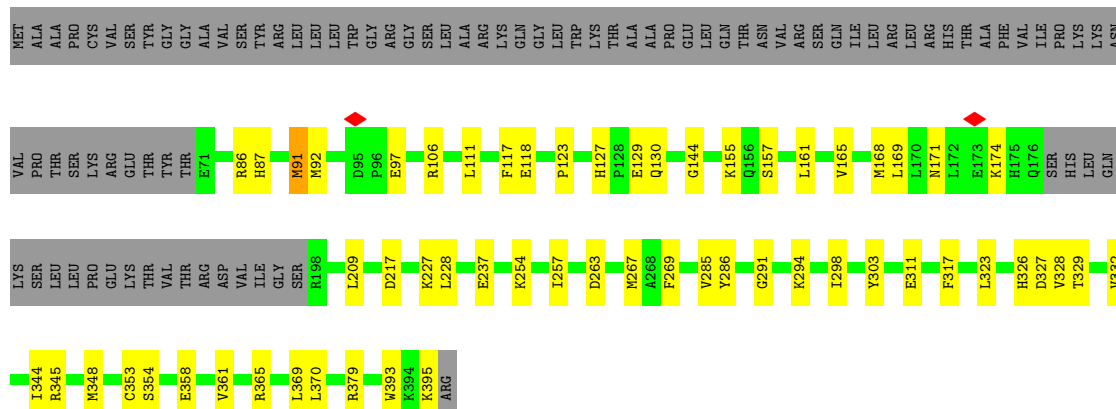
- Molecule 57: Small ribosomal subunit protein uS7m

Chain SG: 64% 18% 17% .



- Molecule 58: Small ribosomal subunit protein uS9m

Chain SI: 62% 15% 23% .

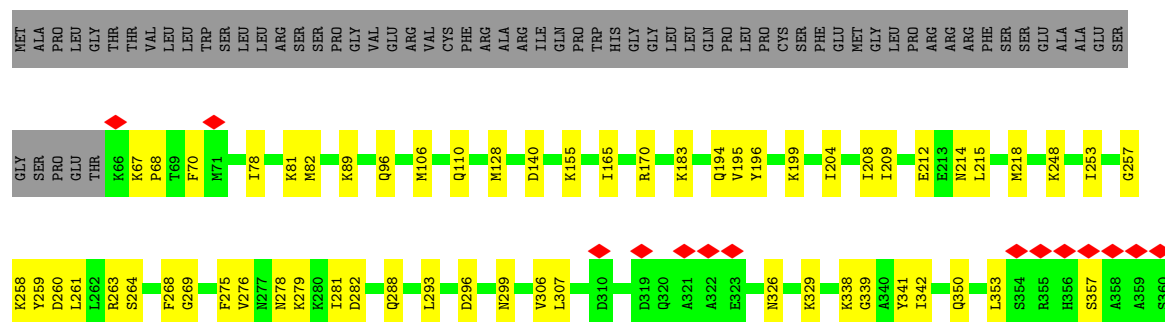


- Molecule 59: Small ribosomal subunit protein uS10m

Chain SJ: 35% 25% 39% .



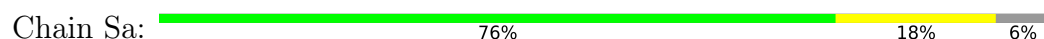




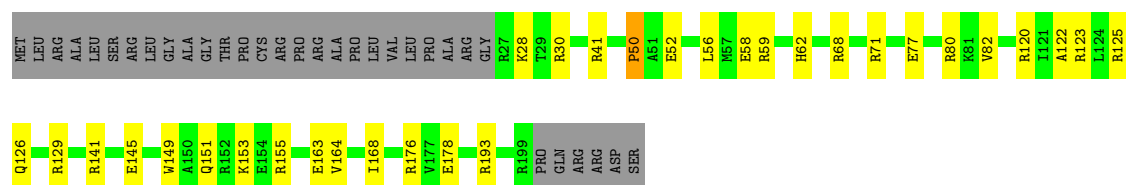
- Molecule 70: Small ribosomal subunit protein mS23



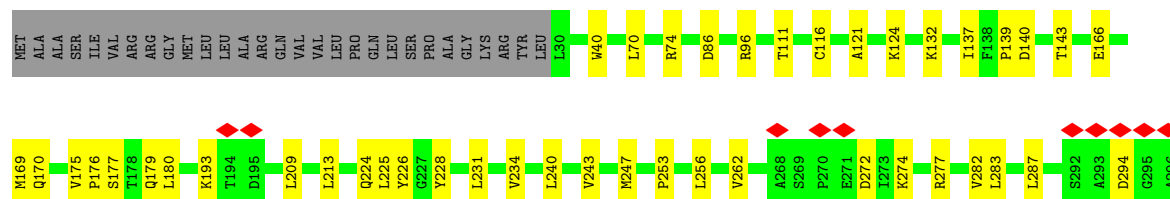
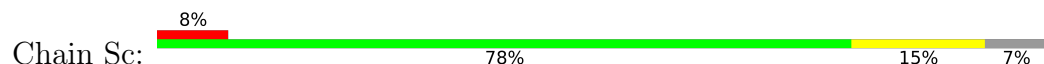
- Molecule 71: Small ribosomal subunit protein mS25

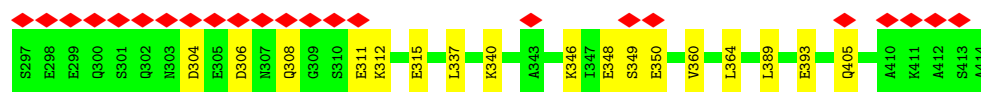


- Molecule 72: Small ribosomal subunit protein mS26



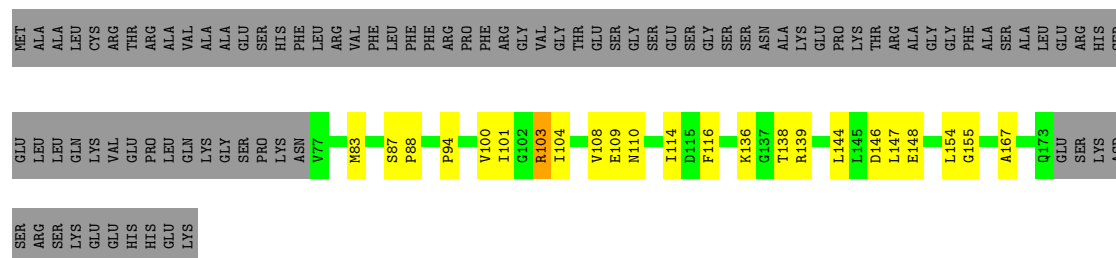
- Molecule 73: Small ribosomal subunit protein mS27





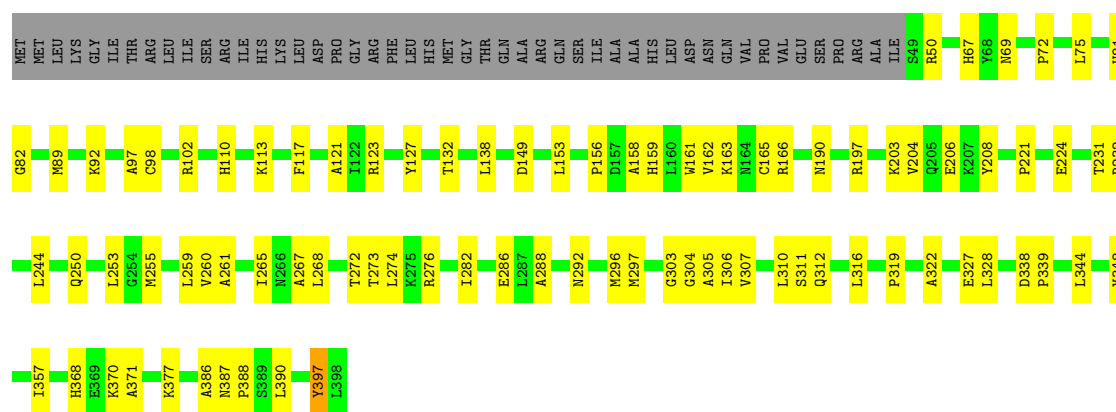
- Molecule 74: Small ribosomal subunit protein bS1m

Chain Sd: 40% 12% 48%



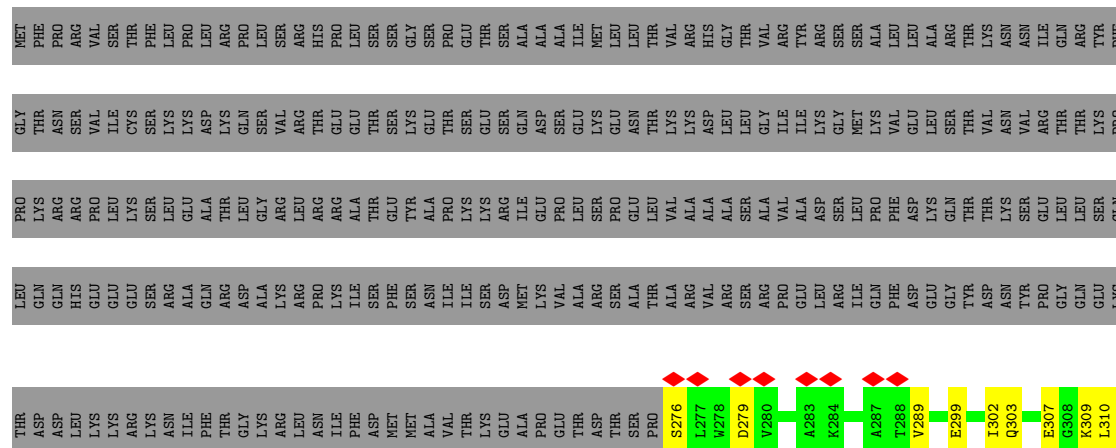
- Molecule 75: Small ribosomal subunit protein mS29

Chain Se: 66% 22% 12%



- Molecule 76: Small ribosomal subunit protein mS31

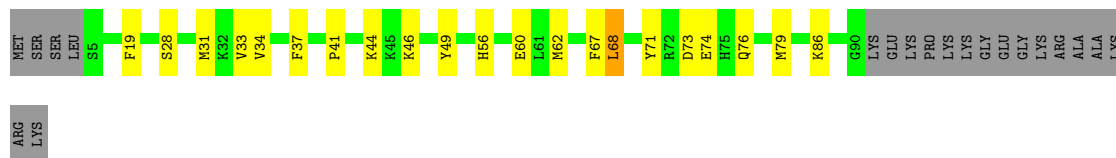
Chain Sg: 20% 7% 73%





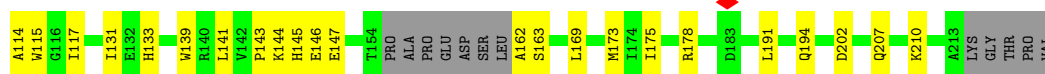
- Molecule 77: Small ribosomal subunit protein mS33

Chain Si: 61% 19% 19%



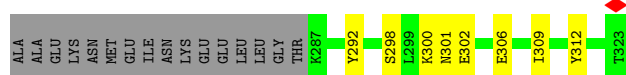
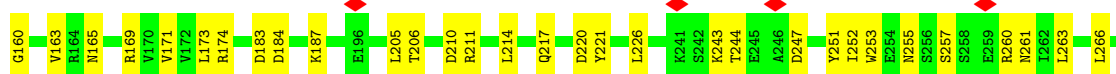
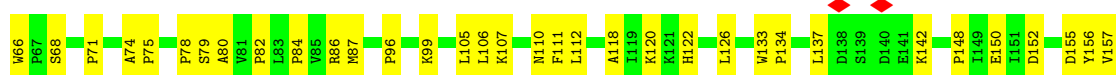
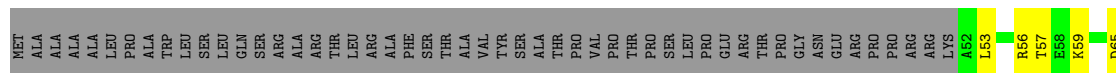
- Molecule 78: Small ribosomal subunit protein mS34

Chain Sj: 67% 26% 8%



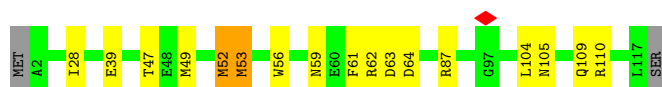
- Molecule 79: Small ribosomal subunit protein mS35

Chain Sk: 55% 24% 21%



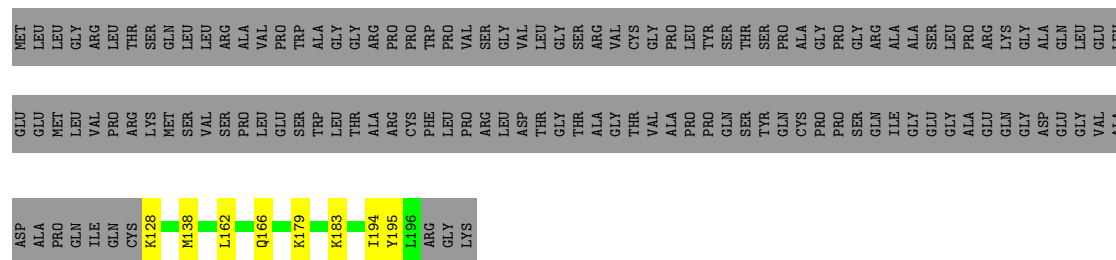
- Molecule 80: Small ribosomal subunit protein mS37

Chain Sm: 84% 13% 3%



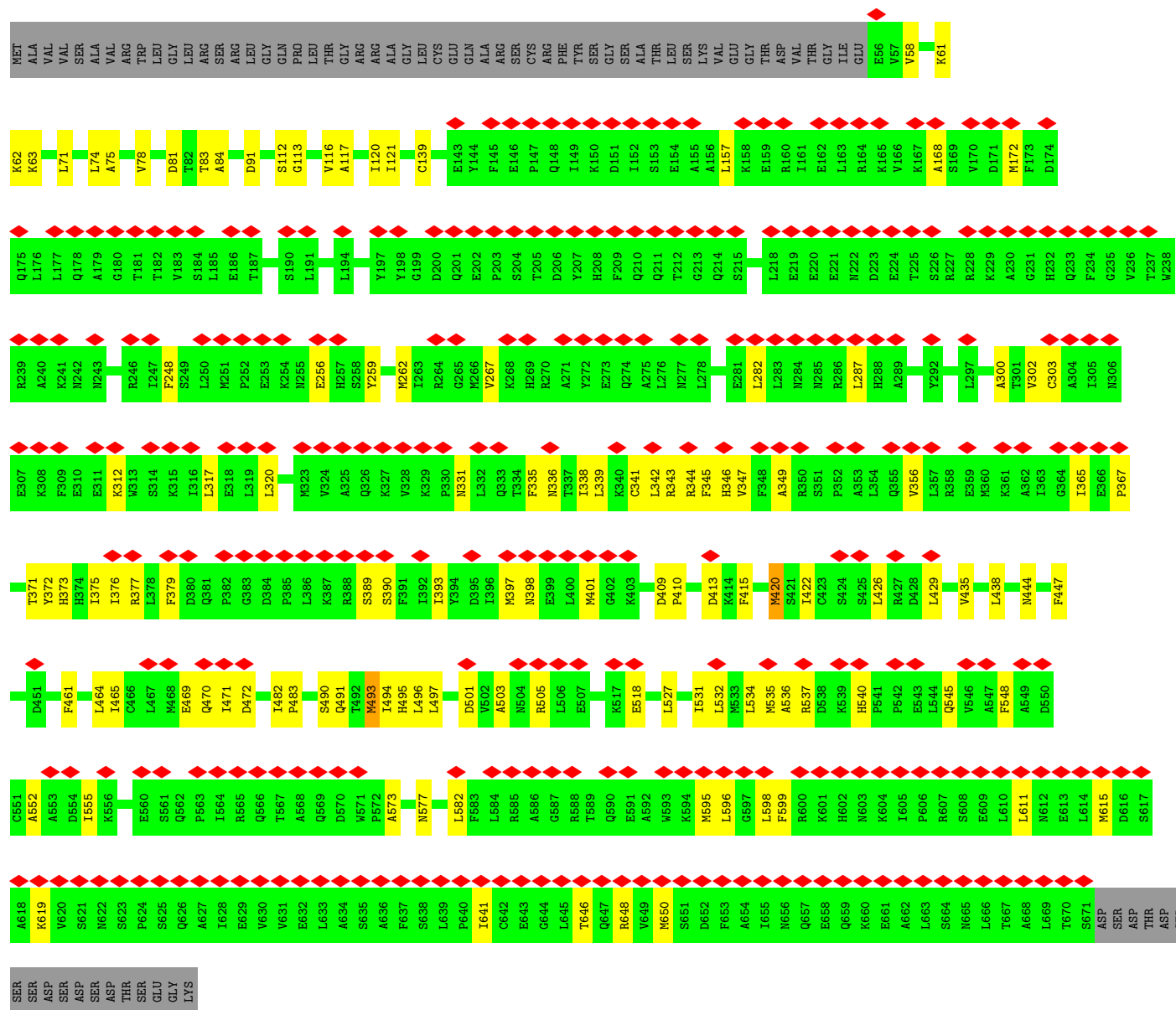
• Molecule 81: Small ribosomal subunit protein mS38

Chain Sn:  31% 65%



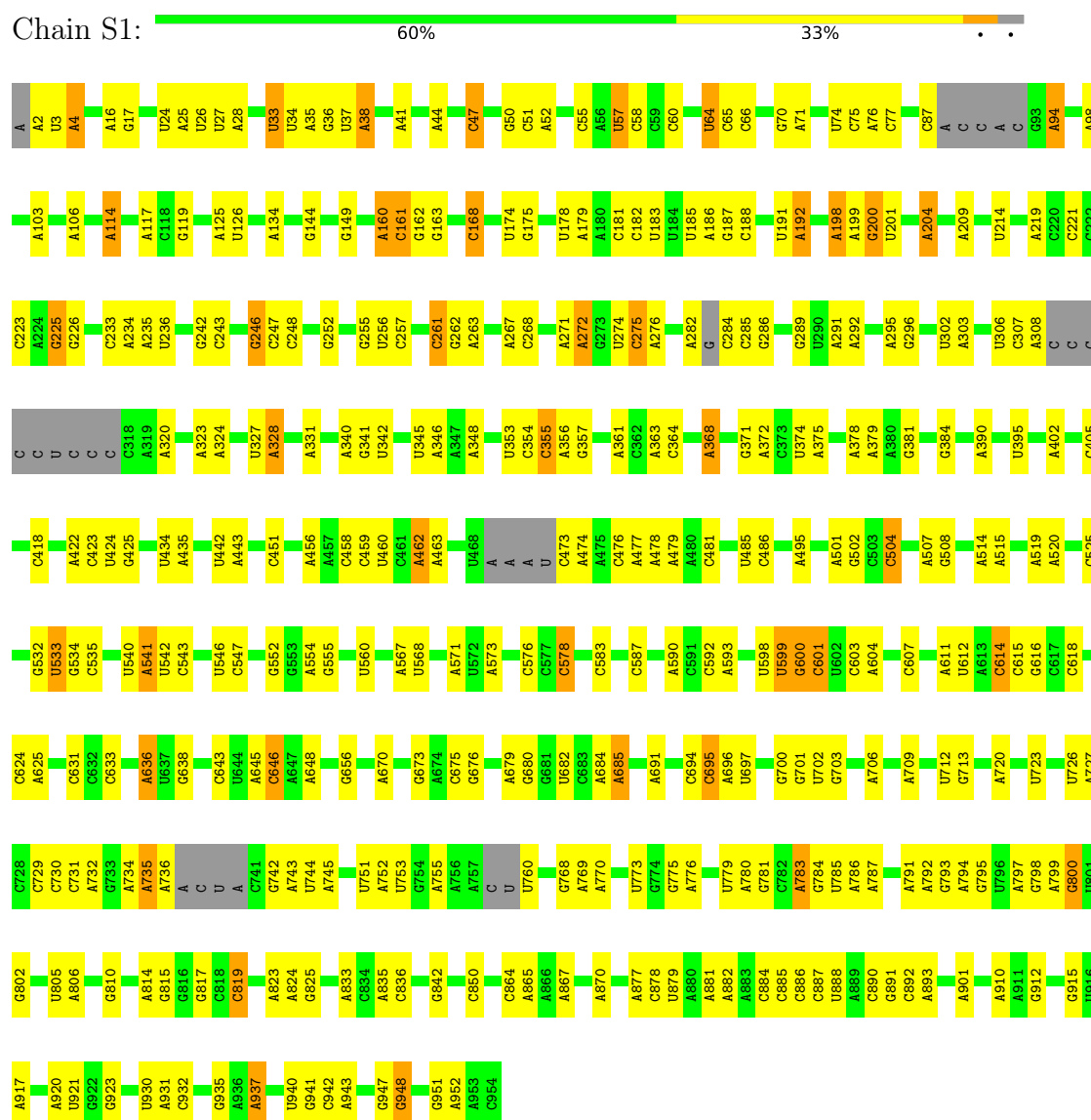
• Molecule 82: Small ribosomal subunit protein mS39

Chain So:  45% 72% 17% 11%



● Molecule 83: 12s rRNA

Chain S1:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112982	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T1C, 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	L1	0.41	0/35628	0.44	0/55448
2	L2	0.16	0/1328	0.30	0/2056
3	LB	0.37	0/1888	0.55	2/2538 (0.1%)
4	LC	0.35	0/2462	0.57	0/3340
5	LD	0.38	0/2071	0.62	2/2817 (0.1%)
6	LI	0.29	0/798	0.58	0/1073
7	LJ	0.45	0/1308	0.94	2/1761 (0.1%)
8	LK	0.27	0/1340	0.52	0/1802
9	LM	0.37	0/1495	0.56	0/2029
10	LN	0.34	0/904	0.53	0/1218
11	LO	0.35	0/2359	0.51	0/3185
12	LP	0.32	0/1826	0.51	0/2458
13	LQ	0.34	0/1269	0.52	0/1708
14	LR	0.31	0/1215	0.49	1/1645 (0.1%)
15	LS	0.30	0/1863	0.52	0/2509
16	LT	0.42	0/1174	0.55	0/1572
17	LU	0.37	0/1311	0.58	0/1778
18	LV	0.37	0/1402	0.53	0/1886
19	LW	0.36	0/1217	0.57	1/1644 (0.1%)
20	LX	0.31	1/1697 (0.1%)	0.58	0/2302
21	La	0.38	0/893	0.47	0/1204
22	Lb	0.32	0/2090	0.53	0/2825
23	Lu	0.35	0/1552	0.54	0/2079
24	Ld	0.38	0/1003	0.56	0/1354
25	Lf	0.32	0/895	0.48	0/1201
26	Lg	0.30	0/438	0.53	0/583
27	Lh	0.46	0/382	0.52	0/507
28	Li	0.39	0/852	0.48	0/1136
29	Lj	0.33	0/349	0.53	0/461
30	Lk	0.28	0/3305	0.48	1/4502 (0.0%)
31	Ll	0.27	0/3042	0.54	0/4140
32	Lm	0.29	0/2439	0.54	0/3299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ln	0.32	0/855	0.69	0/1152
34	Lo	0.31	0/1025	0.57	0/1379
35	Lp	0.32	0/839	0.56	1/1136 (0.1%)
36	Lq	0.34	0/1202	0.54	0/1626
37	Lr	0.28	0/2264	0.52	0/3059
38	Ls	0.28	0/1800	0.57	1/2436 (0.0%)
39	Lt	0.27	0/1797	0.60	1/2422 (0.0%)
40	Lv	0.38	1/1051 (0.1%)	0.81	2/1422 (0.1%)
41	Lw	0.35	0/1134	0.55	1/1547 (0.1%)
42	Lx	0.40	0/918	0.71	2/1249 (0.2%)
43	Ly	0.43	0/849	0.56	0/1135
44	Lz	0.30	0/747	0.52	0/1005
45	L3	0.31	1/754 (0.1%)	0.64	0/1017
46	L4	0.27	0/722	0.69	0/978
47	L5	0.35	0/379	0.86	1/510 (0.2%)
48	L6	0.39	0/818	0.55	0/1097
49	L7	0.26	0/1071	0.54	2/1433 (0.1%)
50	L8	0.27	0/1107	0.47	1/1498 (0.1%)
51	SR	0.35	0/1238	0.59	0/1676
52	Sf	0.31	0/3114	0.53	0/4225
53	SB	0.33	0/1811	0.62	2/2451 (0.1%)
54	SZ	0.42	1/1112 (0.1%)	0.68	1/1505 (0.1%)
55	SE	0.29	0/2590	0.57	1/3477 (0.0%)
56	SF	0.30	0/989	0.58	0/1335
57	SG	0.32	1/1708 (0.1%)	0.61	3/2291 (0.1%)
58	SI	0.25	0/2555	0.60	1/3424 (0.0%)
59	SJ	0.43	0/1019	0.84	2/1379 (0.1%)
60	SK	0.27	0/1031	0.51	0/1390
61	SL	0.36	0/854	0.70	2/1148 (0.2%)
62	SN	0.33	0/879	0.78	1/1182 (0.1%)
63	SO	0.37	1/1406 (0.1%)	0.67	1/1878 (0.1%)
64	SP	0.28	0/941	0.62	0/1265
65	SQ	0.25	0/864	0.52	0/1169
66	SS	0.27	0/1580	0.59	0/2150
67	ST	0.36	0/791	0.60	0/1062
68	SW	0.31	0/752	0.58	0/1001
69	SX	0.19	0/2452	0.48	0/3310
70	SY	0.38	0/1069	0.74	3/1441 (0.2%)
71	Sa	0.26	0/1361	0.55	0/1829
72	Sb	0.23	0/1474	0.50	0/1976
73	Sc	0.21	0/3177	0.47	1/4292 (0.0%)
74	Sd	0.32	0/778	0.69	0/1048
75	Se	0.22	0/2908	0.49	1/3936 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Sg	0.26	0/931	0.67	2/1259 (0.2%)
77	Si	0.26	0/748	0.67	3/1000 (0.3%)
78	Sj	0.23	0/1723	0.59	0/2334
79	Sk	0.27	0/2113	0.68	0/2863
80	Sm	0.42	0/939	0.79	6/1256 (0.5%)
81	Sn	0.31	0/621	0.58	0/820
82	So	0.24	0/5093	0.55	2/6891 (0.0%)
83	S1	0.25	0/22053	0.37	0/34324
All	All	0.33	6/173801 (0.0%)	0.52	53/246748 (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	LD	0	2
11	LO	0	1
12	LP	0	1
13	LQ	0	1
33	Ln	0	2
39	Lt	0	1
42	Lx	0	1
46	L4	0	1
59	SJ	0	1
63	SO	0	1
74	Sd	0	1
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	SZ	131	LYS	CG-CD	-8.08	1.28	1.52
63	SO	68	PRO	CA-C	-5.63	1.48	1.52
40	Lv	179	PRO	CG-CD	-5.40	1.32	1.50
45	L3	11	ARG	C-N	5.37	1.37	1.33
57	SG	234	ARG	CB-CG	-5.24	1.36	1.52
20	LX	165	ILE	CG1-CD1	-5.11	1.31	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Lv	179	PRO	CA-N-CD	-12.05	95.14	112.00
82	So	493	MET	CG-SD-CE	-9.68	79.61	100.90
62	SN	85	VAL	N-CA-C	-8.97	104.74	113.53
40	Lv	179	PRO	N-CD-CG	-8.44	90.53	103.20
47	L5	74	MET	CB-CG-SD	-8.03	88.62	112.70
82	So	420	MET	CG-SD-CE	-7.95	83.41	100.90
63	SO	97	MET	CG-SD-CE	-7.62	84.13	100.90
70	SY	117	LEU	CA-CB-CG	7.54	142.70	116.30
42	Lx	120	MET	CG-SD-CE	-7.50	84.41	100.90
53	SB	135	MET	CG-SD-CE	-7.39	84.65	100.90
7	LJ	166	ARG	CB-CG-CD	6.86	127.07	111.30
59	SJ	81	LYS	CD-CE-NZ	-6.65	90.63	111.90
3	LB	227	GLN	CA-C-N	6.59	130.71	120.68
3	LB	227	GLN	C-N-CA	6.59	130.71	120.68
80	Sm	53	MET	N-CA-C	-6.58	105.39	113.41
5	LD	287	SER	CA-C-N	6.45	130.48	120.68
5	LD	287	SER	C-N-CA	6.45	130.48	120.68
19	LW	129	MET	CA-CB-CG	6.43	126.95	114.10
50	L8	128	MET	CB-CG-SD	-5.88	95.08	112.70
35	Lp	93	LYS	CA-CB-CG	5.82	125.74	114.10
53	SB	262	GLU	N-CA-CB	5.64	119.03	110.28
54	SZ	131	LYS	CD-CE-NZ	-5.64	93.84	111.90
75	Se	397	TYR	CA-CB-CG	-5.57	103.87	113.90
80	Sm	52	MET	CA-CB-CG	5.55	125.21	114.10
49	L7	188	LEU	CA-C-N	5.51	128.22	120.28
49	L7	188	LEU	C-N-CA	5.51	128.22	120.28
42	Lx	75	LYS	CB-CG-CD	5.51	123.97	111.30
77	Si	68	LEU	CA-CB-CG	5.51	135.57	116.30
73	Sc	405	GLN	N-CA-CB	5.49	118.79	110.28
58	SI	91	MET	CG-SD-CE	-5.48	88.85	100.90
57	SG	234	ARG	CB-CA-C	-5.47	102.22	110.92
70	SY	116	LYS	CD-CE-NZ	-5.41	94.58	111.90
80	Sm	52	MET	CA-C-N	-5.40	112.42	122.09
80	Sm	52	MET	C-N-CA	-5.40	112.42	122.09
30	Lk	395	ARG	CG-CD-NE	5.35	123.77	112.00
80	Sm	53	MET	CG-SD-CE	-5.35	89.13	100.90
14	LR	111	ILE	N-CA-C	-5.34	107.62	112.96
57	SG	231	GLU	CB-CG-CD	5.29	121.60	112.60
7	LJ	123	MET	CB-CG-SD	5.29	128.56	112.70
61	SL	116	GLN	CA-C-N	5.28	131.63	121.54
61	SL	116	GLN	C-N-CA	5.28	131.63	121.54
38	Ls	172	MET	N-CA-C	-5.26	108.12	114.75
39	Lt	270	ALA	N-CA-C	-5.21	106.44	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Sm	53	MET	CB-CA-C	5.21	118.35	109.24
59	SJ	148	LEU	CD1-CG-CD2	-5.16	99.45	110.80
41	Lw	42	VAL	N-CA-C	-5.15	108.48	113.53
57	SG	115	LEU	CA-CB-CG	5.13	134.24	116.30
76	Sg	323	ASP	CA-C-N	5.10	131.28	121.54
76	Sg	323	ASP	C-N-CA	5.10	131.28	121.54
70	SY	120	GLU	N-CA-CB	5.09	118.14	110.30
55	SE	137	TYR	CA-CB-CG	5.05	122.99	113.90
77	Si	67	PHE	CA-C-N	5.04	127.74	120.38
77	Si	67	PHE	C-N-CA	5.04	127.74	120.38

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	L4	106	THR	Peptide
5	LD	211	ARG	Sidechain
5	LD	234	THR	Peptide
11	LO	39	ARG	Sidechain
12	LP	73	ARG	Sidechain
13	LQ	110	ILE	Peptide
33	Ln	101	ARG	Sidechain
33	Ln	99	ARG	Sidechain
39	Lt	269	LEU	Peptide
42	Lx	95	ARG	Sidechain
59	SJ	169	ALA	Peptide
63	SO	137	ARG	Sidechain
74	Sd	103	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	L1	31847	0	16176	190	0
2	L2	1191	0	607	12	0
3	LB	1851	0	1909	26	0
4	LC	2393	0	2398	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	LD	2013	0	2044	33	0
6	LI	784	0	832	12	0
7	LJ	1283	0	1370	33	0
8	LK	1323	0	1400	17	0
9	LM	1451	0	1448	12	0
10	LN	889	0	941	10	0
11	LO	2305	0	2378	28	0
12	LP	1779	0	1808	21	0
13	LQ	1245	0	1283	15	0
14	LR	1189	0	1180	19	0
15	LS	1822	0	1859	15	0
16	LT	1153	0	1214	10	0
17	LU	1284	0	1354	16	0
18	LV	1368	0	1410	19	0
19	LW	1188	0	1180	22	0
20	LX	1652	0	1658	31	0
21	La	871	0	898	13	0
22	Lb	2035	0	2054	21	0
23	Lu	1517	0	1561	24	0
24	Ld	978	0	1030	12	0
25	Lf	880	0	902	11	0
26	Lg	433	0	475	6	0
27	Lh	376	0	406	3	0
28	Li	831	0	883	10	0
29	Lj	341	0	361	9	0
30	Lk	3210	0	3206	33	0
31	Ll	2947	0	2841	50	0
32	Lm	2382	0	2393	27	0
33	Ln	836	0	844	30	0
34	Lo	997	0	987	22	0
35	Lp	815	0	792	10	0
36	Lq	1178	0	1180	23	0
37	Lr	2217	0	2220	22	0
38	Ls	1754	0	1732	31	0
39	Lt	1762	0	1767	56	0
40	Lv	1035	0	1040	25	0
41	Lw	1097	0	1085	21	0
42	Lx	895	0	881	16	0
43	Ly	827	0	857	8	0
44	Lz	732	0	730	8	0
45	L3	743	0	758	16	0
46	L4	703	0	693	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	L5	372	0	387	9	0
48	L6	797	0	804	14	0
49	L7	1058	0	1083	16	0
50	L8	1076	0	1049	11	0
51	SR	1203	0	1219	21	0
52	Sf	3036	0	3022	36	0
53	SB	1768	0	1765	28	0
54	SZ	1082	0	1088	43	0
55	SE	2540	0	2574	33	0
56	SF	972	0	1001	19	0
57	SG	1668	0	1716	35	0
58	SI	2501	0	2486	47	0
59	SJ	999	0	1024	51	0
60	SK	1011	0	1052	16	0
61	SL	838	0	887	19	0
62	SN	861	0	885	35	0
63	SO	1382	0	1472	23	0
64	SP	920	0	951	25	0
65	SQ	846	0	908	14	0
66	SS	1528	0	1488	33	0
67	ST	774	0	801	20	0
68	SW	740	0	754	21	0
69	SX	2405	0	2425	43	0
70	SY	1042	0	1037	28	0
71	Sa	1330	0	1342	21	0
72	Sb	1454	0	1464	27	0
73	Sc	3116	0	3069	39	0
74	Sd	766	0	785	20	0
75	Se	2836	0	2828	57	0
76	Sg	903	0	843	26	0
77	Si	731	0	734	18	0
78	Sj	1680	0	1674	41	0
79	Sk	2068	0	2087	72	0
80	Sm	925	0	962	17	0
81	Sn	610	0	682	6	0
82	So	4981	0	4959	94	0
83	S1	19716	0	10015	165	0
84	L1	106	0	0	0	0
84	L6	1	0	0	0	0
84	LB	3	0	0	0	0
84	LP	1	0	0	0	0
84	Lw	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	S1	33	0	0	0	0
85	L1	84	0	76	2	0
85	S1	42	0	38	0	0
86	Lf	1	0	0	0	0
86	Lj	1	0	0	0	0
86	SB	1	0	0	0	0
86	SR	1	0	0	0	0
86	SS	1	0	0	0	0
86	ST	1	0	0	0	0
86	Sa	1	0	0	0	0
87	Se	28	0	12	2	0
All	All	165243	0	140473	1925	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 6.

All (1925) 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)
83:S1:77:C:N4	83:S1:103:A:H61	1.46	1.14
83:S1:77:C:H42	83:S1:103:A:N6	1.46	1.12
9:LM:81:THR:O	9:LM:86:GLY:HA3	1.58	1.04
36:Lq:75:VAL:O	36:Lq:86:GLU:HA	1.64	0.96
29:Lj:76:CYS:SG	29:Lj:98:HIS:CE1	2.63	0.92
59:SJ:75:ARG:HA	59:SJ:145:LEU:O	1.74	0.87
73:Sc:360:VAL:O	73:Sc:364:LEU:HB2	1.78	0.82
59:SJ:83:HIS:H	59:SJ:168:VAL:HG23	1.46	0.81
63:SO:115:ILE:HD11	63:SO:181:ILE:HA	1.64	0.80
14:LR:74:ARG:O	14:LR:96:GLN:NE2	2.16	0.78
61:SL:97:GLY:HA3	61:SL:127:ARG:HH12	1.49	0.78
71:Sa:14:GLN:O	71:Sa:18:GLN:HB2	1.83	0.77
82:So:393:ILE:HG13	82:So:422:ILE:HG21	1.65	0.77
5:LD:211:ARG:NH2	42:Lx:56:ARG:O	2.18	0.76
51:SR:101:PRO:HG2	51:SR:104:ILE:HD13	1.67	0.76
59:SJ:174:LYS:NZ	59:SJ:176:GLN:OE1	2.18	0.76
82:So:336:ASN:ND2	82:So:409:ASP:OD2	2.19	0.75
37:Lr:160:LEU:HD21	37:Lr:223:MET:HB3	1.68	0.75
38:Ls:119:GLN:HB3	38:Ls:123:ARG:HH12	1.50	0.75
42:Lx:88:ASP:OD1	42:Lx:124:ARG:NH2	2.20	0.73
31:Ll:179:VAL:O	31:Ll:183:ASP:HB3	1.87	0.73
76:Sg:289:VAL:HG11	82:So:410:PRO:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sk:260:ARG:NH2	79:Sk:292:TYR:OH	2.22	0.73
70:SY:70:ILE:HD11	70:SY:100:VAL:HG23	1.72	0.72
20:LX:80:ILE:HB	20:LX:85:TRP:HB2	1.72	0.72
75:Se:67:HIS:HB3	75:Se:98:CYS:HB3	1.72	0.72
25:Lf:129:LYS:NZ	38:Ls:289:PRO:O	2.21	0.72
59:SJ:76:LEU:O	59:SJ:145:LEU:HB3	1.90	0.71
36:Lq:77:ALA:O	36:Lq:84:VAL:HA	1.90	0.71
62:SN:98:ARG:HH21	83:S1:583:C:H5'	1.54	0.71
1:L1:973:G:O2'	1:L1:975:G:OP2	2.08	0.71
20:LX:177:THR:HG22	34:Lo:71:LYS:H	1.54	0.71
1:L1:1343:G:HO2'	29:Lj:66:PHE:N	1.87	0.71
40:Lv:77:VAL:HG22	40:Lv:78:ARG:HE	1.56	0.70
72:Sb:68:ARG:HD2	72:Sb:71:ARG:HH21	1.55	0.70
79:Sk:174:ARG:HA	79:Sk:205:LEU:O	1.92	0.70
1:L1:746:U:H5	52:Sf:165:ARG:HH12	1.40	0.70
22:Lb:7:PRO:HD2	22:Lb:10:LEU:HD12	1.74	0.70
1:L1:412:G:N2	24:Ld:88:MET:SD	2.65	0.70
60:SK:129:GLN:HE22	80:Sm:47:THR:HG22	1.55	0.70
39:Lt:177:GLU:O	39:Lt:190:ARG:NH2	2.25	0.69
1:L1:523:U:C2	1:L1:525:A:N7	2.60	0.69
4:LC:198:PHE:HB3	4:LC:202:GLN:HE22	1.57	0.69
52:Sf:113:VAL:HG21	52:Sf:257:VAL:HG11	1.73	0.69
79:Sk:68:SER:HA	82:So:78:VAL:HG23	1.73	0.69
45:L3:46:ASN:ND2	45:L3:49:CYS:SG	2.66	0.69
54:SZ:68:TRP:HZ2	62:SN:124:GLN:HE22	1.41	0.69
18:LV:55:ASN:ND2	18:LV:74:TYR:O	2.26	0.68
68:SW:57:TYR:OH	83:S1:951:G:OP1	2.12	0.68
68:SW:72:ILE:HD12	80:Sm:104:LEU:HD22	1.75	0.68
70:SY:114:GLU:HA	70:SY:117:LEU:HD23	1.75	0.68
24:Ld:101:LYS:NZ	44:Lz:83:GLU:OE2	2.25	0.68
23:Lu:87:CYS:SG	23:Lu:144:LYS:NZ	2.66	0.68
10:LN:128:ARG:HB2	15:LS:125:TYR:HB3	1.76	0.68
62:SN:126:ALA:HB1	62:SN:128:TRP:HE1	1.58	0.68
65:SQ:13:ILE:HD12	65:SQ:30:VAL:HG21	1.76	0.68
66:SS:215:ARG:HG3	66:SS:218:ARG:HH21	1.59	0.68
56:SF:37:ARG:NH1	56:SF:69:TYR:OH	2.27	0.67
31:Ll:215:THR:OG1	31:Ll:275:GLN:NE2	2.27	0.67
53:SB:262:GLU:HB2	53:SB:265:GLN:HE21	1.60	0.67
17:LU:174:PHE:HA	17:LU:180:PHE:O	1.93	0.67
1:L1:394:A:OP1	21:La:101:LYS:NZ	2.28	0.67
70:SY:52:ARG:HH12	70:SY:59:PRO:HD3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sk:211:ARG:NH1	79:Sk:221:TYR:OH	2.27	0.67
4:LC:80:LEU:HA	4:LC:84:PRO:HG3	1.76	0.67
54:SZ:84:GLU:HA	54:SZ:87:VAL:HG12	1.77	0.67
79:Sk:56:ARG:HA	79:Sk:59:LYS:HB3	1.77	0.67
16:LT:111:LYS:NZ	17:LU:139:ASP:OD1	2.28	0.67
18:LV:61:PRO:HG2	38:Ls:182:ARG:HH21	1.60	0.66
1:L1:523:U:O2	1:L1:525:A:N7	2.28	0.66
75:Se:163:LYS:HB3	75:Se:316:LEU:HD11	1.78	0.66
83:S1:533:U:OP1	83:S1:923:G:N2	2.27	0.66
49:L7:133:LEU:HD21	49:L7:157:MET:HE1	1.76	0.66
54:SZ:109:VAL:HB	54:SZ:120:CYS:HB3	1.78	0.66
1:L1:263:C:OP1	30:Lk:395:ARG:NH2	2.27	0.66
40:Lv:119:ILE:HD11	40:Lv:166:PHE:HE2	1.61	0.66
1:L1:608:A:OP1	43:Ly:51:ARG:NH1	2.28	0.66
45:L3:13:VAL:HA	45:L3:68:PHE:HA	1.78	0.66
76:Sg:334:LEU:O	76:Sg:338:LEU:HB2	1.96	0.66
4:LC:129:VAL:O	4:LC:190:GLY:N	2.28	0.65
76:Sg:276:SER:N	76:Sg:279:ASP:OD2	2.29	0.65
54:SZ:103:CYS:HB3	54:SZ:126:GLN:HE22	1.61	0.65
75:Se:123:ARG:NH1	75:Se:297:MET:O	2.29	0.65
54:SZ:69:LEU:HD23	79:Sk:107:LYS:HD2	1.79	0.65
83:S1:77:C:N3	83:S1:103:A:N1	2.43	0.65
58:SI:123:PRO:HB3	79:Sk:87:MET:HE1	1.78	0.65
36:Lq:88:SER:O	36:Lq:92:LYS:NZ	2.30	0.65
78:Sj:57:ASP:OD2	83:S1:58:C:N4	2.30	0.65
67:ST:142:GLU:H	68:SW:28:ARG:HH21	1.45	0.65
82:So:531:ILE:O	82:So:535:MET:HB2	1.97	0.65
79:Sk:251:TYR:O	79:Sk:300:LYS:NZ	2.30	0.65
1:L1:667:A:H5"	34:Lo:28:ARG:HE	1.61	0.65
1:L1:740:U:OP2	52:Sf:160:ARG:NH2	2.22	0.65
55:SE:95:ALA:HB2	77:Si:74:GLU:HB3	1.78	0.65
57:SG:114:THR:HG21	57:SG:205:LEU:HD22	1.79	0.65
1:L1:652:C:OP1	25:Lf:139:ARG:NH1	2.30	0.65
69:SX:258:LYS:HB3	69:SX:261:LEU:HB2	1.77	0.65
1:L1:438:G:N7	12:LP:67:LYS:NZ	2.45	0.64
28:Li:146:GLU:OE2	31:Ll:364:ARG:NH1	2.26	0.64
39:Lt:266:PRO:O	39:Lt:270:ALA:N	2.31	0.64
56:SF:32:ARG:HH21	56:SF:81:HIS:HB2	1.62	0.64
1:L1:179:C:OP2	11:LO:53:HIS:NE2	2.28	0.64
60:SK:151:VAL:HG21	60:SK:158:ARG:HG3	1.78	0.64
14:LR:38:VAL:HG12	14:LR:40:ASN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Sf:319:GLN:HA	52:Sf:322:VAL:HB	1.79	0.64
79:Sk:298:SER:O	79:Sk:302:GLU:HB3	1.98	0.64
18:LV:190:LYS:NZ	18:LV:198:GLU:OE1	2.28	0.64
42:Lx:72:SER:HA	42:Lx:75:LYS:HE2	1.80	0.64
55:SE:139:PHE:HD2	77:Si:68:LEU:HD13	1.61	0.64
71:Sa:21:VAL:HG22	71:Sa:103:ARG:HB3	1.79	0.64
83:S1:836:C:N3	83:S1:920:A:N1	2.45	0.64
60:SK:182:PRO:O	68:SW:42:ARG:NH1	2.31	0.63
32:Lm:247:ASN:ND2	32:Lm:251:ILE:O	2.31	0.63
64:SP:19:ILE:HG22	64:SP:87:MET:HE3	1.80	0.63
57:SG:88:ASP:HB3	57:SG:91:ILE:HB	1.81	0.63
23:Lu:70:ASP:OD2	23:Lu:72:LYS:HG2	1.98	0.63
79:Sk:298:SER:O	79:Sk:301:ASN:O	2.16	0.63
82:So:397:MET:HE1	82:So:435:VAL:HA	1.79	0.63
4:LC:129:VAL:HB	4:LC:191:THR:HG22	1.80	0.63
54:SZ:40:ALA:HB3	54:SZ:59:PRO:HD3	1.81	0.63
65:SQ:93:ASP:O	65:SQ:97:GLY:HA2	1.97	0.63
83:S1:57:U:OP1	83:S1:198:A:N6	2.32	0.63
20:LX:76:VAL:HA	20:LX:88:VAL:HA	1.81	0.63
31:Ll:218:LEU:HB3	31:Ll:235:TRP:HB3	1.81	0.63
64:SP:59:ASN:HB2	64:SP:62:GLY:H	1.64	0.63
54:SZ:145:TYR:HD2	82:So:121:ILE:HD13	1.64	0.62
59:SJ:177:LEU:HG	59:SJ:179:GLN:HE22	1.63	0.62
78:Sj:133:HIS:O	78:Sj:139:TRP:NE1	2.32	0.62
39:Lt:138:THR:OG1	39:Lt:150:ASN:O	2.17	0.62
52:Sf:239:ASN:HB2	52:Sf:299:PHE:HB2	1.80	0.62
59:SJ:154:ASP:OD2	82:So:62:LYS:NZ	2.24	0.62
63:SO:167:LEU:HD11	63:SO:187:ILE:HD12	1.80	0.62
1:L1:211:A:OP2	41:Lw:111:ARG:NH2	2.32	0.62
6:LI:115:LYS:O	6:LI:118:LEU:O	2.16	0.62
25:Lf:155:GLU:HB3	25:Lf:172:LYS:HD2	1.82	0.62
32:Lm:114:ASP:HB2	32:Lm:117:LYS:HB2	1.81	0.62
53:SB:177:THR:HA	53:SB:215:MET:HE3	1.80	0.62
59:SJ:104:ILE:HG12	59:SJ:148:LEU:HG	1.80	0.62
76:Sg:299:GLU:O	76:Sg:303:GLN:NE2	2.33	0.62
10:LN:129:LYS:HG3	15:LS:125:TYR:CE2	2.35	0.62
37:Lr:48:GLN:HA	37:Lr:51:LEU:HG	1.80	0.62
72:Sb:122:ALA:HA	72:Sb:125:ARG:HD2	1.81	0.62
83:S1:583:C:N4	83:S1:799:A:O2'	2.33	0.62
7:LJ:80:ARG:HB3	7:LJ:84:ARG:HH12	1.64	0.62
59:SJ:65:ILE:HD13	82:So:63:LYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:875:U:H5''	1:L1:876:G:H5'	1.82	0.62
5:LD:167:MET:SD	5:LD:279:ARG:NH1	2.73	0.62
7:LJ:101:ASN:OD1	7:LJ:109:LYS:NZ	2.32	0.62
57:SG:142:TYR:O	57:SG:146:HIS:ND1	2.33	0.62
71:Sa:6:ARG:NH2	83:S1:306:U:OP1	2.33	0.62
73:Sc:228:TYR:HE2	73:Sc:262:VAL:HG21	1.65	0.62
32:Lm:167:VAL:HG12	32:Lm:168:ARG:HG3	1.82	0.61
52:Sf:227:ASP:OD1	52:Sf:230:ARG:NH2	2.32	0.61
31:Ll:233:LEU:HD21	31:Ll:236:LEU:HB2	1.83	0.61
32:Lm:150:MET:HE3	32:Lm:181:TYR:HB2	1.82	0.61
4:LC:127:CYS:HB2	4:LC:193:LEU:HB2	1.82	0.61
47:L5:51:LEU:HB3	47:L5:67:ARG:HB3	1.83	0.61
56:SF:69:TYR:HB3	63:SO:97:MET:HE1	1.83	0.61
76:Sg:330:GLU:HB3	76:Sg:366:VAL:HG21	1.82	0.61
20:LX:170:TRP:HD1	34:Lo:77:LEU:HG	1.64	0.61
73:Sc:311:GLU:OE2	78:Sj:60:ARG:NH1	2.34	0.61
77:Si:86:LYS:NZ	83:S1:691:A:OP2	2.33	0.61
81:Sn:138:MET:HE1	83:S1:937:A:H5'	1.82	0.61
39:Lt:49:GLY:HA2	39:Lt:232:PHE:HB3	1.82	0.61
56:SF:33:GLY:O	63:SO:91:ARG:NH2	2.32	0.61
66:SS:214:SER:HA	66:SS:217:ARG:HE	1.63	0.61
82:So:117:ALA:HA	82:So:120:ILE:HG22	1.83	0.61
9:LM:154:ARG:HG2	51:SR:127:LEU:HA	1.83	0.61
1:L1:991:U:OP2	4:LC:238:ARG:NH2	2.34	0.61
4:LC:217:GLY:HA2	4:LC:258:PRO:HB3	1.82	0.61
37:Lr:259:ARG:HB2	37:Lr:271:PHE:HB2	1.83	0.61
69:SX:70:PHE:HZ	69:SX:128:MET:HE3	1.66	0.61
22:Lb:10:LEU:HD22	50:L8:45:LEU:HD23	1.83	0.60
75:Se:244:LEU:HG	75:Se:296:MET:HE3	1.82	0.60
14:LR:62:ARG:NH2	21:La:137:LYS:O	2.31	0.60
33:Ln:88:PHE:HA	47:L5:45:ARG:HH22	1.66	0.60
78:Sj:63:ARG:NH2	78:Sj:110:ASP:OD2	2.34	0.60
82:So:471:ILE:HB	82:So:505:ARG:HH21	1.66	0.60
7:LJ:165:VAL:HG12	7:LJ:169:ARG:HE	1.64	0.60
41:Lw:73:GLN:HB3	41:Lw:162:LEU:HD11	1.83	0.60
62:SN:28:HIS:N	83:S1:601:C:O2	2.34	0.60
79:Sk:156:TYR:O	79:Sk:165:ASN:ND2	2.34	0.60
81:Sn:162:LEU:HD22	81:Sn:195:TYR:HB3	1.83	0.60
83:S1:881:A:H2'	83:S1:882:A:H8	1.67	0.60
1:L1:743:C:OP1	30:Lk:83:LYS:NZ	2.34	0.60
40:Lv:127:MET:HB3	40:Lv:154:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Sb:120:ARG:HG2	72:Sb:123:ARG:HH12	1.65	0.60
76:Sg:338:LEU:O	76:Sg:377:ARG:NH2	2.34	0.60
80:Sm:49:MET:O	80:Sm:53:MET:HB2	2.00	0.60
58:SI:91:MET:HE1	79:Sk:66:TRP:CD2	2.35	0.60
66:SS:211:ARG:NH2	78:Sj:90:ASP:OD2	2.33	0.60
60:SK:158:ARG:NH2	60:SK:177:ASP:OD2	2.34	0.60
1:L1:1236:C:N3	26:Lg:19:ARG:NH1	2.50	0.60
14:LR:53:ARG:NH1	31:Ll:155:TYR:OH	2.35	0.60
15:LS:120:THR:HB	15:LS:173:GLU:HG3	1.84	0.60
79:Sk:59:LYS:NZ	82:So:83:THR:O	2.35	0.60
1:L1:433:A:HO2'	24:Ld:35:LYS:N	1.98	0.60
23:Lu:116:GLU:HG2	23:Lu:126:MET:SD	2.42	0.60
73:Sc:70:LEU:HD11	73:Sc:389:LEU:HB3	1.83	0.60
78:Sj:99:ARG:HB2	78:Sj:115:TRP:HB2	1.82	0.60
12:LP:205:ARG:NH2	12:LP:249:LYS:O	2.35	0.60
16:LT:122:ARG:NH1	16:LT:126:GLU:OE2	2.35	0.60
62:SN:51:ARG:HH21	62:SN:78:LEU:HD22	1.67	0.60
78:Sj:96:ARG:HB3	78:Sj:117:ILE:HB	1.84	0.60
79:Sk:74:ALA:O	79:Sk:110:ASN:ND2	2.35	0.60
7:LJ:168:LEU:HD13	7:LJ:176:LEU:HB2	1.84	0.59
19:LW:74:HIS:HB2	34:Lo:24:LYS:HE3	1.84	0.59
58:SI:291:GLY:HA2	58:SI:326:HIS:O	2.01	0.59
53:SB:82:ARG:HD2	74:Sd:83:MET:HE3	1.85	0.59
82:So:259:TYR:HB3	82:So:282:LEU:HD12	1.83	0.59
58:SI:344:ILE:HG22	58:SI:348:MET:HE1	1.83	0.59
59:SJ:104:ILE:HG21	59:SJ:148:LEU:HD12	1.83	0.59
64:SP:29:ARG:NH1	71:Sa:147:VAL:O	2.35	0.59
69:SX:165:ILE:O	69:SX:170:ARG:NH1	2.36	0.59
4:LC:216:GLN:HG3	4:LC:261:MET:HE2	1.85	0.59
32:Lm:106:ALA:HB3	32:Lm:113:TRP:HB3	1.84	0.59
33:Ln:174:GLU:HB2	40:Lv:183:ARG:NH1	2.17	0.59
69:SX:67:LYS:NZ	69:SX:306:VAL:O	2.36	0.59
18:LV:107:GLU:OE1	18:LV:118:LYS:NZ	2.33	0.59
75:Se:261:ALA:HA	75:Se:307:VAL:O	2.03	0.59
8:LK:56:ARG:NH1	8:LK:80:ILE:O	2.36	0.59
18:LV:157:ARG:HB2	18:LV:167:MET:HG3	1.85	0.59
75:Se:50:ARG:HG2	75:Se:67:HIS:HB2	1.84	0.59
77:Si:76:GLN:NE2	77:Si:79:MET:SD	2.76	0.59
83:S1:451:C:OP1	83:S1:504:C:N4	2.36	0.59
60:SK:101:SER:OG	60:SK:105:GLU:OE1	2.20	0.59
62:SN:116:ASP:OD1	62:SN:125:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:So:312:LYS:HD2	82:So:345:PHE:HZ	1.66	0.59
45:L3:77:ARG:HH21	51:SR:48:ILE:HG23	1.68	0.59
70:SY:116:LYS:HA	70:SY:119:VAL:HG22	1.85	0.59
83:S1:50:G:H21	83:S1:204:A:N6	2.01	0.59
17:LU:95:LEU:HD23	17:LU:138:ALA:HB2	1.83	0.58
25:Lf:108:ASP:OD1	32:Lm:102:LYS:NZ	2.36	0.58
82:So:596:LEU:HA	82:So:599:PHE:HD2	1.68	0.58
38:Ls:91:PRO:HG2	38:Ls:94:ASP:HB2	1.85	0.58
52:Sf:304:ASP:HB2	52:Sf:307:ARG:HH21	1.67	0.58
58:SI:345:ARG:HH11	58:SI:369:LEU:HD23	1.68	0.58
83:S1:50:G:N2	83:S1:204:A:C6	2.70	0.58
1:L1:507:U:N3	1:L1:510:A:OP2	2.33	0.58
1:L1:733:G:OP2	3:LB:105:ARG:NH2	2.34	0.58
10:LN:45:ALA:O	10:LN:49:SER:HB2	2.03	0.58
31:Ll:187:VAL:HG13	31:Ll:319:PHE:HB3	1.84	0.58
53:SB:178:ASN:O	53:SB:182:LEU:HB2	2.02	0.58
65:SQ:29:ARG:HD3	65:SQ:46:ARG:HD2	1.85	0.58
82:So:595:MET:HA	82:So:598:LEU:HG	1.85	0.58
1:L1:292:A:OP2	1:L1:831:C:N4	2.36	0.58
1:L1:421:A:OP2	28:Li:156:LYS:NZ	2.35	0.58
5:LD:70:ARG:HA	5:LD:196:PRO:HD3	1.83	0.58
78:Sj:7:ARG:NH2	83:S1:864:C:OP1	2.36	0.58
78:Sj:77:GLY:O	78:Sj:96:ARG:NH2	2.37	0.58
9:LM:25:MET:HB3	9:LM:149:ARG:HH21	1.67	0.58
55:SE:335:LYS:HE2	83:S1:2:A:H5''	1.85	0.58
63:SO:195:TYR:OH	83:S1:134:A:OP2	2.21	0.58
78:Sj:78:ARG:HB3	78:Sj:97:LEU:HD12	1.85	0.58
55:SE:189:ARG:NH2	55:SE:197:SER:O	2.36	0.58
31:Ll:79:GLY:O	31:Ll:81:LYS:NZ	2.36	0.58
75:Se:338:ASP:O	79:Sk:312:TYR:OH	2.22	0.58
82:So:390:SER:HB3	82:So:426:LEU:HD11	1.84	0.58
31:Ll:233:LEU:HD11	31:Ll:236:LEU:HD22	1.86	0.58
54:SZ:142:LEU:HD23	82:So:121:ILE:HD11	1.85	0.58
67:ST:135:VAL:HG23	72:Sb:193:ARG:HD2	1.86	0.58
71:Sa:78:PHE:HB2	71:Sa:86:VAL:HB	1.85	0.58
76:Sg:328:PHE:HE1	79:Sk:221:TYR:HD1	1.50	0.58
56:SF:115:GLU:OE1	56:SF:116:LYS:NZ	2.37	0.58
7:LJ:111:LEU:HA	7:LJ:114:HIS:HD1	1.68	0.58
63:SO:132:LEU:HD12	63:SO:166:MET:HE1	1.86	0.58
1:L1:725:A:H4'	30:Lk:350:ARG:HH12	1.69	0.57
11:LO:44:ARG:HG3	11:LO:45:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Lt:82:SER:OG	39:Lt:83:LEU:N	2.36	0.57
58:SI:358:GLU:HA	58:SI:361:VAL:HG12	1.86	0.57
66:SS:124:GLU:HA	66:SS:127:VAL:HG12	1.86	0.57
2:L2:8:U:O2	2:L2:15:A:N6	2.37	0.57
62:SN:53:ARG:O	62:SN:56:SER:OG	2.21	0.57
82:So:438:LEU:O	82:So:444:ASN:ND2	2.36	0.57
83:S1:592:C:H2'	83:S1:593:A:H8	1.69	0.57
1:L1:652:C:H4'	1:L1:653:A:H5''	1.86	0.57
2:L2:6:U:H3	2:L2:63:G:H1	1.52	0.57
65:SQ:83:GLU:OE2	71:Sa:85:GLN:NE2	2.33	0.57
69:SX:78:ILE:HG12	69:SX:299:ASN:HD21	1.69	0.57
82:So:611:LEU:HD12	82:So:641:ILE:HD11	1.86	0.57
47:L5:56:LEU:O	47:L5:63:THR:HA	2.05	0.57
58:SI:111:LEU:HD22	79:Sk:112:LEU:HD23	1.85	0.57
61:SL:70:PRO:HB3	61:SL:117:ASP:HB3	1.86	0.57
62:SN:128:TRP:HH2	83:S1:805:U:H5''	1.68	0.57
4:LC:210:THR:HG22	4:LC:290:PRO:HB3	1.87	0.57
19:LW:49:THR:OG1	19:LW:52:ASP:OD1	2.22	0.57
33:Ln:99:ARG:NH2	33:Ln:101:ARG:O	2.35	0.57
9:LM:143:GLU:OE1	36:Lq:136:LYS:NZ	2.37	0.57
51:SR:166:GLY:O	51:SR:171:ARG:NH1	2.38	0.57
54:SZ:60:HIS:HA	62:SN:125:ARG:HG3	1.86	0.57
79:Sk:57:THR:HG23	79:Sk:82:PRO:HA	1.85	0.57
1:L1:623:A:H2'	11:LO:39:ARG:HH12	1.69	0.57
22:Lb:118:ILE:O	22:Lb:168:ARG:NH1	2.38	0.57
23:Lu:86:THR:HB	23:Lu:89:GLN:HG3	1.84	0.57
42:Lx:87:GLN:HB3	42:Lx:124:ARG:HE	1.69	0.57
57:SG:85:VAL:HG13	75:Se:370:LYS:HE2	1.87	0.57
64:SP:36:ALA:HB2	64:SP:51:LEU:HD11	1.86	0.57
82:So:303:CYS:SG	82:So:344:ARG:NH1	2.78	0.57
83:S1:356:A:H2'	83:S1:357:G:H8	1.70	0.57
83:S1:541:A:N6	83:S1:547:C:C2	2.72	0.57
30:Lk:216:GLU:OE2	30:Lk:367:ASN:ND2	2.37	0.57
31:Ll:255:LEU:HD12	31:Ll:256:PRO:HD2	1.85	0.57
32:Lm:73:THR:HG1	32:Lm:99:TYR:HH	1.52	0.57
53:SB:60:ASP:O	53:SB:64:ASN:HB2	2.05	0.57
75:Se:312:GLN:NE2	75:Se:319:PRO:O	2.38	0.57
76:Sg:317:ASN:HA	79:Sk:163:VAL:HG12	1.86	0.57
82:So:342:LEU:HA	82:So:345:PHE:HB2	1.87	0.57
72:Sb:41:ARG:O	78:Sj:49:ARG:NH2	2.37	0.57
83:S1:795:G:H22	83:S1:800:G:H22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:124:A:OP1	5:LD:142:ARG:NH2	2.29	0.56
33:Ln:101:ARG:NH2	39:Lt:82:SER:O	2.30	0.56
34:Lo:100:ILE:HG12	34:Lo:117:TYR:CE2	2.40	0.56
56:SF:35:ILE:HD11	63:SO:92:LEU:HD13	1.85	0.56
83:S1:578:C:HO2'	83:S1:802:G:HO2'	1.52	0.56
3:LB:255:ARG:NH1	3:LB:257:ILE:HD11	2.20	0.56
31:Ll:261:ARG:HH12	49:L7:125:ASN:HA	1.70	0.56
59:SJ:75:ARG:NH2	79:Sk:150:GLU:OE1	2.38	0.56
66:SS:190:ALA:HB3	66:SS:193:LEU:HD23	1.87	0.56
1:L1:858:G:H3'	3:LB:208:ARG:NH2	2.19	0.56
35:Lp:141:ASP:OD2	36:Lq:117:LYS:NZ	2.37	0.56
36:Lq:138:THR:OG1	37:Lr:259:ARG:NH2	2.38	0.56
45:L3:19:GLN:HA	45:L3:54:ASP:HB3	1.86	0.56
62:SN:60:ASN:HB3	77:Si:33:VAL:HG21	1.86	0.56
4:LC:45:SER:O	32:Lm:307:ARG:NH2	2.38	0.56
31:Ll:67:ALA:O	31:Ll:75:ARG:NH2	2.39	0.56
32:Lm:162:TYR:CD2	32:Lm:189:LEU:HD11	2.40	0.56
40:Lv:122:GLU:N	40:Lv:158:GLN:O	2.39	0.56
79:Sk:243:LYS:HE3	79:Sk:247:ASP:HB3	1.86	0.56
83:S1:442:U:H2'	83:S1:443:A:H8	1.69	0.56
1:L1:724:A:O2'	30:Lk:300:ARG:NH2	2.38	0.56
19:LW:16:GLN:HG2	34:Lo:55:GLU:HA	1.88	0.56
53:SB:262:GLU:HA	53:SB:265:GLN:HG3	1.86	0.56
57:SG:123:PHE:O	57:SG:127:HIS:ND1	2.29	0.56
64:SP:112:ARG:NH1	72:Sb:52:GLU:OE2	2.38	0.56
67:ST:58:TYR:CE2	74:Sd:94:PRO:HD3	2.41	0.56
82:So:615:MET:O	82:So:648:ARG:NH2	2.39	0.56
1:L1:801:G:O2'	1:L1:984:U:O4	2.23	0.56
34:Lo:91:LEU:O	34:Lo:95:ALA:HB3	2.06	0.56
51:SR:37:GLU:O	51:SR:51:GLY:HA2	2.06	0.56
65:SQ:67:ARG:NH1	65:SQ:80:GLU:OE2	2.38	0.56
1:L1:520:C:OP2	46:L4:120:ARG:NH1	2.39	0.56
1:L1:1074:U:O2'	1:L1:1076:U:O4	2.23	0.56
19:LW:29:VAL:HG23	19:LW:41:GLN:HB3	1.88	0.56
24:Ld:101:LYS:HE3	44:Lz:80:LEU:HD22	1.88	0.56
53:SB:172:ARG:HB2	53:SB:175:MET:HE3	1.87	0.56
68:SW:50:ARG:NH2	83:S1:948:G:O6	2.32	0.56
73:Sc:132:LYS:NZ	78:Sj:70:ARG:O	2.38	0.56
83:S1:174:U:H2'	83:S1:175:G:H8	1.68	0.56
1:L1:551:C:O2'	1:L1:553:A:N6	2.39	0.56
1:L1:746:U:H4'	34:Lo:52:GLN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LJ:162:LYS:C	7:LJ:166:ARG:HE	2.13	0.56
78:Sj:65:LEU:HG	78:Sj:112:GLY:H	1.71	0.56
82:So:501:ASP:OD1	82:So:537:ARG:NH1	2.39	0.56
54:SZ:44:VAL:HG22	54:SZ:167:LEU:HD22	1.86	0.56
59:SJ:176:GLN:NE2	79:Sk:152:ASP:OD1	2.39	0.56
5:LD:193:LEU:HB3	5:LD:230:ILE:HD13	1.87	0.56
9:LM:28:PRO:HG3	9:LM:65:ILE:HD12	1.87	0.56
58:SI:263:ASP:HB3	58:SI:269:PHE:HE1	1.70	0.56
82:So:75:ALA:O	82:So:78:VAL:O	2.24	0.56
33:Ln:172:GLU:HB3	40:Lv:183:ARG:HH21	1.70	0.55
54:SZ:124:LEU:HD23	54:SZ:158:VAL:HG23	1.87	0.55
1:L1:77:G:OP2	1:L1:79:C:N4	2.39	0.55
40:Lv:87:GLU:HG2	40:Lv:163:SER:HA	1.88	0.55
52:Sf:419:LEU:HA	52:Sf:422:VAL:HG22	1.88	0.55
55:SE:141:TRP:CE3	82:So:116:VAL:HG22	2.40	0.55
57:SG:234:ARG:HG2	80:Sm:53:MET:HE2	1.88	0.55
73:Sc:348:GLU:HG2	73:Sc:350:GLU:H	1.71	0.55
76:Sg:338:LEU:HD11	76:Sg:351:MET:HB3	1.88	0.55
79:Sk:173:LEU:HD21	79:Sk:226:LEU:HD22	1.88	0.55
79:Sk:252:ILE:O	79:Sk:255:ASN:ND2	2.38	0.55
1:L1:216:G:H1	43:Ly:61:GLY:HA3	1.71	0.55
61:SL:117:ASP:OD2	83:S1:248:C:N4	2.39	0.55
76:Sg:358:LEU:HA	76:Sg:361:ASN:HD22	1.71	0.55
82:So:465:ILE:O	82:So:469:GLU:HB2	2.07	0.55
1:L1:2:C:O2'	18:LV:149:ARG:O	2.24	0.55
78:Sj:99:ARG:O	78:Sj:114:ALA:HA	2.06	0.55
18:LV:69:ARG:NH1	38:Ls:228:PHE:O	2.38	0.55
31:Ll:173:LEU:HD13	31:Ll:272:LEU:HD22	1.88	0.55
55:SE:368:LEU:HD12	69:SX:106:MET:C	2.31	0.55
63:SO:115:ILE:HD12	63:SO:184:GLY:HA3	1.88	0.55
71:Sa:11:ARG:HH21	83:S1:285:C:H5	1.53	0.55
18:LV:91:ALA:O	18:LV:94:ILE:O	2.24	0.55
61:SL:55:ARG:HG2	83:S1:179:A:H62	1.72	0.55
75:Se:348:TYR:HB2	75:Se:386:ALA:HB1	1.89	0.55
82:So:493:MET:HA	82:So:496:LEU:HG	1.89	0.55
5:LD:113:LYS:HG3	5:LD:157:GLY:H	1.72	0.55
18:LV:133:ASN:O	38:Ls:230:ARG:NH2	2.39	0.55
59:SJ:109:HIS:HB3	59:SJ:142:CYS:HB3	1.88	0.55
82:So:379:PHE:HB3	82:So:389:SER:HB2	1.89	0.55
21:La:83:VAL:HA	21:La:88:CYS:O	2.06	0.55
21:La:121:PRO:HA	31:Ll:50:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Lj:90:VAL:HB	29:Lj:100:GLN:HB2	1.87	0.55
31:Ll:219:THR:HG22	31:Ll:233:LEU:HA	1.89	0.55
32:Lm:189:LEU:O	32:Lm:295:ARG:NH2	2.39	0.55
59:SJ:126:ILE:HG22	59:SJ:127:TYR:H	1.72	0.55
60:SK:152:LYS:HG3	60:SK:180:PRO:HD3	1.88	0.55
1:L1:911:A:O2'	1:L1:912:A:N7	2.34	0.55
11:LO:286:THR:O	41:Lw:37:ARG:NH2	2.40	0.55
53:SB:148:ASN:HD21	53:SB:197:HIS:CE1	2.25	0.55
83:S1:760:U:H1'	83:S1:798:G:H21	1.72	0.55
12:LP:203:GLU:O	12:LP:207:ARG:HG3	2.06	0.55
49:L7:72:PRO:HB2	49:L7:75:ARG:HB2	1.89	0.55
57:SG:156:ILE:HD11	80:Sm:49:MET:HE2	1.89	0.55
66:SS:185:SER:O	69:SX:183:LYS:NZ	2.39	0.55
4:LC:234:THR:O	4:LC:236:THR:N	2.40	0.54
5:LD:114:THR:O	5:LD:156:ARG:NH1	2.40	0.54
18:LV:133:ASN:ND2	38:Ls:226:ASP:OD1	2.34	0.54
54:SZ:108:LEU:HD21	54:SZ:119:ILE:HG23	1.89	0.54
69:SX:82:MET:HG3	69:SX:268:PHE:HE2	1.72	0.54
1:L1:346:C:OP2	11:LO:59:ARG:NH1	2.39	0.54
1:L1:622:G:O2'	16:LT:11:ARG:O	2.24	0.54
4:LC:213:LYS:HG3	4:LC:261:MET:HE3	1.89	0.54
31:Ll:45:LEU:HD23	31:Ll:48:LEU:HD12	1.88	0.54
31:Ll:214:TRP:HB2	31:Ll:240:ILE:HB	1.88	0.54
36:Lq:44:ARG:NH2	48:L6:99:LYS:O	2.40	0.54
54:SZ:61:TYR:HB3	54:SZ:65:ARG:HB2	1.88	0.54
56:SF:23:LYS:O	56:SF:27:GLU:HG2	2.07	0.54
82:So:540:HIS:O	82:So:545:GLN:NE2	2.41	0.54
83:S1:805:U:H2'	83:S1:806:A:H8	1.72	0.54
66:SS:94:CYS:HB2	66:SS:108:CYS:SG	2.48	0.54
71:Sa:91:GLU:OE2	72:Sb:123:ARG:NH2	2.40	0.54
79:Sk:87:MET:HE3	79:Sk:105:LEU:HD21	1.90	0.54
5:LD:206:LEU:HD21	5:LD:210:ARG:HH11	1.72	0.54
59:SJ:76:LEU:HD13	59:SJ:175:THR:HG22	1.88	0.54
79:Sk:257:SER:HB2	79:Sk:260:ARG:HH21	1.72	0.54
1:L1:144:A:N3	1:L1:192:U:O2'	2.39	0.54
1:L1:395:A:OP1	40:Lv:48:TYR:N	2.41	0.54
41:Lw:144:THR:HG22	41:Lw:146:THR:HG23	1.90	0.54
58:SI:327:ASP:N	58:SI:327:ASP:OD1	2.39	0.54
82:So:335:PHE:HD2	82:So:356:VAL:HG13	1.72	0.54
1:L1:1540:C:O2'	4:LC:47:THR:O	2.23	0.54
6:LI:120:ARG:NH1	22:Lb:136:ASP:OD2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Lt:264:LEU:HD22	39:Lt:269:LEU:HB3	1.89	0.54
59:SJ:84:ASP:HB3	59:SJ:168:VAL:HG21	1.88	0.54
78:Sj:207:GLN:HA	78:Sj:210:LYS:HB2	1.89	0.54
79:Sk:71:PRO:HG3	82:So:78:VAL:HG21	1.90	0.54
4:LC:198:PHE:HB3	4:LC:202:GLN:NE2	2.22	0.54
24:Ld:73:LYS:HD3	48:L6:38:ARG:HH21	1.72	0.54
30:Lk:201:ARG:HG2	30:Lk:232:THR:HG22	1.89	0.54
32:Lm:276:PHE:HB2	32:Lm:304:VAL:HG22	1.90	0.54
54:SZ:75:ASN:ND2	62:SN:121:SER:OG	2.30	0.54
60:SK:150:VAL:HG22	60:SK:176:THR:HB	1.90	0.54
1:L1:105:A:H4'	16:LT:10:LEU:HD13	1.90	0.54
1:L1:646:U:H3	13:LQ:115:LEU:HD21	1.73	0.54
59:SJ:123:SER:HG	83:S1:618:C:HO2'	1.53	0.54
78:Sj:162:ALA:O	78:Sj:194:GLN:NE2	2.40	0.54
31:Ll:49:GLU:OE2	31:Ll:52:ARG:NH2	2.41	0.54
53:SB:159:ALA:O	53:SB:162:CYS:O	2.26	0.54
82:So:573:ALA:O	82:So:577:ASN:ND2	2.39	0.54
1:L1:283:A:O2'	1:L1:793:A:OP1	2.25	0.54
66:SS:64:TYR:OH	66:SS:125:GLN:OE1	2.23	0.54
70:SY:86:ASP:HA	74:Sd:101:ILE:HG22	1.90	0.54
79:Sk:263:LEU:HD12	79:Sk:266:LEU:HD11	1.89	0.54
28:Li:101:LYS:HB3	28:Li:103:LYS:HD3	1.89	0.53
57:SG:110:LEU:HD13	57:SG:201:MET:HG2	1.90	0.53
58:SI:155:LYS:NZ	58:SI:217:ASP:OD2	2.40	0.53
59:SJ:106:ILE:HD13	59:SJ:145:LEU:HD12	1.90	0.53
1:L1:213:G:OP2	11:LO:109:ARG:NH2	2.40	0.53
7:LJ:101:ASN:HB3	7:LJ:150:HIS:HB3	1.91	0.53
23:Lu:187:PRO:HD2	23:Lu:190:LEU:HD12	1.90	0.53
1:L1:719:C:H5''	30:Lk:301:PRO:HB3	1.91	0.53
42:Lx:123:VAL:HA	42:Lx:126:VAL:HG23	1.89	0.53
51:SR:39:VAL:HG22	51:SR:52:ARG:HH12	1.72	0.53
62:SN:43:MET:HE1	62:SN:81:ASP:HB3	1.90	0.53
72:Sb:123:ARG:O	72:Sb:126:GLN:HG3	2.09	0.53
79:Sk:244:THR:HB	79:Sk:247:ASP:HB2	1.90	0.53
80:Sm:63:ASP:OD1	80:Sm:64:ASP:N	2.41	0.53
1:L1:1398:G:OP2	1:L1:1398:G:N2	2.39	0.53
5:LD:175:LYS:HG2	5:LD:273:LEU:HD13	1.90	0.53
31:Ll:157:LEU:O	31:Ll:161:LEU:N	2.40	0.53
46:L4:76:ASN:HD22	46:L4:82:GLN:H	1.56	0.53
58:SI:365:ARG:HB2	58:SI:370:LEU:HD12	1.90	0.53
59:SJ:123:SER:OG	83:S1:618:C:O2'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sn:166:GLN:NE2	81:Sn:194:ILE:O	2.41	0.53
5:LD:218:LEU:HD13	5:LD:230:ILE:HD11	1.91	0.53
14:LR:82:VAL:HG11	14:LR:157:MET:HE1	1.91	0.53
62:SN:40:ARG:NH2	83:S1:587:C:O3'	2.42	0.53
6:LI:115:LYS:O	6:LI:118:LEU:C	2.52	0.53
14:LR:73:SER:O	14:LR:146:GLN:NE2	2.41	0.53
22:Lb:240:GLN:OE1	22:Lb:241:GLN:NE2	2.41	0.53
32:Lm:69:HIS:HB2	32:Lm:79:PHE:HE2	1.74	0.53
72:Sb:151:GLN:HG3	72:Sb:155:ARG:HH21	1.72	0.53
4:LC:68:GLU:O	4:LC:72:GLN:HG3	2.08	0.53
33:Ln:159:ALA:O	33:Ln:163:LYS:NZ	2.41	0.53
39:Lt:98:LEU:HD21	75:Se:232:ARG:HH22	1.74	0.53
66:SS:158:ARG:HG3	66:SS:163:LEU:HD23	1.89	0.53
67:ST:102:LYS:O	67:ST:106:GLU:HG3	2.09	0.53
83:S1:37:U:H2'	83:S1:38:A:H8	1.73	0.53
12:LP:36:VAL:HG23	46:L4:128:ARG:HD2	1.90	0.53
45:L3:15:GLN:HG3	45:L3:67:LEU:HB3	1.90	0.53
64:SP:111:ARG:NH2	66:SS:233:GLU:O	2.41	0.53
75:Se:265:ILE:HD12	75:Se:268:LEU:HD12	1.91	0.53
78:Sj:41:LEU:HD21	78:Sj:55:TRP:HA	1.91	0.53
83:S1:694:C:H5''	83:S1:695:C:H4'	1.91	0.53
7:LJ:86:ILE:HA	7:LJ:89:VAL:HG22	1.91	0.53
32:Lm:112:PRO:HB2	32:Lm:267:PRO:HG3	1.89	0.53
57:SG:112:ILE:HA	75:Se:397:TYR:CE1	2.44	0.53
62:SN:112:ARG:NH2	83:S1:618:C:OP1	2.42	0.53
75:Se:153:LEU:HB3	75:Se:260:VAL:HG12	1.91	0.53
1:L1:220:C:OP2	28:Li:168:ARG:NH1	2.42	0.53
12:LP:114:ASP:HB3	12:LP:118:MET:HE3	1.91	0.53
33:Ln:163:LYS:HD3	40:Lv:86:TYR:HE2	1.74	0.53
66:SS:192:THR:O	66:SS:195:SER:C	2.51	0.53
73:Sc:337:LEU:HA	73:Sc:340:LYS:HG2	1.90	0.53
77:Si:19:PHE:O	79:Sk:211:ARG:NH1	2.42	0.53
79:Sk:86:ARG:HB3	79:Sk:96:PRO:HB2	1.89	0.53
1:L1:1191:A:H4'	21:La:65:ASN:HD22	1.73	0.52
39:Lt:70:MET:HG2	39:Lt:74:LEU:HG	1.92	0.52
64:SP:20:ARG:HB2	83:S1:192:A:H5'	1.91	0.52
69:SX:67:LYS:HD2	69:SX:307:LEU:HD12	1.89	0.52
71:Sa:29:VAL:HB	71:Sa:79:TYR:HB2	1.90	0.52
79:Sk:298:SER:O	79:Sk:301:ASN:C	2.52	0.52
19:LW:81:ASP:HB3	19:LW:87:ILE:HD11	1.91	0.52
20:LX:60:ASP:OD2	20:LX:122:LEU:HD11	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Lm:159:LYS:HA	35:Lp:93:LYS:HE3	1.92	0.52
47:L5:74:MET:SD	47:L5:74:MET:N	2.82	0.52
56:SF:3:ARG:HB3	56:SF:99:THR:HG21	1.91	0.52
72:Sb:168:ILE:HG12	72:Sb:176:ARG:HG2	1.90	0.52
77:Si:31:MET:HA	77:Si:34:VAL:HG12	1.90	0.52
79:Sk:56:ARG:NH2	82:So:91:ASP:O	2.39	0.52
1:L1:214:G:N3	1:L1:225:C:O2'	2.42	0.52
1:L1:237:A:N3	1:L1:1260:U:O2'	2.37	0.52
8:LK:149:ARG:HH12	46:L4:104:PRO:HD3	1.74	0.52
63:SO:145:LYS:HD2	63:SO:146:HIS:CD2	2.43	0.52
4:LC:68:GLU:OE1	32:Lm:315:LYS:NZ	2.41	0.52
34:Lo:100:ILE:HG12	34:Lo:117:TYR:HE2	1.74	0.52
55:SE:274:ARG:NH1	83:S1:633:C:OP2	2.43	0.52
1:L1:395:A:H5'	21:La:74:ARG:HE	1.74	0.52
13:LQ:74:ARG:NH2	15:LS:266:GLU:OE2	2.43	0.52
20:LX:126:MET:SD	20:LX:127:ASP:N	2.82	0.52
53:SB:141:ILE:HB	53:SB:190:PRO:HA	1.91	0.52
69:SX:212:GLU:OE2	69:SX:248:LYS:NZ	2.42	0.52
76:Sg:334:LEU:HB2	76:Sg:355:THR:HG23	1.91	0.52
78:Sj:67:LEU:HD13	78:Sj:141:LEU:HB2	1.92	0.52
83:S1:780:A:H2'	83:S1:781:G:C8	2.45	0.52
8:LK:187:GLU:HG3	8:LK:191:LYS:HE3	1.91	0.52
12:LP:142:GLY:O	21:La:38:SER:OG	2.26	0.52
16:LT:107:ILE:HD13	18:LV:211:THR:HG21	1.92	0.52
1:L1:802:A:OP1	10:LN:56:ARG:NH2	2.38	0.52
5:LD:188:HIS:HB2	5:LD:260:VAL:HG22	1.90	0.52
13:LQ:25:ARG:NH2	13:LQ:51:GLU:OE1	2.39	0.52
81:Sn:128:LYS:NZ	83:S1:460:U:O4	2.39	0.52
83:S1:784:G:O2'	83:S1:810:G:O6	2.27	0.52
1:L1:237:A:OP1	5:LD:126:LYS:NZ	2.36	0.52
7:LJ:128:ASN:HB3	7:LJ:132:LYS:HD2	1.92	0.52
73:Sc:175:VAL:HG22	73:Sc:177:SER:H	1.75	0.52
78:Sj:207:GLN:O	78:Sj:210:LYS:C	2.52	0.52
39:Lt:64:THR:H	39:Lt:67:GLN:NE2	2.08	0.52
42:Lx:120:MET:HE1	42:Lx:126:VAL:N	2.24	0.52
59:SJ:135:GLU:HG3	62:SN:124:GLN:HB2	1.92	0.52
80:Sm:105:ASN:O	80:Sm:109:GLN:HG3	2.10	0.52
83:S1:178:U:O4	83:S1:181:C:N3	2.43	0.52
28:Li:106:THR:HG23	28:Li:162:THR:HA	1.92	0.52
39:Lt:146:ARG:HA	39:Lt:151:ARG:HD3	1.92	0.52
45:L3:36:THR:HG21	45:L3:87:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SY:85:PHE:HB2	74:Sd:100:VAL:HG22	1.91	0.52
83:S1:751:U:H2'	83:S1:752:A:H8	1.74	0.52
4:LC:102:LEU:HD13	4:LC:125:GLN:HE21	1.76	0.51
7:LJ:47:LEU:HD22	12:LP:226:ILE:HG12	1.92	0.51
7:LJ:62:PRO:HA	7:LJ:65:LEU:HB2	1.91	0.51
37:Lr:228:LEU:HB2	37:Lr:307:PHE:CD2	2.45	0.51
75:Se:288:ALA:O	75:Se:292:ASN:ND2	2.43	0.51
1:L1:247:A:O2'	1:L1:313:U:O4	2.23	0.51
8:LK:188:GLU:HG3	8:LK:191:LYS:HD2	1.92	0.51
18:LV:57:ILE:O	38:Ls:227:ARG:NH1	2.39	0.51
39:Lt:97:ARG:HA	39:Lt:100:LYS:HE2	1.91	0.51
52:Sf:307:ARG:HG3	52:Sf:310:ARG:H	1.75	0.51
59:SJ:173:THR:OG1	79:Sk:155:ASP:OD1	2.27	0.51
66:SS:228:SER:OG	66:SS:229:GLY:N	2.42	0.51
70:SY:106:LEU:HD23	70:SY:109:LEU:HD21	1.92	0.51
75:Se:110:HIS:HA	75:Se:113:LYS:HD2	1.92	0.51
78:Sj:25:LEU:HD21	83:S1:884:C:H2'	1.92	0.51
83:S1:355:C:H2'	83:S1:356:A:H8	1.74	0.51
33:Ln:136:ILE:HD11	40:Lv:173:ILE:HG13	1.92	0.51
57:SG:97:MET:HE1	57:SG:184:MET:HB2	1.92	0.51
58:SI:228:LEU:HD21	58:SI:237:GLU:HB3	1.92	0.51
63:SO:176:ASP:OD1	63:SO:177:VAL:N	2.42	0.51
82:So:548:PHE:HB3	82:So:582:LEU:HD22	1.93	0.51
23:Lu:230:LYS:HA	23:Lu:233:ILE:HD12	1.91	0.51
46:L4:110:LEU:HD13	46:L4:117:TYR:HA	1.92	0.51
53:SB:220:VAL:HG22	53:SB:234:TYR:HB2	1.91	0.51
54:SZ:76:LEU:O	62:SN:103:ARG:NH2	2.42	0.51
55:SE:141:TRP:HE3	55:SE:142:PRO:HD2	1.76	0.51
61:SL:74:ASN:ND2	61:SL:117:ASP:OD1	2.43	0.51
69:SX:259:TYR:O	69:SX:263:ARG:HG3	2.11	0.51
83:S1:700:G:H2'	83:S1:701:G:H8	1.75	0.51
5:LD:282:PRO:O	5:LD:290:TYR:OH	2.21	0.51
19:LW:27:GLN:HG2	23:Lu:113:LEU:HB3	1.92	0.51
33:Ln:168:LEU:HA	39:Lt:203:LYS:HE2	1.93	0.51
38:Ls:171:ASP:OD1	38:Ls:171:ASP:N	2.43	0.51
49:L7:78:ILE:HG12	49:L7:101:VAL:HG22	1.92	0.51
70:SY:77:VAL:HG11	70:SY:118:PHE:CZ	2.45	0.51
76:Sg:361:ASN:ND2	77:Si:37:PHE:O	2.44	0.51
82:So:256:GLU:HG2	82:So:287:LEU:HB3	1.93	0.51
1:L1:586:U:O2'	17:LU:118:ASN:ND2	2.44	0.51
20:LX:73:GLN:NE2	20:LX:128:ARG:O	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Lu:151:ASP:OD1	23:Lu:154:ARG:NH2	2.38	0.51
38:Ls:200:SER:OG	38:Ls:201:SER:N	2.43	0.51
49:L7:97:SER:O	49:L7:146:ASN:ND2	2.44	0.51
10:LN:46:LEU:HD12	10:LN:78:LYS:HD3	1.93	0.51
30:Lk:275:ASN:HD21	30:Lk:326:ARG:HH11	1.58	0.51
57:SG:88:ASP:OD2	57:SG:146:HIS:NE2	2.44	0.51
63:SO:211:ILE:O	63:SO:215:GLN:HG3	2.11	0.51
3:LB:109:PHE:CE1	3:LB:208:ARG:HD2	2.46	0.51
29:Lj:72:LEU:HD13	29:Lj:90:VAL:HG23	1.93	0.51
41:Lw:41:SER:OG	41:Lw:43:ASP:OD1	2.28	0.51
46:L4:105:LYS:HG3	46:L4:110:LEU:HG	1.92	0.51
61:SL:51:PRO:O	61:SL:89:ARG:NH2	2.44	0.51
70:SY:104:THR:HG22	70:SY:108:LYS:HZ3	1.76	0.51
73:Sc:225:LEU:HB3	73:Sc:283:LEU:HD11	1.92	0.51
79:Sk:71:PRO:HB3	82:So:78:VAL:HG11	1.93	0.51
83:S1:16:A:H2'	83:S1:17:G:C8	2.46	0.51
1:L1:1397:U:OP1	4:LC:234:THR:OG1	2.27	0.51
57:SG:234:ARG:HG2	80:Sm:53:MET:CE	2.40	0.51
1:L1:1016:G:H5'	1:L1:1434:U:H4'	1.92	0.51
3:LB:126:VAL:HA	3:LB:142:VAL:HG12	1.93	0.51
7:LJ:84:ARG:NH2	46:L4:113:GLU:OE2	2.43	0.51
26:Lg:34:ARG:HD3	26:Lg:41:LEU:HG	1.93	0.51
31:Ll:133:ASP:OD1	31:Ll:134:ALA:N	2.44	0.51
32:Lm:44:ARG:HB3	32:Lm:261:ILE:HD12	1.93	0.51
38:Ls:157:HIS:O	38:Ls:161:HIS:ND1	2.44	0.51
45:L3:76:MET:HG2	51:SR:49:ILE:HD11	1.93	0.51
60:SK:71:SER:O	60:SK:74:ARG:NH1	2.44	0.51
66:SS:216:LEU:HD22	72:Sb:50:PRO:HA	1.93	0.51
78:Sj:144:LYS:HA	78:Sj:147:GLU:HG2	1.93	0.51
82:So:531:ILE:O	82:So:535:MET:CB	2.58	0.51
1:L1:429:U:H2'	1:L1:430:C:C6	2.46	0.50
9:LM:43:HIS:NE2	9:LM:55:ASP:OD2	2.43	0.50
29:Lj:69:LYS:HB2	29:Lj:72:LEU:HD23	1.93	0.50
38:Ls:187:GLU:O	38:Ls:218:THR:OG1	2.29	0.50
54:SZ:134:PHE:HD2	54:SZ:135:LEU:HD22	1.76	0.50
17:LU:119:GLU:HG2	17:LU:189:PRO:HB2	1.93	0.50
20:LX:64:ILE:O	20:LX:71:GLY:N	2.43	0.50
39:Lt:273:ARG:HA	39:Lt:276:VAL:HG12	1.92	0.50
42:Lx:116:ARG:O	42:Lx:120:MET:HG2	2.10	0.50
48:L6:12:ILE:HG13	48:L6:23:ARG:HB2	1.94	0.50
59:SJ:165:PRO:HG3	79:Sk:111:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SY:88:PHE:HE1	74:Sd:116:PHE:C	2.19	0.50
82:So:339:LEU:HD23	82:So:342:LEU:HD21	1.93	0.50
1:L1:1172:C:OP2	12:LP:64:ARG:NH2	2.43	0.50
13:LQ:108:LEU:HD23	25:Lf:122:LEU:HD11	1.93	0.50
42:Lx:74:VAL:HA	42:Lx:77:VAL:HG12	1.93	0.50
46:L4:133:SER:HA	46:L4:136:LYS:HB2	1.92	0.50
55:SE:426:LYS:N	66:SS:88:GLN:OE1	2.43	0.50
58:SI:286:TYR:HB2	58:SI:327:ASP:OD1	2.11	0.50
69:SX:275:PHE:O	69:SX:279:LYS:HA	2.11	0.50
73:Sc:139:PRO:HD2	73:Sc:170:GLN:HE22	1.77	0.50
83:S1:242:G:N2	83:S1:255:G:OP1	2.38	0.50
83:S1:712:U:H2'	83:S1:713:G:H8	1.75	0.50
83:S1:817:G:H21	83:S1:819:C:H42	1.59	0.50
30:Lk:229:ARG:NH1	30:Lk:231:SER:OG	2.44	0.50
57:SG:174:LEU:O	57:SG:179:ARG:NH2	2.45	0.50
75:Se:310:LEU:HD12	75:Se:328:LEU:HB2	1.93	0.50
1:L1:385:U:H2'	1:L1:386:G:H8	1.76	0.50
1:L1:667:A:H5'	34:Lo:28:ARG:HH21	1.76	0.50
40:Lv:137:LEU:HB2	40:Lv:145:LEU:HG	1.92	0.50
69:SX:209:ILE:HD12	69:SX:214:ASN:HB3	1.94	0.50
69:SX:326:ASN:HA	69:SX:329:LYS:HD2	1.94	0.50
82:So:398:ASN:HA	82:So:401:MET:HE1	1.93	0.50
83:S1:735:A:H3'	83:S1:736:A:H8	1.76	0.50
4:LC:220:LYS:HG2	4:LC:261:MET:HE1	1.93	0.50
21:La:62:HIS:HA	21:La:94:GLU:HG3	1.93	0.50
33:Ln:96:ASP:N	39:Lt:84:TYR:OH	2.45	0.50
45:L3:67:LEU:HD13	45:L3:73:ARG:HG2	1.93	0.50
57:SG:231:GLU:HG3	80:Sm:61:PHE:CZ	2.46	0.50
62:SN:101:LYS:HG2	62:SN:104:TRP:HZ3	1.76	0.50
72:Sb:71:ARG:NH1	83:S1:87:C:O3'	2.44	0.50
79:Sk:56:ARG:NH2	79:Sk:79:SER:OG	2.45	0.50
11:LO:31:PRO:HG2	48:L6:86:ARG:HH12	1.77	0.50
11:LO:197:GLY:HA3	50:L8:62:ALA:HB2	1.93	0.50
12:LP:123:ARG:NH1	12:LP:162:GLU:OE1	2.43	0.50
12:LP:218:ILE:HG23	12:LP:223:MET:HB2	1.93	0.50
52:Sf:51:MET:HE1	52:Sf:65:ARG:HB2	1.94	0.50
55:SE:139:PHE:CD2	77:Si:68:LEU:HD13	2.45	0.50
58:SI:317:PHE:HB3	58:SI:323:LEU:HA	1.94	0.50
59:SJ:149:THR:HG1	79:Sk:133:TRP:CD1	2.29	0.50
59:SJ:181:PRO:HD3	79:Sk:148:PRO:HD2	1.93	0.50
66:SS:96:ARG:NH1	83:S1:272:A:OP2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sj:22:ARG:NH2	83:S1:161:C:O2'	2.44	0.50
78:Sj:30:ASP:OD2	78:Sj:113:LYS:NZ	2.41	0.50
82:So:490:SER:HA	82:So:493:MET:HE2	1.92	0.50
54:SZ:75:ASN:ND2	62:SN:121:SER:O	2.45	0.50
58:SI:87:HIS:O	58:SI:91:MET:HG2	2.11	0.50
58:SI:171:ASN:HA	58:SI:174:LYS:HG2	1.93	0.50
58:SI:291:GLY:CA	58:SI:326:HIS:O	2.59	0.50
61:SL:99:GLY:O	61:SL:127:ARG:NH2	2.44	0.50
66:SS:192:THR:O	66:SS:195:SER:O	2.29	0.50
75:Se:204:VAL:HB	75:Se:208:TYR:HE2	1.76	0.50
7:LJ:124:LYS:HA	7:LJ:124:LYS:HE3	1.93	0.50
10:LN:45:ALA:O	10:LN:49:SER:CB	2.60	0.50
42:Lx:73:TYR:CE1	42:Lx:103:HIS:HB3	2.47	0.50
70:SY:86:ASP:OD2	70:SY:89:ASN:ND2	2.43	0.50
74:Sd:104:ILE:HD12	74:Sd:138:THR:HB	1.93	0.50
1:L1:75:U:H5'	22:Lb:55:LYS:HE2	1.94	0.49
1:L1:1070:A:H2'	1:L1:1071:A:C8	2.46	0.49
9:LM:135:GLU:HG2	9:LM:139:LYS:HZ2	1.76	0.49
18:LV:212:LEU:O	35:Lp:142:ARG:NH2	2.44	0.49
19:LW:129:MET:HE3	38:Ls:82:ALA:HB2	1.94	0.49
31:Ll:217:LEU:O	31:Ll:270:PHE:HA	2.12	0.49
38:Ls:160:LEU:O	38:Ls:164:VAL:HB	2.12	0.49
49:L7:135:LEU:HD22	49:L7:153:LYS:HE3	1.94	0.49
52:Sf:142:LEU:HD21	52:Sf:187:LEU:HD22	1.94	0.49
8:LK:59:ASP:OD1	46:L4:77:ILE:HG13	2.11	0.49
20:LX:126:MET:SD	20:LX:152:ARG:NH1	2.85	0.49
39:Lt:74:LEU:HD22	47:L5:42:ARG:HB3	1.95	0.49
63:SO:115:ILE:HG23	63:SO:116:VAL:HG13	1.94	0.49
1:L1:409:C:O2	48:L6:60:ARG:NH1	2.46	0.49
4:LC:107:MET:HE2	4:LC:121:LEU:HD11	1.93	0.49
20:LX:69:ASP:HB3	20:LX:72:LYS:HD2	1.94	0.49
28:Li:172:TYR:HB2	28:Li:175:ASP:HB2	1.94	0.49
37:Lr:44:GLU:OE1	37:Lr:47:ARG:NH2	2.45	0.49
37:Lr:245:LEU:HD12	37:Lr:253:PRO:HD3	1.94	0.49
42:Lx:120:MET:HE1	42:Lx:125:ASP:C	2.37	0.49
44:Lz:45:GLU:OE2	44:Lz:70:ARG:NH2	2.34	0.49
57:SG:190:GLU:HG3	57:SG:208:LYS:HZ3	1.78	0.49
58:SI:353:CYS:SG	58:SI:354:SER:N	2.86	0.49
75:Se:273:THR:HG23	75:Se:316:LEU:HD13	1.93	0.49
79:Sk:152:ASP:O	79:Sk:171:VAL:HA	2.13	0.49
82:So:339:LEU:HA	82:So:342:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1057:C:H2'	1:L1:1058:C:C6	2.47	0.49
5:LD:130:GLN:HE22	5:LD:137:ARG:HD2	1.77	0.49
10:LN:129:LYS:HG3	15:LS:125:TYR:HE2	1.76	0.49
13:LQ:77:ASP:O	13:LQ:83:LYS:NZ	2.45	0.49
29:Lj:76:CYS:SG	29:Lj:98:HIS:HE1	2.18	0.49
51:SR:111:GLU:O	51:SR:115:ILE:HG12	2.13	0.49
54:SZ:123:VAL:O	54:SZ:157:THR:HA	2.12	0.49
55:SE:283:GLU:OE2	70:SY:21:ARG:NH2	2.45	0.49
58:SI:92:MET:HE2	58:SI:106:ARG:HH12	1.77	0.49
58:SI:332:VAL:HG21	58:SI:344:ILE:HD11	1.94	0.49
62:SN:113:HIS:O	62:SN:117:HIS:ND1	2.45	0.49
69:SX:253:ILE:O	69:SX:257:GLY:HA2	2.12	0.49
74:Sd:146:ASP:OD1	74:Sd:147:LEU:N	2.43	0.49
1:L1:19:C:H5''	22:Lb:5:LYS:HG2	1.93	0.49
23:Lu:172:ILE:HD13	27:Lh:70:LEU:HD22	1.95	0.49
30:Lk:136:VAL:HG12	30:Lk:416:ALA:HB1	1.94	0.49
33:Ln:172:GLU:HB3	40:Lv:183:ARG:NH2	2.28	0.49
40:Lv:178:LEU:HD21	40:Lv:184:LEU:HD22	1.94	0.49
56:SF:94:VAL:HG11	67:ST:117:MET:HE1	1.94	0.49
1:L1:488:U:OP1	51:SR:182:ARG:NH2	2.45	0.49
1:L1:1247:G:O6	11:LO:77:ARG:NH2	2.43	0.49
4:LC:345:ILE:HG13	15:LS:169:PRO:HB2	1.95	0.49
7:LJ:79:ILE:HB	7:LJ:83:ARG:HH12	1.77	0.49
31:Ll:241:PRO:HG2	31:Ll:244:ARG:HG3	1.94	0.49
32:Lm:221:VAL:HG21	32:Lm:254:LEU:HD12	1.93	0.49
52:Sf:142:LEU:HD13	52:Sf:422:VAL:HG11	1.93	0.49
59:SJ:85:LYS:NZ	59:SJ:110:GLU:OE2	2.46	0.49
60:SK:149:VAL:HG21	60:SK:162:MET:HE2	1.94	0.49
76:Sg:358:LEU:HD11	76:Sg:372:HIS:HD2	1.78	0.49
83:S1:24:U:H2'	83:S1:25:A:H8	1.78	0.49
83:S1:174:U:H2'	83:S1:175:G:C8	2.47	0.49
83:S1:356:A:H2'	83:S1:357:G:C8	2.47	0.49
83:S1:793:G:H2'	83:S1:794:A:C8	2.47	0.49
11:LO:119:THR:HG21	41:Lw:51:LEU:HD22	1.95	0.49
30:Lk:113:LEU:HD12	30:Lk:311:ALA:HB1	1.94	0.49
59:SJ:152:THR:HA	59:SJ:155:VAL:HG12	1.94	0.49
61:SL:42:PRO:HD3	83:S1:284:C:C4	2.47	0.49
75:Se:81:HIS:CD2	75:Se:190:ASN:HB3	2.47	0.49
75:Se:159:HIS:O	75:Se:163:LYS:HG2	2.13	0.49
4:LC:104:LEU:HG	15:LS:91:LYS:HB2	1.94	0.49
4:LC:111:THR:O	4:LC:114:GLY:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LC:234:THR:HG22	4:LC:235:LYS:H	1.77	0.49
4:LC:322:ASP:OD1	4:LC:322:ASP:N	2.43	0.49
7:LJ:134:PHE:O	7:LJ:138:SER:OG	2.30	0.49
7:LJ:136:GLU:HA	7:LJ:141:GLN:HG3	1.95	0.49
20:LX:36:PRO:HD2	20:LX:39:ILE:HB	1.94	0.49
43:Ly:73:LEU:HD11	50:L8:31:PRO:HG2	1.95	0.49
52:Sf:192:ASN:HB2	52:Sf:426:LEU:HD23	1.94	0.49
53:SB:159:ALA:O	53:SB:162:CYS:C	2.56	0.49
57:SG:44:PRO:HD3	57:SG:75:LYS:HG2	1.94	0.49
70:SY:102:LYS:HA	70:SY:105:GLU:HG3	1.95	0.49
73:Sc:140:ASP:O	73:Sc:143:THR:OG1	2.26	0.49
82:So:429:LEU:HA	82:So:464:LEU:HD21	1.95	0.49
1:L1:648:A:H2'	1:L1:649:A:C8	2.48	0.49
1:L1:1184:U:H4'	28:Li:138:PRO:HG2	1.95	0.49
39:Lt:174:PRO:HB3	39:Lt:195:LEU:HD21	1.95	0.49
48:L6:56:ARG:HA	48:L6:59:GLU:HG2	1.94	0.49
54:SZ:129:PRO:HA	54:SZ:132:TYR:CD1	2.48	0.49
82:So:376:ILE:HG12	82:So:393:ILE:HD12	1.93	0.49
83:S1:616:G:H1	83:S1:682:U:H3	1.60	0.49
3:LB:189:VAL:HG23	3:LB:219:LYS:HE2	1.95	0.49
6:LI:146:LEU:O	6:LI:147:ARG:NE	2.46	0.49
17:LU:76:HIS:ND1	35:Lp:50:ALA:HA	2.28	0.49
19:LW:18:ARG:NH2	20:LX:206:GLU:OE1	2.45	0.49
55:SE:317:HIS:HD2	83:S1:4:A:H5'	1.78	0.49
73:Sc:240:LEU:HA	73:Sc:243:VAL:HG22	1.94	0.49
83:S1:578:C:O2'	83:S1:802:G:O2'	2.26	0.49
1:L1:829:U:OP2	1:L1:834:A:N6	2.36	0.48
33:Ln:178:TYR:O	39:Lt:136:ARG:NH2	2.46	0.48
37:Lr:46:GLU:O	37:Lr:50:LEU:HG	2.12	0.48
40:Lv:135:LEU:HD12	40:Lv:145:LEU:HD13	1.95	0.48
64:SP:108:GLU:HA	64:SP:111:ARG:HG2	1.94	0.48
68:SW:25:THR:O	68:SW:29:ILE:HG12	2.13	0.48
73:Sc:74:ARG:NH2	73:Sc:393:GLU:OE2	2.45	0.48
1:L1:789:A:N6	1:L1:998:A:O2'	2.46	0.48
1:L1:844:C:H2'	1:L1:845:U:H6	1.77	0.48
31:Ll:161:LEU:HG	31:Ll:221:LEU:HD21	1.95	0.48
54:SZ:91:PHE:HD2	54:SZ:92:LEU:HD12	1.78	0.48
60:SK:82:GLU:OE1	60:SK:82:GLU:N	2.47	0.48
66:SS:91:ARG:HH22	66:SS:103:ASN:HB3	1.77	0.48
69:SX:106:MET:HB2	69:SX:110:GLN:HB2	1.96	0.48
71:Sa:95:ASN:O	71:Sa:99:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sj:64:LEU:HD12	78:Sj:139:TRP:CD2	2.49	0.48
79:Sk:214:LEU:HB2	79:Sk:217:GLN:HE21	1.76	0.48
82:So:75:ALA:O	82:So:78:VAL:C	2.56	0.48
82:So:503:ALA:O	82:So:505:ARG:NH1	2.46	0.48
83:S1:35:A:H2'	83:S1:36:G:H8	1.78	0.48
7:LJ:40:MET:HE1	7:LJ:48:MET:HE2	1.95	0.48
31:Ll:213:LEU:HB2	31:Ll:275:GLN:HB2	1.94	0.48
61:SL:64:CYS:HB2	61:SL:82:ARG:HB3	1.95	0.48
64:SP:104:ILE:HD11	72:Sb:59:ARG:HD3	1.95	0.48
73:Sc:277:ARG:HE	73:Sc:349:SER:HB3	1.77	0.48
79:Sk:298:SER:O	79:Sk:302:GLU:CB	2.61	0.48
82:So:302:VAL:HG21	82:So:341:CYS:HB3	1.95	0.48
82:So:471:ILE:HG21	82:So:505:ARG:HE	1.78	0.48
20:LX:21:TYR:CG	20:LX:82:GLN:HG3	2.48	0.48
31:Ll:64:GLU:O	31:Ll:69:HIS:NE2	2.45	0.48
38:Ls:152:LEU:HD11	38:Ls:172:MET:HG2	1.96	0.48
58:SI:257:ILE:HG23	58:SI:354:SER:HA	1.96	0.48
61:SL:62:VAL:HA	61:SL:83:VAL:HG12	1.95	0.48
2:L2:21:A:H2'	2:L2:22:G:C8	2.49	0.48
11:LO:53:HIS:ND1	11:LO:53:HIS:O	2.47	0.48
63:SO:166:MET:HE3	63:SO:166:MET:HB2	1.55	0.48
66:SS:52:LYS:HE3	66:SS:58:TYR:HB2	1.96	0.48
67:ST:78:GLN:HG3	67:ST:129:TYR:CD1	2.49	0.48
70:SY:87:LEU:HD12	74:Sd:88:PRO:HB2	1.95	0.48
73:Sc:274:LYS:HB3	73:Sc:348:GLU:HB2	1.95	0.48
1:L1:26:C:OP2	23:Lu:180:LYS:NZ	2.38	0.48
3:LB:228:LEU:O	3:LB:231:LYS:N	2.46	0.48
14:LR:103:SER:O	14:LR:134:ARG:NH1	2.46	0.48
24:Ld:71:ARG:NH2	24:Ld:92:GLU:O	2.42	0.48
25:Lf:136:GLU:OE2	25:Lf:139:ARG:NH2	2.42	0.48
66:SS:53:ASP:OD1	66:SS:54:GLU:N	2.47	0.48
66:SS:58:TYR:O	66:SS:61:SER:OG	2.31	0.48
78:Sj:169:LEU:O	78:Sj:173:MET:HG2	2.13	0.48
83:S1:592:C:H2'	83:S1:593:A:C8	2.47	0.48
83:S1:616:G:O6	83:S1:682:U:O4	2.31	0.48
2:L2:58:U:H2'	2:L2:59:G:H8	1.78	0.48
24:Ld:84:ASP:O	24:Ld:88:MET:HG3	2.13	0.48
57:SG:120:ARG:NE	75:Se:89:MET:HE2	2.28	0.48
60:SK:85:ILE:HD11	60:SK:148:ARG:HH21	1.78	0.48
75:Se:260:VAL:HG23	75:Se:306:ILE:HA	1.96	0.48
80:Sm:56:TRP:HB3	80:Sm:61:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LJ:111:LEU:HA	7:LJ:114:HIS:ND1	2.29	0.48
32:Lm:142:TYR:OH	32:Lm:301:SER:OG	2.31	0.48
32:Lm:185:LEU:HD12	32:Lm:295:ARG:HH11	1.79	0.48
48:L6:47:TYR:O	48:L6:50:SER:OG	2.28	0.48
62:SN:30:VAL:HG11	62:SN:95:SER:H	1.78	0.48
72:Sb:77:GLU:OE2	72:Sb:80:ARG:NH2	2.44	0.48
83:S1:753:U:O2'	83:S1:797:A:N3	2.44	0.48
1:L1:347:U:O2'	1:L1:1053:A:N1	2.43	0.48
39:Lt:64:THR:H	39:Lt:67:GLN:HE21	1.61	0.48
40:Lv:109:TYR:HE1	47:L5:37:ARG:HH21	1.61	0.48
54:SZ:68:TRP:HZ2	62:SN:124:GLN:NE2	2.09	0.48
54:SZ:131:LYS:HZ3	55:SE:144:LEU:HD22	1.79	0.48
57:SG:176:ASP:HA	57:SG:179:ARG:HG2	1.96	0.48
60:SK:94:ASN:OD1	60:SK:95:THR:N	2.47	0.48
62:SN:48:ALA:HB3	77:Si:44:LYS:HE2	1.96	0.48
83:S1:246:G:HO2'	83:S1:261:C:HO2'	1.61	0.48
1:L1:350:U:O4	11:LO:58:GLN:NE2	2.47	0.48
33:Ln:142:ALA:HB2	39:Lt:274:ARG:HG2	1.96	0.48
52:Sf:63:ILE:HA	52:Sf:66:TRP:CD1	2.49	0.48
62:SN:62:ILE:HD11	76:Sg:349:HIS:HB2	1.96	0.48
73:Sc:308:GLN:O	73:Sc:312:LYS:HB2	2.14	0.48
5:LD:61:PRO:HA	5:LD:84:PRO:HD3	1.96	0.47
30:Lk:125:LYS:HA	30:Lk:253:LEU:HD11	1.96	0.47
38:Ls:95:ALA:HB2	38:Ls:243:LEU:HD22	1.96	0.47
39:Lt:188:ALA:HB2	39:Lt:234:PHE:CD2	2.48	0.47
45:L3:30:THR:HG21	45:L3:62:PRO:HB2	1.95	0.47
51:SR:35:PHE:N	51:SR:56:THR:HG1	2.12	0.47
55:SE:392:ARG:NH1	55:SE:394:ASP:O	2.47	0.47
59:SJ:91:TYR:OH	59:SJ:160:ILE:O	2.32	0.47
65:SQ:46:ARG:NH1	83:S1:302:U:O2'	2.47	0.47
79:Sk:251:TYR:HB3	79:Sk:300:LYS:HD2	1.96	0.47
10:LN:123:ILE:HD12	10:LN:127:LEU:HD12	1.96	0.47
53:SB:100:ARG:NH1	70:SY:52:ARG:HE	2.12	0.47
59:SJ:76:LEU:HD11	59:SJ:173:THR:HB	1.96	0.47
59:SJ:157:LEU:HD11	59:SJ:173:THR:HG21	1.96	0.47
62:SN:91:CYS:HB3	62:SN:94:THR:O	2.14	0.47
66:SS:104:PRO:HB2	66:SS:109:ARG:HB3	1.96	0.47
69:SX:128:MET:HE1	69:SX:269:GLY:HA3	1.96	0.47
79:Sk:66:TRP:NE1	79:Sk:112:LEU:O	2.45	0.47
79:Sk:183:ASP:HB3	79:Sk:187:LYS:HB3	1.95	0.47
1:L1:211:A:H62	41:Lw:111:ARG:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:510:A:H2'	1:L1:514:A:H62	1.79	0.47
8:LK:48:GLN:NE2	8:LK:52:GLU:OE2	2.47	0.47
23:Lu:128:SER:OG	23:Lu:131:ARG:NE	2.29	0.47
36:Lq:77:ALA:HB3	36:Lq:85:ARG:HB3	1.95	0.47
39:Lt:200:MET:HA	39:Lt:241:GLY:HA3	1.96	0.47
40:Lv:130:LYS:HD2	40:Lv:130:LYS:HA	1.61	0.47
53:SB:152:SER:O	53:SB:156:GLU:HG3	2.13	0.47
57:SG:126:TYR:HB2	57:SG:139:ARG:HD3	1.96	0.47
68:SW:62:ARG:O	68:SW:66:MET:HG2	2.14	0.47
71:Sa:14:GLN:O	71:Sa:18:GLN:CB	2.59	0.47
79:Sk:306:GLU:HA	79:Sk:309:ILE:HG22	1.96	0.47
83:S1:515:A:N3	83:S1:850:C:O2'	2.41	0.47
39:Lt:248:ASN:ND2	39:Lt:250:GLY:O	2.47	0.47
44:Lz:99:GLN:HE22	44:Lz:103:ARG:HD2	1.78	0.47
45:L3:22:PRO:HA	45:L3:27:VAL:HG11	1.95	0.47
64:SP:51:LEU:HD21	64:SP:76:TRP:HD1	1.79	0.47
75:Se:387:ASN:HB3	75:Se:390:LEU:HB2	1.96	0.47
82:So:267:VAL:HG22	82:So:300:ALA:HB2	1.95	0.47
82:So:491:GLN:O	82:So:495:HIS:ND1	2.30	0.47
83:S1:942:C:H2'	83:S1:943:A:C8	2.48	0.47
32:Lm:212:LYS:HE2	32:Lm:212:LYS:HB3	1.66	0.47
33:Ln:169:PHE:O	33:Ln:171:PHE:N	2.47	0.47
54:SZ:77:ASP:OD1	54:SZ:78:GLY:N	2.48	0.47
64:SP:42:PRO:HG3	83:S1:66:C:H5'	1.95	0.47
73:Sc:231:LEU:HA	73:Sc:234:VAL:HG12	1.96	0.47
2:L2:42:A:OP1	31:Ll:114:ARG:NH2	2.34	0.47
12:LP:132:THR:O	12:LP:133:ARG:NH1	2.47	0.47
20:LX:54:TRP:NE1	20:LX:56:LEU:O	2.48	0.47
36:Lq:37:GLY:O	36:Lq:44:ARG:NH1	2.39	0.47
37:Lr:246:LYS:HB3	37:Lr:246:LYS:HE2	1.69	0.47
38:Ls:85:PHE:CE2	38:Ls:200:SER:HB2	2.49	0.47
41:Lw:121:GLN:O	41:Lw:125:GLU:HG3	2.15	0.47
54:SZ:145:TYR:CD2	82:So:121:ILE:HD13	2.46	0.47
70:SY:88:PHE:HD2	74:Sd:103:ARG:NH2	2.12	0.47
83:S1:378:A:H2'	83:S1:379:A:C8	2.50	0.47
1:L1:19:C:N4	22:Lb:14:LEU:HB3	2.30	0.47
1:L1:1302:A:H5''	12:LP:184:PRO:HA	1.97	0.47
2:L2:25:C:H4'	33:Ln:133:ARG:HH12	1.79	0.47
3:LB:154:THR:H	3:LB:157:MET:HE3	1.79	0.47
5:LD:191:ASP:OD1	5:LD:191:ASP:N	2.45	0.47
6:LI:123:LEU:HA	6:LI:128:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LO:182:ARG:O	11:LO:186:ILE:HG12	2.15	0.47
11:LO:254:LYS:O	11:LO:258:THR:OG1	2.26	0.47
17:LU:194:ARG:NE	36:Lq:17:ASN:O	2.46	0.47
18:LV:91:ALA:O	18:LV:94:ILE:C	2.58	0.47
20:LX:134:GLU:OE2	20:LX:136:ARG:NE	2.48	0.47
31:Ll:90:ILE:HG21	44:Lz:109:LEU:HD23	1.97	0.47
38:Ls:122:ILE:HD11	38:Ls:197:VAL:HG21	1.96	0.47
39:Lt:214:THR:HB	39:Lt:230:LYS:HD2	1.97	0.47
52:Sf:341:MET:HG2	52:Sf:345:PHE:O	2.15	0.47
54:SZ:88:GLU:HG3	54:SZ:92:LEU:HD13	1.97	0.47
58:SI:169:LEU:HD21	58:SI:228:LEU:HA	1.97	0.47
59:SJ:79:LEU:O	59:SJ:171:GLU:HA	2.14	0.47
59:SJ:81:LYS:HZ1	59:SJ:138:THR:CA	2.28	0.47
61:SL:116:GLN:HE21	83:S1:248:C:H2'	1.80	0.47
63:SO:89:VAL:HG22	72:Sb:164:VAL:HG21	1.96	0.47
68:SW:6:LYS:HD3	68:SW:6:LYS:HA	1.77	0.47
71:Sa:101:HIS:O	71:Sa:105:ILE:HG12	2.15	0.47
73:Sc:137:ILE:HG22	73:Sc:139:PRO:HD3	1.96	0.47
83:S1:424:U:H2'	83:S1:425:G:H8	1.78	0.47
83:S1:554:A:H2'	83:S1:555:G:C8	2.49	0.47
83:S1:554:A:H2'	83:S1:555:G:H8	1.80	0.47
1:L1:1007:A:H2'	1:L1:1008:A:C8	2.49	0.47
2:L2:41:G:H2'	2:L2:42:A:C8	2.49	0.47
7:LJ:78:LEU:HD13	46:L4:118:TRP:CE3	2.50	0.47
7:LJ:108:ASP:O	7:LJ:112:MET:HG2	2.15	0.47
48:L6:68:ARG:O	48:L6:72:GLU:HG2	2.15	0.47
61:SL:58:LEU:HD23	61:SL:85:LEU:HD13	1.97	0.47
65:SQ:57:GLN:O	65:SQ:87:LYS:NZ	2.48	0.47
70:SY:86:ASP:CG	70:SY:89:ASN:HD22	2.23	0.47
70:SY:97:GLN:HA	70:SY:100:VAL:HG12	1.97	0.47
74:Sd:109:GLU:OE2	74:Sd:110:ASN:ND2	2.47	0.47
79:Sk:174:ARG:HG2	79:Sk:206:THR:HG22	1.97	0.47
79:Sk:214:LEU:HB2	79:Sk:217:GLN:HG2	1.96	0.47
82:So:343:ARG:HD2	82:So:377:ARG:HB3	1.97	0.47
83:S1:786:A:H3'	83:S1:787:A:H8	1.80	0.47
1:L1:211:A:OP1	41:Lw:90:ARG:N	2.47	0.47
1:L1:1058:C:H2'	1:L1:1059:U:H6	1.80	0.47
12:LP:163:MET:HE2	12:LP:163:MET:HB3	1.79	0.47
19:LW:46:MET:HE2	34:Lo:36:ARG:HD2	1.97	0.47
22:Lb:177:HIS:O	22:Lb:184:ARG:NH1	2.48	0.47
53:SB:149:ARG:NH2	83:S1:646:C:O2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SE:426:LYS:HB3	66:SS:136:TYR:CE1	2.49	0.47
59:SJ:147:HIS:HA	79:Sk:133:TRP:CH2	2.49	0.47
75:Se:117:PHE:HB3	75:Se:303:GLY:HA2	1.96	0.47
82:So:420:MET:HE1	82:So:461:PHE:N	2.29	0.47
8:LK:149:ARG:HH22	46:L4:104:PRO:HD3	1.80	0.47
16:LT:19:PHE:O	16:LT:23:GLU:HG2	2.14	0.47
31:Ll:136:ARG:NH1	31:Ll:140:GLU:OE2	2.45	0.47
39:Lt:98:LEU:HA	39:Lt:98:LEU:HD23	1.73	0.47
45:L3:15:GLN:NE2	45:L3:65:ASP:OD2	2.47	0.47
54:SZ:125:ARG:HG2	54:SZ:157:THR:HB	1.97	0.47
55:SE:320:ILE:HG23	55:SE:349:LEU:HD11	1.97	0.47
62:SN:41:ARG:NH2	62:SN:88:ARG:O	2.48	0.47
70:SY:111:GLU:HB2	70:SY:116:LYS:NZ	2.30	0.47
74:Sd:103:ARG:HE	74:Sd:139:ARG:CZ	2.28	0.47
82:So:336:ASN:OD1	82:So:371:THR:OG1	2.22	0.47
83:S1:462:A:H2'	83:S1:463:A:H8	1.80	0.47
83:S1:931:A:H2'	83:S1:932:C:C6	2.50	0.47
1:L1:235:C:OP1	5:LD:117:ARG:NH1	2.45	0.46
1:L1:640:G:OP2	25:Lf:94:ARG:NH1	2.40	0.46
4:LC:212:GLY:HA2	4:LC:262:GLY:HA3	1.96	0.46
54:SZ:128:SER:O	54:SZ:131:LYS:HB2	2.14	0.46
75:Se:272:THR:OG1	75:Se:282:ILE:O	2.23	0.46
78:Sj:71:LEU:HD13	78:Sj:78:ARG:HG2	1.97	0.46
79:Sk:84:PRO:HA	79:Sk:99:LYS:HD3	1.97	0.46
83:S1:560:U:H5''	83:S1:571:A:H61	1.79	0.46
1:L1:136:U:H4'	1:L1:137:U:H5'	1.97	0.46
1:L1:143:C:H2'	43:Ly:32:ILE:HG13	1.96	0.46
1:L1:416:A:H2'	1:L1:417:U:C6	2.50	0.46
1:L1:487:U:OP1	51:SR:182:ARG:NH1	2.48	0.46
19:LW:38:ASP:O	19:LW:98:GLN:HA	2.14	0.46
33:Ln:97:LYS:HE3	39:Lt:84:TYR:CD2	2.51	0.46
47:L5:70:GLU:HG2	47:L5:71:PRO:HD2	1.98	0.46
66:SS:73:VAL:HG12	66:SS:106:PRO:HB3	1.97	0.46
71:Sa:141:CYS:HB3	71:Sa:149:CYS:HB2	1.97	0.46
75:Se:276:ARG:NH2	75:Se:286:GLU:OE1	2.45	0.46
79:Sk:56:ARG:HH21	79:Sk:80:ALA:HB2	1.79	0.46
1:L1:1395:U:OP2	4:LC:239:ARG:NH2	2.48	0.46
4:LC:275:ARG:HB3	4:LC:284:TYR:HB2	1.98	0.46
31:Ll:59:ARG:O	31:Ll:63:GLN:HG3	2.14	0.46
39:Lt:202:ALA:HA	39:Lt:239:LEU:H	1.79	0.46
43:Ly:96:LYS:HE2	43:Ly:96:LYS:HB3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SI:157:SER:HB3	58:SI:209:LEU:HD22	1.97	0.46
59:SJ:81:LYS:HZ1	59:SJ:138:THR:C	2.24	0.46
62:SN:58:ARG:NH2	62:SN:71:ALA:O	2.49	0.46
63:SO:152:HIS:NE2	83:S1:390:A:O2'	2.28	0.46
83:S1:47:C:H2'	83:S1:168:C:H41	1.79	0.46
5:LD:75:GLU:HG3	5:LD:210:ARG:HE	1.80	0.46
5:LD:228:GLN:HA	5:LD:231:VAL:HG22	1.97	0.46
13:LQ:131:PRO:HB3	25:Lf:184:TRP:HZ3	1.80	0.46
33:Ln:146:ALA:HB1	39:Lt:209:PRO:HB2	1.97	0.46
48:L6:11:ARG:HH21	48:L6:13:PRO:HA	1.79	0.46
55:SE:179:TRP:HA	55:SE:182:LYS:HG2	1.97	0.46
55:SE:234:LYS:NZ	83:S1:675:C:N3	2.55	0.46
56:SF:15:ARG:NH2	72:Sb:178:GLU:OE1	2.40	0.46
58:SI:92:MET:HE2	58:SI:106:ARG:HH22	1.80	0.46
71:Sa:19:GLY:HA3	71:Sa:54:GLN:HB3	1.97	0.46
81:Sn:183:LYS:HE2	81:Sn:183:LYS:HB2	1.73	0.46
82:So:444:ASN:HA	82:So:447:PHE:HB2	1.96	0.46
83:S1:24:U:H2'	83:S1:25:A:C8	2.51	0.46
1:L1:501:U:C2	1:L1:503:G:H4'	2.50	0.46
1:L1:725:A:O2'	30:Lk:384:GLN:OE1	2.33	0.46
1:L1:755:A:OP1	52:Sf:221:HIS:ND1	2.48	0.46
1:L1:859:U:OP2	3:LB:208:ARG:NE	2.47	0.46
3:LB:140:ALA:HB2	3:LB:153:ALA:HB2	1.96	0.46
14:LR:93:VAL:HB	14:LR:102:VAL:HG12	1.96	0.46
14:LR:125:GLU:OE1	14:LR:159:ARG:NE	2.49	0.46
44:Lz:63:GLN:OE1	44:Lz:66:ARG:NH1	2.49	0.46
53:SB:188:ARG:HD3	58:SI:144:GLY:HA3	1.97	0.46
53:SB:230:CYS:SG	70:SY:47:GLN:N	2.86	0.46
64:SP:111:ARG:HA	66:SS:235:MET:HE1	1.98	0.46
82:So:413:ASP:OD1	82:So:413:ASP:N	2.46	0.46
83:S1:805:U:H2'	83:S1:806:A:C8	2.49	0.46
1:L1:802:A:O2'	1:L1:808:G:N7	2.36	0.46
7:LJ:134:PHE:O	7:LJ:138:SER:CB	2.63	0.46
12:LP:89:ILE:HG13	12:LP:176:LEU:HD22	1.98	0.46
13:LQ:84:ASP:OD2	25:Lf:149:PHE:HA	2.16	0.46
17:LU:112:ASP:O	17:LU:194:ARG:HA	2.16	0.46
52:Sf:84:THR:HB	52:Sf:280:ASN:HB2	1.98	0.46
57:SG:115:LEU:HD13	57:SG:141:PRO:HB2	1.98	0.46
77:Si:28:SER:HA	77:Si:31:MET:HB2	1.97	0.46
79:Sk:217:GLN:HA	79:Sk:220:ASP:HB2	1.98	0.46
79:Sk:257:SER:HA	79:Sk:260:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LU:164:THR:OG1	17:LU:165:GLU:N	2.49	0.46
17:LU:173:ARG:O	17:LU:181:LYS:HA	2.16	0.46
31:Ll:257:PRO:HB3	31:Ll:268:LEU:HD21	1.97	0.46
36:Lq:77:ALA:O	36:Lq:84:VAL:CA	2.63	0.46
39:Lt:151:ARG:NH1	39:Lt:254:TRP:O	2.42	0.46
65:SQ:96:THR:O	65:SQ:98:LYS:N	2.49	0.46
75:Se:132:THR:N	87:Se:500:GDP:O2A	2.49	0.46
83:S1:625:A:N1	83:S1:656:G:O2'	2.37	0.46
30:Lk:215:ARG:NH2	30:Lk:367:ASN:OD1	2.48	0.46
30:Lk:293:LEU:HD12	30:Lk:313:MET:HG2	1.98	0.46
36:Lq:133:PHE:HB3	37:Lr:259:ARG:HH11	1.81	0.46
75:Se:123:ARG:HH21	75:Se:339:PRO:HD2	1.80	0.46
76:Sg:358:LEU:HA	76:Sg:361:ASN:ND2	2.29	0.46
1:L1:791:A:H4'	4:LC:235:LYS:HB3	1.97	0.46
1:L1:1040:C:O2'	1:L1:1550:A:N1	2.38	0.46
4:LC:134:SER:OG	4:LC:137:ASN:OD1	2.34	0.46
37:Lr:148:MET:HG2	37:Lr:305:TYR:HB3	1.97	0.46
69:SX:260:ASP:N	69:SX:260:ASP:OD1	2.48	0.46
73:Sc:304:ASP:OD1	73:Sc:308:GLN:NE2	2.42	0.46
78:Sj:65:LEU:HG	78:Sj:112:GLY:N	2.30	0.46
82:So:342:LEU:HB2	82:So:349:ALA:HB1	1.97	0.46
82:So:494:ILE:HA	82:So:497:LEU:HD12	1.97	0.46
83:S1:930:U:H2'	83:S1:931:A:C8	2.51	0.46
5:LD:113:LYS:HD2	5:LD:157:GLY:HA2	1.98	0.46
14:LR:53:ARG:NE	14:LR:56:GLU:OE2	2.33	0.46
35:Lp:43:TYR:HD2	36:Lq:135:ASN:HA	1.80	0.46
50:L8:128:MET:SD	50:L8:131:MET:HE3	2.56	0.46
59:SJ:161:GLN:HB2	76:Sg:313:PHE:CZ	2.51	0.46
61:SL:33:LEU:HD22	65:SQ:39:LEU:HD22	1.98	0.46
67:ST:126:ASP:HB2	67:ST:129:TYR:HD2	1.81	0.46
68:SW:68:MET:O	68:SW:72:ILE:HG12	2.16	0.46
76:Sg:307:GLU:HB3	76:Sg:309:LYS:HE2	1.98	0.46
83:S1:485:U:H2'	83:S1:486:C:C6	2.50	0.46
83:S1:552:G:N1	83:S1:775:G:OP2	2.46	0.46
1:L1:214:G:H1'	1:L1:225:C:H1'	1.98	0.45
1:L1:552:U:H2'	1:L1:553:A:N3	2.31	0.45
1:L1:858:G:H3'	3:LB:208:ARG:HH21	1.80	0.45
4:LC:202:GLN:O	4:LC:272:LYS:HA	2.16	0.45
4:LC:219:MET:SD	4:LC:238:ARG:HG3	2.56	0.45
7:LJ:82:LEU:HD13	7:LJ:130:VAL:HG21	1.97	0.45
17:LU:142:THR:HG23	35:Lp:62:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Ll:139:TRP:CD1	31:Ll:143:CYS:HG	2.35	0.45
37:Lr:72:ILE:HG23	37:Lr:88:LEU:HD23	1.98	0.45
57:SG:82:THR:HG21	58:SI:311:GLU:HG3	1.98	0.45
78:Sj:145:HIS:HB2	78:Sj:146:GLU:OE1	2.16	0.45
79:Sk:78:PRO:HB2	79:Sk:99:LYS:HE3	1.98	0.45
82:So:367:PRO:HB3	82:So:371:THR:HG21	1.98	0.45
1:L1:187:U:H2'	1:L1:188:G:C8	2.52	0.45
7:LJ:163:GLU:HA	7:LJ:166:ARG:HB2	1.98	0.45
20:LX:122:LEU:HA	20:LX:122:LEU:HD12	1.54	0.45
20:LX:150:SER:HB2	20:LX:152:ARG:NH2	2.31	0.45
38:Ls:213:THR:HG22	38:Ls:247:VAL:HG22	1.98	0.45
54:SZ:52:THR:O	54:SZ:56:ALA:HB2	2.16	0.45
57:SG:103:ASN:HB3	57:SG:106:LEU:HB2	1.98	0.45
59:SJ:81:LYS:NZ	59:SJ:138:THR:HB	2.31	0.45
62:SN:71:ALA:HA	62:SN:74:GLU:HG3	1.97	0.45
63:SO:200:HIS:NE2	83:S1:114:A:OP2	2.48	0.45
68:SW:72:ILE:O	68:SW:76:MET:HG2	2.17	0.45
69:SX:195:VAL:HG23	69:SX:204:ILE:HG21	1.98	0.45
71:Sa:90:VAL:HA	71:Sa:93:LYS:HD2	1.99	0.45
75:Se:259:LEU:HD12	75:Se:305:ALA:HB3	1.97	0.45
1:L1:107:A:N6	1:L1:110:U:OP2	2.44	0.45
4:LC:60:PHE:HB2	13:LQ:153:ARG:HH21	1.81	0.45
7:LJ:95:MET:HG3	7:LJ:164:MET:HE1	1.98	0.45
62:SN:54:ILE:HG21	62:SN:74:GLU:OE2	2.17	0.45
66:SS:136:TYR:HD1	66:SS:138:PRO:HD2	1.81	0.45
74:Sd:144:LEU:HD23	74:Sd:167:ALA:HB2	1.97	0.45
79:Sk:137:LEU:HD12	79:Sk:142:LYS:HG3	1.99	0.45
83:S1:355:C:H2'	83:S1:356:A:C8	2.51	0.45
1:L1:282:U:H2'	1:L1:283:A:C8	2.50	0.45
1:L1:672:U:H5'	19:LW:78:LYS:HD2	1.99	0.45
1:L1:867:G:O2'	1:L1:964:U:OP2	2.32	0.45
34:Lo:46:SER:OG	34:Lo:47:GLY:N	2.45	0.45
43:Ly:102:MET:HE1	43:Ly:110:LEU:HD22	1.99	0.45
73:Sc:226:TYR:HE1	73:Sc:282:VAL:HG21	1.82	0.45
75:Se:159:HIS:HA	75:Se:162:VAL:HG12	1.97	0.45
75:Se:159:HIS:HE1	75:Se:311:SER:HB2	1.81	0.45
78:Sj:52:VAL:HA	78:Sj:55:TRP:CD1	2.52	0.45
82:So:302:VAL:HA	82:So:312:LYS:HD3	1.98	0.45
83:S1:27:U:H2'	83:S1:28:A:H8	1.81	0.45
1:L1:662:C:H42	1:L1:772:U:H3	1.65	0.45
1:L1:1125:U:H2'	1:L1:1126:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1349:G:O2'	1:L1:1455:A:N1	2.45	0.45
30:Lk:395:ARG:HD2	30:Lk:395:ARG:N	2.30	0.45
34:Lo:91:LEU:O	34:Lo:95:ALA:CB	2.64	0.45
39:Lt:198:ASN:HB2	39:Lt:200:MET:HG2	1.98	0.45
39:Lt:266:PRO:HB2	39:Lt:267:LYS:H	1.54	0.45
53:SB:243:PRO:O	53:SB:247:HIS:ND1	2.38	0.45
56:SF:97:PRO:HA	56:SF:100:GLN:HG2	1.97	0.45
70:SY:68:ASP:OD1	70:SY:71:ARG:NH1	2.49	0.45
83:S1:514:A:H2'	83:S1:515:A:H8	1.81	0.45
19:LW:125:ASP:OD2	38:Ls:205:GLN:OE1	2.35	0.45
20:LX:76:VAL:HG12	20:LX:88:VAL:HG22	1.99	0.45
28:Li:180:TYR:OH	31:Ll:367:ASP:OD2	2.28	0.45
29:Lj:72:LEU:HD22	29:Lj:100:GLN:HB3	1.99	0.45
31:Ll:204:VAL:HG11	31:Ll:216:LEU:HD21	1.97	0.45
31:Ll:237:LEU:HB3	31:Ll:240:ILE:HD11	1.98	0.45
34:Lo:54:LYS:HE3	34:Lo:54:LYS:HB3	1.73	0.45
38:Ls:186:VAL:HG21	38:Ls:239:PRO:HB3	1.97	0.45
61:SL:78:ARG:HH21	83:S1:247:C:H41	1.64	0.45
64:SP:101:PRO:HB3	72:Sb:59:ARG:HB3	1.99	0.45
83:S1:35:A:H2'	83:S1:36:G:C8	2.52	0.45
1:L1:405:U:O2'	1:L1:1163:A:N7	2.45	0.45
1:L1:1075:A:O2'	22:Lb:102:LYS:O	2.25	0.45
7:LJ:87:ALA:O	7:LJ:91:GLN:HG3	2.16	0.45
9:LM:39:LEU:HD11	9:LM:125:LEU:HB2	1.98	0.45
18:LV:154:LYS:O	18:LV:155:ARG:NH1	2.49	0.45
31:Ll:374:GLU:OE2	49:L7:140:SER:OG	2.29	0.45
42:Lx:157:SER:O	42:Lx:157:SER:OG	2.32	0.45
43:Ly:71:LYS:HE3	43:Ly:82:GLY:HA3	1.99	0.45
58:SI:294:LYS:HB2	58:SI:329:THR:HA	1.99	0.45
73:Sc:176:PRO:HA	73:Sc:179:GLN:HB2	1.97	0.45
82:So:113:GLY:O	82:So:116:VAL:HB	2.16	0.45
83:S1:160:A:H8	83:S1:161:C:H41	1.64	0.45
1:L1:25:C:OP1	23:Lu:162:ARG:NH2	2.50	0.45
1:L1:789:A:C2	1:L1:1042:G:H5''	2.52	0.45
11:LO:287:ASP:HA	41:Lw:37:ARG:HH21	1.81	0.45
17:LU:125:GLY:N	17:LU:160:VAL:O	2.50	0.45
20:LX:75:LYS:HB2	20:LX:75:LYS:HE3	1.78	0.45
25:Lf:141:ILE:O	25:Lf:145:GLU:HG3	2.17	0.45
32:Lm:64:LYS:HD2	32:Lm:80:VAL:HG12	1.98	0.45
39:Lt:201:GLU:H	39:Lt:241:GLY:HA3	1.81	0.45
50:L8:40:PRO:HG3	50:L8:51:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SF:54:HIS:CD2	56:SF:86:ILE:HA	2.52	0.45
58:SI:269:PHE:HB3	58:SI:286:TYR:CD1	2.51	0.45
59:SJ:81:LYS:HB3	59:SJ:170:MET:HG3	1.98	0.45
79:Sk:53:LEU:HD22	82:So:518:GLU:HB2	1.99	0.45
83:S1:160:A:H1'	83:S1:161:C:H5	1.82	0.45
1:L1:849:G:N7	3:LB:230:SER:OG	2.41	0.45
3:LB:253:ASN:OD1	3:LB:254:LYS:NZ	2.50	0.45
8:LK:39:LEU:HB3	8:LK:44:VAL:HB	1.99	0.45
26:Lg:17:LEU:HB2	26:Lg:65:LEU:HD23	1.99	0.45
57:SG:233:ASN:HB2	57:SG:236:LEU:HD12	1.99	0.45
77:Si:62:MET:HA	77:Si:62:MET:HE3	1.99	0.45
78:Sj:37:ASP:OD2	78:Sj:40:THR:OG1	2.30	0.45
1:L1:9:U:H2'	1:L1:10:A:H8	1.81	0.45
1:L1:534:U:N3	1:L1:537:A:OP2	2.50	0.45
1:L1:934:A:C8	85:L1:1708:T1C:C10	2.99	0.45
13:LQ:52:MET:HE1	13:LQ:123:ILE:HG21	1.99	0.45
31:Ll:157:LEU:HB3	31:Ll:161:LEU:HD12	1.98	0.45
31:Ll:261:ARG:NH1	49:L7:125:ASN:OD1	2.49	0.45
32:Lm:162:TYR:CE2	32:Lm:189:LEU:HD11	2.52	0.45
39:Lt:187:THR:HA	39:Lt:190:ARG:HE	1.81	0.45
46:L4:67:GLN:HA	46:L4:70:THR:HG22	1.98	0.45
50:L8:37:PRO:HG3	50:L8:68:SER:HA	1.99	0.45
58:SI:298:ILE:HD11	58:SI:303:TYR:HD1	1.82	0.45
59:SJ:81:LYS:HG2	59:SJ:170:MET:HE2	1.99	0.45
59:SJ:115:ILE:HA	59:SJ:136:MET:O	2.16	0.45
73:Sc:294:ASP:OD1	73:Sc:294:ASP:N	2.48	0.45
74:Sd:136:LYS:HE2	74:Sd:136:LYS:HB3	1.75	0.45
77:Si:56:HIS:O	77:Si:60:GLU:HB2	2.17	0.45
83:S1:514:A:H2'	83:S1:515:A:C8	2.52	0.45
13:LQ:96:ARG:NH2	25:Lf:155:GLU:OE2	2.50	0.44
42:Lx:153:LYS:HB3	42:Lx:153:LYS:HE3	1.74	0.44
50:L8:80:GLU:HA	50:L8:83:ARG:HE	1.80	0.44
57:SG:92:SER:O	57:SG:96:ASN:ND2	2.50	0.44
57:SG:96:ASN:OD1	57:SG:104:LYS:NZ	2.50	0.44
57:SG:231:GLU:HG3	80:Sm:61:PHE:HZ	1.81	0.44
61:SL:116:GLN:NE2	83:S1:248:C:H2'	2.33	0.44
64:SP:85:LYS:HG2	64:SP:86:PRO:HD3	1.99	0.44
82:So:373:HIS:HB2	82:So:415:PHE:HA	2.00	0.44
83:S1:267:A:H2'	83:S1:268:C:C6	2.51	0.44
1:L1:371:U:H2'	1:L1:372:U:C6	2.52	0.44
2:L2:25:C:O3'	33:Ln:133:ARG:NH2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LC:113:ASP:OD1	4:LC:113:ASP:N	2.50	0.44
17:LU:112:ASP:OD1	17:LU:113:LEU:N	2.51	0.44
20:LX:21:TYR:CD1	20:LX:82:GLN:HG3	2.52	0.44
38:Ls:251:GLN:HG2	38:Ls:254:ASN:HB2	1.98	0.44
39:Lt:187:THR:HA	39:Lt:190:ARG:HG2	1.98	0.44
42:Lx:139:LYS:HD2	42:Lx:139:LYS:HA	1.78	0.44
52:Sf:251:VAL:HG11	52:Sf:255:TYR:CD2	2.52	0.44
53:SB:60:ASP:O	53:SB:64:ASN:CB	2.64	0.44
60:SK:179:THR:H	68:SW:10:ARG:NH2	2.15	0.44
61:SL:59:LYS:HG3	61:SL:130:TYR:HE2	1.82	0.44
66:SS:92:LYS:HA	66:SS:144:VAL:HB	1.99	0.44
67:ST:54:MET:HE2	67:ST:54:MET:HB3	1.88	0.44
71:Sa:76:LEU:HD13	71:Sa:90:VAL:HG11	1.99	0.44
71:Sa:100:GLU:HA	71:Sa:103:ARG:HG2	1.99	0.44
73:Sc:180:LEU:HD13	73:Sc:360:VAL:HG22	1.99	0.44
79:Sk:260:ARG:HH22	79:Sk:292:TYR:HH	1.62	0.44
82:So:112:SER:O	82:So:116:VAL:HG23	2.17	0.44
83:S1:225:G:H2'	83:S1:226:G:C8	2.52	0.44
1:L1:323:A:N3	1:L1:324:A:H5''	2.32	0.44
1:L1:859:U:H6	3:LB:208:ARG:NH2	2.14	0.44
1:L1:1274:C:OP1	48:L6:21:HIS:ND1	2.49	0.44
12:LP:250:ARG:HE	12:LP:250:ARG:HB3	1.63	0.44
21:La:113:ALA:O	21:La:117:ILE:HG12	2.18	0.44
36:Lq:35:ARG:HG3	48:L6:101:TRP:HB2	1.99	0.44
37:Lr:90:THR:HA	37:Lr:93:VAL:HG12	1.99	0.44
53:SB:144:PHE:CG	53:SB:158:MET:HE1	2.53	0.44
53:SB:219:THR:HG22	53:SB:232:ILE:HG23	1.98	0.44
58:SI:269:PHE:HB3	58:SI:286:TYR:HD1	1.82	0.44
66:SS:213:LEU:HD23	66:SS:217:ARG:NE	2.33	0.44
69:SX:339:GLY:HA2	69:SX:342:ILE:HG22	2.00	0.44
73:Sc:166:GLU:OE2	73:Sc:170:GLN:NE2	2.41	0.44
74:Sd:155:GLY:HA3	80:Sm:28:ILE:HG23	1.99	0.44
75:Se:138:LEU:HD11	75:Se:261:ALA:HB1	1.99	0.44
75:Se:319:PRO:HG2	75:Se:322:ALA:HB2	1.99	0.44
83:S1:261:C:H2'	83:S1:262:G:H8	1.82	0.44
1:L1:192:U:H2'	1:L1:193:A:C8	2.53	0.44
1:L1:640:G:O2'	1:L1:1005:G:O6	2.35	0.44
5:LD:291:SER:N	41:Lw:53:PRO:O	2.47	0.44
6:LI:79:VAL:HA	22:Lb:89:GLN:HB2	1.99	0.44
12:LP:200:LYS:HD3	12:LP:200:LYS:N	2.32	0.44
19:LW:126:LEU:O	19:LW:129:MET:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lq:16:HIS:HB3	36:Lq:19:LEU:HD12	1.99	0.44
39:Lt:121:GLU:HA	39:Lt:124:TRP:CE3	2.52	0.44
39:Lt:213:TYR:HB2	39:Lt:233:PHE:HE2	1.82	0.44
41:Lw:43:ASP:OD1	41:Lw:43:ASP:N	2.46	0.44
59:SJ:106:ILE:HD11	59:SJ:143:LEU:HG	1.99	0.44
68:SW:13:MET:HE3	68:SW:13:MET:HB3	1.90	0.44
72:Sb:149:TRP:O	72:Sb:153:LYS:HG2	2.16	0.44
83:S1:702:U:H2'	83:S1:703:G:C8	2.53	0.44
83:S1:814:A:H5'	83:S1:815:G:H5'	1.98	0.44
1:L1:241:C:H2'	1:L1:242:A:C8	2.52	0.44
4:LC:273:VAL:HG22	4:LC:285:VAL:HG22	2.00	0.44
6:LI:134:PRO:O	6:LI:138:LYS:HG3	2.18	0.44
15:LS:241:LYS:HB2	15:LS:241:LYS:HE2	1.77	0.44
19:LW:46:MET:HE1	19:LW:72:VAL:HG22	1.99	0.44
28:Li:151:ASN:HB2	28:Li:154:GLN:HG3	1.99	0.44
53:SB:194:ILE:HA	53:SB:220:VAL:O	2.16	0.44
55:SE:216:GLU:OE1	55:SE:216:GLU:N	2.50	0.44
57:SG:92:SER:O	57:SG:95:THR:OG1	2.33	0.44
62:SN:109:ILE:HD11	83:S1:685:A:C4	2.53	0.44
68:SW:67:GLU:HG3	74:Sd:154:LEU:HB2	1.99	0.44
76:Sg:302:ILE:HD11	82:So:71:LEU:HB2	2.00	0.44
76:Sg:310:LEU:HD12	76:Sg:311:TRP:H	1.81	0.44
79:Sk:65:ASP:OD1	79:Sk:68:SER:N	2.49	0.44
3:LB:223:THR:HG22	3:LB:296:VAL:HG11	2.00	0.44
3:LB:292:MET:HE2	3:LB:292:MET:HB3	1.84	0.44
9:LM:178:LEU:HD12	51:SR:100:LEU:HD21	1.98	0.44
30:Lk:229:ARG:HH21	30:Lk:288:PRO:HG3	1.82	0.44
32:Lm:106:ALA:O	32:Lm:113:TRP:N	2.48	0.44
33:Ln:163:LYS:HB2	39:Lt:207:ASN:HB3	1.99	0.44
40:Lv:106:TYR:OH	40:Lv:174:ILE:O	2.35	0.44
49:L7:185:ARG:O	49:L7:189:ARG:HB2	2.17	0.44
54:SZ:52:THR:O	54:SZ:56:ALA:CB	2.65	0.44
56:SF:44:GLU:CD	56:SF:60:ARG:HH21	2.26	0.44
60:SK:94:ASN:ND2	83:S1:342:U:OP1	2.45	0.44
68:SW:15:GLN:O	68:SW:16:GLU:HG3	2.18	0.44
68:SW:20:GLU:OE2	68:SW:24:ARG:NE	2.50	0.44
69:SX:338:LYS:HG3	69:SX:341:TYR:HB3	1.98	0.44
72:Sb:58:GLU:O	72:Sb:62:HIS:ND1	2.37	0.44
75:Se:368:HIS:HB3	75:Se:371:ALA:HB2	1.99	0.44
83:S1:824:A:H2'	83:S1:825:G:C8	2.53	0.44
1:L1:164:U:C4	18:LV:206:ARG:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:335:C:H2'	1:L1:336:C:C6	2.53	0.44
4:LC:221:ARG:HA	4:LC:261:MET:SD	2.58	0.44
8:LK:103:GLN:HB3	8:LK:106:LYS:HD2	2.00	0.44
14:LR:143:MET:HE2	14:LR:143:MET:HB3	1.81	0.44
54:SZ:115:ASN:HD21	76:Sg:310:LEU:HA	1.82	0.44
58:SI:285:VAL:HB	58:SI:328:VAL:HG22	1.99	0.44
62:SN:54:ILE:HD11	76:Sg:375:TRP:CH2	2.52	0.44
62:SN:112:ARG:HH22	83:S1:618:C:P	2.41	0.44
69:SX:82:MET:SD	69:SX:288:GLN:NE2	2.90	0.44
73:Sc:209:LEU:HD11	73:Sc:228:TYR:CE1	2.53	0.44
1:L1:74:A:OP1	11:LO:87:HIS:NE2	2.46	0.44
1:L1:209:G:OP1	5:LD:92:ARG:NH1	2.40	0.44
1:L1:1394:A:H2'	1:L1:1431:A:H62	1.83	0.44
33:Ln:117:LEU:HD23	39:Lt:73:LEU:HD22	1.99	0.44
34:Lo:91:LEU:HD23	34:Lo:91:LEU:HA	1.88	0.44
40:Lv:162:LEU:HD11	40:Lv:167:ALA:HA	2.00	0.44
46:L4:76:ASN:ND2	46:L4:82:GLN:H	2.14	0.44
57:SG:35:SER:N	83:S1:783:A:OP2	2.51	0.44
58:SI:379:ARG:HH11	58:SI:379:ARG:HG3	1.81	0.44
82:So:493:MET:HE2	82:So:493:MET:HB2	1.72	0.44
1:L1:1064:A:H2'	1:L1:1065:G:H8	1.82	0.44
30:Lk:142:ASP:OD1	30:Lk:144:ARG:NH2	2.51	0.44
33:Ln:99:ARG:CZ	33:Ln:102:PRO:HA	2.48	0.44
37:Lr:161:THR:O	37:Lr:192:GLN:NE2	2.51	0.44
41:Lw:64:GLU:OE1	41:Lw:64:GLU:N	2.45	0.44
46:L4:75:VAL:HG21	46:L4:84:VAL:HG12	2.00	0.44
46:L4:76:ASN:HB2	46:L4:83:ASP:HA	2.00	0.44
54:SZ:134:PHE:CD1	55:SE:143:GLY:HA3	2.53	0.44
55:SE:192:GLY:C	55:SE:194:SER:H	2.26	0.44
75:Se:132:THR:HA	75:Se:388:PRO:HD2	2.00	0.44
75:Se:327:GLU:OE1	75:Se:327:GLU:N	2.48	0.44
78:Sj:56:ALA:O	78:Sj:60:ARG:HG2	2.18	0.44
83:S1:625:A:N6	83:S1:673:G:O2'	2.49	0.44
1:L1:362:G:O2'	1:L1:1195:C:O2	2.28	0.43
14:LR:85:THR:HG23	14:LR:88:HIS:H	1.83	0.43
19:LW:36:PRO:HD3	52:Sf:270:LYS:HB3	2.00	0.43
22:Lb:226:LEU:HD12	23:Lu:155:LEU:HB3	2.00	0.43
30:Lk:60:PHE:HB3	30:Lk:67:VAL:HG12	2.00	0.43
36:Lq:27:GLN:OE1	36:Lq:28:ARG:NH2	2.51	0.43
40:Lv:178:LEU:HD11	40:Lv:184:LEU:HD22	1.99	0.43
52:Sf:89:MET:O	52:Sf:230:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SZ:70:SER:HA	54:SZ:110:LEU:O	2.18	0.43
54:SZ:77:ASP:HB3	59:SJ:138:THR:HG21	2.00	0.43
54:SZ:114:GLY:O	79:Sk:160:GLY:N	2.51	0.43
58:SI:393:TRP:NE1	58:SI:395:LYS:O	2.48	0.43
59:SJ:81:LYS:HD3	59:SJ:140:TYR:CD1	2.53	0.43
62:SN:29:TYR:HE2	62:SN:38:VAL:HG11	1.82	0.43
1:L1:424:G:O2'	1:L1:595:A:N3	2.48	0.43
1:L1:858:G:OP1	3:LB:135:ARG:NH2	2.49	0.43
5:LD:160:SER:HB2	43:Ly:80:LEU:HD22	2.01	0.43
5:LD:237:LEU:O	50:L8:25:TYR:N	2.50	0.43
12:LP:89:ILE:HB	12:LP:161:VAL:HG22	1.99	0.43
12:LP:90:LEU:HD13	12:LP:159:LEU:HD23	2.00	0.43
20:LX:133:ILE:HD11	20:LX:145:ARG:HB3	2.00	0.43
20:LX:170:TRP:CD1	34:Lo:77:LEU:HG	2.50	0.43
30:Lk:329:TYR:HD2	30:Lk:334:LYS:HZ1	1.64	0.43
35:Lp:37:SER:OG	35:Lp:39:LEU:O	2.32	0.43
54:SZ:106:ASP:OD1	54:SZ:106:ASP:N	2.52	0.43
58:SI:227:LYS:HE2	58:SI:227:LYS:HB3	1.83	0.43
82:So:168:ALA:O	82:So:172:MET:HG3	2.18	0.43
82:So:335:PHE:HA	82:So:338:ILE:HD12	2.00	0.43
83:S1:424:U:H2'	83:S1:425:G:C8	2.52	0.43
2:L2:2:A:N6	2:L2:68:G:O6	2.52	0.43
33:Ln:101:ARG:HH22	39:Lt:82:SER:C	2.22	0.43
49:L7:51:GLU:OE1	49:L7:51:GLU:N	2.51	0.43
79:Sk:253:TRP:HH2	79:Sk:261:ASN:HD22	1.66	0.43
82:So:552:ALA:HA	82:So:555:ILE:HD12	2.00	0.43
12:LP:104:MET:HE3	12:LP:104:MET:HB3	1.86	0.43
13:LQ:143:THR:HG22	32:Lm:135:PRO:HG2	2.00	0.43
18:LV:144:GLU:HG3	18:LV:177:LYS:HD3	2.01	0.43
19:LW:11:ARG:NH2	23:Lu:185:VAL:HG13	2.34	0.43
31:Ll:229:ASP:HB3	31:Ll:299:ARG:HH12	1.83	0.43
33:Ln:137:ARG:O	33:Ln:141:GLU:HG2	2.18	0.43
37:Lr:220:ILE:HA	37:Lr:223:MET:HG2	2.01	0.43
53:SB:259:ARG:HA	53:SB:262:GLU:CD	2.43	0.43
54:SZ:68:TRP:CD1	62:SN:121:SER:HA	2.53	0.43
59:SJ:74:LYS:O	59:SJ:176:GLN:HB2	2.18	0.43
62:SN:113:HIS:CE1	62:SN:117:HIS:HE1	2.37	0.43
63:SO:71:THR:HB	63:SO:95:LEU:HD12	2.00	0.43
66:SS:105:CYS:HB2	66:SS:142:VAL:HA	1.99	0.43
67:ST:124:TYR:HE2	68:SW:4:HIS:HB3	1.84	0.43
69:SX:350:GLN:HA	69:SX:353:LEU:HD12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Sb:52:GLU:O	72:Sb:56:LEU:HB2	2.19	0.43
1:L1:469:U:O4	24:Ld:77:ARG:NH1	2.46	0.43
3:LB:110:LEU:HD22	30:Lk:30:ALA:HB2	2.01	0.43
35:Lp:69:TYR:CD2	37:Lr:278:LYS:HG2	2.53	0.43
36:Lq:33:VAL:O	36:Lq:67:SER:HA	2.18	0.43
40:Lv:87:GLU:OE2	40:Lv:162:LEU:N	2.46	0.43
50:L8:111:GLU:OE1	50:L8:114:ARG:NH1	2.52	0.43
53:SB:142:ILE:HB	53:SB:164:GLU:HG3	1.99	0.43
54:SZ:156:GLN:HE21	79:Sk:78:PRO:HD2	1.83	0.43
55:SE:241:ILE:HG21	55:SE:264:ARG:HG3	1.99	0.43
63:SO:123:ARG:HD2	63:SO:123:ARG:HA	1.83	0.43
70:SY:52:ARG:NH1	70:SY:57:LYS:O	2.51	0.43
75:Se:166:ARG:NH2	83:S1:734:A:O2'	2.49	0.43
77:Si:71:TYR:HE2	77:Si:73:ASP:HB3	1.83	0.43
83:S1:191:U:H2'	83:S1:192:A:H8	1.83	0.43
83:S1:599:U:O2	83:S1:600:G:N1	2.51	0.43
83:S1:700:G:H2'	83:S1:701:G:C8	2.54	0.43
1:L1:1134:A:H2'	1:L1:1135:A:C8	2.54	0.43
16:LT:85:ALA:O	16:LT:89:ASN:ND2	2.36	0.43
19:LW:16:GLN:NE2	34:Lo:54:LYS:O	2.46	0.43
53:SB:177:THR:HG21	83:S1:633:C:H5'	2.00	0.43
69:SX:82:MET:HG3	69:SX:268:PHE:CE2	2.54	0.43
69:SX:276:VAL:HG22	69:SX:281:ILE:HG21	2.00	0.43
71:Sa:151:SER:OG	83:S1:37:U:O2'	2.29	0.43
75:Se:159:HIS:CD2	75:Se:267:ALA:HB2	2.54	0.43
1:L1:783:G:O2'	13:LQ:116:ASP:OD2	2.32	0.43
7:LJ:61:HIS:CE1	7:LJ:63:SER:HB2	2.54	0.43
11:LO:100:ARG:HH21	11:LO:126:GLY:HA2	1.84	0.43
31:Ll:195:PRO:HA	31:Ll:198:ALA:HB3	2.00	0.43
39:Lt:164:LYS:HG2	39:Lt:169:ASP:HB3	2.00	0.43
51:SR:90:SER:HA	51:SR:93:ILE:HG12	2.01	0.43
56:SF:21:THR:HA	56:SF:24:ARG:HE	1.83	0.43
58:SI:91:MET:HE1	79:Sk:66:TRP:CE2	2.53	0.43
69:SX:89:LYS:HD2	69:SX:264:SER:HB2	2.00	0.43
1:L1:743:C:C4	52:Sf:162:ARG:HD3	2.54	0.43
5:LD:218:LEU:HD23	5:LD:260:VAL:HB	2.01	0.43
9:LM:17:ILE:O	9:LM:55:ASP:HB3	2.18	0.43
39:Lt:255:VAL:HG23	39:Lt:259:GLU:HB2	2.01	0.43
41:Lw:144:THR:O	41:Lw:146:THR:N	2.51	0.43
41:Lw:154:ASP:N	41:Lw:154:ASP:OD1	2.51	0.43
42:Lx:71:GLU:HG2	42:Lx:86:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SZ:129:PRO:HA	54:SZ:132:TYR:HD1	1.83	0.43
72:Sb:82:VAL:HG11	83:S1:94:A:H5'	2.00	0.43
74:Sd:104:ILE:HG12	74:Sd:114:ILE:HG13	2.01	0.43
75:Se:72:PRO:HA	75:Se:75:LEU:HD12	2.00	0.43
75:Se:165:CYS:HB2	75:Se:274:LEU:HD11	2.00	0.43
79:Sk:169:ARG:HH12	79:Sk:210:ASP:C	2.27	0.43
1:L1:457:A:H4'	1:L1:581:A:C5	2.54	0.43
4:LC:99:LEU:HD13	4:LC:124:VAL:HG21	2.00	0.43
39:Lt:83:LEU:O	47:L5:49:ALA:HA	2.19	0.43
53:SB:85:PHE:HZ	74:Sd:87:SER:HB2	1.84	0.43
56:SF:65:LEU:HD21	67:ST:75:LYS:HE3	2.00	0.43
73:Sc:40:TRP:HE1	73:Sc:111:THR:HG22	1.82	0.43
76:Sg:315:ILE:HD11	79:Sk:157:VAL:HG22	2.01	0.43
1:L1:19:C:H42	22:Lb:14:LEU:HB3	1.84	0.43
3:LB:217:LEU:HD11	3:LB:227:GLN:HB2	2.00	0.43
7:LJ:118:LYS:HB2	7:LJ:118:LYS:HE2	1.66	0.43
22:Lb:221:LYS:HD2	22:Lb:221:LYS:HA	1.86	0.43
30:Lk:377:ASP:OD1	30:Lk:380:GLN:NE2	2.52	0.43
31:Ll:183:ASP:HA	49:L7:192:ARG:HH21	1.84	0.43
33:Ln:101:ARG:NE	39:Lt:79:ILE:O	2.52	0.43
38:Ls:261:MET:HE2	38:Ls:261:MET:HB3	1.85	0.43
52:Sf:316:CYS:HB3	52:Sf:319:GLN:HB2	2.01	0.43
71:Sa:42:GLU:CD	71:Sa:45:ARG:HH21	2.26	0.43
79:Sk:134:PRO:HB3	82:So:58:VAL:H	1.83	0.43
82:So:317:LEU:HD23	82:So:320:LEU:HD21	2.01	0.43
83:S1:775:G:H2'	83:S1:776:A:C8	2.54	0.43
1:L1:774:A:H5'	1:L1:775:U:C6	2.54	0.42
8:LK:48:GLN:HA	8:LK:51:LYS:HD2	2.00	0.42
15:LS:143:ARG:HA	15:LS:143:ARG:HD3	1.87	0.42
21:La:60:TYR:OH	21:La:94:GLU:OE1	2.36	0.42
23:Lu:198:ARG:NH1	27:Lh:70:LEU:O	2.43	0.42
33:Ln:97:LYS:HD2	33:Ln:97:LYS:O	2.19	0.42
36:Lq:76:VAL:HG13	36:Lq:84:VAL:HG13	2.01	0.42
38:Ls:160:LEU:HD22	38:Ls:169:PHE:CD2	2.54	0.42
50:L8:117:ARG:O	50:L8:121:ILE:HG12	2.19	0.42
54:SZ:42:VAL:HG21	54:SZ:51:VAL:HG21	2.00	0.42
57:SG:94:PHE:HE2	57:SG:205:LEU:HD11	1.83	0.42
67:ST:130:LEU:O	67:ST:131:LYS:HD2	2.19	0.42
69:SX:209:ILE:HA	69:SX:214:ASN:HD22	1.84	0.42
69:SX:293:LEU:HB3	69:SX:296:ASP:HB2	2.01	0.42
73:Sc:169:MET:HE1	73:Sc:247:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Sc:272:ASP:HA	73:Sc:346:LYS:HE2	2.01	0.42
78:Sj:163:SER:OG	78:Sj:191:LEU:O	2.37	0.42
82:So:157:LEU:HB2	82:So:172:MET:HE1	2.01	0.42
83:S1:477:A:H2'	83:S1:478:A:H2'	2.01	0.42
1:L1:629:U:H5''	1:L1:630:G:H5''	2.00	0.42
15:LS:106:LEU:O	15:LS:108:ILE:HG13	2.19	0.42
24:Ld:53:HIS:O	24:Ld:57:GLY:HA2	2.20	0.42
30:Lk:289:HIS:ND1	30:Lk:290:THR:OG1	2.49	0.42
32:Lm:228:GLU:HA	32:Lm:231:GLN:NE2	2.34	0.42
40:Lv:166:PHE:CD1	40:Lv:169:ILE:HD12	2.54	0.42
56:SF:54:HIS:NE2	56:SF:85:ASP:O	2.53	0.42
64:SP:110:LEU:HA	64:SP:113:LYS:HG2	2.01	0.42
67:ST:103:LYS:HA	67:ST:103:LYS:HD3	1.78	0.42
69:SX:282:ASP:N	69:SX:282:ASP:OD1	2.48	0.42
82:So:312:LYS:HD2	82:So:345:PHE:CZ	2.52	0.42
82:So:470:GLN:HE22	82:So:472:ASP:HB2	1.85	0.42
83:S1:823:A:H2'	83:S1:824:A:H8	1.84	0.42
1:L1:307:U:H2'	1:L1:308:A:H8	1.83	0.42
1:L1:542:C:H2'	1:L1:543:A:H8	1.84	0.42
1:L1:1445:U:H2'	1:L1:1446:C:C6	2.53	0.42
1:L1:1531:A:H2'	1:L1:1532:U:O4'	2.19	0.42
5:LD:62:VAL:HG23	5:LD:82:LEU:HB2	2.00	0.42
16:LT:50:PHE:HD2	17:LU:172:MET:HE2	1.85	0.42
20:LX:72:LYS:HG2	38:Ls:256:TYR:CE2	2.54	0.42
30:Lk:209:PHE:CZ	30:Lk:224:GLY:HA3	2.54	0.42
36:Lq:2:THR:HG22	36:Lq:5:GLY:H	1.83	0.42
38:Ls:246:VAL:HG12	38:Ls:264:LYS:HB3	2.01	0.42
49:L7:128:ASN:OD1	49:L7:129:ARG:N	2.52	0.42
50:L8:150:LYS:HA	50:L8:150:LYS:HD2	1.74	0.42
55:SE:142:PRO:HB2	55:SE:148:LEU:HD23	2.01	0.42
59:SJ:171:GLU:OE1	59:SJ:171:GLU:N	2.52	0.42
65:SQ:98:LYS:HZ3	65:SQ:109:PRO:HA	1.83	0.42
70:SY:87:LEU:HD12	70:SY:87:LEU:HA	1.84	0.42
80:Sm:39:GLU:HG2	80:Sm:87:ARG:HH21	1.84	0.42
82:So:71:LEU:HD23	82:So:74:LEU:HD12	2.00	0.42
1:L1:490:A:H2'	29:Lj:88:TRP:CE2	2.54	0.42
1:L1:704:A:N6	52:Sf:272:PRO:O	2.48	0.42
4:LC:157:LYS:HD3	4:LC:157:LYS:HA	1.77	0.42
7:LJ:52:GLU:OE2	12:LP:250:ARG:NH1	2.51	0.42
14:LR:127:ILE:HD13	14:LR:127:ILE:HA	1.92	0.42
15:LS:148:THR:HG22	15:LS:165:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Lb:6:TYR:CD2	22:Lb:14:LEU:HD11	2.55	0.42
23:Lu:132:LEU:HA	23:Lu:132:LEU:HD12	1.70	0.42
39:Lt:69:GLU:O	39:Lt:72:SER:OG	2.30	0.42
49:L7:110:TRP:CD1	49:L7:110:TRP:H	2.37	0.42
77:Si:31:MET:HE3	77:Si:31:MET:HB3	1.93	0.42
77:Si:46:LYS:HA	77:Si:49:TYR:CE2	2.54	0.42
83:S1:779:U:H2'	83:S1:780:A:C8	2.54	0.42
3:LB:255:ARG:HH12	3:LB:257:ILE:HD11	1.83	0.42
4:LC:199:ARG:HD3	4:LC:199:ARG:HA	1.69	0.42
7:LJ:161:VAL:HA	7:LJ:164:MET:SD	2.60	0.42
8:LK:58:LYS:HA	8:LK:58:LYS:HD3	1.75	0.42
18:LV:97:MET:HE1	18:LV:105:GLN:HG3	2.01	0.42
20:LX:177:THR:HG21	23:Lu:85:TRP:HZ2	1.85	0.42
30:Lk:181:VAL:O	30:Lk:185:ILE:HG12	2.20	0.42
39:Lt:123:MET:O	39:Lt:126:GLN:HG3	2.20	0.42
49:L7:179:ARG:HG2	49:L7:183:MET:HE3	2.01	0.42
55:SE:193:TRP:CE3	55:SE:199:GLY:HA3	2.54	0.42
58:SI:168:MET:HE3	58:SI:228:LEU:HD11	2.00	0.42
61:SL:44:ARG:HH12	83:S1:282:A:H4'	1.84	0.42
69:SX:214:ASN:O	69:SX:218:MET:HG2	2.19	0.42
72:Sb:41:ARG:NH2	83:S1:55:C:OP1	2.53	0.42
79:Sk:252:ILE:HG22	79:Sk:253:TRP:H	1.85	0.42
83:S1:823:A:H2'	83:S1:824:A:C8	2.54	0.42
1:L1:241:C:H2'	1:L1:242:A:H8	1.84	0.42
1:L1:1499:C:H2'	1:L1:1500:C:C6	2.54	0.42
4:LC:208:ALA:HB2	4:LC:297:VAL:HG12	2.00	0.42
19:LW:148:PRO:HG2	38:Ls:224:ILE:HD13	2.01	0.42
21:La:107:HIS:ND1	21:La:109:ARG:HG2	2.34	0.42
21:La:122:LYS:HA	31:Ll:51:TYR:CZ	2.54	0.42
31:Ll:260:ALA:O	31:Ll:263:SER:OG	2.36	0.42
39:Lt:178:TRP:NE1	39:Lt:182:GLU:O	2.43	0.42
40:Lv:120:LYS:HD2	40:Lv:160:SER:HB3	2.02	0.42
45:L3:5:LEU:HD12	45:L3:5:LEU:HA	1.91	0.42
49:L7:157:MET:HA	49:L7:160:GLU:HG2	2.00	0.42
52:Sf:73:ALA:O	52:Sf:79:LYS:NZ	2.50	0.42
52:Sf:143:ARG:HH21	52:Sf:415:ASP:HB3	1.84	0.42
53:SB:198:THR:O	53:SB:206:HIS:HB2	2.19	0.42
59:SJ:75:ARG:HH22	79:Sk:150:GLU:CD	2.28	0.42
59:SJ:76:LEU:HA	59:SJ:174:LYS:O	2.19	0.42
66:SS:210:GLU:OE2	66:SS:217:ARG:NH2	2.52	0.42
67:ST:94:ARG:HH12	83:S1:371:G:P	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SW:83:PRO:HA	74:Sd:108:VAL:HG21	2.02	0.42
75:Se:149:ASP:HA	75:Se:197:ARG:HH21	1.82	0.42
81:Sn:179:LYS:HD2	81:Sn:179:LYS:HA	1.79	0.42
1:L1:517:C:H2'	1:L1:518:A:C8	2.55	0.42
3:LB:257:ILE:HG23	3:LB:257:ILE:HD12	1.83	0.42
7:LJ:116:LEU:HB3	7:LJ:121:ILE:HB	2.02	0.42
24:Ld:134:MET:HE2	44:Lz:78:VAL:HG21	2.01	0.42
39:Lt:86:ASP:OD1	39:Lt:86:ASP:N	2.52	0.42
39:Lt:94:GLU:HA	39:Lt:97:ARG:HG2	2.01	0.42
52:Sf:415:ASP:N	52:Sf:415:ASP:OD1	2.53	0.42
54:SZ:79:GLU:CD	54:SZ:81:HIS:H	2.27	0.42
57:SG:111:MET:HE3	75:Se:397:TYR:OH	2.19	0.42
65:SQ:12:TRP:HE3	65:SQ:65:LEU:HD21	1.83	0.42
75:Se:127:TYR:CZ	75:Se:344:LEU:HB3	2.55	0.42
83:S1:327:U:O2'	83:S1:328:A:N7	2.44	0.42
1:L1:181:G:H2'	1:L1:1023:A:N7	2.34	0.42
1:L1:266:A:OP1	1:L1:267:A:N6	2.53	0.42
1:L1:712:A:H2'	1:L1:713:U:C6	2.55	0.42
8:LK:188:GLU:HA	8:LK:191:LYS:HD2	2.01	0.42
14:LR:38:VAL:HB	14:LR:41:GLU:HG3	2.01	0.42
23:Lu:101:LEU:HD22	34:Lo:70:LEU:HD13	2.02	0.42
26:Lg:43:LEU:O	26:Lg:55:LEU:HA	2.20	0.42
36:Lq:66:ASN:ND2	36:Lq:68:ARG:HD3	2.34	0.42
37:Lr:301:LEU:HD23	37:Lr:301:LEU:HA	1.90	0.42
39:Lt:65:PRO:HA	39:Lt:68:GLU:HG2	2.02	0.42
39:Lt:188:ALA:HB2	39:Lt:234:PHE:HD2	1.84	0.42
41:Lw:138:THR:HA	41:Lw:148:ARG:O	2.19	0.42
54:SZ:111:LYS:HE3	59:SJ:166:GLU:HG3	2.02	0.42
58:SI:161:LEU:O	58:SI:165:VAL:HG23	2.20	0.42
59:SJ:65:ILE:HD11	82:So:63:LYS:HE3	2.02	0.42
64:SP:15:GLY:HA2	64:SP:39:ASN:HD21	1.84	0.42
64:SP:100:HIS:HB3	64:SP:103:MET:HG3	2.02	0.42
68:SW:42:ARG:HH22	83:S1:368:A:H4'	1.84	0.42
69:SX:215:LEU:HD23	69:SX:215:LEU:HA	1.93	0.42
70:SY:103:TYR:CZ	70:SY:117:LEU:HG	2.55	0.42
75:Se:231:THR:HG22	75:Se:232:ARG:NH1	2.35	0.42
76:Sg:309:LYS:NZ	82:So:139:CYS:SG	2.70	0.42
78:Sj:95:TRP:CE2	78:Sj:131:ILE:HG23	2.54	0.42
2:L2:2:A:H2'	2:L2:3:G:C8	2.55	0.42
2:L2:62:C:H2'	2:L2:63:G:H8	1.84	0.42
3:LB:198:SER:HB3	3:LB:206:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LC:218:VAL:HG13	4:LC:258:PRO:HD3	2.02	0.42
17:LU:114:ILE:HD12	17:LU:116:ILE:HD11	2.01	0.42
24:Ld:53:HIS:CE1	24:Ld:60:PRO:HG3	2.54	0.42
30:Lk:219:LEU:HD12	30:Lk:219:LEU:HA	1.82	0.42
30:Lk:354:PHE:HB3	30:Lk:417:LEU:HD21	2.00	0.42
31:Ll:99:ARG:HA	31:Ll:99:ARG:HD2	1.85	0.42
52:Sf:66:TRP:O	52:Sf:69:THR:OG1	2.27	0.42
55:SE:225:VAL:HG22	55:SE:243:VAL:HG12	2.02	0.42
57:SG:180:ARG:O	57:SG:184:MET:HG3	2.19	0.42
58:SI:285:VAL:HA	58:SI:327:ASP:O	2.19	0.42
67:ST:111:ILE:HG12	67:ST:120:MET:HE1	2.02	0.42
69:SX:326:ASN:OD1	69:SX:326:ASN:N	2.52	0.42
75:Se:221:PRO:HG2	75:Se:224:GLU:HG3	2.01	0.42
82:So:497:LEU:HB3	82:So:534:LEU:HD12	2.01	0.42
83:S1:836:C:O2	83:S1:920:A:N6	2.49	0.42
1:L1:1078:A:H2'	1:L1:1079:A:C8	2.54	0.42
1:L1:1384:G:H2'	1:L1:1385:U:C6	2.55	0.42
10:LN:125:THR:HG22	10:LN:144:PHE:HB3	2.02	0.42
14:LR:105:SER:OG	14:LR:108:GLU:OE1	2.30	0.42
15:LS:76:LEU:HD12	15:LS:76:LEU:HA	1.75	0.42
15:LS:97:LYS:O	15:LS:101:GLU:HG2	2.20	0.42
15:LS:182:ARG:HD2	15:LS:218:ASN:HB3	2.02	0.42
39:Lt:52:CYS:HB3	39:Lt:235:LYS:HA	2.01	0.42
45:L3:21:CYS:O	45:L3:24:GLU:HG3	2.20	0.42
52:Sf:111:LYS:NZ	52:Sf:384:ASP:OD1	2.50	0.42
57:SG:120:ARG:HE	75:Se:89:MET:HE2	1.85	0.42
65:SQ:98:LYS:NZ	65:SQ:111:SER:OG	2.43	0.42
66:SS:227:GLU:HG3	66:SS:228:SER:H	1.84	0.42
69:SX:70:PHE:CZ	69:SX:128:MET:HE3	2.51	0.42
73:Sc:86:ASP:OD1	73:Sc:124:LYS:NZ	2.53	0.42
78:Sj:133:HIS:HB2	78:Sj:139:TRP:HZ2	1.84	0.42
79:Sk:75:PRO:HB2	79:Sk:106:LEU:HD12	2.01	0.42
83:S1:33:U:H2'	83:S1:34:U:H6	1.83	0.42
1:L1:815:U:H1'	1:L1:981:A:H2	1.85	0.41
4:LC:244:ALA:HB1	4:LC:248:ILE:HD11	2.01	0.41
4:LC:266:ARG:HE	4:LC:266:ARG:HB3	1.73	0.41
22:Lb:96:LYS:HB2	22:Lb:96:LYS:HE2	1.85	0.41
24:Ld:73:LYS:HB3	24:Ld:116:LEU:HA	2.02	0.41
48:L6:10:GLY:HA3	51:SR:167:PRO:HG3	2.01	0.41
54:SZ:65:ARG:HG3	58:SI:118:GLU:HG3	2.02	0.41
57:SG:69:LYS:HA	57:SG:72:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SI:328:VAL:HG21	58:SI:348:MET:HG3	2.02	0.41
59:SJ:99:ALA:HA	59:SJ:102:LEU:HD12	2.01	0.41
59:SJ:155:VAL:HG22	79:Sk:126:LEU:HD13	2.02	0.41
66:SS:150:LEU:O	66:SS:154:ILE:HG12	2.20	0.41
67:ST:94:ARG:NH1	83:S1:371:G:P	2.93	0.41
72:Sb:30:ARG:NH2	83:S1:64:U:O2	2.49	0.41
75:Se:69:ASN:HA	75:Se:97:ALA:O	2.20	0.41
82:So:248:PHE:HB2	82:So:262:MET:HE3	2.02	0.41
82:So:302:VAL:O	82:So:312:LYS:NZ	2.40	0.41
1:L1:1203:A:H4'	21:La:90:TYR:CZ	2.55	0.41
6:LI:78:ARG:NH1	22:Lb:87:LEU:O	2.52	0.41
16:LT:141:ILE:HG22	35:Lp:51:LEU:HD12	2.01	0.41
32:Lm:165:ASN:HB2	32:Lm:184:VAL:HB	2.03	0.41
38:Ls:216:MET:HB2	38:Ls:244:GLU:HG2	2.01	0.41
42:Lx:93:ASP:OD1	42:Lx:96:LEU:HB2	2.20	0.41
54:SZ:64:HIS:HA	58:SI:117:PHE:HB2	2.02	0.41
66:SS:67:ARG:HD2	66:SS:68:TYR:CE2	2.54	0.41
82:So:619:LYS:HG3	82:So:648:ARG:NH2	2.35	0.41
83:S1:323:A:H2'	83:S1:324:A:C8	2.55	0.41
1:L1:599:G:N7	11:LO:45:ARG:NH2	2.69	0.41
1:L1:1394:A:H2'	1:L1:1431:A:N6	2.35	0.41
3:LB:138:ASP:OD1	3:LB:249:ASN:ND2	2.52	0.41
5:LD:110:SER:O	5:LD:158:PRO:HA	2.20	0.41
9:LM:59:ILE:HB	9:LM:127:LEU:HD23	2.02	0.41
14:LR:79:ARG:NH2	14:LR:94:GLU:OE1	2.50	0.41
20:LX:57:PHE:HD1	20:LX:145:ARG:NH2	2.18	0.41
30:Lk:104:CYS:HA	30:Lk:219:LEU:HB3	2.01	0.41
31:Ll:53:SER:HB3	31:Ll:56:ARG:HB2	2.01	0.41
31:Ll:139:TRP:O	31:Ll:144:GLY:N	2.46	0.41
31:Ll:229:ASP:HB2	31:Ll:299:ARG:HH22	1.86	0.41
34:Lo:90:GLN:O	34:Lo:94:GLU:HG2	2.20	0.41
42:Lx:87:GLN:CB	42:Lx:124:ARG:HH21	2.33	0.41
55:SE:220:THR:HG22	55:SE:247:VAL:HG22	2.02	0.41
55:SE:282:ILE:HD12	55:SE:353:LEU:HB3	2.02	0.41
56:SF:38:ASP:OD1	56:SF:39:LEU:N	2.53	0.41
59:SJ:158:GLU:O	59:SJ:162:ARG:HG3	2.20	0.41
61:SL:78:ARG:NH2	83:S1:247:C:H41	2.18	0.41
64:SP:67:ALA:HB2	69:SX:196:TYR:CZ	2.55	0.41
67:ST:94:ARG:NH1	83:S1:371:G:OP2	2.53	0.41
69:SX:275:PHE:O	69:SX:278:ASN:O	2.39	0.41
70:SY:88:PHE:HD2	74:Sd:103:ARG:HH22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Se:357:ILE:HG21	75:Se:377:LYS:HG2	2.02	0.41
76:Sg:366:VAL:HG13	76:Sg:367:LYS:HD3	2.01	0.41
78:Sj:202:ASP:OD1	78:Sj:202:ASP:N	2.52	0.41
1:L1:1280:U:H2'	1:L1:1281:A:C8	2.55	0.41
6:LI:100:GLN:NE2	6:LI:128:LEU:HG	2.36	0.41
22:Lb:8:VAL:O	22:Lb:11:TRP:HB2	2.21	0.41
23:Lu:186:ILE:HD12	23:Lu:190:LEU:HB2	2.03	0.41
36:Lq:41:ARG:O	36:Lq:45:GLU:HG2	2.20	0.41
38:Ls:267:PRO:HG2	38:Ls:270:ALA:HB2	2.01	0.41
58:SI:86:ARG:HH12	58:SI:97:GLU:HA	1.85	0.41
67:ST:67:LEU:HD21	67:ST:79:LEU:HD11	2.01	0.41
73:Sc:116:CYS:O	73:Sc:121:ALA:N	2.47	0.41
75:Se:102:ARG:HD2	87:Se:500:GDP:HN21	1.84	0.41
82:So:646:THR:HB	82:So:650:MET:HE1	2.02	0.41
83:S1:614:C:H2'	83:S1:615:C:H6	1.85	0.41
1:L1:567:A:OP1	51:SR:171:ARG:NH2	2.36	0.41
4:LC:144:THR:HB	4:LC:178:ILE:HG23	2.02	0.41
6:LI:92:GLU:OE1	6:LI:92:GLU:N	2.53	0.41
11:LO:149:THR:O	11:LO:149:THR:OG1	2.36	0.41
29:Lj:87:ARG:HH21	29:Lj:101:ARG:HD3	1.85	0.41
30:Lk:144:ARG:NH1	30:Lk:144:ARG:HB2	2.35	0.41
40:Lv:64:LYS:HE2	40:Lv:64:LYS:HB2	1.90	0.41
66:SS:181:HIS:HB3	66:SS:184:VAL:HG12	2.01	0.41
71:Sa:65:MET:HE3	71:Sa:65:MET:HB2	1.90	0.41
73:Sc:193:LYS:HA	73:Sc:193:LYS:HD2	1.84	0.41
73:Sc:209:LEU:HA	73:Sc:209:LEU:HD12	1.67	0.41
75:Se:121:ALA:HA	75:Se:304:GLY:O	2.20	0.41
78:Sj:31:SER:HB3	78:Sj:106:ALA:HB2	2.01	0.41
78:Sj:78:ARG:HH21	78:Sj:143:PRO:HA	1.85	0.41
79:Sk:120:LYS:HA	79:Sk:120:LYS:HD2	1.72	0.41
83:S1:501:A:H2'	83:S1:502:G:C8	2.55	0.41
83:S1:791:A:H2'	83:S1:792:A:H8	1.84	0.41
83:S1:940:U:H2'	83:S1:941:G:H8	1.85	0.41
1:L1:437:G:OP1	12:LP:144:LYS:HE3	2.20	0.41
3:LB:260:ALA:O	3:LB:264:ARG:HG2	2.20	0.41
4:LC:96:ARG:NH2	4:LC:197:HIS:O	2.49	0.41
4:LC:128:HIS:HA	4:LC:191:THR:O	2.21	0.41
5:LD:99:VAL:HG21	5:LD:173:GLY:HA3	2.02	0.41
5:LD:275:TRP:O	5:LD:279:ARG:HB2	2.21	0.41
5:LD:277:ASP:O	41:Lw:90:ARG:NH1	2.53	0.41
8:LK:175:LEU:HD23	8:LK:175:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LM:74:GLN:HA	51:SR:161:PRO:HA	2.03	0.41
17:LU:107:LYS:HD3	18:LV:212:LEU:HD11	2.02	0.41
22:Lb:221:LYS:NZ	22:Lb:222:ASP:O	2.54	0.41
30:Lk:139:LEU:HD11	30:Lk:423:ALA:HB3	2.02	0.41
33:Ln:178:TYR:HD2	33:Ln:179:THR:HG23	1.84	0.41
60:SK:78:LYS:HE2	60:SK:82:GLU:HG3	2.03	0.41
70:SY:71:ARG:HG2	70:SY:96:CYS:SG	2.61	0.41
73:Sc:213:LEU:HA	73:Sc:224:GLN:HE21	1.85	0.41
78:Sj:57:ASP:HA	78:Sj:61:GLU:OE1	2.20	0.41
79:Sk:118:ALA:O	79:Sk:122:HIS:HB3	2.20	0.41
1:L1:191:U:H2'	1:L1:192:U:C6	2.56	0.41
1:L1:488:U:OP2	51:SR:195:TYR:OH	2.30	0.41
3:LB:130:ARG:NH1	3:LB:131:TYR:O	2.54	0.41
4:LC:80:LEU:HD11	4:LC:320:PHE:HB3	2.03	0.41
5:LD:200:PRO:HB3	5:LD:237:LEU:HG	2.03	0.41
11:LO:236:LEU:HD12	11:LO:236:LEU:HA	1.86	0.41
14:LR:40:ASN:ND2	31:Ll:337:MET:HE3	2.35	0.41
33:Ln:177:HIS:CE1	47:L5:64:ILE:HG23	2.56	0.41
36:Lq:75:VAL:O	36:Lq:86:GLU:CA	2.53	0.41
57:SG:140:ASN:O	57:SG:144:ILE:HG12	2.20	0.41
58:SI:127:HIS:CE1	58:SI:130:GLN:HG3	2.56	0.41
67:ST:140:TYR:OH	68:SW:33:ASP:OD1	2.22	0.41
71:Sa:155:LEU:HD12	71:Sa:156:PRO:HD2	2.01	0.41
80:Sm:110:ARG:HE	80:Sm:110:ARG:HB3	1.74	0.41
83:S1:226:G:H1'	83:S1:274:U:H1'	2.03	0.41
83:S1:485:U:H2'	83:S1:486:C:H6	1.85	0.41
83:S1:534:G:H2'	83:S1:535:C:C6	2.56	0.41
83:S1:541:A:N6	83:S1:547:C:O2	2.54	0.41
1:L1:142:C:O4'	37:Lr:52:ARG:NH1	2.54	0.41
1:L1:795:U:H2'	1:L1:796:A:C8	2.56	0.41
7:LJ:143:LEU:HD22	7:LJ:146:LEU:HD22	2.02	0.41
8:LK:20:ILE:HD11	8:LK:42:ARG:HG2	2.03	0.41
8:LK:130:PHE:O	8:LK:133:GLN:O	2.39	0.41
19:LW:9:LEU:N	23:Lu:183:GLN:OE1	2.52	0.41
33:Ln:87:ASP:OD2	40:Lv:129:THR:HG21	2.19	0.41
37:Lr:87:LEU:HA	37:Lr:90:THR:HG22	2.01	0.41
44:Lz:46:LEU:HD23	44:Lz:46:LEU:HA	1.91	0.41
46:L4:87:LYS:HB3	46:L4:91:GLU:OE2	2.21	0.41
52:Sf:242:ARG:HG2	52:Sf:335:TRP:HZ2	1.86	0.41
53:SB:94:LYS:N	74:Sd:148:GLU:OE1	2.54	0.41
55:SE:376:GLU:HA	69:SX:96:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SE:394:ASP:N	55:SE:394:ASP:OD1	2.54	0.41
59:SJ:69:PRO:HA	82:So:61:LYS:HA	2.01	0.41
64:SP:37:ALA:HB1	64:SP:41:CYS:SG	2.61	0.41
67:ST:63:LYS:HE3	67:ST:63:LYS:HB3	1.87	0.41
69:SX:81:LYS:HE2	69:SX:81:LYS:HB3	1.83	0.41
69:SX:140:ASP:HB2	69:SX:183:LYS:HD3	2.03	0.41
73:Sc:240:LEU:HD21	73:Sc:253:PRO:HB3	2.02	0.41
80:Sm:59:ASN:O	80:Sm:62:ARG:HG2	2.20	0.41
83:S1:50:G:N2	83:S1:204:A:N6	2.68	0.41
1:L1:36:C:H1'	19:LW:9:LEU:HD11	2.02	0.41
1:L1:231:C:OP1	11:LO:37:GLU:HG3	2.21	0.41
1:L1:484:A:O2'	1:L1:485:A:H5'	2.21	0.41
1:L1:842:A:O2'	1:L1:871:C:OP1	2.30	0.41
1:L1:859:U:C6	3:LB:208:ARG:NH2	2.89	0.41
1:L1:1024:A:C6	1:L1:1315:C:H1'	2.56	0.41
1:L1:1540:C:H2'	1:L1:1541:C:O4'	2.21	0.41
5:LD:91:PRO:HB3	11:LO:16:LEU:HD11	2.02	0.41
6:LI:94:LEU:HD12	6:LI:94:LEU:HA	1.94	0.41
8:LK:66:LEU:HD23	8:LK:66:LEU:HA	1.95	0.41
10:LN:94:PRO:O	10:LN:97:THR:OG1	2.33	0.41
11:LO:14:ASP:OD1	11:LO:17:ARG:NH2	2.54	0.41
11:LO:268:GLY:HA3	41:Lw:47:PHE:CG	2.56	0.41
13:LQ:53:ARG:O	13:LQ:57:GLU:HG2	2.20	0.41
20:LX:52:GLU:O	20:LX:143:ARG:NH2	2.50	0.41
23:Lu:134:LYS:NZ	34:Lo:76:TYR:OH	2.54	0.41
28:Li:110:VAL:HG13	28:Li:158:LEU:HD22	2.03	0.41
31:Ll:240:ILE:HD13	31:Ll:248:GLY:HA3	2.02	0.41
33:Ln:99:ARG:NH2	33:Ln:102:PRO:HA	2.36	0.41
34:Lo:65:LEU:HD23	34:Lo:65:LEU:HA	1.92	0.41
38:Ls:86:ASP:HB3	38:Ls:198:ARG:HG2	2.03	0.41
41:Lw:45:TYR:HD2	41:Lw:49:GLU:OE2	2.04	0.41
41:Lw:94:ILE:HA	41:Lw:95:PRO:HD3	1.87	0.41
45:L3:10:LEU:HD22	45:L3:42:VAL:HB	2.03	0.41
51:SR:79:HIS:HB3	51:SR:184:ASN:HA	2.03	0.41
51:SR:161:PRO:HG2	51:SR:163:TYR:CE2	2.55	0.41
52:Sf:51:MET:HG2	52:Sf:61:ARG:HE	1.85	0.41
52:Sf:105:TRP:HZ3	52:Sf:268:PRO:HA	1.85	0.41
55:SE:377:CYS:SG	55:SE:378:GLY:N	2.93	0.41
56:SF:96:HIS:HA	56:SF:97:PRO:HD3	1.96	0.41
72:Sb:28:LYS:HE2	83:S1:52:A:C8	2.56	0.41
75:Se:89:MET:HA	75:Se:92:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Sg:354:VAL:HG22	77:Si:37:PHE:CE2	2.56	0.41
82:So:482:ILE:HA	82:So:483:PRO:HA	1.88	0.41
82:So:532:LEU:HD23	82:So:532:LEU:HA	1.93	0.41
82:So:619:LYS:HG3	82:So:648:ARG:HH21	1.86	0.41
83:S1:200:G:H2'	83:S1:201:U:C6	2.56	0.41
1:L1:605:U:H2'	1:L1:606:C:C6	2.56	0.41
5:LD:218:LEU:HD12	5:LD:234:THR:HG21	2.02	0.41
7:LJ:162:LYS:HA	7:LJ:162:LYS:HD2	1.78	0.41
11:LO:12:ALA:HB2	48:L6:88:ILE:HD12	2.03	0.41
11:LO:154:ILE:HG23	11:LO:174:VAL:HG23	2.03	0.41
13:LQ:97:TYR:OH	13:LQ:126:LYS:O	2.27	0.41
14:LR:132:ALA:O	14:LR:136:LEU:HG	2.21	0.41
19:LW:137:ARG:NH1	20:LX:106:GLY:O	2.54	0.41
31:Ll:179:VAL:HG13	31:Ll:183:ASP:OD2	2.21	0.41
39:Lt:162:ARG:HB3	39:Lt:251:HIS:HB2	2.03	0.41
52:Sf:191:HIS:O	52:Sf:428:ARG:NH2	2.49	0.41
55:SE:285:TYR:OH	55:SE:372:GLU:OE1	2.39	0.41
58:SI:267:MET:HE2	58:SI:286:TYR:HB3	2.03	0.41
60:SK:181:ILE:HD11	68:SW:39:ILE:HD11	2.03	0.41
63:SO:173:THR:HG22	65:SQ:101:ALA:HB1	2.03	0.41
64:SP:59:ASN:H	64:SP:62:GLY:HA2	1.84	0.41
64:SP:114:ARG:HA	64:SP:117:GLU:HG3	2.03	0.41
75:Se:206:GLU:HB2	75:Se:208:TYR:CZ	2.55	0.41
75:Se:253:LEU:HD12	75:Se:255:MET:HE1	2.03	0.41
1:L1:9:U:H2'	1:L1:10:A:C8	2.56	0.40
1:L1:431:C:H2'	1:L1:432:A:C8	2.56	0.40
1:L1:1015:U:O2'	1:L1:1434:U:H5'	2.21	0.40
1:L1:1182:C:H5	26:Lg:32:THR:HG21	1.85	0.40
1:L1:1521:A:H4'	51:SR:123:HIS:HB3	2.03	0.40
85:L1:1707:T1C:H953	85:L1:1707:T1C:H921	1.88	0.40
14:LR:114:HIS:CE1	31:Ll:131:PRO:HG2	2.56	0.40
23:Lu:173:PHE:CZ	27:Lh:70:LEU:HD21	2.56	0.40
39:Lt:191:THR:O	39:Lt:195:LEU:HG	2.21	0.40
52:Sf:165:ARG:HD3	52:Sf:307:ARG:HH12	1.86	0.40
55:SE:141:TRP:CH2	82:So:116:VAL:HA	2.55	0.40
59:SJ:161:GLN:HB2	76:Sg:313:PHE:HZ	1.86	0.40
61:SL:32:THR:O	61:SL:36:MET:HG3	2.21	0.40
63:SO:126:GLU:HG2	63:SO:177:VAL:HG21	2.02	0.40
63:SO:132:LEU:HD12	63:SO:166:MET:CE	2.51	0.40
67:ST:96:ILE:HG22	67:ST:136:CYS:HB3	2.03	0.40
75:Se:158:ALA:HA	75:Se:161:TRP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Se:203:LYS:O	75:Se:250:GLN:NE2	2.54	0.40
80:Sm:104:LEU:HD23	80:Sm:104:LEU:HA	1.84	0.40
82:So:331:ASN:HA	82:So:365:ILE:HD13	2.03	0.40
83:S1:261:C:H2'	83:S1:262:G:C8	2.56	0.40
1:L1:384:U:C5	48:L6:75:LYS:HG2	2.56	0.40
1:L1:411:U:H2'	1:L1:412:G:C8	2.57	0.40
1:L1:739:A:O2'	30:Lk:270:ILE:O	2.39	0.40
1:L1:1330:A:H2'	1:L1:1331:G:C8	2.56	0.40
2:L2:26:C:H2'	2:L2:27:C:H6	1.86	0.40
6:LI:139:LEU:O	6:LI:142:GLU:HG3	2.21	0.40
13:LQ:52:MET:HE3	13:LQ:52:MET:HB3	1.77	0.40
15:LS:194:LEU:HB2	15:LS:197:TYR:HD2	1.87	0.40
20:LX:80:ILE:HG23	20:LX:82:GLN:NE2	2.37	0.40
22:Lb:235:ILE:HD13	22:Lb:235:ILE:HA	1.98	0.40
30:Lk:384:GLN:N	30:Lk:404:VAL:O	2.54	0.40
33:Ln:164:ARG:H	40:Lv:86:TYR:HD2	1.69	0.40
45:L3:14:LYS:NZ	45:L3:68:PHE:O	2.53	0.40
56:SF:37:ARG:NH2	72:Sb:163:GLU:OE2	2.54	0.40
64:SP:71:ASP:OD1	64:SP:72:ARG:N	2.53	0.40
65:SQ:78:LYS:HB2	65:SQ:78:LYS:HE3	1.78	0.40
69:SX:67:LYS:HD3	69:SX:68:PRO:HD2	2.03	0.40
69:SX:194:GLN:HE22	69:SX:199:LYS:H	1.69	0.40
70:SY:33:ASP:OD1	70:SY:34:VAL:N	2.54	0.40
78:Sj:175:ILE:O	78:Sj:178:ARG:HG2	2.21	0.40
80:Sm:52:MET:HE2	80:Sm:56:TRP:CZ2	2.56	0.40
82:So:346:HIS:HB3	82:So:347:VAL:H	1.62	0.40
82:So:372:TYR:HA	82:So:375:ILE:HG12	2.04	0.40
82:So:596:LEU:HD23	82:So:599:PHE:CD2	2.56	0.40
83:S1:186:A:H2'	83:S1:187:G:C8	2.56	0.40
83:S1:191:U:H2'	83:S1:192:A:C8	2.56	0.40
83:S1:726:U:H2'	83:S1:727:A:C8	2.56	0.40
83:S1:817:G:H21	83:S1:819:C:N4	2.18	0.40
1:L1:575:A:H2'	51:SR:189:ARG:HE	1.85	0.40
1:L1:1338:C:O2'	1:L1:1381:A:N3	2.44	0.40
7:LJ:133:PRO:HA	7:LJ:136:GLU:CD	2.46	0.40
11:LO:184:LEU:HA	11:LO:187:VAL:HG12	2.02	0.40
20:LX:209:LYS:HA	20:LX:209:LYS:HD3	1.83	0.40
30:Lk:73:PRO:HG2	30:Lk:75:PHE:CZ	2.55	0.40
37:Lr:191:LEU:HD12	37:Lr:191:LEU:HA	1.89	0.40
39:Lt:70:MET:HA	39:Lt:73:LEU:HB3	2.04	0.40
39:Lt:160:LEU:HG	39:Lt:171:TRP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:L7:138:GLU:OE1	49:L7:138:GLU:N	2.54	0.40
52:Sf:341:MET:HE2	52:Sf:341:MET:HB3	1.97	0.40
58:SI:127:HIS:ND1	58:SI:129:GLU:HB3	2.35	0.40
58:SI:254:LYS:HE3	58:SI:254:LYS:HB2	1.85	0.40
62:SN:52:LEU:HD12	77:Si:41:PRO:HB3	2.03	0.40
64:SP:18:THR:HG22	64:SP:20:ARG:HB3	2.03	0.40
64:SP:64:LYS:HB2	69:SX:155:LYS:O	2.20	0.40
69:SX:353:LEU:O	69:SX:357:SER:HB3	2.22	0.40
70:SY:66:HIS:HA	70:SY:69:ARG:HG3	2.02	0.40
72:Sb:126:GLN:HA	72:Sb:129:ARG:HG2	2.04	0.40
72:Sb:141:ARG:O	72:Sb:145:GLU:HG3	2.21	0.40
73:Sc:228:TYR:CE2	73:Sc:262:VAL:HG21	2.51	0.40
79:Sk:184:ASP:O	79:Sk:187:LYS:HG2	2.22	0.40
82:So:81:ASP:HB3	82:So:84:ALA:HB3	2.03	0.40
82:So:497:LEU:HD11	82:So:527:LEU:HD12	2.04	0.40
82:So:536:ALA:HB2	82:So:582:LEU:HG	2.03	0.40
83:S1:25:A:H2'	83:S1:26:U:C6	2.56	0.40
83:S1:34:U:H2'	83:S1:35:A:H8	1.85	0.40
11:LO:104:LEU:HD11	11:LO:126:GLY:HA3	2.03	0.40
16:LT:17:ARG:O	16:LT:21:ILE:HG12	2.21	0.40
19:LW:144:ARG:HA	19:LW:144:ARG:HD2	1.80	0.40
20:LX:177:THR:HG23	34:Lo:73:TYR:O	2.21	0.40
22:Lb:83:GLU:HG2	22:Lb:107:PRO:HB3	2.03	0.40
23:Lu:112:LEU:O	23:Lu:116:GLU:HG3	2.20	0.40
32:Lm:204:LYS:HB2	35:Lp:95:ARG:HH12	1.86	0.40
37:Lr:100:SER:O	37:Lr:104:LYS:HG2	2.21	0.40
39:Lt:120:LEU:HB3	39:Lt:124:TRP:CH2	2.57	0.40
45:L3:76:MET:HE1	45:L3:90:PHE:HB2	2.03	0.40
52:Sf:119:PRO:HG3	52:Sf:394:TRP:CD2	2.57	0.40
57:SG:185:LYS:HA	57:SG:185:LYS:HD2	1.95	0.40
63:SO:86:ASP:OD1	63:SO:87:ASP:N	2.54	0.40
64:SP:51:LEU:HD21	64:SP:76:TRP:CD1	2.56	0.40
68:SW:67:GLU:OE1	68:SW:70:ARG:NH2	2.42	0.40
73:Sc:315:GLU:OE2	78:Sj:60:ARG:NH2	2.53	0.40
75:Se:82:GLY:HA2	75:Se:156:PRO:HB3	2.03	0.40
83:S1:33:U:H2'	83:S1:34:U:C6	2.57	0.40
83:S1:262:G:H2'	83:S1:263:A:H8	1.86	0.40
1:L1:197:A:N1	1:L1:349:G:O2'	2.53	0.40
1:L1:1058:C:H2'	1:L1:1059:U:C6	2.55	0.40
4:LC:96:ARG:H	4:LC:96:ARG:HG2	1.77	0.40
8:LK:118:TYR:HE2	46:L4:93:PRO:HG2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LX:48:PRO:HD3	23:Lu:234:LEU:HD21	2.03	0.40
26:Lg:20:MET:HE3	26:Lg:20:MET:HB3	1.94	0.40
36:Lq:133:PHE:CG	37:Lr:259:ARG:HD2	2.56	0.40
38:Ls:213:THR:HG22	38:Ls:247:VAL:HG13	2.04	0.40
41:Lw:96:VAL:HG22	41:Lw:110:ILE:HG12	2.03	0.40
52:Sf:373:GLN:NE2	52:Sf:375:ASN:OD1	2.53	0.40
55:SE:305:MET:HA	55:SE:333:TYR:O	2.21	0.40
58:SI:169:LEU:HD23	58:SI:169:LEU:HA	1.91	0.40
63:SO:132:LEU:HD23	63:SO:132:LEU:HA	1.82	0.40
69:SX:208:ILE:O	69:SX:214:ASN:ND2	2.54	0.40
73:Sc:96:ARG:HH12	78:Sj:74:PHE:HE1	1.68	0.40
73:Sc:256:LEU:HD11	73:Sc:287:LEU:HD13	2.04	0.40
73:Sc:306:ASP:OD1	73:Sc:306:ASP:N	2.54	0.40
83:S1:162:G:H2'	83:S1:163:G:C8	2.57	0.40
83:S1:275:C:H2'	83:S1:276:A:N7	2.36	0.40
83:S1:473:C:H3'	83:S1:636:A:H61	1.87	0.40
83:S1:791:A:H2'	83:S1:792:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	6 (3%)	1 (0%)	30	62
4	LC	302/348 (87%)	283 (94%)	19 (6%)	0	100	100
5	LD	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
6	LI	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
7	LJ	154/261 (59%)	139 (90%)	15 (10%)	0	100	100
8	LK	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
9	LM	175/178 (98%)	162 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LN	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
11	LO	285/296 (96%)	274 (96%)	11 (4%)	0	100	100
12	LP	219/251 (87%)	214 (98%)	5 (2%)	0	100	100
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	18	52
14	LR	144/179 (80%)	143 (99%)	1 (1%)	0	100	100
15	LS	217/292 (74%)	205 (94%)	12 (6%)	0	100	100
16	LT	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	LU	158/205 (77%)	151 (96%)	7 (4%)	0	100	100
18	LV	164/212 (77%)	153 (93%)	11 (7%)	0	100	100
19	LW	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
20	LX	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
21	La	109/148 (74%)	107 (98%)	2 (2%)	0	100	100
22	Lb	241/256 (94%)	232 (96%)	9 (4%)	0	100	100
23	Lu	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
24	Ld	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
25	Lf	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
26	Lg	50/65 (77%)	50 (100%)	0	0	100	100
27	Lh	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	Li	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	Lj	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
30	Lk	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
31	Ll	352/380 (93%)	327 (93%)	25 (7%)	0	100	100
32	Lm	291/338 (86%)	279 (96%)	12 (4%)	0	100	100
33	Ln	97/206 (47%)	85 (88%)	12 (12%)	0	100	100
34	Lo	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
35	Lp	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
36	Lq	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
37	Lr	271/332 (82%)	265 (98%)	6 (2%)	0	100	100
38	Ls	210/306 (69%)	200 (95%)	10 (5%)	0	100	100
39	Lt	211/279 (76%)	187 (89%)	23 (11%)	1 (0%)	24	59
40	Lv	125/212 (59%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Lw	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
42	Lx	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
43	Ly	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
44	Lz	90/123 (73%)	86 (96%)	4 (4%)	0	100	100
45	L3	94/112 (84%)	85 (90%)	9 (10%)	0	100	100
46	L4	81/138 (59%)	75 (93%)	6 (7%)	0	100	100
47	L5	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
48	L6	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	L7	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
50	L8	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
51	SR	140/196 (71%)	139 (99%)	1 (1%)	0	100	100
52	Sf	366/439 (83%)	351 (96%)	13 (4%)	2 (0%)	24	59
53	SB	215/296 (73%)	204 (95%)	11 (5%)	0	100	100
54	SZ	130/167 (78%)	117 (90%)	13 (10%)	0	100	100
55	SE	314/430 (73%)	295 (94%)	19 (6%)	0	100	100
56	SF	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
57	SG	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
58	SI	300/396 (76%)	271 (90%)	29 (10%)	0	100	100
59	SJ	120/201 (60%)	103 (86%)	17 (14%)	0	100	100
60	SK	134/194 (69%)	123 (92%)	11 (8%)	0	100	100
61	SL	106/138 (77%)	96 (91%)	8 (8%)	2 (2%)	6	33
62	SN	99/128 (77%)	89 (90%)	10 (10%)	0	100	100
63	SO	162/257 (63%)	156 (96%)	6 (4%)	0	100	100
64	SP	114/137 (83%)	107 (94%)	7 (6%)	0	100	100
65	SQ	105/130 (81%)	95 (90%)	10 (10%)	0	100	100
66	SS	183/258 (71%)	167 (91%)	16 (9%)	0	100	100
67	ST	94/142 (66%)	88 (94%)	6 (6%)	0	100	100
68	SW	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
69	SX	293/360 (81%)	282 (96%)	11 (4%)	0	100	100
70	SY	124/190 (65%)	119 (96%)	5 (4%)	0	100	100
71	Sa	160/173 (92%)	150 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Sb	171/205 (83%)	167 (98%)	3 (2%)	1 (1%)	21	56
73	Sc	383/414 (92%)	374 (98%)	9 (2%)	0	100	100
74	Sd	95/187 (51%)	87 (92%)	8 (8%)	0	100	100
75	Se	348/398 (87%)	332 (95%)	16 (5%)	0	100	100
76	Sg	106/395 (27%)	98 (92%)	8 (8%)	0	100	100
77	Si	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
78	Sj	197/218 (90%)	171 (87%)	26 (13%)	0	100	100
79	Sk	252/323 (78%)	226 (90%)	26 (10%)	0	100	100
80	Sm	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
81	Sn	67/199 (34%)	65 (97%)	2 (3%)	0	100	100
82	So	614/689 (89%)	595 (97%)	19 (3%)	0	100	100
All	All	13557/17977 (75%)	12863 (95%)	686 (5%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Lt	266	PRO
61	SL	117	ASP
52	Sf	250	PHE
61	SL	72	LYS
52	Sf	260	GLU
13	LQ	111	PRO
72	Sb	50	PRO
3	LB	207	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	LB	191/245 (78%)	191 (100%)	0	100	100
4	LC	258/290 (89%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LD	217/262 (83%)	217 (100%)	0	100	100
6	LI	86/228 (38%)	86 (100%)	0	100	100
7	LJ	145/232 (62%)	145 (100%)	0	100	100
8	LK	137/150 (91%)	137 (100%)	0	100	100
9	LM	155/156 (99%)	155 (100%)	0	100	100
10	LN	98/124 (79%)	98 (100%)	0	100	100
11	LO	245/249 (98%)	245 (100%)	0	100	100
12	LP	188/211 (89%)	188 (100%)	0	100	100
13	LQ	133/150 (89%)	133 (100%)	0	100	100
14	LR	128/154 (83%)	128 (100%)	0	100	100
15	LS	201/256 (78%)	201 (100%)	0	100	100
16	LT	118/126 (94%)	118 (100%)	0	100	100
17	LU	145/180 (81%)	145 (100%)	0	100	100
18	LV	146/182 (80%)	146 (100%)	0	100	100
19	LW	128/135 (95%)	128 (100%)	0	100	100
20	LX	180/191 (94%)	180 (100%)	0	100	100
21	La	91/119 (76%)	91 (100%)	0	100	100
22	Lb	219/229 (96%)	219 (100%)	0	100	100
23	Lu	159/223 (71%)	159 (100%)	0	100	100
24	Ld	111/147 (76%)	111 (100%)	0	100	100
25	Lf	97/164 (59%)	97 (100%)	0	100	100
26	Lg	49/60 (82%)	49 (100%)	0	100	100
27	Lh	40/72 (56%)	40 (100%)	0	100	100
28	Li	88/166 (53%)	88 (100%)	0	100	100
29	Lj	37/89 (42%)	37 (100%)	0	100	100
30	Lk	353/368 (96%)	353 (100%)	0	100	100
31	Ll	313/332 (94%)	313 (100%)	0	100	100
32	Lm	269/303 (89%)	269 (100%)	0	100	100
33	Ln	91/190 (48%)	91 (100%)	0	100	100
34	Lo	104/112 (93%)	104 (100%)	0	100	100
35	Lp	93/133 (70%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lq	130/186 (70%)	130 (100%)	0	100	100
37	Lr	241/288 (84%)	241 (100%)	0	100	100
38	Ls	196/274 (72%)	196 (100%)	0	100	100
39	Lt	188/236 (80%)	188 (100%)	0	100	100
40	Lv	116/188 (62%)	116 (100%)	0	100	100
41	Lw	122/148 (82%)	122 (100%)	0	100	100
42	Lx	104/148 (70%)	104 (100%)	0	100	100
43	Ly	86/110 (78%)	86 (100%)	0	100	100
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	81 (100%)	0	100	100
46	L4	78/116 (67%)	78 (100%)	0	100	100
47	L5	40/113 (35%)	40 (100%)	0	100	100
48	L6	80/87 (92%)	80 (100%)	0	100	100
49	L7	117/181 (65%)	117 (100%)	0	100	100
50	L8	110/178 (62%)	110 (100%)	0	100	100
51	SR	133/169 (79%)	133 (100%)	0	100	100
52	Sf	326/381 (86%)	326 (100%)	0	100	100
53	SB	191/249 (77%)	191 (100%)	0	100	100
54	SZ	115/143 (80%)	115 (100%)	0	100	100
55	SE	267/357 (75%)	267 (100%)	0	100	100
56	SF	104/107 (97%)	104 (100%)	0	100	100
57	SG	178/209 (85%)	178 (100%)	0	100	100
58	SI	263/342 (77%)	263 (100%)	0	100	100
59	SJ	112/180 (62%)	112 (100%)	0	100	100
60	SK	104/147 (71%)	104 (100%)	0	100	100
61	SL	93/118 (79%)	93 (100%)	0	100	100
62	SN	91/113 (80%)	91 (100%)	0	100	100
63	SO	152/226 (67%)	152 (100%)	0	100	100
64	SP	95/113 (84%)	95 (100%)	0	100	100
65	SQ	93/115 (81%)	93 (100%)	0	100	100
66	SS	166/230 (72%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	ST	87/123 (71%)	87 (100%)	0	100	100
68	SW	78/79 (99%)	78 (100%)	0	100	100
69	SX	263/318 (83%)	263 (100%)	0	100	100
70	SY	109/164 (66%)	109 (100%)	0	100	100
71	Sa	150/157 (96%)	150 (100%)	0	100	100
72	Sb	148/174 (85%)	148 (100%)	0	100	100
73	Sc	338/364 (93%)	338 (100%)	0	100	100
74	Sd	84/158 (53%)	84 (100%)	0	100	100
75	Se	310/351 (88%)	310 (100%)	0	100	100
76	Sg	97/357 (27%)	97 (100%)	0	100	100
77	Si	79/95 (83%)	79 (100%)	0	100	100
78	Sj	175/190 (92%)	175 (100%)	0	100	100
79	Sk	235/291 (81%)	235 (100%)	0	100	100
80	Sm	99/101 (98%)	99 (100%)	0	100	100
81	Sn	63/166 (38%)	63 (100%)	0	100	100
82	So	548/609 (90%)	548 (100%)	0	100	100
All	All	12121/15564 (78%)	12121 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
3	LB	156	ASN
4	LC	202	GLN
5	LD	98	GLN
5	LD	103	GLN
5	LD	105	ASN
7	LJ	128	ASN
8	LK	48	GLN
8	LK	84	GLN
9	LM	9	GLN
9	LM	61	ASN
9	LM	64	HIS
9	LM	94	GLN
9	LM	117	HIS

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Mol	Chain	Res	Type
9	LM	147	GLN
9	LM	160	GLN
10	LN	64	ASN
10	LN	80	GLN
10	LN	104	ASN
11	LO	102	GLN
11	LO	153	ASN
14	LR	96	GLN
15	LS	158	GLN
15	LS	172	GLN
16	LT	22	GLN
17	LU	91	GLN
18	LV	62	GLN
18	LV	75	HIS
21	La	41	ASN
21	La	62	HIS
21	La	72	HIS
22	Lb	241	GLN
23	Lu	88	GLN
23	Lu	92	ASN
23	Lu	179	HIS
27	Lh	77	GLN
28	Li	151	ASN
28	Li	170	ASN
30	Lk	119	GLN
30	Lk	150	GLN
30	Lk	160	HIS
30	Lk	165	GLN
30	Lk	280	GLN
30	Lk	302	HIS
30	Lk	338	GLN
31	Ll	163	HIS
31	Ll	275	GLN
31	Ll	359	HIS
32	Lm	69	HIS
33	Ln	127	GLN
33	Ln	144	GLN
36	Lq	129	GLN
37	Lr	42	GLN
37	Lr	73	GLN
37	Lr	80	GLN
39	Lt	67	GLN

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Mol	Chain	Res	Type
39	Lt	75	GLN
39	Lt	130	GLN
39	Lt	248	ASN
40	Lv	175	GLN
44	Lz	99	GLN
45	L3	46	ASN
46	L4	76	ASN
46	L4	124	GLN
46	L4	135	ASN
49	L7	104	HIS
49	L7	152	GLN
50	L8	136	GLN
50	L8	138	GLN
50	L8	139	GLN
52	Sf	96	GLN
52	Sf	339	GLN
52	Sf	343	GLN
52	Sf	373	GLN
52	Sf	375	ASN
52	Sf	420	GLN
53	SB	113	HIS
53	SB	201	ASN
53	SB	265	GLN
54	SZ	57	HIS
54	SZ	126	GLN
55	SE	369	HIS
56	SF	57	GLN
56	SF	59	ASN
57	SG	122	GLN
57	SG	215	ASN
57	SG	238	HIS
58	SI	156	GLN
58	SI	265	GLN
59	SJ	83	HIS
60	SK	129	GLN
62	SN	89	ASN
62	SN	117	HIS
65	SQ	44	ASN
65	SQ	76	HIS
66	SS	125	GLN
66	SS	225	GLN
67	ST	71	HIS

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Mol	Chain	Res	Type
69	SX	86	ASN
69	SX	96	GLN
69	SX	214	ASN
69	SX	224	HIS
69	SX	299	ASN
69	SX	315	GLN
69	SX	350	GLN
72	Sb	117	HIS
72	Sb	131	GLN
73	Sc	308	GLN
73	Sc	358	GLN
73	Sc	381	GLN
73	Sc	388	GLN
73	Sc	394	GLN
75	Se	67	HIS
75	Se	228	GLN
75	Se	235	ASN
75	Se	358	GLN
78	Sj	88	GLN
78	Sj	89	HIS
79	Sk	218	ASN
79	Sk	301	ASN
80	Sm	59	ASN
80	Sm	109	GLN
81	Sn	158	GLN
81	Sn	166	GLN
82	So	136	HIS
82	So	243	ASN
82	So	295	ASN
82	So	333	GLN
82	So	373	HIS
82	So	436	HIS
82	So	452	GLN
82	So	504	ASN
82	So	602	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	358 (24%)	13 (0%)
2	L2	52/69 (75%)	15 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
83	S1	921/954 (96%)	195 (21%)	10 (1%)
All	All	2464/2582 (95%)	568 (23%)	23 (0%)

All (568) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	A
1	L1	8	C
1	L1	9	U
1	L1	11	G
1	L1	19	C
1	L1	20	C
1	L1	23	C
1	L1	24	U
1	L1	29	C
1	L1	30	U
1	L1	31	U
1	L1	34	U
1	L1	38	A
1	L1	39	G
1	L1	41	C
1	L1	44	C
1	L1	45	C
1	L1	46	U
1	L1	47	U
1	L1	54	A
1	L1	57	A
1	L1	58	U
1	L1	66	A
1	L1	67	A
1	L1	78	G
1	L1	91	A
1	L1	100	G
1	L1	101	C
1	L1	103	A
1	L1	104	U
1	L1	110	U
1	L1	111	A
1	L1	121	G
1	L1	124	A
1	L1	127	G
1	L1	134	A

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Mol	Chain	Res	Type
1	L1	135	A
1	L1	137	U
1	L1	138	A
1	L1	139	U
1	L1	147	C
1	L1	153	A
1	L1	157	C
1	L1	158	A
1	L1	159	A
1	L1	162	A
1	L1	166	A
1	L1	167	C
1	L1	174	A
1	L1	179	C
1	L1	184	U
1	L1	186	A
1	L1	189	A
1	L1	197	A
1	L1	198	G
1	L1	199	A
1	L1	200	A
1	L1	201	A
1	L1	203	A
1	L1	208	U
1	L1	212	A
1	L1	213	G
1	L1	215	A
1	L1	217	A
1	L1	220	C
1	L1	223	A
1	L1	232	C
1	L1	233	C
1	L1	248	G
1	L1	266	A
1	L1	267	A
1	L1	270	A
1	L1	274	C
1	L1	298	G
1	L1	302	A
1	L1	304	A
1	L1	305	U
1	L1	315	G

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Mol	Chain	Res	Type
1	L1	317	G
1	L1	322	C
1	L1	323	A
1	L1	324	A
1	L1	330	C
1	L1	331	C
1	L1	332	G
1	L1	342	A
1	L1	345	G
1	L1	346	C
1	L1	351	U
1	L1	352	G
1	L1	359	A
1	L1	361	A
1	L1	362	G
1	L1	364	A
1	L1	366	C
1	L1	367	U
1	L1	369	A
1	L1	375	A
1	L1	383	U
1	L1	385	U
1	L1	390	A
1	L1	395	A
1	L1	404	A
1	L1	413	U
1	L1	415	A
1	L1	423	U
1	L1	427	A
1	L1	429	U
1	L1	443	G
1	L1	454	A
1	L1	455	C
1	L1	456	U
1	L1	463	A
1	L1	464	A
1	L1	465	A
1	L1	466	C
1	L1	471	U
1	L1	472	A
1	L1	477	G
1	L1	489	U

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Mol	Chain	Res	Type
1	L1	493	A
1	L1	496	C
1	L1	498	U
1	L1	501	U
1	L1	503	G
1	L1	507	U
1	L1	510	A
1	L1	511	A
1	L1	512	G
1	L1	519	C
1	L1	522	A
1	L1	526	A
1	L1	527	G
1	L1	528	A
1	L1	530	A
1	L1	537	A
1	L1	540	C
1	L1	545	C
1	L1	550	A
1	L1	551	C
1	L1	552	U
1	L1	553	A
1	L1	555	C
1	L1	557	A
1	L1	558	A
1	L1	563	U
1	L1	565	C
1	L1	567	A
1	L1	569	A
1	L1	571	A
1	L1	572	U
1	L1	573	A
1	L1	575	A
1	L1	576	A
1	L1	582	C
1	L1	592	C
1	L1	593	C
1	L1	614	C
1	L1	615	U
1	L1	620	A
1	L1	627	A
1	L1	629	U

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Mol	Chain	Res	Type
1	L1	630	G
1	L1	652	C
1	L1	653	A
1	L1	654	U
1	L1	662	C
1	L1	672	U
1	L1	675	G
1	L1	694	C
1	L1	699	A
1	L1	700	A
1	L1	701	U
1	L1	704	A
1	L1	711	A
1	L1	720	A
1	L1	723	C
1	L1	724	A
1	L1	730	C
1	L1	731	A
1	L1	737	U
1	L1	744	C
1	L1	745	C
1	L1	746	U
1	L1	756	C
1	L1	757	C
1	L1	762	A
1	L1	773	C
1	L1	774	A
1	L1	775	U
1	L1	777	A
1	L1	779	G
1	L1	794	G
1	L1	808	G
1	L1	809	C
1	L1	819	C
1	L1	823	C
1	L1	830	A
1	L1	832	C
1	L1	834	A
1	L1	836	A
1	L1	837	A
1	L1	838	C
1	L1	841	C

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Mol	Chain	Res	Type
1	L1	842	A
1	L1	850	C
1	L1	851	A
1	L1	853	C
1	L1	854	A
1	L1	857	A
1	L1	860	A
1	L1	861	U
1	L1	870	C
1	L1	874	C
1	L1	887	C
1	L1	888	A
1	L1	889	U
1	L1	890	G
1	L1	900	C
1	L1	904	G
1	L1	907	C
1	L1	911	A
1	L1	912	A
1	L1	913	C
1	L1	922	G
1	L1	923	G
1	L1	924	U
1	L1	926	G
1	L1	929	U
1	L1	930	A
1	L1	931	A
1	L1	933	C
1	L1	936	U
1	L1	948	U
1	L1	956	U
1	L1	958	U
1	L1	960	U
1	L1	962	A
1	L1	963	A
1	L1	964	U
1	L1	965	G
1	L1	975	G
1	L1	984	U
1	L1	985	G
1	L1	986	U
1	L1	990	U

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Mol	Chain	Res	Type
1	L1	1013	C
1	L1	1014	C
1	L1	1016	G
1	L1	1024	A
1	L1	1026	A
1	L1	1028	G
1	L1	1032	G
1	L1	1036	A
1	L1	1039	A
1	L1	1048	C
1	L1	1049	G
1	L1	1053	A
1	L1	1054	G
1	L1	1055	A
1	L1	1056	C
1	L1	1062	G
1	L1	1069	U
1	L1	1073	U
1	L1	1075	A
1	L1	1087	A
1	L1	1088	G
1	L1	1140	G
1	L1	1161	G
1	L1	1162	A
1	L1	1163	A
1	L1	1172	C
1	L1	1177	C
1	L1	1184	U
1	L1	1185	G
1	L1	1191	A
1	L1	1194	U
1	L1	1195	C
1	L1	1222	A
1	L1	1223	A
1	L1	1225	U
1	L1	1226	G
1	L1	1236	C
1	L1	1240	A
1	L1	1241	C
1	L1	1242	C
1	L1	1243	A
1	L1	1246	G

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Mol	Chain	Res	Type
1	L1	1247	G
1	L1	1248	A
1	L1	1249	A
1	L1	1252	A
1	L1	1256	A
1	L1	1257	C
1	L1	1258	C
1	L1	1262	G
1	L1	1265	A
1	L1	1286	A
1	L1	1292	C
1	L1	1293	A
1	L1	1301	A
1	L1	1305	G
1	L1	1308	U
1	L1	1309	U
1	L1	1311	A
1	L1	1315	C
1	L1	1319	G
1	L1	1320	A
1	L1	1322	G
1	L1	1323	U
1	L1	1324	U
1	L1	1335	A
1	L1	1337	C
1	L1	1346	G
1	L1	1351	C
1	L1	1352	G
1	L1	1371	U
1	L1	1372	U
1	L1	1383	A
1	L1	1384	G
1	L1	1386	C
1	L1	1389	A
1	L1	1390	C
1	L1	1391	G
1	L1	1393	G
1	L1	1399	A
1	L1	1416	U
1	L1	1419	A
1	L1	1426	U
1	L1	1430	U

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Mol	Chain	Res	Type
1	L1	1438	U
1	L1	1439	U
1	L1	1442	A
1	L1	1444	U
1	L1	1452	U
1	L1	1461	G
1	L1	1480	U
1	L1	1485	C
1	L1	1487	C
1	L1	1488	A
1	L1	1490	A
1	L1	1492	C
1	L1	1498	C
1	L1	1499	C
1	L1	1502	C
1	L1	1504	U
1	L1	1506	A
1	L1	1510	A
1	L1	1513	U
1	L1	1520	A
1	L1	1522	C
1	L1	1537	A
1	L1	1539	A
1	L1	1540	C
1	L1	1542	C
1	L1	1547	A
1	L1	1548	A
1	L1	1558	U
2	L2	4	A
2	L2	7	G
2	L2	9	A
2	L2	10	G
2	L2	12	U
2	L2	13	U
2	L2	14	A
2	L2	39	A
2	L2	40	G
2	L2	43	G
2	L2	47	U
2	L2	49	A
2	L2	50	A
2	L2	68	G

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Mol	Chain	Res	Type
2	L2	69	A
83	S1	3	U
83	S1	4	A
83	S1	33	U
83	S1	38	A
83	S1	41	A
83	S1	44	A
83	S1	47	C
83	S1	51	C
83	S1	57	U
83	S1	60	C
83	S1	64	U
83	S1	65	C
83	S1	71	A
83	S1	74	U
83	S1	75	C
83	S1	76	A
83	S1	94	A
83	S1	98	A
83	S1	106	A
83	S1	114	A
83	S1	117	A
83	S1	119	G
83	S1	125	A
83	S1	126	U
83	S1	144	G
83	S1	149	G
83	S1	160	A
83	S1	161	C
83	S1	168	C
83	S1	182	C
83	S1	183	U
83	S1	185	U
83	S1	188	C
83	S1	192	A
83	S1	198	A
83	S1	199	A
83	S1	200	G
83	S1	204	A
83	S1	209	A
83	S1	214	U
83	S1	219	A

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Mol	Chain	Res	Type
83	S1	221	C
83	S1	223	C
83	S1	225	G
83	S1	233	C
83	S1	234	A
83	S1	235	A
83	S1	236	U
83	S1	243	C
83	S1	246	G
83	S1	252	G
83	S1	256	U
83	S1	257	C
83	S1	261	C
83	S1	271	A
83	S1	272	A
83	S1	275	C
83	S1	286	G
83	S1	289	G
83	S1	291	A
83	S1	292	A
83	S1	295	A
83	S1	296	G
83	S1	303	A
83	S1	307	C
83	S1	308	A
83	S1	320	A
83	S1	328	A
83	S1	331	A
83	S1	340	A
83	S1	341	G
83	S1	345	U
83	S1	346	A
83	S1	348	A
83	S1	353	U
83	S1	354	C
83	S1	355	C
83	S1	361	A
83	S1	363	A
83	S1	364	C
83	S1	368	A
83	S1	372	A
83	S1	375	A

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Mol	Chain	Res	Type
83	S1	381	G
83	S1	384	G
83	S1	395	U
83	S1	402	A
83	S1	405	C
83	S1	418	C
83	S1	422	A
83	S1	423	C
83	S1	434	U
83	S1	435	A
83	S1	456	A
83	S1	458	C
83	S1	459	C
83	S1	462	A
83	S1	474	A
83	S1	476	C
83	S1	479	A
83	S1	481	C
83	S1	495	A
83	S1	504	C
83	S1	507	A
83	S1	508	G
83	S1	519	A
83	S1	520	A
83	S1	525	C
83	S1	532	G
83	S1	533	U
83	S1	540	U
83	S1	541	A
83	S1	542	U
83	S1	543	C
83	S1	546	U
83	S1	567	A
83	S1	568	U
83	S1	573	A
83	S1	576	C
83	S1	578	C
83	S1	590	A
83	S1	598	U
83	S1	599	U
83	S1	600	G
83	S1	601	C

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Mol	Chain	Res	Type
83	S1	603	C
83	S1	604	A
83	S1	607	C
83	S1	612	U
83	S1	614	C
83	S1	624	C
83	S1	631	C
83	S1	636	A
83	S1	638	G
83	S1	643	C
83	S1	645	A
83	S1	646	C
83	S1	648	A
83	S1	670	A
83	S1	676	G
83	S1	679	A
83	S1	680	G
83	S1	685	A
83	S1	695	C
83	S1	696	A
83	S1	697	U
83	S1	706	A
83	S1	709	A
83	S1	720	A
83	S1	723	U
83	S1	729	C
83	S1	730	C
83	S1	731	C
83	S1	732	A
83	S1	735	A
83	S1	742	G
83	S1	743	A
83	S1	744	U
83	S1	745	A
83	S1	755	A
83	S1	768	G
83	S1	769	A
83	S1	770	A
83	S1	773	U
83	S1	783	A
83	S1	785	U
83	S1	800	G

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Mol	Chain	Res	Type
83	S1	819	C
83	S1	833	A
83	S1	835	A
83	S1	842	G
83	S1	865	A
83	S1	867	A
83	S1	870	A
83	S1	877	A
83	S1	878	C
83	S1	879	U
83	S1	885	C
83	S1	886	C
83	S1	888	U
83	S1	890	C
83	S1	891	G
83	S1	892	C
83	S1	893	A
83	S1	901	A
83	S1	910	A
83	S1	912	G
83	S1	915	G
83	S1	917	A
83	S1	921	U
83	S1	935	G
83	S1	937	A
83	S1	947	G
83	S1	948	G
83	S1	952	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	33	C
1	L1	304	A
1	L1	324	A
1	L1	551	C
1	L1	575	A
1	L1	837	A
1	L1	853	C
1	L1	860	A
1	L1	889	U
1	L1	929	U

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Mol	Chain	Res	Type
1	L1	1235	A
1	L1	1319	G
1	L1	1371	U
83	S1	70	G
83	S1	374	U
83	S1	519	A
83	S1	542	U
83	S1	599	U
83	S1	611	A
83	S1	684	A
83	S1	768	G
83	S1	887	C
83	S1	890	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 156 ligands modelled in this entry, 152 are monoatomic - leaving 4 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	$\# Z > 2$
85	T1C	S1	1034	84	45,45,45	1.30	5 (11%)	56,72,72	1.35	6 (10%)
87	GDP	Se	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.89	9 (20%)
85	T1C	L1	1707	84	45,45,45	1.19	4 (8%)	56,72,72	1.13	4 (7%)
85	T1C	L1	1708	84	45,45,45	1.16	4 (8%)	56,72,72	0.72	1 (1%)

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
85	T1C	S1	1034	84	-	15/22/80/80	0/4/4/4
87	GDP	Se	500	-	-	2/16/32/32	0/3/3/3
85	T1C	L1	1707	84	-	11/22/80/80	0/4/4/4
85	T1C	L1	1708	84	-	16/22/80/80	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L1	1707	T1C	C21-N21	5.19	1.48	1.33
85	L1	1708	T1C	C21-N21	5.01	1.47	1.33
85	S1	1034	T1C	C21-N21	4.64	1.46	1.33
85	S1	1034	T1C	C1C-C41	-3.50	1.50	1.53
87	Se	500	GDP	C5-C4	3.12	1.47	1.38
85	L1	1707	T1C	C4-N4	2.69	1.53	1.47
87	Se	500	GDP	C6-N1	-2.51	1.34	1.38
85	S1	1034	T1C	C4-N4	2.41	1.52	1.47
85	L1	1708	T1C	C4-N4	2.38	1.52	1.47
85	L1	1708	T1C	O11-C11	2.25	1.27	1.23
85	L1	1707	T1C	O11-C11	2.21	1.27	1.23
85	L1	1707	T1C	C7-N7	2.15	1.48	1.42
87	Se	500	GDP	C5-N7	-2.15	1.34	1.39
85	S1	1034	T1C	O11-C11	2.12	1.27	1.23
85	L1	1708	T1C	C7-N7	2.11	1.48	1.42
85	S1	1034	T1C	C2-C1	-2.10	1.40	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	Se	500	GDP	C5-C4-N3	-6.62	117.85	128.39
85	S1	1034	T1C	C1-C1C-C12	6.34	117.31	109.88
87	Se	500	GDP	C2-N3-C4	5.34	121.51	112.30
87	Se	500	GDP	N9-C4-N3	5.10	136.16	125.95
85	L1	1707	T1C	C1C-C41-C4	5.04	118.53	111.64
85	S1	1034	T1C	C11-C1B-C12	3.16	121.30	118.80
85	L1	1707	T1C	C1-C1C-C12	3.06	113.47	109.88
85	S1	1034	T1C	C61-C6-C51	-2.99	109.17	113.12
87	Se	500	GDP	C6-C5-N7	2.87	135.52	130.29
87	Se	500	GDP	C3'-C2'-C1'	2.60	106.37	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S1	1034	T1C	C41-C1C-C1	-2.59	108.08	111.05
85	S1	1034	T1C	C51-C5-C41	-2.47	106.17	110.38
87	Se	500	GDP	O6-C6-C5	-2.46	120.04	126.53
85	L1	1707	T1C	C11-C1B-C12	2.44	120.73	118.80
87	Se	500	GDP	C4-C5-N7	-2.32	106.99	110.67
85	L1	1707	T1C	C1C-C1-C2	2.21	119.26	115.75
85	L1	1708	T1C	C11-C1B-C12	2.08	120.44	118.80
87	Se	500	GDP	C2'-C1'-N9	-2.06	107.52	113.25
85	S1	1034	T1C	C1C-C12-C1B	-2.05	120.98	123.06
87	Se	500	GDP	C5-C6-N1	2.03	118.41	113.25

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L1	1707	T1C	C41-C4-N4-C43
85	L1	1707	T1C	C3-C4-N4-C43
85	L1	1707	T1C	C3-C4-N4-C42
85	L1	1707	T1C	C3-C2-C21-O21
85	L1	1708	T1C	C41-C4-N4-C43
85	L1	1708	T1C	C3-C4-N4-C43
85	L1	1708	T1C	C3-C4-N4-C42
85	L1	1708	T1C	C3-C2-C21-O21
85	L1	1708	T1C	C3-C2-C21-N21
85	L1	1708	T1C	C1-C2-C21-O21
85	L1	1708	T1C	C1-C2-C21-N21
85	S1	1034	T1C	C94-C93-N92-C92
85	S1	1034	T1C	C95-C93-N92-C92
85	S1	1034	T1C	C92-C91-N9-C9
85	S1	1034	T1C	C41-C4-N4-C43
85	S1	1034	T1C	C3-C4-N4-C43
85	S1	1034	T1C	C3-C4-N4-C42
85	S1	1034	T1C	C3-C2-C21-O21
85	S1	1034	T1C	C3-C2-C21-N21
85	S1	1034	T1C	C1-C2-C21-O21
87	Se	500	GDP	O4'-C1'-N9-C8
87	Se	500	GDP	O4'-C1'-N9-C4
85	S1	1034	T1C	O91-C91-N9-C9
85	L1	1708	T1C	C96-C93-N92-C92
85	S1	1034	T1C	C96-C93-N92-C92
85	L1	1708	T1C	C92-C91-N9-C9
85	L1	1707	T1C	O91-C91-C92-N92

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Mol	Chain	Res	Type	Atoms
85	L1	1707	T1C	N9-C91-C92-N92
85	L1	1708	T1C	C95-C93-N92-C92
85	L1	1708	T1C	O91-C91-N9-C9
85	S1	1034	T1C	N9-C91-C92-N92
85	S1	1034	T1C	O91-C91-C92-N92
85	L1	1707	T1C	C10-C9-N9-C91
85	L1	1707	T1C	C41-C4-N4-C42
85	L1	1707	T1C	C3-C2-C21-N21
85	L1	1708	T1C	C41-C4-N4-C42
85	S1	1034	T1C	C41-C4-N4-C42
85	L1	1708	T1C	C94-C93-N92-C92
85	L1	1707	T1C	C1-C2-C21-N21
85	S1	1034	T1C	C1-C2-C21-N21
85	L1	1708	T1C	N9-C91-C92-N92
85	L1	1707	T1C	C8-C9-N9-C91
85	L1	1708	T1C	O91-C91-C92-N92
85	L1	1708	T1C	C61-C7-N7-C71

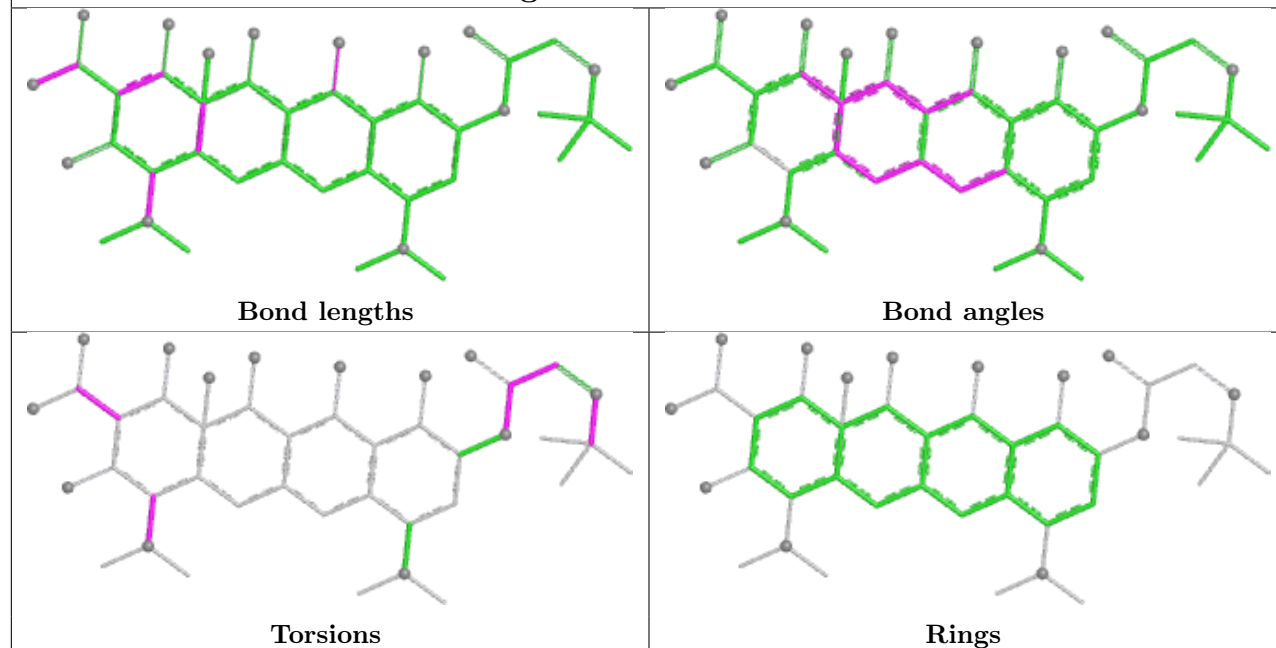
There are no ring outliers.

3 monomers are involved in 4 short contacts:

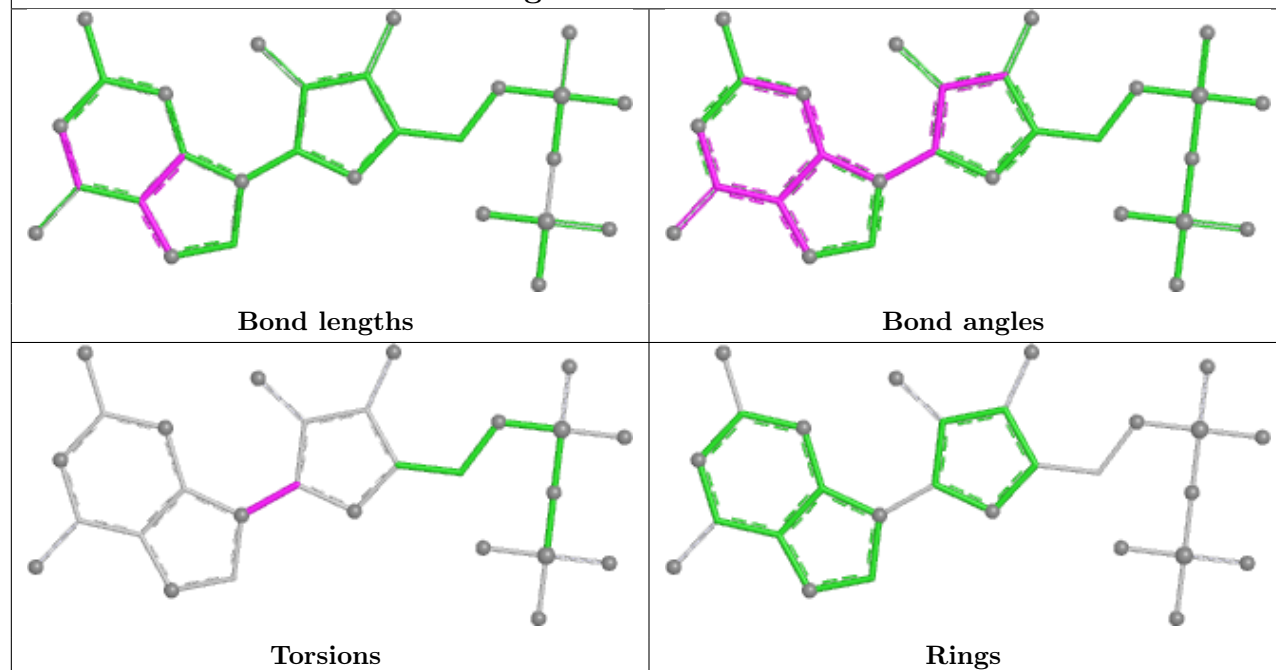
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	Se	500	GDP	2	0
85	L1	1707	T1C	1	0
85	L1	1708	T1C	1	0

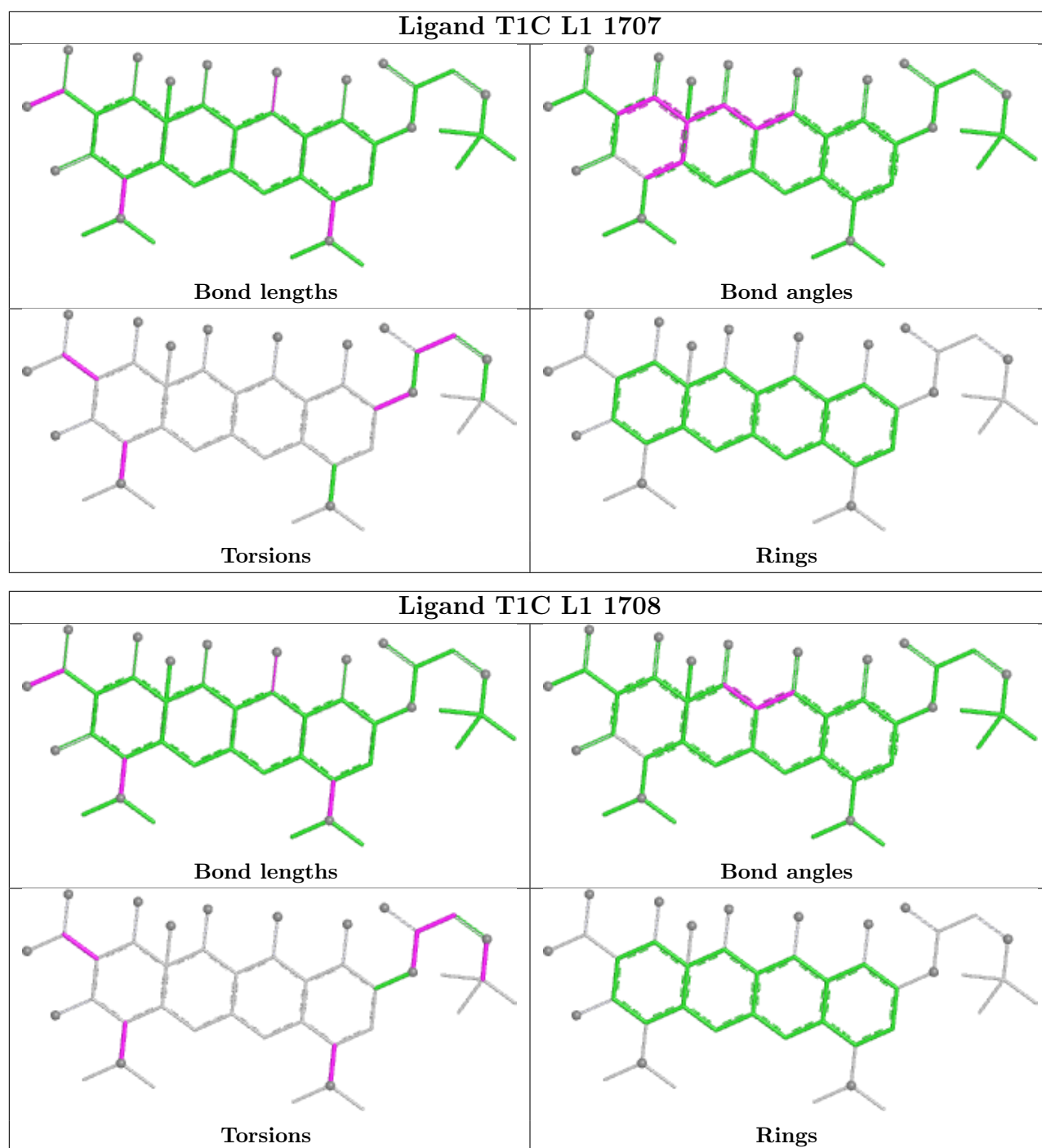
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand T1C S1 1034



Ligand GDP Se 500





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.

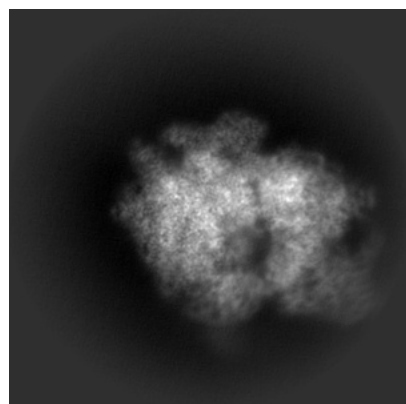
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38632. These allow visual inspection of the internal detail of the map and identification of artifacts.

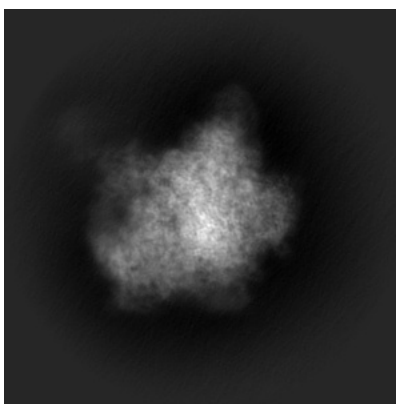
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

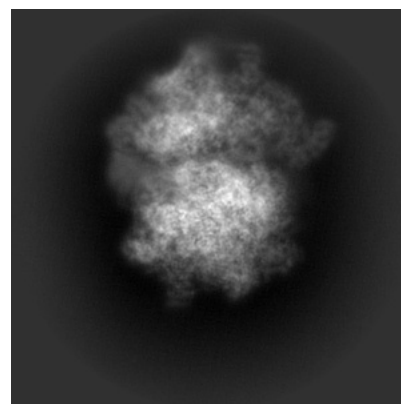
6.1.1 Primary map



X

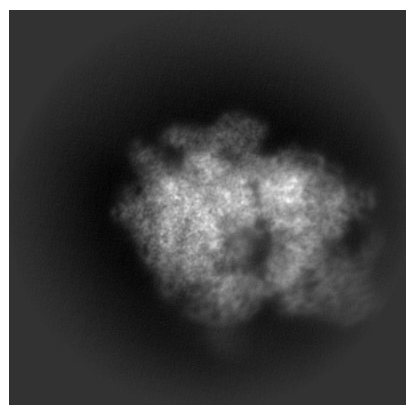


Y

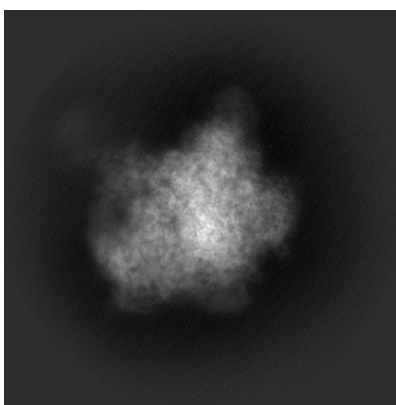


Z

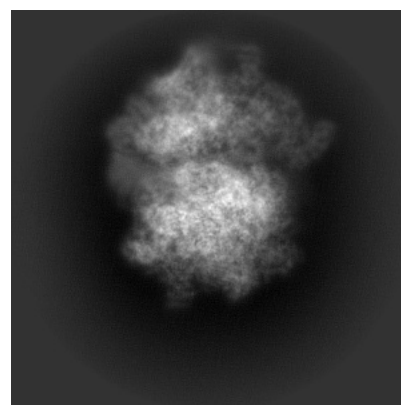
6.1.2 Raw map



X



Y

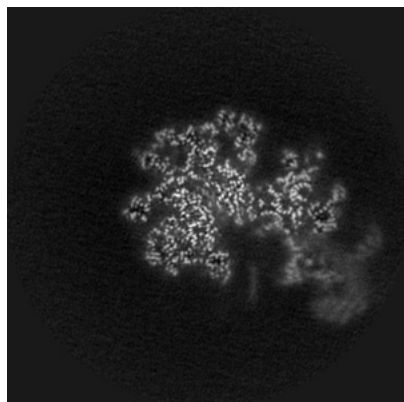


Z

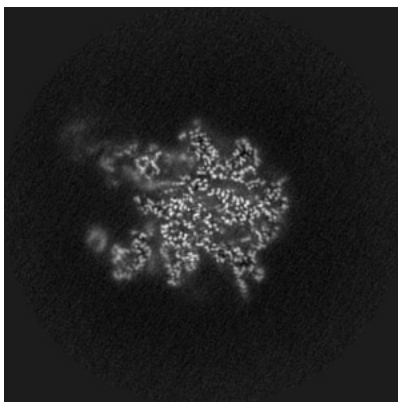
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

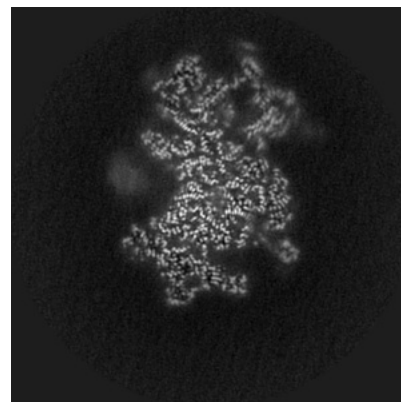
6.2.1 Primary map



X Index: 210

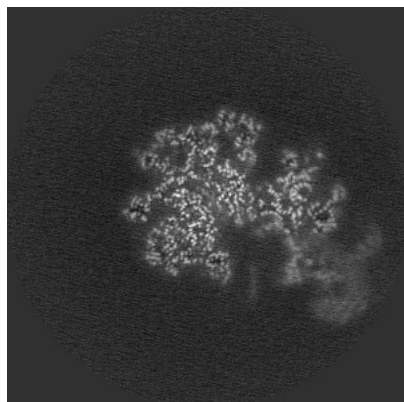


Y Index: 210

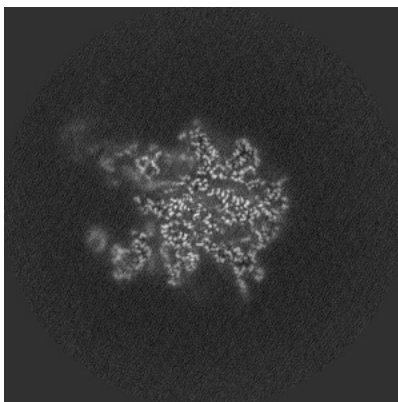


Z Index: 210

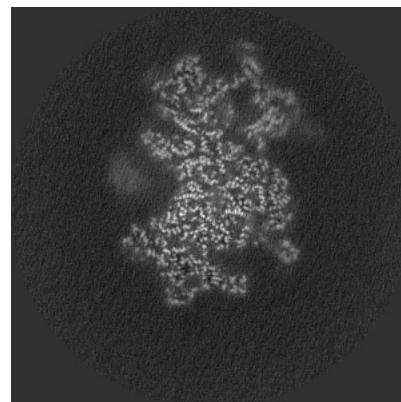
6.2.2 Raw map



X Index: 210



Y Index: 210

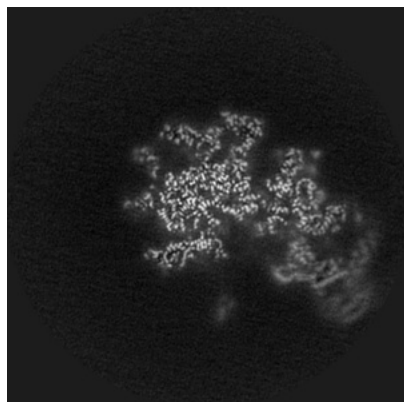


Z Index: 210

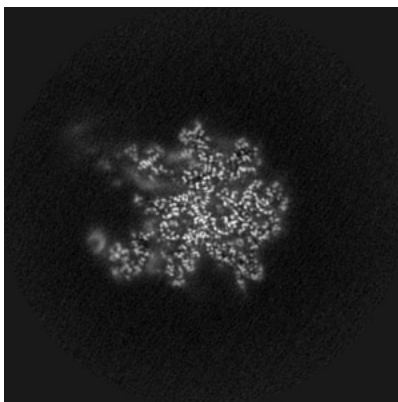
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

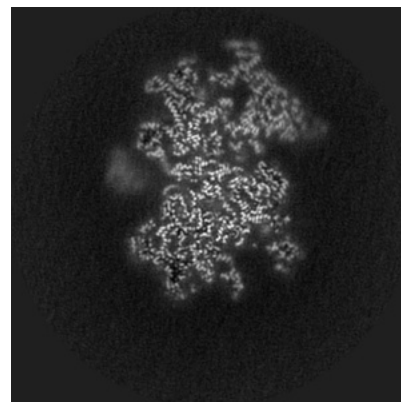
6.3.1 Primary map



X Index: 199

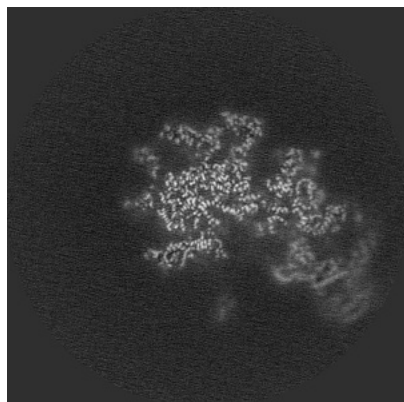


Y Index: 207

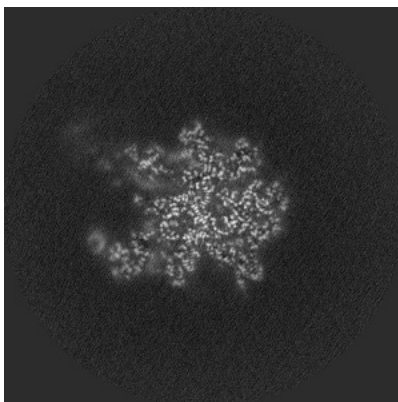


Z Index: 218

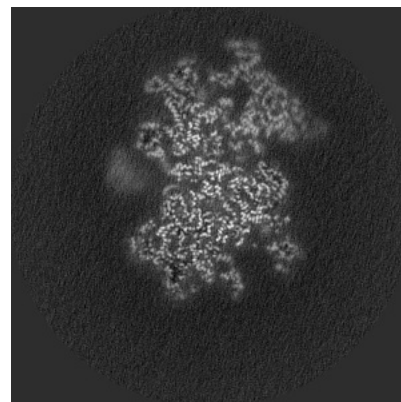
6.3.2 Raw map



X Index: 199



Y Index: 207

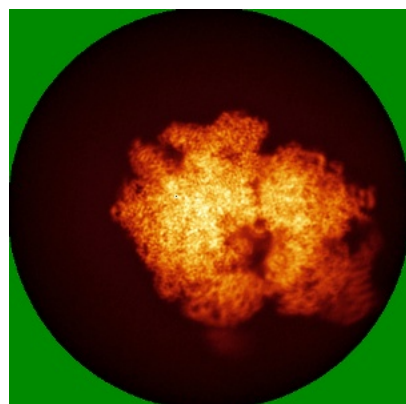


Z Index: 218

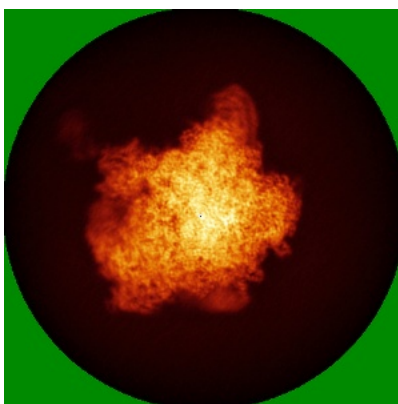
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

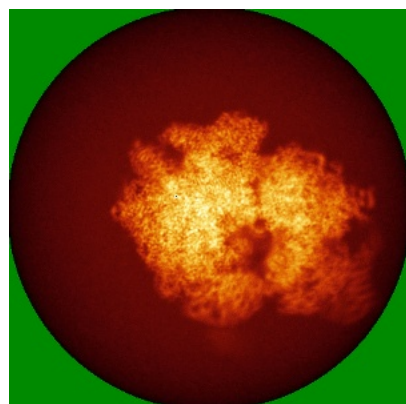


Y

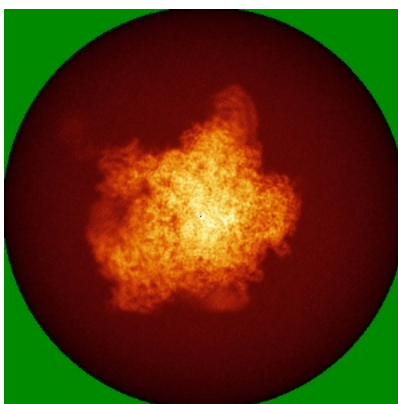


Z

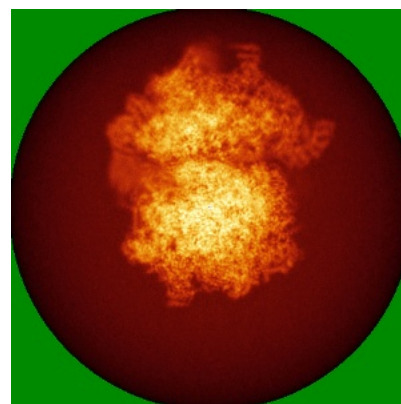
6.4.2 Raw map



X



Y

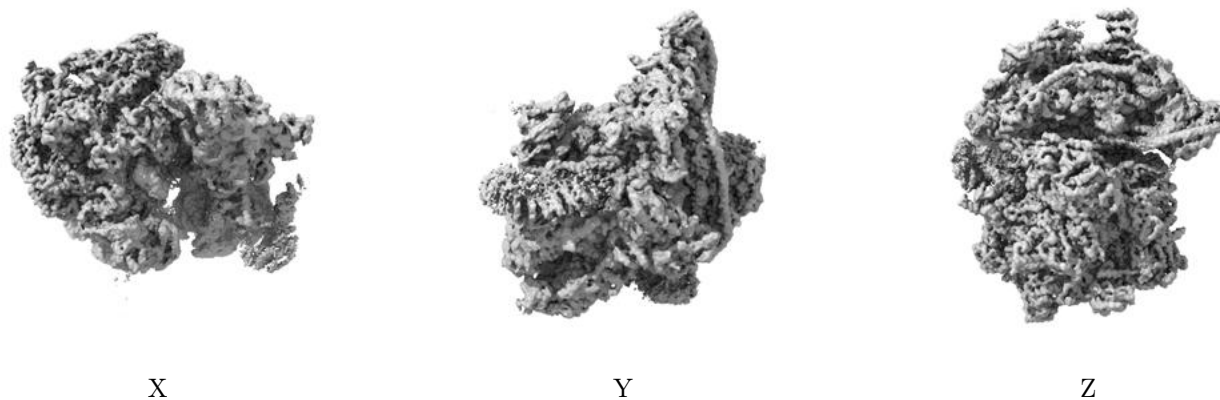


Z

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.

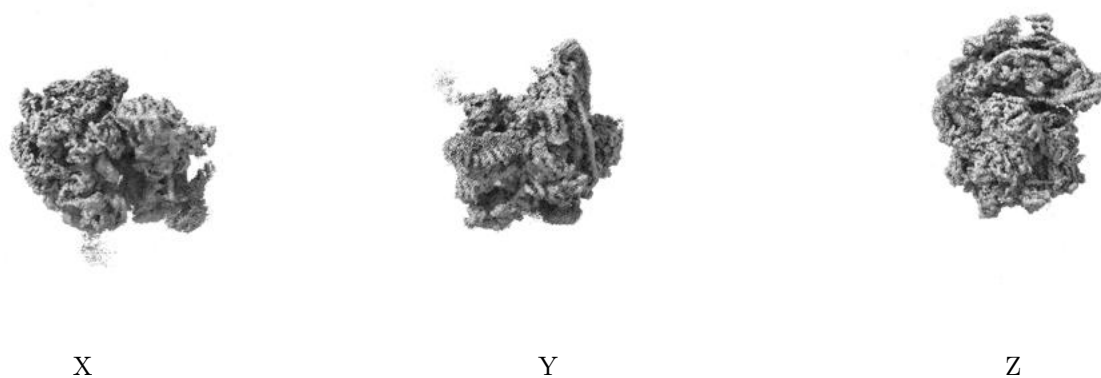
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

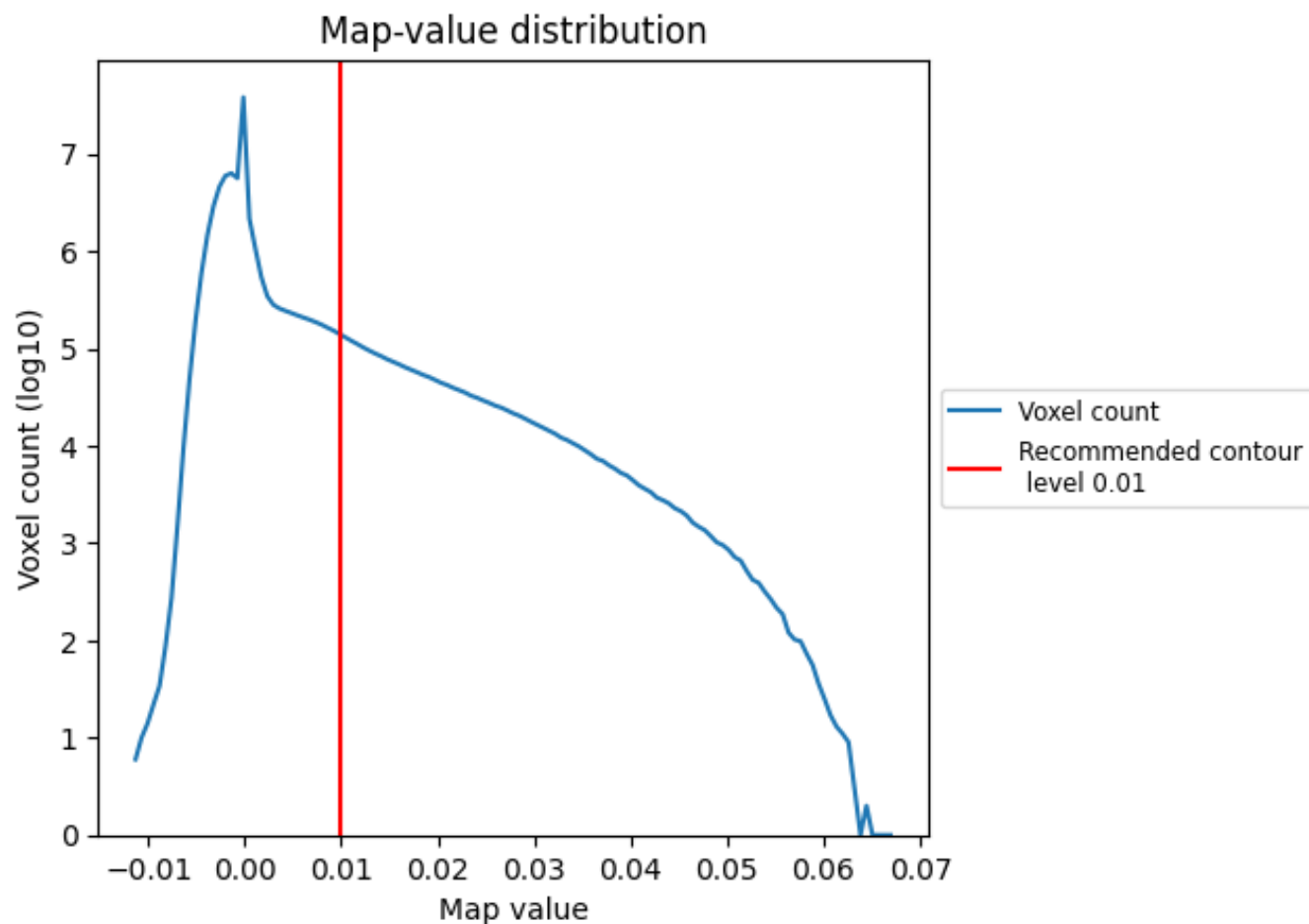
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

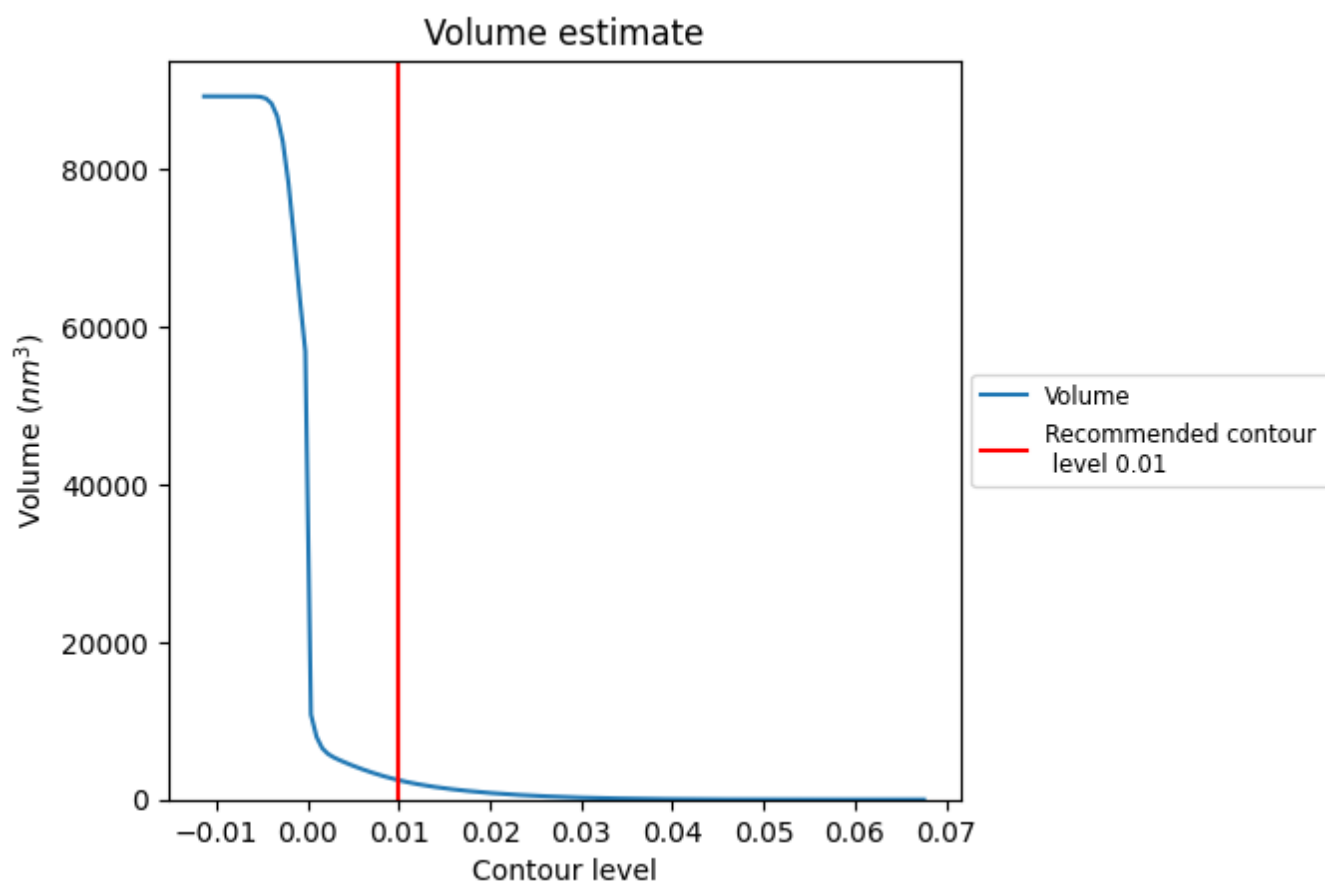
This section contains the results of statistical analysis of the map.

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.

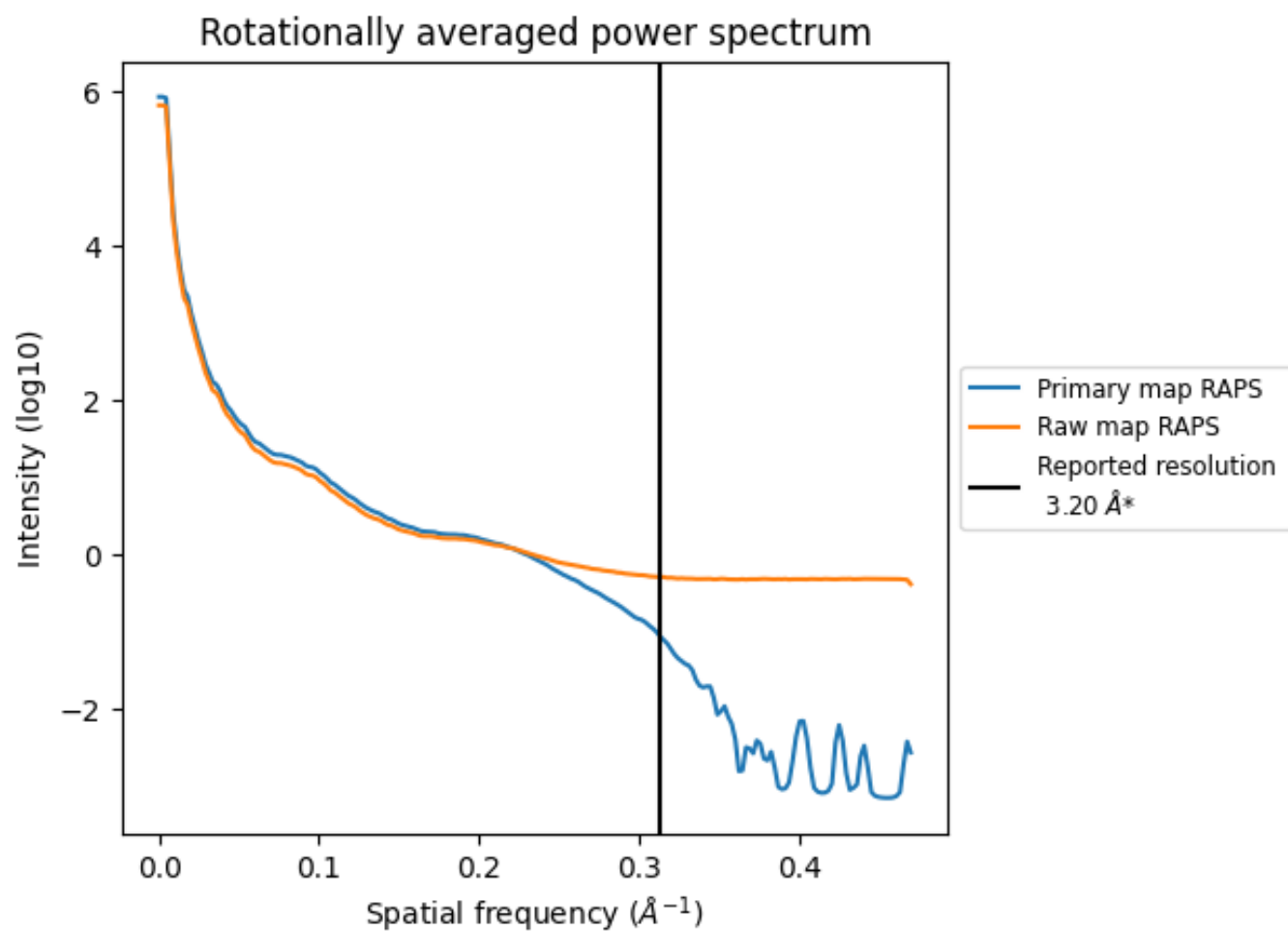
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2465 nm³; this corresponds to an approximate mass of 2227 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 ⓘ

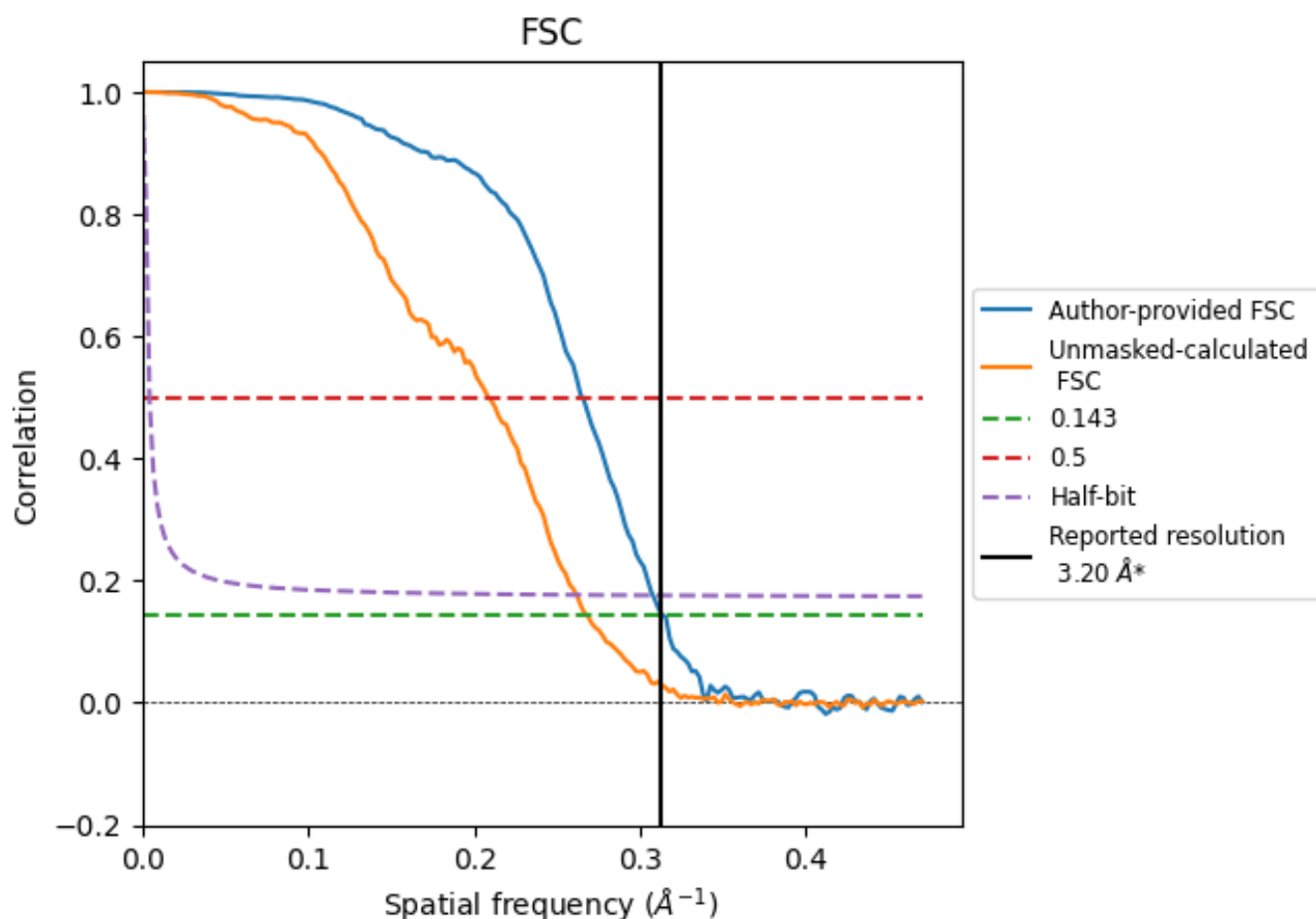


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

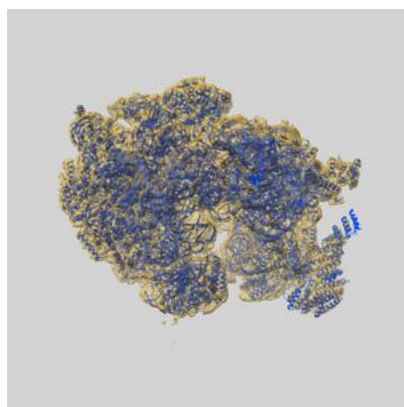
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.77	3.25
Unmasked-calculated*	3.73	4.79	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.2 by more than 10 %

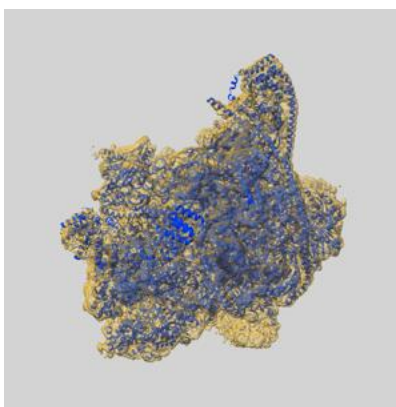
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38632 and PDB model 8XT0. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

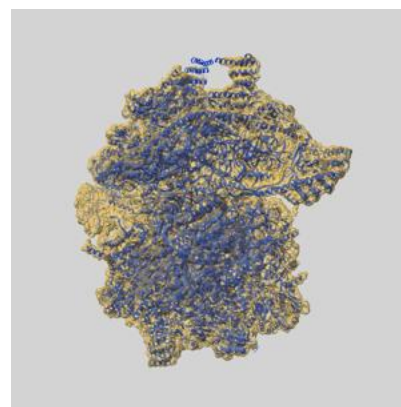
9.1 Map-model overlay [i](#)



X



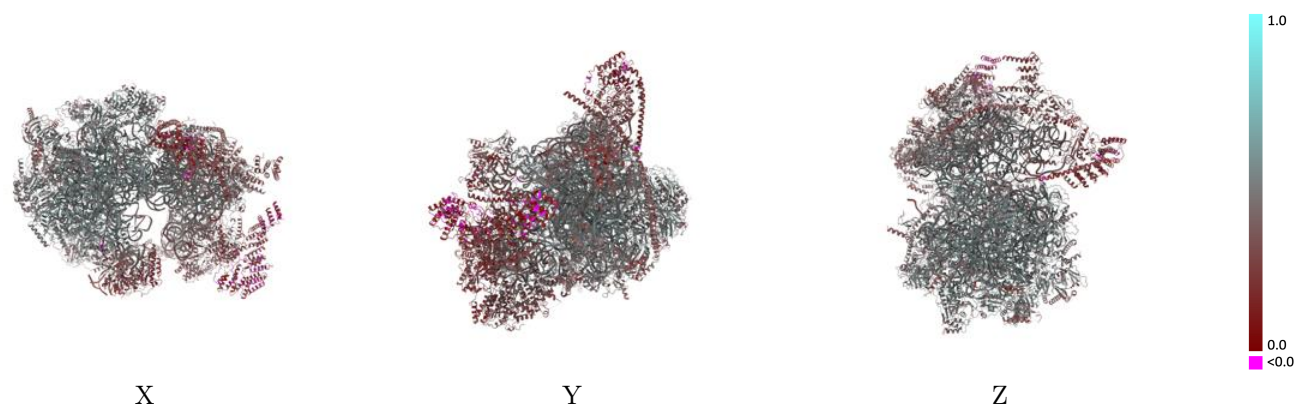
Y



Z

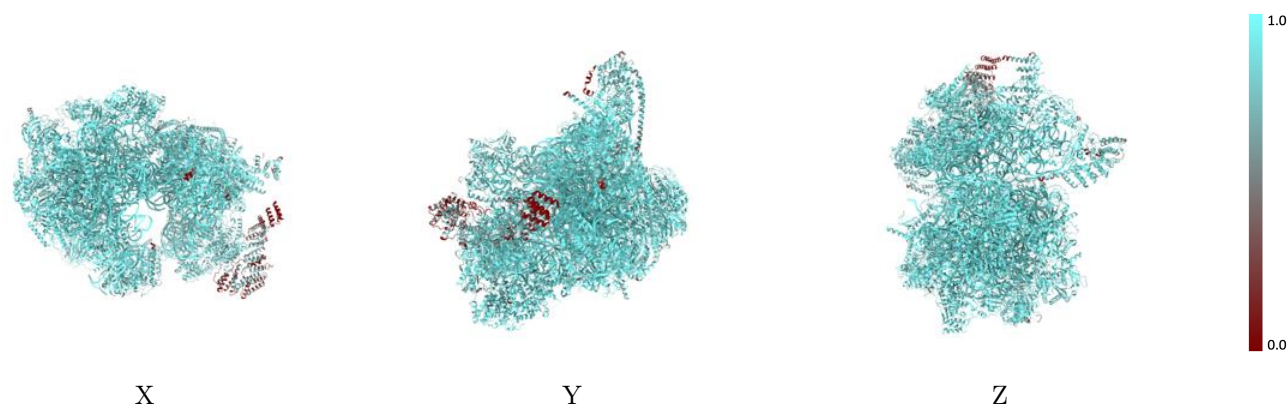
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



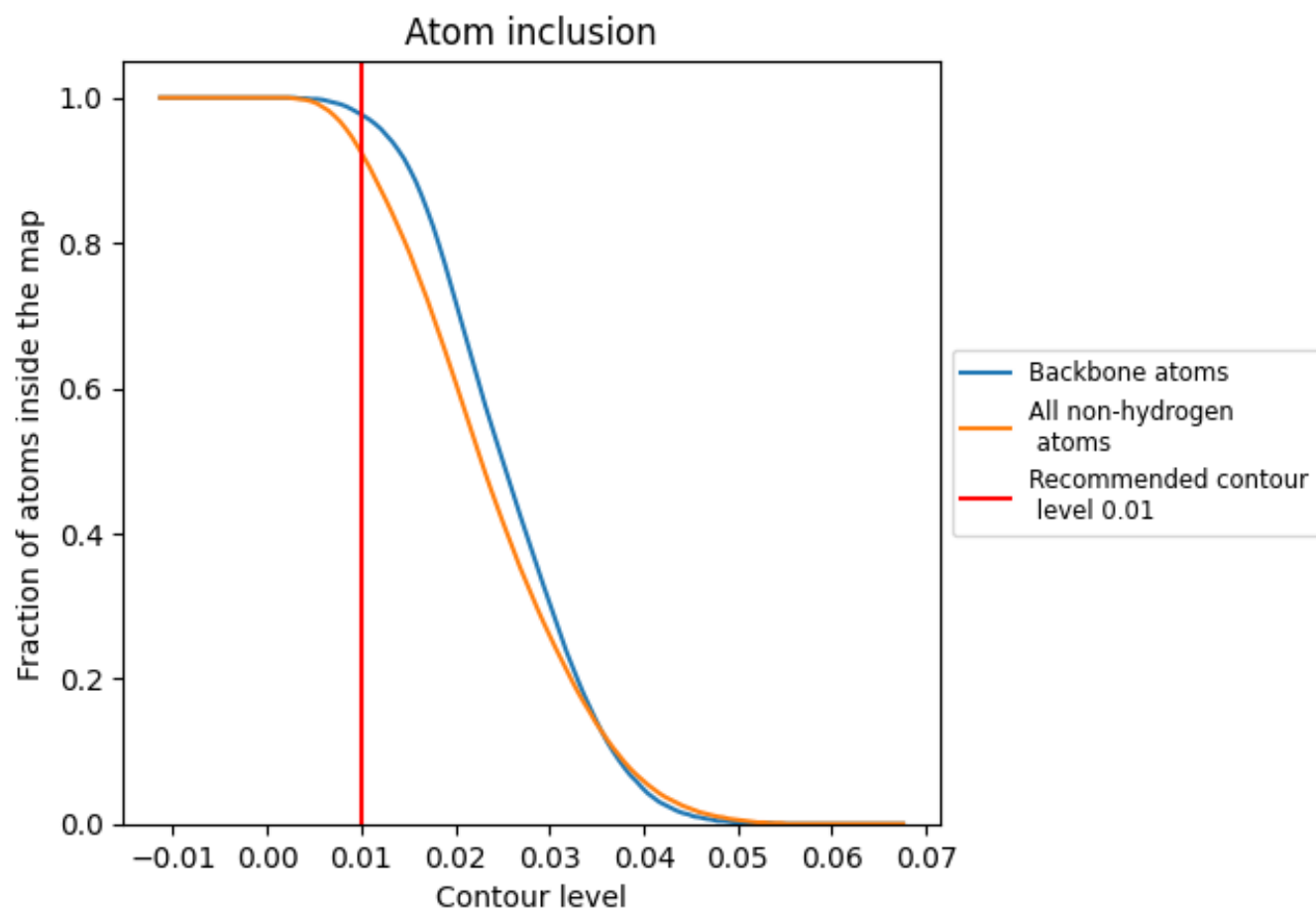
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.4340
L1	 0.9980	 0.5100
L2	 0.9790	 0.3420
L3	 0.8950	 0.3630
L4	 0.7860	 0.2920
L5	 0.9580	 0.3790
L6	 0.9690	 0.5140
L7	 0.9010	 0.4340
L8	 0.9100	 0.4230
LB	 0.9800	 0.5310
LC	 0.9580	 0.4980
LD	 0.9560	 0.5130
LI	 0.9080	 0.4410
LJ	 0.8450	 0.3500
LK	 0.7890	 0.2580
LM	 0.9710	 0.5100
LN	 0.9710	 0.5020
LO	 0.9530	 0.5040
LP	 0.9480	 0.4970
LQ	 0.9560	 0.4990
LR	 0.9320	 0.4640
LS	 0.9320	 0.4800
LT	 0.9590	 0.5140
LU	 0.9390	 0.5120
LV	 0.9590	 0.5170
LW	 0.9220	 0.4860
LX	 0.9020	 0.4410
La	 0.9730	 0.5290
Lb	 0.9240	 0.4730
Ld	 0.9550	 0.5180
Lf	 0.9400	 0.4900
Lg	 0.9740	 0.4920
Lh	 1.0000	 0.5440
Li	 0.9880	 0.5390
Lj	 0.9850	 0.5250



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Chain	Atom inclusion	Q-score
Lk	 0.9390	 0.4810
Ll	 0.9140	 0.4310
Lm	 0.8820	 0.4270
Ln	 0.8630	 0.2960
Lo	 0.9170	 0.4650
Lp	 0.9200	 0.4780
Lq	 0.9570	 0.5170
Lr	 0.9150	 0.4690
Ls	 0.8360	 0.4150
Lt	 0.8240	 0.2640
Lu	 0.9450	 0.4820
Lv	 0.8910	 0.3720
Lw	 0.9450	 0.4940
Lx	 0.8950	 0.4390
Ly	 0.9700	 0.5270
Lz	 0.9210	 0.4670
S1	 0.9970	 0.4500
SB	 0.9360	 0.4410
SE	 0.9210	 0.4170
SF	 0.9160	 0.4640
SG	 0.9250	 0.3770
SI	 0.8940	 0.3450
SJ	 0.9160	 0.3130
SK	 0.9610	 0.4650
SL	 0.9550	 0.4570
SN	 0.9380	 0.3160
SO	 0.9110	 0.4250
SP	 0.9030	 0.3600
SQ	 0.9640	 0.4650
SR	 0.9720	 0.4930
SS	 0.9200	 0.3640
ST	 0.9240	 0.4580
SW	 0.9560	 0.4780
SX	 0.8340	 0.3130
SY	 0.8770	 0.3790
SZ	 0.8990	 0.3500
Sa	 0.9220	 0.4170
Sb	 0.8730	 0.3270
Sc	 0.7470	 0.2090
Sd	 0.8890	 0.4330
Se	 0.8770	 0.3180
Sf	 0.9530	 0.4910

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Chain	Atom inclusion	Q-score
Sg	 0.8000	 0.2380
Si	 0.9150	 0.2860
Sj	 0.8930	 0.3020
Sk	 0.8300	 0.2570
Sm	 0.9260	 0.4200
Sn	 0.9710	 0.4910
So	 0.4260	 0.1380