



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:19 AM UTC

PDB ID : 8K2C / pdb_00008k2c
EMDB ID : EMD-36838
Title : Cryo-EM structure of the human 80S ribosome with Tigecycline
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2023-07-12
Resolution : 2.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

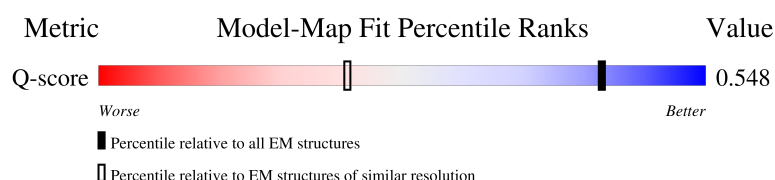
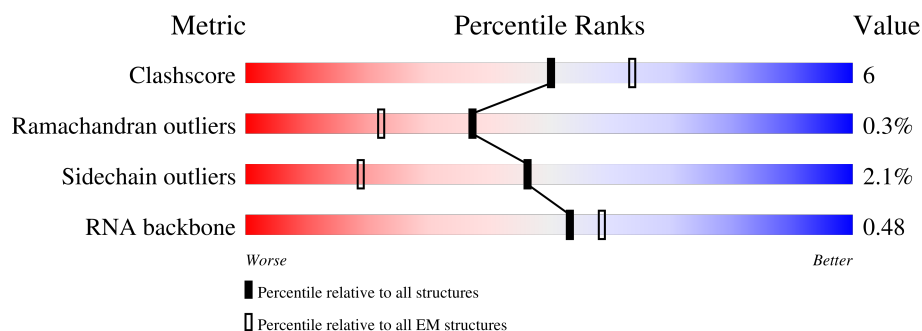
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.



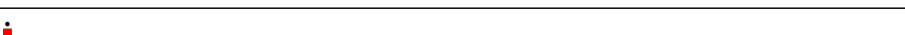
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	L5	5070	5% 50% 21% • 26%
2	L7	121	83% 15% ••
3	L8	157	5% 69% 27% ••

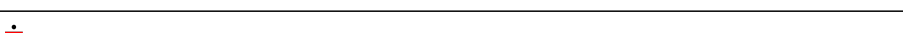
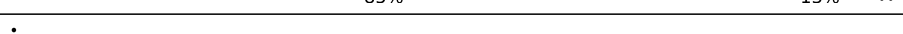
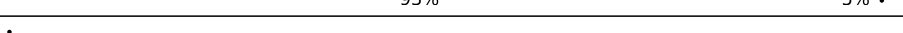
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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

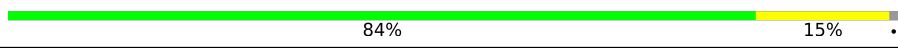
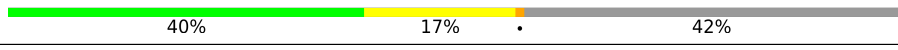
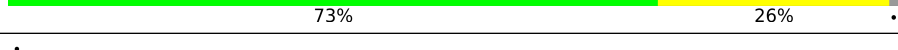
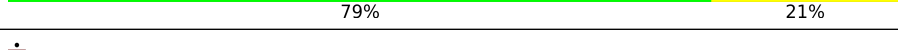
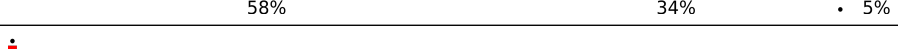
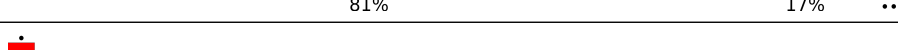
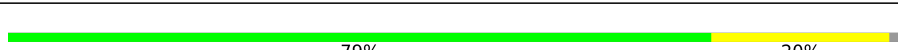
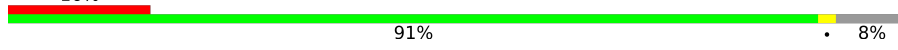
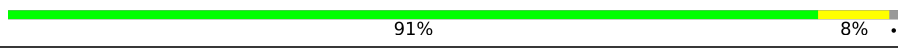
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Mol	Chain	Length	Quality of chain
29	La	148	 89% 10% ..
30	Lb	159	 57% 12% 31%
31	Lc	115	 71% 14% 15%
32	Ld	125	 71% 14% 14%
33	Le	135	 79% 15% . 5%
34	Lf	110	 91% 8% .
35	Lg	117	 91% 7% .
36	Lh	123	 85% 15% .
37	Li	105	 84% 13% .
38	Lj	97	 79% 9% 11%
39	Lk	70	 79% 20% .
40	Ll	51	 67% 31% .
41	Lm	128	 36% . . 59%
42	Ln	25	 88% 8% .
43	Lo	106	 85% 13% ..
44	Lp	92	 93% 5% .
45	Lr	137	 78% 13% 9%
46	Ls	317	 35% 47% 15% 38%
47	Lt	165	 58% 29% . 15%
48	Lz	217	 57% 91% . 6%
49	S2	1869	 59% 30% . 7%
50	SA	295	 62% 13% 25%
51	SB	264	 65% 16% 19%
52	SD	243	 77% 16% 7%
53	SE	263	 84% 15%

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Mol	Chain	Length	Quality of chain
54	SF	204	
55	SH	194	
56	SI	208	
57	SK	165	
58	SL	158	
59	SP	145	
60	SQ	146	
61	SR	135	
62	SS	152	
63	ST	145	
64	SU	119	
65	SV	83	
66	SX	143	
67	Sa	115	
68	Sc	69	
69	Sd	56	
70	Sg	317	
71	SC	293	
72	SG	249	
73	SJ	194	
74	SM	132	
75	SN	151	
76	SO	151	
77	SW	130	
78	SY	133	

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Mol	Chain	Length	Quality of chain
79	SZ	125	
80	Sb	84	
81	Se	59	
82	Sf	156	
83	CA	394	
84	CB	408	
85	CC	75	
86	CE	223	

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 223987 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3771	Total	C	N	O	P	0	0
			80096	35636	14582	26108	3770		

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

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

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

- Molecule 9 is a protein called 60S ribosomal protein L7.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

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

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lz	205	Total	C	N	O	S	0	0
			1018	607	205	206			

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S2	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

- Molecule 50 is a protein called 40S ribosomal protein SA.

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 52 is a protein called 40S ribosomal protein S3.

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

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S7.

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

- Molecule 56 is a protein called 40S ribosomal protein S8.

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

- Molecule 57 is a protein called 40S ribosomal protein S10.

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

- Molecule 58 is a protein called 40S ribosomal protein S11.

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

- Molecule 59 is a protein called 40S ribosomal protein S15.

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

- Molecule 60 is a protein called 40S ribosomal protein S16.

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

- Molecule 61 is a protein called 40S ribosomal protein S17.

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

- Molecule 62 is a protein called 40S ribosomal protein S18.

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

- Molecule 63 is a protein called 40S ribosomal protein S19.

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

- Molecule 64 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 65 is a protein called 40S ribosomal protein S21.

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

- Molecule 66 is a protein called 40S ribosomal protein S23.

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

- Molecule 67 is a protein called 40S ribosomal protein S26.

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

- Molecule 68 is a protein called 40S ribosomal protein S28.

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

- Molecule 69 is a protein called 40S ribosomal protein S29.

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

- Molecule 70 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 71 is a protein called 40S ribosomal protein S2.

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

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called 40S ribosomal protein S9.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

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

- Molecule 79 is a protein called 40S ribosomal protein S25.

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

- Molecule 80 is a protein called 40S ribosomal protein S27.

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

- Molecule 81 is a protein called 40S ribosomal protein S30.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 83 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 84 is a protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CB	16	Total	C	N	O	S	0	0
			127	80	22	24	1		

- Molecule 85 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CC	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		

- Molecule 86 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	CE	73	Total	C	N	O	S	0	0
			613	369	122	121	1		

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

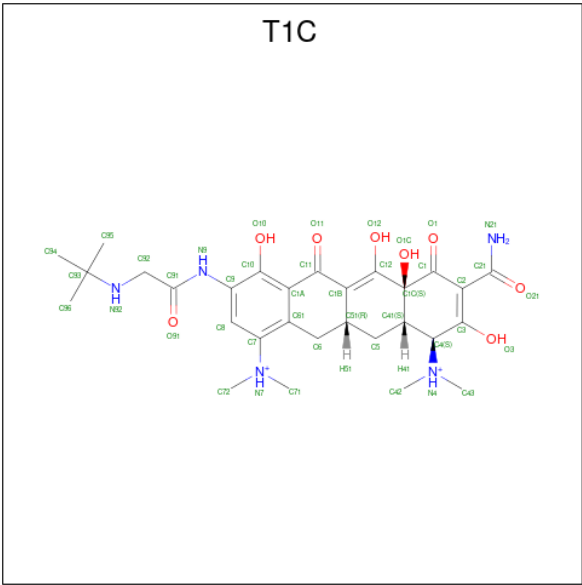
Mol	Chain	Residues	Atoms		AltConf
87	L5	215	Total	Mg	0
			215	215	
87	L7	3	Total	Mg	0
			3	3	
87	L8	4	Total	Mg	0
			4	4	
87	LA	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	2	Total	Mg	0
			2	2	
87	Lg	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	S2	29	Total	Mg	0
			29	29	
87	SG	1	Total	Mg	0
			1	1	

- Molecule 88 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈).

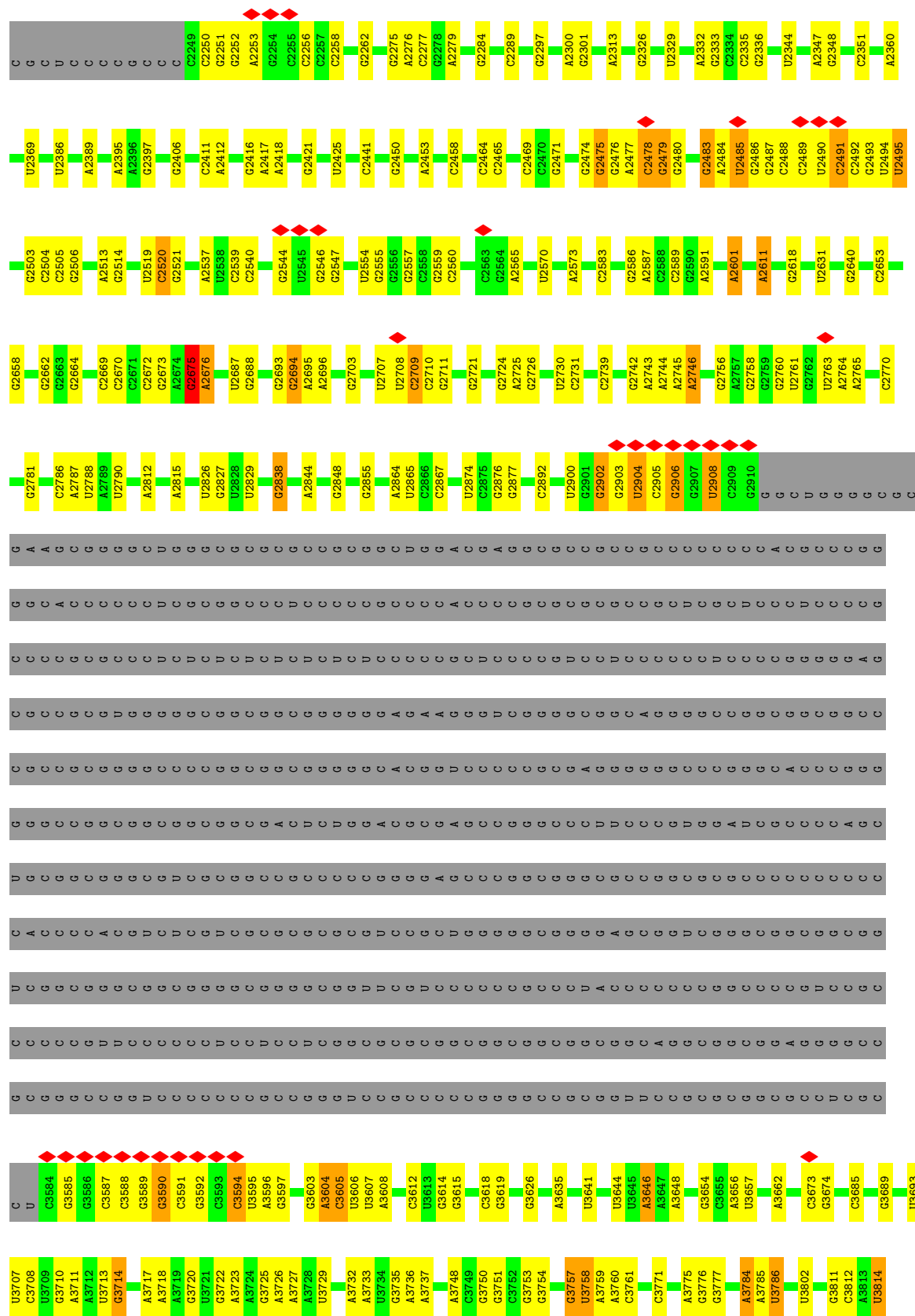


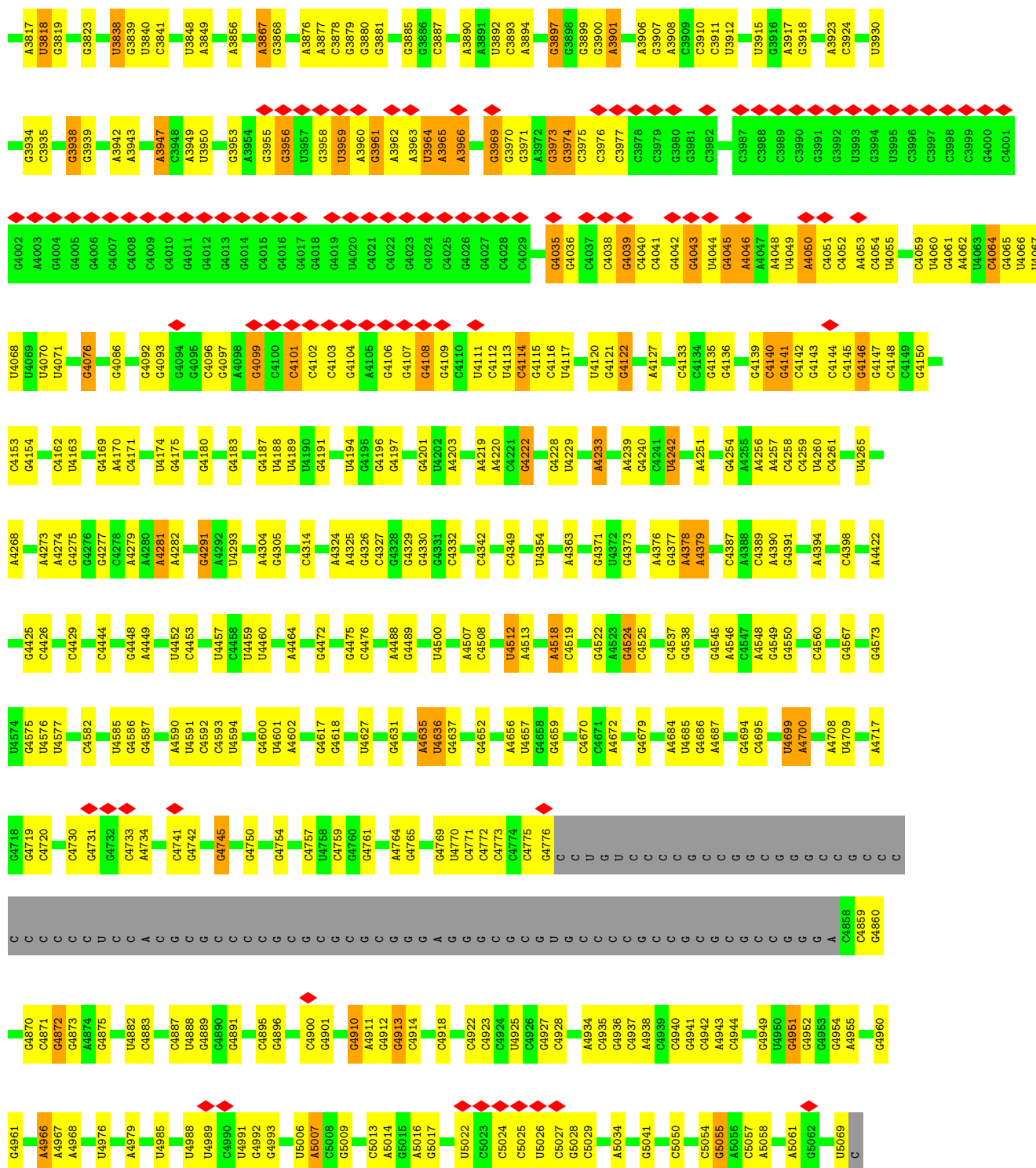
Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	S2	1	Total	C	N	O	0
			42	29	5	8	
88	CC	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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





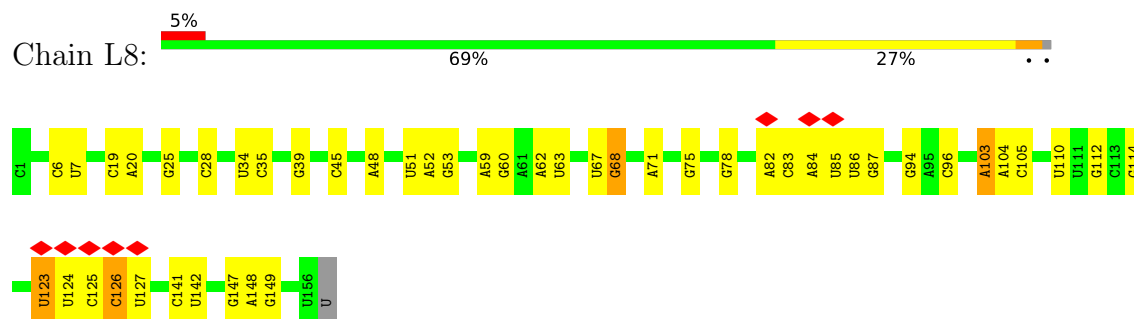


• Molecule 2: 5S rRNA

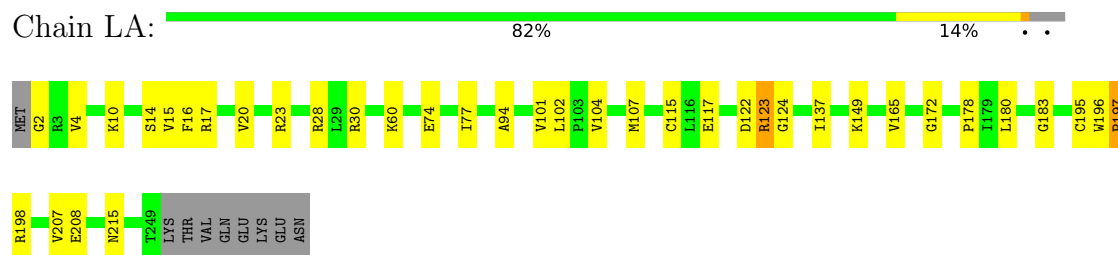
Chain L7: 83% 15% ..



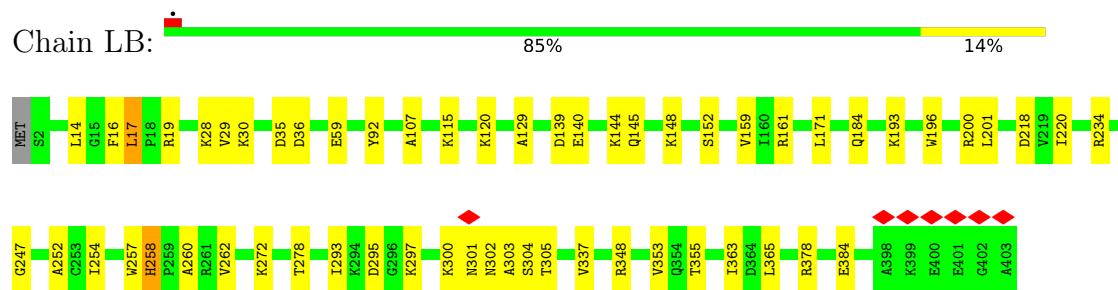
- Molecule 3: 5.8S rRNA



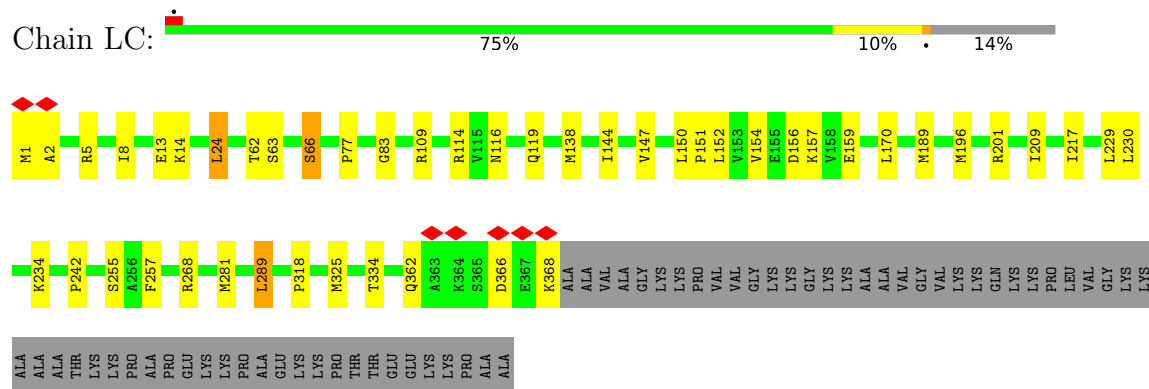
- Molecule 4: 60S ribosomal protein L8



- Molecule 5: 60S ribosomal protein L3



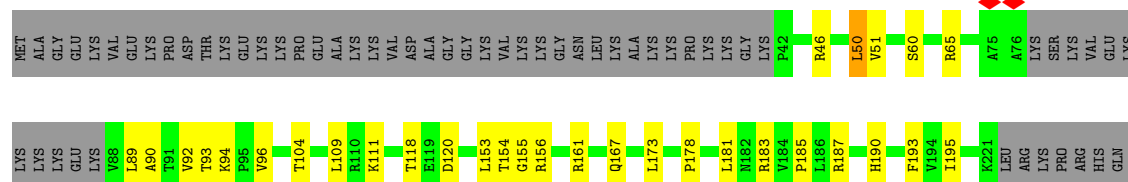
- Molecule 6: 60S ribosomal protein L4



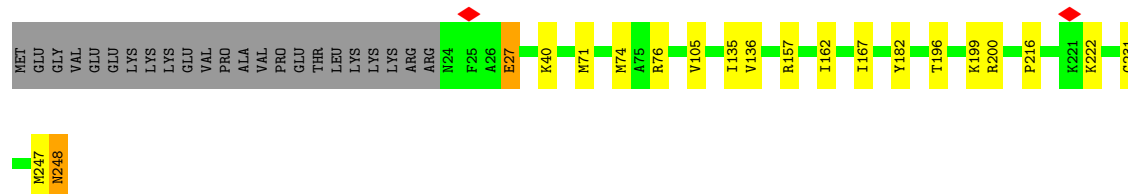
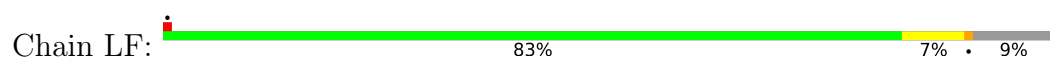
- Molecule 7: 60S ribosomal protein L5



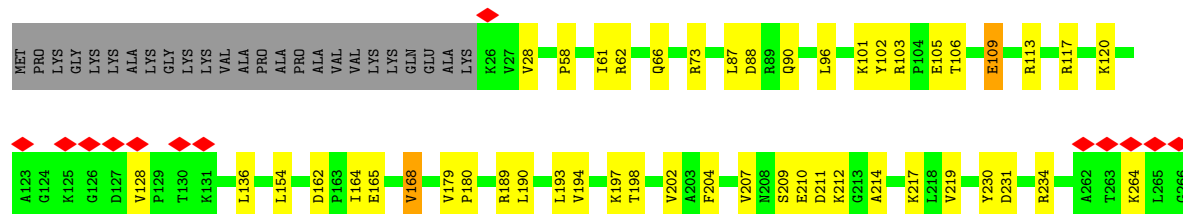
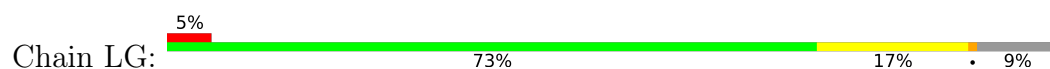
- Molecule 8: 60S ribosomal protein L6



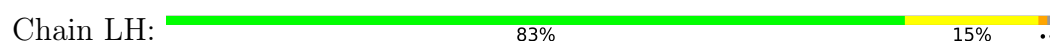
- Molecule 9: 60S ribosomal protein L7



- Molecule 10: 60S ribosomal protein L7a

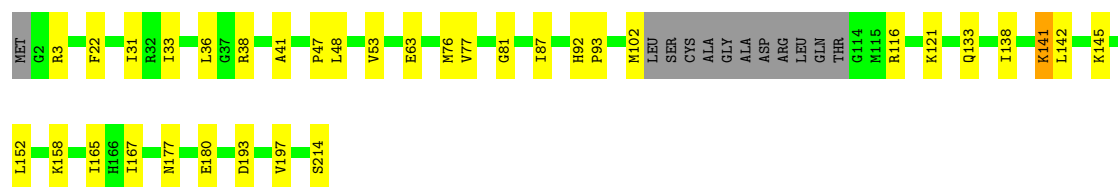


- Molecule 11: 60S ribosomal protein L9



- Molecule 12: Large ribosomal subunit protein uL16

Chain LI:  79% 15% 6%



- Molecule 13: 60S ribosomal protein L11

Chain LJ:  80% 18% ..



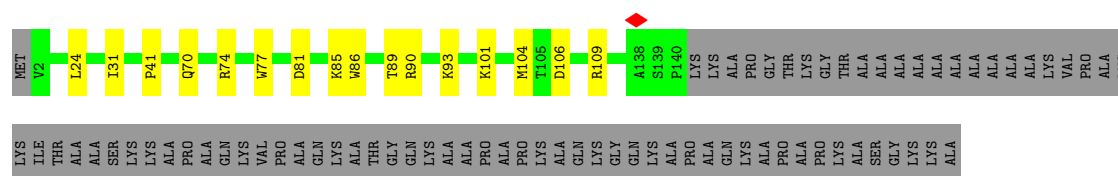
- Molecule 14: 60S ribosomal protein L13

Chain LL:  86% 12% .



- Molecule 15: 60S ribosomal protein L14

Chain LM:  57% 7% 35%



- Molecule 16: 60S ribosomal protein L15

Chain LN:  85% 13% .

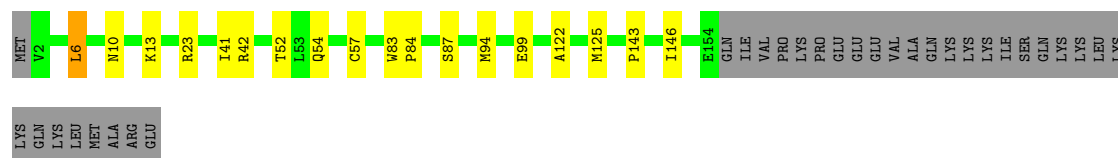
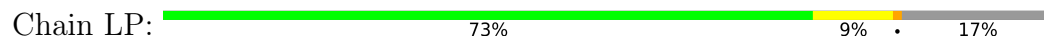


- Molecule 17: 60S ribosomal protein L13a

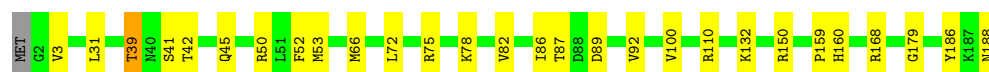
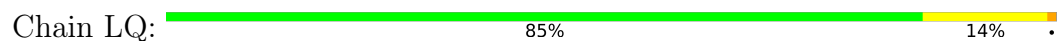
Chain LO:  86% 11% ..



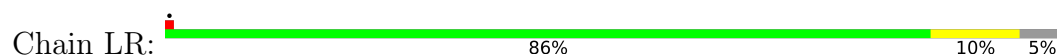
- Molecule 18: 60S ribosomal protein L17



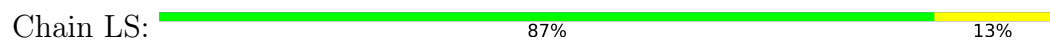
- Molecule 19: 60S ribosomal protein L18



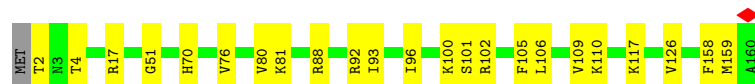
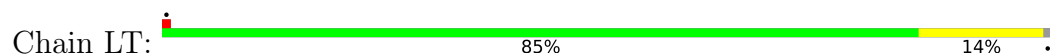
- Molecule 20: 60S ribosomal protein L19



- Molecule 21: 60S ribosomal protein L18a



- Molecule 22: 60S ribosomal protein L21

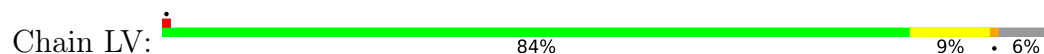


- Molecule 23: 60S ribosomal protein L22

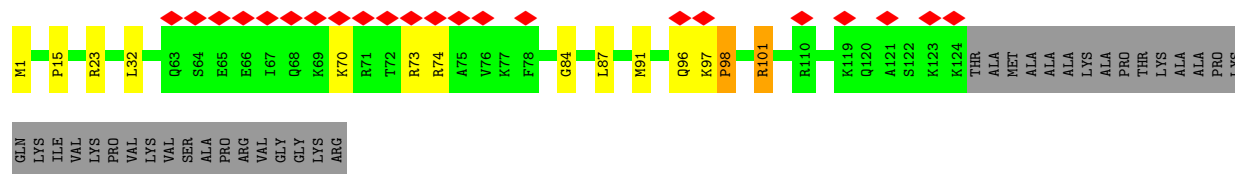




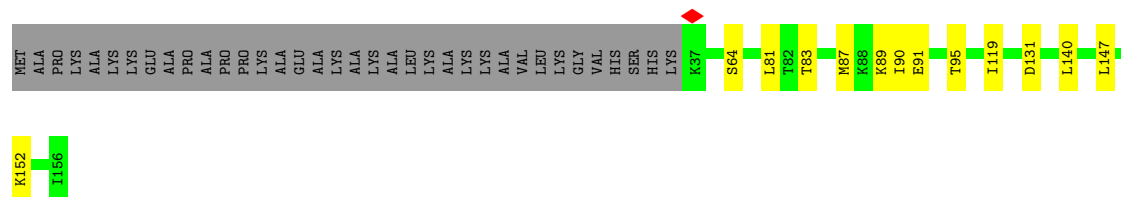
- Molecule 24: 60S ribosomal protein L23



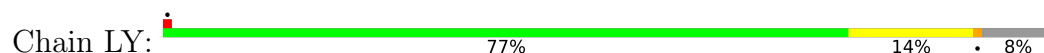
- Molecule 25: 60S ribosomal protein L24



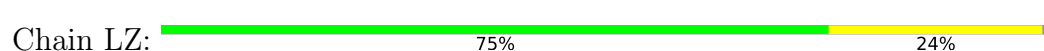
- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26

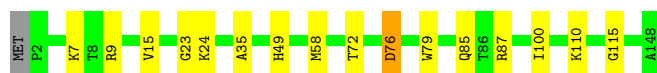


- Molecule 28: 60S ribosomal protein L27

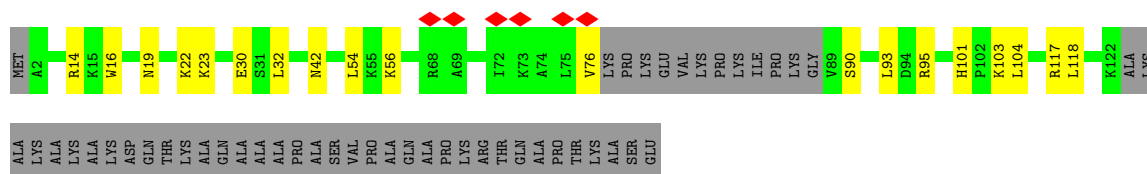


- Molecule 29: 60S ribosomal protein L27a

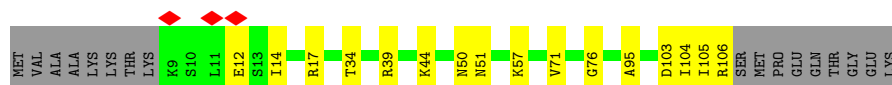




- Molecule 30: 60S ribosomal protein L29



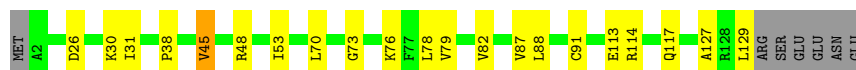
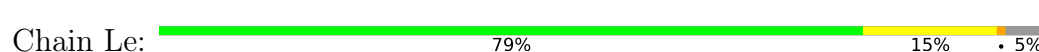
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



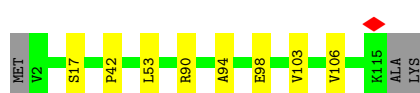
- Molecule 33: 60S ribosomal protein L32



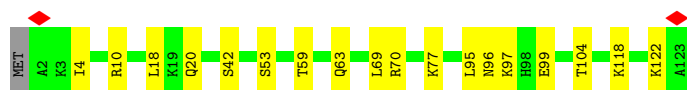
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



• Molecule 36: 60S ribosomal protein L35

Chain Lh:  85% 15%

• Molecule 37: 60S ribosomal protein L36

Chain Li:  84% 13%

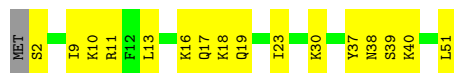
• Molecule 38: 60S ribosomal protein L37

Chain Lj:  79% 9% 11%

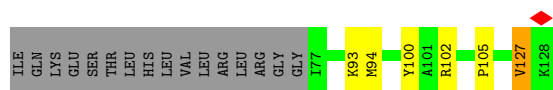
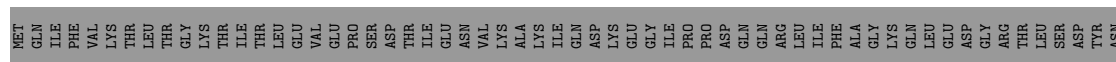
• Molecule 39: 60S ribosomal protein L38

Chain Lk:  79% 20%

• Molecule 40: 60S ribosomal protein L39

Chain Ll:  67% 31%

• Molecule 41: Ubiquitin-60S ribosomal protein L40

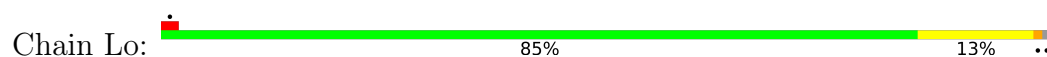
Chain Lm:  36% 59%

• Molecule 42: 60S ribosomal protein L41

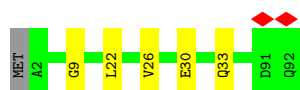
Chain Ln:  88% 8%



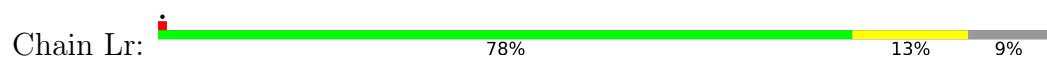
- Molecule 43: 60S ribosomal protein L36a



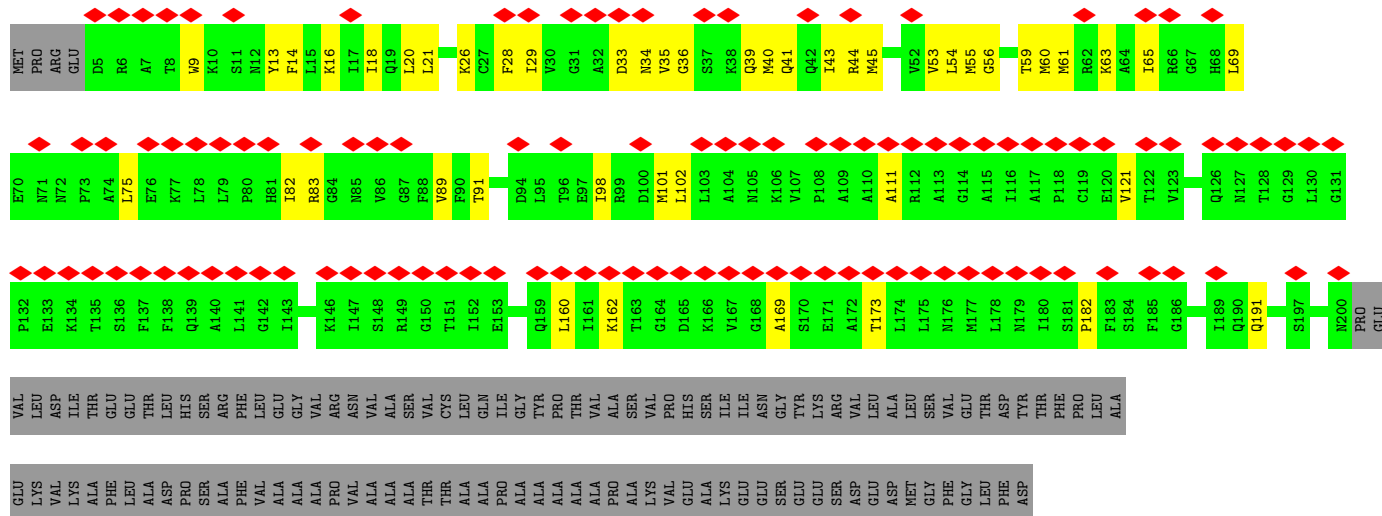
- Molecule 44: 60S ribosomal protein L37a



- Molecule 45: 60S ribosomal protein L28



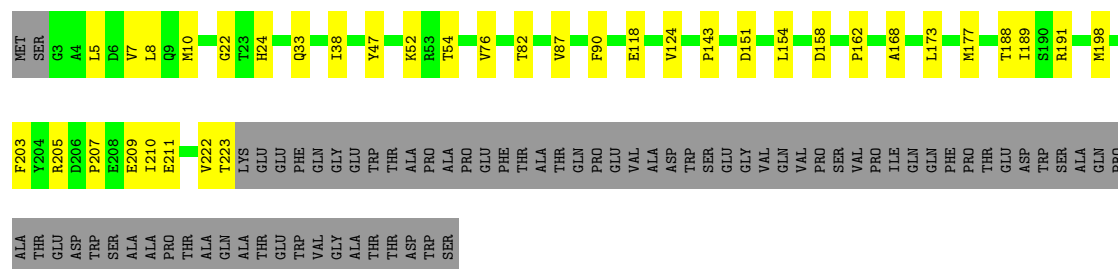
- Molecule 46: Large ribosomal subunit protein uL10



- Molecule 47: 60S ribosomal protein L12

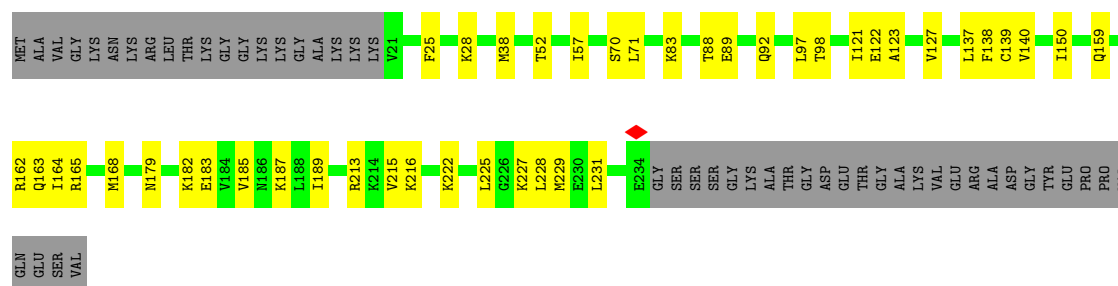






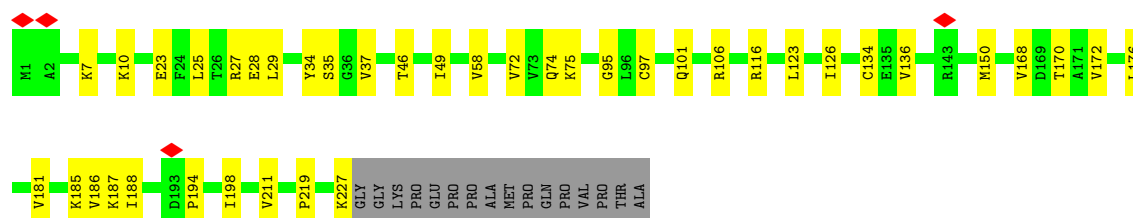
- Molecule 51: 40S ribosomal protein S3a

Chain SB: 65% 16% 19%



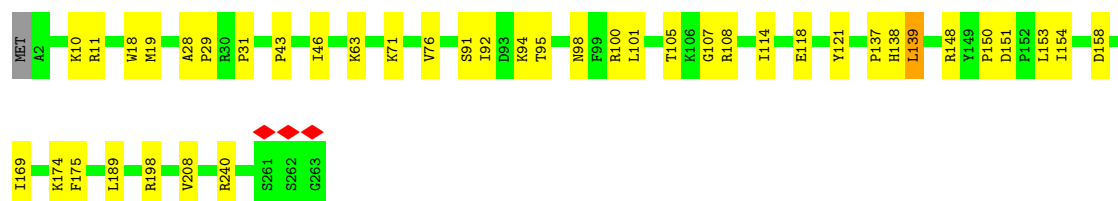
- Molecule 52: 40S ribosomal protein S3

Chain SD: 77% 16% 7%



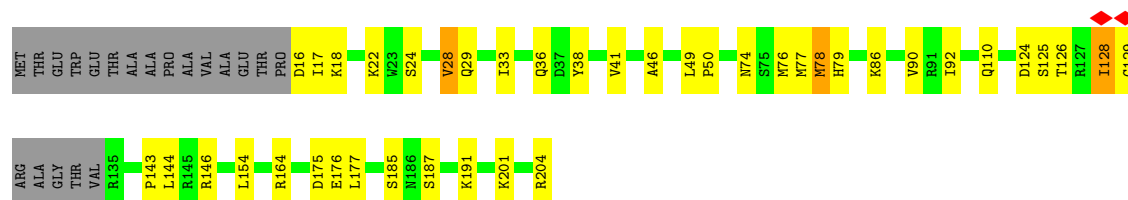
- Molecule 53: 40S ribosomal protein S4, X isoform

Chain SE: 84% 15%

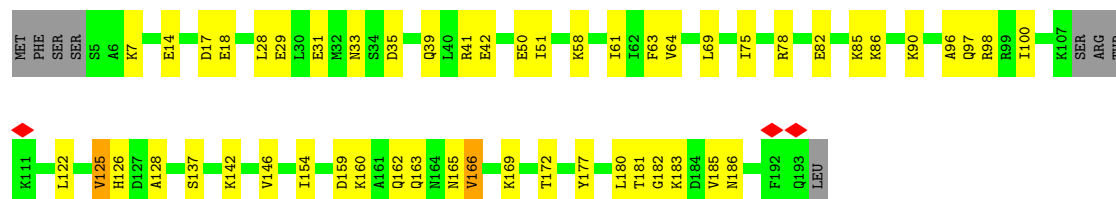


- Molecule 54: 40S ribosomal protein S5

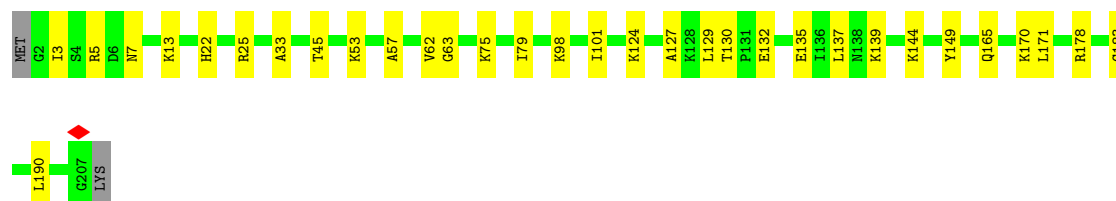
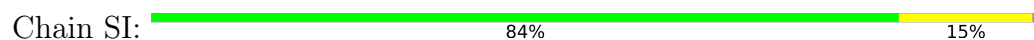
Chain SF: 70% 19% 10%



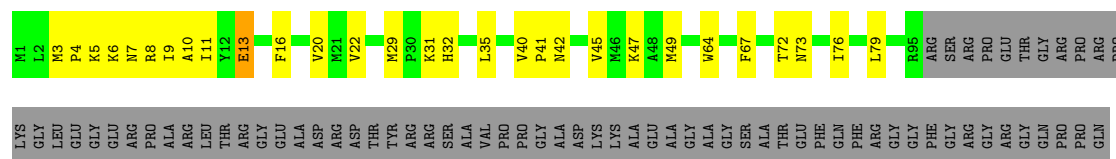
- Molecule 55: 40S ribosomal protein S7



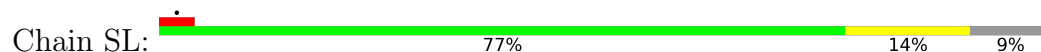
- Molecule 56: 40S ribosomal protein S8



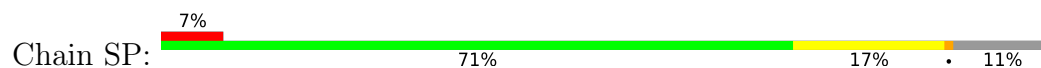
- Molecule 57: 40S ribosomal protein S10

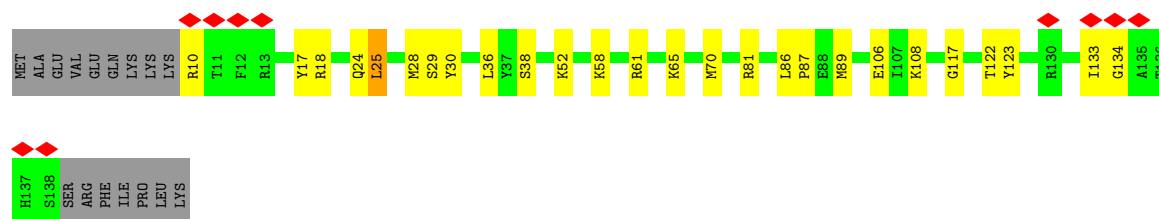


- Molecule 58: 40S ribosomal protein S11

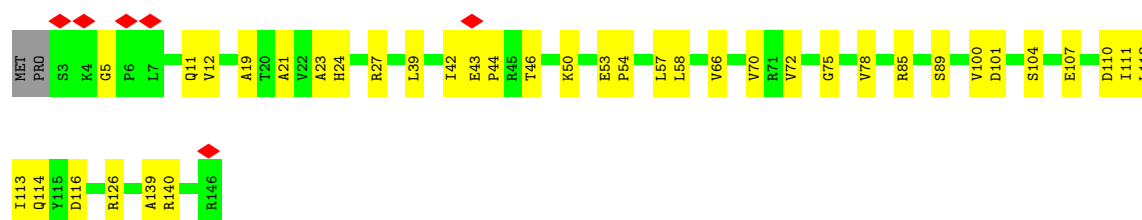
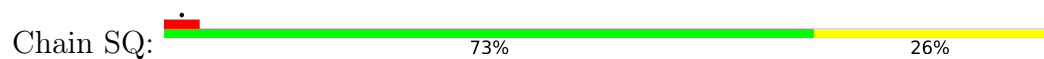


- Molecule 59: 40S ribosomal protein S15

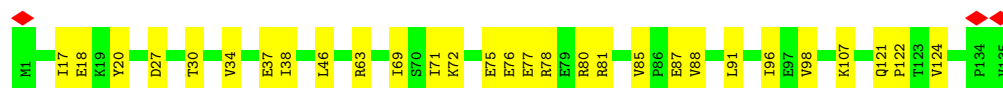
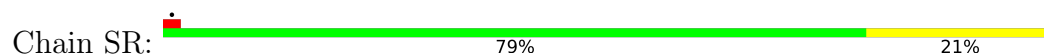




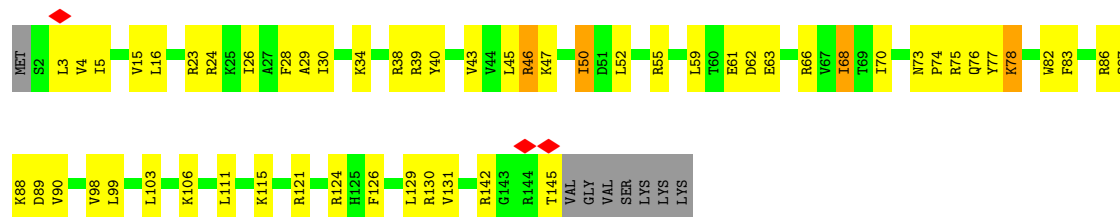
- Molecule 60: 40S ribosomal protein S16



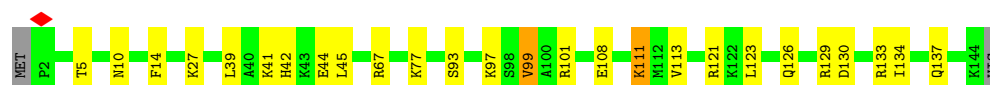
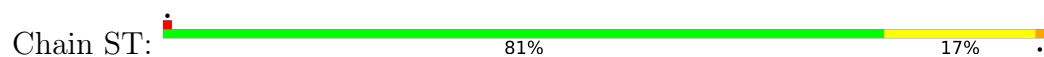
- Molecule 61: 40S ribosomal protein S17



- Molecule 62: 40S ribosomal protein S18



- Molecule 63: 40S ribosomal protein S19



- Molecule 64: 40S ribosomal protein S20

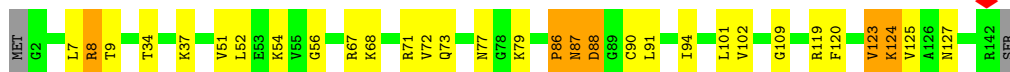
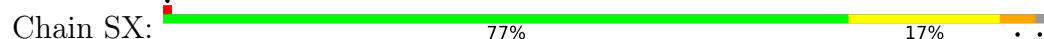




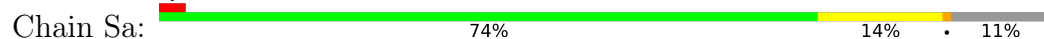
- Molecule 65: 40S ribosomal protein S21



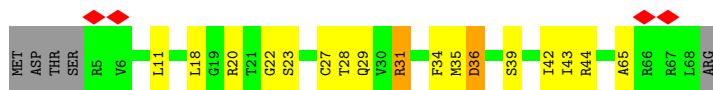
- Molecule 66: 40S ribosomal protein S23



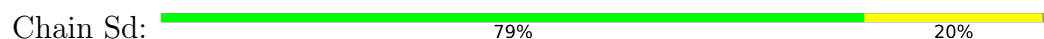
- Molecule 67: 40S ribosomal protein S26



- Molecule 68: 40S ribosomal protein S28

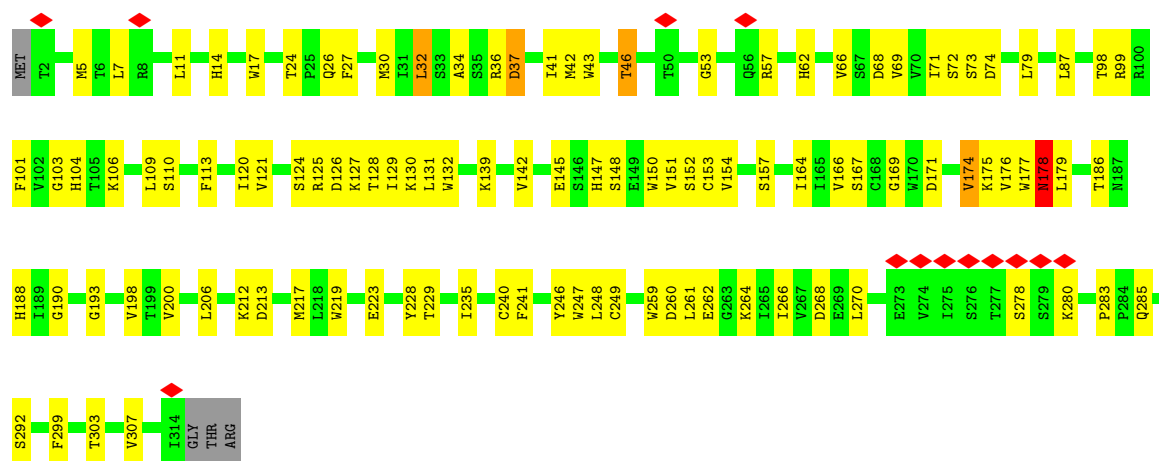


- Molecule 69: 40S ribosomal protein S29

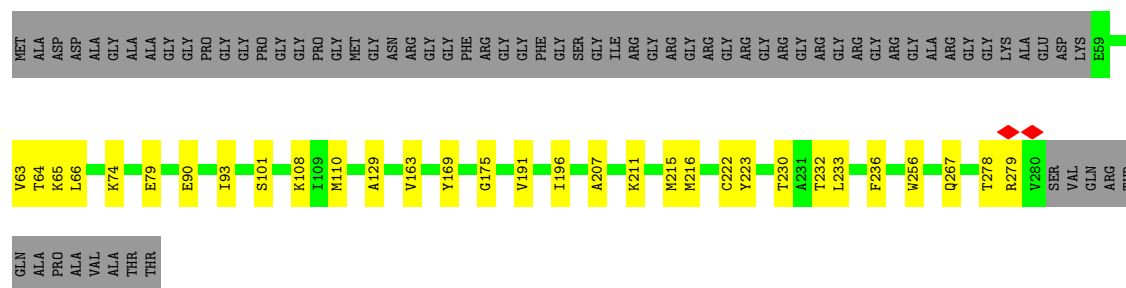


- Molecule 70: Receptor of activated protein C kinase 1

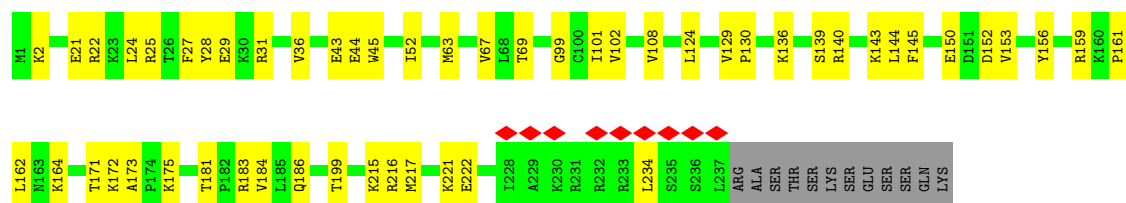
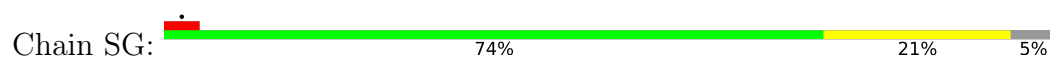




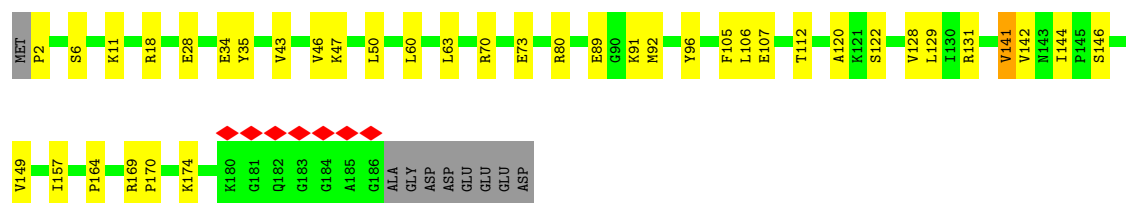
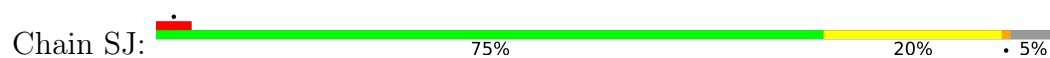
- Molecule 71: 40S ribosomal protein S2



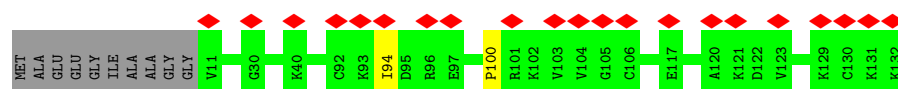
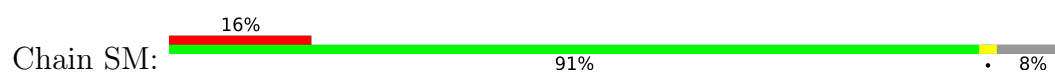
- Molecule 72: 40S ribosomal protein S6



- Molecule 73: 40S ribosomal protein S9



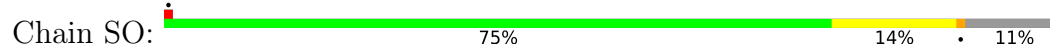
- Molecule 74: 40S ribosomal protein S12



- Molecule 75: 40S ribosomal protein S13



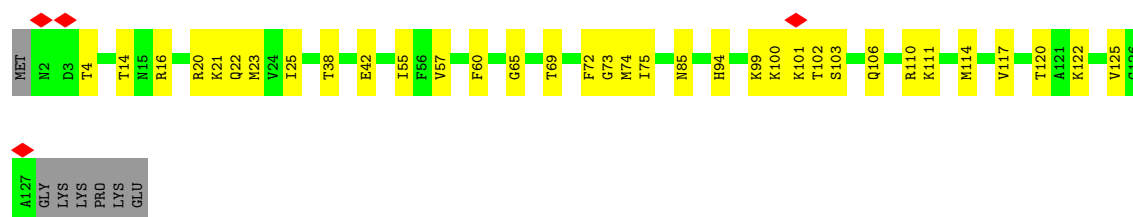
- Molecule 76: 40S ribosomal protein S14



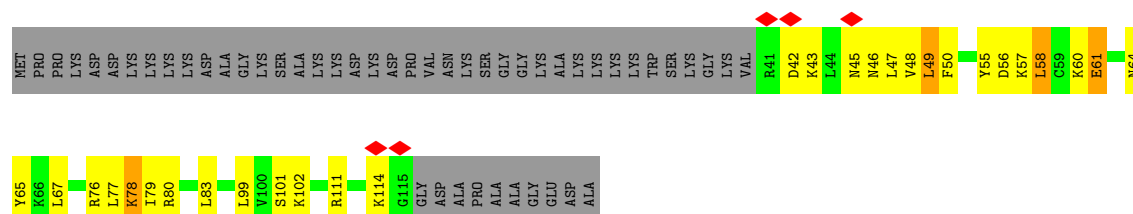
- Molecule 77: 40S ribosomal protein S15a



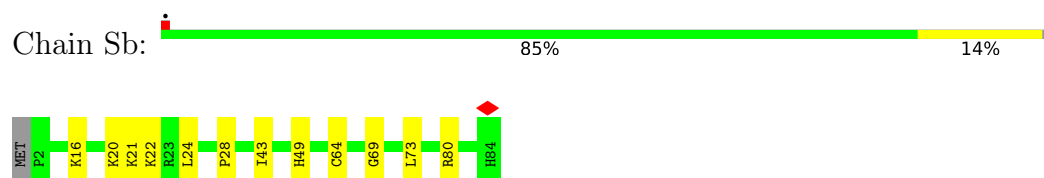
- Molecule 78: 40S ribosomal protein S24



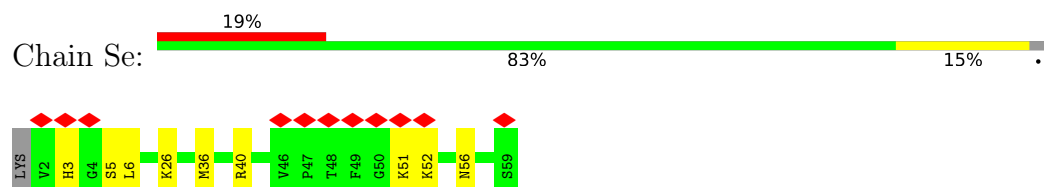
- Molecule 79: 40S ribosomal protein S25



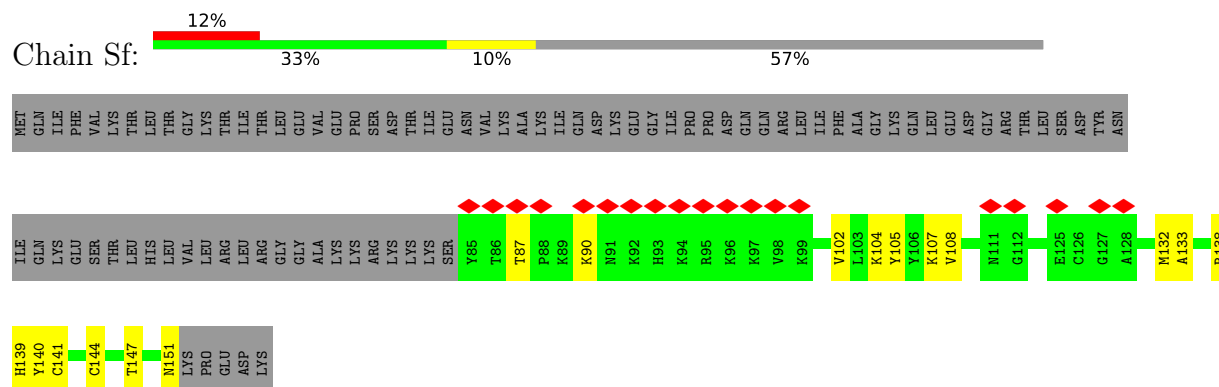
- Molecule 80: 40S ribosomal protein S27



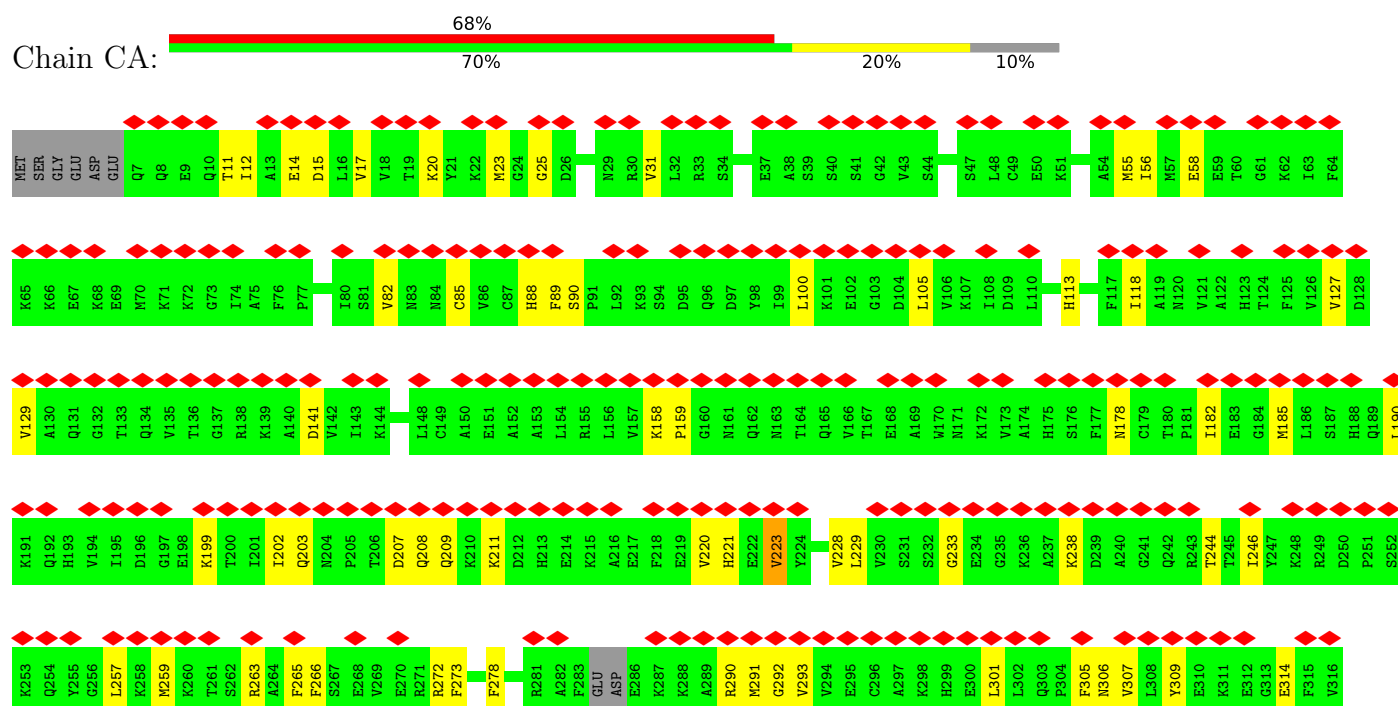
- Molecule 81: 40S ribosomal protein S30

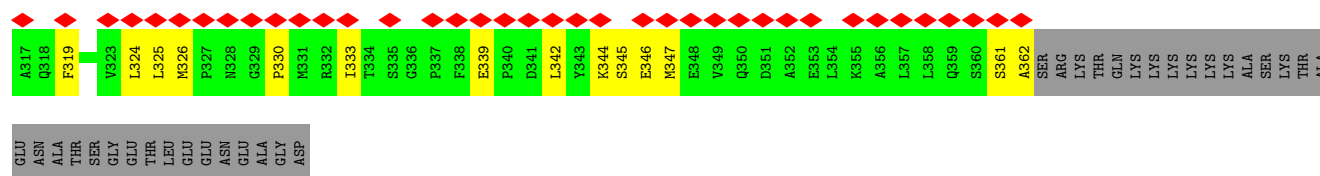


- Molecule 82: Ubiquitin-40S ribosomal protein S27a

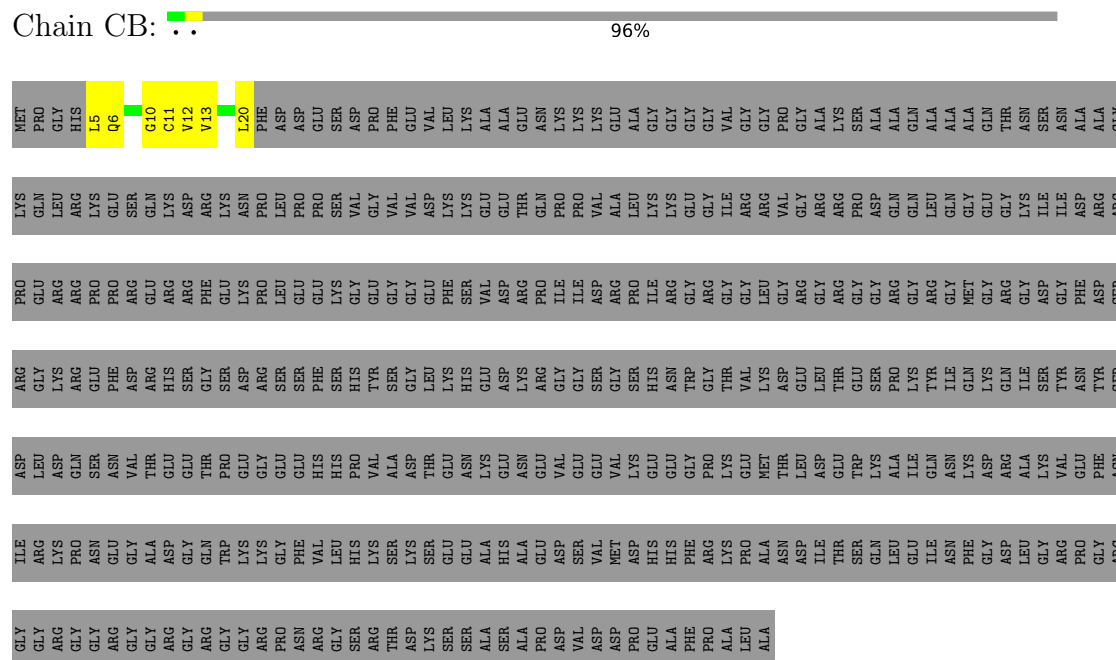


- Molecule 83: Proliferation-associated protein 2G4

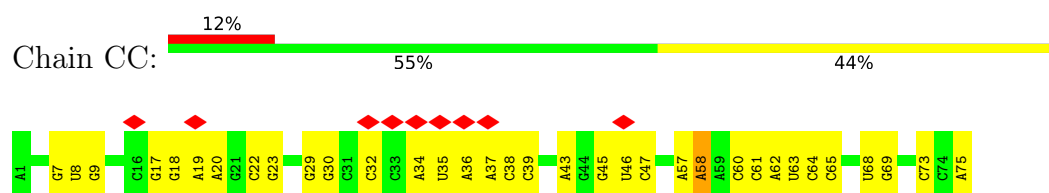




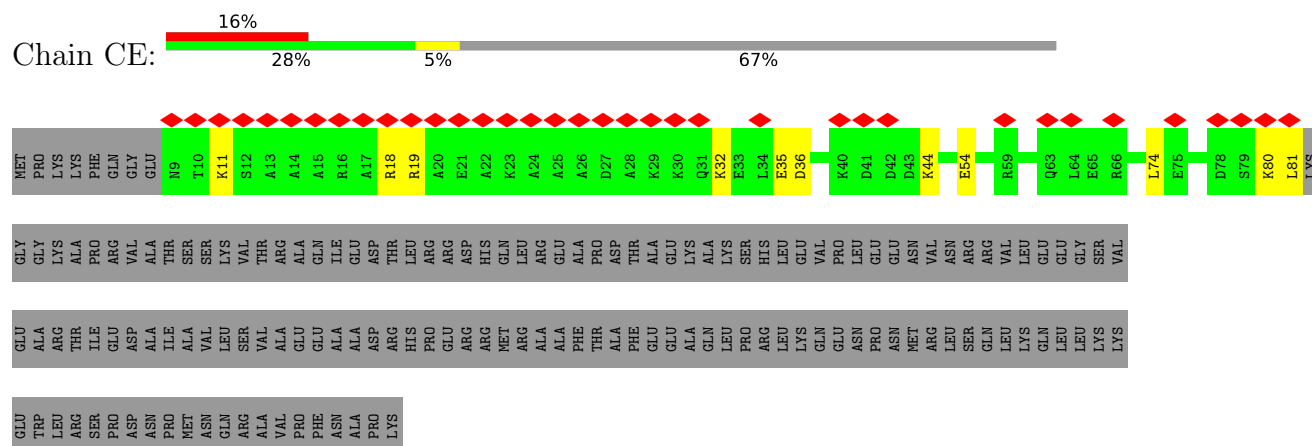
• Molecule 84: SERPINE1 mRNA-binding protein 1



• Molecule 85: tRNA-Met



• Molecule 86: Coiled-coil domain-containing protein 124



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157229	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	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.625	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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, MLZ, T1C

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	L5	0.29	0/89548	0.44	5/139613 (0.0%)
2	L7	0.31	0/2861	0.42	0/4459
3	L8	0.31	0/3701	0.43	0/5766
4	LA	0.72	0/1936	1.05	5/2596 (0.2%)
5	LB	0.50	0/3306	0.74	1/4424 (0.0%)
6	LC	0.53	0/2981	0.85	5/4002 (0.1%)
7	LD	0.55	0/2428	0.80	1/3252 (0.0%)
8	LE	0.53	0/1808	0.80	2/2425 (0.1%)
9	LF	0.39	0/1905	0.68	0/2539
10	LG	0.49	0/1960	0.75	0/2637
11	LH	0.52	0/1537	0.78	0/2066
12	LI	0.50	0/1677	0.74	1/2237 (0.0%)
13	LJ	0.60	0/1433	0.89	1/1915 (0.1%)
14	LL	0.57	0/1732	0.85	1/2315 (0.0%)
15	LM	0.52	0/1161	0.86	2/1554 (0.1%)
16	LN	0.37	0/1746	0.62	2/2338 (0.1%)
17	LO	0.53	0/1682	0.79	0/2250
18	LP	0.51	0/1268	0.83	0/1701
19	LQ	0.60	0/1537	0.84	1/2052 (0.0%)
20	LR	0.42	0/1582	0.64	0/2091
21	LS	0.64	0/1493	1.00	1/2003 (0.0%)
22	LT	0.69	0/1326	0.95	0/1770
23	LU	0.67	0/830	0.99	1/1114 (0.1%)
24	LV	0.60	0/993	0.82	1/1332 (0.1%)
25	LW	0.36	0/1030	0.61	0/1364
26	LX	0.26	0/1002	0.46	0/1345
27	LY	0.53	0/1123	0.76	1/1493 (0.1%)
28	LZ	0.61	0/1130	0.87	1/1507 (0.1%)
29	La	0.54	0/1191	0.82	1/1591 (0.1%)
30	Lb	0.40	0/889	0.66	0/1175
31	Lc	0.67	0/774	0.99	0/1038
32	Ld	0.55	0/903	0.75	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.60	0/1071	0.88	0/1429
34	Lf	0.66	0/895	0.86	0/1198
35	Lg	0.64	0/916	0.82	0/1220
36	Lh	0.51	0/1023	0.76	0/1351
37	Li	0.63	0/843	0.76	0/1115
38	Lj	0.59	0/720	0.87	0/952
39	Lk	0.68	0/575	0.81	0/761
40	Ll	0.75	0/454	0.90	0/599
41	Lm	0.42	0/425	0.65	0/561
42	Ln	0.50	0/231	0.71	0/294
43	Lo	0.65	0/876	0.83	0/1156
44	Lp	0.55	0/718	0.71	0/953
45	Lr	0.75	0/1017	0.96	0/1364
46	Ls	0.46	0/1519	0.69	0/2052
47	Lt	0.40	0/1058	0.85	4/1430 (0.3%)
48	Lz	0.57	0/1017	0.89	1/1416 (0.1%)
49	S2	0.26	0/41241	0.40	3/64258 (0.0%)
50	SA	0.69	0/1778	0.91	0/2416
51	SB	0.40	0/1765	0.64	0/2362
52	SD	0.53	0/1793	0.78	0/2414
53	SE	0.43	0/2118	0.62	0/2849
54	SF	0.72	0/1481	0.95	0/1988
55	SH	0.52	0/1519	0.93	2/2033 (0.1%)
56	SI	0.59	0/1715	0.76	0/2287
57	SK	0.66	0/823	1.02	3/1111 (0.3%)
58	SL	0.71	0/1202	0.84	0/1606
59	SP	0.33	0/1082	0.69	1/1446 (0.1%)
60	SQ	0.75	0/1160	0.96	1/1553 (0.1%)
61	SR	0.70	0/1105	0.95	0/1484
62	SS	0.59	0/1208	0.96	2/1618 (0.1%)
63	ST	0.47	0/1131	0.71	1/1515 (0.1%)
64	SU	0.65	0/831	0.82	0/1115
65	SV	0.69	0/643	0.87	0/860
66	SX	0.69	0/1116	0.99	2/1490 (0.1%)
67	Sa	0.51	0/836	0.70	0/1121
68	Sc	0.87	0/508	1.05	2/680 (0.3%)
69	Sd	0.24	0/470	0.57	0/623
70	Sg	0.62	0/2493	0.87	0/3394
71	SC	0.54	0/1762	0.81	1/2381 (0.0%)
72	SG	0.49	0/1946	0.76	1/2590 (0.0%)
73	SJ	0.62	1/1550 (0.1%)	0.79	0/2069
74	SM	0.39	0/603	0.72	0/837
75	SN	0.49	0/1232	0.69	1/1656 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SO	0.67	0/1023	0.87	0/1372
77	SW	0.63	0/1051	0.92	2/1406 (0.1%)
78	SY	0.55	0/1044	0.79	2/1388 (0.1%)
79	SZ	0.59	0/604	0.87	0/810
80	Sb	0.56	0/665	0.80	0/891
81	Se	0.40	0/465	0.64	0/612
82	Sf	0.24	0/560	0.60	0/745
83	CA	0.22	0/2810	0.55	0/3780
84	CB	0.92	0/128	1.08	0/171
85	CC	0.21	0/1798	0.38	0/2802
86	CE	0.42	0/616	0.61	0/812
All	All	0.42	1/239706 (0.0%)	0.60	62/351576 (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	LB	0	1
34	Lf	0	1
54	SF	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	SJ	2	PRO	N-CD	-8.90	1.35	1.47

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	SH	14	GLU	CA-C-N	12.41	138.86	121.61
55	SH	14	GLU	C-N-CA	12.41	138.86	121.61
47	Lt	9	GLU	CA-C-N	9.32	131.29	121.97
47	Lt	9	GLU	C-N-CA	9.32	131.29	121.97
8	LE	156	ARG	N-CA-C	-8.71	102.66	113.38
21	LS	155	PRO	N-CA-C	8.69	125.61	113.53
48	Lz	200	ASN	N-CA-C	8.44	120.16	110.97
68	Sc	36	ASP	N-CA-C	-8.26	103.03	113.43
6	LC	151	PRO	N-CA-C	-8.19	95.59	112.47
14	LL	50	PRO	N-CA-C	7.87	128.69	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	SK	67	PHE	CA-CB-CG	7.52	121.32	113.80
4	LA	197	PRO	CB-CA-C	7.46	123.87	111.56
4	LA	122	ASP	CA-CB-CG	7.13	119.73	112.60
4	LA	123	ARG	CB-CA-C	6.64	123.63	110.42
49	S2	688	U	C2'-C3'-O3'	6.51	119.27	109.50
12	LI	81	GLY	CA-C-O	-6.46	117.80	122.45
49	S2	291	G	C2'-C3'-O3'	6.41	123.31	113.70
60	SQ	114	GLN	CA-CB-CG	6.39	126.89	114.10
19	LQ	52	PHE	CA-CB-CG	6.14	119.94	113.80
63	ST	111	LYS	CA-CB-CG	6.07	126.25	114.10
72	SG	139	SER	N-CA-C	-6.05	107.72	114.62
57	SK	13	GLU	CA-CB-CG	6.02	126.15	114.10
4	LA	195	CYS	CB-CA-C	-6.00	100.13	109.80
1	L5	2675	G	C2'-C3'-O3'	5.99	118.48	109.50
49	S2	112	U	C2'-C3'-O3'	5.93	122.60	113.70
13	LJ	123	ILE	CA-CB-CG1	5.92	120.47	110.40
57	SK	13	GLU	N-CA-CB	5.92	119.41	110.30
62	SS	46	ARG	N-CA-C	-5.87	106.24	113.41
78	SY	94	HIS	CB-CA-C	5.82	120.11	110.74
6	LC	2	ALA	CA-C-N	5.80	132.13	121.70
6	LC	2	ALA	C-N-CA	5.80	132.13	121.70
8	LE	50	LEU	N-CA-C	-5.72	106.34	113.55
59	SP	70	MET	CB-CG-SD	5.70	129.79	112.70
68	Sc	22	GLY	CA-C-O	-5.67	118.37	122.45
77	SW	59	GLY	CA-C-O	-5.61	118.36	122.23
1	L5	2033	A	C2'-C3'-O3'	5.60	117.90	109.50
4	LA	197	PRO	N-CA-C	-5.58	100.97	112.47
1	L5	417	G	O4'-C1'-N9	5.53	116.50	108.20
15	LM	31	ILE	CA-C-N	5.47	130.13	122.36
15	LM	31	ILE	C-N-CA	5.47	130.13	122.36
24	LV	40	ILE	N-CA-C	-5.45	107.05	113.42
47	Lt	10	ILE	N-CA-CB	5.44	117.02	109.84
23	LU	33	ILE	N-CA-C	-5.37	107.58	113.43
75	SN	136	PRO	O-C-N	-5.36	118.84	121.31
66	SX	8	ARG	CB-CG-CD	5.32	123.53	111.30
27	LY	53	ASP	CA-CB-CG	5.32	117.92	112.60
6	LC	63	SER	CA-C-N	-5.25	113.09	122.07
6	LC	63	SER	C-N-CA	-5.25	113.09	122.07
77	SW	50	PHE	CA-CB-CG	5.25	119.05	113.80
28	LZ	76	ASN	CA-CB-CG	5.24	117.84	112.60
1	L5	2033	A	C4'-C3'-O3'	5.22	117.23	109.40
16	LN	122	GLY	CA-C-N	-5.20	111.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	LN	122	GLY	C-N-CA	-5.20	111.60	121.54
1	L5	4913	G	C2'-C3'-O3'	5.18	117.28	109.50
78	SY	94	HIS	N-CA-C	-5.17	98.98	108.02
5	LB	120	LYS	N-CA-C	-5.16	107.15	113.50
66	SX	86	PRO	CA-C-O	-5.13	115.41	121.67
47	Lt	116	MET	CA-CB-CG	5.12	124.34	114.10
62	SS	52	LEU	N-CA-C	-5.07	107.10	113.28
71	SC	101	SER	N-CA-C	-5.06	108.85	114.62
29	La	76	ASP	CA-CB-CG	5.04	117.64	112.60
7	LD	200	MET	CB-CG-SD	5.00	127.71	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LB	258	HIS	Peptide
34	Lf	106	TYR	Peptide
54	SF	78	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	80096	0	40359	454	0
2	L7	2561	0	1295	8	0
3	L8	3314	0	1683	15	0
4	LA	1898	0	1993	23	0
5	LB	3238	0	3376	37	0
6	LC	2927	0	3104	38	0
7	LD	2382	0	2410	18	0
8	LE	1774	0	1930	30	0
9	LF	1870	0	1996	16	0
10	LG	1927	0	2074	35	0
11	LH	1518	0	1601	21	0
12	LI	1639	0	1687	23	0
13	LJ	1410	0	1441	23	0
14	LL	1701	0	1818	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	LM	1138	0	1204	13	0
16	LN	1701	0	1749	26	0
17	LO	1650	0	1794	24	0
18	LP	1242	0	1269	9	0
19	LQ	1513	0	1628	23	0
20	LR	1566	0	1729	13	0
21	LS	1453	0	1490	11	0
22	LT	1298	0	1366	16	0
23	LU	816	0	842	17	0
24	LV	979	0	1039	11	0
25	LW	1015	0	1079	12	0
26	LX	985	0	1066	13	0
27	LY	1106	0	1192	12	0
28	LZ	1107	0	1182	35	0
29	La	1162	0	1213	10	0
30	Lb	876	0	948	15	0
31	Lc	764	0	804	23	0
32	Ld	888	0	930	13	0
33	Le	1053	0	1147	12	0
34	Lf	876	0	912	5	0
35	Lg	906	0	998	6	0
36	Lh	1015	0	1148	14	0
37	Li	832	0	917	11	0
38	Lj	705	0	736	4	0
39	Lk	569	0	637	10	0
40	Ll	444	0	483	14	0
41	Lm	430	0	466	5	0
42	Ln	230	0	276	2	0
43	Lo	862	0	929	12	0
44	Lp	708	0	756	4	0
45	Lr	1002	0	1068	17	0
46	Ls	1496	0	1540	84	0
47	Lt	1046	0	1076	39	0
48	Lz	1018	0	448	3	0
49	S2	36896	0	18603	246	0
50	SA	1741	0	1746	28	0
51	SB	1738	0	1809	25	0
52	SD	1765	0	1865	25	0
53	SE	2076	0	2177	31	0
54	SF	1461	0	1511	31	0
55	SH	1497	0	1590	46	0
56	SI	1686	0	1772	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	SK	799	0	823	25	0
58	SL	1182	0	1253	23	0
59	SP	1061	0	1107	18	0
60	SQ	1142	0	1213	24	0
61	SR	1090	0	1149	40	0
62	SS	1190	0	1249	36	0
63	ST	1112	0	1146	25	0
64	SU	821	0	883	27	0
65	SV	636	0	637	9	0
66	SX	1098	0	1167	30	0
67	Sa	821	0	870	14	0
68	Sc	506	0	536	13	0
69	Sd	459	0	450	7	0
70	Sg	2436	0	2393	100	0
71	SC	1725	0	1813	23	0
72	SG	1923	0	2088	42	0
73	SJ	1525	0	1640	29	0
74	SM	604	0	281	1	0
75	SN	1208	0	1294	9	0
76	SO	1010	0	1034	16	0
77	SW	1034	0	1080	8	0
78	SY	1027	0	1093	31	0
79	SZ	598	0	656	27	0
80	Sb	651	0	672	10	0
81	Se	459	0	503	11	0
82	Sf	548	0	551	11	0
83	CA	2764	0	2779	74	0
84	CB	127	0	120	24	0
85	CC	1607	0	815	8	0
86	CE	613	0	625	11	0
87	L5	215	0	0	0	0
87	L7	3	0	0	0	0
87	L8	4	0	0	0	0
87	LA	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	2	0	0	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	29	0	0	0	0
87	SG	1	0	0	0	0
88	CC	42	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L5	294	0	266	7	0
88	S2	42	0	38	1	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	0	0
89	Sf	1	0	0	0	0
All	All	223987	0	166163	2138	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 (2138) 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)
46:Ls:13:TYR:CE2	46:Ls:60:MET:HE2	1.54	1.43
1:L5:1998:A:C4	46:Ls:55:MET:HE2	1.58	1.39
70:Sg:42:MET:CE	70:Sg:57:ARG:HB3	1.48	1.38
1:L5:1998:A:C5	46:Ls:55:MET:HE2	1.63	1.33
58:SL:104:LYS:CE	66:SX:8:ARG:HH21	1.44	1.29
70:Sg:42:MET:HE3	70:Sg:57:ARG:CB	1.61	1.29
81:Se:36:MET:HE3	81:Se:40:ARG:NH2	1.49	1.25
11:LH:142:ASP:OD1	11:LH:142:ASP:O	1.55	1.24
59:SP:24:GLN:O	59:SP:28:MET:HG3	1.40	1.21
1:L5:1998:A:C4	46:Ls:55:MET:CE	2.22	1.21
84:CB:6:GLN:NE2	84:CB:13:VAL:H	1.38	1.20
58:SL:104:LYS:CE	66:SX:8:ARG:NH2	2.05	1.18
23:LU:18:VAL:O	23:LU:19:LEU:HD12	1.44	1.16
23:LU:29:VAL:HG21	23:LU:68:SER:OG	1.45	1.16
84:CB:6:GLN:HE22	84:CB:13:VAL:N	1.43	1.15
70:Sg:32:LEU:HD11	70:Sg:42:MET:HG2	1.15	1.15
31:Lc:106:ARG:HH21	84:CB:10:GLY:CA	1.58	1.15
46:Ls:20:LEU:CD1	46:Ls:54:LEU:HD13	1.76	1.14
1:L5:1998:A:N9	46:Ls:55:MET:CE	2.11	1.13
70:Sg:42:MET:CE	70:Sg:57:ARG:CB	2.19	1.11
1:L5:1998:A:C8	46:Ls:55:MET:HE3	1.86	1.09
49:S2:84:A:H5"	78:SY:122:LYS:HD2	1.27	1.09
1:L5:1378:C:C6	14:LL:158:ARG:NH1	2.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ls:39:GLN:NE2	46:Ls:40:MET:SD	2.26	1.08
79:SZ:46:ASN:O	79:SZ:47:LEU:CD2	2.00	1.08
46:Ls:60:MET:HE1	46:Ls:61:MET:HG2	1.33	1.08
70:Sg:32:LEU:CD1	70:Sg:42:MET:HG2	1.83	1.08
6:LC:189:MET:HE1	6:LC:201:ARG:HG2	1.37	1.07
49:S2:1756:C:H42	49:S2:1776:G:N2	1.49	1.07
46:Ls:13:TYR:HE2	46:Ls:60:MET:CE	1.67	1.07
49:S2:1756:C:N4	49:S2:1776:G:H22	1.52	1.07
46:Ls:55:MET:SD	46:Ls:56:GLY:N	2.28	1.06
1:L5:1998:A:C8	46:Ls:55:MET:CE	2.37	1.06
31:Lc:106:ARG:HH21	84:CB:10:GLY:HA3	0.96	1.06
56:SI:135:GLU:CG	56:SI:139:LYS:HE2	1.85	1.06
46:Ls:20:LEU:HD11	46:Ls:54:LEU:HD13	1.31	1.05
58:SL:104:LYS:HE3	66:SX:8:ARG:HH21	1.11	1.05
49:S2:886:A:N6	49:S2:901:G:C4	2.25	1.04
54:SF:128:ILE:HG22	54:SF:129:GLY:N	1.57	1.04
1:L5:1176:C:N4	1:L5:1184:A:H61	1.55	1.04
31:Lc:106:ARG:NH2	84:CB:10:GLY:HA3	1.69	1.04
58:SL:104:LYS:HE2	66:SX:8:ARG:HH21	1.21	1.03
1:L5:1176:C:H42	1:L5:1184:A:N6	1.54	1.03
70:Sg:30:MET:O	70:Sg:30:MET:HE3	1.57	1.03
46:Ls:98:ILE:O	46:Ls:101:MET:HE3	1.57	1.02
24:LV:36:ASN:HD21	24:LV:66:LYS:HB2	1.18	1.02
58:SL:104:LYS:HE2	66:SX:8:ARG:NH2	1.67	1.02
54:SF:128:ILE:CG2	54:SF:129:GLY:H	1.71	1.01
25:LW:1:MET:HG3	25:LW:1:MET:O	1.56	1.01
46:Ls:13:TYR:CZ	46:Ls:60:MET:HE2	1.95	1.01
83:CA:290:ARG:O	83:CA:293:VAL:CG1	2.08	1.01
46:Ls:101:MET:HE1	46:Ls:102:LEU:HD23	1.40	1.00
24:LV:36:ASN:ND2	24:LV:66:LYS:HB2	1.76	1.00
40:Ll:23:ILE:HD12	40:Ll:23:ILE:O	1.59	1.00
56:SI:135:GLU:HG2	56:SI:139:LYS:CE	1.91	1.00
28:LZ:102:ARG:HB3	28:LZ:102:ARG:HH11	1.24	0.99
46:Ls:60:MET:SD	46:Ls:60:MET:C	2.46	0.98
56:SI:135:GLU:CG	56:SI:139:LYS:CE	2.40	0.98
1:L5:1378:C:C5	14:LL:158:ARG:NH1	2.30	0.98
70:Sg:32:LEU:HD11	70:Sg:42:MET:CG	1.91	0.98
58:SL:104:LYS:HE3	66:SX:8:ARG:NH2	1.73	0.98
54:SF:128:ILE:HG22	54:SF:129:GLY:H	0.84	0.98
46:Ls:13:TYR:CE2	46:Ls:60:MET:CE	2.43	0.97
46:Ls:60:MET:CE	46:Ls:61:MET:HG2	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LZ:102:ARG:HB3	28:LZ:102:ARG:NH1	1.80	0.97
7:LD:208:MET:O	7:LD:212:MET:HG2	1.66	0.96
80:Sb:80:ARG:HG2	80:Sb:80:ARG:HH11	1.29	0.96
81:Se:36:MET:HE3	81:Se:40:ARG:HH21	1.04	0.96
79:SZ:46:ASN:O	79:SZ:47:LEU:HD23	1.62	0.95
58:SL:18:GLN:HG2	58:SL:33:LEU:HD11	1.48	0.95
83:CA:290:ARG:O	83:CA:293:VAL:HG13	1.64	0.95
1:L5:1175:A:C2	1:L5:1185:G:N1	2.33	0.95
10:LG:210:GLU:OE1	10:LG:210:GLU:N	2.00	0.94
70:Sg:42:MET:HE2	70:Sg:57:ARG:HB3	1.49	0.94
1:L5:1175:A:H2	1:L5:1185:G:H1	1.12	0.94
46:Ls:101:MET:SD	46:Ls:102:LEU:N	2.40	0.94
1:L5:1976:G:N1	1:L5:1991:A:C2	2.35	0.94
55:SH:35:ASP:OD2	55:SH:78:ARG:NH2	2.00	0.93
56:SI:135:GLU:HG2	56:SI:139:LYS:HE3	1.49	0.93
70:Sg:42:MET:HE3	70:Sg:57:ARG:HB3	0.94	0.93
31:Lc:50:ASN:OD1	31:Lc:51:ASN:N	2.02	0.92
83:CA:290:ARG:C	83:CA:293:VAL:HG12	1.95	0.91
50:SA:143:PRO:HB2	65:SV:34:MET:HE3	1.49	0.91
68:Sc:20:ARG:HD3	68:Sc:28:THR:HG22	1.53	0.91
1:L5:1095:A:H2	1:L5:1200:G:H1	1.19	0.90
1:L5:1175:A:H2	1:L5:1185:G:N1	1.66	0.90
56:SI:135:GLU:HG3	56:SI:139:LYS:HE2	1.52	0.90
79:SZ:46:ASN:O	79:SZ:47:LEU:HD22	1.69	0.90
71:SC:129:ALA:HB1	71:SC:216:MET:HE1	1.51	0.90
39:Lk:27:LYS:CE	39:Lk:68:GLU:OE2	2.20	0.90
56:SI:62:VAL:HG11	56:SI:75:LYS:CE	2.02	0.89
49:S2:1673:U:H5'	60:SQ:78:VAL:HG12	1.53	0.89
43:Lo:71:GLU:OE1	43:Lo:80:LYS:NZ	2.04	0.89
61:SR:77:GLU:CD	61:SR:81:ARG:HH12	1.81	0.88
54:SF:128:ILE:CG2	54:SF:129:GLY:N	2.33	0.88
46:Ls:20:LEU:HD11	46:Ls:54:LEU:CD1	2.03	0.88
1:L5:1341:U:O3'	16:LN:204:ARG:NH1	2.08	0.87
72:SG:63:MET:HG2	72:SG:99:GLY:O	1.74	0.87
31:Lc:14:ILE:HD11	84:CB:11:CYS:CB	2.05	0.87
46:Ls:61:MET:HE3	46:Ls:82:ILE:HD11	1.57	0.87
55:SH:35:ASP:CG	55:SH:78:ARG:HH21	1.82	0.87
83:CA:290:ARG:HA	83:CA:293:VAL:CG1	2.05	0.87
28:LZ:102:ARG:NH1	28:LZ:102:ARG:CB	2.38	0.86
62:SS:3:LEU:HG	62:SS:4:VAL:N	1.89	0.86
1:L5:1707:C:C2	30:Lb:103:LYS:NZ	2.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:175:MET:HA	17:LO:175:MET:HE2	1.57	0.86
39:Lk:27:LYS:HE2	39:Lk:68:GLU:OE2	1.75	0.86
1:L5:4148:C:OP1	28:LZ:59:LYS:HE3	1.76	0.85
56:SI:62:VAL:HG11	56:SI:75:LYS:HE2	1.58	0.84
8:LE:120:ASP:OD2	45:Lr:112:ARG:NH2	2.09	0.84
59:SP:86:LEU:H	59:SP:89:MET:HE3	1.41	0.84
46:Ls:61:MET:HE3	46:Ls:82:ILE:CD1	2.08	0.83
23:LU:18:VAL:HG11	23:LU:78:PHE:H	1.42	0.83
1:L5:493:G:H1	1:L5:660:A:H2	1.26	0.83
46:Ls:61:MET:CE	46:Ls:82:ILE:HD11	2.09	0.83
71:SC:129:ALA:CB	71:SC:216:MET:HE1	2.08	0.83
61:SR:18:GLU:OE2	61:SR:69:ILE:HA	1.78	0.83
1:L5:1998:A:C5	46:Ls:55:MET:CE	2.53	0.83
26:LX:131:ASP:O	26:LX:131:ASP:OD1	1.97	0.83
63:ST:111:LYS:NZ	63:ST:126:GLN:HB3	1.94	0.83
68:Sc:43:ILE:HG22	68:Sc:65:ALA:HB3	1.61	0.82
56:SI:129:LEU:HD13	56:SI:137:LEU:HD12	1.60	0.82
23:LU:29:VAL:CG2	23:LU:68:SER:OG	2.26	0.82
47:Lt:38:SER:OG	47:Lt:39:PRO:HD3	1.78	0.82
31:Lc:14:ILE:HD11	84:CB:11:CYS:HB2	1.61	0.81
49:S2:84:A:C5'	78:SY:122:LYS:HD2	2.10	0.81
56:SI:45:THR:HG23	56:SI:53:LYS:HG3	1.63	0.81
49:S2:834:C:H42	49:S2:839:C:H42	1.29	0.81
49:S2:925:G:H1	49:S2:1017:U:H3	1.25	0.81
70:Sg:32:LEU:HD12	70:Sg:42:MET:HA	1.63	0.81
83:CA:88:HIS:O	83:CA:307:VAL:CG2	2.29	0.81
25:LW:97:LYS:HA	25:LW:101:ARG:HG3	1.63	0.81
64:SU:46:LYS:HZ1	64:SU:97:ILE:HB	1.46	0.81
83:CA:290:ARG:CA	83:CA:293:VAL:HG12	2.11	0.81
19:LQ:159:PRO:HD3	19:LQ:188:ASN:HD21	1.46	0.80
83:CA:290:ARG:HA	83:CA:293:VAL:HG12	1.63	0.80
46:Ls:60:MET:SD	46:Ls:61:MET:N	2.54	0.80
10:LG:106:THR:OG1	10:LG:109:GLU:HG3	1.83	0.79
6:LC:189:MET:CE	6:LC:201:ARG:HG2	2.11	0.79
63:ST:111:LYS:HZ2	63:ST:126:GLN:HB3	1.45	0.79
10:LG:214:ALA:HA	10:LG:217:LYS:HE2	1.65	0.79
24:LV:36:ASN:HD21	24:LV:66:LYS:CB	1.95	0.79
1:L5:1378:C:N1	14:LL:158:ARG:NH1	2.30	0.79
1:L5:1378:C:C4	14:LL:158:ARG:NH1	2.50	0.79
1:L5:2483:G:H1	1:L5:2495:U:H3	1.29	0.79
78:SY:23:MET:HE1	78:SY:75:ILE:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SU:87:ARG:HG2	64:SU:87:ARG:HH11	1.48	0.79
83:CA:220:VAL:HG23	83:CA:221:HIS:CD2	2.17	0.78
83:CA:290:ARG:O	83:CA:293:VAL:HG12	1.82	0.78
52:SD:123:LEU:HD12	52:SD:134:CYS:SG	2.23	0.78
80:Sb:80:ARG:HG2	80:Sb:80:ARG:NH1	1.94	0.78
28:LZ:84:ARG:HD3	84:CB:20:LEU:HD13	1.66	0.78
6:LC:156:ASP:OD2	6:LC:255:SER:OG	2.02	0.78
49:S2:1673:U:H5''	60:SQ:78:VAL:CG1	2.12	0.78
77:SW:111:MET:SD	77:SW:115:GLU:HG2	2.23	0.77
67:Sa:45:VAL:HG11	67:Sa:64:LEU:HD13	1.66	0.77
64:SU:46:LYS:NZ	64:SU:97:ILE:HB	1.98	0.77
78:SY:110:ARG:O	78:SY:114:MET:HG3	1.85	0.77
50:SA:211:GLU:C	50:SA:211:GLU:OE1	2.27	0.77
83:CA:263:ARG:HB2	83:CA:263:ARG:HH11	1.48	0.77
49:S2:384:U:O4	56:SI:5:ARG:NH2	2.18	0.76
8:LE:90:ALA:O	8:LE:109:LEU:HD12	1.85	0.76
19:LQ:159:PRO:CD	19:LQ:188:ASN:HD21	1.97	0.76
46:Ls:55:MET:SD	46:Ls:55:MET:C	2.68	0.76
66:SX:51:VAL:HA	66:SX:72:VAL:HG22	1.66	0.76
1:L5:1998:A:N9	46:Ls:55:MET:HE1	1.99	0.76
1:L5:1378:C:C2	14:LL:158:ARG:NH1	2.53	0.76
70:Sg:30:MET:O	70:Sg:30:MET:CE	2.31	0.76
70:Sg:212:LYS:HA	70:Sg:235:ILE:HG13	1.65	0.76
70:Sg:42:MET:HE3	70:Sg:57:ARG:HB2	1.66	0.75
70:Sg:206:LEU:C	70:Sg:206:LEU:HD12	2.11	0.75
55:SH:35:ASP:CG	55:SH:78:ARG:NH2	2.42	0.75
74:SM:94:ILE:HA	74:SM:100:PRO:HA	1.68	0.75
4:LA:14:SER:HA	4:LA:17:ARG:HH11	1.52	0.75
79:SZ:50:PHE:CZ	79:SZ:58:LEU:HD22	2.21	0.75
64:SU:28:ASN:HD21	64:SU:30:LYS:HD3	1.50	0.74
49:S2:563:G:H1	49:S2:592:C:H5	1.35	0.74
58:SL:33:LEU:HD12	58:SL:34:PRO:HD2	1.69	0.74
70:Sg:217:MET:HG2	70:Sg:229:THR:OG1	1.86	0.74
46:Ls:40:MET:HE3	46:Ls:43:ILE:CG1	2.18	0.74
79:SZ:77:LEU:HD12	79:SZ:79:ILE:HD11	1.69	0.74
1:L5:512:U:H3	1:L5:647:G:H1	1.35	0.74
43:Lo:102:GLN:HA	43:Lo:102:GLN:NE2	2.01	0.74
70:Sg:206:LEU:HD11	70:Sg:241:PHE:CZ	2.21	0.74
46:Ls:13:TYR:HE2	46:Ls:60:MET:HE2	0.97	0.73
1:L5:1762:C:N4	1:L5:1770:A:C2	2.56	0.73
8:LE:153:LEU:HD11	8:LE:195:ILE:HG13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SJ:89:GLU:CD	73:SJ:92:MET:HE2	2.13	0.73
50:SA:158:ASP:HB3	65:SV:69:ILE:HD13	1.68	0.73
13:LJ:17:ILE:HD11	13:LJ:165:TRP:CH2	2.22	0.73
46:Ls:36:GLY:O	46:Ls:40:MET:HG2	1.88	0.73
73:SJ:89:GLU:OE1	73:SJ:92:MET:HE2	1.89	0.73
1:L5:1479:G:H21	14:LL:184:MET:HE3	1.54	0.73
40:Ll:9:ILE:HG23	40:Ll:51:LEU:HD21	1.70	0.73
61:SR:80:ARG:HH11	61:SR:80:ARG:HG3	1.53	0.73
1:L5:1998:A:C4	46:Ls:55:MET:HE1	2.20	0.73
7:LD:291:GLN:HE22	12:LI:214:SER:HA	1.53	0.73
59:SP:24:GLN:O	59:SP:28:MET:CG	2.31	0.72
64:SU:25:THR:HB	64:SU:86:LYS:HG3	1.70	0.72
70:Sg:68:ASP:OD1	70:Sg:69:VAL:N	2.22	0.72
70:Sg:217:MET:CE	70:Sg:219:TRP:CZ2	2.73	0.72
72:SG:67:VAL:HG12	72:SG:69:THR:HG22	1.71	0.72
11:LH:52:LYS:HE3	11:LH:54:ARG:HH12	1.53	0.72
83:CA:88:HIS:O	83:CA:307:VAL:HG22	1.89	0.72
61:SR:107:LYS:HB2	61:SR:107:LYS:NZ	2.03	0.72
47:Lt:113:ALA:HA	47:Lt:116:MET:HE3	1.71	0.72
31:Lc:104:ILE:HG23	31:Lc:105:ILE:HG13	1.71	0.71
9:LF:71:MET:HA	9:LF:74:MET:HE3	1.72	0.71
36:Lh:96:ASN:OD1	36:Lh:99:GLU:HG2	1.90	0.71
49:S2:886:A:N6	49:S2:901:G:C5	2.58	0.71
52:SD:194:PRO:HG3	52:SD:198:ILE:HG13	1.71	0.71
1:L5:2469:C:H5	1:L5:2471:G:H1	1.38	0.71
79:SZ:49:LEU:H	79:SZ:83:LEU:HD22	1.56	0.71
10:LG:103:ARG:HH11	10:LG:193:LEU:HA	1.55	0.71
60:SQ:23:ALA:HB2	60:SQ:70:VAL:HG22	1.71	0.71
1:L5:499:G:H2'	1:L5:504:G:H22	1.55	0.71
31:Lc:14:ILE:HD11	84:CB:11:CYS:HB3	1.72	0.71
68:Sc:43:ILE:CG2	68:Sc:65:ALA:HB3	2.20	0.71
78:SY:23:MET:HE1	78:SY:75:ILE:CD1	2.20	0.71
31:Lc:50:ASN:ND2	31:Lc:76:GLY:O	2.24	0.71
46:Ls:101:MET:CE	46:Ls:102:LEU:HD23	2.20	0.71
1:L5:352:G:C6	6:LC:196:MET:HE2	2.25	0.71
12:LI:77:VAL:HG21	86:CE:81:LEU:HD21	1.72	0.71
61:SR:76:GLU:OE1	61:SR:76:GLU:HA	1.91	0.71
4:LA:94:ALA:HB3	4:LA:102:LEU:CD2	2.20	0.70
26:LX:131:ASP:OD1	40:Ll:18:LYS:HD3	1.91	0.70
49:S2:1314:U:H6	57:SK:5:LYS:HZ1	1.37	0.70
70:Sg:124:SER:OG	70:Sg:126:ASP:OD1	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Lc:34:THR:HG23	31:Lc:95:ALA:HB2	1.74	0.70
62:SS:34:LYS:HG2	62:SS:103:LEU:HD23	1.74	0.70
1:L5:1996:C:H42	1:L5:2000:G:N2	1.88	0.70
1:L5:3713:U:OP2	1:L5:3714:G:N2	2.25	0.70
49:S2:547:G:H1'	49:S2:549:C:H41	1.57	0.70
62:SS:26:ILE:O	62:SS:30:ILE:HG23	1.90	0.70
60:SQ:42:ILE:HG22	60:SQ:44:PRO:HD2	1.72	0.70
75:SN:104:ARG:NE	75:SN:104:ARG:HA	2.06	0.70
39:Lk:17:ARG:HD2	39:Lk:19:ASP:OD1	1.91	0.70
1:L5:86:U:OP1	19:LQ:168:ARG:NH1	2.20	0.70
11:LH:37:ASP:OD1	11:LH:39:ASN:ND2	2.25	0.70
83:CA:290:ARG:C	83:CA:293:VAL:CG1	2.61	0.70
84:CB:20:LEU:C	84:CB:20:LEU:HD12	2.16	0.70
72:SG:31:ARG:HG2	72:SG:101:ILE:HD13	1.74	0.70
46:Ls:55:MET:SD	46:Ls:56:GLY:CA	2.80	0.70
62:SS:3:LEU:HG	62:SS:4:VAL:H	1.56	0.70
1:L5:1976:G:C6	1:L5:1991:A:N1	2.60	0.69
1:L5:480:C:OP1	45:Lr:67:ARG:NH1	2.26	0.69
70:Sg:42:MET:CE	70:Sg:57:ARG:CG	2.70	0.69
83:CA:17:VAL:HA	83:CA:20:LYS:HG2	1.75	0.69
14:LL:123:LYS:HD2	14:LL:155:MET:HE2	1.74	0.69
70:Sg:30:MET:SD	70:Sg:30:MET:C	2.75	0.69
1:L5:4873:G:N3	17:LO:175:MET:HG2	2.08	0.69
49:S2:84:A:H5''	78:SY:122:LYS:CD	2.14	0.69
29:La:79:TRP:CE3	29:La:87:ARG:HG3	2.27	0.69
31:Lc:44:LYS:HB2	31:Lc:105:ILE:HD13	1.74	0.69
1:L5:4242:U:H3	1:L5:4281:A:H2	1.40	0.69
7:LD:27:LYS:HG2	13:LJ:147:ARG:HD3	1.74	0.69
46:Ls:13:TYR:OH	46:Ls:60:MET:HE2	1.93	0.69
46:Ls:101:MET:SD	46:Ls:101:MET:C	2.75	0.68
45:Lr:56:ASP:OD2	45:Lr:58:LYS:NZ	2.26	0.68
78:SY:20:ARG:HH21	78:SY:22:GLN:HE22	1.39	0.68
83:CA:88:HIS:O	83:CA:307:VAL:HG23	1.91	0.68
1:L5:2020:U:H2'	1:L5:2021:G:H8	1.59	0.68
61:SR:107:LYS:HB2	61:SR:107:LYS:HZ3	1.58	0.68
83:CA:20:LYS:HB2	83:CA:23:MET:HE3	1.74	0.68
49:S2:959:G:OP1	76:SO:104:ARG:NH2	2.27	0.68
36:Lh:95:LEU:HB3	36:Lh:99:GLU:HG3	1.76	0.68
1:L5:3751:G:H21	1:L5:3775:A:H8	1.39	0.68
83:CA:203:GLN:HE22	83:CA:228:VAL:HA	1.57	0.68
70:Sg:11:LEU:HG	70:Sg:53:GLY:HA3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CA:263:ARG:HB2	83:CA:263:ARG:NH1	2.09	0.68
1:L5:1176:C:N3	1:L5:1184:A:N1	2.42	0.67
5:LB:107:ALA:HB2	5:LB:201:LEU:HG	1.76	0.67
13:LJ:17:ILE:HD11	13:LJ:165:TRP:HH2	1.58	0.67
39:Lk:27:LYS:HE3	39:Lk:68:GLU:OE2	1.93	0.67
55:SH:50:GLU:OE1	55:SH:58:LYS:HE2	1.94	0.67
61:SR:72:LYS:O	61:SR:76:GLU:HG2	1.94	0.67
12:LI:48:LEU:HB2	12:LI:142:LEU:HD23	1.76	0.67
56:SI:135:GLU:HG3	56:SI:139:LYS:CE	2.18	0.67
84:CB:6:GLN:OE1	84:CB:11:CYS:O	2.13	0.67
1:L5:2709:C:H2'	83:CA:263:ARG:NE	2.09	0.67
50:SA:38:ILE:HD12	50:SA:47:TYR:HB3	1.77	0.67
37:Li:93:VAL:O	37:Li:97:MET:HG3	1.95	0.67
53:SE:139:LEU:C	53:SE:139:LEU:HD12	2.19	0.67
56:SI:62:VAL:HG11	56:SI:75:LYS:HE3	1.77	0.67
61:SR:87:GLU:OE1	61:SR:87:GLU:N	2.20	0.67
46:Ls:69:LEU:HD23	46:Ls:75:LEU:HD11	1.77	0.67
70:Sg:42:MET:HE2	70:Sg:57:ARG:CB	2.16	0.67
1:L5:184:U:H3	1:L5:253:G:H1	1.40	0.67
83:CA:290:ARG:HA	83:CA:293:VAL:HG11	1.77	0.66
1:L5:1629:G:H1	4:LA:208:GLU:HG2	1.60	0.66
1:L5:2658:G:N2	1:L5:2676:A:OP2	2.27	0.66
4:LA:94:ALA:HB3	4:LA:102:LEU:HD22	1.76	0.66
16:LN:124:ASP:HB3	16:LN:127:TYR:H	1.60	0.66
45:Lr:26:SER:HB3	45:Lr:28:GLU:OE1	1.95	0.66
47:Lt:50:THR:HG21	47:Lt:72:GLU:HB2	1.78	0.66
49:S2:885:U:H3	49:S2:901:G:H1	1.41	0.66
56:SI:135:GLU:CG	56:SI:139:LYS:HE3	2.17	0.66
33:Le:113:GLU:OE2	33:Le:117:GLN:NE2	2.27	0.66
49:S2:818:A:OP1	73:SJ:80:ARG:NH2	2.29	0.66
49:S2:940:U:H3	49:S2:1002:U:H3	1.41	0.66
64:SU:87:ARG:HG2	64:SU:87:ARG:NH1	2.10	0.66
46:Ls:53:VAL:HG12	46:Ls:89:VAL:HG22	1.77	0.66
19:LQ:66:MET:HE1	19:LQ:86:ILE:HD13	1.75	0.66
3:L8:96:C:OP1	36:Lh:70:ARG:NH1	2.29	0.66
86:CE:35:GLU:OE1	86:CE:35:GLU:HA	1.96	0.66
49:S2:1314:U:H1'	57:SK:5:LYS:NZ	2.11	0.66
83:CA:199:LYS:HE2	83:CA:199:LYS:HA	1.77	0.66
55:SH:42:GLU:OE1	55:SH:42:GLU:N	2.24	0.66
1:L5:466:A:C6	1:L5:468:U:C4	2.85	0.65
7:LD:204:VAL:HB	7:LD:236:MET:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1636:G:O2'	54:SF:164:ARG:NH1	2.29	0.65
28:LZ:102:ARG:CZ	28:LZ:102:ARG:HB2	2.27	0.65
55:SH:181:THR:HG22	55:SH:183:LYS:HG2	1.77	0.65
49:S2:1751:C:H42	49:S2:1782:G:H21	1.45	0.65
1:L5:2611:A:H5'	1:L5:2688:G:H4'	1.77	0.65
8:LE:93:THR:HG22	8:LE:104:THR:OG1	1.96	0.65
13:LJ:112:HIS:HD2	13:LJ:126:TYR:H	1.44	0.65
12:LI:102:MET:SD	12:LI:102:MET:N	2.68	0.65
17:LO:197:LYS:NZ	17:LO:203:VAL:OXT	2.29	0.65
25:LW:1:MET:SD	25:LW:15:PRO:HG3	2.37	0.65
55:SH:51:ILE:HG12	55:SH:61:ILE:HD11	1.78	0.65
8:LE:90:ALA:C	8:LE:109:LEU:HD12	2.21	0.65
16:LN:123:GLU:HB3	16:LN:128:LYS:HG3	1.78	0.65
47:Lt:125:LEU:HD13	47:Lt:127:GLY:H	1.60	0.65
70:Sg:217:MET:HE3	70:Sg:219:TRP:CZ2	2.32	0.65
17:LO:92:THR:HG22	17:LO:95:GLY:H	1.61	0.65
50:SA:10:MET:HE1	50:SA:52:LYS:HA	1.77	0.65
1:L5:4220:A:OP2	22:LT:2:THR:OG1	2.15	0.64
13:LJ:160:GLU:HA	13:LJ:163:MET:HE2	1.79	0.64
46:Ls:20:LEU:HD13	46:Ls:54:LEU:HD13	1.76	0.64
70:Sg:206:LEU:HD11	70:Sg:241:PHE:CE2	2.32	0.64
1:L5:1095:A:C2	1:L5:1200:G:N1	2.57	0.64
55:SH:39:GLN:OE1	55:SH:75:ILE:CG2	2.45	0.64
63:ST:134:ILE:HA	63:ST:137:GLN:HG3	1.79	0.64
1:L5:729:G:H5''	9:LF:76:ARG:HD2	1.79	0.64
12:LI:36:LEU:HD12	86:CE:74:LEU:HD11	1.78	0.64
32:Ld:46:LEU:CD2	32:Ld:72:VAL:HG11	2.27	0.64
49:S2:3:C:O2	73:SJ:18:ARG:NH1	2.30	0.64
62:SS:115:LYS:HD3	62:SS:126:PHE:HB2	1.78	0.64
7:LD:120:GLU:O	7:LD:248:ARG:NH1	2.30	0.64
46:Ls:28:PHE:HB2	46:Ls:89:VAL:HB	1.80	0.64
70:Sg:42:MET:HE2	70:Sg:57:ARG:CG	2.27	0.64
46:Ls:36:GLY:O	46:Ls:39:GLN:NE2	2.28	0.64
49:S2:396:U:OP2	58:SL:79:LYS:NZ	2.31	0.64
1:L5:493:G:O6	1:L5:660:A:N1	2.31	0.64
9:LF:157:ARG:HG3	9:LF:248:ASN:ND2	2.13	0.64
28:LZ:24:VAL:HG21	28:LZ:87:VAL:HG23	1.79	0.64
52:SD:7:LYS:HE2	64:SU:25:THR:HG21	1.78	0.64
67:Sa:51:ARG:HH22	68:Sc:39:SER:HB2	1.63	0.64
50:SA:211:GLU:OE1	50:SA:211:GLU:O	2.16	0.63
1:L5:2557:G:H1	1:L5:2570:U:H3	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Lr:108:MET:HE3	45:Lr:112:ARG:HH11	1.64	0.63
70:Sg:206:LEU:HD12	70:Sg:206:LEU:O	1.96	0.63
1:L5:1971:C:O2	46:Ls:41:GLN:NE2	2.32	0.63
10:LG:190:LEU:O	10:LG:194:VAL:HG22	1.98	0.63
28:LZ:102:ARG:CB	28:LZ:102:ARG:CZ	2.76	0.63
72:SG:152:ASP:O	72:SG:156:TYR:CD2	2.50	0.63
1:L5:1187:G:N2	1:L5:1187:G:OP2	2.32	0.63
11:LH:52:LYS:HE3	11:LH:54:ARG:NH1	2.13	0.63
31:Lc:106:ARG:HH21	84:CB:10:GLY:HA2	1.58	0.63
81:Se:36:MET:CE	81:Se:40:ARG:HH21	1.96	0.63
1:L5:4093:G:N1	1:L5:4114:C:C2	2.67	0.63
1:L5:4546:A:N7	4:LA:215:ASN:ND2	2.46	0.63
1:L5:1998:A:N7	46:Ls:55:MET:HE2	2.10	0.63
72:SG:27:PHE:HE1	72:SG:36:VAL:HG13	1.63	0.63
40:Ll:37:TYR:CZ	40:Ll:39:SER:HA	2.34	0.63
46:Ls:101:MET:SD	46:Ls:102:LEU:CA	2.87	0.63
1:L5:171:U:O2'	1:L5:265:C:N4	2.31	0.62
20:LR:105:LEU:HD13	20:LR:135:LYS:HD2	1.80	0.62
55:SH:39:GLN:OE1	55:SH:75:ILE:HG21	1.99	0.62
5:LB:14:LEU:HB3	5:LB:17:LEU:HD22	1.81	0.62
32:Ld:29:ILE:O	32:Ld:33:ILE:HG23	1.99	0.62
49:S2:943:U:OP2	51:SB:216:LYS:NZ	2.32	0.62
53:SE:91:SER:OG	53:SE:98:ASN:OD1	2.18	0.62
11:LH:1:MET:HE2	21:LS:140:PRO:HB2	1.81	0.62
72:SG:43:GLU:OE1	72:SG:43:GLU:N	2.32	0.62
50:SA:158:ASP:HB3	65:SV:69:ILE:CD1	2.29	0.62
49:S2:1314:U:H1'	57:SK:5:LYS:HZ1	1.65	0.62
67:Sa:51:ARG:NH2	68:Sc:39:SER:HB2	2.15	0.62
78:SY:20:ARG:HE	78:SY:22:GLN:NE2	1.98	0.62
1:L5:1998:A:C8	46:Ls:55:MET:HE2	2.21	0.62
6:LC:189:MET:HE1	6:LC:201:ARG:CG	2.23	0.62
47:Lt:113:ALA:CA	47:Lt:116:MET:HE3	2.29	0.62
70:Sg:278:SER:HB2	70:Sg:280:LYS:HE3	1.81	0.62
57:SK:10:ALA:HA	57:SK:13:GLU:OE1	1.99	0.62
63:ST:129:ARG:HD2	63:ST:133:ARG:HH21	1.64	0.62
1:L5:3947:A:H61	1:L5:4066:U:H3	1.48	0.62
1:L5:1342:A:P	16:LN:204:ARG:HH11	2.22	0.62
46:Ls:16:LYS:O	46:Ls:20:LEU:HG	1.99	0.62
14:LL:145:LYS:HG3	14:LL:146:LEU:HG	1.81	0.61
53:SE:43:PRO:HG2	53:SE:46:ILE:HD12	1.80	0.61
83:CA:290:ARG:CA	83:CA:293:VAL:CG1	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1996:C:H42	1:L5:2000:G:H22	1.48	0.61
46:Ls:61:MET:CE	46:Ls:82:ILE:CD1	2.74	0.61
50:SA:211:GLU:C	50:SA:211:GLU:CD	2.68	0.61
1:L5:1095:A:N1	1:L5:1200:G:O6	2.33	0.61
10:LG:210:GLU:H	10:LG:210:GLU:CD	2.00	0.61
54:SF:18:LYS:HE3	54:SF:22:LYS:HA	1.81	0.61
8:LE:288:PHE:CD2	34:Lf:110:ILE:HD12	2.35	0.61
28:LZ:95:VAL:HG13	28:LZ:109:LYS:HG2	1.80	0.61
55:SH:69:LEU:HG	55:SH:96:ALA:HB2	1.80	0.61
71:SC:211:LYS:HG2	71:SC:215:MET:HE2	1.80	0.61
79:SZ:57:LYS:HA	79:SZ:60:LYS:NZ	2.16	0.61
46:Ls:14:PHE:CE1	46:Ls:60:MET:HG2	2.36	0.61
59:SP:28:MET:HE1	59:SP:36:LEU:HD22	1.82	0.61
1:L5:4040:C:H5'	1:L5:4045:G:H22	1.66	0.61
8:LE:185:PRO:HG2	8:LE:187:ARG:HG3	1.81	0.61
10:LG:103:ARG:HG2	10:LG:193:LEU:O	2.00	0.61
25:LW:84:GLY:HA2	72:SG:161:PRO:HD3	1.82	0.61
31:Lc:106:ARG:NH2	84:CB:10:GLY:CA	2.42	0.61
63:ST:111:LYS:NZ	63:ST:126:GLN:CB	2.63	0.61
81:Se:36:MET:CE	81:Se:40:ARG:NH2	2.45	0.61
10:LG:136:LEU:HD23	10:LG:193:LEU:HD13	1.83	0.61
12:LI:36:LEU:CD1	86:CE:74:LEU:HD11	2.30	0.61
35:Lg:103:VAL:HB	84:CB:20:LEU:HD23	1.82	0.61
39:Lk:11:PHE:CE1	39:Lk:36:VAL:HG23	2.36	0.61
58:SL:104:LYS:HE3	66:SX:8:ARG:CZ	2.31	0.61
63:ST:111:LYS:HZ1	63:ST:126:GLN:CB	2.14	0.61
19:LQ:66:MET:HE3	19:LQ:100:VAL:HG11	1.83	0.60
1:L5:1:C:H3'	1:L5:2:G:H8	1.66	0.60
10:LG:193:LEU:HD11	10:LG:202:VAL:HG11	1.83	0.60
23:LU:66:SER:O	23:LU:67:LYS:HB2	2.02	0.60
35:Lg:42:PRO:HB2	35:Lg:53:LEU:HD12	1.83	0.60
46:Ls:40:MET:HE3	46:Ls:40:MET:HA	1.83	0.60
70:Sg:26:GLN:NE2	70:Sg:73:SER:O	2.34	0.60
76:SO:59:GLY:HA2	76:SO:68:GLU:HG2	1.84	0.60
1:L5:280:G:OP2	16:LN:14:LYS:NZ	2.35	0.60
64:SU:94:PRO:HD2	64:SU:97:ILE:HD11	1.84	0.60
1:L5:4066:U:H4'	37:Li:59:GLU:HG3	1.82	0.60
26:LX:131:ASP:OD1	26:LX:131:ASP:C	2.45	0.60
46:Ls:13:TYR:HE2	46:Ls:60:MET:SD	2.23	0.60
49:S2:928:G:H1	49:S2:1013:U:H3	1.49	0.60
46:Ls:40:MET:HE3	46:Ls:43:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Sg:217:MET:HE1	70:Sg:219:TRP:CZ2	2.36	0.60
23:LU:18:VAL:O	23:LU:19:LEU:CD1	2.36	0.60
49:S2:1644:C:H4'	60:SQ:140:ARG:HB2	1.84	0.60
56:SI:135:GLU:CD	56:SI:139:LYS:HE2	2.27	0.60
70:Sg:206:LEU:CD1	70:Sg:241:PHE:CZ	2.85	0.60
57:SK:29:MET:SD	57:SK:42:ASN:ND2	2.74	0.60
67:Sa:39:PHE:CE2	67:Sa:41:ILE:HD11	2.37	0.60
84:CB:6:GLN:HE22	84:CB:13:VAL:H	0.70	0.60
1:L5:35:U:OP2	16:LN:83:LYS:NZ	2.35	0.60
1:L5:3938:G:OP1	16:LN:24:ARG:NH1	2.34	0.60
40:L1:13:LEU:O	40:L1:17:GLN:HG2	2.02	0.60
45:Lr:62:VAL:HG12	45:Lr:64:ILE:CD1	2.31	0.60
1:L5:1976:G:O6	1:L5:1991:A:N1	2.35	0.60
1:L5:1998:A:C1'	46:Ls:55:MET:HE1	2.32	0.60
1:L5:3589:G:N2	1:L5:3590:G:N7	2.50	0.59
1:L5:4472:G:O2'	41:Lm:100:TYR:O	2.20	0.59
51:SB:88:THR:HG22	51:SB:98:THR:HG22	1.82	0.59
55:SH:41:ARG:HB3	55:SH:41:ARG:CZ	2.32	0.59
79:SZ:65:TYR:HA	79:SZ:111:ARG:HH21	1.67	0.59
1:L5:1342:A:P	16:LN:204:ARG:NH1	2.74	0.59
1:L5:1342:A:OP1	16:LN:204:ARG:NH1	2.35	0.59
1:L5:1998:A:H4'	46:Ls:9:TRP:HZ2	1.67	0.59
6:LC:150:LEU:O	6:LC:152:LEU:N	2.35	0.59
11:LH:7:ASN:HB3	11:LH:58:ASP:OD1	2.02	0.59
13:LJ:35:ARG:NH1	13:LJ:123:ILE:O	2.35	0.59
19:LQ:42:THR:HA	19:LQ:45:GLN:HE21	1.66	0.59
53:SE:139:LEU:HD21	53:SE:169:ILE:HD11	1.83	0.59
61:SR:87:GLU:H	61:SR:87:GLU:CD	2.10	0.59
49:S2:83:A:H2	78:SY:120:THR:CG2	2.15	0.59
1:L5:135:G:C6	36:Lh:97:LYS:HE3	2.38	0.59
61:SR:71:ILE:O	61:SR:75:GLU:HG2	2.02	0.59
78:SY:55:ILE:HG12	78:SY:75:ILE:HG12	1.84	0.59
83:CA:182:ILE:HG12	83:CA:229:LEU:HB3	1.84	0.59
23:LU:29:VAL:HG21	23:LU:68:SER:HG	1.63	0.59
47:Lt:125:LEU:CD1	47:Lt:127:GLY:H	2.15	0.59
1:L5:1175:A:N1	1:L5:1185:G:O6	2.36	0.59
1:L5:1507:C:H5''	6:LC:114:ARG:HG3	1.84	0.59
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.84	0.59
57:SK:7:ASN:HD22	57:SK:40:VAL:HB	1.68	0.59
64:SU:55:ARG:HH11	64:SU:87:ARG:HE	1.48	0.59
40:L1:23:ILE:HD12	40:L1:23:ILE:C	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:54:A:OP1	78:SY:111:LYS:NZ	2.34	0.59
62:SS:86:ARG:HG3	62:SS:106:LYS:HD2	1.84	0.59
72:SG:44:GLU:HG2	72:SG:45:TRP:CD1	2.37	0.59
76:SO:34:PHE:HB3	76:SO:41:PHE:HB2	1.84	0.59
83:CA:263:ARG:NH1	83:CA:263:ARG:CB	2.66	0.59
1:L5:4942:C:H5''	8:LE:155:GLY:HA2	1.83	0.59
22:LT:51:GLY:HA3	22:LT:92:ARG:HG3	1.85	0.59
46:Ls:13:TYR:OH	46:Ls:60:MET:CE	2.51	0.59
49:S2:1228:A:H2'	49:S2:1229:G:C8	2.38	0.59
55:SH:160:LYS:HA	55:SH:163:GLN:HB2	1.85	0.59
5:LB:92:TYR:HB2	5:LB:159:VAL:HB	1.85	0.59
10:LG:209:SER:HA	10:LG:212:LYS:HG3	1.85	0.59
26:LX:87:MET:HB2	83:CA:259:MET:HE1	1.85	0.59
47:Lt:113:ALA:HA	47:Lt:116:MET:CE	2.32	0.59
70:Sg:42:MET:CE	70:Sg:57:ARG:HG2	2.33	0.59
1:L5:1762:C:N4	1:L5:1770:A:H2	2.01	0.59
9:LF:182:TYR:HB3	9:LF:200:ARG:HG3	1.85	0.58
33:Le:82:VAL:HG13	33:Le:114:ARG:HG2	1.85	0.58
1:L5:935:A:H61	15:LM:70:GLN:HE22	1.51	0.58
54:SF:78:MET:HG2	54:SF:79:HIS:HD2	1.68	0.58
72:SG:152:ASP:O	72:SG:156:TYR:HD2	1.86	0.58
72:SG:159:ARG:HD2	72:SG:173:ALA:HB2	1.84	0.58
1:L5:500:G:H1'	1:L5:504:G:H3'	1.86	0.58
1:L5:4279:A:H5'	1:L5:4281:A:H1'	1.84	0.58
60:SQ:11:GLN:HG2	60:SQ:24:HIS:HD2	1.68	0.58
1:L5:1996:C:N4	1:L5:2000:G:H22	2.00	0.58
8:LE:287:VAL:O	15:LM:109:ARG:NH2	2.36	0.58
49:S2:1563:G:OP1	63:ST:121:ARG:NH1	2.36	0.58
66:SX:52:LEU:HD11	66:SX:73:GLN:HB2	1.84	0.58
19:LQ:75:ARG:HA	19:LQ:78:LYS:HE2	1.86	0.58
55:SH:63:PHE:HB3	55:SH:97:GLN:HG2	1.86	0.58
73:SJ:170:PRO:HB2	73:SJ:174:LYS:HD2	1.86	0.58
1:L5:1503:A:H62	19:LQ:87:THR:HG21	1.67	0.58
17:LO:27:VAL:HG13	17:LO:98:ALA:HB1	1.84	0.58
59:SP:123:TYR:OH	62:SS:124:ARG:NH1	2.37	0.58
17:LO:14:HIS:CE1	17:LO:119:VAL:HG22	2.39	0.58
49:S2:1230:C:OP1	62:SS:130:ARG:NH2	2.36	0.58
1:L5:1785:C:OP1	12:LI:133:GLN:NE2	2.35	0.58
32:Ld:46:LEU:HD12	32:Ld:64:ILE:HD12	1.84	0.58
50:SA:189:ILE:HG22	50:SA:191:ARG:H	1.69	0.58
57:SK:4:PRO:HA	57:SK:5:LYS:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SY:103:SER:OG	78:SY:106:GLN:HG3	2.04	0.58
1:L5:6:C:H5''	10:LG:197:LYS:HG2	1.85	0.58
1:L5:4093:G:N1	1:L5:4114:C:N3	2.52	0.58
49:S2:688:U:O2	55:SH:122:LEU:HD13	2.03	0.58
49:S2:834:C:N4	49:S2:839:C:H42	2.00	0.58
52:SD:123:LEU:CD1	52:SD:134:CYS:SG	2.92	0.58
70:Sg:87:LEU:HB3	70:Sg:101:PHE:HD1	1.69	0.58
83:CA:266:PHE:CE2	83:CA:301:LEU:HD13	2.39	0.58
31:Lc:14:ILE:HG12	31:Lc:17:ARG:HH21	1.69	0.58
49:S2:1600:G:H5'	79:SZ:43:LYS:HG3	1.85	0.58
49:S2:1756:C:N3	49:S2:1776:G:N1	2.47	0.58
6:LC:189:MET:HE1	6:LC:201:ARG:NH1	2.19	0.57
10:LG:231:ASP:O	10:LG:234:ARG:HG2	2.04	0.57
46:Ls:40:MET:HA	46:Ls:43:ILE:HG13	1.85	0.57
83:CA:223:VAL:HG12	83:CA:324:LEU:HD13	1.84	0.57
1:L5:28:C:OP2	16:LN:189:ARG:NH1	2.37	0.57
1:L5:4429:C:N3	12:LI:158:LYS:NZ	2.51	0.57
49:S2:1158:G:H5''	77:SW:76:SER:HB3	1.86	0.57
49:S2:1314:U:O3'	57:SK:3:MET:HE3	2.04	0.57
82:Sf:132:MET:HE2	82:Sf:139:HIS:HB3	1.86	0.57
8:LE:46:ARG:O	8:LE:65:ARG:NH1	2.37	0.57
1:L5:375:G:OP1	6:LC:62:THR:HG22	2.05	0.57
1:L5:1706:A:H5'	1:L5:1707:C:C4	2.39	0.57
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.85	0.57
57:SK:3:MET:HE2	57:SK:8:ARG:NH2	2.19	0.57
1:L5:137:G:H2'	1:L5:138:G:C8	2.40	0.57
47:Lt:130:LYS:NZ	47:Lt:157:SER:OG	2.38	0.57
52:SD:97:CYS:O	52:SD:101:GLN:HG2	2.04	0.57
64:SU:18:HIS:HB3	64:SU:117:ALA:HB2	1.85	0.57
64:SU:28:ASN:HD21	64:SU:30:LYS:CD	2.18	0.57
66:SX:101:LEU:HB3	66:SX:123:VAL:O	2.05	0.57
78:SY:100:LYS:NZ	78:SY:101:LYS:O	2.36	0.57
1:L5:1513:U:H4'	14:LL:4:SER:HB2	1.85	0.57
6:LC:209:ILE:HB	6:LC:229:LEU:HD13	1.86	0.57
8:LE:281:ILE:HB	8:LE:286:LEU:HD21	1.86	0.57
9:LF:71:MET:SD	9:LF:74:MET:HE3	2.45	0.57
17:LO:178:ARG:NH1	17:LO:182:GLU:OE2	2.38	0.57
49:S2:1256:G:H8	64:SU:66:ARG:HB2	1.69	0.57
55:SH:185:VAL:C	55:SH:186:ASN:HD22	2.13	0.57
70:Sg:126:ASP:OD1	70:Sg:128:THR:HG22	2.03	0.57
78:SY:57:VAL:HB	78:SY:60:PHE:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LZ:29:ILE:HG22	28:LZ:32:GLY:H	1.70	0.57
45:Lr:108:MET:HE3	45:Lr:112:ARG:NH1	2.20	0.57
53:SE:100:ARG:HH12	53:SE:118:GLU:HG2	1.70	0.57
72:SG:22:ARG:HH12	72:SG:25:ARG:HD2	1.69	0.57
17:LO:14:HIS:HE1	17:LO:119:VAL:HG22	1.69	0.57
28:LZ:74:VAL:HG23	28:LZ:101:PHE:CE2	2.40	0.57
65:SV:35:ASN:ND2	71:SC:267:GLN:OE1	2.38	0.57
5:LB:220:ILE:HG12	5:LB:278:THR:HG23	1.87	0.57
11:LH:54:ARG:HG3	11:LH:54:ARG:HH11	1.70	0.57
55:SH:17:ASP:OD1	55:SH:18:GLU:N	2.38	0.57
62:SS:142:ARG:HG2	62:SS:142:ARG:HH11	1.70	0.57
1:L5:1339:U:H2'	1:L5:1340:C:C6	2.40	0.56
6:LC:66:SER:HA	6:LC:77:PRO:HA	1.87	0.56
10:LG:136:LEU:CD2	10:LG:193:LEU:HD13	2.35	0.56
23:LU:41:GLN:NE2	23:LU:45:GLU:OE2	2.38	0.56
54:SF:17:ILE:HG21	54:SF:46:ALA:HB1	1.87	0.56
72:SG:181:THR:HG22	72:SG:183:ARG:H	1.69	0.56
1:L5:466:A:C2	1:L5:468:U:C5	2.93	0.56
1:L5:3930:U:H3	1:L5:4180:G:H1	1.52	0.56
52:SD:23:GLU:OE1	52:SD:27:ARG:NH2	2.39	0.56
52:SD:29:LEU:HB2	52:SD:34:TYR:HB2	1.88	0.56
54:SF:28:VAL:HA	54:SF:110:GLN:HG2	1.87	0.56
54:SF:126:THR:HG21	68:Sc:27:CYS:SG	2.45	0.56
70:Sg:176:VAL:HB	70:Sg:186:THR:HB	1.87	0.56
75:SN:17:PRO:HG3	80:Sb:28:PRO:HG3	1.86	0.56
19:LQ:66:MET:CE	19:LQ:100:VAL:HG11	2.35	0.56
49:S2:1228:A:H2'	49:S2:1229:G:H8	1.70	0.56
53:SE:158:ASP:OD2	53:SE:174:LYS:NZ	2.34	0.56
55:SH:137:SER:OG	55:SH:159:ASP:OD1	2.21	0.56
57:SK:29:MET:HB3	57:SK:42:ASN:HB2	1.87	0.56
59:SP:86:LEU:H	59:SP:89:MET:CE	2.16	0.56
23:LU:18:VAL:HG11	23:LU:78:PHE:N	2.18	0.56
56:SI:135:GLU:OE2	56:SI:139:LYS:HE2	2.05	0.56
1:L5:3961:G:N2	1:L5:3964:U:O3'	2.39	0.56
49:S2:433:A:H5''	56:SI:22:HIS:HB3	1.87	0.56
19:LQ:50:ARG:HA	19:LQ:53:MET:SD	2.46	0.56
49:S2:1292:C:N3	82:Sf:138:ARG:NH2	2.49	0.56
64:SU:30:LYS:H	64:SU:30:LYS:HD2	1.71	0.56
1:L5:4873:G:C4	17:LO:175:MET:HG2	2.41	0.56
8:LE:161:ARG:NH1	8:LE:273:SER:OG	2.38	0.56
18:LP:84:PRO:HB2	18:LP:87:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SR:121:GLN:OE1	61:SR:122:PRO:HD2	2.06	0.56
4:LA:115:CYS:SG	4:LA:124:GLY:HA3	2.46	0.56
20:LR:176:ARG:NH2	49:S2:909:G:OP1	2.39	0.56
46:Ls:169:ALA:O	46:Ls:173:THR:OG1	2.20	0.56
47:Lt:82:ILE:HG21	47:Lt:137:GLN:HG3	1.88	0.56
49:S2:351:G:OP1	56:SI:7:ASN:ND2	2.39	0.56
49:S2:1658:G:OP2	49:S2:1660:C:N4	2.38	0.56
62:SS:24:ARG:HB2	62:SS:29:ALA:HB2	1.88	0.56
31:Lc:12:GLU:H	31:Lc:12:GLU:CD	2.13	0.55
49:S2:697:G:OP2	49:S2:733:C:N4	2.39	0.55
10:LG:180:PRO:HG3	10:LG:219:VAL:HG13	1.88	0.55
49:S2:1232:U:H2'	49:S2:1233:G:H8	1.72	0.55
55:SH:166:VAL:HG23	55:SH:169:LYS:HB2	1.88	0.55
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	1.89	0.55
66:SX:34:THR:HA	66:SX:37:LYS:HE3	1.88	0.55
11:LH:142:ASP:OD1	11:LH:142:ASP:C	2.43	0.55
54:SF:16:ASP:N	54:SF:24:SER:HG	2.04	0.55
1:L5:4092:G:N7	1:L5:4114:C:N4	2.54	0.55
1:L5:4139:G:H21	1:L5:4140:C:H41	1.55	0.55
49:S2:695:C:N4	49:S2:736:C:O2'	2.40	0.55
70:Sg:41:ILE:HG21	70:Sg:43:TRP:CE2	2.42	0.55
70:Sg:217:MET:HG2	70:Sg:229:THR:HG23	1.88	0.55
1:L5:2000:G:N2	1:L5:2000:G:OP2	2.38	0.55
28:LZ:121:ARG:HH11	28:LZ:127:ASN:HD21	1.54	0.55
49:S2:981:A:H2'	49:S2:982:G:C8	2.41	0.55
79:SZ:111:ARG:HD3	79:SZ:114:LYS:HE2	1.89	0.55
27:LY:64:GLY:HA3	27:LY:66:GLN:NE2	2.21	0.55
53:SE:19:MET:SD	53:SE:108:ARG:HD2	2.46	0.55
64:SU:80:PHE:HB3	69:Sd:52:PHE:HB3	1.88	0.55
70:Sg:42:MET:HE2	70:Sg:57:ARG:HG2	1.87	0.55
1:L5:1958:A:O2'	1:L5:2025:A:N1	2.36	0.55
5:LB:257:TRP:O	5:LB:260:ALA:HA	2.06	0.55
49:S2:126:G:H2'	72:SG:199:THR:HG21	1.88	0.55
60:SQ:23:ALA:CB	60:SQ:70:VAL:HG22	2.37	0.55
5:LB:218:ASP:OD2	5:LB:348:ARG:NH2	2.36	0.55
1:L5:461:G:H2'	1:L5:462:G:H8	1.72	0.55
1:L5:4099:G:H2'	1:L5:4101:C:H41	1.70	0.55
62:SS:55:ARG:HD2	79:SZ:48:VAL:HG11	1.89	0.55
66:SX:94:ILE:HG12	66:SX:125:VAL:HG21	1.88	0.55
72:SG:221:LYS:HZ1	72:SG:222:GLU:HG3	1.71	0.55
21:LS:82:LEU:C	21:LS:127:MET:HE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Lk:5:ILE:HD11	39:Lk:43:TYR:HB3	1.89	0.55
49:S2:928:G:H2'	49:S2:929:G:C8	2.42	0.55
62:SS:142:ARG:HB3	62:SS:142:ARG:CZ	2.37	0.55
46:Ls:101:MET:SD	46:Ls:102:LEU:HB3	2.47	0.54
68:Sc:18:LEU:HB2	68:Sc:29:GLN:HB2	1.89	0.54
70:Sg:217:MET:CG	70:Sg:229:THR:OG1	2.54	0.54
1:L5:137:G:H2'	1:L5:138:G:H8	1.72	0.54
1:L5:208:A:C2	1:L5:233:U:H5'	2.42	0.54
18:LP:10:ASN:ND2	18:LP:13:LYS:HD2	2.23	0.54
25:LW:74:ARG:NH1	49:S2:1749:G:N7	2.52	0.54
30:Lb:90:SER:OG	30:Lb:95:ARG:NH2	2.40	0.54
49:S2:886:A:C6	49:S2:901:G:N3	2.75	0.54
70:Sg:32:LEU:CD1	70:Sg:42:MET:CG	2.66	0.54
78:SY:72:PHE:CE2	78:SY:74:MET:HE3	2.41	0.54
1:L5:466:A:C6	1:L5:468:U:O4	2.60	0.54
1:L5:1998:A:N7	46:Ls:55:MET:CE	2.66	0.54
1:L5:4274:A:H2'	1:L5:4275:G:C8	2.42	0.54
8:LE:93:THR:CG2	8:LE:104:THR:OG1	2.55	0.54
47:Lt:117:ARG:HH12	47:Lt:129:ILE:HG23	1.72	0.54
51:SB:182:LYS:HG3	51:SB:231:LEU:HD21	1.89	0.54
70:Sg:206:LEU:C	70:Sg:206:LEU:CD1	2.80	0.54
11:LH:114:ILE:HB	11:LH:124:ARG:HG3	1.90	0.54
46:Ls:101:MET:HE1	46:Ls:102:LEU:CD2	2.26	0.54
57:SK:5:LYS:HE2	57:SK:5:LYS:N	2.23	0.54
70:Sg:87:LEU:HB3	70:Sg:101:PHE:CD1	2.42	0.54
1:L5:1976:G:C6	1:L5:1991:A:C2	2.95	0.54
1:L5:4769:G:H5''	17:LO:176:ARG:HD3	1.89	0.54
12:LI:53:VAL:HG11	22:LT:158:PHE:HZ	1.72	0.54
46:Ls:40:MET:CE	46:Ls:43:ILE:HG12	2.38	0.54
55:SH:41:ARG:HB3	55:SH:41:ARG:NH1	2.22	0.54
1:L5:188:G:H1	88:L5:5315:T1C:H92	1.54	0.54
1:L5:1730:U:H4'	22:LT:100:LYS:HB2	1.90	0.54
6:LC:14:LYS:HE2	6:LC:14:LYS:HA	1.90	0.54
28:LZ:84:ARG:CD	84:CB:20:LEU:HD13	2.35	0.54
46:Ls:45:MET:HA	46:Ls:45:MET:HE3	1.90	0.54
70:Sg:5:MET:HG3	70:Sg:268:ASP:OD2	2.08	0.54
79:SZ:65:TYR:OH	79:SZ:76:ARG:NH1	2.41	0.54
1:L5:1503:A:N6	19:LQ:87:THR:HG21	2.23	0.54
1:L5:2486:G:O6	1:L5:2493:G:O6	2.25	0.54
10:LG:117:ARG:NH1	10:LG:128:VAL:O	2.40	0.54
24:LV:99:GLU:OE1	25:LW:23:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SU:23:THR:HB	64:SU:113:GLU:HB2	1.90	0.54
1:L5:1959:U:H4'	1:L5:1960:A:H5''	1.90	0.54
15:LM:41:PRO:O	15:LM:74:ARG:NH1	2.41	0.54
72:SG:27:PHE:HE1	72:SG:36:VAL:CG1	2.21	0.54
28:LZ:97:ASN:O	28:LZ:100:VAL:HG22	2.07	0.54
37:Li:26:HIS:O	37:Li:29:ARG:HG3	2.08	0.54
59:SP:17:TYR:OH	59:SP:18:ARG:NH1	2.41	0.54
70:Sg:217:MET:HG2	70:Sg:229:THR:CB	2.37	0.54
1:L5:437:G:H4'	33:Le:53:ILE:HA	1.88	0.54
1:L5:4942:C:H4'	8:LE:154:THR:HG23	1.90	0.54
28:LZ:102:ARG:HH11	28:LZ:102:ARG:CB	2.01	0.54
56:SI:13:LYS:HG3	58:SL:137:THR:HG21	1.89	0.54
63:ST:39:LEU:HD12	63:ST:99:VAL:HG21	1.88	0.54
70:Sg:17:TRP:H	70:Sg:36:ARG:HB2	1.73	0.54
70:Sg:109:LEU:HD11	70:Sg:125:ARG:HG3	1.90	0.54
10:LG:58:PRO:HD2	10:LG:61:ILE:HD12	1.90	0.53
40:Ll:37:TYR:CE2	40:Ll:38:ASN:O	2.61	0.53
49:S2:1075:C:OP1	75:SN:107:LYS:NZ	2.41	0.53
49:S2:1861:G:H5''	67:Sa:3:LYS:HA	1.90	0.53
1:L5:1095:A:H2	1:L5:1200:G:N1	1.97	0.53
1:L5:2838:G:H5'	5:LB:247:GLY:HA2	1.91	0.53
1:L5:3868:G:H22	1:L5:3900:G:H1'	1.73	0.53
49:S2:1670:C:H2'	49:S2:1671:G:C8	2.42	0.53
58:SL:49:GLU:HG2	58:SL:118:ARG:HD2	1.90	0.53
1:L5:1767:A:N7	59:SP:10:ARG:NH1	2.56	0.53
5:LB:16:PHE:HB2	5:LB:19:ARG:HH21	1.73	0.53
5:LB:378:ARG:HG2	25:LW:32:LEU:HD21	1.90	0.53
21:LS:2:LYS:HE2	21:LS:35:PRO:HD3	1.90	0.53
51:SB:159:GLN:O	51:SB:163:GLN:HG3	2.09	0.53
61:SR:27:ASP:OD2	61:SR:30:THR:OG1	2.20	0.53
1:L5:198:A:OP2	27:LY:126:ARG:NH2	2.40	0.53
1:L5:4508:C:N3	1:L5:4512:U:H5	2.05	0.53
11:LH:15:ASN:OD1	11:LH:15:ASN:N	2.42	0.53
54:SF:143:PRO:HA	54:SF:146:ARG:HG2	1.91	0.53
57:SK:31:LYS:HA	57:SK:41:PRO:HA	1.91	0.53
67:Sa:100:ARG:HE	67:Sa:102:ARG:HH22	1.56	0.53
1:L5:935:A:N6	15:LM:70:GLN:HE22	2.06	0.53
1:L5:1100:U:O3'	1:L5:1167:C:N4	2.41	0.53
1:L5:4060:U:H2'	1:L5:4061:G:C8	2.44	0.53
50:SA:54:THR:HA	50:SA:162:PRO:HG2	1.91	0.53
55:SH:181:THR:CG2	55:SH:183:LYS:HG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SC:211:LYS:CG	71:SC:215:MET:HE2	2.38	0.53
85:CC:22:C:H2'	85:CC:23:G:H8	1.74	0.53
86:CE:32:LYS:HD3	86:CE:36:ASP:OD2	2.09	0.53
10:LG:117:ARG:HA	10:LG:120:LYS:HE2	1.90	0.53
15:LM:90:ARG:HA	15:LM:93:LYS:HG2	1.89	0.53
24:LV:65:VAL:HG22	24:LV:73:ARG:HA	1.90	0.53
61:SR:76:GLU:OE1	61:SR:76:GLU:CA	2.52	0.53
63:ST:111:LYS:HZ1	63:ST:126:GLN:HB2	1.73	0.53
70:Sg:41:ILE:CG2	70:Sg:43:TRP:CE2	2.92	0.53
1:L5:469:C:H2'	1:L5:470:A:C8	2.43	0.53
1:L5:1548:G:O2'	1:L5:2812:A:N3	2.35	0.53
1:L5:4717:A:OP2	5:LB:30:LYS:NZ	2.35	0.53
49:S2:83:A:C2	78:SY:120:THR:HG22	2.43	0.53
70:Sg:11:LEU:HB2	70:Sg:307:VAL:HB	1.91	0.53
1:L5:989:U:O2	1:L5:1064:G:O6	2.26	0.53
1:L5:5055:G:H21	32:Ld:118:GLN:HE22	1.56	0.53
8:LE:258:LEU:HD12	8:LE:262:LYS:HE2	1.91	0.53
59:SP:106:GLU:OE2	59:SP:108:LYS:HG3	2.08	0.53
73:SJ:89:GLU:O	73:SJ:92:MET:HG3	2.09	0.53
75:SN:104:ARG:HA	75:SN:104:ARG:HE	1.74	0.53
1:L5:4872:G:C2	17:LO:203:VAL:HG23	2.44	0.53
3:L8:45:C:H4'	40:Ll:11:ARG:HD2	1.90	0.53
35:Lg:94:ALA:O	35:Lg:98:GLU:HG2	2.09	0.53
46:Ls:29:ILE:HB	46:Ls:191:GLN:HB2	1.90	0.53
51:SB:121:ILE:HD13	51:SB:164:ILE:HG21	1.91	0.53
60:SQ:53:GLU:HG3	60:SQ:54:PRO:HD3	1.89	0.53
1:L5:1968:G:H2'	1:L5:1969:G:C8	2.43	0.53
1:L5:4537:C:H2'	1:L5:4538:G:C8	2.44	0.53
10:LG:62:ARG:O	10:LG:66:GLN:HG3	2.08	0.53
11:LH:52:LYS:HG3	11:LH:54:ARG:HH11	1.74	0.53
26:LX:90:ILE:HG22	26:LX:147:LEU:HD22	1.91	0.53
66:SX:77:ASN:O	66:SX:79:LYS:N	2.41	0.53
79:SZ:57:LYS:HA	79:SZ:60:LYS:HZ2	1.73	0.53
83:CA:246:ILE:HB	83:CA:305:PHE:HB2	1.90	0.53
13:LJ:67:LYS:O	13:LJ:68:ILE:HD13	2.09	0.52
16:LN:138:PHE:HA	16:LN:143:ARG:HD2	1.90	0.52
49:S2:1536:G:H2'	49:S2:1537:A:H8	1.73	0.52
49:S2:1580:A:C8	64:SU:56:MET:SD	3.03	0.52
49:S2:1580:A:H8	64:SU:56:MET:SD	2.33	0.52
62:SS:4:VAL:HG13	62:SS:5:ILE:N	2.24	0.52
4:LA:104:VAL:HA	4:LA:107:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LI:38:ARG:HG2	12:LI:41:ALA:HB2	1.91	0.52
13:LJ:112:HIS:CD2	13:LJ:126:TYR:H	2.27	0.52
45:Lr:28:GLU:HG2	45:Lr:31:ASN:HB2	1.90	0.52
55:SH:169:LYS:O	55:SH:172:THR:HG22	2.09	0.52
70:Sg:57:ARG:HG2	70:Sg:57:ARG:HH11	1.74	0.52
70:Sg:87:LEU:HB2	70:Sg:101:PHE:HB2	1.90	0.52
7:LD:213:GLU:HA	7:LD:213:GLU:OE1	2.09	0.52
12:LI:87:ILE:HG12	12:LI:138:ILE:HG12	1.91	0.52
51:SB:71:LEU:HD11	51:SB:189:ILE:HG23	1.92	0.52
60:SQ:58:LEU:HD11	60:SQ:112:LEU:HD11	1.91	0.52
72:SG:221:LYS:HZ1	72:SG:222:GLU:CG	2.23	0.52
1:L5:1559:G:OP1	20:LR:126:LYS:NZ	2.42	0.52
1:L5:3717:A:H2'	1:L5:3718:A:C8	2.44	0.52
6:LC:13:GLU:OE2	6:LC:157:LYS:HE3	2.08	0.52
28:LZ:30:ASP:O	28:LZ:39:SER:OG	2.26	0.52
46:Ls:55:MET:SD	46:Ls:56:GLY:HA2	2.49	0.52
49:S2:828:G:OP1	73:SJ:6:SER:OG	2.26	0.52
49:S2:1705:C:H2'	49:S2:1706:G:C8	2.44	0.52
53:SE:11:ARG:HA	53:SE:28:ALA:HB2	1.92	0.52
70:Sg:217:MET:HG2	70:Sg:229:THR:CG2	2.39	0.52
79:SZ:64:ASN:OD1	79:SZ:64:ASN:N	2.42	0.52
1:L5:667:A:H5''	1:L5:668:C:H5''	1.91	0.52
1:L5:1942:A:H2'	1:L5:1943:A:C8	2.45	0.52
12:LI:3:ARG:HD2	12:LI:63:GLU:OE2	2.09	0.52
49:S2:993:G:OP1	49:S2:1131:G:N2	2.40	0.52
58:SL:75:GLY:HA3	58:SL:88:ILE:HD12	1.92	0.52
81:Se:36:MET:HE3	81:Se:40:ARG:HH22	1.60	0.52
1:L5:109:G:OP2	14:LL:74:ARG:NH2	2.39	0.52
1:L5:679:C:H2'	1:L5:680:G:C8	2.45	0.52
1:L5:4873:G:C2	17:LO:175:MET:HG2	2.45	0.52
53:SE:18:TRP:HH2	53:SE:31:PRO:HD3	1.74	0.52
59:SP:58:LYS:HG2	59:SP:61:ARG:HH22	1.74	0.52
9:LF:157:ARG:HG3	9:LF:248:ASN:HD22	1.72	0.52
20:LR:74:ARG:O	20:LR:76:MET:HG2	2.09	0.52
54:SF:185:SER:O	54:SF:191:LYS:NZ	2.43	0.52
55:SH:146:VAL:HG12	77:SW:42:MET:HE1	1.92	0.52
60:SQ:139:ALA:O	60:SQ:140:ARG:NH1	2.43	0.52
45:Lr:108:MET:CE	45:Lr:112:ARG:NH1	2.73	0.52
49:S2:1256:G:C8	64:SU:66:ARG:HB2	2.45	0.52
49:S2:1513:C:H2'	49:S2:1514:G:H8	1.75	0.52
54:SF:124:ASP:CG	54:SF:125:SER:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SH:98:ARG:NH1	55:SH:128:ALA:HB1	2.25	0.52
58:SL:109:MET:HG3	58:SL:111:VAL:HG13	1.91	0.52
82:Sf:140:TYR:HB2	82:Sf:147:THR:HG22	1.91	0.52
83:CA:265:PHE:CD2	83:CA:292:GLY:HA3	2.44	0.52
84:CB:6:GLN:NE2	84:CB:13:VAL:N	2.22	0.52
85:CC:61:C:H2'	85:CC:62:A:H8	1.74	0.52
31:Lc:50:ASN:OD1	31:Lc:50:ASN:C	2.53	0.52
49:S2:640:A:H2'	49:S2:641:A:C8	2.45	0.52
49:S2:747:U:N3	49:S2:796:G:N1	2.58	0.52
52:SD:116:ARG:HG2	52:SD:150:MET:HE1	1.91	0.52
62:SS:3:LEU:CG	62:SS:4:VAL:N	2.69	0.52
1:L5:1814:C:O2'	30:Lb:42:ASN:OD1	2.24	0.52
3:L8:123:U:O2'	3:L8:126:C:N4	2.43	0.52
20:LR:158:GLN:O	20:LR:162:ARG:HG3	2.09	0.52
53:SE:100:ARG:HB2	53:SE:114:ILE:HD13	1.92	0.52
56:SI:130:THR:OG1	56:SI:132:GLU:HG3	2.10	0.52
83:CA:25:GLY:HA3	83:CA:333:ILE:HG13	1.90	0.52
1:L5:1969:G:H4'	46:Ls:36:GLY:HA2	1.92	0.51
11:LH:4:ILE:HG12	11:LH:61:TRP:CH2	2.44	0.51
14:LL:54:PRO:HB2	14:LL:97:SER:HB3	1.92	0.51
27:LY:2:LYS:HD3	27:LY:7:VAL:HG13	1.92	0.51
47:Lt:115:GLN:O	47:Lt:119:ARG:NH1	2.42	0.51
49:S2:367:U:H4'	49:S2:371:A:C8	2.46	0.51
49:S2:1756:C:H42	49:S2:1776:G:H22	0.70	0.51
67:Sa:60:ASP:OD1	67:Sa:60:ASP:N	2.39	0.51
73:SJ:120:ALA:HB2	73:SJ:129:LEU:HD12	1.91	0.51
1:L5:3720:G:H22	1:L5:3733:A:H2	1.58	0.51
10:LG:165:GLU:OE2	16:LN:26:ARG:NH2	2.40	0.51
13:LJ:35:ARG:HD2	13:LJ:123:ILE:HA	1.93	0.51
21:LS:173:ASN:ND2	21:LS:175:PHE:O	2.42	0.51
28:LZ:77:TYR:HD2	31:Lc:39:ARG:HD3	1.76	0.51
34:Lf:78:HIS:HB2	34:Lf:85:ARG:HG2	1.92	0.51
71:SC:256:TRP:CD2	77:SW:68:ARG:HD3	2.46	0.51
79:SZ:50:PHE:CZ	79:SZ:58:LEU:CD2	2.93	0.51
14:LL:125:ILE:HD11	36:Lh:122:LYS:HB3	1.93	0.51
50:SA:8:LEU:HD11	65:SV:39:VAL:HG21	1.93	0.51
57:SK:7:ASN:HB3	57:SK:40:VAL:HB	1.91	0.51
78:SY:20:ARG:HE	78:SY:22:GLN:HE21	1.57	0.51
1:L5:2101:C:H2'	1:L5:2102:G:C8	2.46	0.51
1:L5:4992:G:H2'	1:L5:4993:G:C8	2.45	0.51
8:LE:178:PRO:O	8:LE:181:LEU:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:888:U:H2'	49:S2:900:C:H42	1.75	0.51
49:S2:1536:G:H2'	49:S2:1537:A:C8	2.45	0.51
64:SU:49:LYS:HE2	64:SU:92:HIS:CD2	2.46	0.51
81:Se:3:HIS:NE2	81:Se:5:SER:OG	2.42	0.51
8:LE:190:HIS:HB3	8:LE:193:PHE:HD2	1.76	0.51
22:LT:106:LEU:O	22:LT:110:LYS:HG3	2.10	0.51
47:Lt:104:ILE:HD11	47:Lt:140:GLY:HA3	1.92	0.51
49:S2:380:G:H1'	56:SI:5:ARG:CZ	2.40	0.51
49:S2:787:G:H5''	72:SG:234:LEU:HD22	1.91	0.51
50:SA:209:GLU:OE1	50:SA:209:GLU:C	2.53	0.51
6:LC:318:PRO:HB2	6:LC:325:MET:HE2	1.93	0.51
13:LJ:104:ASN:HD22	13:LJ:134:LEU:H	1.58	0.51
50:SA:82:THR:HG23	50:SA:168:ALA:HA	1.93	0.51
1:L5:1332:C:H2'	1:L5:1333:A:H8	1.74	0.51
1:L5:1812:C:H5''	30:Lb:56:LYS:HE2	1.92	0.51
8:LE:92:VAL:HG23	8:LE:94:LYS:HG3	1.93	0.51
24:LV:36:ASN:C	24:LV:36:ASN:OD1	2.53	0.51
51:SB:52:THR:HG23	51:SB:57:ILE:HA	1.93	0.51
57:SK:64:TRP:HB3	69:Sd:23:VAL:HA	1.93	0.51
79:SZ:47:LEU:HG	79:SZ:78:LYS:HB3	1.93	0.51
1:L5:138:G:H2'	1:L5:139:G:C8	2.45	0.51
4:LA:178:PRO:HG2	44:Lp:26:VAL:HG13	1.92	0.51
47:Lt:18:THR:HA	47:Lt:58:ILE:HG13	1.93	0.51
53:SE:63:LYS:HE2	78:SY:85:ASN:HA	1.93	0.51
70:Sg:174:VAL:HB	70:Sg:188:HIS:HB2	1.93	0.51
1:L5:4092:G:H3'	1:L5:4093:G:H21	1.76	0.51
49:S2:67:C:C5	72:SG:164:LYS:HB2	2.46	0.51
49:S2:1498:A:OP2	52:SD:27:ARG:NH1	2.39	0.51
61:SR:80:ARG:HG3	61:SR:80:ARG:NH1	2.24	0.51
10:LG:136:LEU:HD23	10:LG:193:LEU:CD1	2.41	0.51
21:LS:71:SER:O	21:LS:76:LYS:NZ	2.44	0.51
39:Lk:52:LYS:HA	39:Lk:55:LYS:HE3	1.92	0.51
46:Ls:65:ILE:HG23	46:Ls:75:LEU:HD22	1.93	0.51
49:S2:1650:A:H5''	60:SQ:139:ALA:HB2	1.93	0.51
49:S2:1669:G:OP1	64:SU:79:ARG:NH1	2.43	0.51
73:SJ:34:GLU:HG2	73:SJ:35:TYR:CD2	2.45	0.51
6:LC:154:VAL:HG21	6:LC:170:LEU:HD11	1.93	0.50
8:LE:195:ILE:HD13	34:Lf:110:ILE:HD11	1.93	0.50
49:S2:1232:U:H2'	49:S2:1233:G:C8	2.46	0.50
50:SA:7:VAL:HG13	50:SA:8:LEU:HG	1.92	0.50
1:L5:655:C:OP2	6:LC:268:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1374:G:H1'	6:LC:234:LYS:HD3	1.94	0.50
1:L5:3969:G:O2'	1:L5:4054:C:N4	2.44	0.50
31:Lc:50:ASN:CG	31:Lc:76:GLY:O	2.55	0.50
49:S2:165:G:OP2	49:S2:165:G:N2	2.36	0.50
49:S2:1801:A:H2'	49:S2:1802:C:C6	2.46	0.50
1:L5:456:C:H2'	1:L5:457:G:H8	1.76	0.50
1:L5:2848:G:O2'	1:L5:3838:U:O4	2.28	0.50
1:L5:4591:U:H2'	1:L5:4592:C:C6	2.46	0.50
5:LB:115:LYS:NZ	5:LB:129:ALA:O	2.45	0.50
17:LO:7:LEU:HD23	17:LO:33:VAL:HG22	1.94	0.50
39:Lk:11:PHE:CE1	39:Lk:36:VAL:CG2	2.94	0.50
46:Ls:13:TYR:CE2	46:Ls:60:MET:HG3	2.46	0.50
47:Lt:57:ARG:O	47:Lt:59:THR:OG1	2.27	0.50
55:SH:154:ILE:HB	55:SH:185:VAL:HG12	1.93	0.50
80:Sb:49:HIS:ND1	80:Sb:69:GLY:O	2.44	0.50
83:CA:307:VAL:CG1	83:CA:309:TYR:HE1	2.24	0.50
1:L5:3619:G:H4'	20:LR:79:GLY:O	2.12	0.50
7:LD:265:ARG:NH1	7:LD:267:ASN:O	2.43	0.50
12:LI:145:LYS:HE2	12:LI:167:ILE:HG13	1.94	0.50
43:Lo:26:TYR:HB3	43:Lo:67:VAL:HB	1.94	0.50
49:S2:1550:G:H3'	49:S2:1579:A:H61	1.76	0.50
62:SS:39:ARG:HG3	62:SS:83:PHE:CZ	2.47	0.50
1:L5:1175:A:H2	1:L5:1185:G:C2	2.29	0.50
6:LC:138:MET:SD	6:LC:144:ILE:HG13	2.52	0.50
14:LL:111:GLN:O	14:LL:115:GLN:HG2	2.12	0.50
39:Lk:24:LYS:HB3	39:Lk:69:LEU:HD11	1.94	0.50
49:S2:5:U:H2'	49:S2:6:G:H8	1.77	0.50
1:L5:1558:A:H2'	1:L5:1559:G:C8	2.47	0.50
46:Ls:82:ILE:O	46:Ls:83:ARG:NH1	2.45	0.50
49:S2:380:G:O6	56:SI:178:ARG:NH2	2.43	0.50
49:S2:672:A:N6	49:S2:1027:A:OP1	2.29	0.50
51:SB:123:ALA:HB2	51:SB:165:ARG:HG3	1.93	0.50
1:L5:1705:G:H2'	1:L5:1706:A:O4'	2.12	0.50
1:L5:1878:G:OP2	30:Lb:14:ARG:NH2	2.45	0.50
3:L8:75:G:C8	40:Ll:30:LYS:HG2	2.46	0.50
28:LZ:113:GLU:OE2	28:LZ:117:LYS:NZ	2.42	0.50
36:Lh:4:ILE:HG21	36:Lh:20:GLN:HE22	1.76	0.50
49:S2:886:A:C6	49:S2:901:G:C4	2.97	0.50
1:L5:417:G:OP1	1:L5:2329:U:O2'	2.28	0.50
1:L5:1762:C:N3	1:L5:1770:A:N1	2.60	0.50
1:L5:4260:U:H2'	1:L5:4261:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4281:A:H2'	1:L5:4282:A:H2'	1.93	0.50
1:L5:4363:A:H5''	43:Lo:36:GLN:HG2	1.93	0.50
10:LG:101:LYS:HE2	10:LG:211:ASP:OD1	2.11	0.50
12:LI:76:MET:HE2	12:LI:138:ILE:HG21	1.93	0.50
15:LM:70:GLN:OE1	15:LM:74:ARG:NH2	2.45	0.50
46:Ls:43:ILE:HD12	46:Ls:44:ARG:N	2.25	0.50
49:S2:996:A:H2'	49:S2:997:A:C8	2.47	0.50
52:SD:25:LEU:HA	52:SD:28:GLU:HB2	1.93	0.50
70:Sg:37:ASP:OD1	70:Sg:37:ASP:N	2.38	0.50
72:SG:67:VAL:HB	72:SG:99:GLY:HA2	1.92	0.50
80:Sb:64:CYS:HB3	80:Sb:73:LEU:HD23	1.94	0.50
1:L5:46:U:H5''	14:LL:16:LYS:HG2	1.94	0.50
1:L5:208:A:H2	1:L5:233:U:H5'	1.76	0.50
1:L5:493:G:N1	1:L5:660:A:C2	2.70	0.50
8:LE:92:VAL:HG13	8:LE:109:LEU:HD11	1.92	0.50
67:Sa:53:ILE:HD12	76:SO:116:LEU:HD22	1.94	0.50
1:L5:136:C:N4	36:Lh:77:LYS:O	2.39	0.49
1:L5:172:C:H2'	14:LL:129:ARG:HD3	1.93	0.49
1:L5:460:C:H2'	1:L5:461:G:H8	1.76	0.49
1:L5:2601:A:N6	1:L5:2744:A:OP2	2.43	0.49
47:Lt:105:THR:HG22	47:Lt:107:ASP:HB2	1.93	0.49
58:SL:111:VAL:HG12	58:SL:140:PHE:HB2	1.94	0.49
67:Sa:5:ARG:HB3	67:Sa:7:ASN:O	2.11	0.49
83:CA:266:PHE:CZ	83:CA:301:LEU:HB3	2.47	0.49
1:L5:238:C:OP2	27:LY:45:ARG:NH2	2.45	0.49
1:L5:1730:U:H1'	22:LT:101:SER:HB3	1.94	0.49
1:L5:2034:G:H2'	1:L5:2035:C:C6	2.47	0.49
26:LX:91:GLU:OE2	83:CA:259:MET:SD	2.71	0.49
49:S2:145:G:H2'	49:S2:146:G:C8	2.47	0.49
49:S2:1512:C:H5''	69:Sd:8:TRP:HZ3	1.77	0.49
51:SB:139:CYS:SG	51:SB:168:MET:HE3	2.53	0.49
70:Sg:5:MET:HB2	70:Sg:270:LEU:HD21	1.94	0.49
70:Sg:247:TRP:CD1	70:Sg:260:ASP:HB3	2.46	0.49
83:CA:207:ASP:OD1	83:CA:208:GLN:N	2.45	0.49
1:L5:5006:U:H4'	1:L5:5007:A:H5'	1.94	0.49
12:LI:152:LEU:HB3	12:LI:165:ILE:HD12	1.94	0.49
26:LX:91:GLU:OE2	83:CA:291:MET:HE3	2.12	0.49
41:Lm:93:LYS:HD3	41:Lm:102:ARG:HG2	1.94	0.49
49:S2:617:G:H4'	66:SX:88:ASP:HA	1.94	0.49
49:S2:874:G:H2'	49:S2:875:A:H8	1.77	0.49
60:SQ:100:VAL:HG12	60:SQ:101:ASP:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CA:14:GLU:N	83:CA:14:GLU:OE1	2.45	0.49
6:LC:189:MET:CE	6:LC:201:ARG:NH1	2.76	0.49
13:LJ:20:LEU:HD11	13:LJ:83:LEU:HD13	1.93	0.49
31:Lc:103:ASP:OD1	31:Lc:103:ASP:N	2.42	0.49
45:Lr:62:VAL:HG12	45:Lr:64:ILE:HD12	1.93	0.49
49:S2:944:A:H5'	76:SO:134:PRO:HB3	1.94	0.49
49:S2:1005:G:OP2	51:SB:162:ARG:NH1	2.45	0.49
56:SI:124:LYS:HB2	56:SI:127:ALA:HB2	1.95	0.49
70:Sg:79:LEU:HD22	70:Sg:120:ILE:HD12	1.93	0.49
83:CA:12:ILE:HG23	83:CA:326:MET:HE1	1.94	0.49
63:ST:111:LYS:HD2	63:ST:111:LYS:O	2.13	0.49
84:CB:6:GLN:NE2	84:CB:12:VAL:HA	2.27	0.49
1:L5:1:C:H3'	1:L5:2:G:C8	2.47	0.49
1:L5:1333:A:H2'	1:L5:1334:A:C8	2.48	0.49
1:L5:2520:C:O2	1:L5:2640:G:N2	2.45	0.49
7:LD:236:MET:HA	7:LD:239:MET:HE2	1.94	0.49
15:LM:106:ASP:OD1	15:LM:109:ARG:NH1	2.45	0.49
31:Lc:14:ILE:HG12	31:Lc:17:ARG:NH2	2.28	0.49
49:S2:107:A:H2'	49:S2:108:G:C8	2.47	0.49
49:S2:377:G:H5'	56:SI:98:LYS:HB3	1.93	0.49
57:SK:3:MET:HG2	57:SK:8:ARG:HH21	1.78	0.49
61:SR:87:GLU:N	61:SR:87:GLU:CD	2.69	0.49
48:Lz:195:LYS:C	48:Lz:197:ASN:H	2.20	0.49
49:S2:385:G:H3'	58:SL:136:LYS:HB2	1.95	0.49
49:S2:618:C:H41	66:SX:67:ARG:NH2	2.09	0.49
49:S2:1679:A:OP1	68:Sc:20:ARG:NH2	2.46	0.49
1:L5:95:G:N7	14:LL:11:LYS:NZ	2.50	0.49
1:L5:435:A:O2'	33:Le:26:ASP:OD1	2.31	0.49
1:L5:1308:C:H2'	1:L5:1309:C:C6	2.48	0.49
1:L5:4537:C:H2'	1:L5:4538:G:H8	1.78	0.49
49:S2:1217:A:H2'	49:S2:1218:C:H6	1.78	0.49
49:S2:1533:A:H62	49:S2:1602:U:H3	1.60	0.49
55:SH:122:LEU:HD21	55:SH:126:HIS:CE1	2.48	0.49
71:SC:196:ILE:HB	71:SC:223:TYR:HB2	1.94	0.49
1:L5:1602:U:OP1	38:Lj:2:THR:OG1	2.24	0.49
1:L5:4582:C:OP2	5:LB:28:LYS:NZ	2.46	0.49
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.94	0.49
10:LG:264:LYS:HE2	51:SB:92:GLN:HE22	1.77	0.49
21:LS:83:ARG:HG3	21:LS:125:GLN:HB2	1.95	0.49
31:Lc:71:VAL:H	84:CB:13:VAL:HG13	1.76	0.49
32:Ld:64:ILE:HG23	32:Ld:68:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SX:51:VAL:HG22	66:SX:72:VAL:CG2	2.43	0.49
66:SX:51:VAL:CA	66:SX:72:VAL:HG22	2.41	0.49
66:SX:54:LYS:HE3	66:SX:91:LEU:HG	1.92	0.49
70:Sg:246:TYR:CD2	70:Sg:261:LEU:HD13	2.48	0.49
73:SJ:164:PRO:HB3	73:SJ:170:PRO:HA	1.95	0.49
1:L5:1175:A:N1	1:L5:1185:G:C6	2.81	0.49
7:LD:209:ARG:O	7:LD:213:GLU:HG2	2.13	0.49
16:LN:68:ARG:NH1	16:LN:124:ASP:O	2.45	0.49
22:LT:101:SER:O	22:LT:102:ARG:C	2.55	0.49
49:S2:534:G:H2'	49:S2:535:G:H8	1.77	0.49
62:SS:15:VAL:HG13	62:SS:68:ILE:HG12	1.95	0.49
70:Sg:120:ILE:HB	70:Sg:132:TRP:HB2	1.95	0.49
72:SG:181:THR:HB	72:SG:184:VAL:HG23	1.95	0.49
83:CA:347:MET:SD	83:CA:347:MET:N	2.85	0.49
1:L5:280:G:H5''	16:LN:14:LYS:NZ	2.28	0.48
1:L5:3654:G:O2'	1:L5:3693:U:OP1	2.26	0.48
5:LB:36:ASP:N	5:LB:36:ASP:OD1	2.44	0.48
49:S2:691:G:OP2	49:S2:691:G:N2	2.45	0.48
49:S2:1528:G:O2'	49:S2:1666:C:OP1	2.29	0.48
54:SF:33:ILE:HA	54:SF:36:GLN:OE1	2.13	0.48
70:Sg:24:THR:HG23	70:Sg:27:PHE:H	1.78	0.48
73:SJ:149:VAL:HG11	73:SJ:157:ILE:HD11	1.95	0.48
21:LS:15:ARG:HB3	21:LS:27:LEU:HD23	1.95	0.48
47:Lt:53:TRP:HE3	47:Lt:56:LEU:HG	1.78	0.48
49:S2:4:C:H4'	71:SC:207:ALA:HB2	1.94	0.48
82:Sf:133:ALA:N	82:Sf:140:TYR:O	2.46	0.48
1:L5:452:A:H4'	1:L5:453:G:H5'	1.96	0.48
1:L5:4327:C:OP1	22:LT:70:HIS:NE2	2.45	0.48
4:LA:117:GLU:HG2	4:LA:123:ARG:O	2.14	0.48
10:LG:88:ASP:OD1	10:LG:90:GLN:NE2	2.46	0.48
10:LG:154:LEU:HB3	10:LG:204:PHE:HB2	1.96	0.48
61:SR:75:GLU:CD	61:SR:78:ARG:HH12	2.21	0.48
62:SS:82:TRP:CD1	62:SS:82:TRP:H	2.31	0.48
83:CA:220:VAL:HG23	83:CA:221:HIS:HD2	1.75	0.48
16:LN:84:PRO:HA	16:LN:87:HIS:CG	2.48	0.48
22:LT:93:ILE:HA	22:LT:96:ILE:HG12	1.95	0.48
46:Ls:61:MET:HE3	46:Ls:82:ILE:HD13	1.93	0.48
55:SH:169:LYS:C	55:SH:172:THR:HG22	2.38	0.48
70:Sg:152:SER:H	70:Sg:169:GLY:HA2	1.79	0.48
1:L5:1662:C:H2'	1:L5:1663:C:C6	2.48	0.48
1:L5:3736:A:H2'	1:L5:3737:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3956:G:O5'	1:L5:3966:A:N6	2.47	0.48
5:LB:234:ARG:HG3	5:LB:272:LYS:HB2	1.96	0.48
16:LN:146:PRO:HB2	36:Lh:104:THR:HG23	1.95	0.48
31:Lc:14:ILE:CD1	84:CB:11:CYS:HB3	2.43	0.48
46:Ls:40:MET:HE3	46:Ls:43:ILE:HG13	1.96	0.48
49:S2:1565:C:H5	63:ST:101:ARG:HH12	1.62	0.48
50:SA:118:GLU:HB3	71:SC:65:LYS:HD2	1.94	0.48
54:SF:154:LEU:HD22	54:SF:177:LEU:HD23	1.96	0.48
72:SG:25:ARG:NH1	72:SG:25:ARG:HB2	2.28	0.48
6:LC:13:GLU:OE2	6:LC:157:LYS:CE	2.61	0.48
15:LM:24:LEU:HD11	15:LM:86:TRP:CG	2.49	0.48
28:LZ:102:ARG:NH1	28:LZ:102:ARG:HB2	2.20	0.48
29:La:72:THR:HG22	29:La:110:LYS:HB3	1.95	0.48
46:Ls:60:MET:SD	46:Ls:61:MET:HA	2.53	0.48
50:SA:76:VAL:HG11	50:SA:90:PHE:CD1	2.48	0.48
51:SB:122:GLU:HG2	51:SB:140:VAL:HG23	1.94	0.48
73:SJ:34:GLU:HG2	73:SJ:35:TYR:CE2	2.48	0.48
73:SJ:91:LYS:HD3	73:SJ:96:TYR:CE2	2.49	0.48
79:SZ:49:LEU:N	79:SZ:83:LEU:HD22	2.25	0.48
1:L5:2478:C:N3	1:L5:2591:A:O2'	2.46	0.48
1:L5:3725:G:N7	37:Li:67:LYS:NZ	2.50	0.48
7:LD:75:VAL:O	7:LD:112:ARG:NH1	2.47	0.48
10:LG:234:ARG:NH2	37:Li:46:GLU:CD	2.72	0.48
20:LR:115:ILE:HB	20:LR:119:MET:HG2	1.95	0.48
45:Lr:32:LEU:HD23	45:Lr:113:ARG:HD3	1.94	0.48
46:Ls:60:MET:SD	46:Ls:61:MET:CA	3.01	0.48
49:S2:921:G:C6	80:Sb:22:LYS:HA	2.49	0.48
49:S2:1144:A:H2'	49:S2:1145:A:C8	2.48	0.48
49:S2:1310:U:OP2	82:Sf:105:TYR:OH	2.28	0.48
1:L5:2258:C:N3	8:LE:89:LEU:HA	2.29	0.48
5:LB:139:ASP:OD1	5:LB:140:GLU:N	2.47	0.48
5:LB:145:GLN:OE1	5:LB:148:LYS:NZ	2.46	0.48
8:LE:288:PHE:CE2	34:Lf:110:ILE:CD1	2.97	0.48
32:Ld:37:GLY:O	32:Ld:41:ARG:HG3	2.13	0.48
51:SB:138:PHE:O	51:SB:213:ARG:N	2.47	0.48
51:SB:187:LYS:HB3	51:SB:187:LYS:HE2	1.67	0.48
52:SD:170:THR:HG23	52:SD:187:LYS:HG2	1.96	0.48
70:Sg:206:LEU:CD1	70:Sg:241:PHE:HZ	2.26	0.48
83:CA:100:LEU:HD21	83:CA:127:VAL:HG11	1.94	0.48
85:CC:22:C:H2'	85:CC:23:G:C8	2.49	0.48
1:L5:4457:U:H1'	5:LB:252:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L8:71:A:OP1	27:LY:27:ARG:NH1	2.46	0.48
47:Lt:18:THR:O	47:Lt:61:LYS:NZ	2.45	0.48
53:SE:240:ARG:HH11	53:SE:240:ARG:HG3	1.79	0.48
58:SL:55:TYR:CD1	58:SL:115:PRO:HG2	2.49	0.48
83:CA:118:ILE:HB	83:CA:190:LEU:HD11	1.95	0.48
1:L5:1095:A:N1	1:L5:1200:G:C6	2.82	0.48
1:L5:1332:C:H2'	1:L5:1333:A:C8	2.49	0.48
1:L5:4220:A:H2'	1:L5:4222:G:H5''	1.96	0.48
33:Le:78:LEU:HB3	45:Lr:20:ARG:HD3	1.96	0.48
49:S2:102:A:H4'	49:S2:104:A:C8	2.49	0.48
49:S2:1037:G:H4'	49:S2:1845:A:H4'	1.94	0.48
49:S2:1314:U:H4'	57:SK:3:MET:HE1	1.96	0.48
49:S2:1415:C:H5''	63:ST:129:ARG:HB2	1.96	0.48
50:SA:207:PRO:HA	50:SA:210:ILE:HB	1.96	0.48
62:SS:39:ARG:HG3	62:SS:83:PHE:HZ	1.79	0.48
70:Sg:110:SER:CB	70:Sg:153:CYS:HA	2.43	0.48
73:SJ:170:PRO:CB	73:SJ:174:LYS:HD2	2.43	0.48
78:SY:99:LYS:HB2	78:SY:101:LYS:HZ2	1.79	0.48
78:SY:117:VAL:HG21	78:SY:125:VAL:HG21	1.95	0.48
83:CA:202:ILE:HD13	83:CA:209:GLN:HB3	1.96	0.48
1:L5:182:G:N2	88:L5:5317:T1C:H712	2.29	0.47
1:L5:691:C:H2'	1:L5:692:A:C8	2.49	0.47
1:L5:1558:A:H2'	1:L5:1559:G:H8	1.79	0.47
1:L5:3959:U:O2'	1:L5:3961:G:N7	2.47	0.47
4:LA:196:TRP:O	4:LA:197:PRO:C	2.55	0.47
14:LL:16:LYS:O	14:LL:17:ASP:C	2.57	0.47
23:LU:31:ASP:OD1	23:LU:31:ASP:N	2.47	0.47
23:LU:43:LEU:HD12	23:LU:47:ILE:HD11	1.95	0.47
23:LU:91:LEU:HB3	23:LU:97:ARG:HB3	1.96	0.47
33:Le:70:LEU:HD11	33:Le:76:LYS:HB3	1.95	0.47
49:S2:1588:A:H2'	49:S2:1589:A:C8	2.49	0.47
78:SY:38:THR:O	78:SY:42:GLU:HG2	2.15	0.47
28:LZ:88:ASP:OD1	28:LZ:88:ASP:N	2.43	0.47
49:S2:83:A:C2	78:SY:120:THR:CG2	2.97	0.47
49:S2:534:G:H2'	49:S2:535:G:C8	2.49	0.47
49:S2:1568:C:H2'	49:S2:1569:A:C8	2.49	0.47
49:S2:1647:A:N6	49:S2:1676:U:H5	2.12	0.47
58:SL:126:VAL:HG12	58:SL:145:VAL:HG22	1.96	0.47
59:SP:133:ILE:HD12	59:SP:134:GLY:N	2.29	0.47
1:L5:138:G:H2'	1:L5:139:G:H8	1.77	0.47
1:L5:4459:U:H2'	1:L5:4460:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L8:67:U:H2'	3:L8:68:G:H8	1.79	0.47
7:LD:217:ASP:N	7:LD:217:ASP:OD1	2.41	0.47
25:LW:1:MET:O	25:LW:1:MET:CG	2.39	0.47
50:SA:5:LEU:HD13	65:SV:41:LYS:HA	1.97	0.47
54:SF:74:ASN:OD1	54:SF:86:LYS:HE3	2.14	0.47
72:SG:162:LEU:HD11	72:SG:172:LYS:HD2	1.96	0.47
83:CA:233:GLY:N	83:CA:314:GLU:OE2	2.35	0.47
1:L5:1498:G:OP1	19:LQ:150:ARG:NH1	2.43	0.47
1:L5:2020:U:H2'	1:L5:2021:G:C8	2.43	0.47
1:L5:3973:G:N2	1:L5:3974:G:O6	2.45	0.47
1:L5:4153:C:H2'	1:L5:4154:G:C8	2.49	0.47
4:LA:20:VAL:HA	4:LA:23:ARG:HG3	1.95	0.47
19:LQ:39:THR:HG23	19:LQ:132:LYS:HD3	1.95	0.47
28:LZ:7:PRO:HD3	28:LZ:28:ASN:ND2	2.28	0.47
47:Lt:115:GLN:HE22	47:Lt:162:CYS:HA	1.79	0.47
49:S2:1660:C:H4'	49:S2:1663:A:H62	1.79	0.47
83:CA:158:LYS:HD3	83:CA:330:PRO:HD3	1.96	0.47
10:LG:230:TYR:OH	37:Li:46:GLU:OE2	2.32	0.47
19:LQ:39:THR:HG22	19:LQ:41:SER:H	1.80	0.47
46:Ls:111:ALA:H	46:Ls:182:PRO:HG2	1.78	0.47
49:S2:688:U:C2	55:SH:122:LEU:HD13	2.49	0.47
49:S2:1639:G:O2'	49:S2:1640:A:O4'	2.32	0.47
55:SH:39:GLN:OE1	55:SH:75:ILE:HG22	2.13	0.47
55:SH:61:ILE:HG21	55:SH:180:LEU:HD11	1.97	0.47
62:SS:63:GLU:HG2	62:SS:66:ARG:HH21	1.79	0.47
71:SC:211:LYS:O	71:SC:215:MET:HG3	2.15	0.47
1:L5:86:U:P	19:LQ:168:ARG:HH12	2.33	0.47
1:L5:2904:U:O4	1:L5:3592:G:N2	2.46	0.47
42:Ln:11:ARG:NH2	49:S2:1844:U:OP1	2.48	0.47
49:S2:4:C:O2'	73:SJ:18:ARG:NH2	2.40	0.47
54:SF:17:ILE:CG2	54:SF:46:ALA:HB1	2.43	0.47
61:SR:17:ILE:HB	61:SR:69:ILE:HG21	1.96	0.47
86:CE:11:LYS:HE2	86:CE:11:LYS:HB3	1.78	0.47
1:L5:1239:C:H5	8:LE:60:SER:HB3	1.79	0.47
1:L5:4699:U:H1'	1:L5:4700:A:H5''	1.95	0.47
11:LH:54:ARG:NH1	11:LH:54:ARG:HG3	2.29	0.47
47:Lt:11:LYS:HA	47:Lt:11:LYS:HD2	1.74	0.47
48:Lz:86:ASP:O	48:Lz:90:LEU:N	2.48	0.47
49:S2:527:C:H2'	49:S2:528:A:H8	1.79	0.47
49:S2:785:C:OP2	49:S2:887:U:O2'	2.33	0.47
49:S2:1013:U:OP1	49:S2:1129:G:O2'	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1016:U:OP2	80:Sb:20:LYS:NZ	2.38	0.47
49:S2:1217:A:H2'	49:S2:1218:C:C6	2.49	0.47
49:S2:1457:U:H2'	49:S2:1458:G:C8	2.50	0.47
50:SA:203:PHE:HZ	61:SR:91:LEU:HD11	1.80	0.47
52:SD:35:SER:O	52:SD:35:SER:OG	2.29	0.47
53:SE:139:LEU:HD12	53:SE:139:LEU:O	2.14	0.47
62:SS:47:LYS:HD2	62:SS:77:TYR:O	2.15	0.47
70:Sg:148:SER:OG	70:Sg:171:ASP:OD2	2.30	0.47
73:SJ:142:VAL:HG12	73:SJ:144:ILE:H	1.79	0.47
1:L5:188:G:H2'	88:L5:5315:T1C:H62C	1.96	0.47
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.50	0.47
1:L5:3910:C:H2'	1:L5:3911:C:C6	2.50	0.47
8:LE:167:GLN:HG3	8:LE:173:LEU:HD23	1.97	0.47
13:LJ:164:ARG:O	13:LJ:168:GLN:HG3	2.14	0.47
49:S2:293:C:O2'	49:S2:294:U:H3'	2.15	0.47
49:S2:1757:G:H8	49:S2:1758:G:H1'	1.80	0.47
51:SB:89:GLU:OE2	51:SB:228:LEU:HD13	2.15	0.47
54:SF:50:PRO:HG2	54:SF:90:VAL:HG22	1.96	0.47
1:L5:466:A:N1	1:L5:468:U:C4	2.83	0.47
1:L5:1051:G:N2	1:L5:1064:G:OP1	2.48	0.47
1:L5:2864:A:H2'	1:L5:2865:U:C6	2.49	0.47
1:L5:4954:G:H2'	1:L5:4955:A:C8	2.50	0.47
1:L5:3880:G:H2'	1:L5:3881:G:C8	2.50	0.47
1:L5:3897:G:H4'	5:LB:254:ILE:HG12	1.96	0.47
1:L5:4233:A:H4'	43:Lo:98:LYS:HE3	1.96	0.47
14:LL:7:GLY:O	29:La:49:HIS:NE2	2.38	0.47
48:Lz:67:VAL:HA	48:Lz:68:LEU:HA	1.61	0.47
49:S2:562:U:H2'	49:S2:563:G:C8	2.50	0.47
49:S2:681:U:H4'	66:SX:9:THR:HG22	1.97	0.47
1:L5:494:U:H2'	1:L5:495:C:C6	2.50	0.46
1:L5:1503:A:H4'	1:L5:1504:G:H5'	1.97	0.46
1:L5:3641:U:H5	1:L5:3646:A:N7	2.12	0.46
4:LA:60:LYS:HB3	4:LA:60:LYS:NZ	2.29	0.46
49:S2:12:U:H2'	49:S2:13:C:C6	2.50	0.46
49:S2:326:C:O2	49:S2:327:G:N2	2.48	0.46
49:S2:613:G:N2	49:S2:626:G:OP1	2.43	0.46
57:SK:16:PHE:HD2	57:SK:79:LEU:HD23	1.80	0.46
60:SQ:85:ARG:NH2	60:SQ:116:ASP:OD2	2.43	0.46
61:SR:17:ILE:CG2	61:SR:69:ILE:HG21	2.45	0.46
63:ST:113:VAL:HG12	63:ST:123:LEU:HD23	1.97	0.46
67:Sa:3:LYS:NZ	67:Sa:8:ASN:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1976:G:N1	1:L5:1991:A:H2	2.04	0.46
1:L5:2902:G:O6	1:L5:3594:C:N4	2.47	0.46
1:L5:3976:C:N4	1:L5:4035:G:OP2	2.48	0.46
14:LL:48:PRO:HG3	36:Lh:118:LYS:HE3	1.97	0.46
22:LT:159:MET:HE3	22:LT:159:MET:HB2	1.83	0.46
49:S2:851:C:H5''	49:S2:852:G:H5'	1.97	0.46
54:SF:201:LYS:O	54:SF:204:ARG:HG2	2.14	0.46
68:Sc:34:PHE:C	68:Sc:36:ASP:H	2.24	0.46
70:Sg:217:MET:SD	70:Sg:229:THR:OG1	2.71	0.46
1:L5:1958:A:H1'	1:L5:1962:A:H1'	1.98	0.46
1:L5:3604:A:H2'	1:L5:3605:C:O4'	2.16	0.46
1:L5:4745:G:H1	1:L5:4955:A:H61	1.64	0.46
6:LC:8:ILE:HD11	6:LC:257:PHE:CE2	2.49	0.46
27:LY:19:PHE:O	27:LY:26:ARG:NH2	2.48	0.46
46:Ls:121:VAL:HG13	46:Ls:160:LEU:HD23	1.96	0.46
51:SB:38:MET:HE2	51:SB:185:VAL:HG11	1.97	0.46
51:SB:92:GLN:HG2	51:SB:97:LEU:HD11	1.98	0.46
52:SD:187:LYS:HB3	52:SD:187:LYS:HE3	1.71	0.46
64:SU:68:THR:O	69:Sd:40:ARG:NH1	2.47	0.46
68:Sc:31:ARG:O	68:Sc:31:ARG:HG3	2.10	0.46
1:L5:1440:U:H2'	1:L5:1441:C:C6	2.50	0.46
1:L5:4135:G:H2'	1:L5:4136:G:C8	2.50	0.46
6:LC:144:ILE:HD13	6:LC:150:LEU:HD13	1.98	0.46
12:LI:47:PRO:HD2	12:LI:141:LYS:HA	1.97	0.46
22:LT:88:ARG:HH22	30:Lb:30:GLU:CD	2.24	0.46
25:LW:97:LYS:HE3	25:LW:101:ARG:HE	1.80	0.46
49:S2:455:A:H2'	49:S2:456:C:C6	2.51	0.46
51:SB:225:LEU:HD23	51:SB:229:MET:HG2	1.98	0.46
61:SR:69:ILE:HD13	61:SR:71:ILE:CD1	2.45	0.46
62:SS:45:LEU:HD13	62:SS:50:ILE:HD11	1.97	0.46
72:SG:216:ARG:O	72:SG:217:MET:HG3	2.15	0.46
83:CA:263:ARG:CB	83:CA:263:ARG:CZ	2.94	0.46
85:CC:68:U:H2'	85:CC:69:G:C8	2.51	0.46
4:LA:10:LYS:HA	4:LA:16:PHE:CD2	2.51	0.46
14:LL:135:LYS:HE2	14:LL:135:LYS:HB2	1.60	0.46
20:LR:21:LYS:HE3	20:LR:55:VAL:HA	1.97	0.46
37:Li:53:TYR:HB2	37:Li:76:ARG:HG3	1.98	0.46
49:S2:1220:A:H2'	49:S2:1221:G:O4'	2.15	0.46
55:SH:41:ARG:HG2	55:SH:41:ARG:HH11	1.79	0.46
55:SH:41:ARG:HH11	55:SH:41:ARG:CG	2.28	0.46
59:SP:81:ARG:NH2	59:SP:117:GLY:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SV:27:LYS:HD3	71:SC:163:VAL:HG12	1.97	0.46
72:SG:27:PHE:CE1	72:SG:36:VAL:CG1	2.98	0.46
83:CA:90:SER:O	83:CA:90:SER:OG	2.32	0.46
83:CA:263:ARG:CZ	83:CA:263:ARG:HB3	2.45	0.46
1:L5:1995:G:H4'	47:Lt:128:THR:HB	1.97	0.46
1:L5:4139:G:O6	1:L5:4141:G:N2	2.48	0.46
6:LC:156:ASP:CG	6:LC:255:SER:OG	2.58	0.46
28:LZ:92:ASP:OD1	28:LZ:94:THR:N	2.47	0.46
46:Ls:44:ARG:HE	46:Ls:53:VAL:HG23	1.81	0.46
55:SH:169:LYS:HA	55:SH:172:THR:HG22	1.98	0.46
69:Sd:3:HIS:CE1	69:Sd:5:GLN:HB2	2.51	0.46
70:Sg:32:LEU:HD12	70:Sg:42:MET:CA	2.41	0.46
1:L5:1258:G:H2'	1:L5:1259:G:C8	2.51	0.46
1:L5:2520:C:H2'	1:L5:2521:G:H8	1.80	0.46
1:L5:4966:A:H2'	1:L5:4967:A:O4'	2.15	0.46
1:L5:5055:G:H21	32:Ld:118:GLN:NE2	2.13	0.46
60:SQ:5:GLY:O	60:SQ:27:ARG:NH2	2.49	0.46
70:Sg:30:MET:O	70:Sg:30:MET:SD	2.74	0.46
70:Sg:46:THR:O	70:Sg:46:THR:OG1	2.33	0.46
83:CA:272:ARG:C	83:CA:273:PHE:CD1	2.94	0.46
1:L5:703:G:H2'	1:L5:704:C:H4'	1.98	0.46
49:S2:528:A:H2'	49:S2:529:A:H8	1.80	0.46
52:SD:34:TYR:OH	52:SD:37:VAL:HG13	2.15	0.46
71:SC:108:LYS:HZ3	71:SC:110:MET:HB3	1.80	0.46
81:Se:26:LYS:HE2	81:Se:26:LYS:HB3	1.73	0.46
1:L5:433:A:C2	1:L5:3867:A:H4'	2.51	0.46
1:L5:505:G:H1	1:L5:653:U:H3	1.64	0.46
1:L5:1442:C:H2'	1:L5:1443:A:C8	2.50	0.46
1:L5:2284:G:OP1	29:La:7:LYS:NZ	2.41	0.46
1:L5:2745:A:H2'	1:L5:2746:A:C8	2.51	0.46
1:L5:3923:A:H2'	1:L5:3924:C:C6	2.50	0.46
1:L5:4389:C:H2'	1:L5:4390:A:C8	2.51	0.46
4:LA:14:SER:HA	4:LA:17:ARG:NH1	2.26	0.46
11:LH:89:ARG:NH1	11:LH:147:GLU:OE2	2.49	0.46
26:LX:64:SER:HB2	36:Lh:69:LEU:HD13	1.98	0.46
28:LZ:88:ASP:O	28:LZ:121:ARG:NH2	2.39	0.46
36:Lh:10:ARG:HH12	36:Lh:63:GLN:HG3	1.81	0.46
49:S2:690:G:H8	55:SH:182:GLY:HA3	1.80	0.46
61:SR:63:ARG:HB2	61:SR:63:ARG:HH11	1.81	0.46
70:Sg:223:GLU:OE1	70:Sg:223:GLU:N	2.48	0.46
81:Se:52:LYS:HE2	81:Se:52:LYS:HB3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:25:A:H2'	1:L5:26:C:H6	1.81	0.46
1:L5:1645:C:H2'	1:L5:1646:A:C8	2.50	0.46
1:L5:1749:A:H2'	1:L5:1750:G:C8	2.51	0.46
1:L5:1949:U:H5'	11:LH:64:ARG:HD3	1.98	0.46
1:L5:3656:A:H2'	1:L5:3657:U:H6	1.81	0.46
1:L5:4635:A:OP1	1:L5:4636:U:O2'	2.26	0.46
14:LL:8:MET:HE3	14:LL:8:MET:HB2	1.92	0.46
18:LP:122:ALA:HB3	18:LP:143:PRO:HB2	1.98	0.46
36:Lh:59:THR:O	36:Lh:63:GLN:HG2	2.15	0.46
45:Lr:32:LEU:HD22	45:Lr:110:ALA:HA	1.98	0.46
47:Lt:16:ARG:HD2	47:Lt:28:LEU:HD12	1.97	0.46
49:S2:902:G:O2'	49:S2:903:A:H8	1.99	0.46
49:S2:1458:G:H5''	70:Sg:280:LYS:HD3	1.98	0.46
53:SE:151:ASP:OD2	72:SG:216:ARG:NH2	2.49	0.46
62:SS:23:ARG:O	62:SS:55:ARG:NH1	2.49	0.46
63:ST:111:LYS:HD2	63:ST:111:LYS:C	2.41	0.46
70:Sg:34:ALA:HB1	70:Sg:66:VAL:HG23	1.97	0.46
82:Sf:104:LYS:O	82:Sf:104:LYS:HD2	2.17	0.46
83:CA:361:SER:OG	83:CA:362:ALA:N	2.49	0.46
1:L5:651:C:O2	29:La:85:GLN:NE2	2.49	0.45
1:L5:2458:C:H5''	16:LN:67:ARG:HD2	1.97	0.45
1:L5:2520:C:H2'	1:L5:2521:G:C8	2.51	0.45
1:L5:3966:A:H1'	1:L5:4046:A:H61	1.81	0.45
3:L8:19:C:H2'	3:L8:20:A:C8	2.51	0.45
5:LB:262:VAL:O	17:LO:64:THR:HG23	2.16	0.45
9:LF:196:THR:O	9:LF:196:THR:OG1	2.29	0.45
17:LO:54:TYR:OH	17:LO:73:PHE:O	2.34	0.45
49:S2:528:A:H2'	49:S2:529:A:C8	2.51	0.45
49:S2:656:G:H5'	49:S2:662:G:N2	2.31	0.45
52:SD:7:LYS:HA	52:SD:10:LYS:HG2	1.98	0.45
58:SL:80:MET:HE2	58:SL:80:MET:HB3	1.68	0.45
64:SU:56:MET:HE2	64:SU:88:LEU:HD11	1.96	0.45
70:Sg:217:MET:CE	70:Sg:219:TRP:HZ2	2.28	0.45
1:L5:2479:G:H2'	1:L5:2480:G:C8	2.51	0.45
16:LN:191:ALA:O	16:LN:195:ARG:HG2	2.16	0.45
27:LY:112:ASP:N	27:LY:112:ASP:OD1	2.50	0.45
43:Lo:102:GLN:HA	43:Lo:102:GLN:HE21	1.77	0.45
49:S2:1394:G:H21	49:S2:1475:G:H1'	1.81	0.45
49:S2:1777:G:H2'	49:S2:1778:C:C6	2.51	0.45
59:SP:29:SER:OG	59:SP:30:TYR:N	2.47	0.45
1:L5:1327:C:H2'	1:L5:1328:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1846:G:H2'	1:L5:1847:C:C6	2.51	0.45
1:L5:1976:G:C2	1:L5:1991:A:C2	3.02	0.45
1:L5:4061:G:H2'	1:L5:4062:A:C8	2.52	0.45
1:L5:4258:C:H2'	1:L5:4259:C:H6	1.82	0.45
6:LC:66:SER:O	6:LC:66:SER:OG	2.33	0.45
9:LF:71:MET:SD	9:LF:74:MET:CE	3.04	0.45
28:LZ:135:ARG:HA	28:LZ:135:ARG:HD2	1.72	0.45
49:S2:352:U:H2'	49:S2:353:C:C6	2.52	0.45
53:SE:138:HIS:HD2	53:SE:148:ARG:HG2	1.81	0.45
58:SL:21:LYS:HA	58:SL:21:LYS:HD2	1.68	0.45
73:SJ:28:GLU:HB2	73:SJ:43:VAL:HG11	1.99	0.45
1:L5:461:G:H2'	1:L5:462:G:C8	2.51	0.45
1:L5:1464:C:H5''	30:Lb:32:LEU:HD12	1.99	0.45
1:L5:1802:A:H5''	1:L5:1803:G:H5'	1.97	0.45
6:LC:13:GLU:OE2	6:LC:157:LYS:NZ	2.49	0.45
56:SI:101:ILE:HD12	56:SI:190:LEU:HD11	1.97	0.45
64:SU:98:VAL:HA	64:SU:101:ILE:HB	1.98	0.45
1:L5:456:C:H2'	1:L5:457:G:C8	2.51	0.45
1:L5:469:C:H2'	1:L5:470:A:H8	1.82	0.45
1:L5:3911:C:H2'	1:L5:3912:U:C6	2.52	0.45
1:L5:3917:A:H2'	1:L5:3918:G:H8	1.81	0.45
1:L5:4685:U:H2'	1:L5:4686:G:C8	2.51	0.45
14:LL:123:LYS:HD2	14:LL:155:MET:CE	2.44	0.45
24:LV:10:SER:OG	24:LV:11:GLY:N	2.46	0.45
49:S2:51:U:H2'	49:S2:52:G:C8	2.51	0.45
49:S2:1275:G:N2	49:S2:1506:A:OP2	2.38	0.45
49:S2:1287:A:H62	49:S2:1312:G:H21	1.63	0.45
49:S2:1611:G:O2'	62:SS:87:GLN:O	2.24	0.45
60:SQ:21:ALA:HB2	60:SQ:72:VAL:HG23	1.97	0.45
61:SR:37:GLU:OE2	70:Sg:150:TRP:NE1	2.45	0.45
61:SR:75:GLU:OE1	61:SR:78:ARG:NH1	2.49	0.45
63:ST:97:LYS:HB2	63:ST:97:LYS:HE2	1.69	0.45
70:Sg:41:ILE:HG22	70:Sg:43:TRP:NE1	2.31	0.45
1:L5:717:U:H2'	1:L5:718:C:C6	2.51	0.45
1:L5:4618:G:H5''	24:LV:15:ARG:HB2	1.99	0.45
26:LX:152:LYS:HE3	26:LX:152:LYS:HB3	1.70	0.45
37:Li:76:ARG:HD3	37:Li:76:ARG:HA	1.69	0.45
46:Ls:26:LYS:HB2	46:Ls:91:THR:HG23	1.97	0.45
47:Lt:121:LEU:HB3	47:Lt:123:ARG:HB3	1.99	0.45
49:S2:1298:G:H21	59:SP:52:LYS:NZ	2.15	0.45
65:SV:12:TYR:HB3	71:SC:79:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Sd:6:LEU:HA	69:Sd:9:SER:HB2	1.99	0.45
78:SY:102:THR:OG1	78:SY:106:GLN:OE1	2.33	0.45
1:L5:407:A:O2'	1:L5:410:A:OP1	2.28	0.45
2:L7:55:A:H4'	13:LJ:155:HIS:HB2	1.99	0.45
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	1.98	0.45
5:LB:353:VAL:HG12	5:LB:355:THR:HG23	1.99	0.45
26:LX:89:LYS:HB3	26:LX:95:THR:OG1	2.17	0.45
47:Lt:57:ARG:HD3	47:Lt:83:LYS:HD3	1.99	0.45
50:SA:173:LEU:HD11	50:SA:177:MET:HE2	1.99	0.45
58:SL:16:ILE:HG23	58:SL:34:PRO:HG2	1.97	0.45
70:Sg:41:ILE:HG22	70:Sg:43:TRP:CD1	2.52	0.45
70:Sg:262:GLU:OE1	70:Sg:262:GLU:N	2.49	0.45
78:SY:100:LYS:HA	78:SY:100:LYS:HD2	1.79	0.45
79:SZ:99:LEU:HD21	79:SZ:102:LYS:HB2	1.97	0.45
83:CA:15:ASP:OD1	83:CA:15:ASP:N	2.50	0.45
1:L5:2709:C:H1'	20:LR:39:GLN:HB3	1.98	0.45
1:L5:2906:G:H1'	1:L5:2908:U:H1'	1.97	0.45
13:LJ:113:ILE:HG21	13:LJ:119:TYR:HB2	1.99	0.45
37:Li:63:VAL:HG12	37:Li:65:LYS:HG3	1.98	0.45
45:Lr:28:GLU:OE2	45:Lr:31:ASN:ND2	2.50	0.45
49:S2:527:C:H2'	49:S2:528:A:C8	2.52	0.45
49:S2:532:C:H2'	49:S2:533:A:H8	1.82	0.45
49:S2:750:C:H41	49:S2:793:G:H21	1.65	0.45
60:SQ:43:GLU:HB3	60:SQ:44:PRO:HD3	1.98	0.45
70:Sg:129:ILE:CD1	70:Sg:154:VAL:HG11	2.46	0.45
72:SG:136:LYS:NZ	72:SG:175:LYS:O	2.44	0.45
1:L5:21:G:H1'	3:L8:103:A:N3	2.32	0.45
5:LB:29:VAL:HA	5:LB:220:ILE:HD13	1.99	0.45
28:LZ:103:ASP:OD2	28:LZ:106:LEU:HD13	2.17	0.45
47:Lt:115:GLN:HA	47:Lt:119:ARG:HH22	1.82	0.45
49:S2:201:C:H3'	49:S2:202:G:H21	1.81	0.45
49:S2:1047:C:H5'	76:SO:143:LYS:HB2	1.99	0.45
49:S2:1101:U:H2'	49:S2:1102:G:C8	2.52	0.45
83:CA:12:ILE:HG12	83:CA:324:LEU:HD21	1.99	0.45
83:CA:307:VAL:CG1	83:CA:309:TYR:CE1	3.00	0.45
1:L5:2279:A:O2'	33:Le:48:ARG:NH2	2.50	0.45
7:LD:232:THR:H	7:LD:235:MET:HG2	1.82	0.45
8:LE:50:LEU:HD23	8:LE:50:LEU:H	1.82	0.45
36:Lh:4:ILE:HD11	36:Lh:53:SER:HB3	1.99	0.45
49:S2:222:U:H5''	58:SL:17:PHE:CG	2.52	0.45
49:S2:300:U:H2'	49:S2:301:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:33:GLN:HB3	50:SA:154:LEU:HD12	1.99	0.45
53:SE:153:LEU:O	53:SE:174:LYS:NZ	2.50	0.45
56:SI:165:GLN:HG3	56:SI:171:LEU:HD23	1.98	0.45
71:SC:230:THR:C	71:SC:232:THR:H	2.25	0.45
1:L5:908:G:H2'	1:L5:909:A:H8	1.82	0.44
1:L5:962:C:H2'	1:L5:1702:C:H5	1.82	0.44
1:L5:1514:U:H2'	1:L5:1515:A:C8	2.52	0.44
1:L5:4067:U:H2'	1:L5:4068:U:C6	2.52	0.44
8:LE:239:LYS:HB3	8:LE:241:GLU:OE2	2.17	0.44
26:LX:119:ILE:HD12	26:LX:140:LEU:HD22	1.99	0.44
32:Ld:50:ARG:O	32:Ld:54:MET:HG3	2.18	0.44
41:Lm:94:MET:HG2	41:Lm:105:PRO:HA	1.98	0.44
49:S2:15:U:H2'	49:S2:16:G:O4'	2.18	0.44
88:S2:1930:T1C:H953	88:S2:1930:T1C:H921	1.75	0.44
53:SE:151:ASP:HB3	53:SE:154:ILE:HG13	1.99	0.44
62:SS:3:LEU:CG	62:SS:4:VAL:H	2.26	0.44
63:ST:42:HIS:HB3	63:ST:93:SER:HB2	1.99	0.44
72:SG:31:ARG:HH11	72:SG:31:ARG:HG3	1.81	0.44
1:L5:162:A:H2'	1:L5:163:A:C8	2.52	0.44
1:L5:163:A:H2'	1:L5:164:G:H8	1.82	0.44
1:L5:3603:G:H2'	1:L5:3604:A:H5''	1.98	0.44
1:L5:4507:A:H2'	1:L5:4508:C:C6	2.53	0.44
4:LA:196:TRP:O	4:LA:198:ARG:N	2.51	0.44
5:LB:302:ASN:O	5:LB:304:SER:N	2.45	0.44
10:LG:102:TYR:OH	10:LG:207:VAL:HG13	2.17	0.44
10:LG:165:GLU:HA	10:LG:168:VAL:HG22	2.00	0.44
20:LR:8:LYS:HB2	20:LR:8:LYS:HE3	1.83	0.44
49:S2:1394:G:H5''	60:SQ:126:ARG:NH1	2.32	0.44
52:SD:219:PRO:HB2	70:Sg:190:GLY:HA2	1.98	0.44
53:SE:101:LEU:HD23	53:SE:101:LEU:HA	1.90	0.44
66:SX:71:ARG:HD2	66:SX:71:ARG:HA	1.81	0.44
70:Sg:259:TRP:HE1	70:Sg:266:ILE:HG22	1.83	0.44
1:L5:318:A:H2'	1:L5:319:A:C8	2.53	0.44
23:LU:19:LEU:O	23:LU:73:THR:HA	2.17	0.44
23:LU:96:LEU:HB3	23:LU:100:LEU:HD12	1.98	0.44
49:S2:67:C:C5	72:SG:162:LEU:HB3	2.52	0.44
49:S2:522:A:OP1	73:SJ:146:SER:OG	2.19	0.44
49:S2:1413:G:H2'	49:S2:1414:A:H8	1.82	0.44
51:SB:227:LYS:HE2	51:SB:227:LYS:HB3	1.71	0.44
57:SK:3:MET:O	57:SK:5:LYS:NZ	2.48	0.44
66:SX:109:GLY:O	66:SX:119:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SZ:42:ASP:OD1	79:SZ:42:ASP:N	2.41	0.44
82:Sf:87:THR:O	82:Sf:90:LYS:NZ	2.43	0.44
83:CA:141:ASP:HA	83:CA:345:SER:HB2	1.98	0.44
1:L5:182:G:H22	88:L5:5317:T1C:H712	1.81	0.44
1:L5:4324:A:H2'	1:L5:4325:A:C8	2.51	0.44
15:LM:101:LYS:HG3	15:LM:104:MET:HE2	1.99	0.44
25:LW:73:ARG:NH2	49:S2:1781:A:OP2	2.50	0.44
46:Ls:13:TYR:CE2	46:Ls:60:MET:SD	3.07	0.44
47:Lt:53:TRP:CE3	47:Lt:56:LEU:HG	2.52	0.44
49:S2:71:G:H2'	49:S2:72:C:H4'	1.99	0.44
49:S2:379:C:H5'	56:SI:33:ALA:HA	2.00	0.44
49:S2:441:C:H2'	49:S2:442:C:C6	2.53	0.44
49:S2:975:G:OP1	76:SO:98:ARG:NH1	2.48	0.44
49:S2:1610:G:OP1	62:SS:121:ARG:NH2	2.50	0.44
54:SF:38:TYR:HD2	54:SF:144:LEU:HD13	1.82	0.44
54:SF:176:GLU:OE2	54:SF:187:SER:OG	2.32	0.44
70:Sg:153:CYS:SG	70:Sg:198:VAL:N	2.83	0.44
72:SG:52:ILE:HG21	72:SG:102:VAL:HG21	2.00	0.44
75:SN:119:GLU:HG2	75:SN:141:TYR:CE2	2.52	0.44
76:SO:103:ASN:HD21	76:SO:140:THR:HG22	1.82	0.44
83:CA:31:VAL:HG21	83:CA:56:ILE:HD11	1.99	0.44
1:L5:390:C:H5'	83:CA:211:LYS:HE2	1.99	0.44
1:L5:1359:G:H4'	16:LN:203:TYR:HB2	1.99	0.44
1:L5:4425:G:OP1	41:Lm:100:TYR:OH	2.32	0.44
1:L5:4910:G:N2	17:LO:106:ASP:O	2.50	0.44
2:L7:111:C:H2'	2:L7:112:U:O4'	2.17	0.44
47:Lt:39:PRO:HG2	47:Lt:70:GLN:HE22	1.83	0.44
47:Lt:48:LYS:HD2	47:Lt:48:LYS:HA	1.84	0.44
47:Lt:121:LEU:HD23	47:Lt:123:ARG:HB3	1.99	0.44
53:SE:138:HIS:CD2	53:SE:148:ARG:HG2	2.53	0.44
55:SH:100:ILE:HG12	55:SH:125:VAL:HG21	2.00	0.44
55:SH:169:LYS:CA	55:SH:172:THR:HG22	2.47	0.44
62:SS:40:TYR:HA	62:SS:43:VAL:HG12	1.99	0.44
66:SX:51:VAL:HA	66:SX:72:VAL:CG2	2.43	0.44
67:Sa:90:GLU:OE1	67:Sa:90:GLU:N	2.48	0.44
80:Sb:24:LEU:HD23	80:Sb:24:LEU:HA	1.78	0.44
84:CB:6:GLN:HE22	84:CB:12:VAL:HA	1.81	0.44
1:L5:38:A:H5''	29:La:35:ALA:HB2	1.98	0.44
1:L5:62:A:N3	1:L5:77:U:O2'	2.45	0.44
1:L5:493:G:C6	1:L5:660:A:N1	2.85	0.44
1:L5:1974:U:H4'	1:L5:1975:G:H3'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2664:G:OP2	20:LR:121:HIS:ND1	2.44	0.44
9:LF:27:GLU:H	9:LF:27:GLU:HG2	1.54	0.44
11:LH:27:VAL:HG23	11:LH:80:MET:HE2	1.99	0.44
15:LM:93:LYS:HE2	15:LM:93:LYS:HB3	1.75	0.44
39:Lk:25:ILE:HD13	39:Lk:57:LYS:HE3	1.98	0.44
47:Lt:82:ILE:HA	47:Lt:85:LEU:HB2	1.99	0.44
49:S2:83:A:H2	78:SY:120:THR:HG21	1.81	0.44
54:SF:33:ILE:HD11	68:Sc:11:LEU:HD23	2.00	0.44
55:SH:41:ARG:CZ	55:SH:41:ARG:CB	2.94	0.44
55:SH:169:LYS:O	55:SH:172:THR:CG2	2.65	0.44
62:SS:28:PHE:HE1	62:SS:38:ARG:HE	1.64	0.44
63:ST:10:ASN:O	63:ST:14:PHE:N	2.46	0.44
72:SG:22:ARG:NH1	72:SG:25:ARG:HD2	2.32	0.44
75:SN:40:LEU:HB3	75:SN:45:LEU:HD12	1.99	0.44
1:L5:1502:G:H1	19:LQ:89:ASP:HA	1.83	0.44
1:L5:1994:C:H2'	1:L5:1995:G:H8	1.83	0.44
1:L5:2539:C:H2'	1:L5:2540:C:C6	2.53	0.44
1:L5:4194:U:O2'	12:LI:116:ARG:NH2	2.51	0.44
5:LB:201:LEU:HD12	5:LB:201:LEU:HA	1.85	0.44
8:LE:183:ARG:HA	8:LE:183:ARG:HD2	1.73	0.44
28:LZ:50:PRO:HD3	28:LZ:68:ILE:HG12	1.98	0.44
49:S2:1313:A:H4'	49:S2:1314:U:O4'	2.17	0.44
55:SH:162:GLN:HG3	55:SH:165:ASN:HB2	1.99	0.44
61:SR:18:GLU:HG2	61:SR:69:ILE:HG22	2.00	0.44
70:Sg:292:SER:HB3	70:Sg:299:PHE:HE2	1.83	0.44
73:SJ:47:LYS:HB2	73:SJ:47:LYS:HE2	1.81	0.44
83:CA:257:LEU:O	83:CA:263:ARG:HD2	2.18	0.44
83:CA:306:ASN:OD1	83:CA:306:ASN:N	2.51	0.44
1:L5:325:U:H2'	1:L5:326:C:C6	2.52	0.44
1:L5:1613:A:H5''	4:LA:183:GLY:HA3	2.00	0.44
5:LB:14:LEU:O	5:LB:17:LEU:HB2	2.18	0.44
7:LD:99:TYR:HE2	7:LD:164:LYS:HG3	1.82	0.44
33:Le:38:PRO:HG2	33:Le:45:VAL:HG22	1.99	0.44
49:S2:857:U:H2'	49:S2:858:A:C8	2.53	0.44
50:SA:151:ASP:OD1	50:SA:151:ASP:N	2.44	0.44
57:SK:6:LYS:HE3	57:SK:6:LYS:HB2	1.73	0.44
71:SC:129:ALA:HB1	71:SC:216:MET:CE	2.37	0.44
72:SG:145:PHE:CD2	72:SG:156:TYR:HB3	2.53	0.44
1:L5:2029:A:H2'	1:L5:2030:A:C8	2.53	0.44
1:L5:2874:U:O2'	1:L5:2876:G:N7	2.46	0.44
5:LB:161:ARG:HG2	5:LB:184:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:362:GLN:NE2	6:LC:366:ASP:OD2	2.51	0.44
29:La:23:GLY:HA3	29:La:24:LYS:HA	1.55	0.44
31:Lc:57:LYS:HB2	31:Lc:57:LYS:HE2	1.74	0.44
46:Ls:60:MET:SD	46:Ls:60:MET:O	2.75	0.44
49:S2:639:C:H2'	49:S2:640:A:C8	2.53	0.44
52:SD:211:VAL:O	61:SR:20:TYR:OH	2.35	0.44
55:SH:142:LYS:HB3	77:SW:54:ASP:HB3	2.00	0.44
73:SJ:131:ARG:HA	73:SJ:131:ARG:HD2	1.80	0.44
86:CE:18:ARG:HH22	86:CE:19:ARG:HH21	1.65	0.44
1:L5:495:C:H2'	1:L5:496:G:C8	2.53	0.43
1:L5:3848:U:H2'	1:L5:3849:A:C8	2.52	0.43
1:L5:4140:C:N3	1:L5:4145:C:O2'	2.46	0.43
11:LH:173:ARG:HB3	41:Lm:127:VAL:HG22	2.00	0.43
19:LQ:159:PRO:HA	19:LQ:160:HIS:HA	1.63	0.43
22:LT:117:LYS:HE3	22:LT:117:LYS:HB2	1.85	0.43
28:LZ:41:ALA:HB2	28:LZ:77:TYR:HE1	1.83	0.43
42:Ln:10:MET:HE2	49:S2:1172:U:H4'	1.99	0.43
46:Ls:18:ILE:HD13	46:Ls:21:LEU:HD21	1.99	0.43
49:S2:1622:U:N3	59:SP:122:THR:OG1	2.45	0.43
50:SA:205:ARG:HB3	50:SA:209:GLU:OE2	2.17	0.43
52:SD:136:VAL:HG22	52:SD:186:VAL:HG22	2.00	0.43
53:SE:118:GLU:HG3	53:SE:121:TYR:OH	2.17	0.43
61:SR:37:GLU:OE1	70:Sg:106:LYS:NZ	2.50	0.43
62:SS:98:VAL:HG21	62:SS:106:LYS:HG3	1.98	0.43
63:ST:27:LYS:HE2	63:ST:27:LYS:HB2	1.89	0.43
70:Sg:228:TYR:HD1	70:Sg:229:THR:N	2.16	0.43
70:Sg:259:TRP:NE1	70:Sg:266:ILE:HG22	2.32	0.43
1:L5:1371:A:N1	3:L8:28:C:O2'	2.50	0.43
1:L5:2673:G:N3	1:L5:2673:G:H5'	2.33	0.43
1:L5:4219:A:H2'	1:L5:4220:A:C8	2.53	0.43
3:L8:78:G:O2'	36:Lh:42:SER:HA	2.18	0.43
6:LC:1:MET:HE3	6:LC:1:MET:HB3	1.82	0.43
8:LE:93:THR:HG22	8:LE:104:THR:CB	2.48	0.43
28:LZ:7:PRO:HD3	28:LZ:28:ASN:HD22	1.81	0.43
49:S2:606:G:H5''	81:Se:56:ASN:HB3	1.99	0.43
53:SE:92:ILE:HG22	53:SE:94:LYS:H	1.82	0.43
70:Sg:32:LEU:HD22	70:Sg:71:ILE:CD1	2.49	0.43
78:SY:14:THR:HA	78:SY:21:LYS:HA	1.99	0.43
82:Sf:132:MET:HG2	82:Sf:141:CYS:HB2	1.99	0.43
1:L5:1354:A:OP2	19:LQ:87:THR:HG23	2.18	0.43
1:L5:3786:U:OP1	1:L5:4550:G:O2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4122:G:H4'	35:Lg:90:ARG:HD2	2.00	0.43
1:L5:5057:C:H2'	1:L5:5058:A:C8	2.54	0.43
9:LF:222:LYS:HB3	9:LF:231:GLY:HA2	2.01	0.43
12:LI:33:ILE:HG21	86:CE:74:LEU:HD13	2.00	0.43
13:LJ:26:VAL:HG22	13:LJ:33:LEU:HD13	2.00	0.43
26:LX:81:LEU:HG	26:LX:83:THR:HG23	2.01	0.43
43:Lo:15:CYS:HB3	43:Lo:17:LYS:HG2	1.99	0.43
46:Ls:162:LYS:HD3	46:Ls:162:LYS:HA	1.80	0.43
47:Lt:57:ARG:HH11	47:Lt:58:ILE:HG23	1.83	0.43
49:S2:750:C:N4	49:S2:752:G:OP2	2.52	0.43
49:S2:1507:G:H22	82:Sf:87:THR:HA	1.83	0.43
52:SD:95:GLY:HA2	52:SD:101:GLN:OE1	2.19	0.43
70:Sg:145:GLU:O	70:Sg:175:LYS:NZ	2.52	0.43
83:CA:158:LYS:HA	83:CA:158:LYS:HD2	1.78	0.43
1:L5:3911:C:H2'	1:L5:3912:U:H6	1.82	0.43
1:L5:3953:G:H22	1:L5:4059:C:H1'	1.84	0.43
1:L5:4076:G:OP1	10:LG:73:ARG:NE	2.46	0.43
25:LW:87:LEU:O	25:LW:91:MET:HG2	2.19	0.43
45:Lr:84:LYS:H	45:Lr:84:LYS:HG2	1.65	0.43
49:S2:508:A:H3'	49:S2:509:G:H8	1.83	0.43
49:S2:532:C:H2'	49:S2:533:A:C8	2.54	0.43
49:S2:1007:C:H2'	49:S2:1008:A:C8	2.54	0.43
49:S2:1124:C:H5''	51:SB:150:ILE:HG12	2.01	0.43
54:SF:33:ILE:HA	54:SF:36:GLN:CD	2.43	0.43
59:SP:25:LEU:HB3	59:SP:87:PRO:HB3	1.99	0.43
61:SR:69:ILE:HD13	61:SR:71:ILE:HD11	2.01	0.43
63:ST:130:ASP:OD1	63:ST:130:ASP:N	2.50	0.43
83:CA:55:MET:HA	83:CA:58:GLU:HG3	2.00	0.43
1:L5:93:G:H2'	1:L5:94:A:C8	2.54	0.43
1:L5:908:G:H2'	1:L5:909:A:C8	2.54	0.43
4:LA:102:LEU:HB2	4:LA:107:MET:HE3	2.01	0.43
10:LG:164:ILE:HG12	10:LG:168:VAL:HG13	1.99	0.43
13:LJ:5:GLN:HA	13:LJ:8:LYS:HE3	2.00	0.43
19:LQ:72:LEU:HB2	19:LQ:75:ARG:HD2	2.00	0.43
28:LZ:84:ARG:HD3	84:CB:20:LEU:CD1	2.42	0.43
46:Ls:35:VAL:HG22	46:Ls:39:GLN:NE2	2.33	0.43
49:S2:1521:C:H5'	62:SS:129:LEU:HD22	2.01	0.43
49:S2:1845:A:H2'	49:S2:1846:G:C8	2.54	0.43
53:SE:240:ARG:HG3	53:SE:240:ARG:NH1	2.33	0.43
57:SK:9:ILE:O	57:SK:13:GLU:OE1	2.36	0.43
61:SR:87:GLU:HG2	61:SR:88:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SS:89:ASP:OD1	62:SS:90:VAL:N	2.52	0.43
70:Sg:104:HIS:CD2	70:Sg:130:LYS:HD2	2.53	0.43
71:SC:90:GLU:HB2	71:SC:93:ILE:HG13	2.00	0.43
1:L5:256:G:C6	88:L5:5317:T1C:H51C	2.54	0.43
1:L5:1994:C:H1'	47:Lt:132:ILE:HA	2.00	0.43
1:L5:3757:G:HO2'	1:L5:3758:U:H6	1.67	0.43
6:LC:144:ILE:HG22	6:LC:147:VAL:HG21	2.00	0.43
15:LM:85:LYS:O	15:LM:89:THR:HG23	2.18	0.43
53:SE:198:ARG:HG3	53:SE:208:VAL:HG12	2.01	0.43
60:SQ:140:ARG:HD3	60:SQ:140:ARG:HA	1.83	0.43
64:SU:98:VAL:O	64:SU:102:THR:HG23	2.19	0.43
73:SJ:63:LEU:HD23	73:SJ:63:LEU:HA	1.91	0.43
82:Sf:107:LYS:HD3	82:Sf:108:VAL:H	1.82	0.43
1:L5:3612:C:H1'	1:L5:5016:A:C8	2.53	0.43
1:L5:3893:C:H2'	1:L5:3894:A:C8	2.54	0.43
1:L5:4935:C:H2'	1:L5:4936:G:C8	2.54	0.43
6:LC:116:ASN:HB2	6:LC:119:GLN:HE21	1.84	0.43
6:LC:230:LEU:HD23	6:LC:230:LEU:HA	1.81	0.43
13:LJ:63:ARG:HH11	13:LJ:63:ARG:HG2	1.82	0.43
15:LM:77:TRP:O	15:LM:81:ASP:HA	2.19	0.43
32:Ld:65:ASP:OD2	32:Ld:67:ARG:HB2	2.18	0.43
49:S2:344:U:H2'	49:S2:345:U:C6	2.54	0.43
49:S2:543:C:H3'	49:S2:544:G:C8	2.54	0.43
49:S2:1627:C:H5''	63:ST:41:LYS:HD2	2.00	0.43
57:SK:47:LYS:HD2	57:SK:47:LYS:HA	1.76	0.43
70:Sg:129:ILE:HD11	70:Sg:154:VAL:HG11	2.01	0.43
73:SJ:60:LEU:HD22	73:SJ:70:ARG:HA	2.00	0.43
85:CC:19:A:O2'	85:CC:58:A:N7	2.42	0.43
1:L5:3726:A:H2'	1:L5:3727:A:C8	2.54	0.43
1:L5:4188:U:H2'	1:L5:4189:U:C6	2.53	0.43
3:L8:148:A:H2'	3:L8:149:G:C8	2.54	0.43
6:LC:289:LEU:HD21	19:LQ:31:LEU:HB2	2.01	0.43
28:LZ:99:ASP:CG	28:LZ:102:ARG:HH21	2.26	0.43
30:Lb:19:ASN:O	30:Lb:22:LYS:NZ	2.52	0.43
46:Ls:59:THR:O	46:Ls:63:LYS:HG2	2.19	0.43
49:S2:1533:A:H2	49:S2:1536:G:N3	2.16	0.43
55:SH:50:GLU:OE2	55:SH:90:LYS:NZ	2.49	0.43
61:SR:63:ARG:HB2	61:SR:63:ARG:NH1	2.34	0.43
61:SR:87:GLU:HG2	61:SR:88:VAL:H	1.83	0.43
61:SR:87:GLU:CG	61:SR:88:VAL:H	2.31	0.43
62:SS:4:VAL:HG23	79:SZ:55:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Sg:131:LEU:HG	70:Sg:139:LYS:HB2	2.01	0.43
70:Sg:164:ILE:HD13	70:Sg:178:ASN:HA	2.01	0.43
70:Sg:259:TRP:CD1	70:Sg:266:ILE:HG22	2.53	0.43
81:Se:51:LYS:HD2	81:Se:51:LYS:HA	1.76	0.43
83:CA:12:ILE:HG21	83:CA:324:LEU:HD11	2.01	0.43
1:L5:1241:C:H2'	1:L5:1242:G:H8	1.83	0.43
1:L5:2326:G:H5''	33:Le:127:ALA:HB2	2.01	0.43
1:L5:4277:G:H5''	22:LT:17:ARG:HG2	2.00	0.43
1:L5:4378:A:O2'	1:L5:4379:A:H2'	2.19	0.43
17:LO:165:LYS:HA	17:LO:165:LYS:HD2	1.76	0.43
28:LZ:95:VAL:CG1	28:LZ:109:LYS:HG2	2.49	0.43
32:Ld:46:LEU:HD23	32:Ld:72:VAL:HG11	2.00	0.43
32:Ld:92:ARG:HB3	32:Ld:94:GLU:HG2	2.01	0.43
43:Lo:69:ARG:HH22	43:Lo:80:LYS:HE3	1.84	0.43
49:S2:190:G:OP1	56:SI:149:TYR:OH	2.25	0.43
49:S2:223:C:H2'	49:S2:224:A:C8	2.53	0.43
49:S2:1426:U:H1'	63:ST:5:THR:HG21	2.00	0.43
51:SB:70:SER:HA	51:SB:83:LYS:HB3	2.01	0.43
52:SD:123:LEU:HD12	52:SD:123:LEU:HA	1.84	0.43
62:SS:86:ARG:HD2	62:SS:86:ARG:HA	1.79	0.43
70:Sg:228:TYR:CD2	70:Sg:264:LYS:HD3	2.54	0.43
73:SJ:11:LYS:HB3	73:SJ:11:LYS:HE2	1.83	0.43
76:SO:63:LYS:HA	76:SO:63:LYS:HD3	1.83	0.43
1:L5:302:C:OP1	16:LN:68:ARG:HB2	2.19	0.43
1:L5:1307:A:H2'	1:L5:1308:C:C6	2.53	0.43
1:L5:4938:A:N6	8:LE:247:LYS:HD3	2.34	0.43
24:LV:36:ASN:OD1	24:LV:36:ASN:O	2.36	0.43
30:Lb:101:HIS:HB3	30:Lb:104:LEU:HB2	2.01	0.43
43:Lo:2:VAL:N	43:Lo:90:HIS:O	2.52	0.43
43:Lo:102:GLN:NE2	43:Lo:102:GLN:CA	2.77	0.43
49:S2:5:U:H2'	49:S2:6:G:C8	2.53	0.43
49:S2:318:A:H61	72:SG:186:GLN:HE22	1.66	0.43
49:S2:382:C:H2'	49:S2:383:G:H8	1.84	0.43
49:S2:448:A:H5''	56:SI:25:ARG:HA	2.01	0.43
49:S2:931:C:H2'	49:S2:932:G:C8	2.54	0.43
53:SE:175:PHE:HE2	53:SE:198:ARG:HD2	1.84	0.43
66:SX:68:LYS:HB3	66:SX:91:LEU:HD22	2.01	0.43
73:SJ:169:ARG:HD2	73:SJ:169:ARG:HA	1.87	0.43
77:SW:111:MET:HE2	77:SW:111:MET:HB3	1.90	0.43
1:L5:171:U:H3'	1:L5:172:C:H4'	2.01	0.42
1:L5:1983:A:H62	1:L5:1987:C:H5''	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2758:G:O2'	1:L5:2765:A:N3	2.41	0.42
1:L5:3949:A:H2	1:L5:4064:C:H41	1.66	0.42
3:L8:67:U:H2'	3:L8:68:G:C8	2.54	0.42
9:LF:199:LYS:HA	9:LF:199:LYS:HD2	1.78	0.42
11:LH:142:ASP:O	11:LH:142:ASP:CG	2.43	0.42
28:LZ:121:ARG:HH11	28:LZ:127:ASN:ND2	2.17	0.42
49:S2:1692:U:H2'	49:S2:1693:G:C8	2.54	0.42
51:SB:137:LEU:HG	51:SB:215:VAL:HG22	2.01	0.42
54:SF:49:LEU:HD12	60:SQ:50:LYS:HG2	2.00	0.42
60:SQ:100:VAL:HG12	60:SQ:104:SER:OG	2.20	0.42
1:L5:985:C:H2'	1:L5:986:C:H6	1.85	0.42
1:L5:1392:A:H2'	1:L5:1393:G:C8	2.54	0.42
1:L5:3965:A:O2'	1:L5:4050:A:OP2	2.26	0.42
9:LF:40:LYS:HB2	9:LF:40:LYS:HE3	1.70	0.42
23:LU:97:ARG:HE	23:LU:97:ARG:HB2	1.67	0.42
47:Lt:62:LEU:HG	47:Lt:75:PRO:HG3	2.01	0.42
49:S2:566:U:H3	49:S2:584:G:H1	1.68	0.42
49:S2:1435:C:O2'	49:S2:1436:C:O4'	2.36	0.42
53:SE:71:LYS:HG2	53:SE:76:VAL:HG22	2.00	0.42
68:Sc:42:ILE:HD11	68:Sc:44:ARG:HD3	2.00	0.42
71:SC:108:LYS:HD3	71:SC:233:LEU:HD13	2.00	0.42
73:SJ:50:LEU:HD13	73:SJ:105:PHE:CE1	2.54	0.42
79:SZ:48:VAL:CG2	79:SZ:80:ARG:HD2	2.49	0.42
83:CA:238:LYS:HB2	83:CA:238:LYS:HE2	1.89	0.42
1:L5:1553:A:O2'	44:Lp:9:GLY:O	2.31	0.42
1:L5:1677:U:H4'	1:L5:1680:G:C2	2.55	0.42
1:L5:1857:C:H2'	1:L5:1858:A:C8	2.54	0.42
1:L5:4601:U:H2'	1:L5:4602:A:H8	1.84	0.42
2:L7:110:G:H2'	2:L7:111:C:C6	2.55	0.42
5:LB:293:ILE:HG12	5:LB:297:LYS:HB3	2.00	0.42
7:LD:239:MET:HE2	7:LD:239:MET:HB3	1.71	0.42
13:LJ:123:ILE:HD12	13:LJ:124:GLY:N	2.34	0.42
17:LO:54:TYR:CE1	17:LO:58:LEU:HD13	2.55	0.42
17:LO:85:ARG:HG3	17:LO:99:LEU:HD11	2.01	0.42
18:LP:94:MET:HE1	18:LP:146:ILE:HB	2.00	0.42
30:Lb:23:LYS:HE3	30:Lb:23:LYS:HB3	1.76	0.42
49:S2:53:C:O2'	49:S2:507:G:N7	2.44	0.42
49:S2:750:C:O2	49:S2:752:G:N1	2.52	0.42
49:S2:1203:G:H2'	49:S2:1204:A:C8	2.53	0.42
56:SI:45:THR:CG2	56:SI:53:LYS:HG3	2.43	0.42
61:SR:81:ARG:HH11	61:SR:81:ARG:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66: SX:127: ASN: HD22	66: SX:127: ASN: HA	1.66	0.42
71: SC:216: MET: HE2	71: SC:216: MET: HB2	1.80	0.42
72: SG:21: GLU: O	72: SG:25: ARG: NH1	2.53	0.42
76: SO:42: VAL: HG11	76: SO:78: ALA: HA	2.01	0.42
79: SZ:56: ASP: OD1	79: SZ:60: LYS: HD3	2.20	0.42
1: L5:502: C: H3'	1: L5:503: C: H3'	2.00	0.42
1: L5:1437: C: H2'	1: L5:1438: U: C6	2.54	0.42
1: L5:1786: A: H2'	1: L5:1789: C: C5	2.55	0.42
1: L5:2631: U: O4	23: LU:51: GLY: N	2.52	0.42
1: L5:3732: A: H2'	1: L5:3733: A: C8	2.55	0.42
1: L5:3786: U: O2	1: L5:3814: U: H4'	2.18	0.42
1: L5:4576: U: H2'	1: L5:4577: U: O4'	2.20	0.42
2: L7:3: C: H2'	2: L7:4: U: C6	2.53	0.42
3: L8:53: G: H4'	40: L1:40: LYS: HE2	2.01	0.42
27: LY:62: TYR: CD2	27: LY:85: VAL: HG13	2.55	0.42
28: LZ:24: VAL: HG21	28: LZ:87: VAL: CG2	2.45	0.42
46: Ls:83: ARG: HD3	46: Ls:83: ARG: HA	1.85	0.42
49: S2:1410: C: H2'	49: S2:1411: G: H8	1.85	0.42
66: SX:56: GLY: HA3	81: Se:6: LEU: HD21	2.02	0.42
71: SC:169: TYR: OH	71: SC:175: GLY: O	2.37	0.42
78: SY:72: PHE: HE2	78: SY:74: MET: HE3	1.82	0.42
1: L5:1590: C: H3'	1: L5:1591: U: H4'	2.02	0.42
1: L5:1726: U: H5'	9: LF:135: ILE: HD11	2.01	0.42
1: L5:1887: G: OP2	34: Lf:19: ARG: NH2	2.51	0.42
1: L5:1994: C: H2'	1: L5:1995: G: C8	2.55	0.42
1: L5:2045: G: C6	17: LO:62: MET: HA	2.54	0.42
1: L5:2275: G: H2'	1: L5:2276: A: C8	2.55	0.42
1: L5:2485: U: H4'	1: L5:2486: G: N2	2.34	0.42
1: L5:3648: A: H1'	1: L5:3785: A: N6	2.35	0.42
6: LC:109: ARG: O	6: LC:109: ARG: HG2	2.20	0.42
16: LN:148: THR: O	16: LN:151: ILE: HG22	2.20	0.42
25: LW:70: LYS: HA	25: LW:70: LYS: HD2	1.79	0.42
37: Li:79: THR: HG22	37: Li:82: ARG: H	1.84	0.42
47: Lt:126: SER: HA	47: Lt:129: ILE: HB	2.01	0.42
49: S2:17: C: H2'	49: S2:18: C: C6	2.55	0.42
49: S2:817: G: H4'	73: SJ:73: GLU: OE1	2.19	0.42
49: S2:1404: U: C2	64: SU:56: MET: HE1	2.54	0.42
54: SF:38: TYR: CD2	54: SF:144: LEU: HD13	2.54	0.42
54: SF:76: MET: HE2	54: SF:92: ILE: HG21	2.00	0.42
54: SF:76: MET: HE3	54: SF:76: MET: HB3	1.93	0.42
56: SI:79: ILE: HD12	56: SI:170: LYS: HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SK:3:MET:CG	57:SK:8:ARG:HH21	2.33	0.42
70:Sg:193:GLY:N	70:Sg:213:ASP:OD1	2.53	0.42
75:SN:13:GLN:HG3	80:Sb:21:LYS:HE3	2.02	0.42
1:L5:1171:G:N7	1:L5:1172:C:N4	2.68	0.42
1:L5:1414:C:H2'	1:L5:1415:G:H8	1.85	0.42
1:L5:2475:G:H5''	1:L5:2476:G:C8	2.54	0.42
1:L5:2672:C:O3'	1:L5:2675:G:H5'	2.20	0.42
5:LB:300:LYS:HB2	5:LB:300:LYS:HE2	1.84	0.42
12:LI:92:HIS:HA	12:LI:93:PRO:HD3	1.90	0.42
21:LS:70:LYS:HD3	21:LS:70:LYS:HA	1.62	0.42
38:Lj:39:TYR:O	38:Lj:40:PRO:C	2.63	0.42
38:Lj:83:THR:HA	38:Lj:84:PRO:HD3	1.89	0.42
49:S2:84:A:N3	49:S2:150:A:O2'	2.46	0.42
49:S2:1171:G:O2'	49:S2:1187:G:O6	2.36	0.42
50:SA:10:MET:HE2	50:SA:10:MET:HB2	1.81	0.42
52:SD:227:LYS:HE3	52:SD:227:LYS:HB3	1.87	0.42
76:SO:61:LYS:HA	76:SO:61:LYS:HD2	1.84	0.42
78:SY:72:PHE:HE2	78:SY:74:MET:CE	2.32	0.42
1:L5:2386:U:H5''	20:LR:24:LEU:HD12	2.01	0.42
1:L5:4039:G:N2	1:L5:4050:A:O2'	2.51	0.42
1:L5:4260:U:H2'	1:L5:4261:C:H6	1.85	0.42
1:L5:4489:G:N2	1:L5:4592:C:OP1	2.53	0.42
10:LG:105:GLU:OE1	10:LG:113:ARG:NH1	2.52	0.42
13:LJ:33:LEU:HD12	13:LJ:33:LEU:HA	1.87	0.42
21:LS:5:GLY:O	21:LS:111:ARG:NH2	2.53	0.42
32:Ld:33:ILE:HD11	32:Ld:41:ARG:NH2	2.33	0.42
38:Lj:67:LEU:HD23	38:Lj:67:LEU:HA	1.86	0.42
47:Lt:82:ILE:HD13	47:Lt:137:GLN:HB3	2.01	0.42
49:S2:1579:A:H4'	49:S2:1581:C:H5	1.85	0.42
57:SK:73:ASN:HA	57:SK:76:ILE:HD12	2.01	0.42
61:SR:34:VAL:O	61:SR:38:ILE:HG13	2.19	0.42
80:Sb:16:LYS:HD2	80:Sb:16:LYS:HA	1.68	0.42
1:L5:116:G:H2'	1:L5:117:C:C6	2.54	0.42
1:L5:4070:U:H2'	1:L5:4071:U:C6	2.55	0.42
1:L5:4585:U:H2'	1:L5:4586:G:C8	2.55	0.42
5:LB:301:ASN:N	5:LB:301:ASN:OD1	2.51	0.42
18:LP:42:ARG:NH2	18:LP:99:GLU:OE1	2.53	0.42
49:S2:1199:A:OP1	67:Sa:2:THR:N	2.53	0.42
49:S2:1245:G:O2'	49:S2:1492:U:OP1	2.32	0.42
53:SE:95:THR:HG22	78:SY:16:ARG:HE	1.84	0.42
56:SI:144:LYS:H	56:SI:144:LYS:HG2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SQ:44:PRO:C	60:SQ:46:THR:H	2.28	0.42
61:SR:46:LEU:HD12	61:SR:46:LEU:O	2.20	0.42
62:SS:4:VAL:CG1	62:SS:5:ILE:N	2.82	0.42
72:SG:24:LEU:HB3	72:SG:28:TYR:CZ	2.55	0.42
82:Sf:151:ASN:OD1	82:Sf:151:ASN:N	2.38	0.42
83:CA:185:MET:HE2	83:CA:185:MET:HA	2.02	0.42
83:CA:265:PHE:CD2	83:CA:292:GLY:C	2.98	0.42
1:L5:1179:U:H3'	1:L5:1180:C:H5''	2.01	0.42
1:L5:1577:G:O2'	1:L5:1612:G:H4'	2.19	0.42
1:L5:2744:A:H2'	1:L5:2745:A:C8	2.54	0.42
1:L5:4108:G:H2'	1:L5:4109:G:H8	1.85	0.42
1:L5:4146:G:H2'	1:L5:4147:G:C8	2.55	0.42
1:L5:4389:C:H2'	1:L5:4390:A:H8	1.85	0.42
4:LA:28:ARG:HB2	4:LA:123:ARG:HB3	2.02	0.42
5:LB:258:HIS:HA	5:LB:260:ALA:N	2.35	0.42
49:S2:674:C:H2'	49:S2:675:U:C6	2.55	0.42
49:S2:1779:G:H2'	49:S2:1780:G:C8	2.54	0.42
51:SB:88:THR:HA	51:SB:98:THR:HA	2.01	0.42
73:SJ:107:GLU:HA	73:SJ:112:THR:HG21	2.01	0.42
1:L5:460:C:H2'	1:L5:461:G:C8	2.54	0.42
1:L5:490:C:H2'	1:L5:491:G:C8	2.55	0.42
1:L5:1693:U:H2'	1:L5:1694:C:O4'	2.20	0.42
1:L5:2491:C:O2'	1:L5:2492:C:O4'	2.36	0.42
1:L5:4274:A:H2'	1:L5:4275:G:H8	1.82	0.42
88:L5:5316:T1C:H433	88:L5:5316:T1C:H41	1.89	0.42
6:LC:281:MET:HE2	19:LQ:110:ARG:NE	2.35	0.42
10:LG:103:ARG:NH1	10:LG:193:LEU:HA	2.29	0.42
18:LP:23:ARG:HD2	18:LP:125:MET:HE1	2.02	0.42
24:LV:72:LEU:HD21	24:LV:113:LYS:HE2	2.01	0.42
49:S2:1218:C:H2'	49:S2:1219:C:H6	1.84	0.42
70:Sg:72:SER:OG	70:Sg:74:ASP:OD1	2.32	0.42
71:SC:278:THR:HA	71:SC:279:ARG:HA	1.74	0.42
76:SO:95:ILE:HG13	76:SO:116:LEU:HD21	2.01	0.42
77:SW:39:THR:O	77:SW:43:LYS:HG2	2.20	0.42
83:CA:11:THR:OG1	83:CA:12:ILE:N	2.51	0.42
83:CA:159:PRO:HD3	83:CA:325:LEU:HD11	2.01	0.42
83:CA:345:SER:OG	83:CA:346:GLU:N	2.52	0.42
1:L5:676:C:H2'	1:L5:677:G:C8	2.55	0.41
1:L5:1983:A:OP1	1:L5:2010:A:O2'	2.36	0.41
1:L5:4967:A:H2'	1:L5:4968:A:C8	2.55	0.41
4:LA:2:GLY:HA2	4:LA:207:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:305:THR:OG1	5:LB:365:LEU:O	2.38	0.41
8:LE:244:GLU:O	8:LE:248:ILE:HD12	2.20	0.41
10:LG:136:LEU:HD12	10:LG:136:LEU:HA	1.95	0.41
46:Ls:33:ASP:OD1	46:Ls:34:ASN:N	2.53	0.41
49:S2:118:C:H1'	49:S2:445:A:C5	2.54	0.41
60:SQ:113:ILE:HD13	60:SQ:113:ILE:HA	1.86	0.41
61:SR:18:GLU:OE2	61:SR:69:ILE:CA	2.60	0.41
65:SV:17:CYS:HB2	65:SV:56:CYS:HB3	2.01	0.41
85:CC:64:C:H2'	85:CC:65:C:H6	1.85	0.41
86:CE:44:LYS:HB3	86:CE:44:LYS:HE2	1.64	0.41
1:L5:4587:G:OP1	17:LO:61:ARG:HD2	2.21	0.41
5:LB:35:ASP:OD2	5:LB:193:LYS:NZ	2.52	0.41
9:LF:216:PRO:HD3	9:LF:247:MET:HE3	2.01	0.41
11:LH:173:ARG:HE	11:LH:173:ARG:HB2	1.69	0.41
13:LJ:63:ARG:HG2	13:LJ:63:ARG:NH1	2.35	0.41
13:LJ:87:LEU:HA	13:LJ:90:ARG:HB2	2.02	0.41
45:Lr:84:LYS:HE2	45:Lr:84:LYS:HB3	1.87	0.41
49:S2:1010:G:H2'	49:S2:1011:A:C8	2.55	0.41
50:SA:22:GLY:O	50:SA:24:HIS:N	2.47	0.41
63:ST:108:GLU:OE1	63:ST:113:VAL:HG23	2.20	0.41
64:SU:48:LEU:HD13	64:SU:93:SER:HB2	2.00	0.41
66:SX:87:ASN:HB2	66:SX:90:CYS:SG	2.60	0.41
77:SW:14:ILE:HD11	77:SW:27:ILE:HD11	2.01	0.41
85:CC:61:C:H2'	85:CC:62:A:C8	2.54	0.41
1:L5:74:G:H5''	14:LL:59:VAL:HG22	2.01	0.41
1:L5:1968:G:H2'	1:L5:1969:G:H8	1.86	0.41
1:L5:3856:A:H5''	18:LP:83:TRP:O	2.20	0.41
49:S2:1628:C:H2'	49:S2:1629:C:C6	2.56	0.41
62:SS:142:ARG:HH11	62:SS:142:ARG:CG	2.30	0.41
1:L5:1306:C:H2'	1:L5:1307:A:C8	2.56	0.41
1:L5:3656:A:H2'	1:L5:3657:U:C6	2.55	0.41
1:L5:4524:G:N3	5:LB:252:ALA:HB1	2.36	0.41
2:L7:39:C:H4'	13:LJ:47:THR:HG23	2.03	0.41
22:LT:81:LYS:HB3	30:Lb:16:TRP:CZ3	2.55	0.41
24:LV:22:VAL:O	24:LV:39:ILE:HB	2.20	0.41
27:LY:64:GLY:HA3	27:LY:66:GLN:HE22	1.84	0.41
30:Lb:118:LEU:HD12	30:Lb:118:LEU:HA	1.93	0.41
44:Lp:30:GLU:HA	44:Lp:33:GLN:HG2	2.02	0.41
49:S2:1314:U:H4'	57:SK:3:MET:CE	2.50	0.41
49:S2:1681:U:H2'	49:S2:1682:C:C6	2.55	0.41
49:S2:1810:U:H2'	49:S2:1811:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SF:175:ASP:OD1	54:SF:175:ASP:N	2.53	0.41
55:SH:159:ASP:OD1	55:SH:159:ASP:N	2.53	0.41
61:SR:81:ARG:HG3	61:SR:81:ARG:NH1	2.36	0.41
67:Sa:13:LYS:HD3	67:Sa:13:LYS:HA	1.83	0.41
72:SG:2:LYS:HB2	72:SG:108:VAL:HG23	2.02	0.41
1:L5:18:C:H4'	16:LN:138:PHE:CD1	2.55	0.41
1:L5:173:C:H2'	1:L5:174:C:C6	2.55	0.41
1:L5:1194:G:H2'	1:L5:1195:G:C8	2.55	0.41
1:L5:1273:G:C8	30:Lb:117:ARG:HD2	2.55	0.41
1:L5:2297:G:H4'	6:LC:242:PRO:HB2	2.03	0.41
1:L5:3893:C:O2'	1:L5:4979:A:N1	2.49	0.41
5:LB:144:LYS:HE2	5:LB:148:LYS:HE2	2.02	0.41
5:LB:302:ASN:HB3	5:LB:303:ALA:H	1.74	0.41
17:LO:54:TYR:HE1	17:LO:58:LEU:HD13	1.86	0.41
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.55	0.41
49:S2:747:U:O4	49:S2:796:G:O6	2.39	0.41
49:S2:1415:C:H2'	49:S2:1416:C:C6	2.55	0.41
51:SB:179:ASN:HB3	51:SB:183:GLU:HB3	2.02	0.41
53:SE:137:PRO:HG2	53:SE:150:PRO:HD2	2.03	0.41
54:SF:128:ILE:HD13	68:Sc:23:SER:OG	2.20	0.41
61:SR:96:ILE:HG22	61:SR:98:VAL:HG13	2.02	0.41
66:SX:123:VAL:O	66:SX:124:LYS:HB2	2.21	0.41
70:Sg:99:ARG:HD2	70:Sg:99:ARG:HA	1.72	0.41
70:Sg:147:HIS:HE1	70:Sg:167:SER:OG	2.03	0.41
84:CB:5:LEU:HD12	84:CB:5:LEU:HA	1.93	0.41
86:CE:80:LYS:HB2	86:CE:80:LYS:HE3	1.86	0.41
1:L5:162:A:H2'	1:L5:163:A:H8	1.86	0.41
1:L5:956:A:H1'	1:L5:2076:G:H5''	2.03	0.41
1:L5:1345:A:H2'	1:L5:1346:C:C6	2.56	0.41
1:L5:1788:A:H2'	12:LI:22:PHE:CZ	2.55	0.41
1:L5:2111:G:N2	1:L5:2251:G:O2'	2.53	0.41
1:L5:3722:G:H2'	1:L5:3723:A:H8	1.85	0.41
1:L5:4291:G:H5''	1:L5:4293:U:C6	2.56	0.41
3:L8:141:C:H2'	3:L8:142:U:C6	2.56	0.41
12:LI:177:ASN:HB2	12:LI:180:GLU:HG2	2.02	0.41
47:Lt:63:THR:HG22	47:Lt:72:GLU:HG3	2.03	0.41
49:S2:433:A:H2'	49:S2:434:G:C8	2.55	0.41
49:S2:529:A:OP1	49:S2:548:C:N4	2.53	0.41
49:S2:1499:U:H4'	52:SD:176:LEU:HD13	2.02	0.41
49:S2:1617:G:H4'	69:Sd:14:PHE:CZ	2.55	0.41
52:SD:172:VAL:HG22	52:SD:185:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SP:86:LEU:N	59:SP:89:MET:HE3	2.23	0.41
63:ST:77:LYS:HB2	63:ST:77:LYS:HE3	1.72	0.41
66:SX:86:PRO:O	66:SX:87:ASN:HB2	2.20	0.41
66:SX:102:VAL:CG1	66:SX:120:PHE:HB3	2.51	0.41
67:Sa:51:ARG:NH1	67:Sa:51:ARG:HG2	2.35	0.41
73:SJ:46:VAL:HG11	73:SJ:106:LEU:HD21	2.02	0.41
79:SZ:67:LEU:HD12	79:SZ:67:LEU:HA	1.88	0.41
83:CA:228:VAL:HG12	83:CA:319:PHE:HB2	2.03	0.41
85:CC:38:C:H2'	85:CC:39:C:C6	2.56	0.41
1:L5:4043:G:N2	1:L5:4045:G:N3	2.66	0.41
4:LA:180:LEU:HD21	44:Lp:22:LEU:HB3	2.03	0.41
21:LS:30:MET:HE2	21:LS:30:MET:HB3	1.98	0.41
28:LZ:109:LYS:HE3	28:LZ:109:LYS:HB2	1.77	0.41
49:S2:1277:C:H2'	49:S2:1278:A:H8	1.86	0.41
50:SA:198:MET:SD	61:SR:85:VAL:HG13	2.61	0.41
53:SE:107:GLY:HA2	53:SE:189:LEU:HG	2.02	0.41
55:SH:85:LYS:HB2	55:SH:85:LYS:HE3	1.73	0.41
55:SH:98:ARG:HH11	55:SH:98:ARG:HG3	1.86	0.41
70:Sg:283:PRO:O	70:Sg:285:GLN:NE2	2.51	0.41
71:SC:64:THR:OG1	71:SC:90:GLU:OE2	2.38	0.41
75:SN:119:GLU:HG2	75:SN:141:TYR:HE2	1.85	0.41
76:SO:65:ASP:HA	76:SO:68:GLU:OE2	2.20	0.41
79:SZ:83:LEU:HD12	79:SZ:83:LEU:O	2.21	0.41
1:L5:368:C:O4'	6:LC:83:GLY:HA3	2.20	0.41
1:L5:425:U:H4'	18:LP:6:LEU:HD11	2.02	0.41
1:L5:2693:G:H2'	1:L5:2694:G:N2	2.35	0.41
1:L5:2781:G:H5''	40:Ll:10:LYS:HD3	2.03	0.41
1:L5:4187:G:H4'	16:LN:82:GLY:HA2	2.01	0.41
6:LC:5:ARG:HB3	6:LC:24:LEU:HB3	2.02	0.41
16:LN:158:HIS:HB3	16:LN:161:MET:HG3	2.02	0.41
17:LO:201:LEU:O	17:LO:202:LEU:HB2	2.20	0.41
45:Lr:32:LEU:O	45:Lr:33:LYS:HB2	2.21	0.41
49:S2:1226:G:N1	49:S2:1639:G:OP2	2.36	0.41
49:S2:1589:A:N3	49:S2:1653:U:O2'	2.43	0.41
49:S2:1736:G:H2'	49:S2:1737:G:C8	2.56	0.41
50:SA:222:VAL:HG23	50:SA:223:THR:HG23	2.03	0.41
62:SS:68:ILE:H	62:SS:68:ILE:HG13	1.69	0.41
70:Sg:62:HIS:CD2	70:Sg:66:VAL:HG12	2.56	0.41
70:Sg:240:CYS:HB3	70:Sg:249:CYS:SG	2.60	0.41
76:SO:90:ILE:O	76:SO:124:MET:HE1	2.21	0.41
79:SZ:47:LEU:HB2	79:SZ:78:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SZ:61:GLU:OE2	79:SZ:76:ARG:NH2	2.53	0.41
1:L5:989:U:O2'	1:L5:990:C:O4'	2.37	0.41
1:L5:1504:G:H2'	1:L5:1505:C:C6	2.55	0.41
1:L5:1707:C:N1	30:Lb:103:LYS:NZ	2.69	0.41
1:L5:1907:A:H2'	1:L5:1908:A:C8	2.55	0.41
1:L5:1930:U:OP2	17:LO:49:ARG:NH1	2.48	0.41
1:L5:2347:A:C4	33:Le:31:ILE:HD11	2.56	0.41
1:L5:3899:G:H5''	5:LB:257:TRP:CD1	2.56	0.41
1:L5:3934:G:H2'	1:L5:3935:C:C6	2.56	0.41
1:L5:4174:U:H2'	1:L5:4175:G:H8	1.85	0.41
1:L5:4522:G:O2'	1:L5:4525:C:OP2	2.27	0.41
1:L5:4951:G:H2'	1:L5:4952:G:H8	1.85	0.41
88:L5:5316:T1C:H953	88:L5:5316:T1C:H921	1.90	0.41
2:L7:29:C:H4'	13:LJ:12:MET:HE1	2.02	0.41
10:LG:87:LEU:HD23	10:LG:87:LEU:HA	1.93	0.41
14:LL:55:ILE:HG22	14:LL:96:ILE:HA	2.02	0.41
14:LL:101:ARG:HA	37:Li:25:ARG:HH12	1.85	0.41
14:LL:162:LYS:CA	14:LL:162:LYS:HE3	2.51	0.41
20:LR:133:LYS:HB2	20:LR:133:LYS:HE3	1.88	0.41
22:LT:106:LEU:O	22:LT:109:VAL:HG22	2.20	0.41
26:LX:83:THR:O	26:LX:87:MET:HG2	2.20	0.41
29:La:76:ASP:HB3	29:La:115:GLY:HA3	2.03	0.41
33:Le:87:VAL:HG23	33:Le:88:LEU:HD23	2.03	0.41
40:Ll:37:TYR:OH	40:Ll:39:SER:HA	2.20	0.41
43:Lo:24:THR:OG1	43:Lo:69:ARG:HB3	2.21	0.41
49:S2:75:G:H22	72:SG:171:THR:HG21	1.86	0.41
52:SD:126:ILE:HG21	52:SD:188:ILE:HG12	2.02	0.41
53:SE:10:LYS:HA	53:SE:10:LYS:HD3	1.91	0.41
53:SE:98:ASN:O	53:SE:114:ILE:HG12	2.21	0.41
55:SH:177:TYR:O	55:SH:181:THR:HB	2.21	0.41
59:SP:65:LYS:HE3	59:SP:65:LYS:HB3	1.93	0.41
63:ST:41:LYS:NZ	63:ST:93:SER:OG	2.48	0.41
70:Sg:127:LYS:HA	70:Sg:151:VAL:HG23	2.03	0.41
71:SC:74:LYS:HA	71:SC:74:LYS:HD2	1.84	0.41
72:SG:129:VAL:HA	72:SG:130:PRO:HD3	1.96	0.41
72:SG:215:LYS:HE2	72:SG:215:LYS:HB2	1.91	0.41
72:SG:221:LYS:NZ	72:SG:222:GLU:HG3	2.36	0.41
73:SJ:141:VAL:HG13	78:SY:65:GLY:HA3	2.02	0.41
83:CA:89:PHE:HD1	83:CA:307:VAL:HG21	1.84	0.41
83:CA:339:GLU:HG3	83:CA:342:LEU:HB3	2.02	0.41
1:L5:1324:A:O2'	1:L5:1326:A:OP1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3784:A:O2'	1:L5:3785:A:H3'	2.21	0.41
1:L5:3901:A:H8	1:L5:4518:A:N1	2.19	0.41
1:L5:4169:G:H4'	1:L5:4171:C:C2	2.56	0.41
1:L5:4239:A:H2'	1:L5:4240:G:C8	2.56	0.41
1:L5:4342:C:O3'	43:Lo:37:GLY:HA3	2.21	0.41
27:LY:48:PRO:O	27:LY:115:ARG:NH1	2.48	0.41
27:LY:113:LYS:HE2	27:LY:113:LYS:HB3	1.88	0.41
49:S2:652:U:H2'	49:S2:653:A:C8	2.55	0.41
49:S2:878:G:O6	49:S2:908:A:N1	2.54	0.41
49:S2:1060:A:O2'	49:S2:1062:A:N7	2.47	0.41
49:S2:1201:U:H2'	49:S2:1202:U:C6	2.56	0.41
49:S2:1683:C:H2'	49:S2:1684:C:H6	1.86	0.41
49:S2:1759:G:H21	49:S2:1773:C:H4'	1.85	0.41
53:SE:29:PRO:HG2	53:SE:46:ILE:HD11	2.02	0.41
55:SH:41:ARG:NH1	55:SH:41:ARG:CG	2.84	0.41
71:SC:191:VAL:HG11	71:SC:236:PHE:HA	2.02	0.41
83:CA:344:LYS:HE3	83:CA:344:LYS:HB3	1.91	0.41
1:L5:231:U:H4'	27:LY:100:HIS:CD2	2.56	0.40
1:L5:746:A:H2'	1:L5:747:A:C8	2.56	0.40
1:L5:1348:U:H2'	1:L5:1349:G:H8	1.86	0.40
2:L7:12:U:OP2	2:L7:67:C:O2'	2.39	0.40
7:LD:80:ALA:HA	7:LD:83:LEU:HG	2.03	0.40
9:LF:162:ILE:HD12	9:LF:167:ILE:HB	2.02	0.40
16:LN:178:HIS:HA	16:LN:181:HIS:NE2	2.37	0.40
54:SF:29:GLN:H	54:SF:110:GLN:NE2	2.19	0.40
56:SI:62:VAL:CG1	56:SI:63:GLY:N	2.83	0.40
60:SQ:19:ALA:HB2	60:SQ:75:GLY:HA3	2.02	0.40
62:SS:78:LYS:HE2	62:SS:78:LYS:HB3	1.85	0.40
64:SU:34:LYS:HE3	64:SU:34:LYS:HB3	1.69	0.40
79:SZ:101:SER:OG	79:SZ:102:LYS:N	2.54	0.40
83:CA:273:PHE:CD1	83:CA:273:PHE:N	2.88	0.40
86:CE:18:ARG:NH1	86:CE:19:ARG:HE	2.19	0.40
1:L5:3689:G:O2'	1:L5:3818:U:OP2	2.37	0.40
2:L7:3:C:H2'	2:L7:4:U:H6	1.86	0.40
3:L8:6:C:H2'	3:L8:7:U:C6	2.57	0.40
7:LD:119:TYR:OH	7:LD:139:PRO:O	2.36	0.40
11:LH:118:LEU:HD11	11:LH:167:VAL:HG22	2.03	0.40
12:LI:121:LYS:HA	12:LI:121:LYS:HD3	1.81	0.40
23:LU:36:ALA:HB1	23:LU:65:ARG:HD2	2.03	0.40
30:Lb:93:LEU:HD23	30:Lb:93:LEU:HA	1.93	0.40
47:Lt:59:THR:HG23	47:Lt:80:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lt:152:ILE:HD13	47:Lt:152:ILE:HA	1.93	0.40
49:S2:114:G:O6	49:S2:351:G:H1'	2.21	0.40
57:SK:32:HIS:HB3	57:SK:35:LEU:HD12	2.04	0.40
70:Sg:14:HIS:HB3	70:Sg:41:ILE:HD12	2.01	0.40
72:SG:29:GLU:OE1	72:SG:29:GLU:HA	2.20	0.40
72:SG:140:ARG:HA	72:SG:143:LYS:HE2	2.03	0.40
83:CA:178:ASN:HB2	83:CA:347:MET:HE3	2.02	0.40
1:L5:153:G:H2'	1:L5:154:G:H8	1.87	0.40
1:L5:2476:G:H2'	1:L5:2477:A:C8	2.56	0.40
1:L5:4593:C:H2'	1:L5:4594:U:H6	1.87	0.40
5:LB:196:TRP:CZ2	5:LB:200:ARG:NE	2.90	0.40
5:LB:295:ASP:OD1	5:LB:295:ASP:N	2.55	0.40
6:LC:159:GLU:HA	6:LC:217:ILE:HB	2.03	0.40
11:LH:124:ARG:NH1	11:LH:164:ALA:O	2.53	0.40
14:LL:97:SER:O	14:LL:97:SER:OG	2.32	0.40
15:LM:90:ARG:HA	15:LM:93:LYS:CG	2.50	0.40
16:LN:80:THR:OG1	16:LN:87:HIS:HA	2.21	0.40
19:LQ:179:GLY:HA2	19:LQ:186:TYR:CE2	2.56	0.40
22:LT:105:PHE:O	22:LT:109:VAL:HG13	2.21	0.40
35:Lg:103:VAL:HA	35:Lg:106:VAL:HG22	2.03	0.40
40:Ll:16:LYS:HD2	40:Ll:19:GLN:HE21	1.86	0.40
47:Lt:22:VAL:HA	47:Lt:48:LYS:HG3	2.03	0.40
49:S2:634:A:H2'	49:S2:635:G:H8	1.86	0.40
49:S2:1587:G:C5	63:ST:67:ARG:HD3	2.56	0.40
49:S2:1779:G:H2'	49:S2:1780:G:H8	1.86	0.40
49:S2:1808:U:H2'	49:S2:1809:A:C8	2.57	0.40
60:SQ:107:GLU:O	60:SQ:111:ILE:HD12	2.22	0.40
61:SR:17:ILE:HG21	61:SR:69:ILE:HG12	2.03	0.40
76:SO:19:PRO:HD2	76:SO:89:GLY:HA3	2.03	0.40
83:CA:129:VAL:HG11	83:CA:342:LEU:HD21	2.04	0.40
83:CA:273:PHE:CD2	83:CA:278:PHE:CG	3.09	0.40
84:CB:6:GLN:HE22	84:CB:12:VAL:C	2.17	0.40
1:L5:462:G:H2'	1:L5:463:A:C8	2.57	0.40
1:L5:1767:A:N6	1:L5:1769:G:O2'	2.55	0.40
1:L5:2335:C:H2'	1:L5:2336:G:H8	1.86	0.40
1:L5:2344:U:H2'	29:La:9:ARG:NH2	2.37	0.40
1:L5:2406:G:N7	40:Ll:2:SER:N	2.69	0.40
1:L5:2411:C:H2'	1:L5:2412:A:H8	1.86	0.40
1:L5:2730:U:H2'	1:L5:2731:C:C6	2.57	0.40
1:L5:3607:U:H2'	1:L5:3608:A:C8	2.57	0.40
7:LD:291:GLN:NE2	12:LI:214:SER:HA	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LG:96:LEU:HD11	10:LG:189:ARG:HD2	2.04	0.40
21:LS:98:ARG:HG3	21:LS:142:VAL:HG13	2.03	0.40
28:LZ:99:ASP:OD2	28:LZ:102:ARG:NH2	2.53	0.40
32:Ld:91:LYS:HE3	32:Ld:91:LYS:HB3	1.89	0.40
47:Lt:112:ILE:O	47:Lt:116:MET:HG3	2.21	0.40
49:S2:1731:A:H2'	49:S2:1732:G:C8	2.57	0.40
50:SA:210:ILE:HG21	61:SR:81:ARG:HD3	2.03	0.40
51:SB:25:PHE:HA	51:SB:28:LYS:HG3	2.02	0.40
52:SD:106:ARG:HE	52:SD:106:ARG:HB2	1.75	0.40
55:SH:7:LYS:HG2	55:SH:28:LEU:HG	2.04	0.40
58:SL:104:LYS:HE3	66:SX:8:ARG:NE	2.36	0.40
72:SG:31:ARG:HG3	72:SG:31:ARG:NH1	2.37	0.40
75:SN:110:ASP:O	75:SN:114:ARG:HG2	2.21	0.40
78:SY:25:ILE:HD11	78:SY:73:GLY:HA3	2.03	0.40
1:L5:2514:G:OP1	35:Lg:17:SER:OG	2.38	0.40
1:L5:2844:A:O2'	1:L5:4631:G:H4'	2.21	0.40
4:LA:30:ARG:HA	4:LA:74:GLU:OE1	2.20	0.40
6:LC:368:LYS:HA	6:LC:368:LYS:HD3	1.99	0.40
19:LQ:42:THR:HA	19:LQ:45:GLN:NE2	2.34	0.40
29:La:58:MET:HE3	29:La:58:MET:HB2	1.92	0.40
33:Le:129:LEU:HD23	33:Le:129:LEU:HA	1.90	0.40
49:S2:1513:C:H2'	49:S2:1514:G:C8	2.56	0.40
76:SO:75:MET:HE2	76:SO:75:MET:HB3	1.84	0.40
83:CA:20:LYS:HA	83:CA:23:MET:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	LA	246/257 (96%)	228 (93%)	17 (7%)	1 (0%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LB	400/403 (99%)	385 (96%)	15 (4%)	0	100	100
6	LC	366/427 (86%)	344 (94%)	22 (6%)	0	100	100
7	LD	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
8	LE	215/288 (75%)	197 (92%)	16 (7%)	2 (1%)	14	22
9	LF	223/248 (90%)	214 (96%)	9 (4%)	0	100	100
10	LG	239/266 (90%)	226 (95%)	13 (5%)	0	100	100
11	LH	188/192 (98%)	175 (93%)	11 (6%)	2 (1%)	11	18
12	LI	198/214 (92%)	191 (96%)	7 (4%)	0	100	100
13	LJ	174/178 (98%)	168 (97%)	5 (3%)	1 (1%)	21	32
14	LL	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	12	20
15	LM	137/215 (64%)	131 (96%)	6 (4%)	0	100	100
16	LN	201/204 (98%)	192 (96%)	7 (4%)	2 (1%)	12	20
17	LO	199/203 (98%)	196 (98%)	2 (1%)	1 (0%)	24	37
18	LP	151/184 (82%)	144 (95%)	7 (5%)	0	100	100
19	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	LT	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
23	LU	98/128 (77%)	90 (92%)	7 (7%)	1 (1%)	12	20
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/157 (78%)	115 (94%)	6 (5%)	1 (1%)	16	25
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
28	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
29	La	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
30	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
31	Lc	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
32	Ld	105/125 (84%)	99 (94%)	6 (6%)	0	100	100
33	Le	126/135 (93%)	122 (97%)	3 (2%)	1 (1%)	16	25
34	Lf	107/110 (97%)	96 (90%)	9 (8%)	2 (2%)	6	8
35	Lg	112/117 (96%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	84/97 (87%)	81 (96%)	3 (4%)	0	100	100
39	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
46	Ls	194/317 (61%)	174 (90%)	20 (10%)	0	100	100
47	Lt	137/165 (83%)	106 (77%)	30 (22%)	1 (1%)	18	28
48	Lz	203/217 (94%)	164 (81%)	39 (19%)	0	100	100
50	SA	219/295 (74%)	205 (94%)	14 (6%)	0	100	100
51	SB	212/264 (80%)	198 (93%)	14 (7%)	0	100	100
52	SD	225/243 (93%)	209 (93%)	16 (7%)	0	100	100
53	SE	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
54	SF	180/204 (88%)	164 (91%)	14 (8%)	2 (1%)	11	18
55	SH	182/194 (94%)	175 (96%)	7 (4%)	0	100	100
56	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
57	SK	93/165 (56%)	81 (87%)	12 (13%)	0	100	100
58	SL	140/158 (89%)	128 (91%)	12 (9%)	0	100	100
59	SP	127/145 (88%)	117 (92%)	10 (8%)	0	100	100
60	SQ	142/146 (97%)	129 (91%)	13 (9%)	0	100	100
61	SR	133/135 (98%)	120 (90%)	13 (10%)	0	100	100
62	SS	142/152 (93%)	129 (91%)	12 (8%)	1 (1%)	18	28
63	ST	141/145 (97%)	134 (95%)	6 (4%)	1 (1%)	18	28
64	SU	102/119 (86%)	94 (92%)	8 (8%)	0	100	100
65	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
66	SX	139/143 (97%)	130 (94%)	7 (5%)	2 (1%)	9	13
67	Sa	100/115 (87%)	93 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Sc	62/69 (90%)	58 (94%)	2 (3%)	2 (3%)	3	3
69	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
70	Sg	311/317 (98%)	263 (85%)	45 (14%)	3 (1%)	12	20
71	SC	220/293 (75%)	203 (92%)	17 (8%)	0	100	100
72	SG	235/249 (94%)	222 (94%)	13 (6%)	0	100	100
73	SJ	183/194 (94%)	175 (96%)	7 (4%)	1 (0%)	24	37
74	SM	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
75	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
76	SO	133/151 (88%)	126 (95%)	6 (4%)	1 (1%)	16	25
77	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
78	SY	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
79	SZ	73/125 (58%)	60 (82%)	10 (14%)	3 (4%)	2	2
80	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
81	Se	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
82	Sf	65/156 (42%)	56 (86%)	9 (14%)	0	100	100
83	CA	350/394 (89%)	335 (96%)	15 (4%)	0	100	100
84	CB	14/408 (3%)	14 (100%)	0	0	100	100
86	CE	71/223 (32%)	70 (99%)	1 (1%)	0	100	100
All	All	12250/14412 (85%)	11509 (94%)	708 (6%)	33 (0%)	37	50

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	LE	96	VAL
23	LU	67	LYS
63	ST	45	LEU
79	SZ	45	ASN
79	SZ	78	LYS
4	LA	172	GLY
14	LL	17	ASP
16	LN	124	ASP
25	LW	98	PRO
33	Le	73	GLY
66	SX	87	ASN
66	SX	124	LYS
70	Sg	179	LEU

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Mol	Chain	Res	Type
11	LH	60	TRP
14	LL	50	PRO
34	Lf	83	MET
70	Sg	103	GLY
73	SJ	122	SER
76	SO	140	THR
8	LE	111	LYS
54	SF	128	ILE
62	SS	74	PRO
68	Sc	31	ARG
11	LH	107	GLU
34	Lf	80	ASN
68	Sc	35	MET
70	Sg	178	ASN
17	LO	202	LEU
79	SZ	49	LEU
13	LJ	176	PRO
16	LN	83	LYS
47	Lt	139	VAL
54	SF	41	VAL

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	
4	LA	190/199 (96%)	187 (98%)	3 (2%)	55	76
5	LB	348/349 (100%)	341 (98%)	7 (2%)	48	70
6	LC	306/348 (88%)	302 (99%)	4 (1%)	61	80
7	LD	246/250 (98%)	242 (98%)	4 (2%)	55	76
8	LE	195/252 (77%)	190 (97%)	5 (3%)	40	63
9	LF	194/215 (90%)	192 (99%)	2 (1%)	68	84
10	LG	203/223 (91%)	197 (97%)	6 (3%)	36	58
11	LH	169/171 (99%)	162 (96%)	7 (4%)	27	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LI	172/181 (95%)	168 (98%)	4 (2%)	44	66
13	LJ	148/149 (99%)	144 (97%)	4 (3%)	39	62
14	LL	176/177 (99%)	173 (98%)	3 (2%)	53	74
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	170 (99%)	1 (1%)	78	89
17	LO	173/174 (99%)	169 (98%)	4 (2%)	44	66
18	LP	134/163 (82%)	130 (97%)	4 (3%)	36	58
19	LQ	164/165 (99%)	160 (98%)	4 (2%)	43	65
20	LR	166/175 (95%)	165 (99%)	1 (1%)	78	89
21	LS	156/157 (99%)	154 (99%)	2 (1%)	61	80
22	LT	139/140 (99%)	135 (97%)	4 (3%)	37	60
23	LU	90/115 (78%)	86 (96%)	4 (4%)	25	43
24	LV	101/107 (94%)	100 (99%)	1 (1%)	68	84
25	LW	103/126 (82%)	100 (97%)	3 (3%)	37	60
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	123/135 (91%)	118 (96%)	5 (4%)	27	46
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	118 (98%)	2 (2%)	53	74
30	Lb	88/126 (70%)	86 (98%)	2 (2%)	44	66
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	96 (98%)	2 (2%)	48	70
33	Le	114/121 (94%)	110 (96%)	4 (4%)	32	53
34	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	66
35	Lg	98/100 (98%)	98 (100%)	0	100	100
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	85
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	70 (96%)	3 (4%)	27	46
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	69
42	Ln	23/24 (96%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Lo	93/94 (99%)	91 (98%)	2 (2%)	45	67
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	107 (98%)	2 (2%)	51	73
46	Ls	162/258 (63%)	162 (100%)	0	100	100
47	Lt	112/137 (82%)	109 (97%)	3 (3%)	39	62
50	SA	183/243 (75%)	180 (98%)	3 (2%)	55	76
51	SB	195/231 (84%)	193 (99%)	2 (1%)	68	84
52	SD	190/202 (94%)	182 (96%)	8 (4%)	26	45
53	SE	224/225 (100%)	222 (99%)	2 (1%)	70	85
54	SF	156/170 (92%)	154 (99%)	2 (1%)	61	80
55	SH	166/174 (95%)	158 (95%)	8 (5%)	23	40
56	SI	178/180 (99%)	177 (99%)	1 (1%)	78	89
57	SK	86/136 (63%)	80 (93%)	6 (7%)	14	24
58	SL	130/142 (92%)	130 (100%)	0	100	100
59	SP	115/130 (88%)	113 (98%)	2 (2%)	53	74
60	SQ	119/121 (98%)	113 (95%)	6 (5%)	22	38
61	SR	122/122 (100%)	121 (99%)	1 (1%)	73	86
62	SS	125/132 (95%)	108 (86%)	17 (14%)	3	5
63	ST	113/115 (98%)	111 (98%)	2 (2%)	51	73
64	SU	94/107 (88%)	93 (99%)	1 (1%)	65	82
65	SV	67/67 (100%)	66 (98%)	1 (2%)	57	77
66	SX	113/115 (98%)	110 (97%)	3 (3%)	39	62
67	Sa	89/98 (91%)	87 (98%)	2 (2%)	45	67
68	Sc	57/62 (92%)	57 (100%)	0	100	100
69	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	45
70	Sg	272/275 (99%)	256 (94%)	16 (6%)	18	31
71	SC	188/225 (84%)	185 (98%)	3 (2%)	55	76
72	SG	207/218 (95%)	203 (98%)	4 (2%)	50	71
73	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	81
75	SN	130/131 (99%)	129 (99%)	1 (1%)	73	86
76	SO	105/119 (88%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	SW	112/113 (99%)	110 (98%)	2 (2%)	51	73
78	SY	109/115 (95%)	107 (98%)	2 (2%)	51	73
79	SZ	66/103 (64%)	64 (97%)	2 (3%)	36	58
80	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	80
81	Se	47/48 (98%)	47 (100%)	0	100	100
82	Sf	60/140 (43%)	58 (97%)	2 (3%)	33	55
83	CA	303/336 (90%)	297 (98%)	6 (2%)	48	70
84	CB	14/328 (4%)	14 (100%)	0	100	100
86	CE	62/190 (33%)	61 (98%)	1 (2%)	55	76
All	All	10379/11941 (87%)	10162 (98%)	217 (2%)	46	69

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	4	VAL
4	LA	15	VAL
4	LA	77	ILE
5	LB	17	LEU
5	LB	59	GLU
5	LB	152	SER
5	LB	171	LEU
5	LB	337	VAL
5	LB	363	ILE
5	LB	384	GLU
6	LC	24	LEU
6	LC	66	SER
6	LC	289	LEU
6	LC	334	THR
7	LD	36	LEU
7	LD	88	VAL
7	LD	118	ILE
7	LD	181	PRO
8	LE	51	VAL
8	LE	118	THR
8	LE	251	LYS
8	LE	258	LEU
8	LE	278	THR
9	LF	27	GLU
9	LF	248	ASN

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Mol	Chain	Res	Type
10	LG	28	VAL
10	LG	109	GLU
10	LG	162	ASP
10	LG	168	VAL
10	LG	179	VAL
10	LG	198	THR
11	LH	16	VAL
11	LH	27	VAL
11	LH	85	THR
11	LH	106	GLN
11	LH	146	LEU
11	LH	183	GLU
11	LH	187	VAL
12	LI	31	ILE
12	LI	141	LYS
12	LI	193	ASP
12	LI	197	VAL
13	LJ	15	LEU
13	LJ	22	LEU
13	LJ	26	VAL
13	LJ	132	VAL
14	LL	59	VAL
14	LL	122	SER
14	LL	154	VAL
16	LN	123	GLU
17	LO	27	VAL
17	LO	58	LEU
17	LO	92	THR
17	LO	119	VAL
18	LP	6	LEU
18	LP	41	ILE
18	LP	52	THR
18	LP	57	CYS
19	LQ	3	VAL
19	LQ	39	THR
19	LQ	82	VAL
19	LQ	92	VAL
20	LR	185	ILE
21	LS	16	CYS
21	LS	62	VAL
22	LT	4	THR
22	LT	76	VAL

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Mol	Chain	Res	Type
22	LT	80	VAL
22	LT	126	VAL
23	LU	25	CYS
23	LU	43	LEU
23	LU	80	LYS
23	LU	107	LYS
24	LV	65	VAL
25	LW	96	GLN
25	LW	98	PRO
25	LW	101	ARG
27	LY	7	VAL
27	LY	44	VAL
27	LY	79	VAL
27	LY	86	GLN
27	LY	94	THR
29	La	15	VAL
29	La	100	ILE
30	Lb	54	LEU
30	Lb	76	VAL
32	Ld	95	ASP
32	Ld	122	VAL
33	Le	30	LYS
33	Le	45	VAL
33	Le	79	VAL
33	Le	91	CYS
34	Lf	5	LEU
34	Lf	43	LEU
36	Lh	18	LEU
38	Lj	32	SER
38	Lj	36	LYS
38	Lj	80	GLU
41	Lm	127	VAL
43	Lo	2	VAL
43	Lo	18	HIS
45	Lr	37	SER
45	Lr	49	VAL
47	Lt	126	SER
47	Lt	139	VAL
47	Lt	151	ILE
50	SA	87	VAL
50	SA	124	VAL
50	SA	188	THR

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Mol	Chain	Res	Type
51	SB	127	VAL
51	SB	222	LYS
52	SD	46	THR
52	SD	49	ILE
52	SD	58	VAL
52	SD	72	VAL
52	SD	74	GLN
52	SD	75	LYS
52	SD	168	VAL
52	SD	181	VAL
53	SE	105	THR
53	SE	139	LEU
54	SF	28	VAL
54	SF	77	MET
55	SH	29	GLU
55	SH	31	GLU
55	SH	33	ASN
55	SH	64	VAL
55	SH	82	GLU
55	SH	86	LYS
55	SH	125	VAL
55	SH	166	VAL
56	SI	3	ILE
57	SK	11	ILE
57	SK	20	VAL
57	SK	22	VAL
57	SK	45	VAL
57	SK	49	MET
57	SK	72	THR
59	SP	25	LEU
59	SP	38	SER
60	SQ	12	VAL
60	SQ	39	LEU
60	SQ	57	LEU
60	SQ	66	VAL
60	SQ	89	SER
60	SQ	110	ASP
61	SR	124	VAL
62	SS	16	LEU
62	SS	46	ARG
62	SS	50	ILE
62	SS	59	LEU

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Mol	Chain	Res	Type
62	SS	61	GLU
62	SS	62	ASP
62	SS	68	ILE
62	SS	70	ILE
62	SS	73	ASN
62	SS	75	ARG
62	SS	76	GLN
62	SS	78	LYS
62	SS	88	LYS
62	SS	99	LEU
62	SS	111	LEU
62	SS	131	VAL
62	SS	145	THR
63	ST	44	GLU
63	ST	99	VAL
64	SU	39	LEU
65	SV	66	ASP
66	SX	7	LEU
66	SX	88	ASP
66	SX	123	VAL
67	Sa	18	VAL
67	Sa	45	VAL
69	Sd	30	LEU
69	Sd	39	CYS
70	Sg	7	LEU
70	Sg	32	LEU
70	Sg	37	ASP
70	Sg	46	THR
70	Sg	98	THR
70	Sg	113	PHE
70	Sg	121	VAL
70	Sg	142	VAL
70	Sg	157	SER
70	Sg	166	VAL
70	Sg	174	VAL
70	Sg	177	TRP
70	Sg	178	ASN
70	Sg	200	VAL
70	Sg	248	LEU
70	Sg	303	THR
71	SC	63	VAL
71	SC	66	LEU

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Mol	Chain	Res	Type
71	SC	222	CYS
72	SG	124	LEU
72	SG	144	LEU
72	SG	150	GLU
72	SG	153	VAL
73	SJ	128	VAL
73	SJ	141	VAL
75	SN	150	VAL
77	SW	25	VAL
77	SW	74	VAL
78	SY	4	THR
78	SY	69	THR
79	SZ	58	LEU
79	SZ	61	GLU
80	Sb	43	ILE
82	Sf	102	VAL
82	Sf	144	CYS
83	CA	82	VAL
83	CA	85	CYS
83	CA	105	LEU
83	CA	113	HIS
83	CA	223	VAL
83	CA	244	THR
86	CE	54	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	50	HIS
5	LB	121	ASN
5	LB	204	GLN
5	LB	236	HIS
5	LB	258	HIS
5	LB	302	ASN
6	LC	21	ASN
6	LC	50	GLN
6	LC	61	GLN
6	LC	119	GLN
6	LC	329	ASN
6	LC	347	HIS
7	LD	131	ASN
7	LD	225	GLN

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Mol	Chain	Res	Type
7	LD	275	GLN
7	LD	291	GLN
8	LE	128	HIS
9	LF	39	GLN
9	LF	63	GLN
9	LF	110	GLN
9	LF	248	ASN
10	LG	43	GLN
10	LG	90	GLN
10	LG	195	HIS
11	LH	78	GLN
11	LH	102	ASN
11	LH	169	ASN
13	LJ	65	ASN
13	LJ	97	ASN
13	LJ	98	ASN
13	LJ	104	ASN
14	LL	111	GLN
14	LL	205	GLN
15	LM	33	GLN
15	LM	34	ASN
15	LM	44	GLN
15	LM	70	GLN
17	LO	42	ASN
18	LP	21	ASN
18	LP	28	ASN
19	LQ	7	HIS
19	LQ	21	GLN
19	LQ	45	GLN
19	LQ	188	ASN
20	LR	36	ASN
22	LT	54	HIS
22	LT	79	GLN
22	LT	127	GLN
23	LU	94	ASN
24	LV	135	ASN
25	LW	48	GLN
25	LW	95	ASN
25	LW	96	GLN
25	LW	104	GLN
25	LW	120	GLN
26	LX	111	GLN

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Mol	Chain	Res	Type
27	LY	18	HIS
27	LY	72	GLN
28	LZ	28	ASN
28	LZ	127	ASN
29	La	19	HIS
29	La	67	GLN
29	La	93	ASN
29	La	120	GLN
30	Lb	6	ASN
30	Lb	17	HIS
31	Lc	19	GLN
32	Ld	34	HIS
32	Ld	118	GLN
33	Le	52	GLN
34	Lf	20	ASN
36	Lh	20	GLN
36	Lh	30	GLN
36	Lh	65	GLN
36	Lh	107	GLN
37	Li	15	HIS
37	Li	20	ASN
38	Lj	66	HIS
40	Ll	19	GLN
40	Ll	33	ASN
43	Lo	90	HIS
43	Lo	102	GLN
44	Lp	72	ASN
46	Ls	191	GLN
47	Lt	115	GLN
47	Lt	147	HIS
50	SA	36	GLN
50	SA	193	HIS
51	SB	40	ASN
51	SB	43	ASN
51	SB	147	ASN
51	SB	158	HIS
52	SD	145	GLN
52	SD	207	HIS
53	SE	67	GLN
53	SE	138	HIS
53	SE	197	ASN
53	SE	224	ASN

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Mol	Chain	Res	Type
54	SF	31	ASN
54	SF	79	HIS
54	SF	186	ASN
54	SF	203	ASN
55	SH	76	GLN
55	SH	186	ASN
56	SI	35	ASN
56	SI	88	ASN
56	SI	116	HIS
56	SI	146	GLN
57	SK	32	HIS
57	SK	66	HIS
57	SK	73	ASN
57	SK	84	HIS
58	SL	39	ASN
58	SL	94	HIS
59	SP	41	GLN
59	SP	103	ASN
60	SQ	24	HIS
60	SQ	80	GLN
61	SR	74	GLN
61	SR	118	GLN
62	SS	101	ASN
62	SS	105	ASN
63	ST	85	ASN
64	SU	28	ASN
64	SU	100	GLN
65	SV	2	GLN
65	SV	21	ASN
65	SV	82	ASN
66	SX	61	GLN
66	SX	127	ASN
67	Sa	72	HIS
70	Sg	62	HIS
70	Sg	76	GLN
70	Sg	147	HIS
70	Sg	178	ASN
70	Sg	237	ASN
70	Sg	272	GLN
71	SC	120	GLN
72	SG	202	ASN
72	SG	225	GLN

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Mol	Chain	Res	Type
73	SJ	39	ASN
73	SJ	156	HIS
75	SN	58	HIS
75	SN	62	GLN
75	SN	69	ASN
77	SW	70	ASN
78	SY	22	GLN
78	SY	112	ASN
79	SZ	45	ASN
79	SZ	46	ASN
81	Se	58	ASN
83	CA	120	ASN
83	CA	123	HIS
83	CA	221	HIS
84	CB	6	GLN
86	CE	45	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3703/5070 (73%)	833 (22%)	30 (0%)
2	L7	119/121 (98%)	12 (10%)	0
3	L8	155/157 (98%)	31 (20%)	1 (0%)
49	S2	1715/1869 (91%)	381 (22%)	14 (0%)
85	CC	74/75 (98%)	23 (31%)	0
All	All	5766/7292 (79%)	1280 (22%)	45 (0%)

All (1280) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	15	A
1	L5	17	A
1	L5	25	A
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A

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Mol	Chain	Res	Type
1	L5	66	A
1	L5	69	A
1	L5	71	C
1	L5	73	A
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	112	C
1	L5	119	G
1	L5	120	A
1	L5	128	C
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	136	C
1	L5	137	G
1	L5	139	G
1	L5	152	U
1	L5	159	C
1	L5	165	A
1	L5	171	U
1	L5	172	C
1	L5	173	C
1	L5	177	G
1	L5	181	C
1	L5	182	G
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	186	G
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	210	C
1	L5	216	C
1	L5	218	A
1	L5	219	G
1	L5	233	U

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Mol	Chain	Res	Type
1	L5	234	G
1	L5	253	G
1	L5	261	G
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	269	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	349	A
1	L5	373	G
1	L5	387	G
1	L5	406	C
1	L5	407	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	414	C
1	L5	431	G
1	L5	432	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	464	G
1	L5	466	A
1	L5	467	U
1	L5	468	U
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	497	G
1	L5	498	C

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Mol	Chain	Res	Type
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	504	G
1	L5	505	G
1	L5	506	C
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	517	C
1	L5	518	G
1	L5	643	C
1	L5	645	G
1	L5	646	G
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	696	C
1	L5	703	G
1	L5	704	C
1	L5	706	C
1	L5	708	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	742	G
1	L5	757	G
1	L5	758	G
1	L5	759	G
1	L5	760	G

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Mol	Chain	Res	Type
1	L5	904	C
1	L5	905	C
1	L5	906	C
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	931	C
1	L5	932	A
1	L5	933	G
1	L5	935	A
1	L5	936	C
1	L5	941	C
1	L5	944	A
1	L5	945	U
1	L5	956	A
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	968	C
1	L5	969	C
1	L5	970	G
1	L5	972	C
1	L5	977	C
1	L5	982	U
1	L5	989	U
1	L5	990	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	996	G
1	L5	1048	G
1	L5	1049	C
1	L5	1050	C

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Mol	Chain	Res	Type
1	L5	1051	G
1	L5	1070	G
1	L5	1071	C
1	L5	1074	G
1	L5	1075	G
1	L5	1084	C
1	L5	1094	G
1	L5	1095	A
1	L5	1168	G
1	L5	1171	G
1	L5	1172	C
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1193	C
1	L5	1202	C
1	L5	1203	G
1	L5	1204	C
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1216	C
1	L5	1217	G
1	L5	1219	G
1	L5	1222	A
1	L5	1235	G
1	L5	1240	G
1	L5	1243	C
1	L5	1245	C
1	L5	1246	G
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1258	G
1	L5	1261	G
1	L5	1266	G
1	L5	1267	C

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Mol	Chain	Res	Type
1	L5	1269	G
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1301	C
1	L5	1312	A
1	L5	1326	A
1	L5	1337	A
1	L5	1344	C
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1365	C
1	L5	1366	G
1	L5	1368	A
1	L5	1378	C
1	L5	1387	A
1	L5	1393	G
1	L5	1394	G
1	L5	1397	A
1	L5	1398	A
1	L5	1403	G
1	L5	1404	G
1	L5	1405	C
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1414	C
1	L5	1415	G
1	L5	1417	C
1	L5	1420	A
1	L5	1435	G
1	L5	1438	U
1	L5	1444	G

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Mol	Chain	Res	Type
1	L5	1447	C
1	L5	1457	G
1	L5	1482	G
1	L5	1483	C
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1513	U
1	L5	1517	G
1	L5	1534	A
1	L5	1547	A
1	L5	1562	G
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1624	G
1	L5	1625	G
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	U
1	L5	1678	C
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G
1	L5	1706	A
1	L5	1707	C
1	L5	1708	G
1	L5	1718	C
1	L5	1719	A
1	L5	1726	U
1	L5	1733	G

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Mol	Chain	Res	Type
1	L5	1734	G
1	L5	1741	G
1	L5	1742	A
1	L5	1753	G
1	L5	1755	C
1	L5	1757	U
1	L5	1758	G
1	L5	1760	G
1	L5	1761	G
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1767	A
1	L5	1768	C
1	L5	1770	A
1	L5	1771	U
1	L5	1772	C
1	L5	1775	A
1	L5	1781	U
1	L5	1787	A
1	L5	1804	A
1	L5	1810	G
1	L5	1820	C
1	L5	1821	G
1	L5	1822	U
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1843	A
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1897	A
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G

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Mol	Chain	Res	Type
1	L5	1931	C
1	L5	1932	A
1	L5	1936	C
1	L5	1940	G
1	L5	1948	G
1	L5	1951	G
1	L5	1959	U
1	L5	1960	A
1	L5	1961	G
1	L5	1962	A
1	L5	1972	G
1	L5	1974	U
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1986	U
1	L5	1987	C
1	L5	1988	G
1	L5	1990	A
1	L5	1991	A
1	L5	1992	U
1	L5	1993	C
1	L5	1997	U
1	L5	2001	G
1	L5	2002	A
1	L5	2004	U
1	L5	2014	C
1	L5	2017	A
1	L5	2018	C
1	L5	2024	G
1	L5	2026	A
1	L5	2033	A
1	L5	2034	G
1	L5	2046	G
1	L5	2048	U
1	L5	2052	G
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A

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Mol	Chain	Res	Type
1	L5	2084	C
1	L5	2085	G
1	L5	2089	G
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2106	G
1	L5	2107	C
1	L5	2108	G
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2250	C
1	L5	2252	G
1	L5	2253	A
1	L5	2256	C
1	L5	2262	G
1	L5	2277	C
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	C
1	L5	2360	A
1	L5	2369	U
1	L5	2389	A
1	L5	2395	A
1	L5	2397	G
1	L5	2417	A
1	L5	2418	A
1	L5	2421	G
1	L5	2425	U
1	L5	2441	C
1	L5	2450	G

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Mol	Chain	Res	Type
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2479	G
1	L5	2483	G
1	L5	2484	A
1	L5	2485	U
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2491	C
1	L5	2494	U
1	L5	2495	U
1	L5	2503	G
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2555	G
1	L5	2559	G
1	L5	2560	C
1	L5	2565	A
1	L5	2573	A
1	L5	2583	C
1	L5	2586	G
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2611	A
1	L5	2618	G
1	L5	2653	C

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Mol	Chain	Res	Type
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2721	G
1	L5	2724	G
1	L5	2725	A
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2746	A
1	L5	2756	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2815	A
1	L5	2826	U
1	L5	2827	G
1	L5	2829	U
1	L5	2838	G
1	L5	2855	G
1	L5	2867	C
1	L5	2877	G
1	L5	2892	C
1	L5	2900	U
1	L5	2902	G

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Mol	Chain	Res	Type
1	L5	2903	G
1	L5	2904	U
1	L5	2905	C
1	L5	2906	G
1	L5	2908	U
1	L5	3585	G
1	L5	3587	C
1	L5	3588	C
1	L5	3590	G
1	L5	3591	C
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3604	A
1	L5	3605	C
1	L5	3606	U
1	L5	3615	G
1	L5	3618	C
1	L5	3626	G
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3662	A
1	L5	3673	C
1	L5	3674	G
1	L5	3685	C
1	L5	3710	G
1	L5	3711	A
1	L5	3714	G
1	L5	3729	U
1	L5	3735	G
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3754	G
1	L5	3757	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3761	C
1	L5	3771	C

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Mol	Chain	Res	Type
1	L5	3776	G
1	L5	3777	G
1	L5	3784	A
1	L5	3786	U
1	L5	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3823	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3841	C
1	L5	3867	A
1	L5	3876	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3887	C
1	L5	3890	A
1	L5	3892	U
1	L5	3897	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3938	G
1	L5	3939	G
1	L5	3942	A
1	L5	3943	A
1	L5	3947	A
1	L5	3950	U
1	L5	3955	G
1	L5	3956	G
1	L5	3958	G
1	L5	3959	U
1	L5	3960	A

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Mol	Chain	Res	Type
1	L5	3961	G
1	L5	3962	A
1	L5	3963	A
1	L5	3964	U
1	L5	3965	A
1	L5	3966	A
1	L5	3969	G
1	L5	3970	G
1	L5	3971	G
1	L5	3973	G
1	L5	3974	G
1	L5	3975	C
1	L5	3977	C
1	L5	4035	G
1	L5	4036	G
1	L5	4038	C
1	L5	4039	G
1	L5	4041	C
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4045	G
1	L5	4046	A
1	L5	4048	A
1	L5	4049	U
1	L5	4050	A
1	L5	4051	C
1	L5	4052	C
1	L5	4053	A
1	L5	4055	U
1	L5	4064	C
1	L5	4065	G
1	L5	4076	G
1	L5	4086	G
1	L5	4096	C
1	L5	4097	G
1	L5	4099	G
1	L5	4101	C
1	L5	4102	C
1	L5	4103	C
1	L5	4104	G
1	L5	4106	G

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Mol	Chain	Res	Type
1	L5	4107	G
1	L5	4108	G
1	L5	4111	U
1	L5	4112	C
1	L5	4113	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4120	U
1	L5	4121	G
1	L5	4122	G
1	L5	4127	A
1	L5	4133	C
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4150	G
1	L5	4162	C
1	L5	4163	U
1	L5	4170	A
1	L5	4183	G
1	L5	4191	G
1	L5	4196	G
1	L5	4197	G
1	L5	4201	G
1	L5	4203	A
1	L5	4222	G
1	L5	4228	G
1	L5	4229	U
1	L5	4233	A
1	L5	4242	U
1	L5	4251	A
1	L5	4254	G
1	L5	4256	A
1	L5	4257	A
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A

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Mol	Chain	Res	Type
1	L5	4281	A
1	L5	4291	G
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C
1	L5	4326	G
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4349	C
1	L5	4354	U
1	L5	4371	G
1	L5	4373	G
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4398	C
1	L5	4422	A
1	L5	4426	C
1	L5	4444	C
1	L5	4448	G
1	L5	4449	A
1	L5	4452	U
1	L5	4453	C
1	L5	4464	A
1	L5	4475	G
1	L5	4476	C
1	L5	4488	A
1	L5	4500	U
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4524	G
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4560	C

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Mol	Chain	Res	Type
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4590	A
1	L5	4600	G
1	L5	4617	G
1	L5	4627	U
1	L5	4635	A
1	L5	4636	U
1	L5	4637	G
1	L5	4652	G
1	L5	4656	A
1	L5	4657	U
1	L5	4659	G
1	L5	4670	C
1	L5	4672	A
1	L5	4679	G
1	L5	4684	A
1	L5	4687	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4720	C
1	L5	4730	C
1	L5	4731	G
1	L5	4733	C
1	L5	4734	A
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4750	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4764	A
1	L5	4765	G
1	L5	4770	U
1	L5	4771	C

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Mol	Chain	Res	Type
1	L5	4772	C
1	L5	4773	C
1	L5	4775	C
1	L5	4776	G
1	L5	4859	C
1	L5	4860	G
1	L5	4870	G
1	L5	4871	C
1	L5	4872	G
1	L5	4875	G
1	L5	4882	U
1	L5	4883	C
1	L5	4887	C
1	L5	4888	U
1	L5	4889	G
1	L5	4891	G
1	L5	4895	C
1	L5	4896	G
1	L5	4900	C
1	L5	4901	G
1	L5	4910	G
1	L5	4911	A
1	L5	4912	G
1	L5	4913	G
1	L5	4914	C
1	L5	4918	C
1	L5	4922	C
1	L5	4923	C
1	L5	4925	U
1	L5	4927	G
1	L5	4928	C
1	L5	4934	A
1	L5	4937	C
1	L5	4940	C
1	L5	4941	G
1	L5	4943	A
1	L5	4944	C
1	L5	4949	G
1	L5	4951	G
1	L5	4960	G
1	L5	4961	G
1	L5	4966	A

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Mol	Chain	Res	Type
1	L5	4976	U
1	L5	4985	U
1	L5	4988	U
1	L5	4989	U
1	L5	4991	U
1	L5	5007	A
1	L5	5009	G
1	L5	5013	C
1	L5	5014	A
1	L5	5017	G
1	L5	5022	U
1	L5	5024	C
1	L5	5025	C
1	L5	5026	U
1	L5	5027	C
1	L5	5028	G
1	L5	5029	C
1	L5	5034	A
1	L5	5041	G
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5061	A
1	L5	5069	U
2	L7	33	U
2	L7	38	U
2	L7	42	A
2	L7	53	U
2	L7	54	A
2	L7	64	G
2	L7	97	G
2	L7	100	A
2	L7	106	G
2	L7	109	U
2	L7	110	G
2	L7	111	C
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	39	G
3	L8	48	A
3	L8	51	U

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Mol	Chain	Res	Type
3	L8	52	A
3	L8	59	A
3	L8	60	G
3	L8	62	A
3	L8	63	U
3	L8	68	G
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	104	A
3	L8	105	C
3	L8	110	U
3	L8	112	G
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	147	G
49	S2	23	G
49	S2	33	G
49	S2	45	A
49	S2	46	A
49	S2	56	G
49	S2	58	C
49	S2	59	U
49	S2	64	A
49	S2	65	C
49	S2	67	C
49	S2	68	A
49	S2	72	C
49	S2	73	C
49	S2	74	G
49	S2	76	U
49	S2	103	A
49	S2	113	G

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Mol	Chain	Res	Type
49	S2	114	G
49	S2	115	U
49	S2	116	U
49	S2	121	U
49	S2	126	G
49	S2	129	C
49	S2	130	G
49	S2	143	U
49	S2	147	A
49	S2	149	A
49	S2	160	U
49	S2	162	C
49	S2	163	U
49	S2	175	A
49	S2	190	G
49	S2	198	U
49	S2	199	C
49	S2	200	G
49	S2	203	G
49	S2	204	G
49	S2	206	G
49	S2	207	G
49	S2	211	G
49	S2	214	U
49	S2	291	G
49	S2	292	A
49	S2	293	C
49	S2	294	U
49	S2	295	C
49	S2	302	A
49	S2	306	C
49	S2	307	G
49	S2	308	G
49	S2	309	G
49	S2	311	C
49	S2	318	A
49	S2	319	C
49	S2	322	C
49	S2	323	C
49	S2	324	C
49	S2	325	C
49	S2	326	C

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Mol	Chain	Res	Type
49	S2	327	G
49	S2	328	U
49	S2	329	G
49	S2	332	G
49	S2	339	A
49	S2	340	C
49	S2	347	G
49	S2	351	G
49	S2	360	A
49	S2	362	C
49	S2	364	A
49	S2	368	U
49	S2	370	G
49	S2	385	G
49	S2	386	C
49	S2	407	G
49	S2	408	A
49	S2	409	C
49	S2	417	C
49	S2	418	A
49	S2	428	U
49	S2	438	G
49	S2	448	A
49	S2	449	A
49	S2	450	C
49	S2	452	G
49	S2	464	A
49	S2	471	G
49	S2	472	C
49	S2	473	A
49	S2	474	G
49	S2	482	G
49	S2	487	U
49	S2	488	U
49	S2	492	C
49	S2	496	C
49	S2	503	C
49	S2	512	A
49	S2	523	A
49	S2	525	A
49	S2	529	A
49	S2	530	U

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Mol	Chain	Res	Type
49	S2	540	U
49	S2	541	U
49	S2	542	U
49	S2	545	A
49	S2	546	G
49	S2	547	G
49	S2	548	C
49	S2	554	A
49	S2	555	A
49	S2	563	G
49	S2	564	A
49	S2	576	A
49	S2	583	C
49	S2	585	C
49	S2	589	G
49	S2	591	U
49	S2	592	C
49	S2	596	U
49	S2	597	G
49	S2	604	A
49	S2	608	C
49	S2	614	C
49	S2	623	G
49	S2	627	U
49	S2	628	A
49	S2	629	A
49	S2	631	U
49	S2	643	A
49	S2	644	G
49	S2	655	A
49	S2	660	C
49	S2	664	A
49	S2	668	A
49	S2	669	A
49	S2	671	A
49	S2	672	A
49	S2	673	G
49	S2	687	C
49	S2	688	U
49	S2	689	U
49	S2	692	G
49	S2	693	A

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Mol	Chain	Res	Type
49	S2	695	C
49	S2	696	G
49	S2	697	G
49	S2	698	G
49	S2	732	U
49	S2	733	C
49	S2	736	C
49	S2	738	C
49	S2	749	U
49	S2	751	G
49	S2	752	G
49	S2	753	C
49	S2	788	G
49	S2	791	C
49	S2	792	C
49	S2	798	A
49	S2	799	U
49	S2	810	A
49	S2	821	G
49	S2	822	U
49	S2	830	A
49	S2	834	C
49	S2	835	C
49	S2	836	G
49	S2	837	A
49	S2	838	G
49	S2	839	C
49	S2	840	C
49	S2	841	G
49	S2	842	C
49	S2	847	A
49	S2	869	A
49	S2	870	A
49	S2	873	G
49	S2	874	G
49	S2	878	G
49	S2	880	G
49	S2	883	U
49	S2	887	U
49	S2	888	U
49	S2	889	U
49	S2	891	G

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Mol	Chain	Res	Type
49	S2	896	U
49	S2	897	U
49	S2	898	U
49	S2	899	U
49	S2	900	C
49	S2	901	G
49	S2	906	U
49	S2	913	A
49	S2	920	A
49	S2	922	A
49	S2	930	C
49	S2	933	G
49	S2	934	G
49	S2	943	U
49	S2	955	A
49	S2	963	A
49	S2	971	G
49	S2	990	A
49	S2	992	A
49	S2	999	G
49	S2	1001	A
49	S2	1016	U
49	S2	1017	U
49	S2	1023	A
49	S2	1027	A
49	S2	1028	A
49	S2	1061	U
49	S2	1062	A
49	S2	1067	C
49	S2	1083	A
49	S2	1085	C
49	S2	1089	G
49	S2	1109	C
49	S2	1114	U
49	S2	1115	U
49	S2	1116	C
49	S2	1119	A
49	S2	1121	G
49	S2	1133	A
49	S2	1138	C
49	S2	1153	C
49	S2	1154	U

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Mol	Chain	Res	Type
49	S2	1195	A
49	S2	1203	G
49	S2	1207	G
49	S2	1208	A
49	S2	1212	G
49	S2	1215	C
49	S2	1216	C
49	S2	1217	A
49	S2	1224	G
49	S2	1227	G
49	S2	1242	U
49	S2	1243	U
49	S2	1251	A
49	S2	1253	A
49	S2	1256	G
49	S2	1257	G
49	S2	1259	A
49	S2	1264	C
49	S2	1271	C
49	S2	1274	G
49	S2	1275	G
49	S2	1283	C
49	S2	1284	A
49	S2	1286	G
49	S2	1294	G
49	S2	1295	A
49	S2	1301	A
49	S2	1302	G
49	S2	1303	C
49	S2	1306	U
49	S2	1308	U
49	S2	1312	G
49	S2	1341	C
49	S2	1342	U
49	S2	1343	U
49	S2	1348	G
49	S2	1371	U
49	S2	1373	C
49	S2	1378	A
49	S2	1382	A
49	S2	1396	A
49	S2	1397	U

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Mol	Chain	Res	Type
49	S2	1402	A
49	S2	1404	U
49	S2	1412	C
49	S2	1414	A
49	S2	1416	C
49	S2	1421	A
49	S2	1423	C
49	S2	1431	G
49	S2	1433	C
49	S2	1435	C
49	S2	1436	C
49	S2	1438	A
49	S2	1442	U
49	S2	1449	G
49	S2	1452	A
49	S2	1454	A
49	S2	1462	U
49	S2	1463	U
49	S2	1464	C
49	S2	1480	A
49	S2	1487	A
49	S2	1489	A
49	S2	1490	G
49	S2	1495	G
49	S2	1497	G
49	S2	1498	A
49	S2	1505	U
49	S2	1507	G
49	S2	1509	U
49	S2	1520	G
49	S2	1521	C
49	S2	1533	A
49	S2	1536	G
49	S2	1537	A
49	S2	1544	C
49	S2	1553	C
49	S2	1556	A
49	S2	1558	C
49	S2	1560	U
49	S2	1570	G
49	S2	1575	G
49	S2	1580	A

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Mol	Chain	Res	Type
49	S2	1585	U
49	S2	1587	G
49	S2	1588	A
49	S2	1594	A
49	S2	1601	A
49	S2	1606	G
49	S2	1621	U
49	S2	1623	A
49	S2	1632	G
49	S2	1637	A
49	S2	1638	G
49	S2	1640	A
49	S2	1643	U
49	S2	1644	C
49	S2	1648	G
49	S2	1649	U
49	S2	1654	G
49	S2	1663	A
49	S2	1664	A
49	S2	1665	G
49	S2	1680	G
49	S2	1683	C
49	S2	1686	G
49	S2	1696	C
49	S2	1698	C
49	S2	1699	A
49	S2	1715	A
49	S2	1719	A
49	S2	1721	U
49	S2	1722	G
49	S2	1742	C
49	S2	1743	G
49	S2	1744	G
49	S2	1745	A
49	S2	1752	C
49	S2	1753	C
49	S2	1754	G
49	S2	1757	G
49	S2	1758	G
49	S2	1759	G
49	S2	1760	G
49	S2	1761	U

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Mol	Chain	Res	Type
49	S2	1772	C
49	S2	1773	C
49	S2	1774	C
49	S2	1775	U
49	S2	1776	G
49	S2	1777	G
49	S2	1781	A
49	S2	1783	C
49	S2	1784	G
49	S2	1786	U
49	S2	1798	C
49	S2	1822	A
49	S2	1823	A
49	S2	1824	A
49	S2	1825	A
49	S2	1826	G
49	S2	1829	G
49	S2	1831	A
49	S2	1835	A
49	S2	1838	U
49	S2	1849	G
49	S2	1851	A
49	S2	1852	C
49	S2	1861	G
49	S2	1862	G
49	S2	1863	A
49	S2	1864	U
49	S2	1865	C
85	CC	7	G
85	CC	8	U
85	CC	9	G
85	CC	17	G
85	CC	18	G
85	CC	20	A
85	CC	29	G
85	CC	30	G
85	CC	32	C
85	CC	34	A
85	CC	35	U
85	CC	36	A
85	CC	37	A
85	CC	43	A

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Mol	Chain	Res	Type
85	CC	45	G
85	CC	46	U
85	CC	47	C
85	CC	57	A
85	CC	58	A
85	CC	60	C
85	CC	63	U
85	CC	73	C
85	CC	75	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	184	U
1	L5	406	C
1	L5	412	G
1	L5	413	G
1	L5	493	G
1	L5	504	G
1	L5	914	U
1	L5	968	C
1	L5	1633	G
1	L5	1733	G
1	L5	1919	G
1	L5	1977	C
1	L5	2033	A
1	L5	2056	G
1	L5	2084	C
1	L5	2416	G
1	L5	2675	G
1	L5	2696	A
1	L5	2724	G
1	L5	2760	G
1	L5	2786	C
1	L5	3614	G
1	L5	3673	C
1	L5	3876	A
1	L5	4291	G
1	L5	4378	A
1	L5	4475	G
1	L5	4699	U
1	L5	4913	G

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Mol	Chain	Res	Type
1	L5	4927	G
3	L8	51	U
49	S2	112	U
49	S2	113	G
49	S2	291	G
49	S2	293	C
49	S2	407	G
49	S2	417	C
49	S2	563	G
49	S2	628	A
49	S2	688	U
49	S2	821	G
49	S2	1434	C
49	S2	1488	C
49	S2	1534	C
49	S2	1598	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	MLZ	Lm	98	41	8,9,10	0.83	0	4,9,11	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	MLZ	Lm	98	41	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 267 are monoatomic - leaving 9 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	$\# Z > 2$
88	T1C	L5	5312	87	45,45,45	1.15	4 (8%)	56,72,72	1.06	3 (5%)
88	T1C	L5	5318	-	45,45,45	1.16	4 (8%)	56,72,72	0.99	2 (3%)
88	T1C	L5	5316	-	45,45,45	1.17	4 (8%)	56,72,72	1.27	7 (12%)
88	T1C	CC	101	-	45,45,45	1.15	4 (8%)	56,72,72	1.14	4 (7%)
88	T1C	L5	5317	-	45,45,45	1.19	4 (8%)	56,72,72	1.51	10 (17%)
88	T1C	L5	5313	87	45,45,45	1.15	4 (8%)	56,72,72	1.20	4 (7%)
88	T1C	S2	1930	-	45,45,45	1.17	4 (8%)	56,72,72	1.19	5 (8%)
88	T1C	L5	5315	87	45,45,45	1.18	4 (8%)	56,72,72	1.05	7 (12%)
88	T1C	L5	5314	87	45,45,45	1.16	4 (8%)	56,72,72	0.84	3 (5%)

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
88	T1C	L5	5312	87	-	10/22/80/80	0/4/4/4
88	T1C	L5	5318	-	-	9/22/80/80	0/4/4/4
88	T1C	L5	5316	-	-	10/22/80/80	0/4/4/4
88	T1C	CC	101	-	-	10/22/80/80	0/4/4/4
88	T1C	L5	5317	-	-	9/22/80/80	0/4/4/4
88	T1C	L5	5313	87	-	11/22/80/80	0/4/4/4
88	T1C	S2	1930	-	-	14/22/80/80	0/4/4/4
88	T1C	L5	5315	87	-	11/22/80/80	0/4/4/4
88	T1C	L5	5314	87	-	13/22/80/80	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	L5	5318	T1C	C21-N21	5.10	1.48	1.33
88	S2	1930	T1C	C21-N21	5.07	1.48	1.33
88	L5	5315	T1C	C21-N21	5.07	1.48	1.33
88	L5	5314	T1C	C21-N21	5.05	1.48	1.33
88	L5	5312	T1C	C21-N21	5.04	1.48	1.33
88	L5	5316	T1C	C21-N21	5.04	1.48	1.33
88	CC	101	T1C	C21-N21	5.03	1.47	1.33
88	L5	5313	T1C	C21-N21	5.02	1.47	1.33
88	L5	5317	T1C	C21-N21	5.02	1.47	1.33
88	L5	5318	T1C	C4-N4	2.73	1.53	1.47
88	L5	5317	T1C	C4-N4	2.71	1.53	1.47
88	L5	5314	T1C	C4-N4	2.62	1.52	1.47
88	L5	5315	T1C	C4-N4	2.60	1.52	1.47
88	CC	101	T1C	C4-N4	2.59	1.52	1.47
88	S2	1930	T1C	C4-N4	2.57	1.52	1.47
88	L5	5312	T1C	C4-N4	2.55	1.52	1.47
88	L5	5313	T1C	C4-N4	2.36	1.52	1.47
88	L5	5317	T1C	C7-N7	2.33	1.48	1.42
88	L5	5316	T1C	C4-N4	2.31	1.52	1.47
88	L5	5315	T1C	C7-N7	2.27	1.48	1.42
88	L5	5317	T1C	O11-C11	2.23	1.27	1.23
88	L5	5316	T1C	O11-C11	2.23	1.27	1.23
88	S2	1930	T1C	O11-C11	2.23	1.27	1.23
88	L5	5313	T1C	O11-C11	2.23	1.27	1.23
88	L5	5315	T1C	O11-C11	2.22	1.27	1.23
88	L5	5314	T1C	O11-C11	2.22	1.27	1.23
88	CC	101	T1C	O11-C11	2.22	1.27	1.23
88	L5	5318	T1C	O11-C11	2.21	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	L5	5312	T1C	O11-C11	2.20	1.27	1.23
88	CC	101	T1C	C7-N7	2.17	1.48	1.42
88	L5	5316	T1C	C7-N7	2.16	1.48	1.42
88	L5	5318	T1C	C7-N7	2.16	1.48	1.42
88	S2	1930	T1C	C7-N7	2.15	1.48	1.42
88	L5	5313	T1C	C7-N7	2.13	1.48	1.42
88	L5	5312	T1C	C7-N7	2.11	1.48	1.42
88	L5	5314	T1C	C7-N7	2.03	1.47	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	L5	5316	T1C	C11-C1B-C12	5.27	122.97	118.80
88	CC	101	T1C	C11-C1B-C12	4.74	122.55	118.80
88	L5	5317	T1C	C1C-C1-C2	4.60	123.05	115.75
88	L5	5313	T1C	C1C-C1-C2	4.29	122.56	115.75
88	S2	1930	T1C	C1C-C41-C4	4.07	117.20	111.64
88	L5	5317	T1C	C61-C6-C51	4.01	118.44	113.12
88	L5	5312	T1C	C1C-C1-C2	4.00	122.10	115.75
88	L5	5318	T1C	C1C-C1-C2	3.87	121.91	115.75
88	L5	5317	T1C	C1C-C41-C4	3.76	116.79	111.64
88	L5	5312	T1C	C11-C1B-C12	3.75	121.77	118.80
88	S2	1930	T1C	C11-C1B-C12	3.69	121.72	118.80
88	L5	5313	T1C	C11-C1B-C12	3.60	121.65	118.80
88	L5	5317	T1C	C51-C5-C41	3.43	116.23	110.38
88	S2	1930	T1C	C51-C5-C41	2.95	115.41	110.38
88	L5	5316	T1C	C1C-C12-C1B	-2.93	120.09	123.06
88	L5	5317	T1C	C61-C7-N7	2.90	122.33	118.87
88	L5	5316	T1C	C1C-C41-C4	2.86	115.54	111.64
88	L5	5314	T1C	C11-C1B-C12	2.84	121.05	118.80
88	L5	5315	T1C	C11-C1B-C12	2.84	121.04	118.80
88	CC	101	T1C	O1C-C1C-C12	-2.79	105.68	110.14
88	L5	5317	T1C	C11-C1B-C12	2.78	121.00	118.80
88	L5	5316	T1C	C1C-C1-C2	2.76	120.13	115.75
88	CC	101	T1C	C1C-C1-C2	2.73	120.09	115.75
88	L5	5313	T1C	C5-C41-C4	-2.68	109.86	113.73
88	L5	5315	T1C	C61-C6-C51	2.64	116.62	113.12
88	L5	5318	T1C	C11-C1B-C12	2.64	120.89	118.80
88	L5	5313	T1C	C51-C5-C41	2.60	114.81	110.38
88	L5	5314	T1C	C1C-C1-C2	2.56	119.82	115.75
88	S2	1930	T1C	C1C-C12-C1B	-2.47	120.56	123.06
88	L5	5315	T1C	C1-C1C-C12	2.46	112.77	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	L5	5316	T1C	C5-C41-C4	-2.44	110.21	113.73
88	L5	5316	T1C	C51-C5-C41	2.40	114.47	110.38
88	CC	101	T1C	C1C-C12-C1B	-2.34	120.69	123.06
88	L5	5317	T1C	C8-C7-N7	-2.31	117.29	120.89
88	L5	5317	T1C	C72-N7-C71	-2.27	108.89	116.18
88	L5	5312	T1C	C1-C1C-C12	2.23	112.50	109.88
88	L5	5315	T1C	C61-C7-N7	2.21	121.51	118.87
88	L5	5317	T1C	O1C-C1C-C12	-2.19	106.63	110.14
88	L5	5315	T1C	O1C-C1C-C12	-2.17	106.67	110.14
88	L5	5315	T1C	C1C-C1-C2	2.10	119.09	115.75
88	L5	5316	T1C	O12-C12-C1C	2.09	116.39	113.37
88	L5	5317	T1C	C1C-C12-C1B	2.07	125.16	123.06
88	L5	5314	T1C	C5-C41-C4	-2.06	110.76	113.73
88	L5	5315	T1C	C72-N7-C71	-2.04	109.63	116.18
88	S2	1930	T1C	C1C-C1-C2	2.01	118.95	115.75

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5312	T1C	C92-C91-N9-C9
88	L5	5312	T1C	C1-C2-C21-O21
88	L5	5312	T1C	C1-C2-C21-N21
88	L5	5313	T1C	C94-C93-N92-C92
88	L5	5313	T1C	C95-C93-N92-C92
88	L5	5313	T1C	C96-C93-N92-C92
88	L5	5313	T1C	C92-C91-N9-C9
88	L5	5313	T1C	C1-C2-C21-O21
88	L5	5313	T1C	C1-C2-C21-N21
88	L5	5314	T1C	C92-C91-N9-C9
88	L5	5314	T1C	C1-C2-C21-O21
88	L5	5314	T1C	C1-C2-C21-N21
88	L5	5315	T1C	C91-C92-N92-C93
88	L5	5315	T1C	C3-C4-N4-C43
88	L5	5315	T1C	C1-C2-C21-O21
88	L5	5315	T1C	C1-C2-C21-N21
88	L5	5316	T1C	C92-C91-N9-C9
88	L5	5316	T1C	C41-C4-N4-C43
88	L5	5316	T1C	C1-C2-C21-O21
88	L5	5316	T1C	C1-C2-C21-N21
88	L5	5317	T1C	C1-C2-C21-O21
88	L5	5317	T1C	C1-C2-C21-N21

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Mol	Chain	Res	Type	Atoms
88	L5	5318	T1C	C91-C92-N92-C93
88	L5	5318	T1C	C92-C91-N9-C9
88	L5	5318	T1C	O91-C91-N9-C9
88	L5	5318	T1C	C1-C2-C21-O21
88	L5	5318	T1C	C1-C2-C21-N21
88	S2	1930	T1C	C95-C93-N92-C92
88	S2	1930	T1C	C96-C93-N92-C92
88	S2	1930	T1C	C92-C91-N9-C9
88	S2	1930	T1C	C3-C2-C21-O21
88	S2	1930	T1C	C3-C2-C21-N21
88	S2	1930	T1C	C1-C2-C21-O21
88	S2	1930	T1C	C1-C2-C21-N21
88	CC	101	T1C	C1-C2-C21-O21
88	CC	101	T1C	C1-C2-C21-N21
88	L5	5316	T1C	O91-C91-N9-C9
88	L5	5314	T1C	O91-C91-N9-C9
88	L5	5313	T1C	O91-C91-N9-C9
88	L5	5312	T1C	O91-C91-N9-C9
88	S2	1930	T1C	C94-C93-N92-C92
88	S2	1930	T1C	O91-C91-N9-C9
88	L5	5315	T1C	C92-C91-N9-C9
88	L5	5314	T1C	O91-C91-C92-N92
88	L5	5315	T1C	O91-C91-C92-N92
88	L5	5315	T1C	N9-C91-C92-N92
88	L5	5315	T1C	O91-C91-N9-C9
88	L5	5314	T1C	N9-C91-C92-N92
88	L5	5314	T1C	C10-C9-N9-C91
88	S2	1930	T1C	N9-C91-C92-N92
88	S2	1930	T1C	O91-C91-C92-N92
88	L5	5318	T1C	C10-C9-N9-C91
88	CC	101	T1C	C10-C9-N9-C91
88	L5	5312	T1C	O91-C91-C92-N92
88	CC	101	T1C	O91-C91-N9-C9
88	L5	5312	T1C	N9-C91-C92-N92
88	L5	5316	T1C	C10-C9-N9-C91
88	L5	5317	T1C	C10-C9-N9-C91
88	L5	5314	T1C	C8-C9-N9-C91
88	L5	5313	T1C	C3-C2-C21-N21
88	L5	5315	T1C	C41-C4-N4-C43
88	L5	5315	T1C	C41-C4-N4-C42
88	L5	5315	T1C	C3-C4-N4-C42
88	L5	5317	T1C	C3-C4-N4-C42

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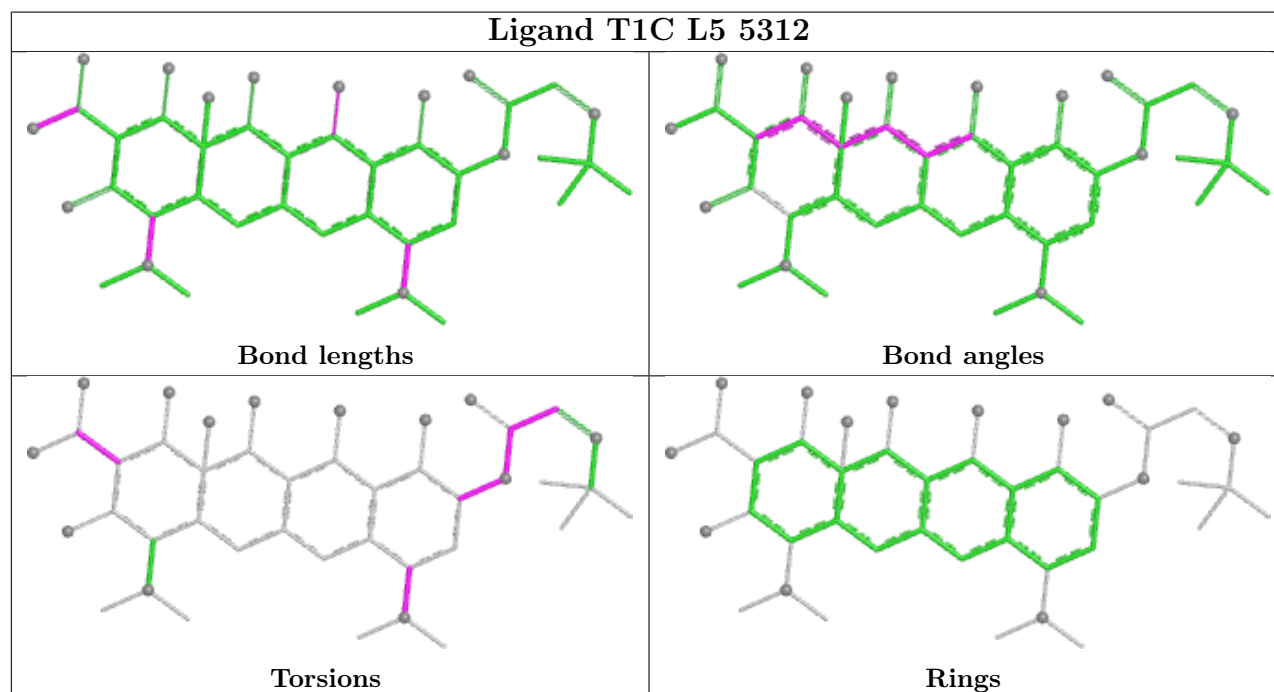
Mol	Chain	Res	Type	Atoms
88	L5	5317	T1C	C3-C2-C21-N21
88	L5	5318	T1C	C41-C4-N4-C42
88	L5	5313	T1C	C3-C2-C21-O21
88	L5	5313	T1C	C91-C92-N92-C93
88	L5	5314	T1C	C91-C92-N92-C93
88	L5	5316	T1C	C91-C92-N92-C93
88	S2	1930	T1C	C91-C92-N92-C93
88	CC	101	T1C	C91-C92-N92-C93
88	L5	5312	T1C	C10-C9-N9-C91
88	CC	101	T1C	C92-C91-N9-C9
88	L5	5317	T1C	O91-C91-C92-N92
88	CC	101	T1C	C8-C9-N9-C91
88	L5	5316	T1C	C8-C9-N9-C91
88	L5	5317	T1C	N9-C91-C92-N92
88	L5	5317	T1C	C8-C9-N9-C91
88	L5	5318	T1C	C8-C9-N9-C91
88	L5	5312	T1C	C61-C7-N7-C71
88	L5	5314	T1C	C61-C7-N7-C72
88	L5	5314	T1C	C61-C7-N7-C71
88	L5	5312	T1C	C61-C7-N7-C72
88	L5	5316	T1C	C61-C7-N7-C71
88	S2	1930	T1C	C61-C7-N7-C72
88	CC	101	T1C	C61-C7-N7-C72
88	L5	5313	T1C	C61-C7-N7-C71
88	L5	5314	T1C	C3-C2-C21-N21
88	L5	5318	T1C	C41-C4-N4-C43
88	CC	101	T1C	C41-C4-N4-C42
88	L5	5312	T1C	C3-C2-C21-O21
88	L5	5314	T1C	C3-C2-C21-O21
88	L5	5317	T1C	C3-C2-C21-O21
88	S2	1930	T1C	C61-C7-N7-C71
88	L5	5316	T1C	C61-C7-N7-C72
88	CC	101	T1C	C61-C7-N7-C71

There are no ring outliers.

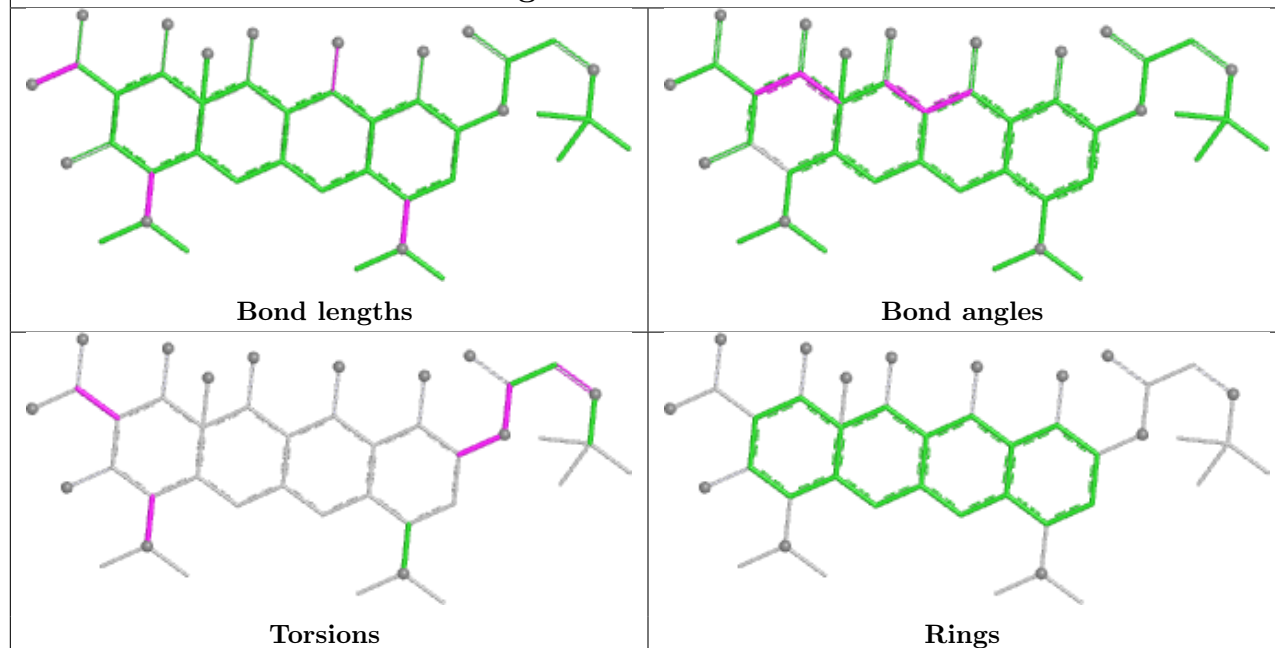
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5316	T1C	2	0
88	L5	5317	T1C	3	0
88	S2	1930	T1C	1	0
88	L5	5315	T1C	2	0

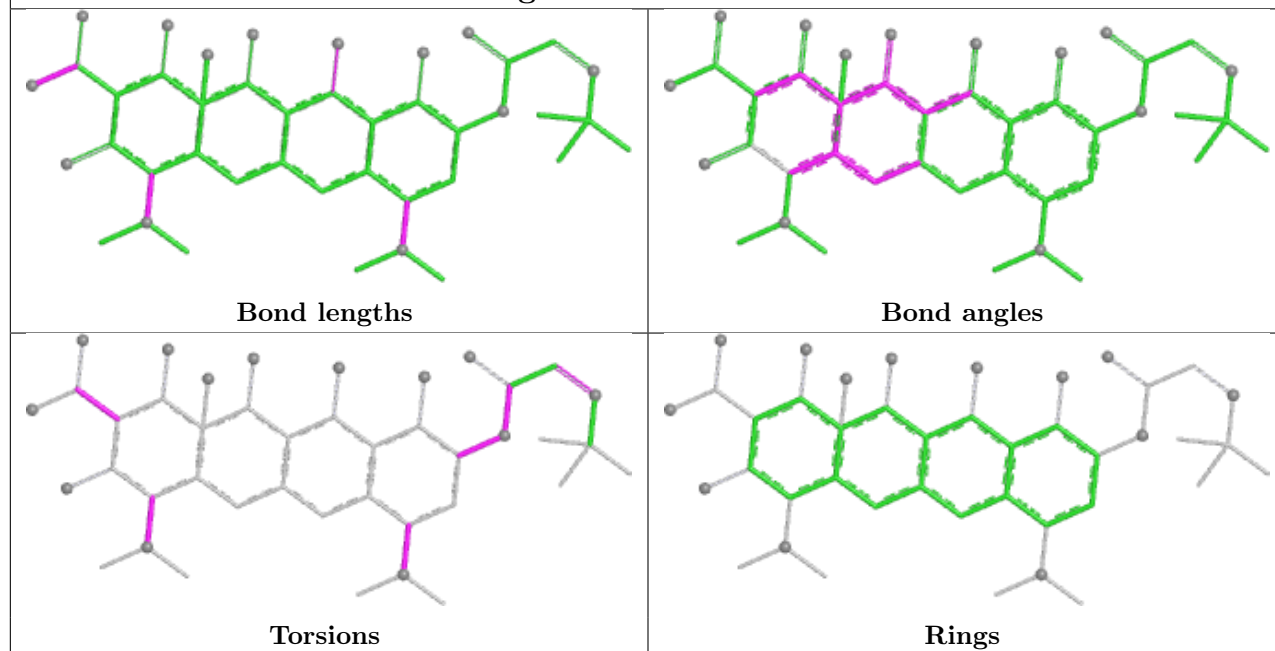
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



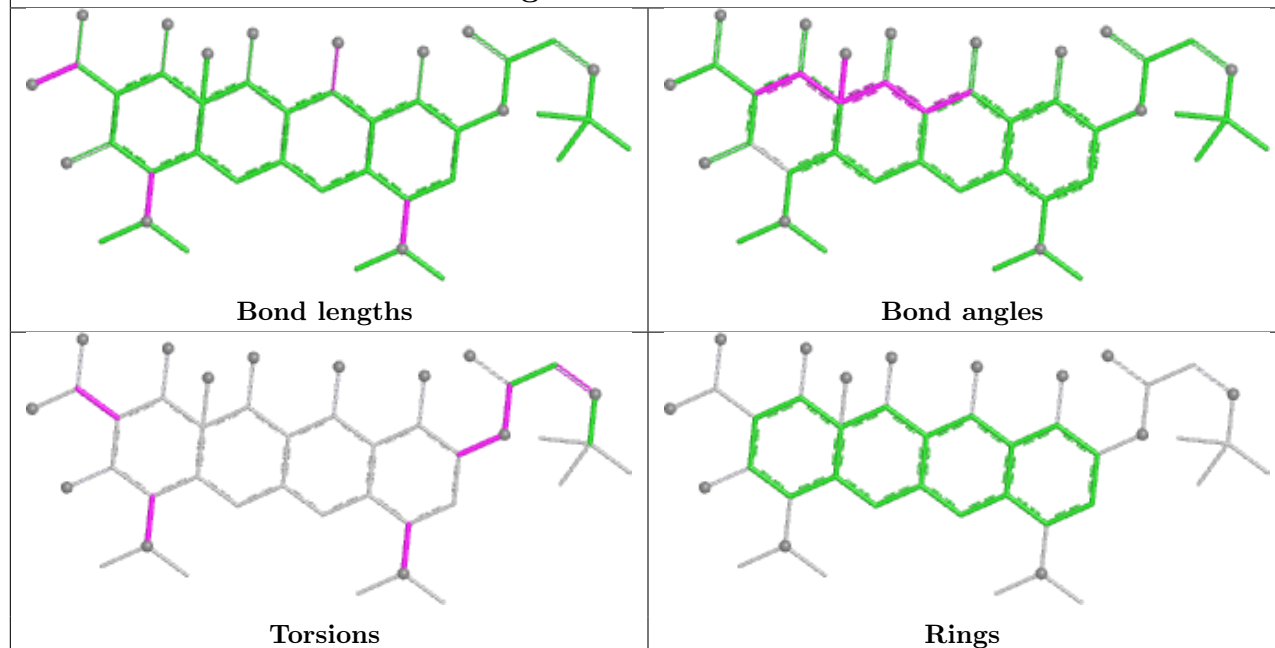
Ligand T1C L5 5318



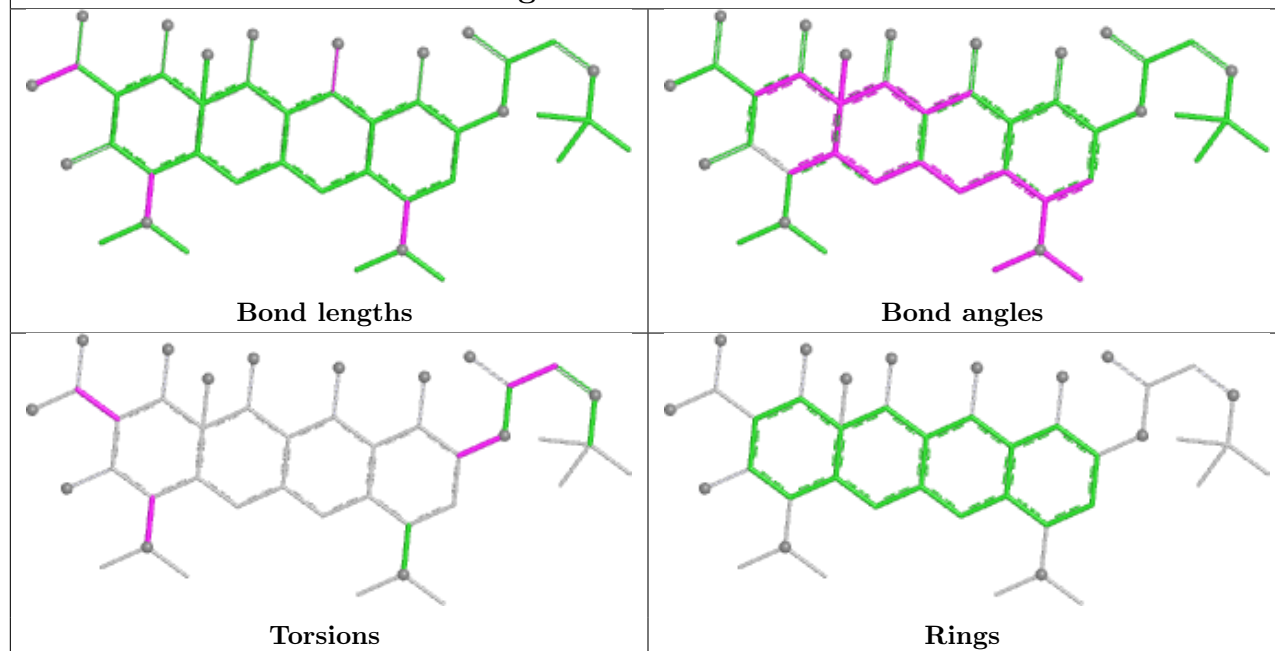
Ligand T1C L5 5316



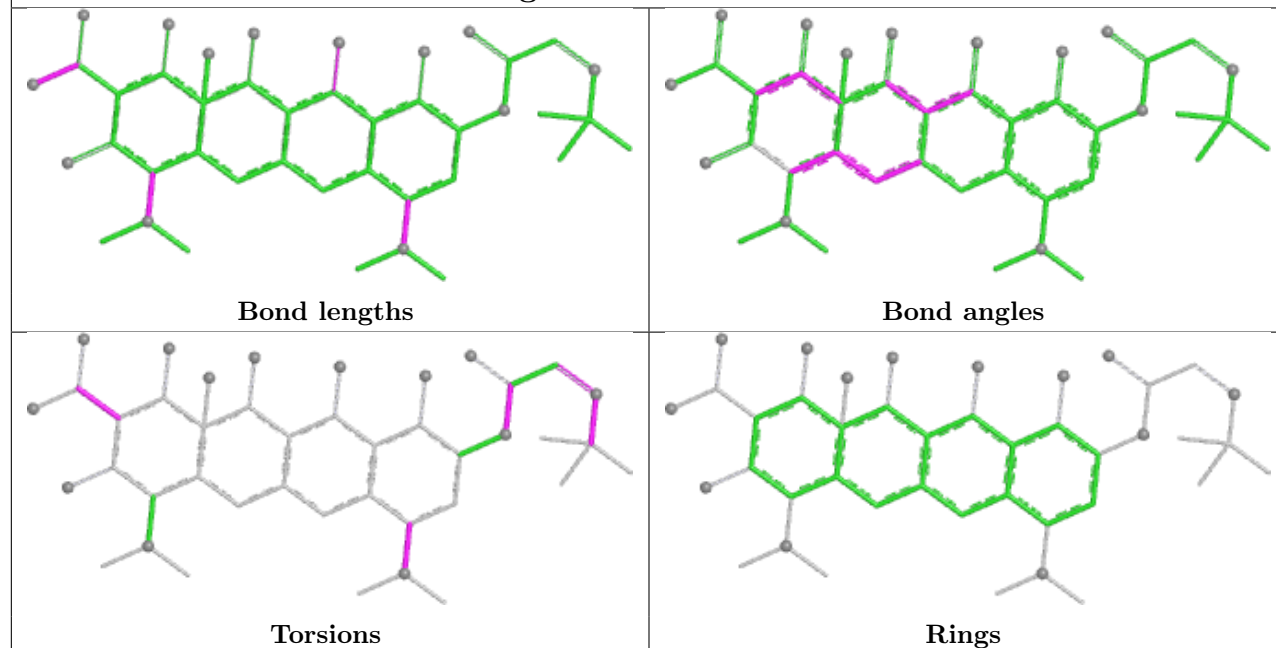
Ligand T1C CC 101



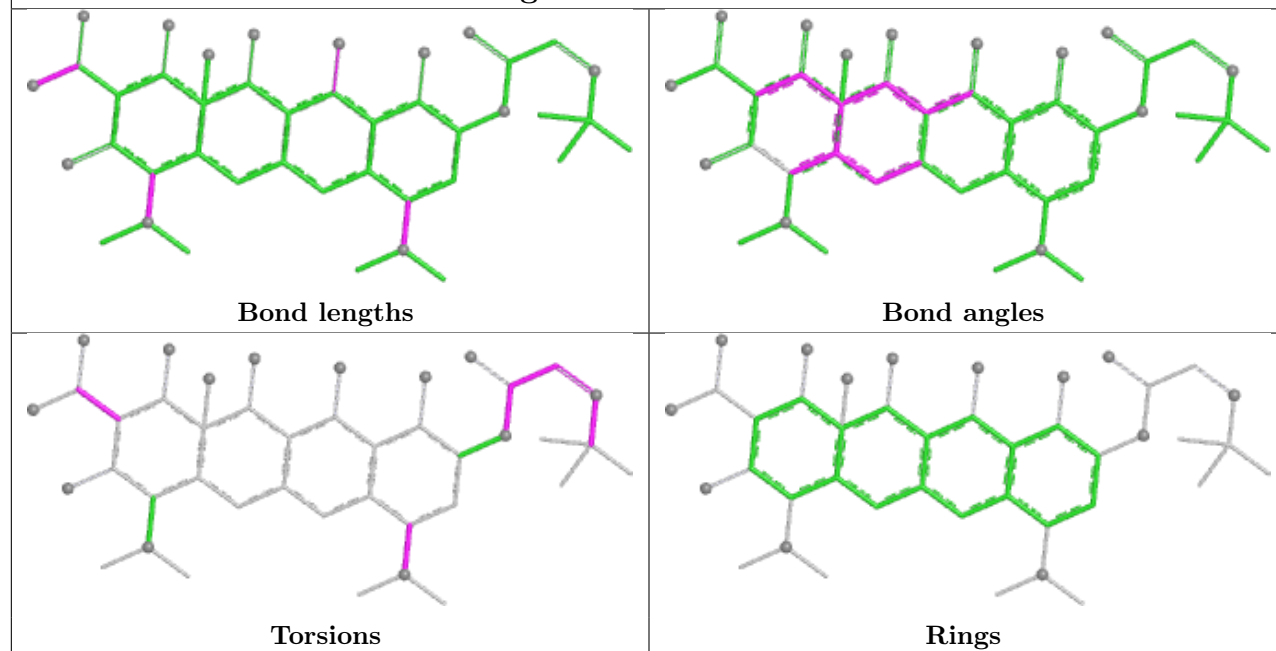
Ligand T1C L5 5317

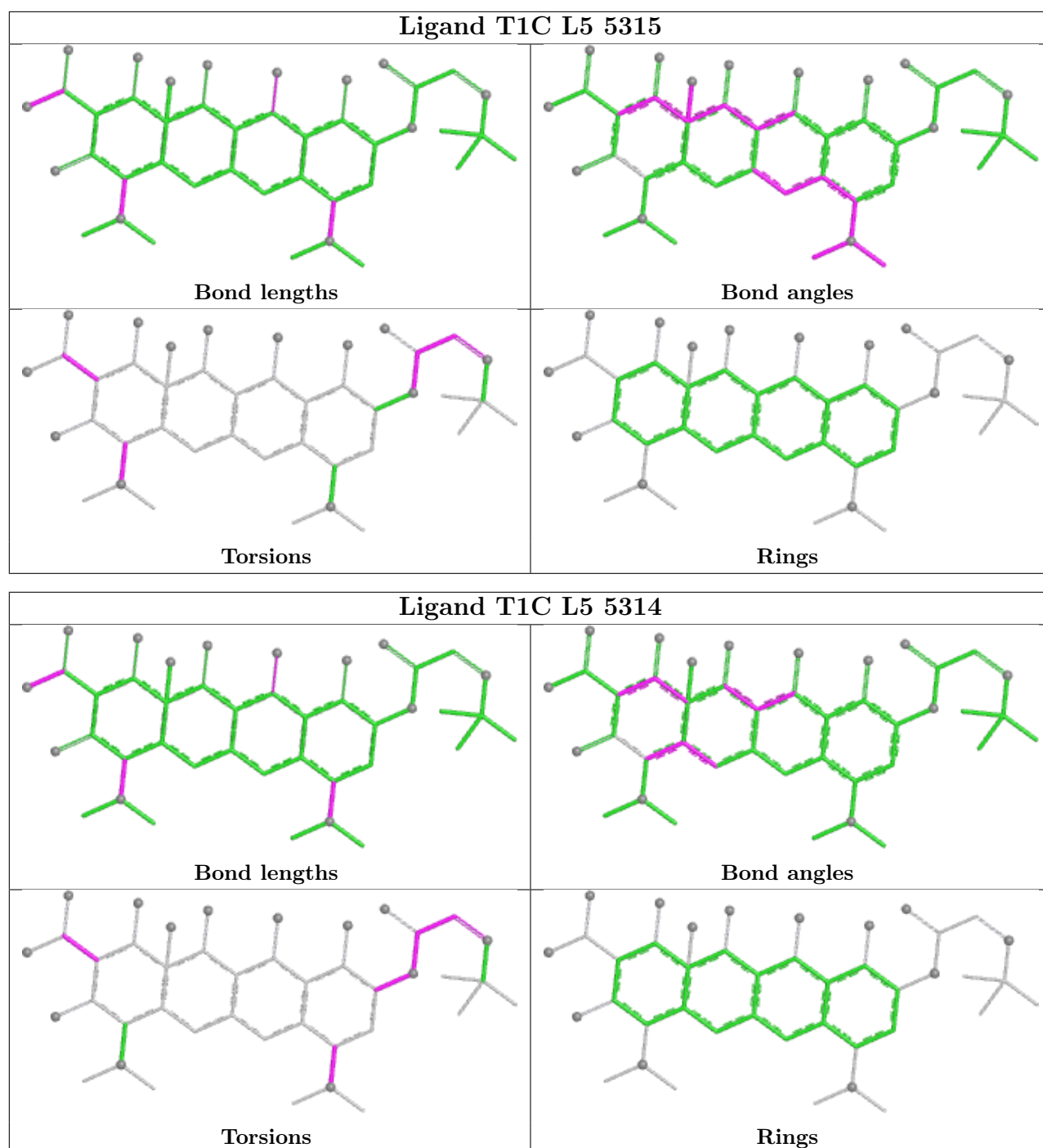


Ligand T1C L5 5313



Ligand T1C S2 1930





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.

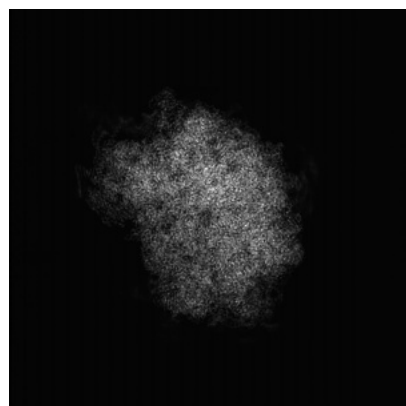
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36838. These allow visual inspection of the internal detail of the map and identification of artifacts.

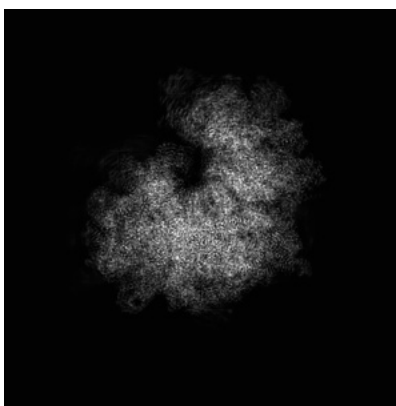
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

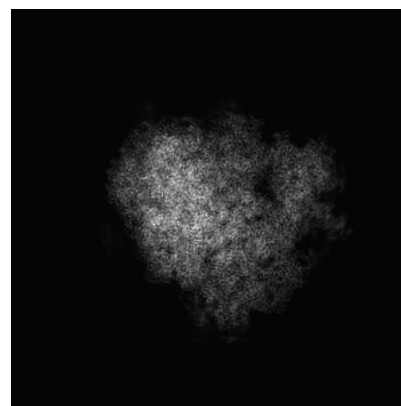
6.1.1 Primary map



X

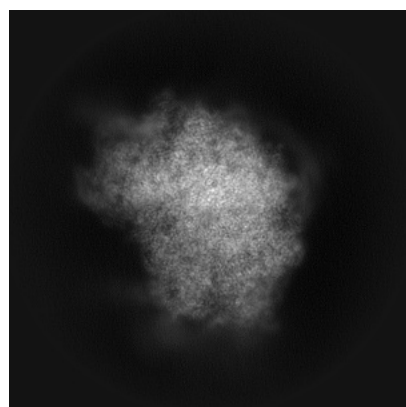


Y

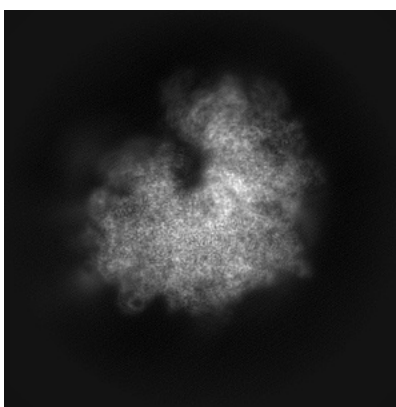


Z

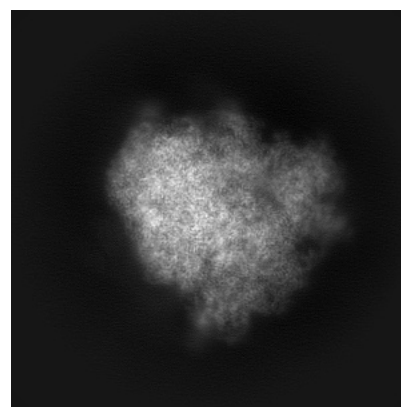
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

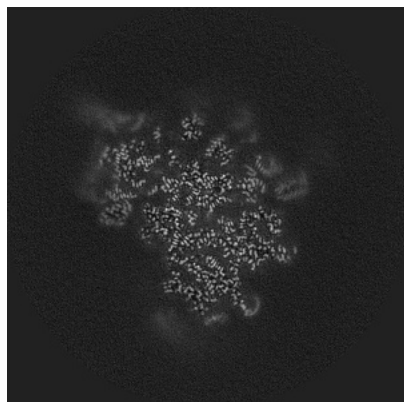


Y Index: 240

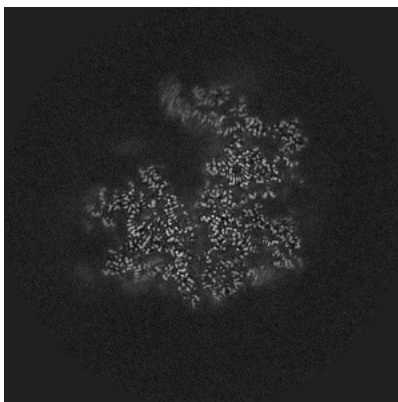


Z Index: 240

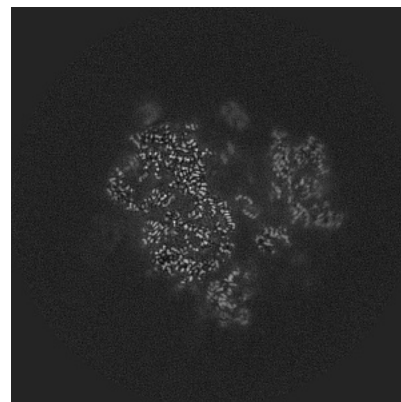
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 215

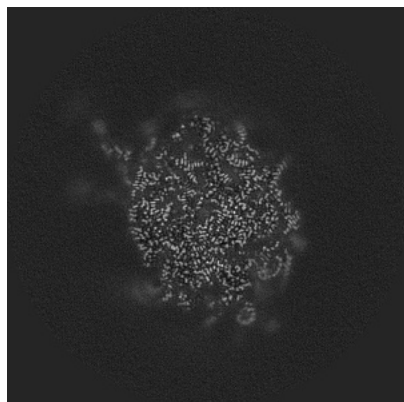


Y Index: 231

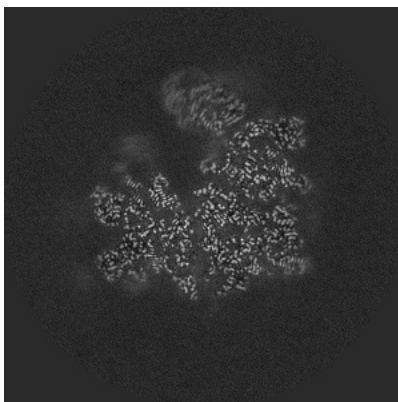


Z Index: 266

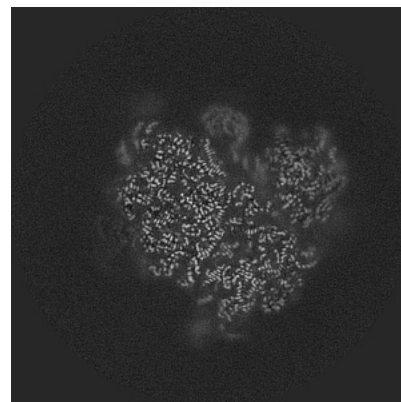
6.3.2 Raw map



X Index: 215



Y Index: 231

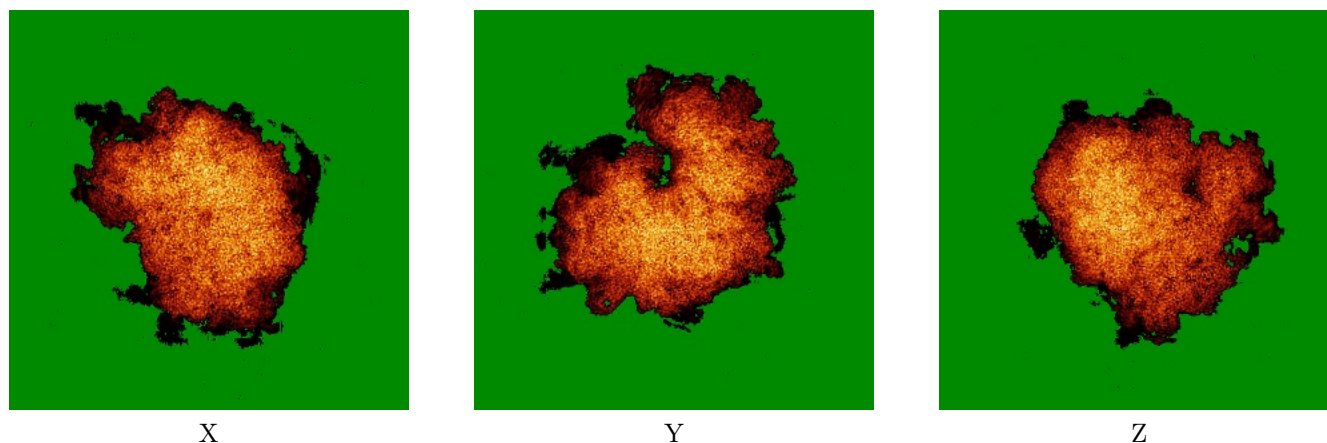


Z Index: 266

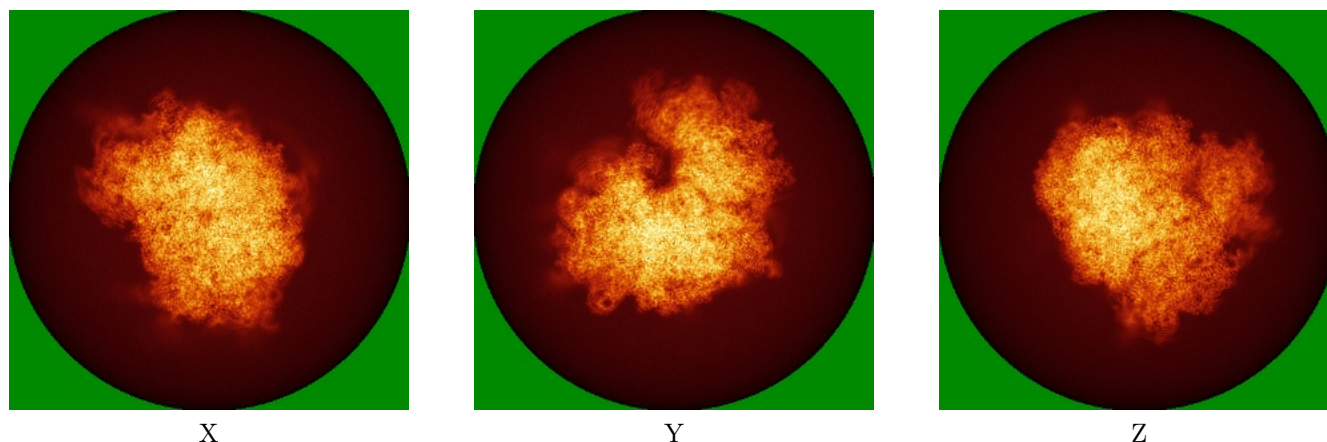
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

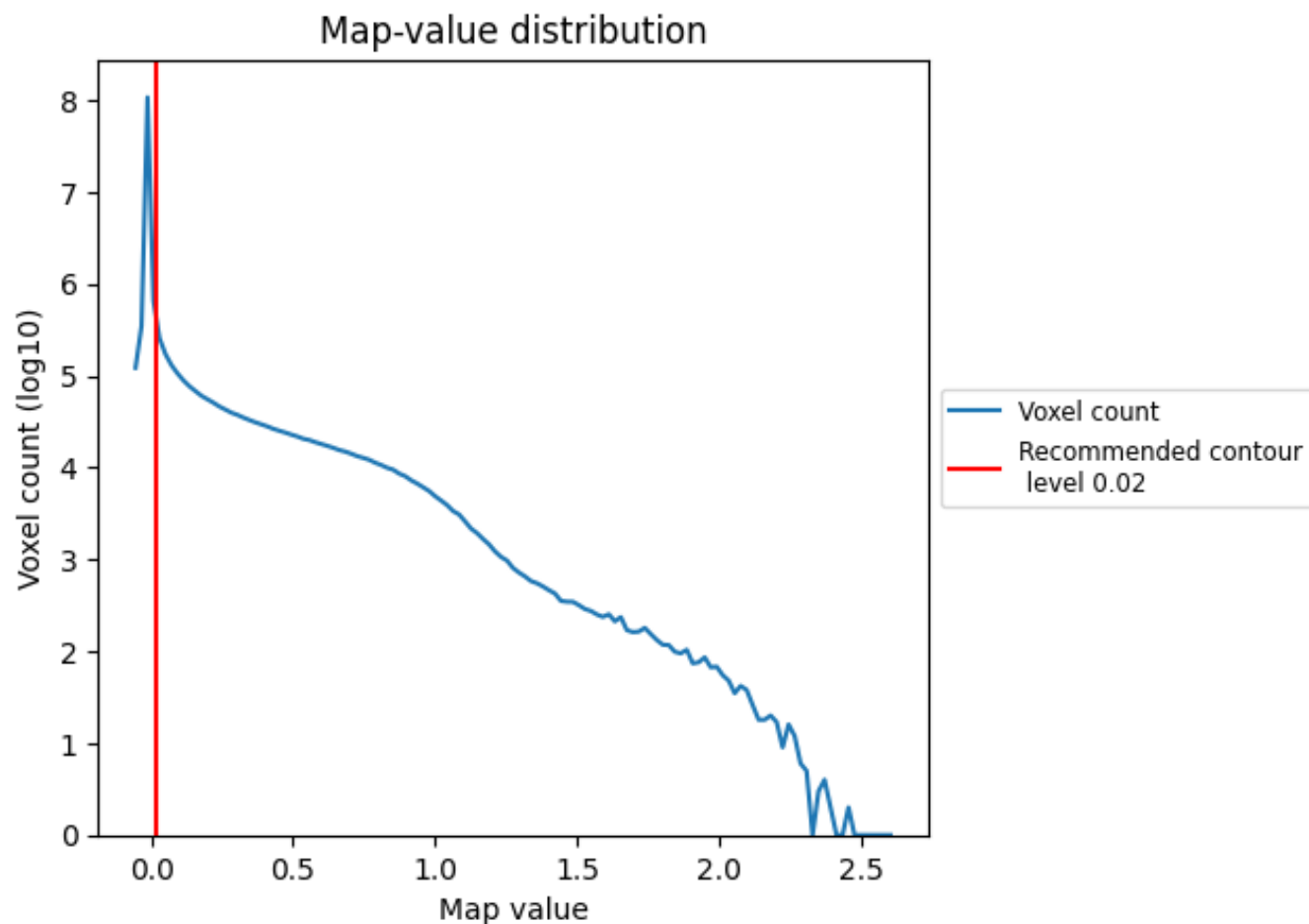
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

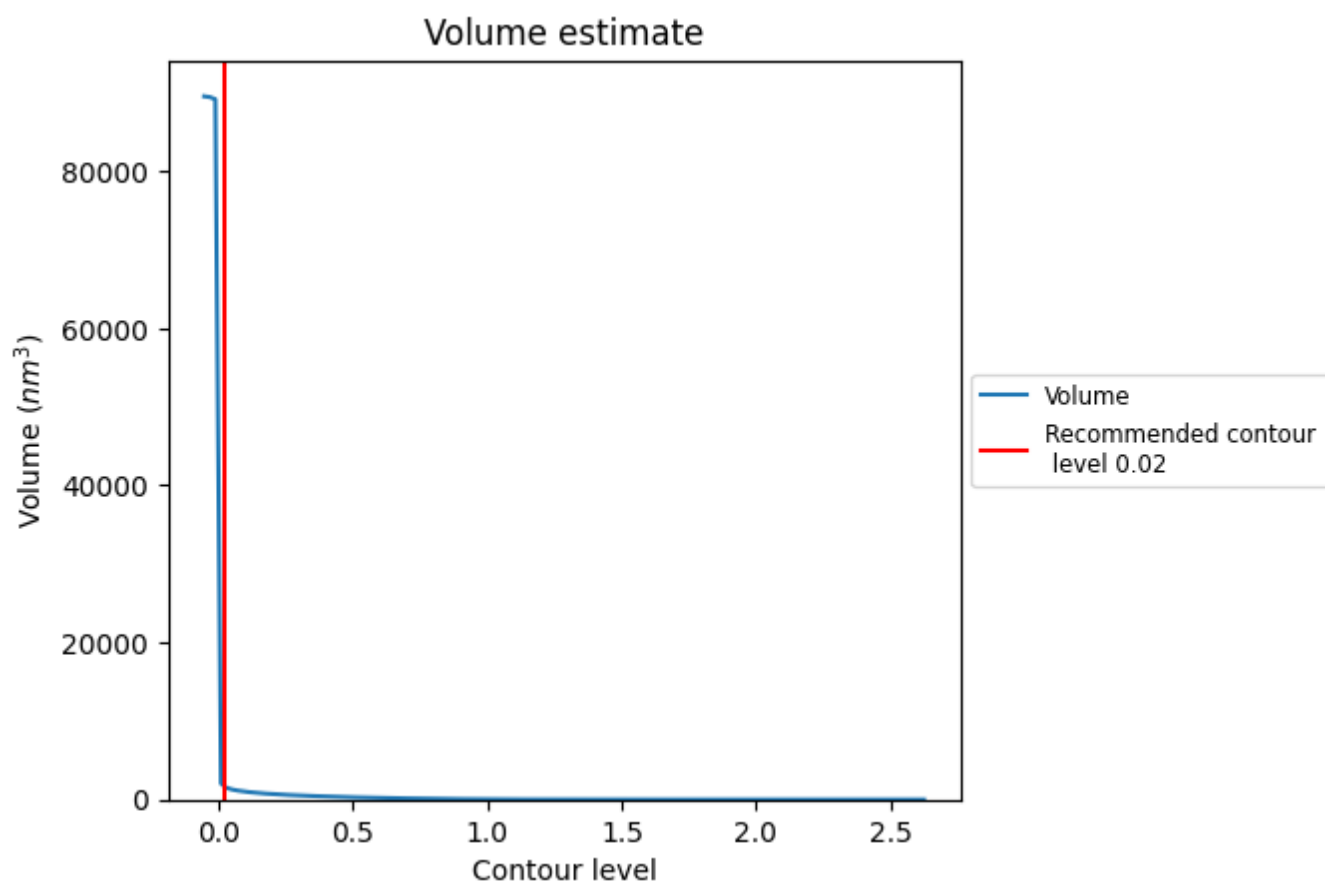
This section contains the results of statistical analysis of the map.

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.

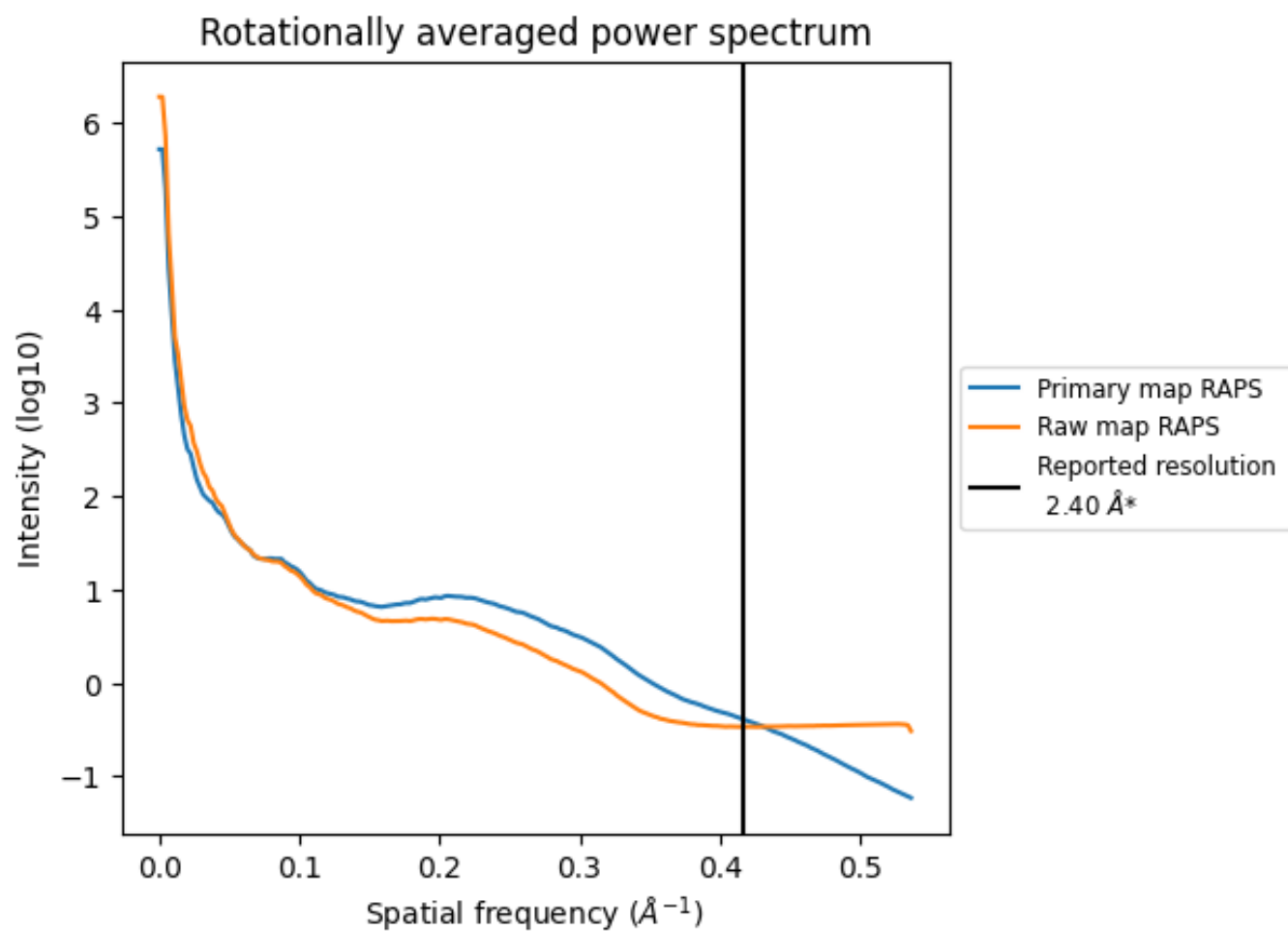
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1717 nm^3 ; this corresponds to an approximate mass of 1551 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 ⓘ

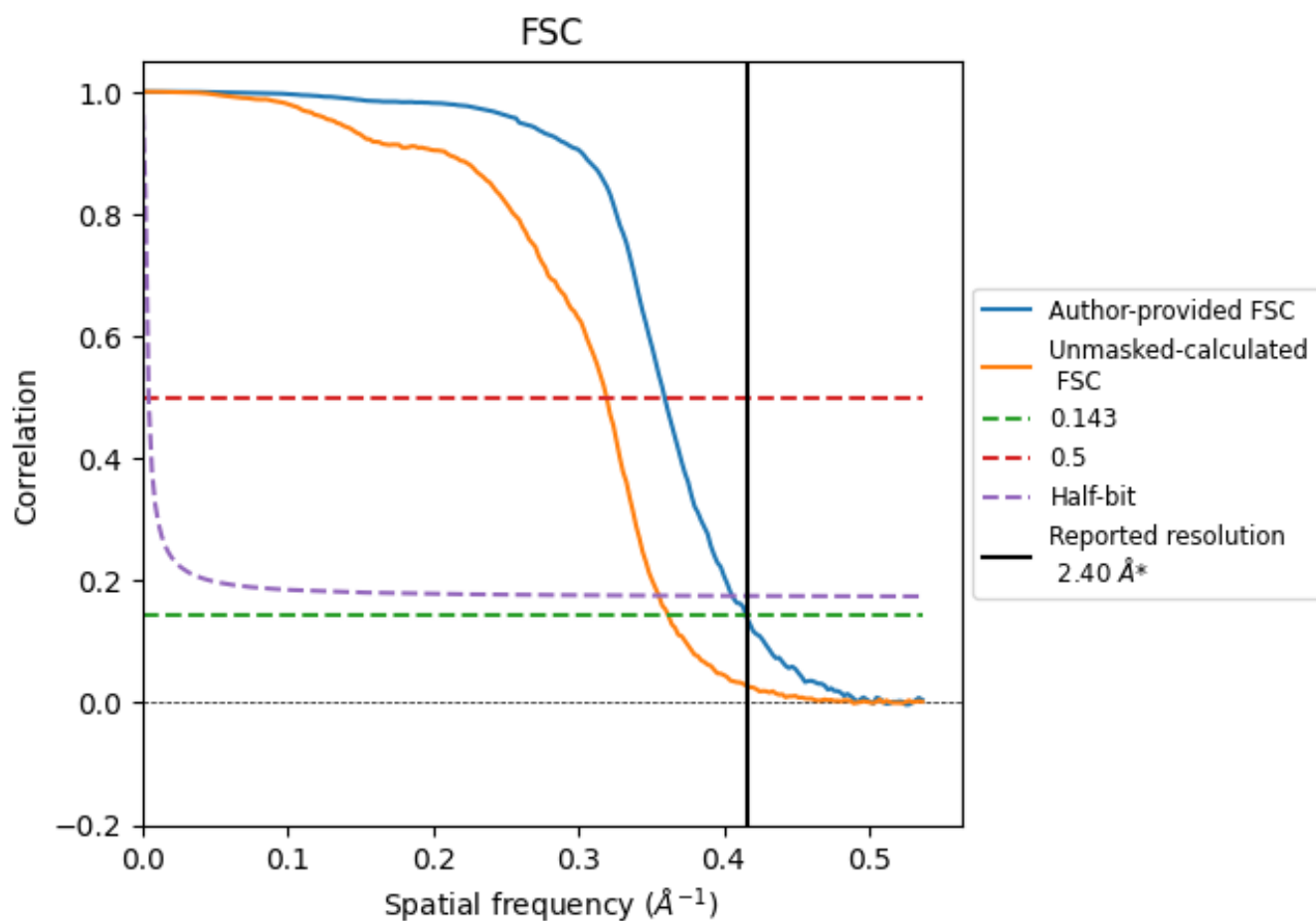


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.41	2.78	2.46
Unmasked-calculated*	2.76	3.13	2.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.4 by more than 10 %

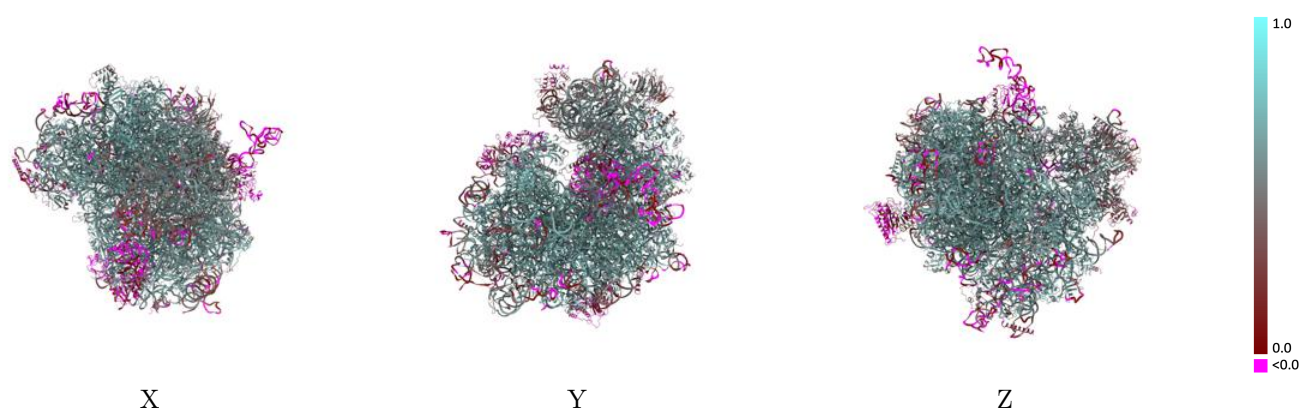
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36838 and PDB model 8K2C. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

This section was not generated.

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

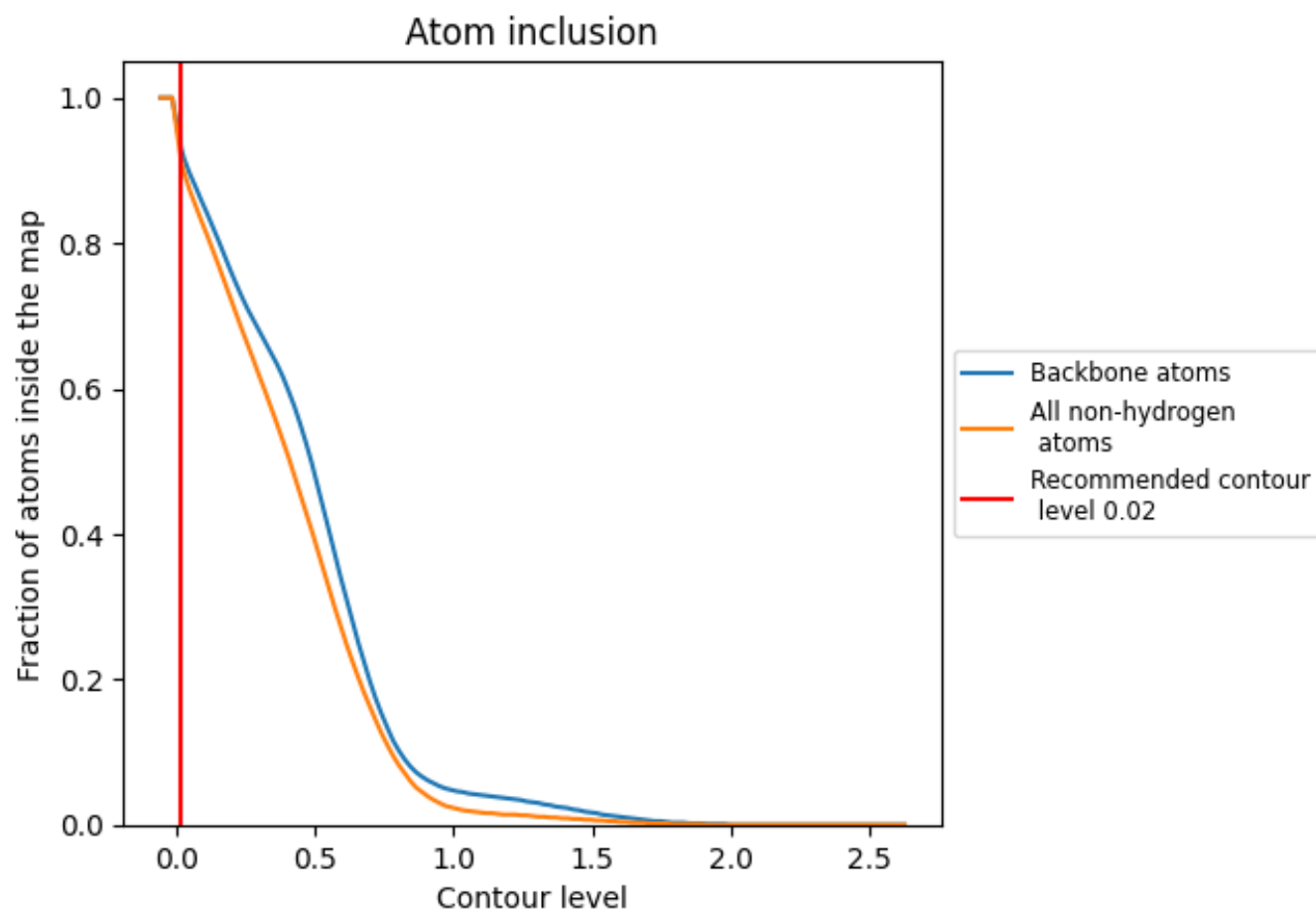


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5480
CA	 0.2330	 0.0850
CB	 0.8560	 0.4860
CC	 0.7710	 0.3860
CE	 0.3980	 0.2590
L5	 0.9180	 0.5490
L7	 0.9970	 0.6440
L8	 0.9450	 0.5880
LA	 0.9850	 0.6690
LB	 0.9590	 0.6380
LC	 0.9630	 0.6340
LD	 0.9590	 0.6140
LE	 0.9460	 0.5760
LF	 0.9690	 0.6540
LG	 0.9110	 0.5740
LH	 0.9610	 0.6190
LI	 0.9630	 0.6410
LJ	 0.9050	 0.5340
LL	 0.9310	 0.5950
LM	 0.9610	 0.6200
LN	 0.9930	 0.6730
LO	 0.9640	 0.6510
LP	 0.9660	 0.6520
LQ	 0.9810	 0.6670
LR	 0.9320	 0.5970
LS	 0.9820	 0.6660
LT	 0.9540	 0.6230
LU	 0.9060	 0.5380
LV	 0.9650	 0.6600
LW	 0.7360	 0.4090
LX	 0.9400	 0.6200
LY	 0.9520	 0.6240
LZ	 0.9700	 0.6330
La	 0.9820	 0.6670
Lb	 0.8850	 0.5480



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Chain	Atom inclusion	Q-score
Lc	 0.9480	 0.6320
Ld	 0.9350	 0.6060
Le	 0.9770	 0.6600
Lf	 0.9860	 0.6710
Lg	 0.9550	 0.6280
Lh	 0.9490	 0.6170
Li	 0.9620	 0.6170
Lj	 0.9820	 0.6560
Lk	 0.8990	 0.5430
Ll	 0.9550	 0.6140
Lm	 0.9500	 0.6290
Ln	 0.9570	 0.6390
Lo	 0.9350	 0.6160
Lp	 0.9450	 0.6360
Lr	 0.9720	 0.6440
Ls	 0.3660	 0.0200
Lt	 0.3050	 0.0050
Lz	 0.4120	 0.0190
S2	 0.9440	 0.5490
SA	 0.9650	 0.6050
SB	 0.9550	 0.6090
SC	 0.9680	 0.6260
SD	 0.8940	 0.4700
SE	 0.9710	 0.6160
SF	 0.9340	 0.5270
SG	 0.8900	 0.4950
SH	 0.9150	 0.5340
SI	 0.9400	 0.5990
SJ	 0.9420	 0.5940
SK	 0.9100	 0.4170
SL	 0.9320	 0.6180
SM	 0.7900	 0.1960
SN	 0.9680	 0.6340
SO	 0.9610	 0.6140
SP	 0.7910	 0.3590
SQ	 0.9170	 0.5130
SR	 0.9100	 0.5320
SS	 0.8940	 0.4720
ST	 0.9210	 0.4810
SU	 0.8840	 0.4390
SV	 0.9730	 0.6140
SW	 0.9810	 0.6500

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Chain	Atom inclusion	Q-score
SX	 0.9560	 0.6260
SY	 0.9280	 0.5520
SZ	 0.8580	 0.4180
Sa	 0.9380	 0.5990
Sb	 0.9330	 0.5770
Sc	 0.8750	 0.4920
Sd	 0.9340	 0.5200
Se	 0.7720	 0.4700
Sf	 0.6270	 0.1760
Sg	 0.8570	 0.3880