



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 11:31 AM EDT

PDB ID : 6OLI / pdb_00006oli
EMDB ID : EMD-0526
Title : Structure of human ribosome nascent chain complex selectively stalled by a drug-like small molecule (USO1-RNC)
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-16
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

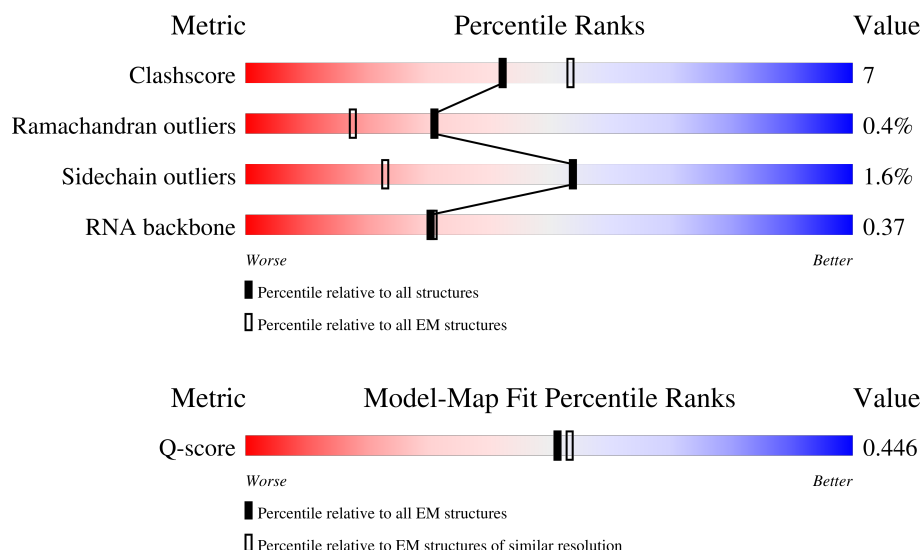
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	S2	1714	12% 55% 36% 9%
2	SA	221	28% 74% 25% •
3	SB	214	21% 73% 26% •

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Mol	Chain	Length	Quality of chain
4	SD	226	
5	SE	259	
6	SF	189	
7	SH	189	
8	SI	204	
9	SK	98	
10	SL	153	
11	SP	127	
12	SQ	146	
13	SR	134	
14	SS	145	
15	ST	143	
16	SU	104	
17	SV	82	
18	SX	141	
19	Sa	102	
20	Sc	64	
21	Sd	55	
22	Sg	312	
23	SC	220	
24	SG	237	
25	SJ	185	
26	SM	118	
27	SN	150	
28	SO	137	

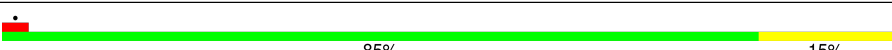
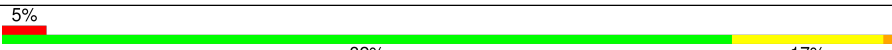
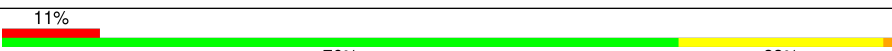
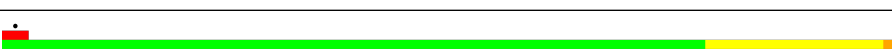
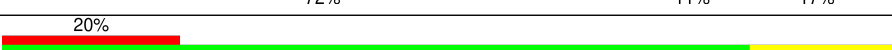
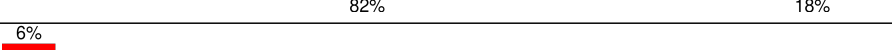
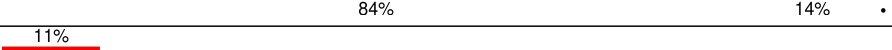
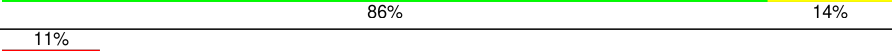
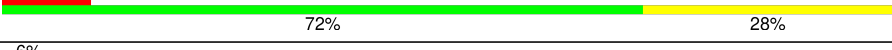
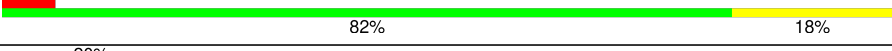
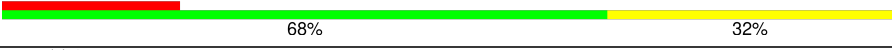
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Mol	Chain	Length	Quality of chain
29	SW	129	
30	SY	131	
31	SZ	73	
32	Sb	82	
33	Se	57	
34	Sf	67	
35	A	252	
36	B	397	
37	C	363	
38	D	157	
39	E	121	
40	F	294	
41	G	247	
42	H	225	
43	I	234	
44	J	191	
45	K	211	
46	L	169	
47	M	205	
48	N	139	
49	O	203	
50	P	195	
51	Q	153	
52	R	187	
53	S	181	

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Mol	Chain	Length	Quality of chain
54	T	175	
55	U	157	
56	V	99	
57	W	129	
58	X	61	
59	Y	117	
60	Z	134	
61	a	134	
62	b	147	
63	c	121	
64	d	103	
65	e	106	
66	f	129	
67	g	109	
68	h	114	
69	i	122	
70	j	97	
71	k	84	
72	l	69	
73	m	50	
74	n	50	
75	o	25	
76	p	105	
77	q	91	
78	r	122	

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Mol	Chain	Length	Quality of chain
79	t	3607	9% 64% 30% 6%
80	u	76	63% 54% 43%
81	v	76	24% 51% 32% 17%
82	w	10	80% 10% 10%
83	y	36	92% 97%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 214867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1714	Total	C	N	O	P	0	0
			36501	16306	6533	11949	1713		

- Molecule 2 is a protein called 40S ribosomal protein SA.

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

- Molecule 3 is a protein called 40S ribosomal protein S3a.

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

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	226	Total	C	N	O	S	0	0
			1757	1120	316	314	7		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

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

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	204	Total	C	N	O	S	0	0
			1673	1050	329	289	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 15 is a protein called 40S ribosomal protein S19.

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

- Molecule 16 is a protein called 40S ribosomal protein S20.

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

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SV	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 40S ribosomal protein S26.

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

- Molecule 20 is a protein called 40S ribosomal protein S28.

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

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sg	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SC	220	Total	C	N	O	S	1	0
			1715	1109	296	300	10		

- Molecule 24 is a protein called 40S ribosomal protein S6.

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

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	118	Total	C	N	O	S	0	0
			912	571	161	173	7		

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 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Se	57	Total	C	N	O	S	0	0
			452	281	99	71	1		

- Molecule 34 is a protein called 40S ribosomal protein S27a.

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

- Molecule 35 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	252	Total	C	N	O	S	0	0
			1930	1209	395	320	6		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	397	Total	C	N	O	S	0	0
			3202	2039	602	547	14		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	D	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	F	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	G	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 42 is a protein called 60S ribosomal protein L7.

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

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	I	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 44 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	J	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 45 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	K	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 48 is a protein called 60S ribosomal protein L14.

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

- Molecule 49 is a protein called 60S ribosomal protein L15.

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

- Molecule 50 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 51 is a protein called 60S ribosomal protein L17.

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

- Molecule 52 is a protein called 60S ribosomal protein L18.

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

- Molecule 53 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 54 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 55 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 56 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 57 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 58 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X	61	Total	C	N	O	S	0	0
			511	327	100	82	2		

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	100	Total	C	N	O	S	0	0
			814	506	179	125	4		

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

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

- Molecule 69 is a protein called 60S ribosomal protein L35.

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

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 71 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

- Molecule 73 is a protein called 60S ribosomal protein L39.

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

- Molecule 74 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 75 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 76 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 79 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t	3607	Total	C	N	O	P	0	0
			77332	34436	14150	25139	3607		

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	u	76	Total	C	N	O	P	0	0
			1613	720	283	535	75		

- Molecule 81 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	v	76	Total	C	N	O	P	0	0
			1618	721	287	534	76		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	w	10	Total	C	N	O	P	0	0
			213	95	37	72	9		

- Molecule 83 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	y	36	Total	C	N	O	0	0
			178	106	36	36		

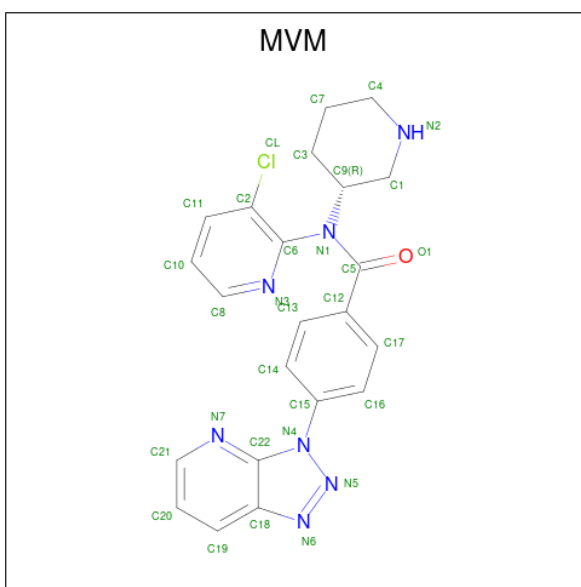
- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	S2	2	Total	Mg	0
			2	2	
84	B	1	Total	Mg	0
			1	1	
84	D	7	Total	Mg	0
			7	7	
84	E	9	Total	Mg	0
			9	9	
84	O	1	Total	Mg	0
			1	1	
84	b	1	Total	Mg	0
			1	1	
84	o	1	Total	Mg	0
			1	1	
84	t	9	Total	Mg	0
			9	9	

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

Mol	Chain	Residues	Atoms		AltConf
85	S2	1	Total	Zn	0
			1	1	
85	Sa	1	Total	Zn	0
			1	1	
85	Sf	1	Total	Zn	0
			1	1	
85	k	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	q	1	Total	Zn	0
			1	1	

- Molecule 86 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (CCD ID: MVM) (formula: C₂₂H₂₀ClN₇O).



Mol	Chain	Residues	Atoms					AltConf
86	t	1	Total 31	C 22	Cl 1	N 7	O 1	0

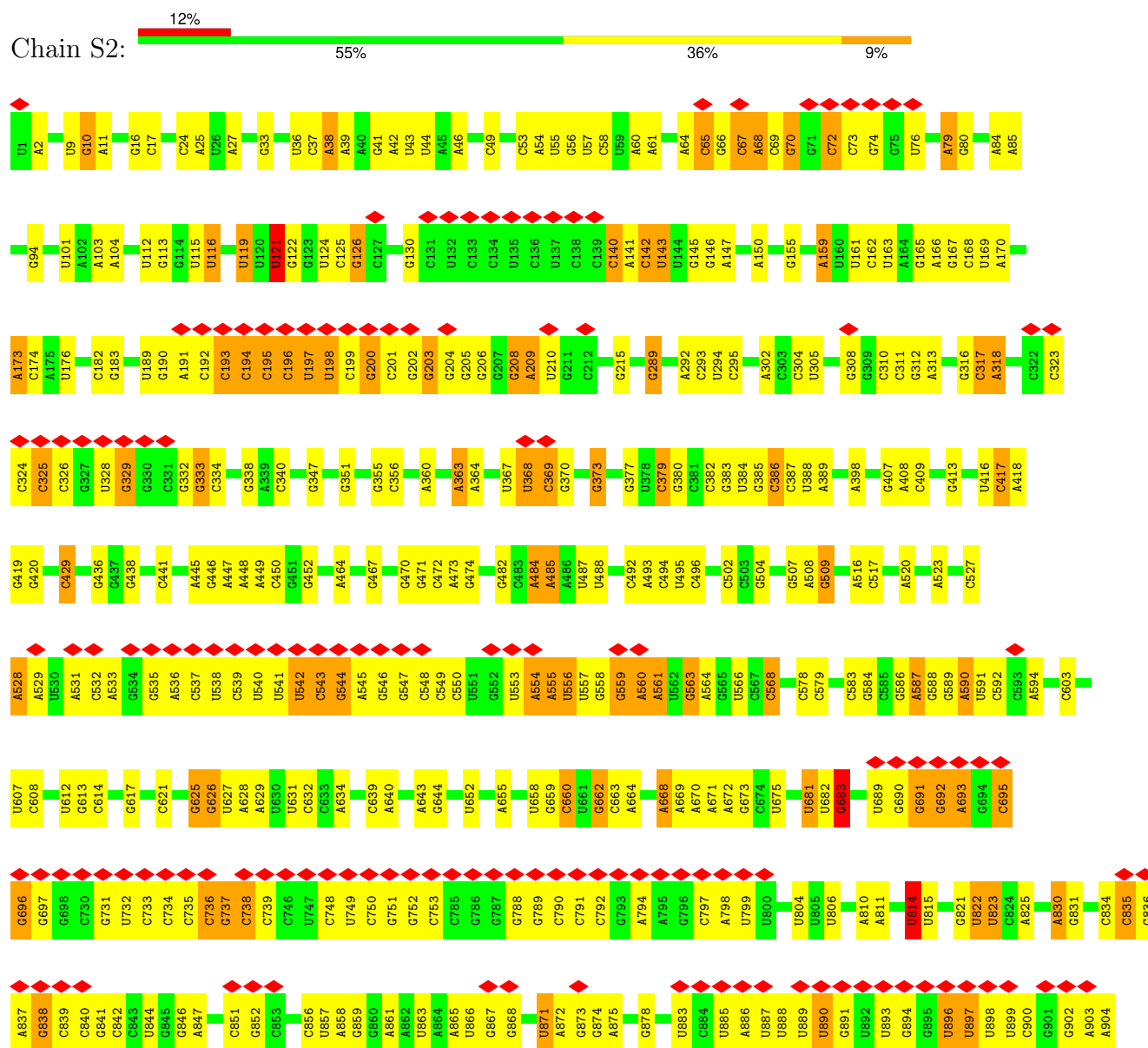
- Molecule 87 is water.

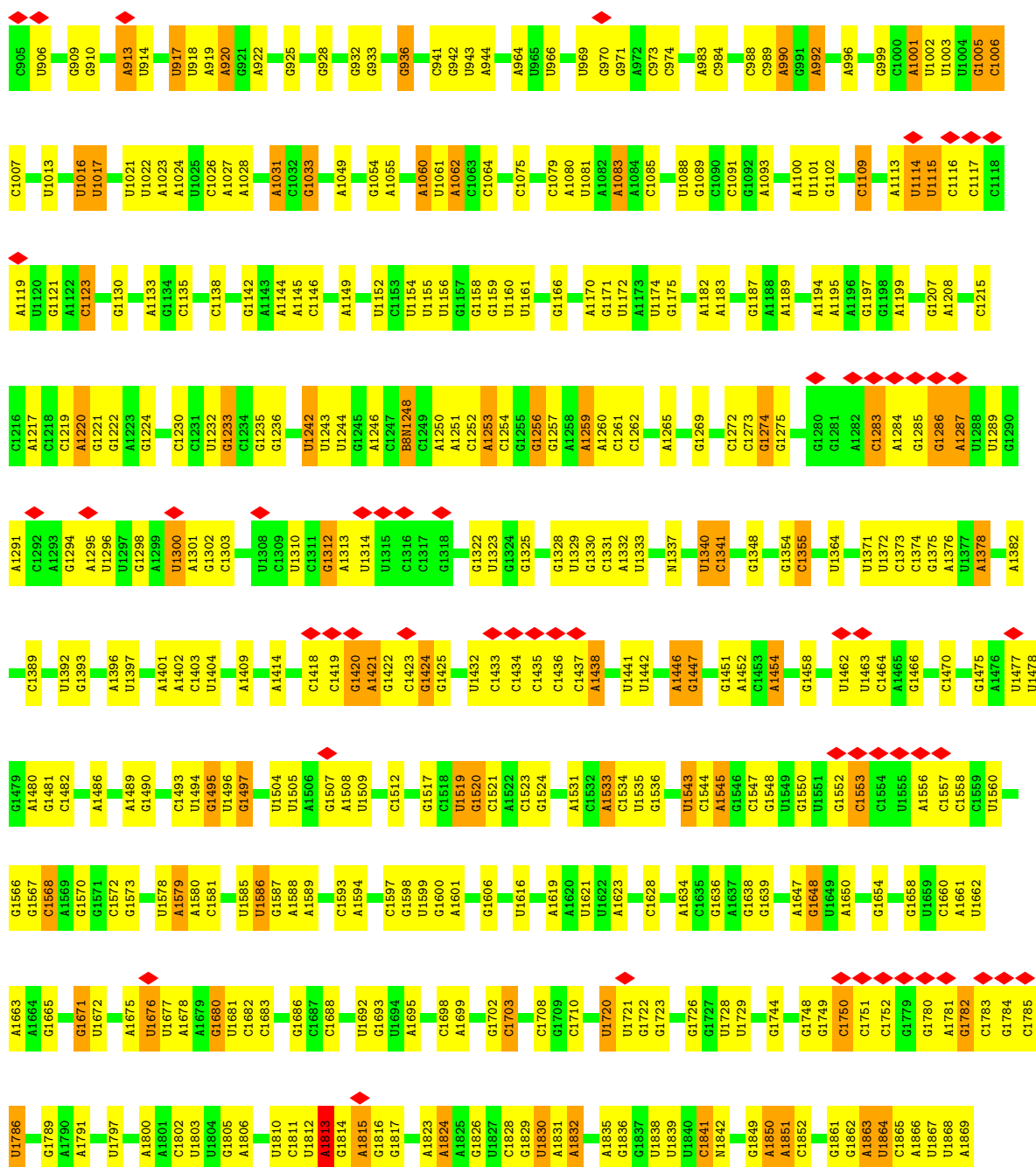
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total 5	O 5	0
87	SP	1	Total 1	O 1	0
87	SQ	1	Total 1	O 1	0
87	SR	1	Total 1	O 1	0
87	SS	1	Total 1	O 1	0
87	SC	1	Total 1	O 1	0
87	SJ	1	Total 1	O 1	0
87	Sb	1	Total 1	O 1	0
87	Sf	1	Total 1	O 1	0
87	u	1	Total 1	O 1	0

3 Residue-property plots

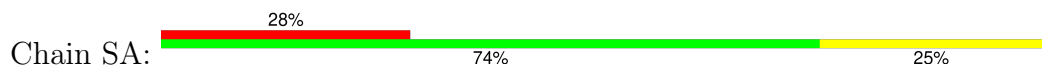
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

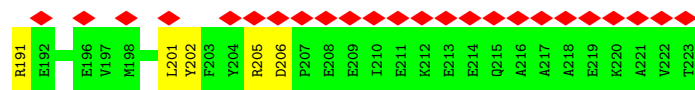
• Molecule 1: 18S ribosomal RNA



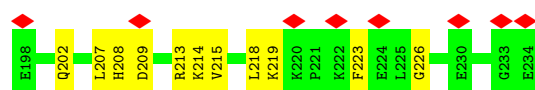
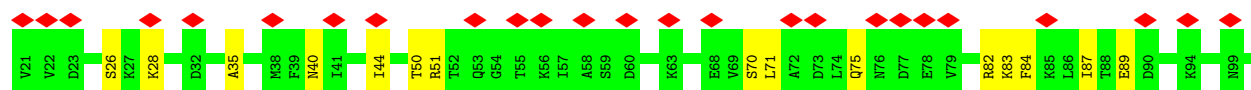
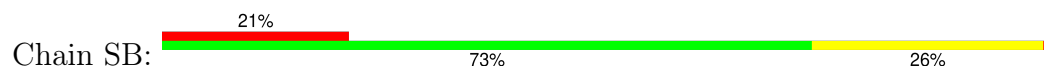


• Molecule 2: 40S ribosomal protein SA

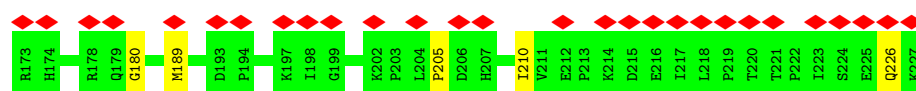
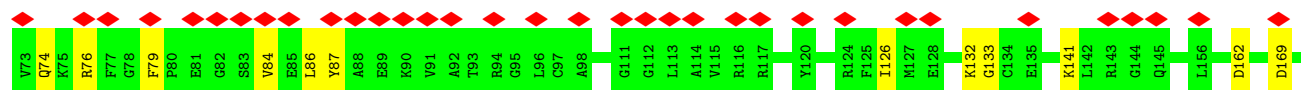
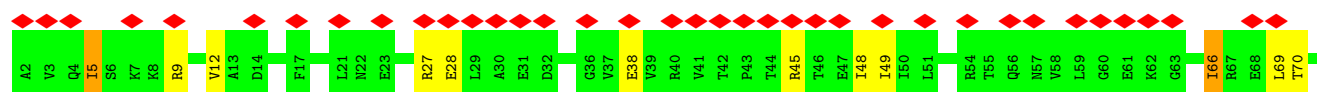
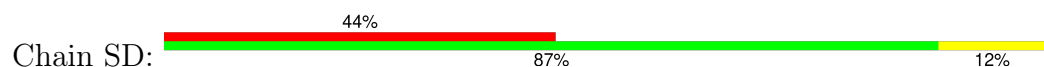




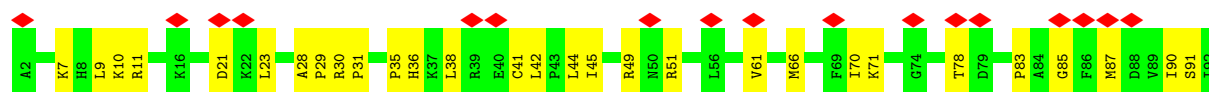
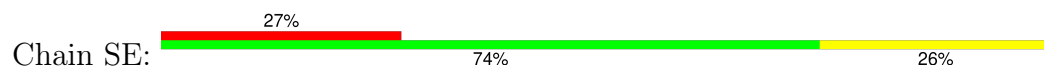
• Molecule 3: 40S ribosomal protein S3a

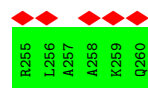


• Molecule 4: 40S ribosomal protein S3

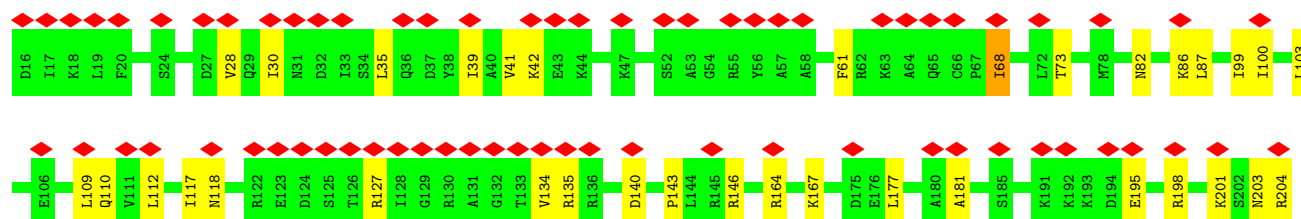
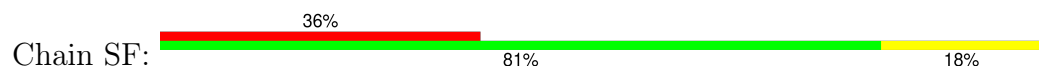


• Molecule 5: 40S ribosomal protein S4, X isoform

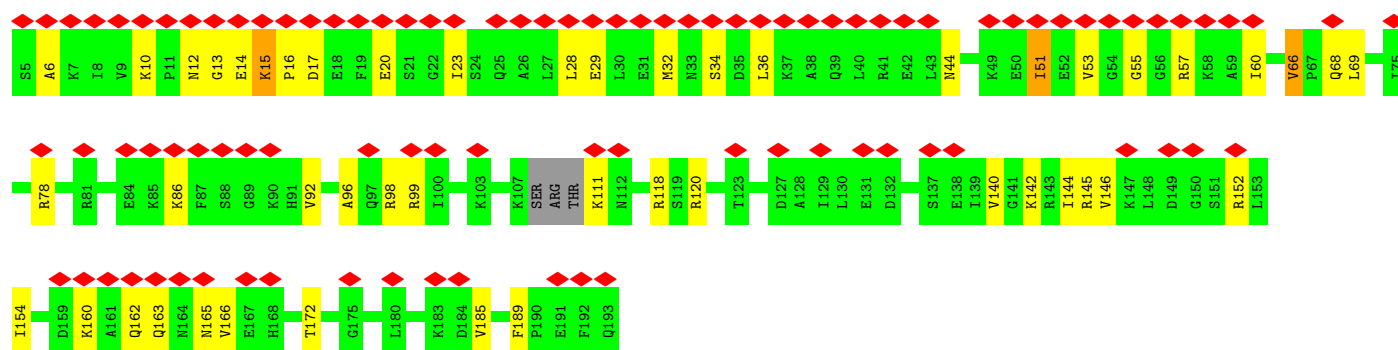
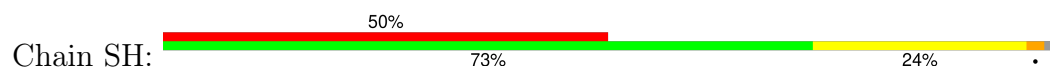




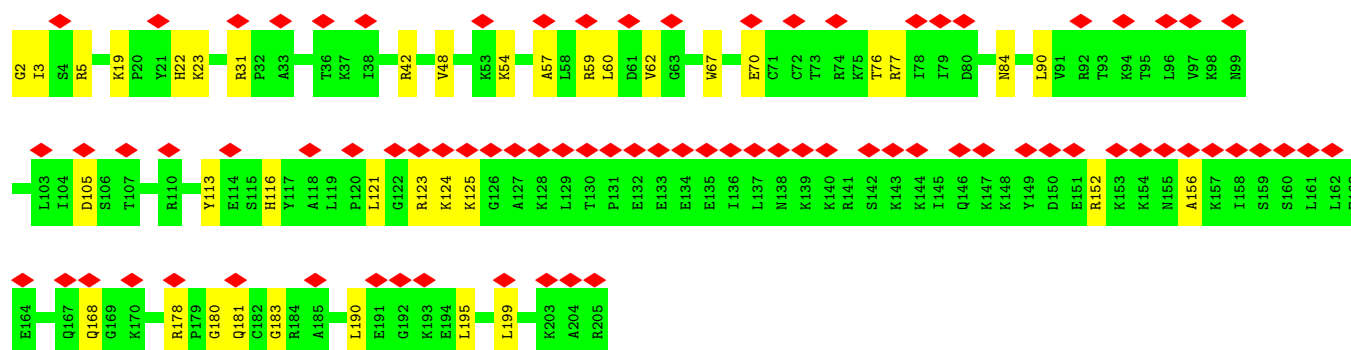
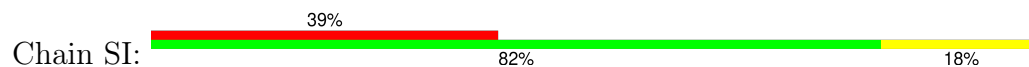
• Molecule 6: 40S ribosomal protein S5



• Molecule 7: 40S ribosomal protein S7

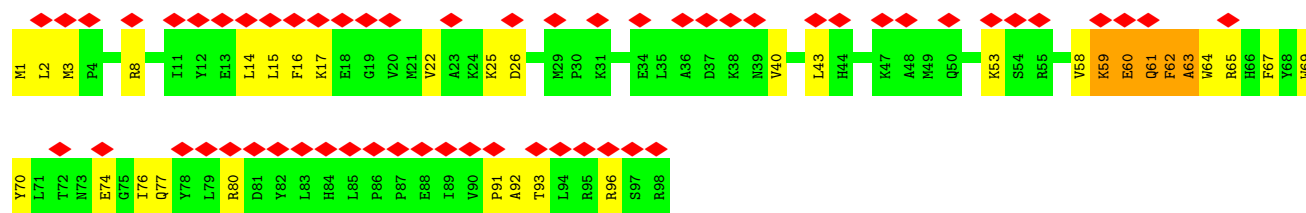


• Molecule 8: 40S ribosomal protein S8

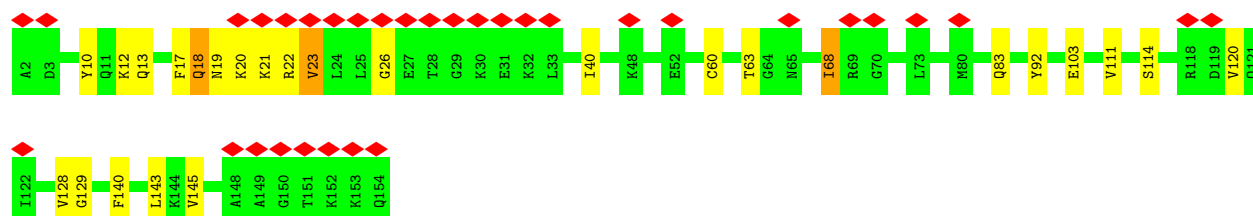
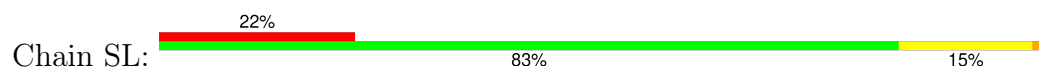


• Molecule 9: 40S ribosomal protein S10

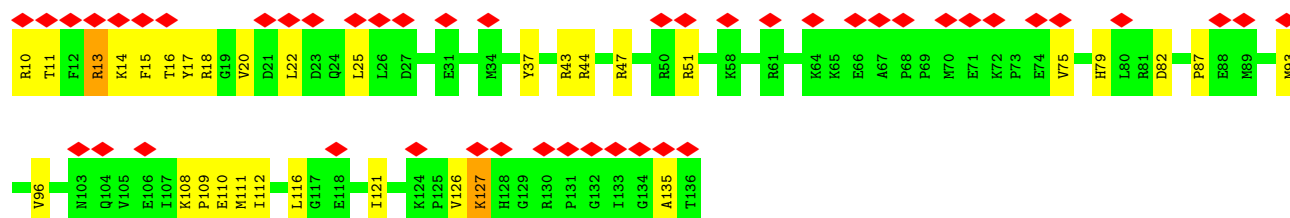
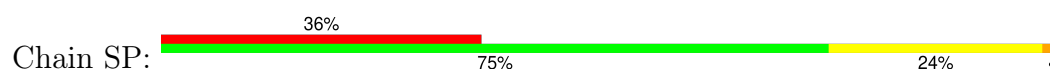




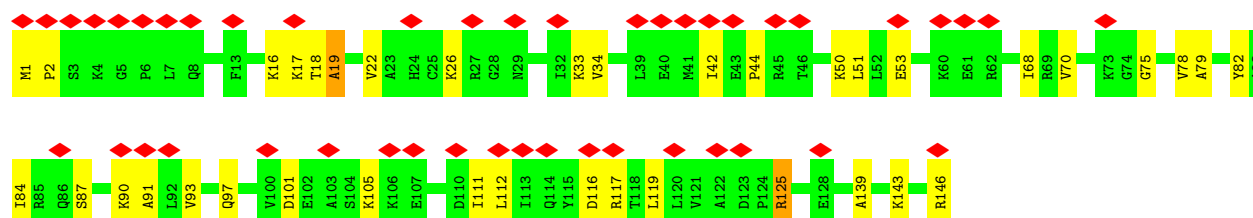
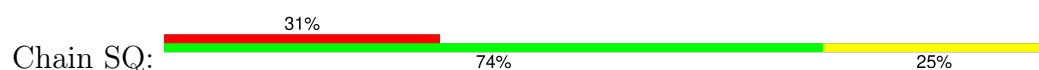
• Molecule 10: 40S ribosomal protein S11



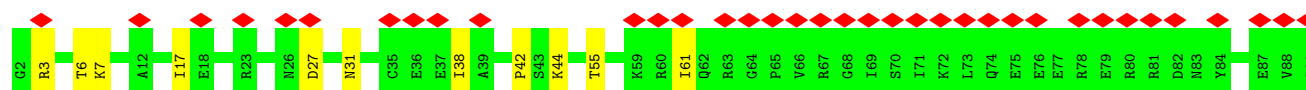
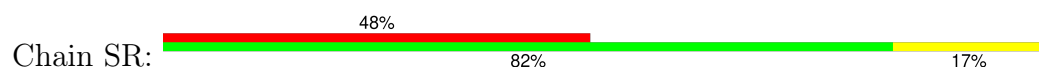
• Molecule 11: 40S ribosomal protein S15

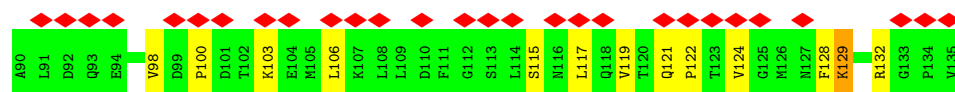


• Molecule 12: 40S ribosomal protein S16

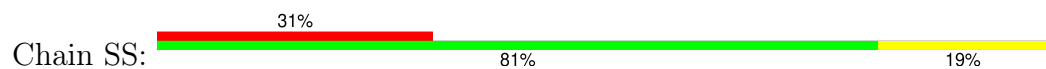


• Molecule 13: 40S ribosomal protein S17

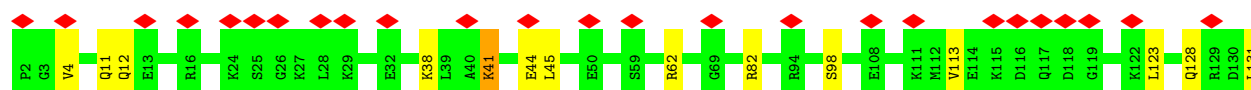
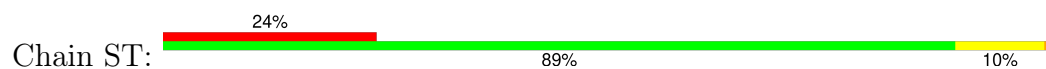




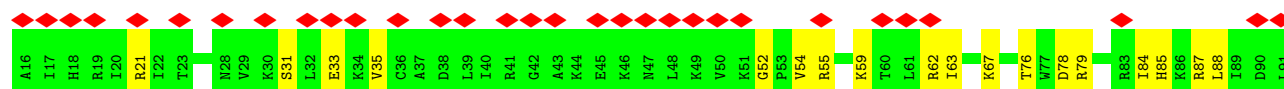
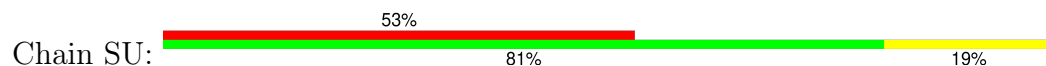
- Molecule 14: 40S ribosomal protein S18



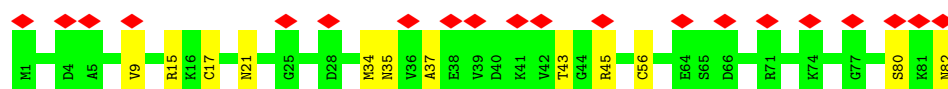
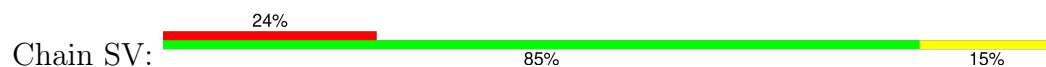
- Molecule 15: 40S ribosomal protein S19



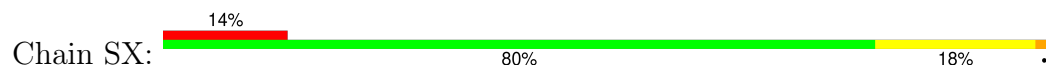
- Molecule 16: 40S ribosomal protein S20

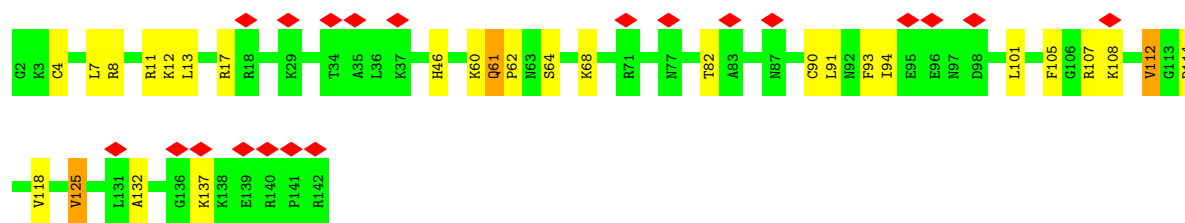


- Molecule 17: 40S ribosomal protein S21

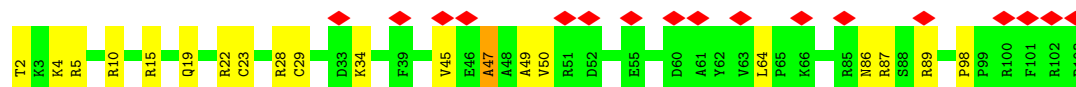
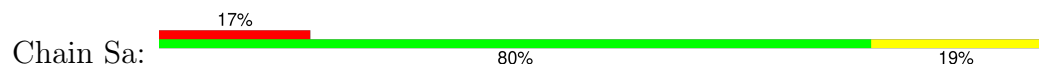


- Molecule 18: 40S ribosomal protein S23

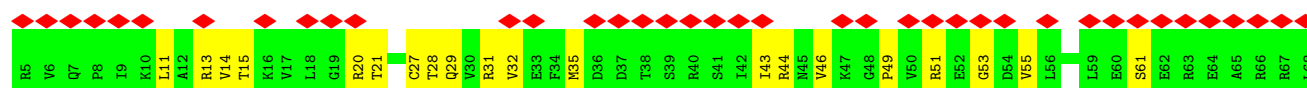




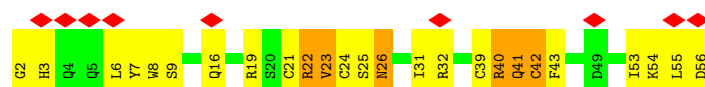
• Molecule 19: 40S ribosomal protein S26



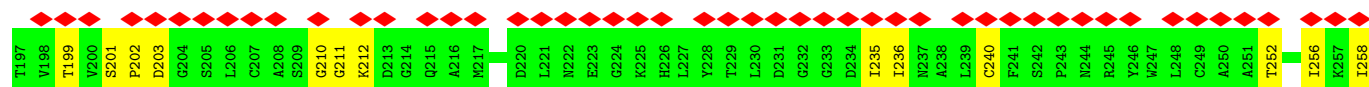
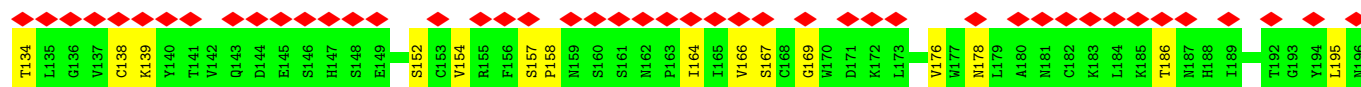
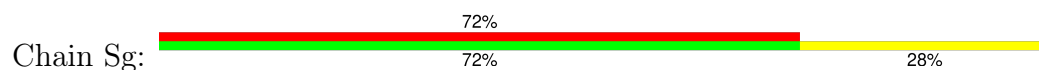
• Molecule 20: 40S ribosomal protein S28

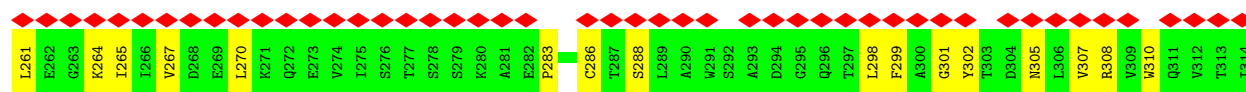


• Molecule 21: 40S ribosomal protein S29

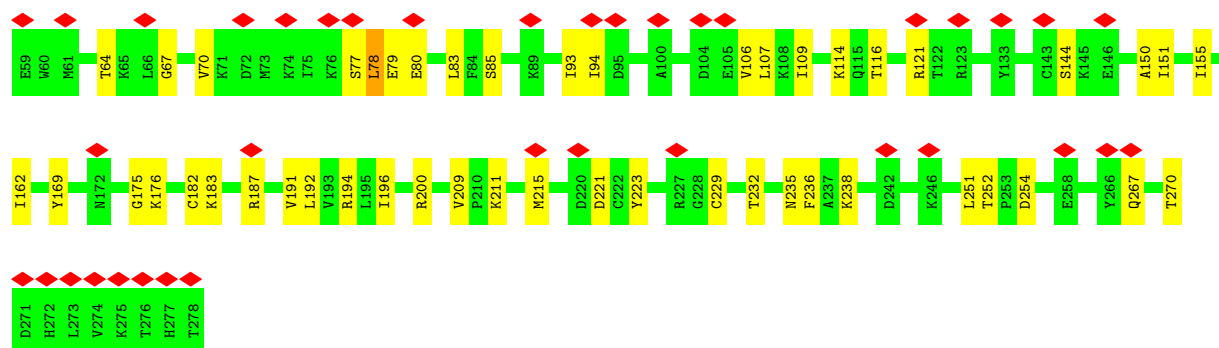
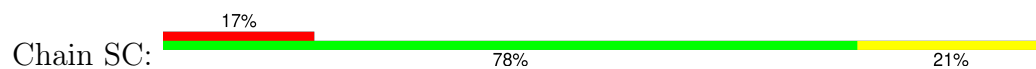


• Molecule 22: Receptor of activated protein C kinase 1

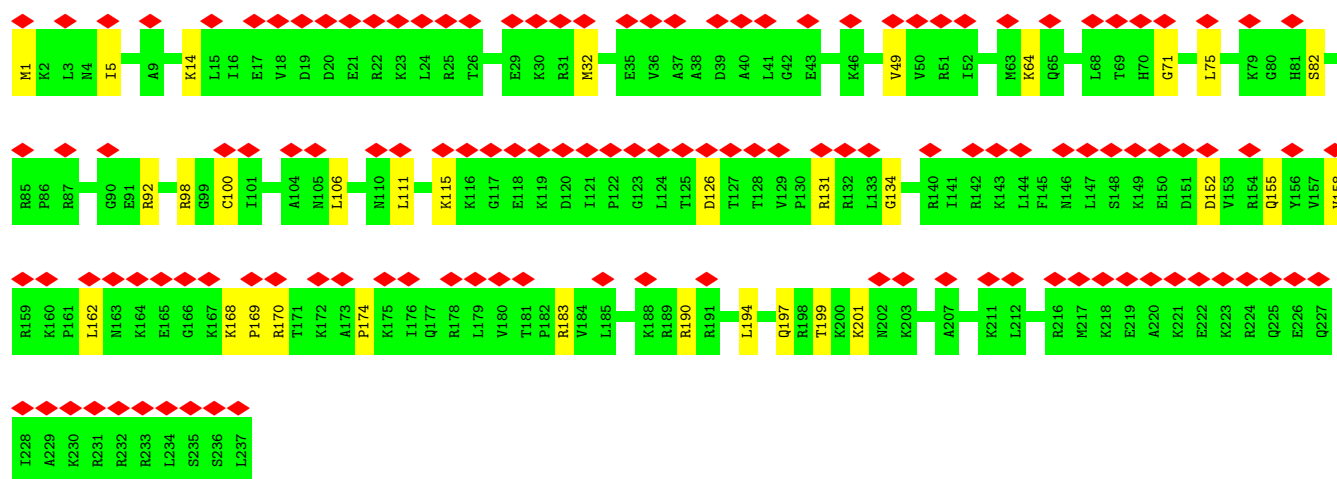
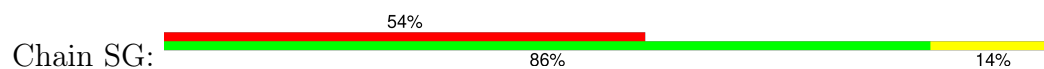




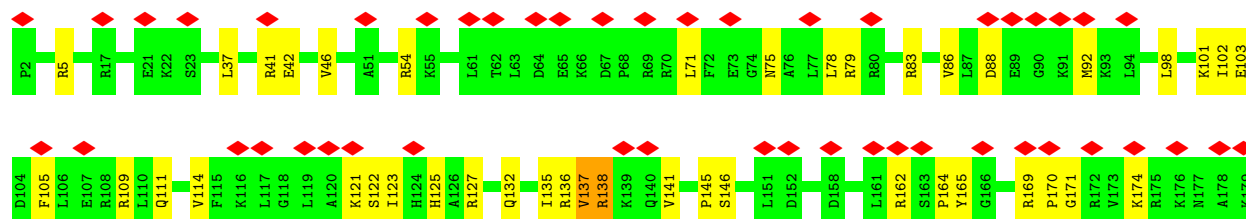
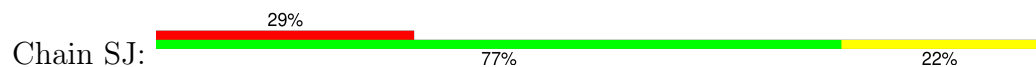
• Molecule 23: 40S ribosomal protein S2

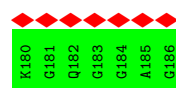


• Molecule 24: 40S ribosomal protein S6

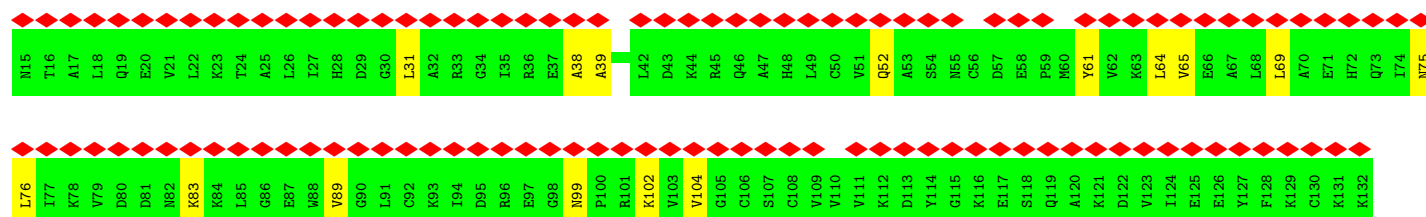
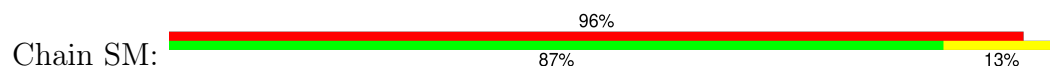


• Molecule 25: 40S ribosomal protein S9

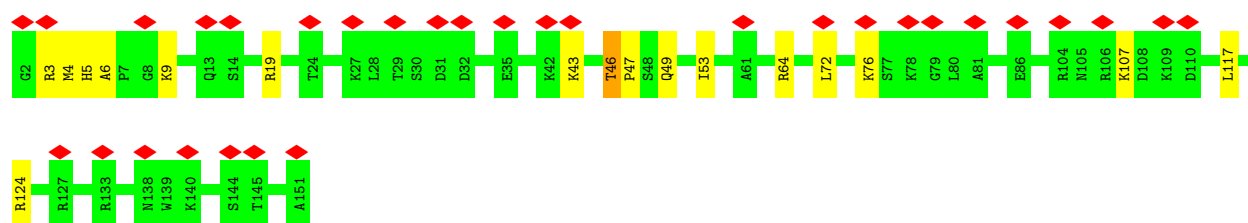
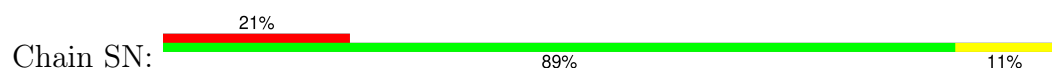




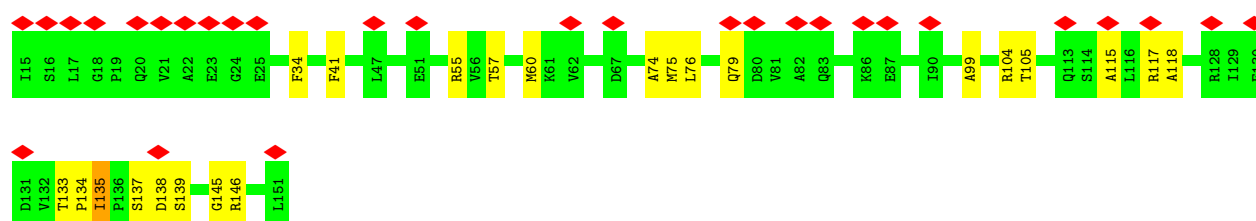
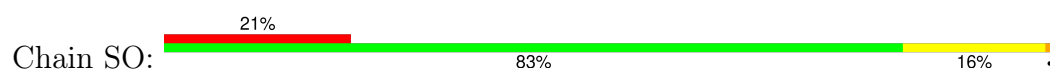
- Molecule 26: 40S ribosomal protein S12



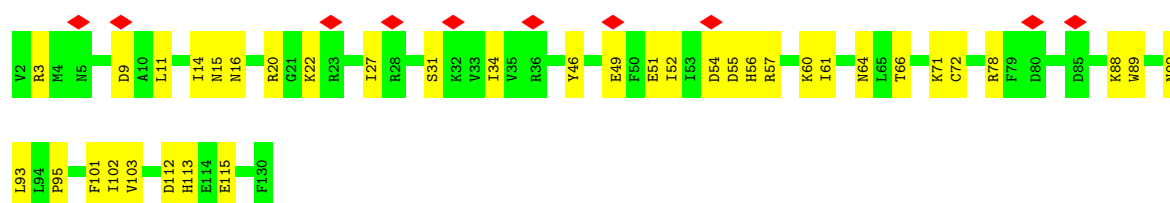
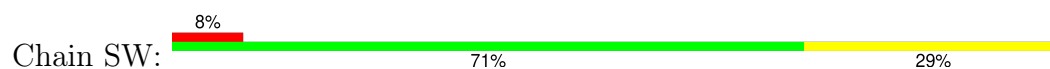
- Molecule 27: 40S ribosomal protein S13



- Molecule 28: 40S ribosomal protein S14

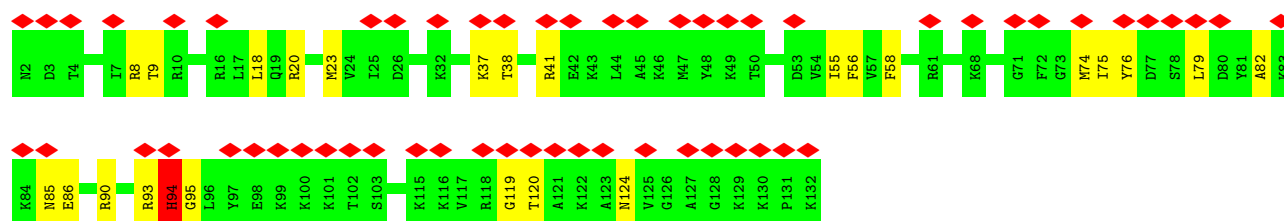


- Molecule 29: 40S ribosomal protein S15a



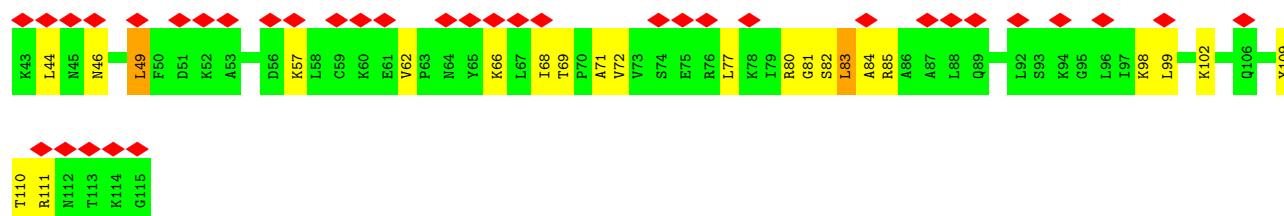
- Molecule 30: 40S ribosomal protein S24

Chain SY: 



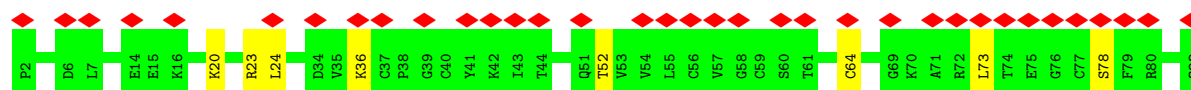
- Molecule 31: 40S ribosomal protein S25

Chain SZ: 

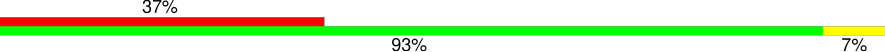


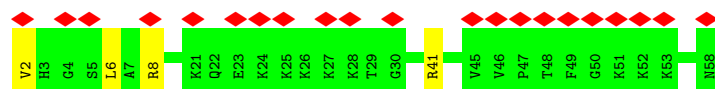
- Molecule 32: 40S ribosomal protein S27

Chain Sb: 



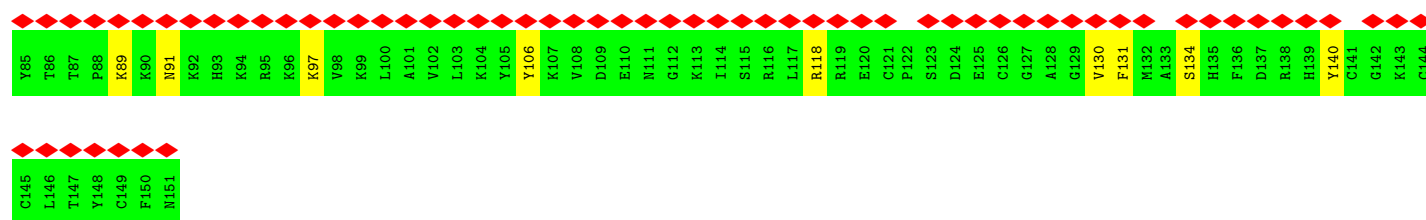
- Molecule 33: 40S ribosomal protein S30

Chain Se: 



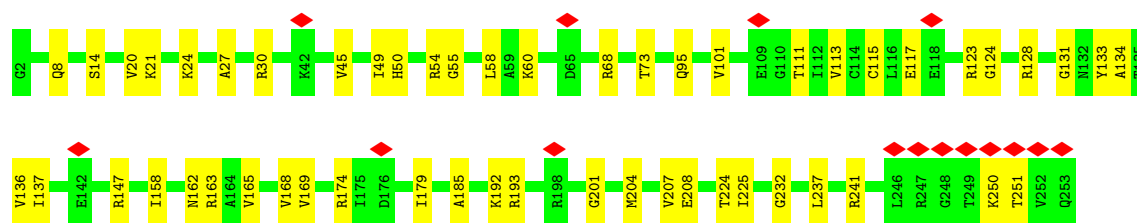
- Molecule 34: 40S ribosomal protein S27a

Chain Sf: 

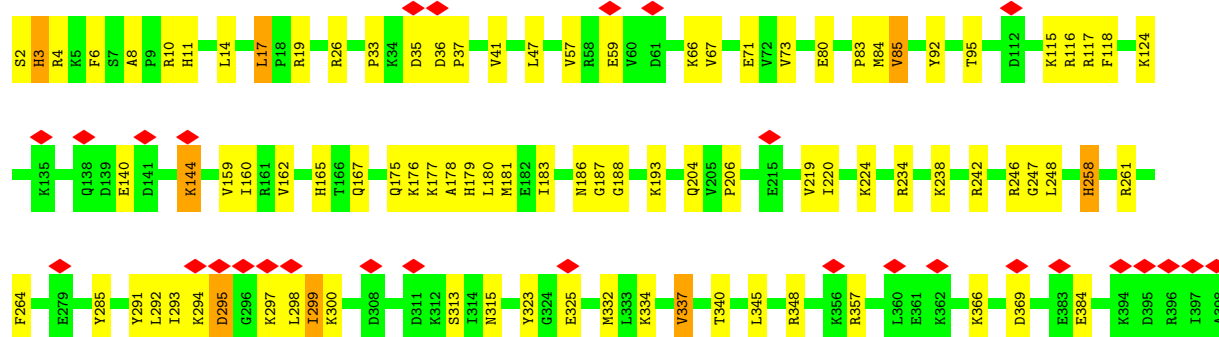
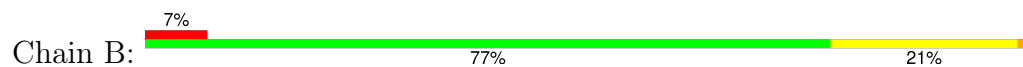


- Molecule 35: 60S ribosomal protein L8

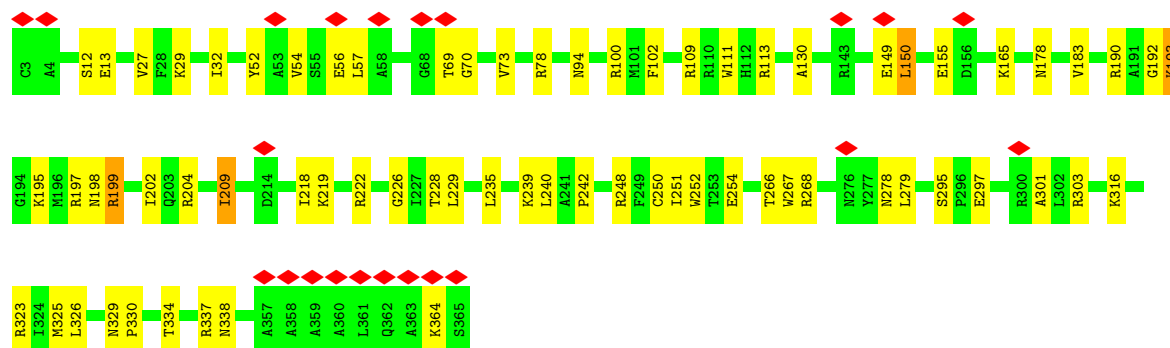
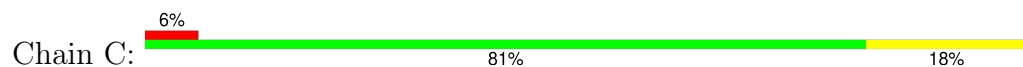
Chain A: 



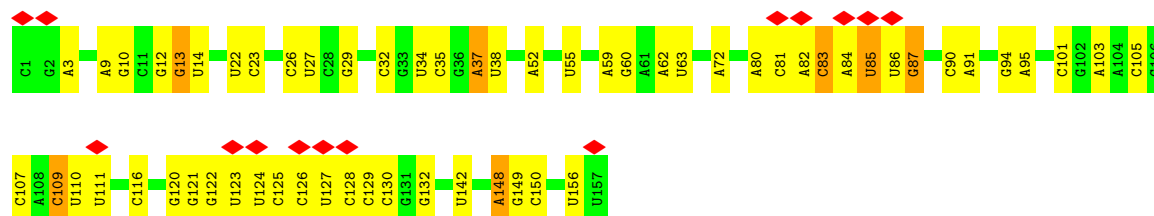
• Molecule 36: 60S ribosomal protein L3



• Molecule 37: 60S ribosomal protein L4

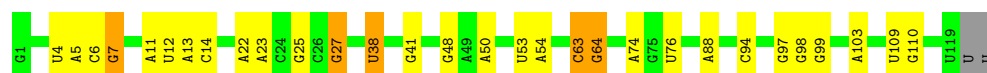


• Molecule 38: 5.8S ribosomal RNA



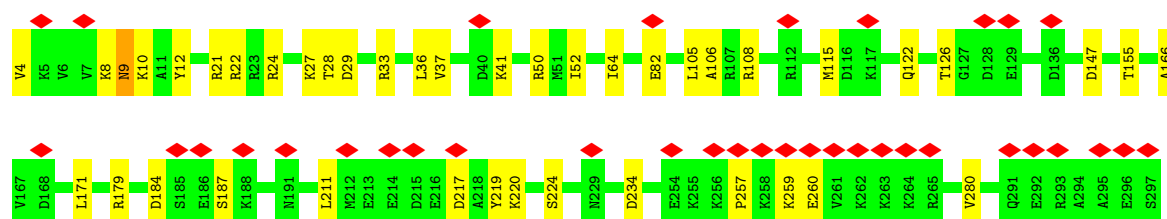
• Molecule 39: 5S ribosomal RNA

Chain E: 



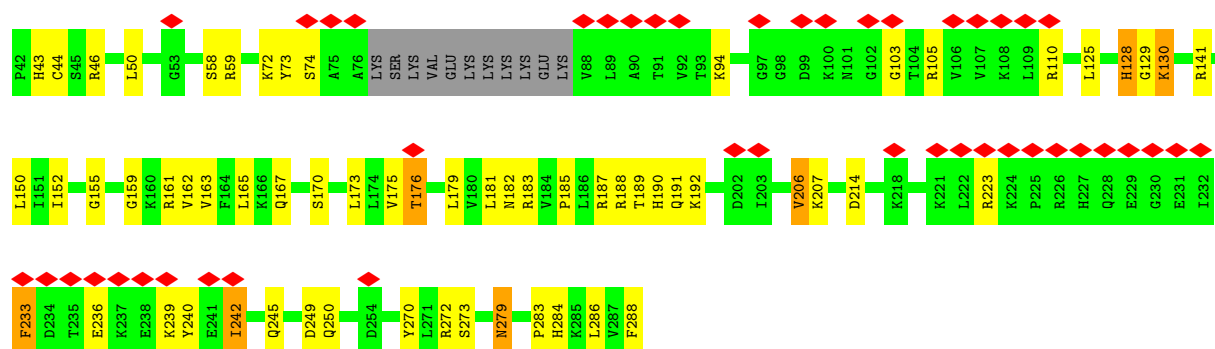
- Molecule 40: 60S ribosomal protein L5

Chain F: 



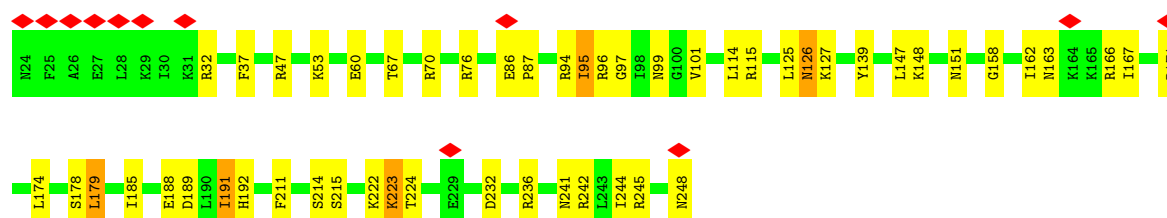
- Molecule 41: 60S ribosomal protein L6

Chain G: 



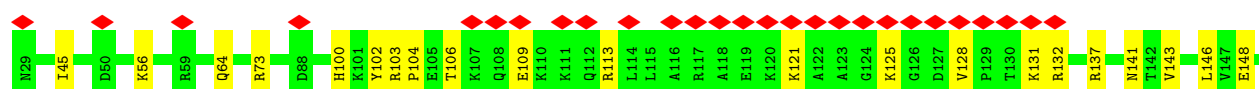
- Molecule 42: 60S ribosomal protein L7

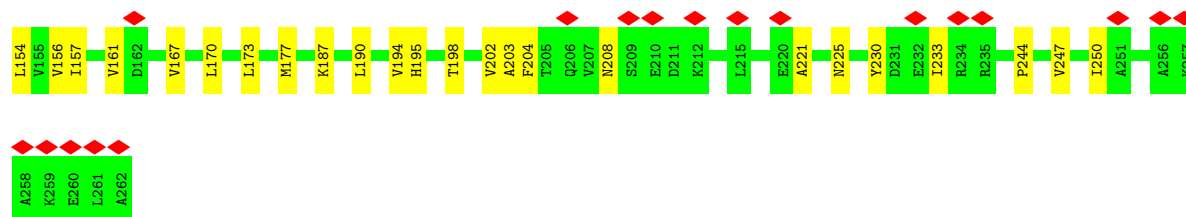
Chain H: 



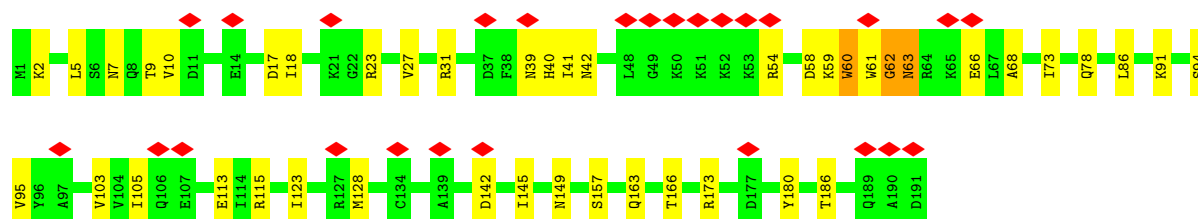
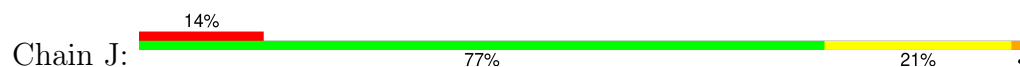
- Molecule 43: 60S ribosomal protein L7a

Chain I: 

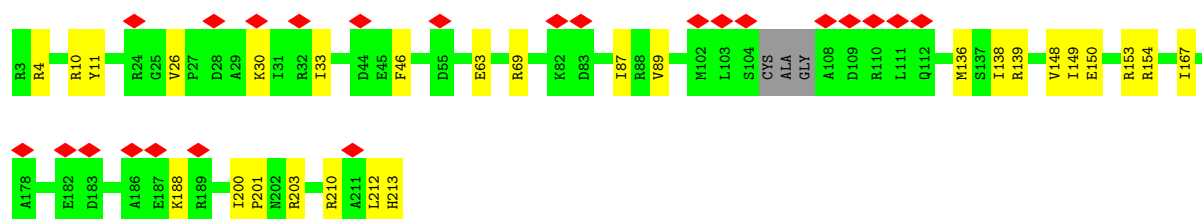
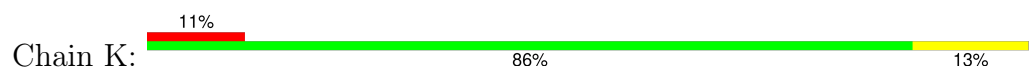




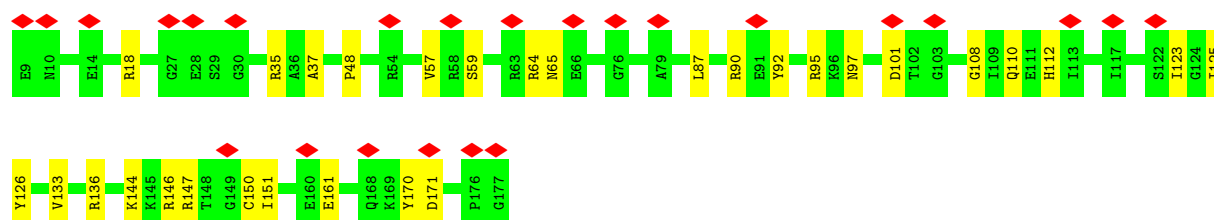
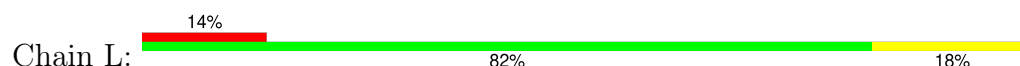
• Molecule 44: 60S ribosomal protein L9



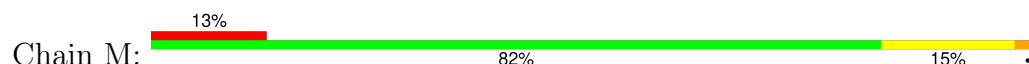
• Molecule 45: 60S ribosomal protein L10

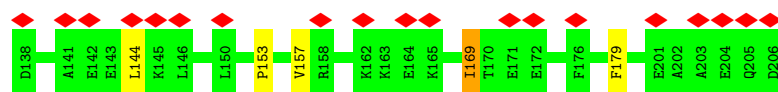


• Molecule 46: 60S ribosomal protein L11

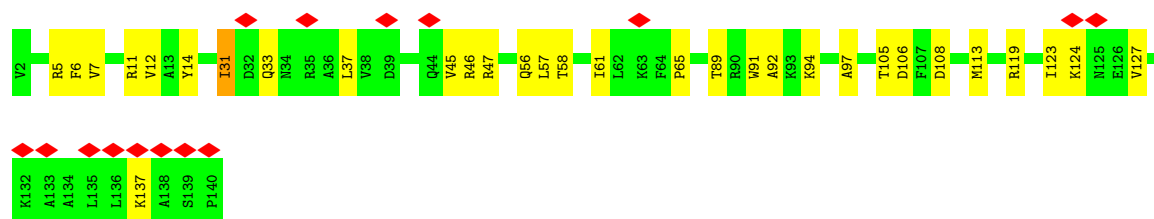
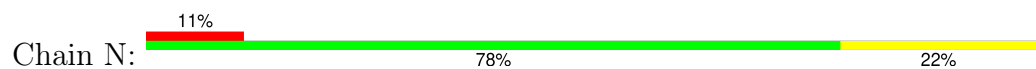


• Molecule 47: 60S ribosomal protein L13

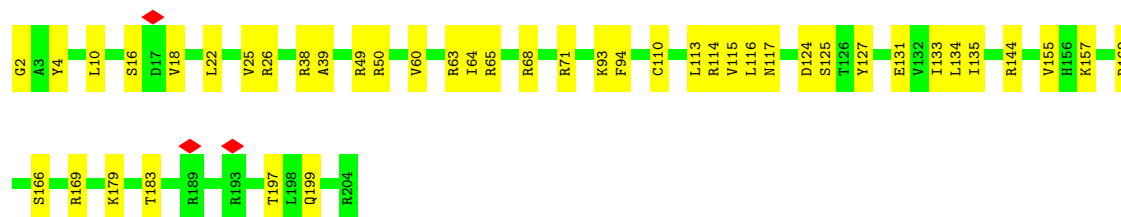
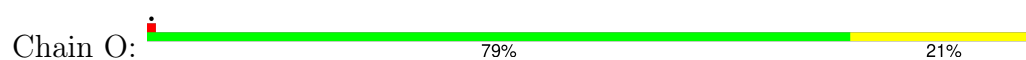




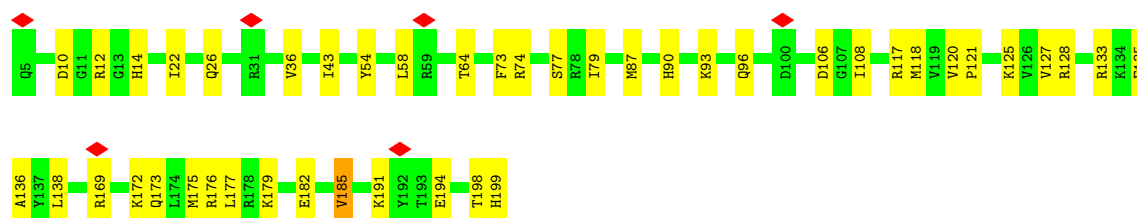
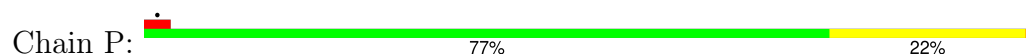
- Molecule 48: 60S ribosomal protein L14



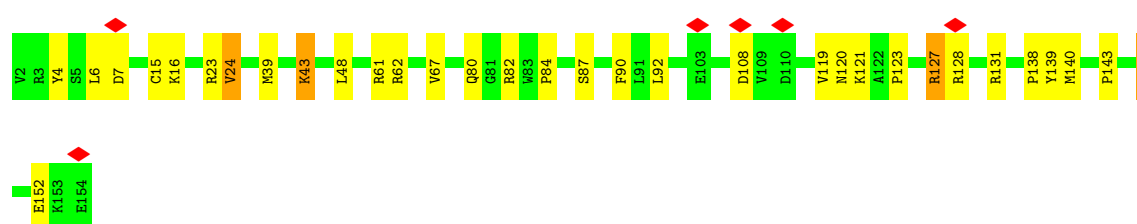
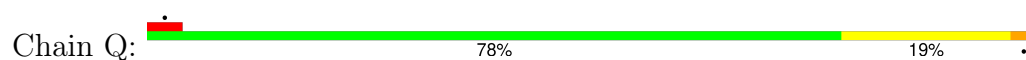
- Molecule 49: 60S ribosomal protein L15



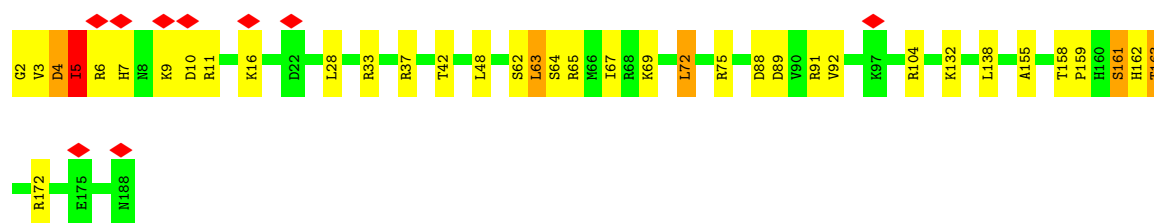
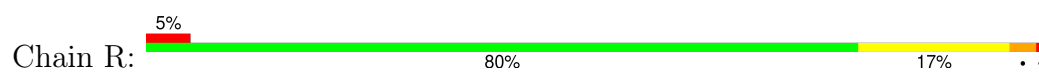
- Molecule 50: 60S ribosomal protein L13a



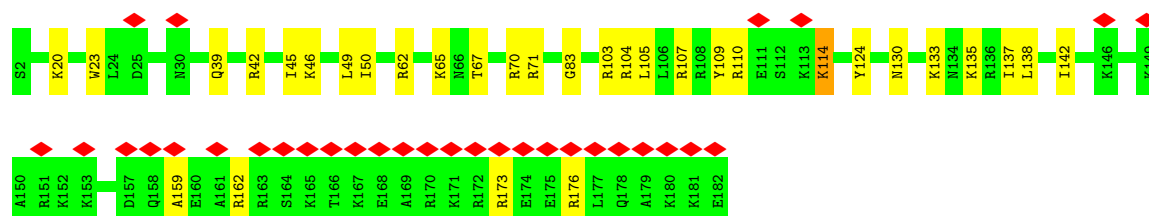
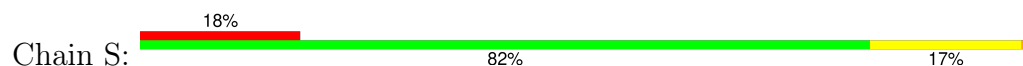
- Molecule 51: 60S ribosomal protein L17



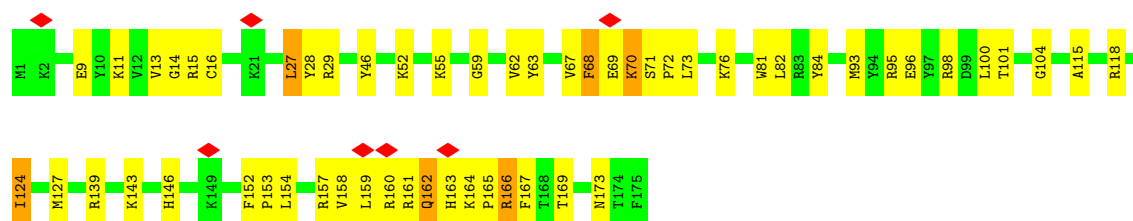
- Molecule 52: 60S ribosomal protein L18



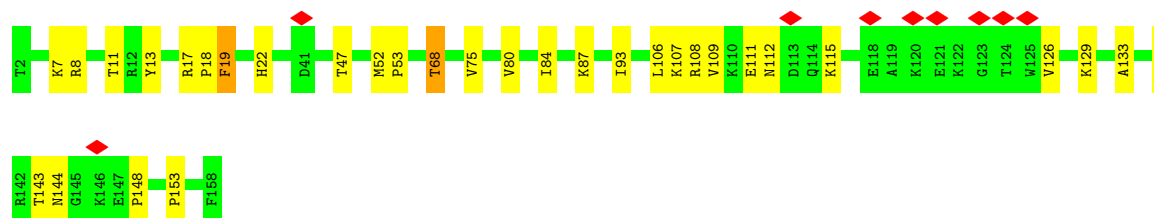
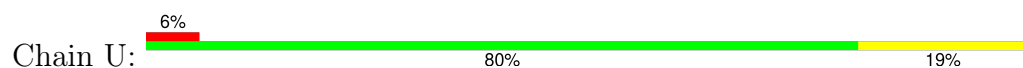
- Molecule 53: 60S ribosomal protein L19



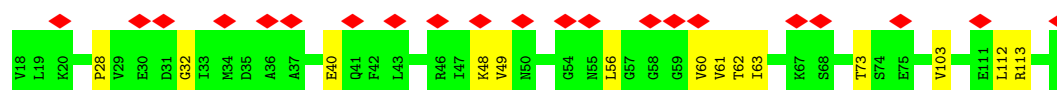
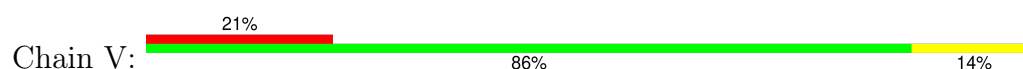
- Molecule 54: 60S ribosomal protein L18a



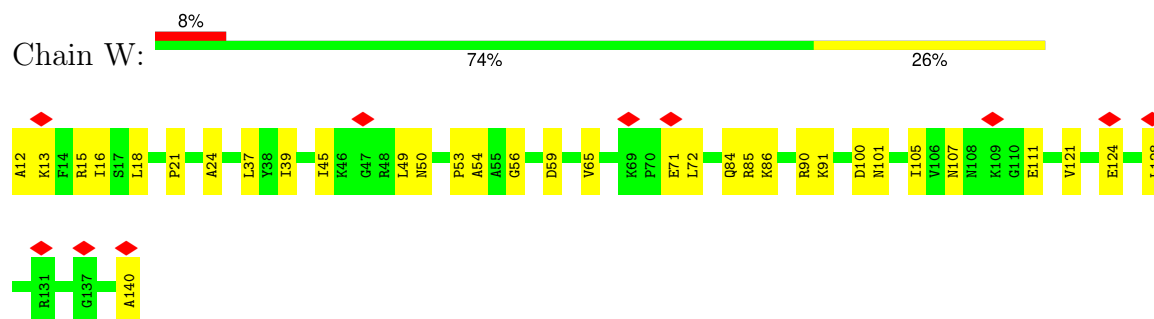
- Molecule 55: 60S ribosomal protein L21



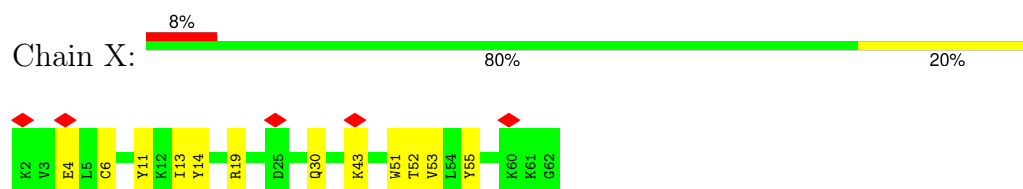
- Molecule 56: 60S ribosomal protein L22



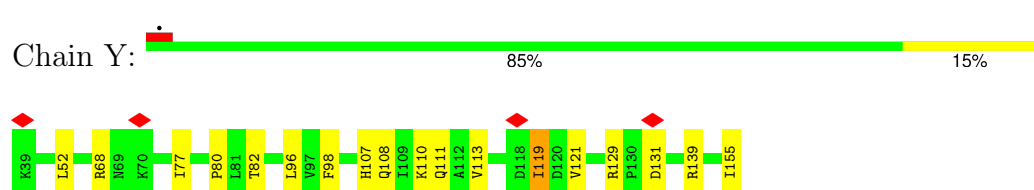
- Molecule 57: 60S ribosomal protein L23



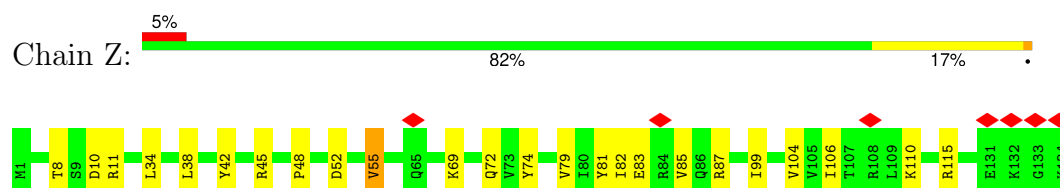
- Molecule 58: 60S ribosomal protein L24



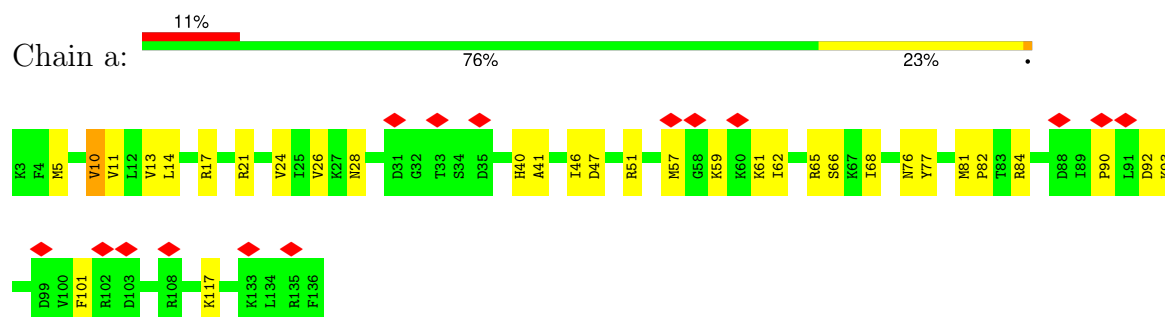
- Molecule 59: 60S ribosomal protein L23a



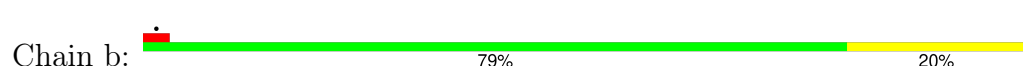
- Molecule 60: 60S ribosomal protein L26

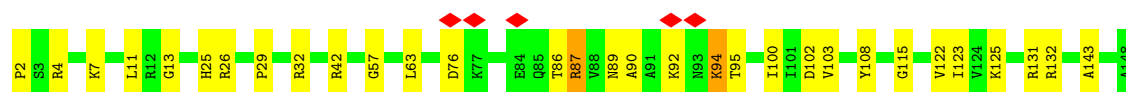


- Molecule 61: 60S ribosomal protein L27

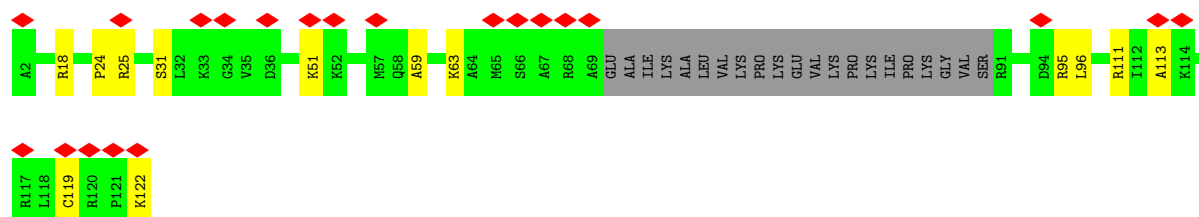


- Molecule 62: 60S ribosomal protein L27a

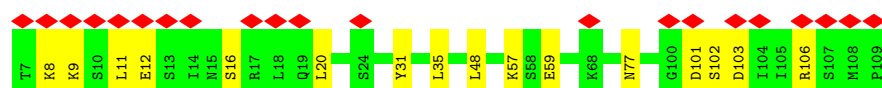
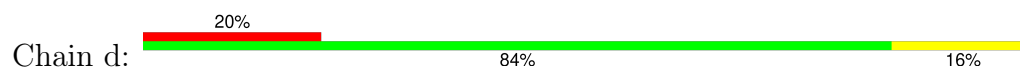




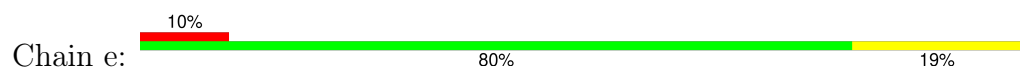
- Molecule 63: 60S ribosomal protein L29



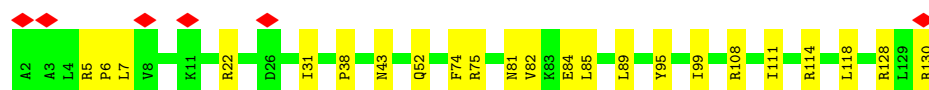
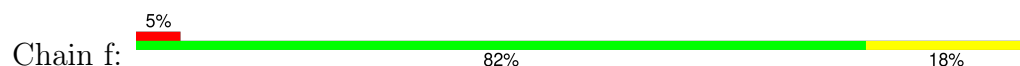
- Molecule 64: 60S ribosomal protein L30



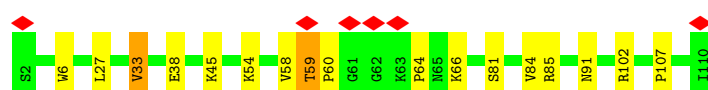
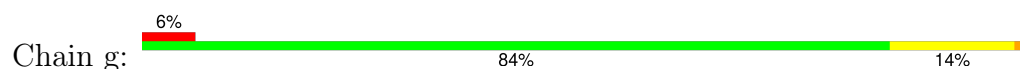
- Molecule 65: 60S ribosomal protein L31



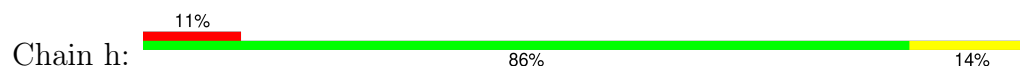
- Molecule 66: 60S ribosomal protein L32



- Molecule 67: 60S ribosomal protein L35a

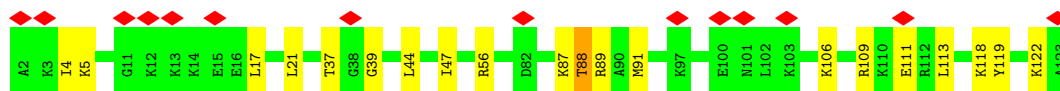
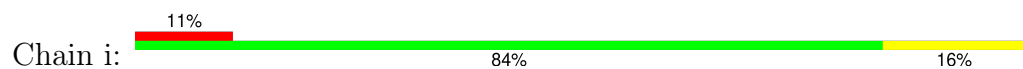


- Molecule 68: 60S ribosomal protein L34

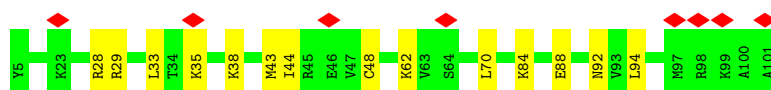
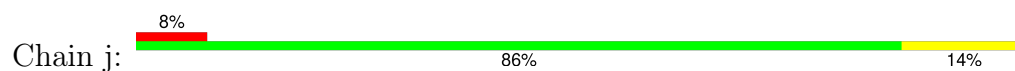




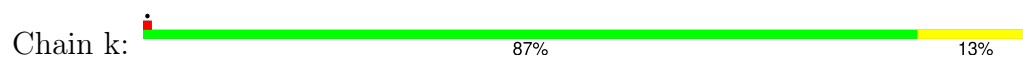
- Molecule 69: 60S ribosomal protein L35



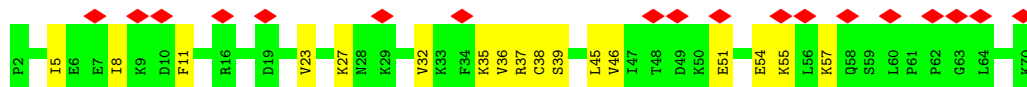
- Molecule 70: 60S ribosomal protein L36



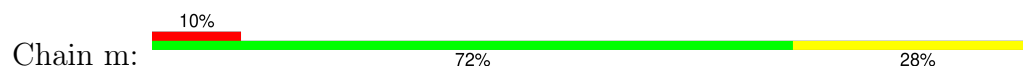
- Molecule 71: 60S ribosomal protein L37



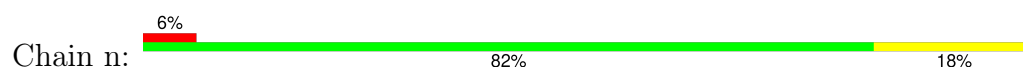
- Molecule 72: 60S ribosomal protein L38



- Molecule 73: 60S ribosomal protein L39



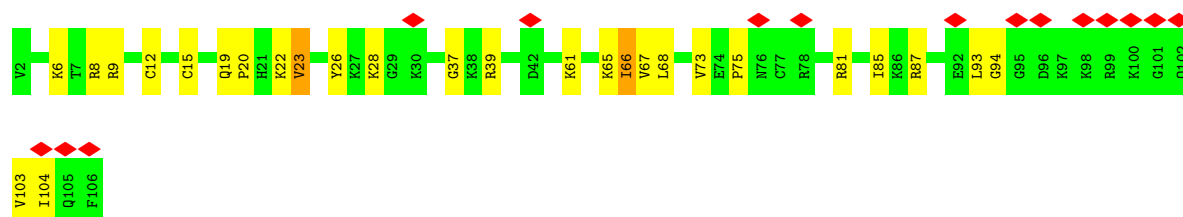
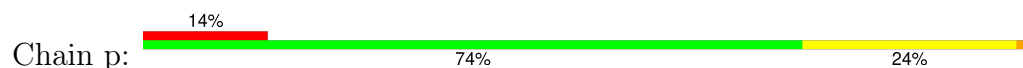
- Molecule 74: 60S ribosomal protein L40



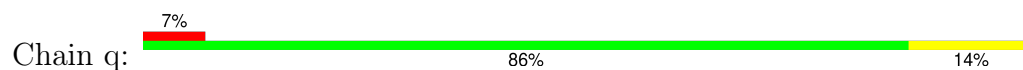
- Molecule 75: 60S ribosomal protein L41



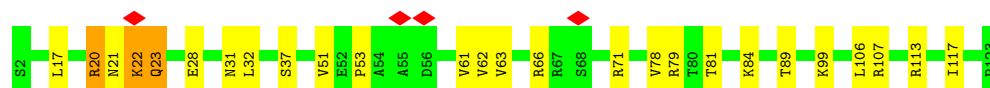
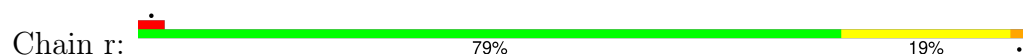
- Molecule 76: 60S ribosomal protein L36a



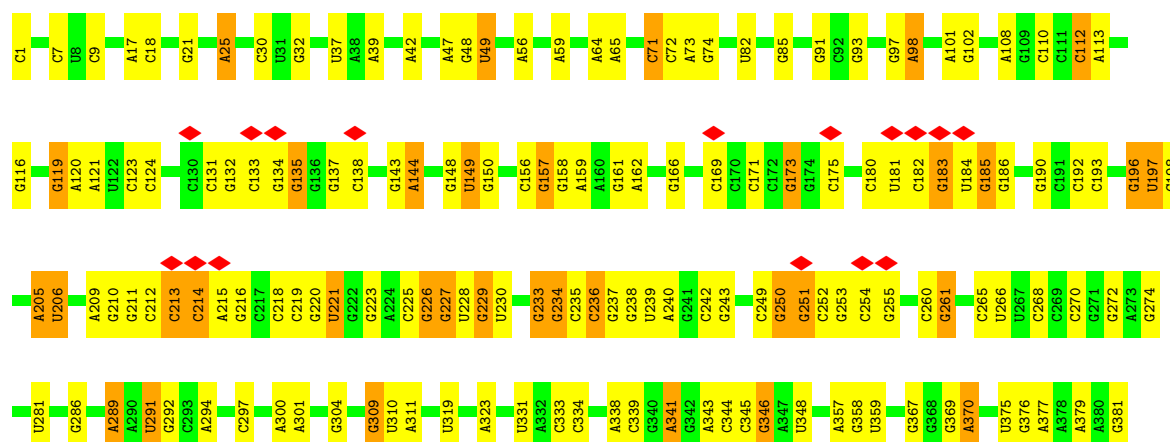
- Molecule 77: 60S ribosomal protein L37a

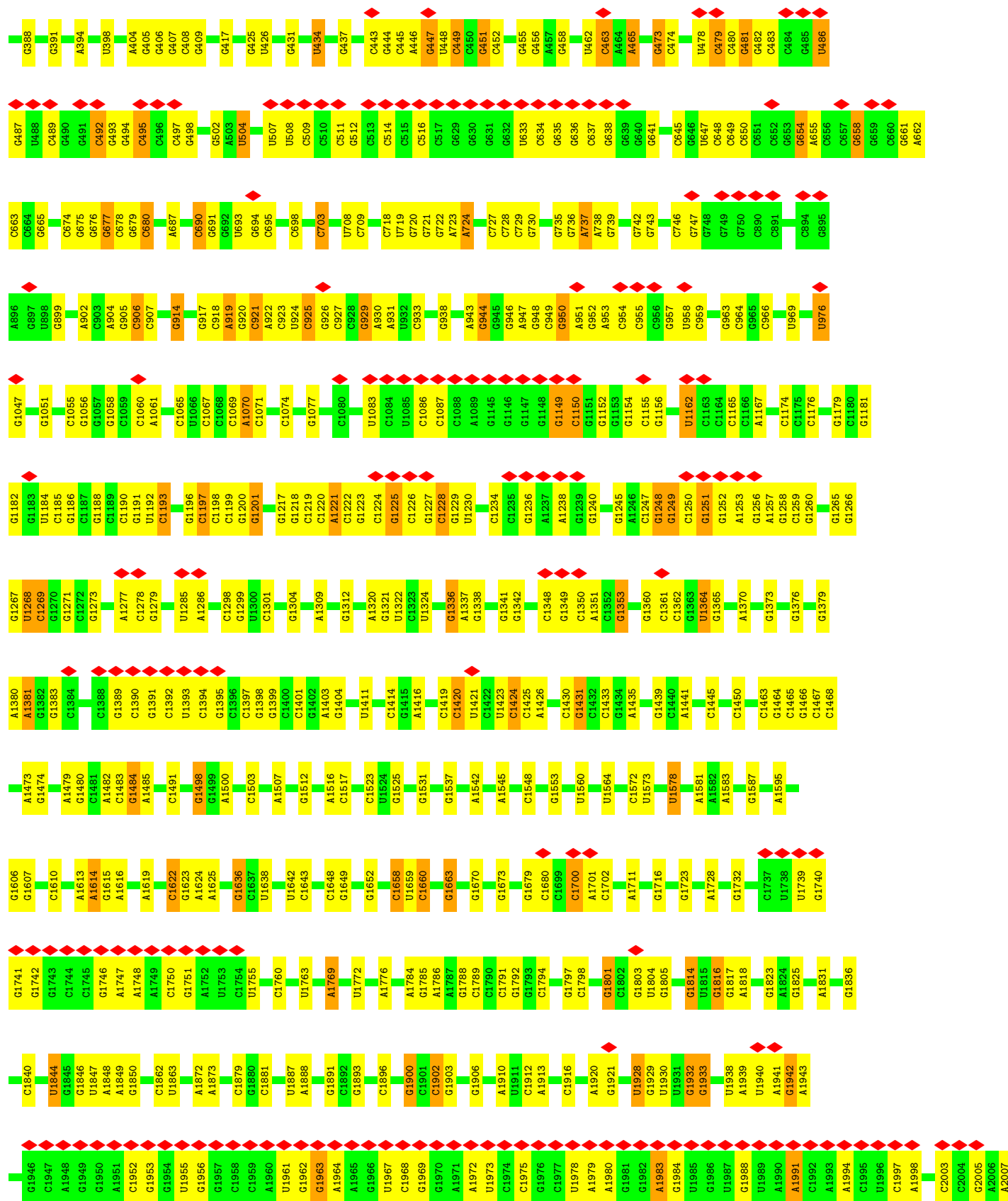


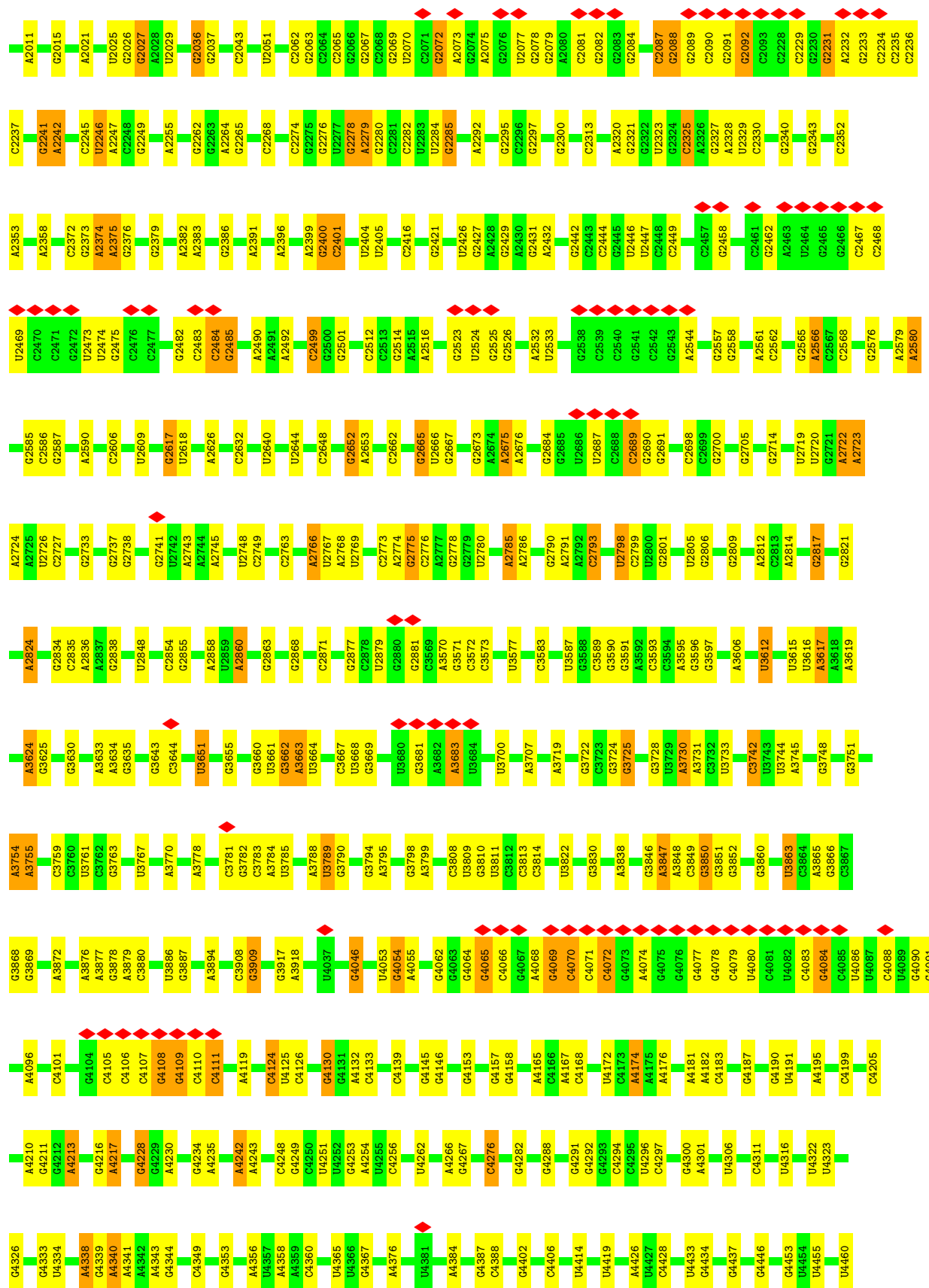
- Molecule 78: 60S ribosomal protein L28

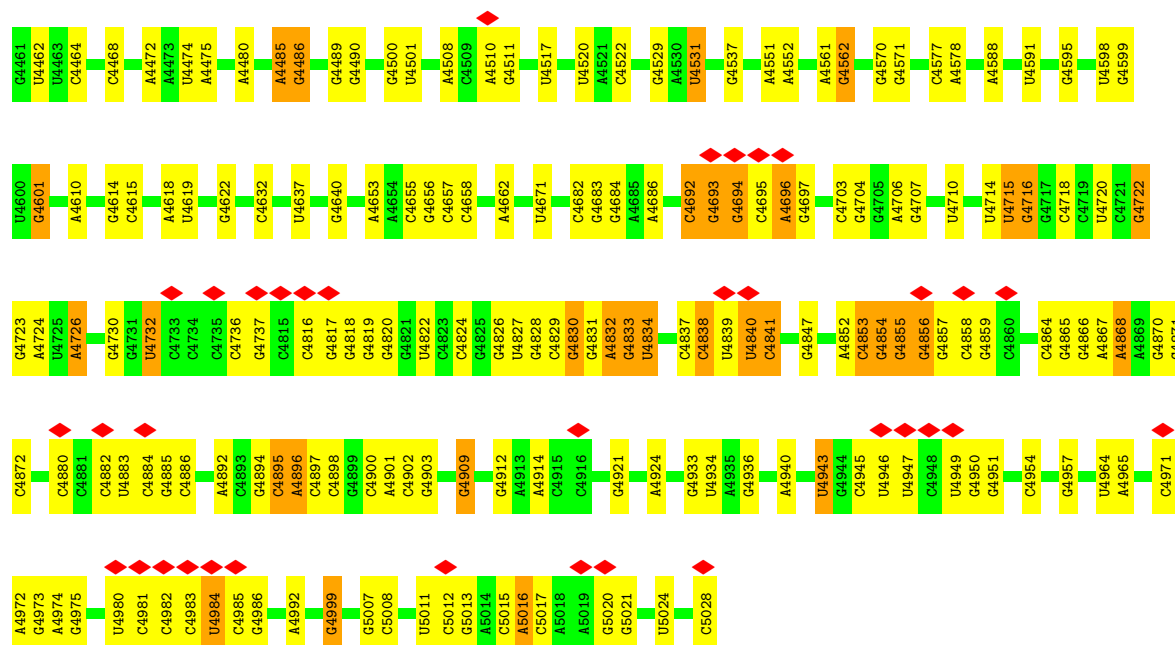


- Molecule 79: 28S ribosomal RNA

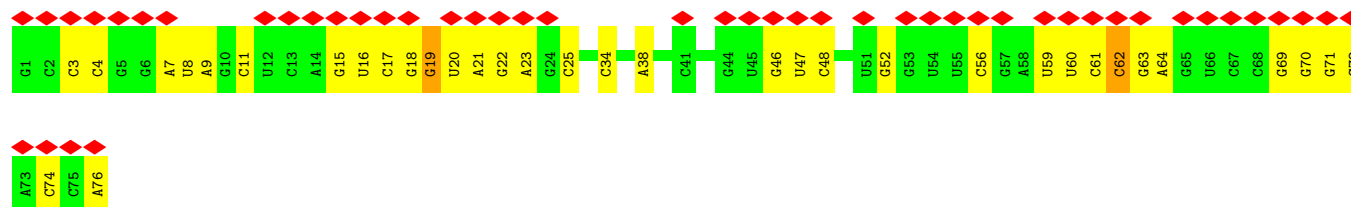




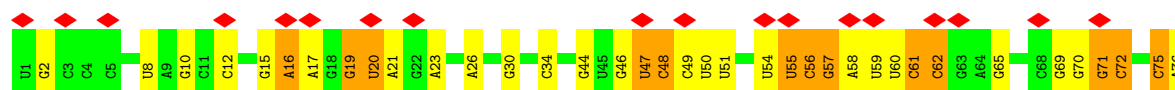




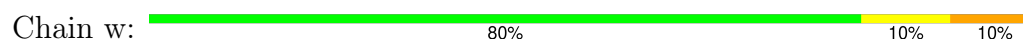
• Molecule 80: tRNA



• Molecule 81: tRNA



• Molecule 82: mRNA



• Molecule 83: Nascent chain



X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39
----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size ($\text{\AA}$)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.15, 1.15, 1.15	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, MA6, A2M, B8N, MG, M7A, OMC, OMG, 4AC, B8Q, 6MZ, PSU, 5MC, OMU, E3C, UR3, 5MU, MVM

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	S2	0.38	0/39959	0.46	3/62253 (0.0%)
2	SA	0.41	0/1778	0.76	0/2416
3	SB	0.39	0/1765	0.71	3/2362 (0.1%)
4	SD	0.37	0/1785	0.73	0/2404
5	SE	0.36	0/2101	0.69	0/2828
6	SF	0.38	0/1516	0.71	0/2037
7	SH	0.42	1/1519 (0.1%)	0.76	1/2033 (0.0%)
8	SI	0.36	0/1702	0.71	0/2271
9	SK	0.44	0/851	0.78	3/1147 (0.3%)
10	SL	0.37	0/1268	0.70	1/1696 (0.1%)
11	SP	0.39	0/1065	0.70	0/1423
12	SQ	0.38	0/1177	0.84	1/1575 (0.1%)
13	SR	0.34	0/1097	0.81	2/1474 (0.1%)
14	SS	0.38	0/1216	0.68	1/1628 (0.1%)
15	ST	0.38	0/1131	0.71	0/1515
16	SU	0.36	0/831	0.77	0/1115
17	SV	0.39	0/631	0.72	0/844
18	SX	0.40	0/1116	0.78	0/1490
19	Sa	0.45	0/836	0.77	0/1121
20	Sc	0.34	0/508	0.76	0/680
21	Sd	0.42	0/470	1.04	4/623 (0.6%)
22	Sg	0.36	1/2486 (0.0%)	0.75	0/3384
23	SC	0.44	0/1755	0.78	3/2371 (0.1%)
24	SG	0.30	0/1946	0.68	0/2590
25	SJ	0.37	0/1561	0.81	1/2083 (0.0%)
26	SM	0.29	0/922	0.66	0/1238
27	SN	0.40	0/1232	0.62	0/1656
28	SO	0.40	0/1037	0.75	0/1391
29	SW	0.47	0/1051	0.70	0/1406
30	SY	0.34	0/1094	0.68	1/1452 (0.1%)
31	SZ	0.37	0/585	0.94	4/785 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.36	0/653	0.69	0/876
33	Se	0.32	0/458	0.78	0/604
34	Sf	0.37	0/560	0.90	2/745 (0.3%)
35	A	0.53	0/1968	0.75	2/2639 (0.1%)
36	B	0.49	0/3270	0.82	2/4377 (0.0%)
37	C	0.56	0/2942	0.83	3/3951 (0.1%)
38	D	0.48	0/3726	0.47	0/5804
39	E	0.44	0/2839	0.42	0/4425
40	F	0.45	0/2437	0.75	4/3262 (0.1%)
41	G	0.47	0/1942	0.94	8/2606 (0.3%)
42	H	0.57	0/1905	0.79	0/2539
43	I	0.47	0/1913	0.73	0/2576
44	J	0.43	0/1545	0.72	2/2077 (0.1%)
45	K	0.45	0/1730	0.73	1/2311 (0.0%)
46	L	0.39	0/1376	0.73	2/1841 (0.1%)
47	M	0.49	0/1688	0.87	3/2260 (0.1%)
48	N	0.47	0/1161	0.75	1/1554 (0.1%)
49	O	0.56	0/1746	0.84	0/2338
50	P	0.49	0/1638	0.73	0/2191
51	Q	0.52	0/1268	0.74	1/1701 (0.1%)
52	R	0.54	0/1537	0.86	4/2052 (0.2%)
53	S	0.47	0/1533	0.75	1/2025 (0.0%)
54	T	0.50	0/1488	0.75	2/1997 (0.1%)
55	U	0.49	0/1312	0.77	1/1753 (0.1%)
56	V	0.38	0/822	0.68	0/1103
57	W	0.50	0/983	0.65	0/1319
58	X	0.49	0/524	0.68	0/698
59	Y	0.46	0/975	0.70	0/1312
60	Z	0.49	0/1132	0.73	2/1504 (0.1%)
61	a	0.45	0/1126	0.77	2/1502 (0.1%)
62	b	0.55	1/1191 (0.1%)	0.85	0/1591
63	c	0.43	0/826	0.80	0/1088
64	d	0.46	0/812	0.75	0/1089
65	e	0.47	0/894	0.79	2/1204 (0.2%)
66	f	0.53	0/1082	0.77	0/1443
67	g	0.57	0/895	0.82	0/1198
68	h	0.47	0/916	0.85	0/1220
69	i	0.47	0/1023	0.79	2/1351 (0.1%)
70	j	0.43	0/805	0.80	0/1065
71	k	0.51	0/703	0.73	0/929
72	l	0.43	0/575	0.67	0/761
73	m	0.52	0/454	0.80	0/599
74	n	0.41	0/417	0.78	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	o	0.41	0/241	0.84	0/305
76	p	0.50	0/877	0.82	2/1156 (0.2%)
77	q	0.51	0/718	0.72	0/953
78	r	0.57	0/995	0.94	3/1334 (0.2%)
79	t	0.46	0/86502	0.48	2/134927 (0.0%)
80	u	0.27	0/1799	0.50	0/2800
81	v	0.32	0/1802	0.49	1/2797 (0.0%)
82	w	0.39	0/235	0.68	0/365
All	All	0.44	3/229950 (0.0%)	0.60	83/337961 (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
25	SJ	0	1
40	F	0	1
47	M	0	1
76	p	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	SH	66	VAL	CA-CB	7.13	1.58	1.53
22	Sg	283	PRO	CA-C	-5.94	1.48	1.52
62	b	132	ARG	NE-CZ	-5.22	1.27	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	G	129	GLY	N-CA-C	10.27	125.05	112.73
52	R	5	ILE	N-CA-C	-9.33	96.53	108.84
21	Sd	23	VAL	N-CA-C	9.10	119.91	110.72
41	G	128	HIS	N-CA-C	9.04	121.22	111.36
31	SZ	84	ALA	N-CA-C	-8.31	102.22	111.28
30	SY	94	HIS	N-CA-C	-8.01	95.46	108.52
3	SB	189	ILE	CA-C-N	7.85	127.41	118.85
3	SB	189	ILE	C-N-CA	7.85	127.41	118.85
13	SR	121	GLN	CA-C-N	7.63	128.22	120.14
13	SR	121	GLN	C-N-CA	7.63	128.22	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	G	233	PHE	CA-C-N	7.47	135.80	121.54
41	G	233	PHE	C-N-CA	7.47	135.80	121.54
54	T	166	ARG	N-CA-C	-7.24	103.39	111.28
31	SZ	83	LEU	N-CA-C	-7.19	104.64	113.41
55	U	80	VAL	N-CA-C	-7.04	99.74	109.46
41	G	130	LYS	N-CA-C	7.02	120.66	110.28
52	R	6	ARG	N-CA-C	6.94	119.79	110.35
9	SK	62	PHE	N-CA-C	6.83	120.81	111.39
25	SJ	137	VAL	N-CA-C	-6.73	100.17	109.46
37	C	150	LEU	CA-C-N	-6.72	111.44	119.84
37	C	150	LEU	C-N-CA	-6.72	111.44	119.84
34	Sf	91	ASN	CA-C-N	6.59	134.13	121.54
34	Sf	91	ASN	C-N-CA	6.59	134.13	121.54
53	S	114	LYS	N-CA-C	6.56	118.43	111.28
7	SH	15	LYS	N-CA-C	6.53	122.43	113.16
44	J	62	GLY	N-CA-C	6.50	120.62	111.00
79	t	3595	A	C2'-C3'-O3'	6.40	119.11	109.50
47	M	78	LEU	N-CA-C	6.35	118.20	111.28
9	SK	61	GLN	N-CA-C	6.19	122.73	114.12
23	SC	78	LEU	CA-CB-CG	6.18	137.93	116.30
52	R	11	ARG	N-CA-C	6.16	118.99	109.07
52	R	161	SER	N-CA-C	6.11	117.61	111.07
21	Sd	41	GLN	N-CA-C	-6.04	104.78	111.36
12	SQ	19	ALA	N-CA-C	5.91	117.83	108.79
40	F	9	ASN	CA-C-N	5.80	132.62	121.54
40	F	9	ASN	C-N-CA	5.80	132.62	121.54
45	K	10	ARG	N-CA-C	-5.75	98.54	110.80
44	J	60	TRP	N-CA-C	5.73	117.60	111.36
3	SB	188	LEU	N-CA-C	5.69	117.49	111.28
14	SS	82	TRP	CA-CB-CG	5.69	124.42	113.60
69	i	87	LYS	CA-C-N	5.67	132.37	121.54
69	i	87	LYS	C-N-CA	5.67	132.37	121.54
36	B	17	LEU	N-CA-C	5.58	120.51	113.25
65	e	94	GLU	CA-C-N	5.50	130.62	122.82
65	e	94	GLU	C-N-CA	5.50	130.62	122.82
47	M	63	THR	CA-C-N	5.49	131.84	121.97
47	M	63	THR	C-N-CA	5.49	131.84	121.97
23	SC	251	LEU	CA-C-N	5.46	139.26	122.71
23	SC	251	LEU	C-N-CA	5.46	139.26	122.71
37	C	57	LEU	N-CA-C	-5.44	104.29	111.96
76	p	75	PRO	CA-C-N	5.44	131.93	121.54
76	p	75	PRO	C-N-CA	5.44	131.93	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	SL	18	GLN	N-CA-C	5.43	117.28	111.36
78	r	20	ARG	CA-C-N	5.33	131.72	121.54
78	r	20	ARG	C-N-CA	5.33	131.72	121.54
21	Sd	3	HIS	CA-C-N	5.32	129.20	120.63
21	Sd	3	HIS	C-N-CA	5.32	129.20	120.63
35	A	250	LYS	CA-C-N	5.31	130.89	122.61
35	A	250	LYS	C-N-CA	5.31	130.89	122.61
54	T	27	LEU	CA-CB-CG	5.31	134.88	116.30
1	S2	1815	A	P-O3'-C3'	5.30	128.15	120.20
46	L	170	TYR	CA-C-N	5.27	131.60	121.54
46	L	170	TYR	C-N-CA	5.27	131.60	121.54
61	a	101	PHE	CA-C-N	5.26	135.12	126.86
61	a	101	PHE	C-N-CA	5.26	135.12	126.86
41	G	242	ILE	N-CA-C	-5.21	106.80	112.80
9	SK	60	GLU	N-CA-C	5.20	117.29	109.23
41	G	206	VAL	CA-C-N	5.19	131.46	121.54
41	G	206	VAL	C-N-CA	5.19	131.46	121.54
79	t	3595	A	P-O3'-C3'	5.18	127.97	120.20
81	v	61	C	C2-N1-C1'	5.18	134.33	118.80
60	Z	42	TYR	CA-C-N	5.16	131.40	121.54
60	Z	42	TYR	C-N-CA	5.16	131.40	121.54
36	B	258	HIS	N-CA-C	5.16	121.22	109.81
48	N	31	ILE	CA-CB-CG1	5.10	119.08	110.40
31	SZ	49	LEU	CA-C-N	5.10	128.91	121.31
31	SZ	49	LEU	C-N-CA	5.10	128.91	121.31
1	S2	1813	A	C2'-C3'-O3'	5.08	117.12	109.50
40	F	259	LYS	CA-C-N	5.05	131.19	121.54
40	F	259	LYS	C-N-CA	5.05	131.19	121.54
1	S2	559	G	P-O3'-C3'	5.05	127.78	120.20
51	Q	6	LEU	CA-CB-CG	5.04	133.94	116.30
78	r	106	LEU	CA-CB-CG	5.02	133.88	116.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	F	257	PRO	Peptide
47	M	130	LYS	Peptide
25	SJ	137	VAL	Peptide
76	p	103	VAL	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	S2	36501	0	18404	325	0
2	SA	1741	0	1746	39	0
3	SB	1738	0	1809	61	0
4	SD	1757	0	1853	24	0
5	SE	2059	0	2164	38	0
6	SF	1495	0	1549	25	0
7	SH	1497	0	1587	39	0
8	SI	1673	0	1756	24	0
9	SK	827	0	852	65	0
10	SL	1247	0	1323	28	0
11	SP	1045	0	1095	44	0
12	SQ	1158	0	1232	59	0
13	SR	1082	0	1137	36	0
14	SS	1198	0	1261	18	0
15	ST	1112	0	1146	11	0
16	SU	821	0	883	14	0
17	SV	625	0	628	8	0
18	SX	1098	0	1167	32	0
19	Sa	821	0	870	17	0
20	Sc	506	0	536	15	0
21	Sd	459	0	448	46	0
22	Sg	2429	0	2386	55	0
23	SC	1715	0	1804	32	0
24	SG	1923	0	2089	23	0
25	SJ	1533	0	1653	26	0
26	SM	912	0	930	10	0
27	SN	1208	0	1294	13	0
28	SO	1024	0	1050	16	0
29	SW	1034	0	1080	27	0
30	SY	1073	0	1155	39	0
31	SZ	579	0	639	17	0
32	Sb	640	0	665	5	0
33	Se	452	0	498	2	0
34	Sf	548	0	552	9	0
35	A	1930	0	2030	29	0
36	B	3202	0	3343	98	0
37	C	2888	0	3064	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	D	3337	0	1692	26	0
39	E	2541	0	1285	12	0
40	F	2392	0	2425	26	0
41	G	1904	0	2055	78	0
42	H	1870	0	1996	40	0
43	I	1880	0	2018	28	0
44	J	1526	0	1605	52	0
45	K	1692	0	1744	14	0
46	L	1353	0	1386	16	0
47	M	1657	0	1764	24	0
48	N	1138	0	1204	32	0
49	O	1701	0	1749	32	0
50	P	1606	0	1745	33	0
51	Q	1242	0	1269	26	0
52	R	1513	0	1628	51	0
53	S	1517	0	1670	27	0
54	T	1449	0	1492	86	0
55	U	1284	0	1352	33	0
56	V	808	0	831	13	0
57	W	969	0	1031	22	0
58	X	511	0	521	8	0
59	Y	958	0	1029	10	0
60	Z	1115	0	1205	13	0
61	a	1103	0	1179	17	0
62	b	1162	0	1213	26	0
63	c	814	0	880	12	0
64	d	801	0	845	14	0
65	e	879	0	924	15	0
66	f	1064	0	1160	19	0
67	g	876	0	912	9	0
68	h	906	0	1002	13	0
69	i	1015	0	1148	14	0
70	j	794	0	870	10	0
71	k	689	0	717	8	0
72	l	569	0	637	9	0
73	m	444	0	483	11	0
74	n	411	0	443	8	0
75	o	240	0	289	6	0
76	p	863	0	931	19	0
77	q	708	0	757	9	0
78	r	980	0	1041	15	0
79	t	77332	0	39076	499	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	u	1613	0	822	6	0
81	v	1618	0	826	13	0
82	w	213	0	109	1	0
83	y	178	0	36	1	0
84	B	1	0	0	0	0
84	D	7	0	0	0	0
84	E	9	0	0	0	0
84	O	1	0	0	0	0
84	S2	2	0	0	0	0
84	b	1	0	0	0	0
84	o	1	0	0	0	0
84	t	9	0	0	0	0
85	S2	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sf	1	0	0	0	0
85	k	1	0	0	0	0
85	p	1	0	0	0	0
85	q	1	0	0	0	0
86	t	31	0	0	0	0
87	S2	5	0	0	1	0
87	SC	1	0	0	0	0
87	SJ	1	0	0	0	0
87	SP	1	0	0	0	0
87	SQ	1	0	0	0	0
87	SR	1	0	0	0	0
87	SS	1	0	0	0	0
87	Sb	1	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	1	0
All	All	214867	0	158674	2272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2272) 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)
41:G:165:LEU:HD11	41:G:176:THR:CG2	1.16	1.61
52:R:7:HIS:CE1	79:t:1648:C:H5''	1.09	1.61
1:S2:814:5MU:C4	1:S2:814:5MU:C5	1.81	1.61
41:G:165:LEU:CG	41:G:176:THR:HG22	1.12	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R:7:HIS:HE1	79:t:1648:C:C5'	1.12	1.55
41:G:165:LEU:CD1	41:G:176:THR:HG22	1.25	1.54
36:B:291:TYR:CA	36:B:298:LEU:HD21	1.37	1.51
41:G:165:LEU:CD1	41:G:176:THR:CG2	1.76	1.50
41:G:165:LEU:HD11	41:G:176:THR:CB	1.36	1.50
54:T:160:ARG:HD3	54:T:163:HIS:CD2	1.43	1.50
1:S2:1109:C:H2'	13:SR:124:VAL:CG2	1.44	1.48
12:SQ:16:LYS:CE	12:SQ:82:TYR:HB2	1.41	1.46
12:SQ:16:LYS:HE2	12:SQ:82:TYR:CB	1.45	1.46
3:SB:185:VAL:CG2	3:SB:188:LEU:HD11	1.41	1.46
3:SB:185:VAL:HG23	3:SB:188:LEU:CD1	1.49	1.40
41:G:165:LEU:CG	41:G:176:THR:CG2	1.91	1.38
36:B:291:TYR:HA	36:B:298:LEU:CD2	1.56	1.36
62:b:89:ASN:OD1	62:b:92:LYS:CE	1.77	1.31
41:G:165:LEU:CD2	41:G:176:THR:CG2	2.07	1.31
41:G:165:LEU:HD21	41:G:176:THR:CG2	1.58	1.31
12:SQ:16:LYS:CE	12:SQ:82:TYR:CB	2.03	1.30
36:B:298:LEU:O	36:B:299:ILE:HG13	1.17	1.30
44:J:60:TRP:CE3	54:T:153:PRO:HD3	1.64	1.29
1:S2:1672:U:OP1	12:SQ:18:THR:HB	1.26	1.29
69:i:44:LEU:O	69:i:47:ILE:HG22	1.23	1.27
54:T:164:LYS:HG2	54:T:165:PRO:CD	1.64	1.27
52:R:7:HIS:CE1	79:t:1648:C:C5'	1.95	1.27
12:SQ:16:LYS:HE2	12:SQ:82:TYR:CG	1.69	1.26
62:b:89:ASN:OD1	62:b:92:LYS:HE3	1.07	1.25
44:J:60:TRP:CE3	54:T:153:PRO:CD	2.22	1.23
30:SY:56:PHE:CE1	30:SY:94:HIS:CE1	2.28	1.20
1:S2:1648:G:C8	12:SQ:17:LYS:HD3	1.77	1.19
1:S2:1495:G:H22	21:Sd:24:CYS:CB	1.54	1.18
1:S2:1194:A:OP1	18:SX:60:LYS:NZ	1.75	1.17
11:SP:17:TYR:OH	11:SP:18:ARG:NH2	1.77	1.17
11:SP:17:TYR:CE2	11:SP:18:ARG:NE	2.13	1.17
54:T:160:ARG:CD	54:T:163:HIS:CD2	2.28	1.17
30:SY:56:PHE:HE1	30:SY:94:HIS:CE1	1.63	1.15
41:G:165:LEU:CD2	41:G:176:THR:HG21	1.72	1.15
1:S2:1495:G:N2	21:Sd:24:CYS:HB2	1.62	1.14
54:T:160:ARG:CD	54:T:163:HIS:HD2	1.60	1.14
54:T:160:ARG:HG2	54:T:163:HIS:HB3	1.19	1.14
1:S2:1109:C:C2'	13:SR:124:VAL:CG2	2.27	1.13
41:G:165:LEU:HD11	41:G:176:THR:HB	1.25	1.13
1:S2:1648:G:N7	12:SQ:17:LYS:HD3	1.61	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:60:TRP:CZ3	54:T:152:PHE:HA	1.85	1.12
11:SP:17:TYR:HE2	11:SP:18:ARG:NE	1.44	1.12
4:SD:28:GLU:HA	9:SK:61:GLN:HE22	1.12	1.10
10:SL:22:ARG:O	10:SL:23:VAL:HG13	1.51	1.09
2:SA:89:LYS:HD3	2:SA:202:TYR:CD1	1.88	1.09
1:S2:1109:C:O2	13:SR:124:VAL:O	1.72	1.08
1:S2:1497:G:C8	9:SK:62:PHE:CE2	2.42	1.08
41:G:165:LEU:HD21	41:G:176:THR:HG21	1.17	1.08
55:U:17:ARG:NH1	55:U:47:THR:CG2	2.16	1.07
36:B:291:TYR:HB3	36:B:298:LEU:HD11	1.37	1.07
1:S2:1495:G:H22	21:Sd:24:CYS:HB2	0.90	1.07
54:T:164:LYS:HG2	54:T:165:PRO:HD3	1.09	1.06
4:SD:28:GLU:CA	9:SK:61:GLN:HE22	1.67	1.06
41:G:165:LEU:HG	41:G:176:THR:HG22	1.13	1.06
12:SQ:16:LYS:HE3	12:SQ:82:TYR:HB2	1.10	1.05
44:J:60:TRP:CZ3	54:T:153:PRO:HD3	1.90	1.05
3:SB:82:ARG:NH2	3:SB:191:ASP:HB2	1.72	1.04
1:S2:1109:C:C2'	13:SR:124:VAL:HG21	1.86	1.03
30:SY:37:LYS:NZ	30:SY:93:ARG:HH21	1.56	1.03
30:SY:56:PHE:CE1	30:SY:94:HIS:HE1	1.68	1.03
1:S2:1109:C:O2	13:SR:124:VAL:CG2	2.05	1.02
1:S2:1672:U:OP1	12:SQ:18:THR:CB	2.06	1.02
54:T:164:LYS:HE2	79:t:4833:G:N1	1.70	1.02
55:U:108:ARG:O	55:U:112:ASN:HB2	1.59	1.02
30:SY:37:LYS:NZ	30:SY:93:ARG:NH2	2.07	1.02
31:SZ:49:LEU:H	31:SZ:83:LEU:HD21	1.24	1.02
52:R:10:ASP:O	79:t:2062:C:O2'	1.79	1.01
44:J:60:TRP:HZ3	54:T:152:PHE:HA	1.24	1.00
1:S2:1109:C:C2	13:SR:124:VAL:HG22	1.96	1.00
41:G:165:LEU:HD11	41:G:176:THR:HG21	1.43	0.99
52:R:155:ALA:O	52:R:161:SER:HB2	1.60	0.99
36:B:298:LEU:O	36:B:299:ILE:CG1	2.11	0.98
52:R:7:HIS:HE1	79:t:1648:C:C4'	1.75	0.98
52:R:7:HIS:NE2	79:t:1648:C:H5''	1.78	0.98
52:R:3:VAL:HG13	52:R:5:ILE:HG12	1.42	0.98
1:S2:1109:C:C2	13:SR:124:VAL:O	2.17	0.98
44:J:2:LYS:HB3	44:J:61:TRP:CZ3	1.99	0.98
4:SD:28:GLU:HA	9:SK:61:GLN:NE2	1.77	0.97
21:Sd:21:CYS:SG	21:Sd:24:CYS:N	2.35	0.97
44:J:2:LYS:HB3	44:J:61:TRP:HZ3	1.27	0.97
69:i:44:LEU:O	69:i:47:ILE:CG2	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1553:C:H41	21:Sd:22:ARG:NH2	1.61	0.97
3:SB:82:ARG:HH22	3:SB:191:ASP:HB2	1.20	0.97
55:U:17:ARG:HH12	55:U:47:THR:HG21	1.30	0.97
30:SY:37:LYS:HZ3	30:SY:93:ARG:NH2	1.61	0.96
55:U:17:ARG:NH1	55:U:47:THR:HG23	1.80	0.96
30:SY:58:PHE:HB3	30:SY:93:ARG:NH1	1.80	0.96
50:P:121:PRO:HD2	54:T:166:ARG:O	1.65	0.96
44:J:60:TRP:CE3	54:T:153:PRO:HD2	2.01	0.95
3:SB:188:LEU:HD23	3:SB:188:LEU:H	1.31	0.95
54:T:160:ARG:HG2	54:T:163:HIS:CB	1.98	0.94
3:SB:189:ILE:HB	3:SB:190:PRO:HD3	1.48	0.94
36:B:35:ASP:HB3	36:B:186:ASN:OD1	1.66	0.94
1:S2:1497:G:N7	9:SK:62:PHE:CZ	2.35	0.94
36:B:291:TYR:CB	36:B:298:LEU:HD21	1.98	0.94
36:B:37:PRO:HA	36:B:188:GLY:HA2	1.50	0.93
36:B:35:ASP:HB3	36:B:186:ASN:CG	1.94	0.92
56:V:56:LEU:O	56:V:60:VAL:CG2	2.17	0.92
30:SY:58:PHE:CB	30:SY:93:ARG:HH12	1.82	0.92
12:SQ:16:LYS:HE2	12:SQ:82:TYR:HB3	1.49	0.92
30:SY:37:LYS:HZ3	30:SY:93:ARG:HH21	0.97	0.92
54:T:70:LYS:HE2	54:T:70:LYS:HA	1.53	0.91
36:B:291:TYR:CA	36:B:298:LEU:CD2	2.29	0.91
1:S2:1553:C:C5	21:Sd:22:ARG:NH2	2.38	0.91
9:SK:62:PHE:CD1	9:SK:67:PHE:CE1	2.59	0.91
9:SK:62:PHE:HD1	9:SK:67:PHE:CE1	1.89	0.90
41:G:165:LEU:CD1	41:G:176:THR:CB	2.29	0.90
1:S2:1109:C:H2'	13:SR:124:VAL:HG21	0.91	0.90
1:S2:1553:C:N4	21:Sd:22:ARG:NH2	2.21	0.89
54:T:164:LYS:CG	54:T:165:PRO:CD	2.50	0.89
1:S2:1272:C:HO2'	21:Sd:2:GLY:N	1.70	0.89
12:SQ:16:LYS:HG2	12:SQ:79:ALA:HA	1.53	0.89
1:S2:1109:C:O2	13:SR:124:VAL:HG22	1.66	0.89
54:T:164:LYS:CG	54:T:165:PRO:HD3	2.00	0.89
12:SQ:16:LYS:CE	12:SQ:82:TYR:CG	2.47	0.88
56:V:49:VAL:HG11	56:V:60:VAL:HG21	1.55	0.88
1:S2:1109:C:C2'	13:SR:124:VAL:HG23	2.01	0.88
1:S2:1648:G:C8	12:SQ:17:LYS:CD	2.56	0.88
1:S2:1553:C:H41	21:Sd:22:ARG:HH21	1.16	0.87
52:R:3:VAL:CG1	52:R:5:ILE:HG12	2.03	0.87
7:SH:14:GLU:OE1	7:SH:14:GLU:N	2.08	0.86
44:J:61:TRP:CH2	48:N:33:GLN:NE2	2.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:164:LYS:CE	79:t:4833:G:N1	2.32	0.86
9:SK:59:LYS:NZ	9:SK:70:TYR:HB2	1.91	0.85
1:S2:1109:C:H2'	13:SR:124:VAL:HG23	1.55	0.85
41:G:130:LYS:H	41:G:130:LYS:HD2	1.40	0.85
47:M:77:SER:O	47:M:81:LEU:HG	1.76	0.85
10:SL:17:PHE:CE2	10:SL:19:ASN:O	2.30	0.85
44:J:60:TRP:CH2	48:N:6:PHE:CE1	2.65	0.85
11:SP:17:TYR:CE1	11:SP:112:ILE:CG2	2.60	0.84
10:SL:22:ARG:O	10:SL:23:VAL:CG1	2.25	0.84
41:G:165:LEU:CD1	41:G:176:THR:HG21	1.89	0.84
41:G:165:LEU:HD21	41:G:176:THR:HG23	1.60	0.84
3:SB:84:PHE:HE2	3:SB:188:LEU:HD12	1.41	0.84
40:F:4:VAL:N	79:t:1760:C:HO2'	1.76	0.83
9:SK:64:TRP:CE3	21:Sd:23:VAL:HG22	2.14	0.83
30:SY:58:PHE:CB	30:SY:93:ARG:NH1	2.41	0.83
2:SA:26:GLY:O	2:SA:46:ILE:HG23	1.77	0.83
79:t:1942:G:HO2'	79:t:2005:G:H1	1.24	0.83
54:T:68:PHE:HE2	79:t:722:G:H1'	1.43	0.83
1:S2:1109:C:O2	13:SR:124:VAL:HG23	1.79	0.82
55:U:17:ARG:HH12	55:U:47:THR:CG2	1.82	0.82
36:B:35:ASP:HB3	36:B:186:ASN:CB	2.10	0.81
36:B:292:LEU:O	36:B:298:LEU:HG	1.80	0.81
36:B:293:ILE:O	36:B:298:LEU:HA	1.80	0.81
41:G:179:LEU:O	41:G:179:LEU:HD13	1.80	0.81
54:T:164:LYS:HG2	54:T:165:PRO:HD2	1.58	0.81
54:T:160:ARG:CG	54:T:163:HIS:HB3	2.06	0.81
9:SK:62:PHE:O	9:SK:63:ALA:O	1.99	0.80
52:R:155:ALA:O	52:R:161:SER:CB	2.29	0.80
44:J:60:TRP:CE3	54:T:152:PHE:HA	2.15	0.80
7:SH:12:ASN:HB2	7:SH:14:GLU:O	1.81	0.80
18:SX:61:GLN:NE2	18:SX:61:GLN:H	1.80	0.80
9:SK:25:LYS:HD2	9:SK:62:PHE:CZ	2.18	0.79
9:SK:65:ARG:HG3	21:Sd:22:ARG:O	1.81	0.79
41:G:130:LYS:HD2	41:G:130:LYS:N	1.96	0.79
44:J:59:LYS:NZ	44:J:66:GLU:HB3	1.97	0.79
41:G:165:LEU:CD1	41:G:176:THR:HB	2.02	0.79
30:SY:58:PHE:HB2	30:SY:93:ARG:HH12	1.45	0.79
30:SY:90:ARG:O	30:SY:93:ARG:HG3	1.82	0.79
1:S2:1109:C:C2	13:SR:124:VAL:CG2	2.64	0.79
74:n:106:ARG:HH22	79:t:4658:C:H4'	1.49	0.78
9:SK:60:GLU:CD	9:SK:69:TRP:HE1	1.91	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SY:37:LYS:HZ2	30:SY:93:ARG:CZ	1.96	0.78
36:B:291:TYR:C	36:B:298:LEU:HD21	2.08	0.78
1:S2:1109:C:N3	13:SR:124:VAL:O	2.16	0.77
2:SA:89:LYS:HB3	2:SA:89:LYS:NZ	1.98	0.77
9:SK:53:LYS:HG3	9:SK:60:GLU:OE2	1.84	0.77
79:t:708:U:H3	79:t:938:G:H1	1.32	0.77
56:V:56:LEU:O	56:V:60:VAL:HG22	1.85	0.77
1:S2:1495:G:N2	21:Sd:24:CYS:CB	2.35	0.77
36:B:291:TYR:HA	36:B:298:LEU:HD21	0.78	0.77
54:T:68:PHE:CE2	79:t:722:G:H1'	2.20	0.77
12:SQ:16:LYS:HG2	12:SQ:79:ALA:CA	2.15	0.77
52:R:158:THR:HG22	52:R:161:SER:HB3	1.66	0.77
3:SB:188:LEU:HG	3:SB:189:ILE:HD12	1.67	0.76
3:SB:188:LEU:H	3:SB:188:LEU:CD2	1.98	0.76
44:J:60:TRP:HE3	54:T:153:PRO:HD2	1.50	0.76
11:SP:17:TYR:CZ	11:SP:18:ARG:NH2	2.51	0.76
12:SQ:16:LYS:CD	12:SQ:82:TYR:HB2	2.16	0.76
13:SR:128:PHE:O	13:SR:129:LYS:HB2	1.83	0.76
1:S2:1553:C:H5	21:Sd:22:ARG:NH2	1.84	0.75
30:SY:56:PHE:CE1	30:SY:94:HIS:NE2	2.54	0.75
56:V:61:VAL:HG23	56:V:73:THR:O	1.86	0.75
54:T:70:LYS:O	79:t:723:A:H4'	1.87	0.75
1:S2:1495:G:N2	21:Sd:24:CYS:SG	2.60	0.74
30:SY:37:LYS:HZ2	30:SY:93:ARG:NH2	1.82	0.74
62:b:89:ASN:OD1	62:b:92:LYS:HE2	1.86	0.74
1:S2:1495:G:H21	21:Sd:26:ASN:HB2	1.53	0.74
1:S2:1497:G:N7	9:SK:62:PHE:CE2	2.54	0.74
54:T:164:LYS:HE2	79:t:4833:G:C6	2.21	0.74
55:U:108:ARG:O	55:U:112:ASN:CB	2.36	0.74
1:S2:1287:A:H62	1:S2:1312:G:H21	1.34	0.74
36:B:36:ASP:O	36:B:187:GLY:O	2.04	0.74
54:T:160:ARG:CG	54:T:163:HIS:CB	2.66	0.73
1:S2:1553:C:H5	21:Sd:22:ARG:HH22	1.35	0.73
54:T:69:GLU:OE2	54:T:72:PRO:HG3	1.88	0.73
11:SP:17:TYR:CE2	11:SP:18:ARG:CZ	2.72	0.73
52:R:37:ARG:NH1	79:t:2067:G:N7	2.36	0.73
9:SK:53:LYS:CG	9:SK:60:GLU:OE2	2.31	0.73
79:t:161:G:H1	79:t:266:U:H3	1.37	0.73
9:SK:62:PHE:HE1	9:SK:67:PHE:CZ	2.07	0.73
36:B:37:PRO:HA	36:B:188:GLY:CA	2.17	0.73
1:S2:1672:U:P	12:SQ:18:THR:HB	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SG:32:MET:HB2	24:SG:100:CYS:HB2	1.68	0.72
41:G:163:VAL:O	41:G:175:VAL:HG23	1.89	0.72
36:B:298:LEU:C	36:B:299:ILE:HG13	2.10	0.72
44:J:61:TRP:HH2	48:N:33:GLN:OE1	1.73	0.72
52:R:7:HIS:ND1	79:t:1648:C:O3'	2.23	0.72
54:T:70:LYS:HE2	54:T:70:LYS:CA	2.19	0.72
52:R:7:HIS:CE1	79:t:1648:C:C4'	2.61	0.72
9:SK:25:LYS:HD2	9:SK:62:PHE:CE1	2.23	0.72
11:SP:17:TYR:HE2	11:SP:18:ARG:CZ	2.03	0.72
37:C:94:ASN:HD22	37:C:102:PHE:HB2	1.53	0.72
55:U:17:ARG:HD2	55:U:17:ARG:N	2.04	0.72
9:SK:59:LYS:HB3	9:SK:59:LYS:HZ3	1.55	0.71
36:B:37:PRO:O	36:B:188:GLY:HA2	1.90	0.71
22:Sg:157:SER:HB3	22:Sg:164:ILE:HG22	1.70	0.71
47:M:79:GLU:OE1	47:M:79:GLU:N	2.19	0.71
52:R:7:HIS:ND1	79:t:1649:G:P	2.63	0.71
7:SH:13:GLY:C	7:SH:14:GLU:OE1	2.33	0.71
3:SB:188:LEU:HD23	3:SB:188:LEU:N	2.05	0.70
36:B:298:LEU:C	36:B:298:LEU:HD23	2.16	0.70
9:SK:60:GLU:HB3	9:SK:69:TRP:CD1	2.26	0.70
54:T:69:GLU:OE1	54:T:69:GLU:N	2.24	0.70
1:S2:533:A:H61	1:S2:550:C:H42	1.38	0.70
37:C:330:PRO:HG3	42:H:47:ARG:HH21	1.57	0.70
66:f:6:PRO:HB3	66:f:74:PHE:CZ	2.25	0.70
1:S2:1723:G:H1	1:S2:1810:U:H3	1.39	0.70
2:SA:89:LYS:HB3	2:SA:89:LYS:HZ1	1.54	0.70
6:SF:61:PHE:HB3	20:Sc:51:ARG:HH21	1.56	0.70
8:SI:124:LYS:HG2	8:SI:125:LYS:HG2	1.73	0.70
22:Sg:195:LEU:HA	22:Sg:211:GLY:HA3	1.73	0.70
52:R:158:THR:OG1	52:R:159:PRO:HD2	1.92	0.70
9:SK:53:LYS:HD3	9:SK:60:GLU:CD	2.15	0.70
11:SP:17:TYR:CD1	11:SP:112:ILE:HG21	2.27	0.70
42:H:232:ASP:HB2	42:H:236:ARG:HH22	1.56	0.70
57:W:85:ARG:HH21	57:W:100:ASP:HA	1.57	0.70
81:v:55:U:H2'	81:v:56:C:H2'	1.74	0.70
79:t:159:A:H61	79:t:268:C:H42	1.39	0.70
1:S2:1553:C:C4	21:Sd:22:ARG:NH2	2.59	0.70
53:S:109:TYR:CD1	53:S:114:LYS:HD2	2.27	0.70
31:SZ:81:GLY:O	31:SZ:82:SER:HB3	1.90	0.69
81:v:50:U:H3	81:v:65:G:H1	1.39	0.69
12:SQ:16:LYS:CE	12:SQ:82:TYR:CD2	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1341:C:N4	1:S2:1486:A:N1	2.41	0.69
11:SP:17:TYR:CE2	11:SP:18:ARG:NH2	2.60	0.69
25:SJ:37:LEU:HD23	25:SJ:42:GLU:HG3	1.75	0.69
56:V:56:LEU:O	56:V:60:VAL:HG23	1.92	0.69
60:Z:52:ASP:HB2	60:Z:110:LYS:HD2	1.74	0.69
44:J:61:TRP:CH2	48:N:33:GLN:CD	2.70	0.69
36:B:33:PRO:O	36:B:186:ASN:ND2	2.26	0.69
53:S:20:LYS:NZ	79:t:2801:G:N7	2.40	0.69
1:S2:1495:G:C2	21:Sd:24:CYS:HB2	2.28	0.68
73:m:27:ILE:HG13	73:m:30:LYS:HD3	1.75	0.68
11:SP:17:TYR:CD1	11:SP:112:ILE:CG2	2.76	0.68
30:SY:56:PHE:HE1	30:SY:94:HIS:HE1	1.02	0.68
36:B:291:TYR:C	36:B:298:LEU:CD2	2.64	0.68
43:I:104:PRO:HG2	43:I:194:VAL:HG23	1.76	0.68
4:SD:49:ILE:HG22	4:SD:87:TYR:HB2	1.74	0.68
9:SK:53:LYS:HD3	9:SK:60:GLU:CG	2.23	0.68
46:L:112:HIS:HD2	46:L:126:TYR:H	1.42	0.68
81:v:19:G:N3	81:v:57:G:N2	2.42	0.68
28:SO:34:PHE:HB3	28:SO:41:PHE:HB2	1.76	0.68
79:t:4710:U:H3	79:t:4909:G:H1	1.42	0.68
54:T:160:ARG:CG	54:T:163:HIS:CD2	2.77	0.68
62:b:42:ARG:NH1	79:t:4338:A:O2'	2.27	0.68
79:t:4951:G:H1	79:t:5016:A:H61	1.40	0.68
46:L:90:ARG:NH2	46:L:108:GLY:O	2.27	0.68
52:R:63:LEU:HB2	52:R:88:ASP:HA	1.76	0.68
3:SB:184:VAL:O	3:SB:188:LEU:HD22	1.85	0.67
9:SK:59:LYS:NZ	9:SK:59:LYS:HB3	2.10	0.67
10:SL:17:PHE:CZ	10:SL:19:ASN:HB2	2.28	0.67
11:SP:17:TYR:HE2	11:SP:18:ARG:HE	0.75	0.67
22:Sg:256:ILE:HB	22:Sg:270:LEU:HB2	1.75	0.67
1:S2:1672:U:P	12:SQ:18:THR:CB	2.83	0.67
79:t:1424:C:H42	79:t:2084:G:H1	1.41	0.67
8:SI:168:GLN:HB2	79:t:4984:U:H5	1.60	0.67
1:S2:1672:U:P	12:SQ:18:THR:OG1	2.52	0.67
53:S:103:ARG:NH1	53:S:124:TYR:OH	2.27	0.67
79:t:123:C:H42	79:t:144:A:H61	1.42	0.67
21:Sd:39:CYS:HB2	21:Sd:41:GLN:OE1	1.93	0.67
44:J:2:LYS:HE2	44:J:61:TRP:CE3	2.29	0.67
53:S:109:TYR:CD1	53:S:114:LYS:CD	2.77	0.67
79:t:2626:A:H62	79:t:2665:G:H8	1.42	0.67
14:SS:90:VAL:HG11	14:SS:113:ARG:HH22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SK:62:PHE:CE1	9:SK:67:PHE:CE1	2.83	0.66
79:t:4433:U:H3	79:t:4446:G:H1	1.44	0.66
22:Sg:298:LEU:HB3	22:Sg:310:TRP:HB2	1.77	0.66
54:T:161:ARG:O	54:T:162:GLN:HB2	1.96	0.66
79:t:4485:A:H5''	79:t:4486:G:H5'	1.77	0.66
52:R:3:VAL:O	52:R:4:ASP:HB3	1.94	0.66
12:SQ:16:LYS:CD	12:SQ:82:TYR:CB	2.74	0.66
36:B:224:LYS:NZ	79:t:4588:A:OP2	2.27	0.66
59:Y:107:HIS:O	59:Y:111:GLN:NE2	2.29	0.66
2:SA:77:ILE:HG22	2:SA:99:ILE:HB	1.77	0.66
35:A:54:ARG:NH2	79:t:3651:U:OP1	2.29	0.66
36:B:37:PRO:CA	36:B:188:GLY:HA2	2.25	0.65
79:t:1069:C:H42	79:t:1193:C:H42	1.44	0.65
11:SP:17:TYR:HE1	11:SP:112:ILE:CG2	2.10	0.65
7:SH:145:ARG:NH1	29:SW:51:GLU:OE2	2.30	0.65
37:C:235:LEU:HD23	37:C:240:LEU:HD11	1.78	0.65
53:S:133:LYS:H	53:S:137:ILE:HD11	1.62	0.65
62:b:123:ILE:HG22	62:b:143:ALA:HB3	1.77	0.65
9:SK:62:PHE:CE1	9:SK:67:PHE:CZ	2.84	0.65
66:f:6:PRO:HB3	66:f:74:PHE:CE1	2.32	0.65
7:SH:154:ILE:HB	7:SH:185:VAL:HG12	1.77	0.65
25:SJ:114:VAL:HG21	25:SJ:135:ILE:HD13	1.78	0.65
48:N:5:ARG:HB2	48:N:11:ARG:HH12	1.60	0.65
41:G:179:LEU:HD13	41:G:179:LEU:C	2.22	0.65
79:t:1320:A:H62	79:t:2325:C:H5	1.43	0.65
79:t:1636:G:N2	79:t:1660:C:OP1	2.29	0.65
53:S:39:GLN:NE2	79:t:2689:C:OP2	2.30	0.65
3:SB:84:PHE:CE2	3:SB:188:LEU:HD12	2.30	0.64
47:M:64:VAL:HG22	79:t:71:C:H5'	1.77	0.64
39:E:6:C:H4'	40:F:52:ILE:HD13	1.80	0.64
3:SB:189:ILE:HD12	3:SB:189:ILE:N	2.12	0.64
3:SB:219:LYS:HE2	77:q:90:LYS:HA	1.79	0.64
60:Z:8:THR:O	79:t:223:G:N2	2.29	0.64
45:K:149:ILE:HD11	45:K:167:ILE:HD11	1.79	0.64
50:P:87:MET:SD	79:t:1893:G:N2	2.70	0.64
54:T:160:ARG:CG	54:T:163:HIS:CG	2.80	0.64
1:S2:1401:A:H4'	16:SU:52:GLY:HA3	1.79	0.64
6:SF:100:ILE:HD11	6:SF:177:LEU:HD21	1.79	0.64
10:SL:22:ARG:NE	10:SL:22:ARG:HA	2.13	0.64
35:A:27:ALA:O	35:A:128:ARG:NH2	2.31	0.64
41:G:165:LEU:HG	41:G:176:THR:CG2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:452:C:H42	79:t:690:C:H42	1.45	0.64
1:S2:1016:U:OP2	32:Sb:20:LYS:NZ	2.31	0.64
11:SP:17:TYR:O	11:SP:18:ARG:HG3	1.98	0.64
30:SY:90:ARG:HA	30:SY:93:ARG:CG	2.28	0.64
79:t:3663:A:H62	79:t:3794:G:H21	1.45	0.64
1:S2:992:A:N7	19:Sa:15:ARG:NH2	2.46	0.64
18:SX:107:ARG:HG2	18:SX:112:VAL:HG12	1.79	0.64
22:Sg:11:LEU:HB2	22:Sg:307:VAL:HB	1.79	0.64
44:J:60:TRP:HZ3	54:T:152:PHE:CA	2.08	0.64
81:v:71:G:H21	81:v:72:C:H42	1.46	0.64
44:J:94:SER:HB3	44:J:142:ASP:HB2	1.80	0.63
1:S2:681:U:O3'	18:SX:8:ARG:NE	2.31	0.63
1:S2:909:G:H5''	53:S:176:ARG:HH12	1.63	0.63
36:B:19:ARG:HB2	36:B:234:ARG:HH21	1.64	0.63
1:S2:523:A:OP1	25:SJ:127:ARG:NH2	2.31	0.63
35:A:21:LYS:HD2	79:t:1523:C:H5''	1.81	0.63
5:SE:41:CYS:SG	5:SE:42:LEU:N	2.69	0.63
40:F:9:ASN:HB2	40:F:12:TYR:HB3	1.81	0.63
79:t:4065:G:N7	79:t:4068:A:N6	2.45	0.63
9:SK:59:LYS:NZ	9:SK:70:TYR:CD2	2.67	0.63
62:b:26:ARG:NH2	79:t:1638:U:OP2	2.32	0.63
1:S2:1006:C:H4'	64:d:11:LEU:HB2	1.81	0.63
1:S2:683:OMG:N1	1:S2:1022:U:OP2	2.28	0.63
36:B:6:PHE:HB3	57:W:49:LEU:HD21	1.79	0.63
44:J:60:TRP:HE3	54:T:153:PRO:CD	2.01	0.63
57:W:24:ALA:HB3	57:W:39:ILE:HD12	1.80	0.63
50:P:118:MET:HG2	54:T:169:THR:HG22	1.81	0.63
1:S2:121:OMU:HM23	5:SE:144:ALA:HB3	1.81	0.62
1:S2:194:C:OP2	1:S2:196:C:N4	2.32	0.62
8:SI:48:VAL:HG11	8:SI:54:LYS:HE3	1.80	0.62
48:N:94:LYS:NZ	79:t:4829:C:OP2	2.30	0.62
54:T:82:LEU:HB2	54:T:93:MET:HB3	1.80	0.62
61:a:14:LEU:HD21	61:a:81:MET:HG2	1.81	0.62
79:t:703:C:H42	79:t:943:A:H61	1.46	0.62
1:S2:1648:G:N7	12:SQ:17:LYS:CD	2.53	0.62
79:t:2372:C:OP2	79:t:2373:G:N2	2.32	0.62
4:SD:28:GLU:N	9:SK:61:GLN:HE22	1.96	0.62
9:SK:64:TRP:CZ3	21:Sd:23:VAL:HG22	2.33	0.62
29:SW:20:ARG:HG2	29:SW:22:LYS:HE2	1.81	0.62
79:t:289:A:N6	79:t:4323:U:O2'	2.31	0.62
1:S2:1310:U:H5''	34:Sf:130:VAL:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1812:U:O4	1:S2:1813:A:N6	2.31	0.62
44:J:61:TRP:CH2	48:N:33:GLN:OE1	2.52	0.62
50:P:90:HIS:O	50:P:96:GLN:NE2	2.29	0.62
41:G:59:ARG:NH2	79:t:964:C:OP2	2.33	0.62
41:G:162:VAL:HB	41:G:175:VAL:HG21	1.81	0.62
54:T:164:LYS:CG	54:T:165:PRO:HD2	2.26	0.62
1:S2:928:G:H1	1:S2:1013:U:H3	1.47	0.62
5:SE:71:LYS:HB2	5:SE:91:SER:HB2	1.80	0.62
11:SP:108:LYS:HG2	11:SP:111:MET:HE3	1.81	0.62
1:S2:561:A:N3	25:SJ:132:GLN:NE2	2.48	0.62
20:Sc:13:ARG:HB2	20:Sc:35:MET:HE2	1.82	0.62
22:Sg:166:VAL:HG12	22:Sg:176:VAL:HG22	1.82	0.62
42:H:245:ARG:NH2	79:t:930:A:OP1	2.32	0.62
79:t:4066:C:O2	79:t:4084:G:N1	2.32	0.62
49:O:179:LYS:NZ	79:t:292:G:OP1	2.32	0.62
1:S2:1230:C:OP1	14:SS:130:ARG:NH2	2.32	0.62
1:S2:1748:G:H1	1:S2:1786:U:H3	1.48	0.62
11:SP:13:ARG:N	11:SP:13:ARG:HD2	2.15	0.62
44:J:63:ASN:H	44:J:66:GLU:HB2	1.65	0.62
52:R:3:VAL:O	52:R:4:ASP:CB	2.48	0.62
9:SK:25:LYS:CD	9:SK:62:PHE:HZ	2.13	0.62
22:Sg:10:THR:HG22	22:Sg:308:ARG:HG2	1.81	0.62
36:B:291:TYR:HB3	36:B:298:LEU:CD1	2.24	0.61
41:G:110:ARG:NH2	79:t:955:C:O4'	2.33	0.61
46:L:18:ARG:HB3	46:L:133:VAL:HG23	1.82	0.61
65:e:44:ARG:NH2	79:t:2812:A:OP2	2.32	0.61
79:t:465:A:H62	79:t:677:G:H21	1.47	0.61
79:t:1074:C:O2	79:t:1188:G:N2	2.32	0.61
1:S2:1628:C:OP1	15:ST:38:LYS:NZ	2.33	0.61
22:Sg:85:GLY:HA2	22:Sg:107:ASP:HA	1.83	0.61
35:A:192:LYS:HB3	35:A:193:ARG:HE	1.65	0.61
42:H:167:ILE:HD13	42:H:174:LEU:HD23	1.82	0.61
44:J:61:TRP:HH2	48:N:33:GLN:CD	2.06	0.61
11:SP:17:TYR:CE1	11:SP:112:ILE:HG23	2.34	0.61
18:SX:61:GLN:H	18:SX:61:GLN:HE21	1.44	0.61
41:G:245:GLN:NE2	41:G:249:ASP:OD2	2.32	0.61
1:S2:1418:C:H3'	1:S2:1419:C:H2'	1.83	0.61
1:S2:1648:G:H5''	12:SQ:125:ARG:HB2	1.82	0.61
50:P:77:SER:HB3	50:P:106:ASP:HB2	1.81	0.61
58:X:19:ARG:NH2	79:t:4591:U:O2'	2.33	0.61
6:SF:135:ARG:O	6:SF:203:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R:172:ARG:HD2	62:b:57:GLY:HA3	1.81	0.61
66:f:75:ARG:HD3	78:r:22:LYS:HZ3	1.65	0.61
18:SX:68:LYS:HB3	18:SX:91:LEU:HD22	1.83	0.61
22:Sg:42:MET:HB2	22:Sg:57:ARG:HB2	1.82	0.61
36:B:246:ARG:NH2	79:t:4520:U:OP2	2.34	0.61
38:D:87:G:OP2	69:i:5:LYS:NZ	2.33	0.61
79:t:3612:U:OP2	79:t:3617:A:N6	2.33	0.61
81:v:60:U:OP1	81:v:62:C:N4	2.33	0.61
26:SM:69:LEU:HD21	26:SM:76:LEU:HD23	1.83	0.61
35:A:174:ARG:NH2	79:t:3655:G:OP1	2.34	0.61
52:R:3:VAL:HG11	52:R:5:ILE:HD11	1.81	0.61
52:R:10:ASP:O	79:t:2063:G:H5'	2.00	0.61
67:g:59:THR:HG23	67:g:60:PRO:HD3	1.83	0.61
23:SC:106:VAL:HG11	23:SC:151:ILE:HD11	1.82	0.61
28:SO:74:ALA:HB1	28:SO:115:ALA:HB2	1.82	0.61
47:M:55:ILE:HG23	47:M:76:PHE:HE2	1.66	0.61
79:t:166:G:H22	79:t:261:G:H22	1.49	0.61
1:S2:925:G:H1	1:S2:1017:U:H3	1.48	0.61
5:SE:207:VAL:HA	5:SE:221:ARG:HA	1.83	0.61
31:SZ:49:LEU:N	31:SZ:83:LEU:HD21	2.07	0.61
37:C:149:GLU:OE2	78:r:71:ARG:NH1	2.34	0.61
79:t:1149:G:N3	79:t:1150:C:O2'	2.33	0.61
36:B:238:LYS:NZ	79:t:3813:C:OP1	2.33	0.60
79:t:2790:G:N1	79:t:2793:C:OP2	2.34	0.60
22:Sg:152:SER:H	22:Sg:169:GLY:HA2	1.67	0.60
22:Sg:210:GLY:HA3	22:Sg:236:ILE:HD11	1.82	0.60
27:SN:46:THR:HG22	27:SN:49:GLN:HG2	1.83	0.60
1:S2:695:C:N4	1:S2:737:G:OP2	2.34	0.60
12:SQ:18:THR:O	12:SQ:18:THR:HG22	2.01	0.60
51:Q:127:ARG:NH2	79:t:2401:C:OP1	2.32	0.60
55:U:87:LYS:NZ	79:t:4262:U:OP1	2.35	0.60
22:Sg:87:LEU:HB2	22:Sg:101:PHE:HB2	1.82	0.60
36:B:298:LEU:O	36:B:298:LEU:HD23	2.01	0.60
76:p:9:ARG:HA	76:p:20:PRO:HA	1.84	0.60
2:SA:163:CYS:SG	2:SA:164:ASN:N	2.74	0.60
30:SY:58:PHE:HB3	30:SY:93:ARG:HH11	1.64	0.60
37:C:195:LYS:NZ	79:t:2313:C:OP2	2.35	0.60
68:h:10:ARG:NH1	79:t:2382:A:OP1	2.33	0.60
28:SO:75:MET:SD	28:SO:79:GLN:NE2	2.75	0.60
40:F:82:GLU:OE2	40:F:108:ARG:NH2	2.34	0.60
50:P:169:ARG:NH2	79:t:4816:C:O3'	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1962:G:O6	79:t:1969:G:N2	2.35	0.60
1:S2:1006:C:OP2	64:d:9:LYS:N	2.28	0.60
41:G:273:SER:HG	79:t:4839:U:HO2'	1.48	0.60
3:SB:185:VAL:CG2	3:SB:188:LEU:CD1	2.36	0.60
6:SF:140:ASP:HB2	20:Sc:46:VAL:HG12	1.83	0.60
29:SW:55:ASP:OD1	29:SW:57:ARG:NH1	2.35	0.60
31:SZ:49:LEU:H	31:SZ:83:LEU:CD2	2.08	0.60
36:B:37:PRO:HA	36:B:188:GLY:C	2.27	0.60
54:T:13:VAL:HG23	54:T:62:VAL:HG23	1.82	0.60
63:c:25:ARG:NH2	79:t:1825:G:OP1	2.35	0.60
76:p:15:CYS:SG	76:p:19:GLN:NE2	2.75	0.60
1:S2:1235:G:H21	11:SP:135:ALA:HB2	1.67	0.60
10:SL:22:ARG:C	10:SL:23:VAL:HG13	2.23	0.60
41:G:283:PRO:O	41:G:284:HIS:ND1	2.34	0.60
47:M:77:SER:O	47:M:81:LEU:CG	2.50	0.60
52:R:65:ARG:NH2	79:t:1441:A:OP1	2.34	0.60
54:T:81:TRP:HB3	54:T:127:MET:HE3	1.83	0.60
1:S2:373:G:H21	10:SL:83:GLN:HE21	1.49	0.59
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.66	0.59
76:p:39:ARG:NH1	79:t:289:A:OP2	2.34	0.59
79:t:166:G:H1	79:t:261:G:H1	1.50	0.59
1:S2:658:U:O2	18:SX:17:ARG:NH2	2.35	0.59
1:S2:1692:U:O2'	19:Sa:86:ASN:ND2	2.35	0.59
4:SD:28:GLU:CA	9:SK:61:GLN:NE2	2.47	0.59
59:Y:113:VAL:HG12	59:Y:119:ILE:HD11	1.83	0.59
41:G:94:LYS:NZ	79:t:680:C:OP1	2.33	0.59
65:e:90:ARG:HD3	65:e:102:LEU:HD13	1.84	0.59
1:S2:289:G:OP1	5:SE:155:LYS:NZ	2.33	0.59
13:SR:124:VAL:O	13:SR:124:VAL:HG22	2.01	0.59
23:SC:64:THR:HG23	23:SC:67:GLY:H	1.67	0.59
31:SZ:81:GLY:O	31:SZ:82:SER:CB	2.49	0.59
32:Sb:36:LYS:HB3	32:Sb:78:SER:HB3	1.84	0.59
41:G:187:ARG:NH1	79:t:4897:C:OP1	2.35	0.59
1:S2:386:C:O2	8:SI:31:ARG:NH1	2.35	0.59
9:SK:59:LYS:O	9:SK:69:TRP:HA	2.03	0.59
44:J:113:GLU:OE2	44:J:115:ARG:NH2	2.35	0.59
78:r:66:ARG:NH1	79:t:473:G:OP1	2.36	0.59
1:S2:613:G:N2	1:S2:626:G:OP1	2.36	0.59
16:SU:59:LYS:HD2	16:SU:84:ILE:HD11	1.84	0.59
41:G:130:LYS:NZ	79:t:703:C:O2	2.36	0.59
41:G:188:ARG:NH1	41:G:214:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:67:THR:OG1	42:H:70:ARG:NH2	2.35	0.59
44:J:173:ARG:NH1	74:n:125:LYS:O	2.36	0.59
51:Q:80:GLN:NE2	79:t:3863:U:O2'	2.35	0.59
68:h:38:VAL:O	68:h:60:ARG:NH2	2.35	0.59
1:S2:1533:A:OP1	6:SF:164:ARG:NH1	2.36	0.59
9:SK:25:LYS:CD	9:SK:62:PHE:CZ	2.85	0.59
30:SY:37:LYS:HZ2	30:SY:93:ARG:NE	1.99	0.59
36:B:295:ASP:OD1	36:B:295:ASP:N	2.36	0.59
57:W:50:ASN:ND2	79:t:4419:U:OP1	2.36	0.59
76:p:81:ARG:HH22	79:t:4256:C:H5''	1.67	0.59
79:t:196:G:N2	79:t:206:U:OP1	2.35	0.59
1:S2:198:U:H4'	1:S2:201:C:H41	1.68	0.59
9:SK:59:LYS:HZ3	9:SK:70:TYR:HB2	1.67	0.59
30:SY:56:PHE:CD1	30:SY:94:HIS:NE2	2.66	0.59
50:P:22:ILE:HG23	54:T:166:ARG:HH21	1.68	0.59
52:R:2:GLY:N	79:t:1879:C:OP1	2.35	0.59
61:a:5:MET:O	61:a:28:ASN:ND2	2.36	0.59
1:S2:495:U:OP1	5:SE:49:ARG:NH1	2.33	0.59
10:SL:17:PHE:HE2	10:SL:19:ASN:O	1.84	0.59
36:B:292:LEU:O	36:B:298:LEU:HA	2.02	0.59
1:S2:379:C:N3	8:SI:31:ARG:NH2	2.50	0.58
22:Sg:164:ILE:HD12	22:Sg:178:ASN:HB3	1.84	0.58
43:I:131:LYS:HG3	43:I:132:ARG:HG2	1.85	0.58
52:R:104:ARG:NH1	79:t:1336:G:N7	2.51	0.58
66:f:130:ARG:NH2	79:t:2284:U:O2	2.36	0.58
1:S2:441:C:OP1	8:SI:2:GLY:N	2.36	0.58
52:R:7:HIS:CE1	79:t:1648:C:C3'	2.85	0.58
71:k:52:LYS:NZ	79:t:369:G:OP2	2.34	0.58
7:SH:144:ILE:HD13	7:SH:154:ILE:HG13	1.86	0.58
30:SY:55:ILE:HG13	30:SY:75:ILE:HG12	1.85	0.58
1:S2:1109:C:O2	13:SR:124:VAL:C	2.45	0.58
3:SB:82:ARG:NH1	3:SB:191:ASP:OD2	2.35	0.58
29:SW:102:ILE:HG13	29:SW:113:HIS:HB3	1.85	0.58
37:C:165:LYS:NZ	79:t:219:C:O2	2.37	0.58
73:m:44:TRP:O	73:m:48:LYS:NZ	2.37	0.58
80:u:9:A:N7	87:u:101:HOH:O	2.31	0.58
7:SH:15:LYS:HD2	7:SH:15:LYS:C	2.28	0.58
79:t:1228:C:H42	79:t:1247:C:H42	1.51	0.58
1:S2:1636:G:O2'	6:SF:164:ARG:NH1	2.29	0.58
17:SV:35:ASN:ND2	23:SC:267:GLN:OE1	2.37	0.58
22:Sg:26:GLN:NE2	22:Sg:73:SER:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:a:21:ARG:NH1	61:a:47:ASP:O	2.36	0.58
78:r:37:SER:OG	79:t:2246:U:OP1	2.21	0.58
53:S:130:ASN:ND2	79:t:1553:G:O2'	2.37	0.58
55:U:17:ARG:HG2	55:U:22:HIS:CE1	2.38	0.58
1:S2:554:A:H8	1:S2:555:A:H1'	1.69	0.58
7:SH:10:LYS:CD	7:SH:17:ASP:OD1	2.52	0.58
13:SR:128:PHE:O	13:SR:129:LYS:CB	2.52	0.58
29:SW:3:ARG:NH2	29:SW:9:ASP:OD2	2.35	0.58
53:S:110:ARG:NH2	79:t:2644:U:OP1	2.37	0.58
79:t:451:G:H1	79:t:691:G:H22	1.52	0.58
79:t:727:C:H42	79:t:914:G:H1	1.51	0.58
79:t:1058:G:N2	79:t:1219:C:O2	2.37	0.58
79:t:4693:G:H1'	79:t:4694:G:H2'	1.85	0.58
36:B:71:GLU:OE2	36:B:366:LYS:NZ	2.37	0.58
37:C:190:ARG:NH1	79:t:2274:C:OP1	2.37	0.58
43:I:121:LYS:HD2	43:I:125:LYS:HA	1.86	0.58
79:t:4839:U:H5''	79:t:4840:U:H3'	1.85	0.58
1:S2:1867:U:H4'	1:S2:1868:U:H5'	1.86	0.57
2:SA:74:VAL:HG12	2:SA:121:LEU:HB3	1.86	0.57
42:H:127:LYS:HB2	55:U:133:ALA:HB3	1.84	0.57
42:H:148:LYS:HD2	79:t:930:A:H3'	1.85	0.57
44:J:18:ILE:HG12	44:J:27:VAL:HG22	1.85	0.57
79:t:2092:G:O2'	79:t:2229:C:N4	2.37	0.57
79:t:4069:G:O2'	79:t:4078:G:N2	2.34	0.57
25:SJ:162:ARG:HH12	25:SJ:169:ARG:HE	1.51	0.57
1:S2:1824:A:OP1	18:SX:61:GLN:HG3	2.04	0.57
35:A:241:ARG:NH1	79:t:3630:G:OP1	2.36	0.57
69:i:106:LYS:NZ	79:t:112:C:OP2	2.35	0.57
79:t:133:C:N4	79:t:135:G:N3	2.53	0.57
79:t:198:C:H42	79:t:209:A:H61	1.52	0.57
79:t:3909:G:N2	79:t:4133:C:OP2	2.37	0.57
1:S2:1170:A:N6	1:S2:1189:A:OP2	2.35	0.57
79:t:2373:G:N2	79:t:2798:U:OP2	2.38	0.57
36:B:8:ALA:HB2	57:W:49:LEU:HD12	1.86	0.57
56:V:49:VAL:CG1	56:V:60:VAL:HG21	2.31	0.57
61:a:11:VAL:HG12	61:a:82:PRO:HA	1.87	0.57
79:t:4726:A:H61	79:t:4826:G:H22	1.52	0.57
3:SB:104:ASP:HB3	3:SB:214:LYS:HG3	1.87	0.57
12:SQ:16:LYS:CE	12:SQ:82:TYR:HB3	2.16	0.57
13:SR:115:SER:HB3	13:SR:117:LEU:HD23	1.85	0.57
21:Sd:39:CYS:O	21:Sd:43:PHE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SY:18:LEU:HD13	30:SY:20:ARG:HH11	1.70	0.57
39:E:7:G:O5'	40:F:33:ARG:NH1	2.37	0.57
79:t:85:G:O2'	79:t:97:G:O6	2.21	0.57
3:SB:26:SER:O	3:SB:51:ARG:NH2	2.36	0.57
11:SP:10:ARG:HG2	11:SP:11:THR:HG23	1.87	0.57
21:Sd:39:CYS:O	21:Sd:42:CYS:CB	2.53	0.57
22:Sg:20:GLN:HE22	22:Sg:22:ALA:HB2	1.70	0.57
38:D:12:G:H21	51:Q:120:ASN:HD22	1.53	0.57
38:D:37:A:OP2	69:i:89:ARG:NH1	2.34	0.57
66:f:128:ARG:NH2	79:t:2285:G:OP1	2.37	0.57
76:p:65:LYS:HE3	76:p:87:ARG:HH21	1.70	0.57
3:SB:189:ILE:N	3:SB:190:PRO:CD	2.68	0.57
8:SI:116:HIS:O	8:SI:152:ARG:NH1	2.37	0.57
10:SL:13:GLN:NE2	10:SL:63:THR:OG1	2.38	0.57
11:SP:87:PRO:HB3	11:SP:112:ILE:HD11	1.87	0.57
27:SN:47:PRO:HG3	27:SN:72:LEU:HD12	1.86	0.57
54:T:154:LEU:HB3	54:T:157:ARG:HD3	1.87	0.57
76:p:81:ARG:NH2	79:t:4256:C:OP1	2.37	0.57
1:S2:1355:C:O2'	23:SC:235:ASN:ND2	2.38	0.57
2:SA:85:ARG:O	2:SA:89:LYS:HG2	2.04	0.57
5:SE:35:PRO:HD2	5:SE:83:PRO:HG2	1.85	0.57
22:Sg:34:ALA:HB2	22:Sg:69:VAL:HG12	1.87	0.57
41:G:162:VAL:HB	41:G:175:VAL:CG2	2.35	0.57
46:L:57:VAL:HG23	46:L:59:SER:H	1.70	0.57
35:A:137:ILE:HG13	35:A:147:ARG:HG3	1.86	0.56
35:A:207:VAL:HG23	35:A:208:GLU:HG3	1.87	0.56
42:H:166:ARG:NH1	79:t:2255:A:OP1	2.37	0.56
44:J:7:ASN:HB3	44:J:58:ASP:HB3	1.87	0.56
52:R:7:HIS:NE2	79:t:1648:C:OP1	2.36	0.56
54:T:28:TYR:OH	54:T:52:LYS:NZ	2.38	0.56
79:t:1056:G:H22	79:t:1221:A:H2	1.53	0.56
79:t:1741:G:H1	79:t:1755:U:H3	1.53	0.56
1:S2:1420:G:N2	1:S2:1421:A:N3	2.52	0.56
41:G:103:GLY:O	41:G:105:ARG:NH1	2.39	0.56
79:t:1416:A:N6	79:t:1433:C:O2'	2.38	0.56
79:t:2590:A:H5'	79:t:2667:G:H4'	1.85	0.56
3:SB:70:SER:HA	3:SB:83:LYS:HA	1.86	0.56
6:SF:127:ARG:H	6:SF:135:ARG:HD3	1.70	0.56
24:SG:64:LYS:NZ	24:SG:82:SER:OG	2.35	0.56
37:C:197:ARG:NH2	79:t:345:C:OP2	2.34	0.56
49:O:39:ALA:HB2	49:O:63:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:P:14:HIS:HE1	50:P:120:VAL:H	1.51	0.56
78:r:61:VAL:HG12	78:r:81:THR:HG22	1.87	0.56
79:t:1953:G:H1	79:t:1975:C:H42	1.53	0.56
79:t:2072:G:O2'	79:t:2241:G:N2	2.35	0.56
79:t:2576:G:H1	79:t:2727:C:H5	1.51	0.56
81:v:26:A:H61	81:v:44:G:H1	1.52	0.56
8:SI:76:THR:OG1	8:SI:105:ASP:OD1	2.21	0.56
11:SP:127:LYS:HB2	11:SP:127:LYS:NZ	2.21	0.56
22:Sg:120:ILE:HB	22:Sg:132:TRP:HB2	1.86	0.56
30:SY:90:ARG:HA	30:SY:93:ARG:HG3	1.85	0.56
31:SZ:46:ASN:HB2	31:SZ:80:ARG:HB3	1.87	0.56
36:B:300:LYS:HB3	36:B:313:SER:HB2	1.87	0.56
48:N:7:VAL:HG12	48:N:57:LEU:HD21	1.88	0.56
49:O:93:LYS:NZ	79:t:281:U:O2	2.38	0.56
54:T:159:LEU:O	54:T:161:ARG:NH1	2.38	0.56
72:l:38:CYS:SG	72:l:39:SER:N	2.78	0.56
1:S2:124:U:OP1	24:SG:201:LYS:NZ	2.38	0.56
1:S2:1130:G:N2	1:S2:1130:G:OP2	2.36	0.56
1:S2:1161:U:OP1	18:SX:12:LYS:NZ	2.38	0.56
2:SA:141:ASN:ND2	23:SC:85:SER:O	2.39	0.56
23:SC:211:LYS:HG2	23:SC:215:MET:HE2	1.88	0.56
36:B:224:LYS:HD3	36:B:340:THR:HG22	1.87	0.56
51:Q:62:ARG:NH1	79:t:417:G:OP1	2.39	0.56
61:a:26:VAL:O	61:a:93:LYS:NZ	2.38	0.56
73:m:40:LYS:NZ	79:t:359:U:O2'	2.38	0.56
1:S2:639:C:H5''	33:Se:41:ARG:HH21	1.69	0.56
3:SB:82:ARG:HH22	3:SB:191:ASP:CB	2.07	0.56
5:SE:87:MET:HE2	5:SE:123:LEU:HB2	1.86	0.56
9:SK:59:LYS:NZ	9:SK:70:TYR:CB	2.66	0.56
10:SL:111:VAL:HG12	10:SL:140:PHE:HB2	1.88	0.56
25:SJ:71:LEU:O	25:SJ:75:ASN:ND2	2.39	0.56
41:G:223:ARG:NH2	79:t:447:G:N3	2.54	0.56
48:N:113:MET:HG3	79:t:4838:C:C4	2.41	0.56
51:Q:127:ARG:NH1	79:t:2399:A:OP2	2.38	0.56
79:t:2383:A:N1	79:t:2766:A:N6	2.54	0.56
12:SQ:16:LYS:HG2	12:SQ:79:ALA:CB	2.35	0.56
22:Sg:4:GLN:NE2	22:Sg:5:MET:O	2.39	0.56
44:J:10:VAL:HG22	44:J:78:GLN:HE21	1.69	0.56
79:t:193:C:O2	79:t:218:C:O2'	2.22	0.56
79:t:1955:U:N3	79:t:1983:A:N7	2.54	0.56
21:Sd:39:CYS:O	21:Sd:42:CYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:D:156:U:H3	79:t:1:C:H42	1.51	0.56
42:H:151:ASN:HA	42:H:191:ILE:HD11	1.87	0.56
52:R:3:VAL:HG11	52:R:5:ILE:CD1	2.35	0.56
72:l:23:VAL:HG22	72:l:36:VAL:HG22	1.88	0.56
79:t:966:C:O2	79:t:1260:G:N2	2.39	0.56
21:Sd:41:GLN:CD	21:Sd:41:GLN:H	2.14	0.56
41:G:181:LEU:O	79:t:4841:C:N4	2.35	0.56
49:O:124:ASP:OD1	79:t:3908:C:O2'	2.24	0.56
51:Q:24:VAL:HG22	51:Q:90:PHE:HD2	1.71	0.56
61:a:40:HIS:HA	61:a:76:ASN:HA	1.88	0.56
79:t:724:A:H62	79:t:918:C:H42	1.54	0.56
79:t:1251:G:H2'	79:t:1252:G:H8	1.71	0.56
2:SA:30:LEU:HD23	2:SA:30:LEU:O	2.06	0.56
8:SI:113:TYR:OH	8:SI:156:ALA:O	2.24	0.56
21:Sd:6:LEU:HA	21:Sd:9:SER:HB3	1.87	0.56
27:SN:53:ILE:HG22	32:Sb:52:THR:HG21	1.86	0.56
29:SW:88:LYS:O	29:SW:92:ASN:ND2	2.39	0.56
62:b:32:ARG:HD2	79:t:37:U:H4'	1.88	0.56
1:S2:1100:A:O3'	13:SR:132:ARG:NH1	2.39	0.55
1:S2:1497:G:C5	9:SK:62:PHE:CZ	2.95	0.55
10:SL:129:GLY:H	10:SL:143:LEU:HD13	1.71	0.55
35:A:50:HIS:HD2	79:t:2720:U:H2'	1.72	0.55
43:I:161:VAL:HG21	43:I:167:VAL:HG21	1.88	0.55
46:L:110:GLN:HG3	79:t:4213:A:H1'	1.86	0.55
53:S:23:TRP:HD1	53:S:50:ILE:HA	1.71	0.55
59:Y:139:ARG:NH1	79:t:2512:C:OP1	2.39	0.55
79:t:190:G:H22	79:t:243:G:H1	1.55	0.55
1:S2:1446:A:H1'	16:SU:55:ARG:HG3	1.89	0.55
47:M:56:ARG:NH1	47:M:74:ARG:O	2.37	0.55
54:T:68:PHE:N	54:T:68:PHE:CD1	2.74	0.55
58:X:52:THR:HG23	58:X:55:TYR:H	1.70	0.55
79:t:1227:G:H21	79:t:1228:C:H41	1.55	0.55
9:SK:3:MET:SD	9:SK:8:ARG:NE	2.79	0.55
14:SS:4:VAL:HG12	14:SS:5:ILE:HG22	1.88	0.55
35:A:123:ARG:NH1	79:t:4053:U:OP1	2.39	0.55
37:C:222:ARG:NH1	79:t:221:U:OP1	2.39	0.55
40:F:211:LEU:HB3	40:F:219:TYR:HB2	1.88	0.55
43:I:157:ILE:HD12	43:I:170:LEU:HD22	1.88	0.55
44:J:2:LYS:CB	44:J:61:TRP:HZ3	2.09	0.55
54:T:115:ALA:O	54:T:118:ARG:NH1	2.38	0.55
79:t:3634:A:N6	79:t:4130:G:O2'	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G:74:SER:HA	79:t:1256:G:H1'	1.89	0.55
53:S:67:THR:HA	53:S:70:ARG:HG2	1.88	0.55
62:b:100:ILE:HG22	62:b:123:ILE:HD11	1.87	0.55
64:d:31:TYR:OH	64:d:59:GLU:OE2	2.22	0.55
65:e:26:THR:HG23	65:e:85:ARG:HH11	1.70	0.55
2:SA:30:LEU:HD22	2:SA:47:TYR:CZ	2.41	0.55
2:SA:36:GLN:O	2:SA:53:ARG:NH1	2.39	0.55
3:SB:189:ILE:HD12	3:SB:189:ILE:H	1.70	0.55
18:SX:60:LYS:HG3	18:SX:114:ASP:O	2.07	0.55
35:A:55:GLY:HA3	35:A:174:ARG:HH11	1.71	0.55
41:G:128:HIS:HE1	79:t:1265:G:OP2	1.90	0.55
56:V:49:VAL:HG11	56:V:60:VAL:CG2	2.34	0.55
61:a:90:PRO:HB2	61:a:117:LYS:HD2	1.89	0.55
1:S2:682:U:H5'	18:SX:8:ARG:HE	1.71	0.55
1:S2:1256:G:O4'	21:Sd:40:ARG:NH1	2.40	0.55
3:SB:138:PHE:HD2	3:SB:214:LYS:HB3	1.72	0.55
28:SO:57:THR:HB	28:SO:60:MET:HG3	1.87	0.55
36:B:160:ILE:HD11	36:B:193:LYS:HG2	1.89	0.55
37:C:199:ARG:NH2	79:t:344:C:OP2	2.39	0.55
41:G:239:LYS:NZ	79:t:4895:C:O2	2.33	0.55
73:m:25:GLN:OE1	73:m:28:ARG:NH1	2.39	0.55
1:S2:1658:G:OP2	1:S2:1660:C:N4	2.40	0.55
38:D:55:U:H3	38:D:62:A:H2	1.53	0.55
41:G:163:VAL:C	41:G:175:VAL:HG23	2.32	0.55
42:H:95:ILE:HD12	42:H:96:ARG:HG2	1.87	0.55
53:S:135:LYS:NZ	79:t:2877:G:OP2	2.39	0.55
22:Sg:78:ALA:O	22:Sg:90:TRP:N	2.36	0.55
36:B:2:SER:O	36:B:3:HIS:ND1	2.40	0.55
48:N:14:TYR:HB3	48:N:56:GLN:HB2	1.89	0.55
79:t:358:G:N2	79:t:370:A:OP2	2.37	0.55
79:t:2738:G:H8	79:t:2743:A:H2	1.55	0.55
1:S2:1075:C:OP1	27:SN:107:LYS:NZ	2.40	0.55
1:S2:1083:A:N7	1:S2:1841:C:O2'	2.38	0.55
6:SF:134:VAL:HG12	6:SF:135:ARG:HG2	1.87	0.55
35:A:14:SER:OG	79:t:1610:C:OP1	2.24	0.55
50:P:54:TYR:OH	50:P:73:PHE:O	2.24	0.55
51:Q:39:MET:HG3	51:Q:43:LYS:HE2	1.88	0.55
66:f:43:ASN:ND2	79:t:1299:G:OP1	2.40	0.55
73:m:45:ARG:HH21	79:t:2775:G:H5'	1.71	0.55
79:t:3668:U:H5''	79:t:3669:G:H5'	1.89	0.55
36:B:264:PHE:N	50:P:64:THR:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:455:G:H22	79:t:687:A:H2	1.55	0.54
1:S2:420:G:O2'	1:S2:660:C:N3	2.38	0.54
1:S2:835:C:H41	30:SY:9:THR:H	1.55	0.54
1:S2:1314:U:O2'	9:SK:2:LEU:O	2.24	0.54
52:R:3:VAL:CG1	52:R:5:ILE:CG1	2.80	0.54
79:t:1732:G:N2	79:t:1763:U:O2	2.40	0.54
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	1.89	0.54
11:SP:17:TYR:OH	11:SP:18:ARG:CZ	2.52	0.54
67:g:33:VAL:HG23	67:g:38:GLU:HG3	1.90	0.54
1:S2:197:U:O2'	1:S2:203:G:N2	2.40	0.54
3:SB:185:VAL:CB	3:SB:188:LEU:HD11	2.28	0.54
11:SP:17:TYR:C	11:SP:17:TYR:CD2	2.86	0.54
26:SM:52:GLN:HG3	26:SM:65:VAL:HG11	1.89	0.54
38:D:109:C:N3	71:k:20:ARG:NH2	2.55	0.54
5:SE:201:HIS:HE1	5:SE:207:VAL:HG12	1.71	0.54
7:SH:32:MET:H	7:SH:36:LEU:HD22	1.71	0.54
24:SG:152:ASP:OD2	24:SG:155:GLN:NE2	2.41	0.54
36:B:37:PRO:C	36:B:188:GLY:HA2	2.32	0.54
36:B:219:VAL:HG11	36:B:337:VAL:HG13	1.89	0.54
39:E:27:G:OP1	46:L:146:ARG:NH2	2.35	0.54
43:I:230:TYR:HA	43:I:233:ILE:HG22	1.90	0.54
49:O:157:LYS:NZ	79:t:56:A:OP1	2.36	0.54
52:R:7:HIS:CE1	79:t:1648:C:O3'	2.61	0.54
54:T:70:LYS:O	54:T:72:PRO:HD3	2.07	0.54
74:n:100:TYR:O	79:t:4434:G:O2'	2.25	0.54
79:t:1789:C:O2	79:t:1814:G:N2	2.41	0.54
42:H:60:GLU:OE2	42:H:192:HIS:NE2	2.37	0.54
49:O:22:LEU:HD12	49:O:26:ARG:HH21	1.73	0.54
1:S2:1259:A:H61	1:S2:1519:U:H5''	1.72	0.54
4:SD:141:LYS:HD3	4:SD:180:GLY:HA3	1.90	0.54
7:SH:55:GLY:H	7:SH:57:ARG:HE	1.54	0.54
9:SK:64:TRP:CD2	21:Sd:23:VAL:HG22	2.43	0.54
55:U:129:LYS:HE2	79:t:1817:G:H4'	1.90	0.54
77:q:37:TYR:HB2	77:q:47:MET:HB2	1.90	0.54
79:t:211:G:OP2	79:t:211:G:N2	2.35	0.54
79:t:2566:A:H5'	79:t:2749:C:H5'	1.88	0.54
1:S2:1589:A:H4'	15:ST:82:ARG:HB2	1.89	0.54
45:K:4:ARG:NH1	79:t:1847:U:O4'	2.41	0.54
62:b:2:PRO:HG2	79:t:1491:C:H5''	1.90	0.54
1:S2:121:OMU:HM22	1:S2:122:G:H5'	1.89	0.54
1:S2:1481:G:N2	21:Sd:56:ASP:OD2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:192:SER:O	3:SB:193:ILE:C	2.49	0.54
36:B:247:GLY:HA2	79:t:2817:G:H5'	1.89	0.54
44:J:115:ARG:HB3	44:J:123:ILE:HG22	1.90	0.54
1:S2:871:U:H5'	27:SN:76:LYS:HE3	1.89	0.54
1:S2:1001:A:N7	19:Sa:19:GLN:NE2	2.55	0.54
12:SQ:34:VAL:HG12	12:SQ:70:VAL:HB	1.90	0.54
1:S2:1547:C:O2'	16:SU:62:ARG:NH2	2.40	0.53
1:S2:1547:C:N4	1:S2:1586:U:O4	2.33	0.53
7:SH:144:ILE:HD11	7:SH:152:ARG:HB2	1.90	0.53
13:SR:103:LYS:HD2	13:SR:119:VAL:HG11	1.89	0.53
14:SS:108:ARG:HH22	46:L:125:ILE:HD11	1.73	0.53
76:p:6:LYS:HE2	76:p:94:GLY:HA3	1.91	0.53
1:S2:1060:A:O2'	1:S2:1062:A:N7	2.34	0.53
1:S2:1283:C:N4	26:SM:102:LYS:O	2.37	0.53
3:SB:192:SER:O	3:SB:195:LYS:N	2.42	0.53
29:SW:27:ILE:HB	29:SW:61:ILE:HB	1.90	0.53
36:B:140:GLU:OE1	36:B:144:LYS:NZ	2.41	0.53
41:G:130:LYS:H	41:G:130:LYS:CD	2.17	0.53
53:S:109:TYR:CD1	53:S:114:LYS:HD3	2.43	0.53
1:S2:1175:G:OP1	75:o:21:ARG:NH2	2.40	0.53
1:S2:1452:A:O2'	1:S2:1475:G:N2	2.41	0.53
48:N:97:ALA:O	50:P:198:THR:OG1	2.23	0.53
49:O:110:CYS:HB3	49:O:113:LEU:HD23	1.90	0.53
81:v:47:U:H3	81:v:50:U:H3'	1.72	0.53
1:S2:384:U:O4	8:SI:5:ARG:NH2	2.31	0.53
9:SK:65:ARG:CG	21:Sd:22:ARG:O	2.55	0.53
23:SC:109:ILE:HD11	23:SC:151:ILE:HD12	1.90	0.53
25:SJ:86:VAL:HG11	25:SJ:105:PHE:HE1	1.74	0.53
55:U:17:ARG:HH11	55:U:47:THR:CG2	2.13	0.53
68:h:60:ARG:HD3	68:h:61:PRO:HD2	1.89	0.53
1:S2:10:G:H21	23:SC:114:LYS:HA	1.73	0.53
1:S2:70:G:O6	24:SG:170:ARG:NH1	2.40	0.53
1:S2:334:C:H5	24:SG:190:ARG:HH12	1.55	0.53
1:S2:692:G:H2'	1:S2:693:A:H8	1.74	0.53
1:S2:1024:A:OP2	27:SN:124:ARG:NH2	2.42	0.53
4:SD:28:GLU:HG2	4:SD:69:LEU:HD21	1.91	0.53
4:SD:205:PRO:HA	13:SR:42:PRO:HG2	1.91	0.53
76:p:8:ARG:NH2	79:t:4254:A:O2'	2.41	0.53
80:u:62:C:N4	80:u:63:G:O6	2.41	0.53
1:S2:539:C:N4	1:S2:542:U:OP2	2.41	0.53
1:S2:695:C:H3'	1:S2:736:C:H42	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:87:MET:HE1	5:SE:236:ILE:HG21	1.89	0.53
37:C:334:THR:O	37:C:338:ASN:ND2	2.41	0.53
1:S2:528:A:N6	1:S2:556:U:O4	2.35	0.53
1:S2:659:G:O2'	1:S2:662:G:O2'	2.25	0.53
8:SI:57:ALA:HB2	8:SI:183:GLY:HA2	1.91	0.53
45:K:188:LYS:HD2	45:K:212:LEU:HD13	1.91	0.53
1:S2:1005:G:OP2	64:d:9:LYS:NZ	2.41	0.53
1:S2:1310:U:OP1	34:Sf:131:PHE:N	2.39	0.53
1:S2:1839:U:H5	19:Sa:28:ARG:HH12	1.57	0.53
7:SH:160:LYS:HA	7:SH:163:GLN:HB2	1.90	0.53
26:SM:83:LYS:HE3	26:SM:104:VAL:HG13	1.89	0.53
35:A:95:GLN:HE21	77:q:87:LYS:HD3	1.74	0.53
36:B:95:THR:HG22	79:t:4868:A:H4'	1.90	0.53
36:B:116:ARG:HG2	36:B:177:LYS:HG2	1.89	0.53
40:F:29:ASP:OD1	40:F:29:ASP:N	2.40	0.53
44:J:59:LYS:CE	44:J:66:GLU:HB3	2.38	0.53
56:V:61:VAL:HG22	56:V:62:THR:N	2.23	0.53
58:X:51:TRP:O	79:t:4999:G:N2	2.42	0.53
62:b:32:ARG:NH1	79:t:1498:G:OP2	2.42	0.53
76:p:39:ARG:HD2	79:t:289:A:H5'	1.91	0.53
30:SY:90:ARG:C	30:SY:93:ARG:HG3	2.34	0.53
42:H:101:VAL:HG13	42:H:139:TYR:HE2	1.73	0.53
48:N:97:ALA:HB1	50:P:198:THR:HG23	1.91	0.53
60:Z:45:ARG:NH2	79:t:234:G:OP2	2.41	0.53
79:t:478:U:H3	79:t:665:G:H22	1.57	0.53
1:S2:104:A:H62	1:S2:356:C:H5	1.56	0.53
41:G:130:LYS:HE3	79:t:1268:U:H1'	1.90	0.53
43:I:137:ARG:HG3	43:I:146:LEU:HD11	1.91	0.53
12:SQ:51:LEU:HB2	12:SQ:84:ILE:HD11	1.91	0.52
13:SR:100:PRO:HD2	13:SR:122:PRO:HD3	1.91	0.52
42:H:188:GLU:OE2	79:t:931:A:N6	2.42	0.52
52:R:10:ASP:C	79:t:2062:C:HO2'	2.00	0.52
3:SB:138:PHE:O	3:SB:213:ARG:N	2.42	0.52
52:R:62:SER:OG	79:t:1484:G:OP2	2.25	0.52
59:Y:110:LYS:NZ	59:Y:121:VAL:O	2.42	0.52
1:S2:146:G:H1	1:S2:173:A:H61	1.57	0.52
1:S2:1680:G:H4'	20:Sc:20:ARG:HH11	1.75	0.52
8:SI:22:HIS:ND1	8:SI:23:LYS:O	2.39	0.52
15:ST:11:GLN:OE1	15:ST:62:ARG:NH2	2.42	0.52
40:F:28:THR:O	79:t:4242:A:N6	2.41	0.52
64:d:20:LEU:HD22	64:d:102:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:67:C:N4	24:SG:168:LYS:O	2.42	0.52
37:C:219:LYS:HD2	37:C:222:ARG:HH21	1.75	0.52
47:M:25:TRP:HE1	49:O:199:GLN:HE21	1.57	0.52
51:Q:119:VAL:HG13	51:Q:146:ILE:HG22	1.91	0.52
56:V:56:LEU:HD23	56:V:61:VAL:HG13	1.90	0.52
78:r:84:LYS:HB2	78:r:89:THR:HB	1.91	0.52
79:t:950:G:N7	79:t:951:A:N6	2.57	0.52
79:t:2484:C:O2'	79:t:2485:G:N2	2.42	0.52
1:S2:936:G:O6	64:d:8:LYS:NZ	2.43	0.52
1:S2:1300:U:H2'	11:SP:51:ARG:HD3	1.91	0.52
11:SP:16:THR:OG1	11:SP:20:VAL:N	2.42	0.52
36:B:293:ILE:O	36:B:298:LEU:CA	2.55	0.52
36:B:293:ILE:C	36:B:294:LYS:HD2	2.34	0.52
37:C:54:VAL:HG22	38:D:27:U:H4'	1.90	0.52
37:C:204:ARG:NH2	79:t:2278:G:OP2	2.35	0.52
68:h:101:LYS:HA	68:h:104:VAL:HG12	1.91	0.52
79:t:4217:A:N6	80:u:19:G:O6	2.43	0.52
1:S2:141:A:H4'	1:S2:142:C:H3'	1.91	0.52
1:S2:1091:C:OP1	27:SN:9:LYS:NZ	2.42	0.52
11:SP:127:LYS:NZ	11:SP:127:LYS:CB	2.73	0.52
23:SC:80:GLU:HA	23:SC:83:LEU:HG	1.92	0.52
25:SJ:46:VAL:HG23	25:SJ:102:ILE:HD11	1.91	0.52
26:SM:64:LEU:HD11	34:Sf:106:TYR:HB2	1.92	0.52
40:F:155:THR:HG22	40:F:179:ARG:HD3	1.91	0.52
50:P:176:ARG:HD3	79:t:4730:G:H5''	1.92	0.52
54:T:70:LYS:CA	54:T:70:LYS:CE	2.87	0.52
79:t:183:G:O2'	79:t:1349:G:N3	2.41	0.52
79:t:226:G:H22	79:t:236:C:H1'	1.73	0.52
1:S2:1220:A:N3	1:S2:1677:U:O2'	2.41	0.52
25:SJ:88:ASP:N	25:SJ:88:ASP:OD1	2.42	0.52
36:B:294:LYS:CD	36:B:294:LYS:N	2.73	0.52
38:D:85:U:H2'	38:D:86:U:H2'	1.92	0.52
43:I:143:VAL:HG22	43:I:203:ALA:HB2	1.91	0.52
48:N:14:TYR:HD2	48:N:56:GLN:HG3	1.73	0.52
76:p:22:LYS:HZ3	76:p:73:VAL:HG23	1.73	0.52
79:t:3625:G:O2'	79:t:3664:U:OP1	2.25	0.52
4:SD:169:ASP:N	4:SD:169:ASP:OD1	2.41	0.52
11:SP:110:GLU:HB3	14:SS:117:ILE:HG21	1.92	0.52
30:SY:38:THR:HA	30:SY:41:ARG:HG2	1.91	0.52
35:A:179:ILE:HG21	35:A:185:ALA:HB2	1.90	0.52
54:T:67:VAL:O	54:T:67:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1963:G:O2'	79:t:1991:A:O2'	2.28	0.52
7:SH:142:LYS:HB3	29:SW:54:ASP:HB3	1.92	0.52
8:SI:57:ALA:H	8:SI:180:GLY:HA2	1.74	0.52
24:SG:1:MET:HE1	24:SG:106:LEU:HB2	1.92	0.52
30:SY:120:THR:O	30:SY:124:ASN:N	2.43	0.52
41:G:46:ARG:NH1	79:t:966:C:OP1	2.42	0.52
42:H:115:ARG:CG	52:R:4:ASP:OD1	2.58	0.52
61:a:92:ASP:N	61:a:92:ASP:OD1	2.43	0.52
79:t:3754:A:H4'	79:t:3755:A:H5'	1.92	0.52
1:S2:85:A:H5'	30:SY:119:GLY:HA2	1.91	0.52
1:S2:1447:G:OP1	16:SU:85:HIS:ND1	2.42	0.52
37:C:192:GLY:O	37:C:195:LYS:NZ	2.37	0.52
37:C:228:THR:OG1	37:C:248:ARG:NH2	2.43	0.52
40:F:22:ARG:HD2	40:F:27:LYS:HB2	1.92	0.52
41:G:155:GLY:HA2	79:t:4900:C:H5''	1.92	0.52
51:Q:15:CYS:SG	51:Q:16:LYS:N	2.83	0.52
1:S2:1114:U:OP2	1:S2:1115:U:O2'	2.27	0.51
10:SL:10:TYR:HE2	10:SL:18:GLN:HE22	1.58	0.51
49:O:166:SER:HA	49:O:169:ARG:HG2	1.93	0.51
67:g:6:TRP:CD2	67:g:102:ARG:HG3	2.45	0.51
79:t:175:C:O2	79:t:254:C:N4	2.43	0.51
79:t:2499:C:H5	79:t:2514:G:H1	1.58	0.51
79:t:4692:C:H5'	79:t:4696:A:H61	1.75	0.51
5:SE:66:MET:SD	5:SE:78:THR:OG1	2.69	0.51
27:SN:5:HIS:HB3	27:SN:117:LEU:HD23	1.92	0.51
41:G:152:ILE:O	41:G:159:GLY:N	2.43	0.51
42:H:171:ASP:HB2	42:H:174:LEU:HD13	1.91	0.51
47:M:79:GLU:H	47:M:79:GLU:CD	2.15	0.51
79:t:25:A:N3	79:t:333:C:O2'	2.39	0.51
2:SA:12:GLU:OE2	13:SR:115:SER:OG	2.27	0.51
33:Se:2:VAL:HG23	33:Se:8:ARG:HH22	1.76	0.51
43:I:173:LEU:HD12	70:j:43:MET:HE2	1.92	0.51
47:M:124:LEU:HD11	69:i:119:TYR:HB2	1.92	0.51
52:R:3:VAL:HG13	52:R:5:ILE:CG1	2.29	0.51
79:t:1572:C:H4'	79:t:2836:A:H5'	1.91	0.51
79:t:4716:G:H22	79:t:4837:C:H1'	1.74	0.51
1:S2:1291:A:O2'	34:Sf:140:TYR:OH	2.22	0.51
35:A:201:GLY:HA2	35:A:204:MET:HE3	1.92	0.51
78:r:107:ARG:NH2	79:t:2242:A:OP1	2.41	0.51
1:S2:94:G:O2'	1:S2:508:A:O2'	2.21	0.51
1:S2:1172:U:OP1	75:o:14:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:41:ARG:HD3	2:SA:45:GLY:HA2	1.93	0.51
31:SZ:99:LEU:HD11	31:SZ:102:LYS:HB2	1.93	0.51
45:K:33:ILE:O	45:K:69:ARG:NH1	2.41	0.51
61:a:59:LYS:HB3	61:a:61:LYS:HG2	1.92	0.51
1:S2:696:G:N2	1:S2:735:C:OP2	2.44	0.51
1:S2:1033:G:N1	1:S2:1080:A:O2'	2.35	0.51
5:SE:11:ARG:HA	5:SE:28:ALA:HB2	1.92	0.51
14:SS:3:LEU:HD12	14:SS:4:VAL:HG23	1.93	0.51
20:Sc:31:ARG:HA	20:Sc:43:ILE:HA	1.92	0.51
36:B:59:GLU:HB2	36:B:366:LYS:HD2	1.93	0.51
49:O:49:ARG:NH2	79:t:150:G:OP2	2.43	0.51
51:Q:4:TYR:OH	79:t:394:A:OP1	2.28	0.51
52:R:64:SER:HA	52:R:67:ILE:HG12	1.92	0.51
55:U:18:PRO:O	55:U:19:PHE:CB	2.59	0.51
69:i:109:ARG:HH21	69:i:113:LEU:HD11	1.76	0.51
2:SA:30:LEU:HA	2:SA:150:THR:HB	1.93	0.51
3:SB:113:MET:HE3	3:SB:209:ASP:HB3	1.91	0.51
31:SZ:57:LYS:HE3	31:SZ:77:LEU:HG	1.92	0.51
36:B:357:ARG:NH1	79:t:4577:C:O3'	2.44	0.51
1:S2:560:A:H2'	25:SJ:164:PRO:HB3	1.92	0.51
5:SE:137:PRO:HG2	5:SE:149:TYR:HA	1.93	0.51
46:L:95:ARG:HH12	46:L:97:ASN:HD21	1.59	0.51
49:O:144:ARG:NH1	79:t:124:C:OP1	2.44	0.51
79:t:1512:G:O6	79:t:1625:A:N6	2.44	0.51
31:SZ:98:LYS:NZ	31:SZ:111:ARG:O	2.40	0.51
44:J:41:ILE:HG21	44:J:73:ILE:HD11	1.92	0.51
44:J:180:TYR:OH	74:n:90:ASN:ND2	2.40	0.51
70:j:70:LEU:HD11	70:j:84:LYS:HG2	1.92	0.51
79:t:1414:C:H42	79:t:1435:A:H61	1.57	0.51
1:S2:1242:U:O2	1:S2:1517:G:O2'	2.23	0.51
2:SA:190:SER:HA	17:SV:45:ARG:HH21	1.76	0.51
10:SL:22:ARG:HA	10:SL:22:ARG:HE	1.74	0.51
26:SM:75:ASN:OD1	26:SM:75:ASN:N	2.44	0.51
50:P:194:GLU:O	50:P:199:HIS:N	2.44	0.51
61:a:57:MET:HE3	61:a:61:LYS:HD2	1.92	0.51
68:h:4:ARG:NH2	79:t:2376:G:O6	2.41	0.51
72:l:37:ARG:NH1	79:t:2516:A:OP2	2.44	0.51
79:t:694:G:OP2	79:t:694:G:N2	2.37	0.51
79:t:2067:G:H1	79:t:2249:G:H1	1.58	0.51
1:S2:317:C:OP2	24:SG:183:ARG:NH2	2.44	0.50
1:S2:1451:G:N7	13:SR:44:LYS:NZ	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SP:108:LYS:HD3	14:SS:117:ILE:HG22	1.92	0.50
20:Sc:14:VAL:HG12	20:Sc:32:VAL:HG12	1.93	0.50
29:SW:31:SER:HB3	29:SW:34:ILE:HG12	1.93	0.50
42:H:76:ARG:NH2	79:t:718:C:OP1	2.44	0.50
65:e:87:ARG:HH21	65:e:109:VAL:HG11	1.76	0.50
79:t:1619:A:OP1	79:t:1622:C:N4	2.42	0.50
1:S2:587:A:H1'	1:S2:590:A:H1'	1.93	0.50
1:S2:944:A:H5''	28:SO:134:PRO:HB3	1.93	0.50
1:S2:1648:G:H8	12:SQ:17:LYS:CD	2.21	0.50
18:SX:61:GLN:HE21	18:SX:61:GLN:N	2.07	0.50
55:U:17:ARG:NH1	55:U:47:THR:HG21	1.98	0.50
58:X:11:TYR:OH	79:t:4999:G:N2	2.41	0.50
64:d:59:GLU:HB3	68:h:96:LEU:HD11	1.93	0.50
77:q:51:ALA:HB3	77:q:54:ILE:HD12	1.93	0.50
20:Sc:11:LEU:HD12	20:Sc:55:VAL:HG11	1.93	0.50
36:B:66:LYS:HD3	57:W:12:ALA:HB3	1.93	0.50
47:M:58:ILE:HG12	47:M:116:ARG:HD2	1.94	0.50
52:R:91:ARG:HG3	62:b:76:ASP:HB3	1.92	0.50
66:f:99:ILE:HD13	66:f:108:ARG:HG3	1.92	0.50
1:S2:964:A:N3	1:S2:1054:G:O2'	2.41	0.50
3:SB:104:ASP:N	3:SB:104:ASP:OD1	2.43	0.50
16:SU:67:LYS:HB3	16:SU:76:THR:HG23	1.93	0.50
31:SZ:68:ILE:HG23	31:SZ:109:TYR:HB2	1.93	0.50
36:B:35:ASP:CB	36:B:186:ASN:OD1	2.50	0.50
37:C:209:ILE:HG13	37:C:251:ILE:HB	1.93	0.50
46:L:37:ALA:HB1	46:L:48:PRO:HG2	1.94	0.50
46:L:150:CYS:SG	46:L:151:ILE:N	2.84	0.50
49:O:16:SER:OG	70:j:48:CYS:SG	2.61	0.50
54:T:101:THR:HG23	54:T:104:GLY:H	1.76	0.50
65:e:32:ARG:NH2	79:t:4954:C:OP1	2.40	0.50
79:t:445:C:N4	79:t:1278:C:N3	2.59	0.50
1:S2:863:U:O3'	29:SW:78:ARG:NH1	2.44	0.50
1:S2:1671:G:O3'	12:SQ:18:THR:OG1	2.29	0.50
1:S2:1791:A:H5''	24:SG:75:LEU:HD11	1.93	0.50
2:SA:67:ALA:HB2	17:SV:37:ALA:HB2	1.94	0.50
3:SB:184:VAL:O	3:SB:188:LEU:CD2	2.59	0.50
11:SP:13:ARG:N	11:SP:13:ARG:CD	2.73	0.50
37:C:250:CYS:SG	37:C:252:TRP:NE1	2.83	0.50
38:D:22:U:O4	79:t:346:G:O2'	2.28	0.50
41:G:206:VAL:HG13	41:G:207:LYS:H	1.76	0.50
54:T:164:LYS:CB	54:T:165:PRO:CD	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:k:56:ARG:NH2	79:t:369:G:N7	2.55	0.50
3:SB:186:ASN:O	3:SB:190:PRO:CD	2.59	0.50
14:SS:30:ILE:HD12	14:SS:71:MET:HE1	1.94	0.50
41:G:141:ARG:HG3	41:G:191:GLN:HE21	1.76	0.50
57:W:15:ARG:NH1	57:W:16:ILE:O	2.44	0.50
63:c:51:LYS:NZ	79:t:1383:G:O3'	2.44	0.50
79:t:729:C:N4	79:t:730:G:O6	2.45	0.50
79:t:2848:U:O2'	79:t:2860:A:N7	2.42	0.50
1:S2:1079:C:O2'	1:S2:1182:A:N1	2.45	0.50
1:S2:1340:U:H3'	1:S2:1341:C:H2'	1.92	0.50
1:S2:1454:A:H5''	13:SR:3:ARG:HG2	1.93	0.50
1:S2:1497:G:C4	9:SK:62:PHE:CD2	2.99	0.50
2:SA:89:LYS:HD3	2:SA:202:TYR:CG	2.42	0.50
11:SP:17:TYR:CE1	11:SP:112:ILE:HG22	2.46	0.50
23:SC:221:ASP:N	23:SC:221:ASP:OD1	2.42	0.50
36:B:80:GLU:OE1	36:B:323:TYR:OH	2.29	0.50
42:H:115:ARG:HG2	52:R:4:ASP:OD1	2.11	0.50
45:K:138:ILE:HD11	45:K:148:VAL:HG22	1.93	0.50
54:T:68:PHE:HE2	79:t:722:G:C1'	2.18	0.50
56:V:48:LYS:NZ	79:t:2609:U:OP1	2.43	0.50
64:d:48:LEU:HD13	64:d:57:LYS:HG3	1.93	0.50
78:r:32:LEU:O	78:r:113:ARG:NH2	2.45	0.50
79:t:102:G:HO2'	79:t:1364:U:HO2'	1.60	0.50
1:S2:1597:C:OP2	31:SZ:85:ARG:NH2	2.36	0.50
16:SU:63:ILE:HD11	21:Sd:31:ILE:HD13	1.93	0.50
25:SJ:170:PRO:HB2	25:SJ:174:LYS:HB3	1.93	0.50
76:p:26:TYR:HB3	76:p:67:VAL:HG23	1.93	0.50
1:S2:193:C:O2'	1:S2:195:C:N4	2.38	0.50
1:S2:890:U:H5'	1:S2:896:U:H3	1.77	0.50
7:SH:34:SER:HB2	7:SH:78:ARG:HD3	1.94	0.50
8:SI:67:TRP:CD1	8:SI:70:GLU:H	2.29	0.50
36:B:384:GLU:OE2	58:X:14:TYR:OH	2.30	0.50
41:G:74:SER:O	79:t:1256:G:O2'	2.27	0.50
42:H:232:ASP:HB2	42:H:236:ARG:NH2	2.25	0.50
44:J:59:LYS:HZ1	44:J:66:GLU:HB3	1.77	0.50
62:b:4:ARG:NH2	79:t:2320:A:OP2	2.45	0.50
79:t:2374:A:O2'	79:t:2786:A:OP2	2.29	0.50
79:t:3663:A:H62	79:t:3794:G:N2	2.09	0.50
79:t:4732:U:H3	79:t:4820:G:H22	1.58	0.50
1:S2:913:A:N7	7:SH:120:ARG:NE	2.55	0.49
36:B:219:VAL:HG13	36:B:345:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G:183:ARG:HB3	79:t:4896:A:H5'	1.94	0.49
43:I:141:ASN:OD1	49:O:2:GLY:N	2.44	0.49
53:S:46:LYS:NZ	79:t:2684:G:O6	2.44	0.49
54:T:82:LEU:HD22	54:T:124:ILE:HD11	1.92	0.49
17:SV:80:SER:OG	17:SV:82:ASN:OD1	2.22	0.49
20:Sc:20:ARG:HE	20:Sc:28:THR:HG22	1.77	0.49
20:Sc:44:ARG:NH2	20:Sc:61:SER:O	2.45	0.49
53:S:42:ARG:HA	53:S:45:ILE:HD12	1.94	0.49
79:t:946:G:O2'	79:t:2242:A:N6	2.42	0.49
1:S2:1101:U:H5'	13:SR:132:ARG:HH12	1.77	0.49
37:C:295:SER:OG	37:C:297:GLU:OE1	2.29	0.49
50:P:127:VAL:HG13	54:T:161:ARG:HE	1.77	0.49
57:W:121:VAL:O	57:W:140:ALA:N	2.41	0.49
70:j:62:LYS:HE3	70:j:94:LEU:HD11	1.93	0.49
79:t:249:C:H2'	79:t:250:G:C8	2.48	0.49
79:t:451:G:H22	79:t:691:G:H22	1.59	0.49
79:t:2838:G:N2	79:t:3808:C:O2	2.34	0.49
1:S2:943:U:O2'	28:SO:135:ILE:O	2.30	0.49
2:SA:104:THR:O	2:SA:107:THR:OG1	2.26	0.49
7:SH:13:GLY:C	7:SH:14:GLU:CD	2.81	0.49
17:SV:43:THR:OG1	17:SV:45:ARG:NH1	2.45	0.49
22:Sg:73:SER:HB2	22:Sg:117:ASN:HD21	1.77	0.49
30:SY:90:ARG:CA	30:SY:93:ARG:HG3	2.43	0.49
36:B:294:LYS:HD2	36:B:294:LYS:N	2.28	0.49
45:K:89:VAL:HG22	45:K:136:MET:HG2	1.94	0.49
50:P:36:VAL:HG12	50:P:108:ILE:HG12	1.94	0.49
54:T:9:GLU:HG2	54:T:67:VAL:CG1	2.43	0.49
69:i:111:GLU:OE1	79:t:171:C:O2'	2.23	0.49
1:S2:1286:G:H22	26:SM:38:ALA:HB3	1.76	0.49
1:S2:1425:G:O3'	12:SQ:33:LYS:NZ	2.45	0.49
3:SB:189:ILE:H	3:SB:189:ILE:CD1	2.25	0.49
12:SQ:51:LEU:HD12	12:SQ:84:ILE:HD11	1.93	0.49
41:G:128:HIS:HB2	79:t:1265:G:C6	2.47	0.49
49:O:125:SER:HB2	79:t:3908:C:H1'	1.93	0.49
79:t:1769:A:N3	79:t:4172:U:O2'	2.43	0.49
79:t:2579:A:N6	79:t:2724:A:OP2	2.38	0.49
1:S2:1109:C:C1'	13:SR:124:VAL:HG23	2.41	0.49
1:S2:1414:A:O2'	15:ST:128:GLN:NE2	2.45	0.49
1:S2:1593:C:O2	15:ST:12:GLN:NE2	2.46	0.49
4:SD:66:ILE:O	4:SD:70:THR:N	2.42	0.49
7:SH:144:ILE:HG23	29:SW:52:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SK:91:PRO:HB2	9:SK:93:THR:HG23	1.94	0.49
38:D:13:G:O2'	51:Q:121:LYS:O	2.30	0.49
38:D:29:G:H5''	47:M:27:ASN:HB3	1.94	0.49
44:J:59:LYS:NZ	44:J:62:GLY:HA3	2.27	0.49
49:O:93:LYS:O	79:t:294:A:O2'	2.30	0.49
62:b:102:ASP:HB3	62:b:125:LYS:HB2	1.93	0.49
64:d:103:ASP:HB2	64:d:106:ARG:HB2	1.95	0.49
79:t:1268:U:O2'	79:t:1269:C:O4'	2.24	0.49
79:t:1298:C:O2	79:t:1312:G:N2	2.45	0.49
29:SW:112:ASP:HB2	29:SW:115:GLU:H	1.77	0.49
36:B:10:ARG:NH1	36:B:11:HIS:O	2.46	0.49
42:H:241:ASN:O	42:H:245:ARG:NH1	2.46	0.49
44:J:59:LYS:HZ2	44:J:66:GLU:HB3	1.76	0.49
44:J:128:MET:SD	44:J:157:SER:OG	2.70	0.49
45:K:188:LYS:HZ1	45:K:213:HIS:H	1.61	0.49
67:g:45:LYS:HD3	67:g:107:PRO:HD2	1.94	0.49
67:g:91:ASN:O	79:t:434:U:O2'	2.30	0.49
77:q:46:LYS:HB3	77:q:58:GLY:H	1.77	0.49
79:t:1070:A:H2	79:t:1191:G:H22	1.60	0.49
1:S2:1512:C:O2'	21:Sd:7:TYR:O	2.27	0.49
14:SS:89:ASP:OD1	14:SS:94:LYS:N	2.43	0.49
29:SW:60:LYS:NZ	32:Sb:23:ARG:O	2.46	0.49
44:J:23:ARG:HE	44:J:39:ASN:HA	1.78	0.49
55:U:7:LYS:O	79:t:4296:U:O2'	2.27	0.49
62:b:29:PRO:HB2	79:t:1663:G:H5'	1.95	0.49
1:S2:1289:U:OP2	34:Sf:97:LYS:NZ	2.45	0.49
2:SA:108:PHE:HB2	2:SA:136:GLU:HG2	1.95	0.49
4:SD:226:GLN:HG3	22:Sg:186:THR:HG22	1.94	0.49
6:SF:61:PHE:O	20:Sc:51:ARG:NH2	2.46	0.49
8:SI:178:ARG:HD3	8:SI:181:GLN:HG2	1.95	0.49
10:SL:20:LYS:C	10:SL:20:LYS:HD3	2.38	0.49
14:SS:98:VAL:HG23	14:SS:103:LEU:HD23	1.94	0.49
44:J:68:ALA:O	79:t:4653:A:O2'	2.29	0.49
48:N:11:ARG:HE	48:N:61:ILE:HG22	1.76	0.49
54:T:160:ARG:HG3	54:T:163:HIS:CG	2.47	0.49
55:U:18:PRO:O	55:U:19:PHE:HB2	2.12	0.49
57:W:21:PRO:HA	57:W:54:ALA:HA	1.94	0.49
63:c:31:SER:HB3	79:t:1445:C:H5''	1.95	0.49
76:p:68:LEU:HD11	76:p:85:ILE:HD11	1.95	0.49
79:t:746:C:H2'	79:t:747:G:H8	1.78	0.49
79:t:1798:C:O2	79:t:1805:G:N2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4857:G:N2	79:t:4880:C:N3	2.60	0.49
1:S2:639:C:H2'	1:S2:640:A:H8	1.77	0.49
1:S2:974:C:O2	28:SO:55:ARG:NH1	2.46	0.49
1:S2:1183:A:OP1	75:o:15:ARG:NH2	2.44	0.49
3:SB:28:LYS:HA	3:SB:50:THR:HA	1.94	0.49
9:SK:53:LYS:HD3	9:SK:60:GLU:HG2	1.95	0.49
13:SR:6:THR:OG1	13:SR:7:LYS:N	2.46	0.49
25:SJ:79:ARG:HH12	25:SJ:83:ARG:HH21	1.61	0.49
26:SM:39:ALA:HB2	26:SM:61:TYR:HE1	1.77	0.49
37:C:178:ASN:OD1	79:t:2279:A:N6	2.46	0.49
42:H:94:ARG:NH2	42:H:97:GLY:O	2.46	0.49
43:I:148:GLU:HA	43:I:177:MET:HG3	1.95	0.49
44:J:91:LYS:HG2	44:J:145:ILE:HG12	1.95	0.49
55:U:84:ILE:HD11	63:c:24:PRO:HD3	1.95	0.49
60:Z:48:PRO:O	60:Z:115:ARG:NH2	2.45	0.49
66:f:52:GLN:O	79:t:431:G:O2'	2.28	0.49
1:S2:682:U:H5'	18:SX:8:ARG:NE	2.28	0.48
10:SL:21:LYS:O	10:SL:23:VAL:HG22	2.13	0.48
10:SL:22:ARG:NH2	10:SL:26:GLY:HA3	2.27	0.48
18:SX:60:LYS:HG3	18:SX:114:ASP:HB2	1.95	0.48
46:L:87:LEU:O	46:L:92:TYR:N	2.45	0.48
58:X:6:CYS:HA	58:X:30:GLN:HB2	1.95	0.48
66:f:38:PRO:HB2	66:f:43:ASN:HD21	1.77	0.48
71:k:14:LYS:HE2	73:m:51:LEU:HD23	1.95	0.48
71:k:82:THR:OG1	71:k:83:THR:N	2.46	0.48
79:t:654:G:H2'	79:t:655:A:H8	1.78	0.48
1:S2:835:C:H5	30:SY:8:ARG:HE	1.58	0.48
1:S2:1160:U:OP1	18:SX:8:ARG:NH1	2.41	0.48
1:S2:1708:C:O2'	79:t:3730:A:N1	2.44	0.48
3:SB:146:ARG:HB2	3:SB:149:GLN:HB2	1.95	0.48
25:SJ:54:ARG:NH2	25:SJ:98:LEU:O	2.42	0.48
50:P:12:ARG:NH2	79:t:4723:G:OP2	2.46	0.48
54:T:70:LYS:C	54:T:72:PRO:HD3	2.37	0.48
79:t:1251:G:H2'	79:t:1252:G:C8	2.48	0.48
1:S2:1497:G:C5	9:SK:62:PHE:CE1	3.01	0.48
3:SB:137:LEU:HD11	3:SB:176:VAL:HG21	1.95	0.48
6:SF:68:ILE:HD13	6:SF:112:LEU:HD22	1.94	0.48
40:F:21:ARG:HA	40:F:24:ARG:HH21	1.77	0.48
41:G:165:LEU:HG	41:G:176:THR:H	1.77	0.48
50:P:172:LYS:HA	50:P:175:MET:HG2	1.93	0.48
52:R:42:THR:HB	79:t:1411:U:H5''	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:o:13:LEU:HD21	75:o:17:ARG:HH21	1.77	0.48
77:q:7:LYS:HE2	79:t:2854:C:H2'	1.96	0.48
79:t:976:U:H3	79:t:1047:G:H1	1.61	0.48
1:S2:1520:G:H21	11:SP:126:VAL:HG11	1.78	0.48
1:S2:1553:C:N4	21:Sd:22:ARG:HH21	1.92	0.48
2:SA:177:MET:SD	2:SA:180:ARG:NH2	2.68	0.48
5:SE:44:LEU:HD11	5:SE:70:ILE:HG21	1.95	0.48
10:SL:68:ILE:HD12	10:SL:143:LEU:HD11	1.96	0.48
10:SL:103:GLU:HG3	18:SX:11:ARG:HB2	1.95	0.48
23:SC:183:LYS:HG2	29:SW:95:PRO:HA	1.95	0.48
54:T:98:ARG:HH22	79:t:737:A:H61	1.61	0.48
79:t:1181:G:H2'	79:t:1182:G:H8	1.79	0.48
79:t:4964:U:H4'	79:t:4965:A:H5'	1.95	0.48
8:SI:5:ARG:HE	8:SI:31:ARG:CZ	2.26	0.48
21:Sd:54:LYS:HD3	21:Sd:55:LEU:H	1.78	0.48
36:B:162:VAL:N	36:B:183:ILE:O	2.46	0.48
37:C:326:LEU:HD23	79:t:963:G:H4'	1.94	0.48
57:W:90:ARG:NE	57:W:124:GLU:OE2	2.45	0.48
67:g:54:LYS:HA	67:g:66:LYS:HE3	1.95	0.48
71:k:34:CYS:SG	71:k:35:GLY:N	2.87	0.48
79:t:162:A:H61	79:t:265:C:H42	1.61	0.48
79:t:1249:G:N2	79:t:1251:G:O6	2.38	0.48
81:v:16:A:H62	81:v:20:U:H5	1.60	0.48
1:S2:1256:G:OP2	21:Sd:40:ARG:NH1	2.47	0.48
3:SB:103:MET:HG3	3:SB:215:VAL:HB	1.94	0.48
3:SB:189:ILE:N	3:SB:190:PRO:HD2	2.29	0.48
7:SH:12:ASN:CB	7:SH:14:GLU:O	2.57	0.48
8:SI:42:ARG:HH21	8:SI:59:ARG:HD3	1.79	0.48
23:SC:191:VAL:HG11	23:SC:236:PHE:HD1	1.78	0.48
36:B:175:GLN:HG3	79:t:4943:U:H4'	1.95	0.48
41:G:240:TYR:HD2	41:G:242:ILE:HG22	1.79	0.48
50:P:79:ILE:HG21	50:P:138:LEU:HD11	1.95	0.48
79:t:173:G:H22	79:t:255:G:H1	1.62	0.48
79:t:742:G:N2	79:t:743:G:N7	2.61	0.48
79:t:4853:C:N4	79:t:4854:G:N3	2.61	0.48
5:SE:201:HIS:ND1	5:SE:205:PHE:O	2.47	0.48
12:SQ:42:ILE:HG23	12:SQ:44:PRO:HD2	1.94	0.48
49:O:4:TYR:OH	79:t:149:U:OP2	2.31	0.48
49:O:114:ARG:O	49:O:135:ILE:N	2.45	0.48
54:T:16:CYS:HA	54:T:59:GLY:HA2	1.95	0.48
55:U:17:ARG:CG	55:U:22:HIS:CE1	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1831:A:N3	79:t:2262:G:O2'	2.46	0.48
79:t:2026:G:N2	79:t:2027:G:N7	2.58	0.48
79:t:4168:C:O2'	79:t:4297:C:O2'	2.32	0.48
79:t:4562:G:O2'	79:t:4571:G:O6	2.28	0.48
1:S2:150:A:N6	1:S2:169:U:O2	2.46	0.48
1:S2:1250:A:OP2	12:SQ:143:LYS:NZ	2.46	0.48
6:SF:118:ASN:ND2	6:SF:181:ALA:O	2.47	0.48
9:SK:62:PHE:C	9:SK:63:ALA:O	2.57	0.48
11:SP:96:VAL:HG11	11:SP:116:LEU:HB3	1.95	0.48
20:Sc:29:GLN:HB3	20:Sc:43:ILE:HD11	1.96	0.48
44:J:58:ASP:OD1	44:J:58:ASP:N	2.43	0.48
69:i:37:THR:HG23	69:i:39:GLY:H	1.79	0.48
79:t:1581:A:OP1	79:t:2774:A:N6	2.40	0.48
79:t:4730:G:H1	79:t:4822:U:H3	1.62	0.48
2:SA:51:LEU:HA	2:SA:54:THR:HG22	1.96	0.48
2:SA:184:ARG:HD3	2:SA:191:ARG:HD3	1.96	0.48
7:SH:15:LYS:C	7:SH:15:LYS:CD	2.85	0.48
23:SC:169:TYR:OH	23:SC:175:GLY:O	2.31	0.48
23:SC:176:LYS:O	23:SC:200[A]:ARG:NH1	2.47	0.48
35:A:117:GLU:HG2	35:A:124:GLY:H	1.79	0.48
41:G:179:LEU:C	41:G:179:LEU:CD1	2.86	0.48
65:e:64:ILE:HD11	79:t:2352:C:H4'	1.95	0.48
79:t:1420:C:O2'	79:t:2079:G:OP2	2.28	0.48
1:S2:910:G:OP2	53:S:176:ARG:NH2	2.47	0.48
5:SE:181:CYS:HA	5:SE:227:VAL:HA	1.96	0.48
8:SI:62:VAL:HA	8:SI:77:ARG:HA	1.95	0.48
34:Sf:118:ARG:HG3	34:Sf:134:SER:HB3	1.95	0.48
36:B:298:LEU:HD23	36:B:299:ILE:O	2.14	0.48
47:M:31:ARG:HH12	79:t:331:U:H5''	1.79	0.48
48:N:105:THR:HG23	48:N:108:ASP:H	1.78	0.48
52:R:67:ILE:HD11	52:R:92:VAL:HG21	1.96	0.48
66:f:5:ARG:NH1	79:t:449:C:H1'	2.28	0.48
79:t:192:C:H42	79:t:240:A:H61	1.62	0.48
79:t:4531:U:O5'	79:t:4940:A:O2'	2.32	0.48
1:S2:917:U:H1'	7:SH:118:ARG:HD2	1.96	0.47
1:S2:1006:C:H5'	64:d:11:LEU:H	1.79	0.47
1:S2:1232:U:H2'	1:S2:1233:G:H8	1.78	0.47
3:SB:35:ALA:HB2	3:SB:44:ILE:HD11	1.96	0.47
7:SH:162:GLN:NE2	7:SH:165:ASN:OD1	2.35	0.47
12:SQ:18:THR:O	12:SQ:75:GLY:CA	2.61	0.47
22:Sg:104:HIS:H	22:Sg:106:LYS:HE3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:144:ASN:OD1	55:U:144:ASN:N	2.47	0.47
79:t:1058:G:H1	79:t:1218:G:H1	1.62	0.47
79:t:1700:C:H5'	79:t:1816:G:H4'	1.95	0.47
1:S2:888:U:O2'	1:S2:897:U:O4	2.32	0.47
3:SB:189:ILE:CB	3:SB:190:PRO:HD3	2.27	0.47
4:SD:45:ARG:NH1	4:SD:84:VAL:O	2.47	0.47
4:SD:76:ARG:HB2	9:SK:22:VAL:HG11	1.96	0.47
5:SE:104:ASP:HB3	5:SE:110:ALA:HB2	1.96	0.47
40:F:184:ASP:HB3	40:F:187:SER:HB3	1.96	0.47
44:J:31:ARG:NH1	44:J:149:ASN:OD1	2.47	0.47
51:Q:67:VAL:HA	51:Q:82:ARG:HH21	1.78	0.47
63:c:122:LYS:O	79:t:1225:G:O2'	2.27	0.47
79:t:976:U:O2	79:t:1047:G:N2	2.31	0.47
79:t:4855:G:H2'	79:t:4856:G:H8	1.79	0.47
1:S2:363:A:O2'	1:S2:398:A:N6	2.48	0.47
37:C:239:LYS:HZ1	79:t:1353:G:H22	1.62	0.47
60:Z:87:ARG:NH2	79:t:398:U:O3'	2.47	0.47
62:b:13:GLY:HA2	79:t:1642:U:H3'	1.95	0.47
78:r:63:VAL:HG12	78:r:79:ARG:HB3	1.96	0.47
79:t:492:C:O2'	79:t:495:C:N4	2.40	0.47
79:t:1482:A:H5''	79:t:1483:C:H5'	1.94	0.47
1:S2:806:U:H3	1:S2:857:U:H3	1.61	0.47
1:S2:1156:U:O4	23:SC:194:ARG:NH1	2.47	0.47
3:SB:189:ILE:N	3:SB:189:ILE:CD1	2.78	0.47
12:SQ:16:LYS:HB3	12:SQ:79:ALA:HB1	1.97	0.47
36:B:291:TYR:C	36:B:298:LEU:HG	2.39	0.47
41:G:223:ARG:HH11	41:G:233:PHE:HD1	1.61	0.47
57:W:13:LYS:HB2	57:W:128:LEU:HD11	1.97	0.47
66:f:22:ARG:HD3	66:f:31:ILE:HG23	1.97	0.47
70:j:28:ARG:HH22	79:t:319:U:P	2.37	0.47
79:t:205:A:N6	79:t:229:G:N7	2.62	0.47
79:t:1379:G:O2'	79:t:1450:C:O2'	2.32	0.47
1:S2:659:G:HO2'	1:S2:662:G:HO2'	1.57	0.47
1:S2:844:U:OP1	5:SE:240:ARG:NH2	2.42	0.47
1:S2:1113:A:H4'	3:SB:202:GLN:HE22	1.79	0.47
1:S2:1524:G:OP2	14:SS:141:ARG:NH2	2.47	0.47
1:S2:1648:G:C8	12:SQ:17:LYS:CE	2.98	0.47
5:SE:29:PRO:HB3	5:SE:45:ILE:HG21	1.97	0.47
19:Sa:23:CYS:HB3	19:Sa:28:ARG:H	1.79	0.47
31:SZ:69:THR:HG22	31:SZ:71:ALA:H	1.80	0.47
55:U:17:ARG:CG	55:U:22:HIS:ND1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:f:89:LEU:HD13	66:f:118:LEU:HD22	1.96	0.47
73:m:27:ILE:O	73:m:33:ASN:ND2	2.47	0.47
79:t:1077:G:H1	79:t:1184:U:H3	1.63	0.47
16:SU:21:ARG:O	16:SU:115:THR:OG1	2.28	0.47
19:Sa:10:ARG:HG2	19:Sa:34:LYS:HB2	1.95	0.47
32:Sb:64:CYS:HB3	32:Sb:73:LEU:HD23	1.96	0.47
40:F:166:ALA:HB1	40:F:171:LEU:HD12	1.96	0.47
49:O:22:LEU:HA	49:O:25:VAL:HG12	1.96	0.47
49:O:68:ARG:NH2	79:t:297:C:OP2	2.48	0.47
49:O:155:VAL:O	49:O:162:ARG:NH2	2.48	0.47
53:S:104:ARG:HH22	79:t:2877:G:H5''	1.79	0.47
54:T:13:VAL:HG22	54:T:63:TYR:HB3	1.97	0.47
67:g:27:LEU:HA	67:g:85:ARG:HA	1.96	0.47
1:S2:1236:G:O6	14:SS:137:LYS:NZ	2.47	0.47
1:S2:1650:A:H5''	12:SQ:139:ALA:HB2	1.96	0.47
2:SA:69:GLU:HB3	23:SC:270:THR:HG21	1.96	0.47
5:SE:31:PRO:HG2	5:SE:38:LEU:HB2	1.96	0.47
6:SF:195:GLU:OE1	6:SF:198:ARG:NH2	2.35	0.47
7:SH:140:VAL:HG12	27:SN:19:ARG:HD3	1.97	0.47
9:SK:60:GLU:CD	9:SK:69:TRP:NE1	2.69	0.47
11:SP:18:ARG:HH22	11:SP:37:TYR:HA	1.80	0.47
22:Sg:46:THR:OG1	22:Sg:51:ASN:O	2.32	0.47
22:Sg:106:LYS:HA	22:Sg:126:ASP:HB2	1.96	0.47
25:SJ:78:LEU:HD23	25:SJ:92:MET:HB2	1.96	0.47
44:J:9:THR:HB	44:J:54:ARG:HD2	1.95	0.47
45:K:46:PHE:HB2	45:K:139:ARG:HH11	1.79	0.47
54:T:71:SER:O	54:T:76:LYS:NZ	2.47	0.47
54:T:173:ASN:HA	79:t:4724:A:H2	1.80	0.47
59:Y:82:THR:HG21	59:Y:155:ILE:HG21	1.97	0.47
68:h:6:THR:HG22	79:t:2379:G:H21	1.79	0.47
75:o:23:ARG:NH1	79:t:3778:A:OP1	2.47	0.47
78:r:28:GLU:HB2	78:r:31:ASN:HB2	1.96	0.47
79:t:82:U:O2'	79:t:1365:G:O2'	2.29	0.47
79:t:1230:U:H3	79:t:1245:G:H1	1.62	0.47
79:t:4500:G:O6	79:t:4508:A:N6	2.48	0.47
1:S2:681:U:O2'	18:SX:8:ARG:NH1	2.48	0.47
3:SB:83:LYS:HE3	3:SB:106:THR:HG22	1.97	0.47
7:SH:6:ALA:HB3	7:SH:28:LEU:HD11	1.97	0.47
18:SX:4:CYS:HB2	18:SX:13:LEU:HD21	1.97	0.47
22:Sg:17:TRP:H	22:Sg:36:ARG:HB3	1.80	0.47
35:A:113:VAL:O	35:A:134:ALA:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:60:TRP:CZ2	48:N:6:PHE:CE1	3.03	0.47
48:N:124:LYS:HA	48:N:127:VAL:HG12	1.96	0.47
60:Z:69:LYS:HG2	60:Z:83:GLU:HG2	1.97	0.47
64:d:101:ASP:OD1	64:d:101:ASP:N	2.48	0.47
1:S2:983:A:H2	28:SO:139:SER:HB2	1.80	0.47
1:S2:1864:U:OP2	19:Sa:5:ARG:NH2	2.46	0.47
3:SB:144:LYS:HD2	3:SB:208:HIS:HB3	1.95	0.47
22:Sg:106:LYS:HE2	22:Sg:130:LYS:HG3	1.96	0.47
22:Sg:110:SER:O	22:Sg:123:GLY:N	2.47	0.47
37:C:325:MET:O	37:C:329:ASN:N	2.47	0.47
50:P:43:ILE:HG23	50:P:136:ALA:HB3	1.95	0.47
69:i:88:THR:HG22	69:i:91:MET:HG2	1.96	0.47
79:t:1067:C:O2	79:t:1197:C:N4	2.47	0.47
79:t:2766:A:H2	79:t:2780:U:H3	1.61	0.47
1:S2:441:C:O2'	24:SG:92:ARG:NH2	2.48	0.47
12:SQ:16:LYS:HE3	12:SQ:82:TYR:CB	1.98	0.47
16:SU:31:SER:OG	16:SU:107:GLU:OE2	2.32	0.47
35:A:133:TYR:HB3	35:A:168:VAL:HG23	1.96	0.47
48:N:47:ARG:HD3	54:T:73:LEU:HD13	1.97	0.47
79:t:1071:C:H42	79:t:1190:C:H42	1.62	0.47
79:t:1739:U:H2'	79:t:1740:G:H8	1.79	0.47
79:t:3583:C:H1'	79:t:4974:A:H8	1.80	0.47
1:S2:318:A:N6	1:S2:333:G:O6	2.48	0.46
1:S2:1866:A:C6	19:Sa:87:ARG:HD2	2.51	0.46
29:SW:46:TYR:O	29:SW:66:THR:OG1	2.31	0.46
35:A:158:ILE:HD12	35:A:162:ASN:HD22	1.80	0.46
37:C:301:ALA:HB1	52:R:132:LYS:HE2	1.97	0.46
42:H:158:GLY:HA2	42:H:211:PHE:HE1	1.80	0.46
44:J:41:ILE:HD13	44:J:73:ILE:HD11	1.96	0.46
54:T:127:MET:HA	55:U:153:PRO:HG2	1.96	0.46
58:X:52:THR:OG1	58:X:53:VAL:N	2.48	0.46
62:b:94:LYS:HE2	62:b:94:LYS:HB2	1.67	0.46
64:d:12:GLU:O	64:d:16:SER:OG	2.33	0.46
66:f:82:VAL:HG23	66:f:111:ILE:HG22	1.96	0.46
79:t:221:U:O3'	79:t:238:G:N2	2.48	0.46
79:t:4105:C:O2'	79:t:4111:C:O2	2.31	0.46
1:S2:1274:G:H5''	9:SK:1:MET:HG3	1.97	0.46
7:SH:44:ASN:OD1	7:SH:68:GLN:NE2	2.48	0.46
22:Sg:138:CYS:SG	22:Sg:139:LYS:N	2.88	0.46
35:A:30:ARG:O	35:A:163:ARG:NH2	2.48	0.46
41:G:185:PRO:HG2	41:G:187:ARG:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:163:ASN:OD1	42:H:163:ASN:N	2.45	0.46
48:N:37:LEU:HD13	54:T:100:LEU:HD21	1.96	0.46
50:P:26:GLN:HG3	54:T:167:PHE:HZ	1.79	0.46
53:S:109:TYR:HD2	53:S:142:ILE:HD13	1.80	0.46
23:SC:77:SER:O	23:SC:79:GLU:N	2.48	0.46
23:SC:114:LYS:HG2	23:SC:121:ARG:HB2	1.96	0.46
49:O:60:VAL:HG13	49:O:134:LEU:HB2	1.97	0.46
49:O:116:LEU:HD22	49:O:135:ILE:HD11	1.97	0.46
51:Q:48:LEU:HB3	51:Q:92:LEU:HD22	1.97	0.46
1:S2:990:A:OP1	3:SB:116:LYS:NZ	2.49	0.46
1:S2:1750:C:N3	1:S2:1782:G:N1	2.58	0.46
23:SC:182:CYS:HB2	29:SW:95:PRO:HB2	1.96	0.46
44:J:59:LYS:HE3	44:J:66:GLU:HB3	1.98	0.46
47:M:179:PHE:CD2	62:b:131:ARG:HB3	2.50	0.46
71:k:22:CYS:SG	71:k:24:SER:OG	2.66	0.46
79:t:502:G:O2'	79:t:504:U:OP1	2.25	0.46
1:S2:200:G:C2	1:S2:201:C:H1'	2.51	0.46
13:SR:98:VAL:HG23	13:SR:119:VAL:HG12	1.98	0.46
42:H:214:SER:OG	42:H:215:SER:N	2.45	0.46
57:W:85:ARG:H	57:W:101:ASN:ND2	2.13	0.46
79:t:3846:G:N1	79:t:3850:G:OP1	2.37	0.46
4:SD:132:LYS:HD3	4:SD:189:MET:HE2	1.98	0.46
20:Sc:13:ARG:NH2	20:Sc:53:GLY:O	2.49	0.46
36:B:115:LYS:HA	36:B:118:PHE:HD2	1.81	0.46
41:G:128:HIS:ND1	79:t:1265:G:C5	2.83	0.46
79:t:462:U:O2'	79:t:463:C:O4'	2.34	0.46
1:S2:1497:G:C5	9:SK:62:PHE:CE2	3.03	0.46
14:SS:51:ASP:OD2	14:SS:53:THR:OG1	2.28	0.46
22:Sg:14:HIS:CE1	22:Sg:18:VAL:HG22	2.51	0.46
22:Sg:35:SER:OG	22:Sg:36:ARG:N	2.49	0.46
23:SC:252:THR:OG1	23:SC:254:ASP:OD1	2.25	0.46
42:H:99:ASN:OD1	42:H:99:ASN:N	2.43	0.46
43:I:113:ARG:NH1	79:t:119:G:N7	2.63	0.46
65:e:60:PRO:HD2	65:e:100:ASN:HD22	1.80	0.46
72:l:8:ILE:HG12	72:l:45:LEU:HD21	1.98	0.46
72:l:54:GLU:HA	72:l:57:LYS:HB3	1.98	0.46
79:t:1928:U:O2	79:t:4655:C:N4	2.48	0.46
79:t:1953:G:N2	79:t:1975:C:N3	2.64	0.46
6:SF:28:VAL:HG11	6:SF:109:LEU:HB2	1.97	0.46
12:SQ:16:LYS:CD	12:SQ:82:TYR:HB3	2.44	0.46
39:E:12:U:O3'	39:E:109:U:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:242:ARG:NH2	79:t:929:G:OP2	2.49	0.46
51:Q:48:LEU:HD23	51:Q:92:LEU:HB2	1.98	0.46
57:W:100:ASP:N	57:W:100:ASP:OD1	2.47	0.46
74:n:111:ARG:HG3	74:n:112:LYS:HD2	1.96	0.46
76:p:66:ILE:H	76:p:66:ILE:HG13	1.53	0.46
77:q:62:LYS:NZ	79:t:4090:G:N7	2.63	0.46
79:t:1997:C:H2'	79:t:1998:A:H8	1.81	0.46
79:t:4707:G:H1	79:t:4912:G:H1	1.63	0.46
1:S2:1199:A:H5''	19:Sa:2:THR:HG22	1.98	0.46
2:SA:25:LEU:HD23	2:SA:48:ILE:HG22	1.98	0.46
5:SE:201:HIS:N	5:SE:206:ASP:OD1	2.42	0.46
6:SF:143:PRO:HA	6:SF:146:ARG:HG2	1.97	0.46
7:SH:29:GLU:OE1	7:SH:86:LYS:NZ	2.47	0.46
8:SI:190:LEU:HB3	8:SI:195:LEU:HD12	1.98	0.46
14:SS:35:GLY:O	14:SS:97:GLN:NE2	2.48	0.46
22:Sg:158:PRO:HG3	22:Sg:202:PRO:HA	1.98	0.46
35:A:8:GLN:HE21	35:A:232:GLY:HA3	1.81	0.46
36:B:35:ASP:HB3	36:B:186:ASN:CA	2.45	0.46
36:B:261:ARG:HB2	50:P:64:THR:HG21	1.97	0.46
36:B:298:LEU:CD2	36:B:298:LEU:C	2.86	0.46
41:G:72:LYS:HD2	63:c:119:CYS:HB2	1.98	0.46
42:H:115:ARG:HB3	52:R:4:ASP:OD1	2.16	0.46
65:e:64:ILE:HG22	65:e:106:VAL:HB	1.98	0.46
79:t:1419:C:O2	79:t:1431:G:N2	2.49	0.46
79:t:1791:C:H2'	79:t:1792:G:H8	1.80	0.46
1:S2:140:C:O2'	1:S2:143:U:OP1	2.33	0.45
1:S2:1432:U:H2'	1:S2:1438:A:C8	2.51	0.45
1:S2:1748:G:H22	1:S2:1786:U:H3	1.61	0.45
3:SB:40:ASN:ND2	3:SB:75:GLN:OE1	2.48	0.45
3:SB:185:VAL:O	3:SB:189:ILE:CD1	2.64	0.45
9:SK:76:ILE:HG22	9:SK:80:ARG:HH21	1.81	0.45
15:ST:44:GLU:HG2	15:ST:45:LEU:HD12	1.98	0.45
36:B:92:TYR:HB2	36:B:159:VAL:HG23	1.97	0.45
37:C:218:ILE:HA	37:C:229:LEU:HD22	1.98	0.45
55:U:107:LYS:O	55:U:111:GLU:HG3	2.16	0.45
79:t:2089:G:H22	79:t:2231:G:H1	1.63	0.45
3:SB:71:LEU:O	3:SB:75:GLN:N	2.50	0.45
19:Sa:89:ARG:HD3	19:Sa:89:ARG:HA	1.74	0.45
22:Sg:199:THR:HG21	22:Sg:240:CYS:HA	1.97	0.45
35:A:224:THR:HG22	35:A:237:LEU:HB2	1.97	0.45
36:B:41:VAL:HA	36:B:187:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G:73:TYR:OH	79:t:969:U:O5'	2.33	0.45
55:U:68:THR:HG21	79:t:4276:C:H4'	1.98	0.45
57:W:107:ASN:ND2	57:W:111:GLU:OE1	2.40	0.45
65:e:24:GLU:HA	65:e:87:ARG:HA	1.99	0.45
79:t:1304:G:H2'	79:t:3847:A:N7	2.32	0.45
1:S2:851:C:H5'	1:S2:852:G:H5'	1.97	0.45
1:S2:984:C:O2'	28:SO:138:ASP:OD2	2.31	0.45
5:SE:194:VAL:N	5:SE:211:LYS:O	2.49	0.45
6:SF:167:LYS:HA	31:SZ:71:ALA:HB1	1.98	0.45
22:Sg:5:MET:HB3	22:Sg:310:TRP:HB3	1.99	0.45
24:SG:126:ASP:OD1	24:SG:126:ASP:N	2.47	0.45
24:SG:134:GLY:HA3	24:SG:158:VAL:HG21	1.98	0.45
30:SY:76:TYR:OH	30:SY:86:GLU:OE1	2.34	0.45
36:B:35:ASP:CB	36:B:186:ASN:CB	2.90	0.45
36:B:315:ASN:OD1	36:B:315:ASN:N	2.48	0.45
44:J:61:TRP:CZ2	48:N:33:GLN:NE2	2.83	0.45
44:J:95:VAL:HG22	74:n:82:LEU:HB3	1.99	0.45
47:M:78:LEU:HD11	79:t:157:G:H1'	1.97	0.45
79:t:4157:G:N2	79:t:4183:C:O2'	2.50	0.45
1:S2:560:A:H4'	25:SJ:174:LYS:HD2	1.98	0.45
1:S2:1093:A:O2'	29:SW:9:ASP:OD1	2.26	0.45
9:SK:26:ASP:N	9:SK:26:ASP:OD1	2.48	0.45
24:SG:5:ILE:HG23	24:SG:14:LYS:HB2	1.98	0.45
37:C:190:ARG:HE	37:C:202:ILE:HG12	1.80	0.45
37:C:218:ILE:HD12	37:C:229:LEU:HD22	1.97	0.45
39:E:4:U:H2'	39:E:5:A:H8	1.80	0.45
41:G:161:ARG:O	41:G:182:ASN:ND2	2.49	0.45
42:H:244:ILE:O	42:H:248:ASN:N	2.39	0.45
43:I:154:LEU:HB3	43:I:204:PHE:HD2	1.82	0.45
54:T:11:LYS:HD2	54:T:29:ARG:HD2	1.99	0.45
79:t:4951:G:H1	79:t:5016:A:N6	2.13	0.45
1:S2:1253:A:H4'	1:S2:1254:C:H5''	1.99	0.45
2:SA:76:VAL:HG22	2:SA:87:VAL:HG23	1.98	0.45
6:SF:61:PHE:CE1	20:Sc:49:PRO:HB2	2.52	0.45
7:SH:69:LEU:HD13	7:SH:96:ALA:HB2	1.99	0.45
8:SI:121:LEU:O	8:SI:123:ARG:NH2	2.50	0.45
24:SG:194:LEU:HD13	24:SG:197:GLN:HE21	1.80	0.45
36:B:85:VAL:HG13	36:B:204:GLN:HG2	1.98	0.45
46:L:64:ARG:NH1	46:L:65:ASN:OD1	2.49	0.45
47:M:169:ILE:H	47:M:169:ILE:HG13	1.44	0.45
51:Q:4:TYR:HE2	51:Q:16:LYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:106:LEU:HA	55:U:109:VAL:HG12	1.98	0.45
4:SD:38:GLU:HB3	4:SD:49:ILE:HD11	1.99	0.45
5:SE:9:LEU:HB2	5:SE:30:ARG:HD3	1.99	0.45
6:SF:73:THR:HG23	6:SF:86:LYS:HE3	1.99	0.45
18:SX:60:LYS:HD2	18:SX:114:ASP:HA	1.98	0.45
36:B:224:LYS:HE3	36:B:224:LYS:HB2	1.81	0.45
36:B:242:ARG:HA	36:B:248:LEU:HD11	1.98	0.45
40:F:36:LEU:HD11	40:F:147:ASP:HB3	1.98	0.45
41:G:233:PHE:CD2	41:G:236:GLU:HG2	2.52	0.45
50:P:14:HIS:CE1	50:P:120:VAL:H	2.33	0.45
51:Q:84:PRO:HB2	51:Q:87:SER:HB3	1.97	0.45
54:T:166:ARG:HD2	79:t:1900:G:C2	2.52	0.45
70:j:62:LYS:HB3	70:j:94:LEU:HD21	1.97	0.45
79:t:185:G:H2'	79:t:186:G:H8	1.81	0.45
79:t:227:G:N2	79:t:234:G:H1	2.15	0.45
79:t:4973:G:H21	79:t:4992:A:H2	1.64	0.45
1:S2:1102:G:OP1	3:SB:151:ARG:NH1	2.50	0.45
1:S2:1142:G:OP2	23:SC:187:ARG:NH2	2.49	0.45
1:S2:1868:U:N3	19:Sa:98:PRO:O	2.50	0.45
5:SE:141:THR:OG1	5:SE:143:ASP:OD1	2.34	0.45
7:SH:20:GLU:HA	7:SH:23:ILE:HB	1.98	0.45
42:H:96:ARG:HD2	42:H:223:LYS:HE3	1.99	0.45
50:P:10:ASP:HB2	50:P:117:ARG:HD3	1.98	0.45
50:P:133:ARG:NH1	79:t:2036:G:OP2	2.43	0.45
60:Z:55:VAL:HG23	60:Z:106:ILE:HA	1.98	0.45
61:a:84:ARG:NH1	68:h:99:GLU:OE1	2.50	0.45
62:b:25:HIS:CD2	79:t:1321:G:H22	2.35	0.45
70:j:88:GLU:O	70:j:92:ASN:ND2	2.49	0.45
72:l:51:GLU:O	72:l:55:LYS:NZ	2.48	0.45
79:t:2373:G:H8	79:t:2799:C:H41	1.65	0.45
79:t:2617:G:H1	79:t:2676:A:H61	1.65	0.45
1:S2:625:G:O6	18:SX:64:SER:N	2.47	0.45
1:S2:1378:A:H61	2:SA:109:THR:HG21	1.82	0.45
7:SH:60:ILE:HD11	7:SH:92:VAL:HG22	1.98	0.45
12:SQ:18:THR:O	12:SQ:75:GLY:N	2.50	0.45
15:ST:38:LYS:HE3	15:ST:41:LYS:HA	1.98	0.45
37:C:52:TYR:HB2	37:C:111:TRP:CH2	2.51	0.45
37:C:190:ARG:HB3	37:C:195:LYS:HG2	1.98	0.45
41:G:279:ASN:HB2	79:t:4715:U:H5	1.81	0.45
49:O:157:LYS:O	49:O:162:ARG:NH1	2.50	0.45
61:a:10:VAL:HB	61:a:24:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1930:U:H5	79:t:2015:G:H1	1.63	0.45
79:t:2297:G:N2	79:t:2300:G:OP2	2.47	0.45
79:t:2868:G:H21	79:t:4992:A:H8	1.64	0.45
4:SD:9:ARG:HA	4:SD:12:VAL:HG22	1.99	0.45
7:SH:66:VAL:HG22	7:SH:96:ALA:HB1	1.97	0.45
12:SQ:101:ASP:N	12:SQ:101:ASP:OD1	2.47	0.45
15:ST:141:ALA:HA	15:ST:144:LYS:HB2	1.99	0.45
38:D:52:A:H4'	73:m:19:GLN:HA	1.97	0.45
39:E:63:C:H5'	39:E:64:G:H5''	1.99	0.45
40:F:41:LYS:HE2	55:U:93:ILE:HG12	1.99	0.45
40:F:64:ILE:HG13	40:F:105:LEU:HD11	1.99	0.45
66:f:81:ASN:N	66:f:81:ASN:OD1	2.48	0.45
79:t:4980:U:H3	79:t:4983:C:N4	2.14	0.45
1:S2:561:A:P	25:SJ:171:GLY:H	2.40	0.45
1:S2:1329:U:O2'	1:S2:1332:A:OP2	2.30	0.45
21:Sd:43:PHE:CD1	21:Sd:43:PHE:O	2.70	0.45
22:Sg:40:ILE:HD11	22:Sg:66:VAL:HG21	2.00	0.45
40:F:115:MET:SD	79:t:1801:G:O2'	2.75	0.45
57:W:18:LEU:HD23	57:W:54:ALA:HB3	1.99	0.45
1:S2:920:A:H4'	29:SW:57:ARG:HG3	1.99	0.44
1:S2:942:G:N2	28:SO:137:SER:O	2.50	0.44
17:SV:15:ARG:NE	23:SC:83:LEU:O	2.50	0.44
21:Sd:39:CYS:O	21:Sd:42:CYS:N	2.49	0.44
23:SC:267:GLN:HA	23:SC:270:THR:HG23	1.99	0.44
24:SG:71:GLY:H	24:SG:98:ARG:NH1	2.16	0.44
36:B:315:ASN:HD22	36:B:325:GLU:HG2	1.83	0.44
39:E:63:C:H1'	40:F:280:VAL:HG11	1.98	0.44
73:m:3:SER:HB2	79:t:2763:C:H41	1.82	0.44
79:t:2462:G:N2	79:t:2474:U:O2	2.35	0.44
1:S2:380:G:N1	1:S2:383:G:OP2	2.34	0.44
1:S2:910:G:O5'	53:S:173:ARG:NH1	2.51	0.44
1:S2:1389:C:O2'	4:SD:162:ASP:OD1	2.25	0.44
36:B:167:GLN:HE22	36:B:204:GLN:NE2	2.15	0.44
45:K:201:PRO:HB2	45:K:203:ARG:HG2	1.99	0.44
48:N:65:PRO:HG3	79:t:906:C:H2'	1.99	0.44
56:V:103:VAL:HG21	56:V:113:ARG:NH1	2.32	0.44
79:t:637:C:H2'	79:t:638:G:H8	1.81	0.44
1:S2:563:G:N7	1:S2:586:G:N2	2.65	0.44
1:S2:1152:U:H1'	29:SW:16:ASN:HD21	1.82	0.44
5:SE:162:ILE:HG22	5:SE:169:ILE:HA	1.99	0.44
9:SK:14:LEU:HA	9:SK:17:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SL:12:LYS:HD2	10:SL:18:GLN:NE2	2.32	0.44
11:SP:127:LYS:HB2	11:SP:127:LYS:HZ2	1.82	0.44
14:SS:84:LEU:HG	14:SS:97:GLN:HB2	1.98	0.44
23:SC:229:CYS:SG	23:SC:232:THR:OG1	2.67	0.44
36:B:248:LEU:N	79:t:2817:G:OP1	2.41	0.44
37:C:155:GLU:HA	37:C:254:GLU:HG3	1.98	0.44
38:D:14:U:H5''	51:Q:123:PRO:HD3	1.99	0.44
50:P:128:ARG:HA	50:P:128:ARG:HD3	1.81	0.44
51:Q:108:ASP:N	51:Q:152:GLU:OE2	2.44	0.44
54:T:14:GLY:HA2	54:T:62:VAL:HG22	2.00	0.44
54:T:161:ARG:C	54:T:162:GLN:HE21	2.25	0.44
69:i:4:ILE:O	69:i:56:ARG:NH1	2.45	0.44
79:t:376:G:N1	79:t:379:A:OP2	2.50	0.44
1:S2:126:G:H8	24:SG:199:THR:HG21	1.83	0.44
35:A:131:GLY:H	35:A:169:VAL:HB	1.82	0.44
36:B:298:LEU:CD2	36:B:299:ILE:O	2.65	0.44
47:M:42:LYS:HE3	47:M:46:ILE:HD11	1.99	0.44
47:M:47:ALA:HB3	47:M:49:ARG:HG3	2.00	0.44
63:c:59:ALA:O	63:c:63:LYS:N	2.49	0.44
11:SP:22:LEU:HD13	11:SP:109:PRO:HB3	1.98	0.44
11:SP:22:LEU:HA	11:SP:25:LEU:HD12	1.99	0.44
12:SQ:19:ALA:HB2	12:SQ:75:GLY:HA3	2.00	0.44
18:SX:105:PHE:CE2	18:SX:112:VAL:HG22	2.53	0.44
28:SO:75:MET:HG2	28:SO:118:ALA:HB2	1.99	0.44
29:SW:11:LEU:HD12	29:SW:72:CYS:HB2	1.99	0.44
29:SW:49:GLU:O	29:SW:64:ASN:ND2	2.50	0.44
41:G:170:SER:OG	41:G:214:ASP:OD2	2.33	0.44
45:K:30:LYS:HD3	45:K:63:GLU:HG2	1.99	0.44
48:N:58:THR:HG22	48:N:91:TRP:HZ3	1.83	0.44
53:S:83:GLY:N	79:t:2791:A:OP1	2.50	0.44
60:Z:72:GLN:HB3	60:Z:81:TYR:HD2	1.83	0.44
77:q:4:ARG:NH2	79:t:1537:G:N7	2.60	0.44
1:S2:165:G:OP2	1:S2:165:G:N2	2.42	0.44
1:S2:325:C:H42	1:S2:329:G:H1'	1.82	0.44
1:S2:904:A:N6	87:S2:2002:HOH:O	2.51	0.44
1:S2:1392:U:H2'	1:S2:1393:G:C8	2.53	0.44
5:SE:234:PRO:HG3	5:SE:238:LEU:HD11	1.98	0.44
18:SX:82:THR:HG23	18:SX:118:VAL:HG23	1.99	0.44
39:E:38:U:N3	39:E:41:G:OP2	2.43	0.44
44:J:5:LEU:HD12	44:J:58:ASP:HB2	2.00	0.44
44:J:40:HIS:CE1	44:J:41:ILE:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:W:56:GLY:N	57:W:59:ASP:OD2	2.47	0.44
79:t:286:G:H22	79:t:309:G:H21	1.65	0.44
79:t:2474:U:H2'	79:t:2475:G:C8	2.52	0.44
1:S2:1545:A:O2'	12:SQ:18:THR:HG21	2.18	0.44
3:SB:82:ARG:CZ	3:SB:191:ASP:HB2	2.44	0.44
5:SE:21:ASP:OD2	5:SE:23:LEU:N	2.48	0.44
9:SK:92:ALA:HA	9:SK:96:ARG:HG3	1.99	0.44
29:SW:11:LEU:HD13	29:SW:14:ILE:HD12	2.00	0.44
37:C:190:ARG:HD3	37:C:202:ILE:HD11	1.98	0.44
37:C:364:LYS:HE3	37:C:364:LYS:HB3	1.88	0.44
39:E:94:C:OP1	54:T:46:TYR:OH	2.31	0.44
44:J:163:GLN:O	44:J:166:THR:OG1	2.30	0.44
45:K:210:ARG:HD3	79:t:1162:U:H5	1.83	0.44
52:R:9:LYS:HD3	52:R:9:LYS:HA	1.58	0.44
76:p:23:VAL:HG23	76:p:68:LEU:HB3	1.99	0.44
79:t:85:G:N2	79:t:98:A:OP2	2.44	0.44
79:t:479:C:H5	79:t:658:G:H5'	1.82	0.44
79:t:1397:C:H2'	79:t:1398:G:C8	2.52	0.44
79:t:2328:A:H5''	79:t:2329:U:H5''	2.00	0.44
79:t:2558:G:N2	79:t:2561:A:OP2	2.38	0.44
1:S2:70:G:H2'	1:S2:79:A:H61	1.83	0.44
12:SQ:16:LYS:HE3	12:SQ:82:TYR:CD2	2.53	0.44
22:Sg:236:ILE:HG22	22:Sg:252:THR:HA	2.00	0.44
30:SY:76:TYR:OH	30:SY:85:ASN:O	2.31	0.44
36:B:26:ARG:NH1	36:B:180:LEU:O	2.46	0.44
37:C:323:ARG:HA	37:C:326:LEU:HB2	2.00	0.44
43:I:190:LEU:HD12	43:I:202:VAL:HG13	1.98	0.44
65:e:60:PRO:HD2	65:e:100:ASN:ND2	2.33	0.44
69:i:17:LEU:O	69:i:21:LEU:N	2.50	0.44
70:j:33:LEU:HG	70:j:38:LYS:HB2	1.99	0.44
79:t:2087:C:N4	79:t:2088:G:O6	2.51	0.44
79:t:4489:G:OP2	79:t:4489:G:N2	2.51	0.44
79:t:4951:G:N2	79:t:5016:A:N1	2.65	0.44
1:S2:67:C:H5	24:SG:162:LEU:HB3	1.83	0.44
1:S2:543:C:O2'	1:S2:544:G:O4'	2.28	0.44
6:SF:201:LYS:HA	6:SF:204:ARG:HB2	2.00	0.44
7:SH:160:LYS:HD2	7:SH:189:PHE:HB3	2.00	0.44
13:SR:31:ASN:HD22	13:SR:55:THR:HG22	1.83	0.44
22:Sg:201:SER:OG	22:Sg:203:ASP:O	2.36	0.44
25:SJ:111:GLN:HG3	25:SJ:145:PRO:HB3	1.99	0.44
36:B:220:ILE:HD11	36:B:348:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:285:TYR:HB2	36:B:332:MET:HG3	1.98	0.44
38:D:148:A:H61	79:t:7:C:H42	1.66	0.44
42:H:94:ARG:NH1	42:H:115:ARG:O	2.51	0.44
57:W:49:LEU:HD23	57:W:49:LEU:HA	1.77	0.44
79:t:1848:A:N3	79:t:4365:U:O2'	2.43	0.44
80:u:3:C:N4	80:u:70:G:O6	2.50	0.44
1:S2:1259:A:N6	1:S2:1519:U:H5''	2.33	0.43
3:SB:134:LEU:HG	3:SB:218:LEU:HD12	2.00	0.43
12:SQ:16:LYS:HD3	12:SQ:82:TYR:CB	2.47	0.43
18:SX:60:LYS:HG3	18:SX:114:ASP:CA	2.48	0.43
22:Sg:265:ILE:H	22:Sg:265:ILE:HG13	1.60	0.43
29:SW:101:PHE:HA	29:SW:113:HIS:CE1	2.53	0.43
36:B:14:LEU:HA	36:B:17:LEU:HG	1.99	0.43
37:C:27:VAL:HA	37:C:279:LEU:HD11	2.00	0.43
38:D:82:A:C5	38:D:87:G:H5''	2.53	0.43
38:D:149:G:H21	43:I:64:GLN:HE22	1.66	0.43
40:F:234:ASP:OD1	40:F:234:ASP:N	2.43	0.43
46:L:101:ASP:N	79:t:4210:A:O2'	2.49	0.43
47:M:76:PHE:O	47:M:80:GLU:OE1	2.36	0.43
48:N:119:ARG:HH22	50:P:191:LYS:NZ	2.15	0.43
52:R:69:LYS:O	52:R:75:ARG:NH1	2.51	0.43
61:a:62:ILE:O	61:a:66:SER:OG	2.31	0.43
79:t:197:U:H5	79:t:210:G:H1	1.66	0.43
79:t:480:C:N4	79:t:481:G:O6	2.51	0.43
79:t:1784:A:H5''	79:t:1785:G:H5'	2.00	0.43
1:S2:1409:A:OP1	12:SQ:26:LYS:NZ	2.50	0.43
1:S2:1454:A:H2'	13:SR:3:ARG:HG3	2.00	0.43
19:Sa:47:ALA:HA	19:Sa:50:VAL:HG23	2.00	0.43
25:SJ:138[A]:ARG:H	25:SJ:138[A]:ARG:HG3	1.40	0.43
41:G:179:LEU:O	41:G:182:ASN:O	2.36	0.43
60:Z:82:ILE:HD12	60:Z:99:ILE:HD11	2.00	0.43
79:t:166:G:N2	79:t:261:G:H22	2.13	0.43
79:t:180:C:O2	79:t:251:G:N2	2.51	0.43
79:t:2386:G:OP2	79:t:2386:G:N2	2.52	0.43
1:S2:167:G:H4'	24:SG:131:ARG:HH11	1.83	0.43
3:SB:121:ILE:HD11	3:SB:207:LEU:HD21	1.98	0.43
3:SB:226:GLY:HA3	79:t:4070:C:H4'	1.99	0.43
5:SE:36:HIS:CE1	5:SE:85:GLY:HA3	2.53	0.43
5:SE:204:SER:OG	5:SE:205:PHE:N	2.51	0.43
22:Sg:124:SER:OG	22:Sg:128:THR:O	2.34	0.43
36:B:291:TYR:C	36:B:298:LEU:CG	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:193:LYS:HD3	79:t:346:G:C8	2.53	0.43
37:C:198:ASN:HD22	60:Z:10:ASP:HB3	1.83	0.43
41:G:272:ARG:HG3	79:t:4841:C:H5	1.83	0.43
42:H:125:LEU:HD23	42:H:125:LEU:HA	1.84	0.43
52:R:3:VAL:HG11	52:R:5:ILE:CG1	2.47	0.43
1:S2:835:C:H42	30:SY:9:THR:HG22	1.83	0.43
1:S2:838:G:O2'	1:S2:840:C:OP2	2.26	0.43
1:S2:1720:U:O2'	79:t:3767:U:O2'	2.28	0.43
1:S2:1832:6MZ:O5'	1:S2:1832:6MZ:H8	2.18	0.43
3:SB:172:MET:HE2	3:SB:172:MET:HB3	1.77	0.43
9:SK:65:ARG:CD	21:Sd:22:ARG:O	2.67	0.43
10:SL:12:LYS:HD2	10:SL:18:GLN:HE21	1.84	0.43
13:SR:27:ASP:O	13:SR:31:ASN:ND2	2.51	0.43
22:Sg:258:ILE:HG22	22:Sg:267:VAL:HB	2.00	0.43
25:SJ:109:ARG:HE	25:SJ:146:SER:HA	1.81	0.43
46:L:144:LYS:NZ	46:L:147:ARG:O	2.48	0.43
53:S:65:LYS:HE2	53:S:65:LYS:HB3	1.90	0.43
78:r:51:VAL:HG12	78:r:62:VAL:HG22	1.98	0.43
79:t:220:G:HO2'	79:t:239:U:HO2'	1.62	0.43
79:t:746:C:H2'	79:t:747:G:C8	2.54	0.43
79:t:4722:G:H2'	79:t:4723:G:C8	2.54	0.43
1:S2:1006:C:P	64:d:8:LYS:H	2.42	0.43
1:S2:1619:A:OP1	11:SP:47:ARG:NE	2.35	0.43
10:SL:17:PHE:CD2	10:SL:19:ASN:O	2.69	0.43
35:A:111:THR:HG22	35:A:136:VAL:HG12	2.01	0.43
53:S:62:ARG:NH2	79:t:4610:A:OP1	2.51	0.43
54:T:15:ARG:HB3	54:T:27:LEU:HA	2.00	0.43
79:t:4819:G:H2'	79:t:4820:G:C8	2.53	0.43
16:SU:33:GLU:OE2	16:SU:87:ARG:NH2	2.50	0.43
20:Sc:15:THR:HG22	20:Sc:31:ARG:O	2.18	0.43
34:Sf:89:LYS:H	34:Sf:89:LYS:HD2	1.84	0.43
38:D:26:C:H42	79:t:341:A:H61	1.66	0.43
57:W:45:ILE:HG21	57:W:53:PRO:HB3	2.00	0.43
63:c:95:ARG:HE	63:c:96:LEU:HD12	1.84	0.43
72:l:5:ILE:HG21	72:l:11:PHE:HB2	2.00	0.43
79:t:1967:U:H3	79:t:1988:G:H22	1.67	0.43
1:S2:355:G:OP1	10:SL:92:TYR:OH	2.29	0.43
6:SF:28:VAL:HG12	6:SF:110:GLN:HB2	2.00	0.43
9:SK:16:PHE:HE1	9:SK:76:ILE:HG23	1.84	0.43
9:SK:62:PHE:HD1	9:SK:67:PHE:CD1	2.34	0.43
14:SS:25:LYS:O	14:SS:29:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sg:14:HIS:HE1	22:Sg:18:VAL:HG22	1.84	0.43
22:Sg:99:ARG:HH12	22:Sg:134:THR:HB	1.84	0.43
22:Sg:261:LEU:HA	22:Sg:264:LYS:HE2	2.00	0.43
22:Sg:302:TYR:HE2	22:Sg:308:ARG:HB2	1.84	0.43
36:B:124:LYS:NZ	79:t:5021:G:N7	2.61	0.43
36:B:293:ILE:O	36:B:297:LYS:C	2.61	0.43
38:D:83:C:H5''	38:D:85:U:H5''	2.00	0.43
42:H:37:PHE:HE2	63:c:113:ALA:HB1	1.83	0.43
48:N:137:LYS:HE3	48:N:137:LYS:HB3	1.87	0.43
79:t:1185:C:H2'	79:t:1186:G:C8	2.52	0.43
80:u:34:C:H42	82:w:21:G:H1	1.67	0.43
1:S2:1648:G:H8	12:SQ:17:LYS:HD3	1.64	0.43
1:S2:1672:U:OP1	12:SQ:17:LYS:O	2.36	0.43
6:SF:103:LEU:HA	31:SZ:66:LYS:HG3	2.00	0.43
8:SI:3:ILE:HG23	8:SI:31:ARG:H	1.84	0.43
11:SP:75:VAL:HG12	11:SP:93:MET:HB3	2.00	0.43
18:SX:90:CYS:HA	18:SX:93:PHE:HD2	1.83	0.43
22:Sg:16:GLY:N	22:Sg:305:ASN:OD1	2.52	0.43
35:A:49:ILE:HG13	35:A:58:LEU:HB2	2.00	0.43
37:C:32:ILE:HD12	37:C:130:ALA:HB2	2.01	0.43
37:C:268:ARG:NH2	79:t:486:U:OP2	2.44	0.43
43:I:56:LYS:HB2	79:t:4055:A:H5''	2.00	0.43
43:I:100:HIS:CE1	43:I:103:ARG:HH21	2.36	0.43
47:M:21:ARG:HB3	49:O:197:THR:HA	2.01	0.43
51:Q:128:ARG:HH21	83:y:17:UNK:CB	2.31	0.43
79:t:213:C:H4'	79:t:214:C:H5	1.84	0.43
79:t:216:G:N2	79:t:233:G:H22	2.17	0.43
79:t:451:G:H22	79:t:691:G:N2	2.16	0.43
79:t:1154:G:H2'	79:t:1155:C:C6	2.54	0.43
1:S2:72:C:C4	24:SG:170:ARG:HA	2.53	0.43
1:S2:72:C:N4	24:SG:169:PRO:O	2.52	0.43
1:S2:84:A:H4'	30:SY:124:ASN:HD22	1.84	0.43
1:S2:566:U:H3	1:S2:584:G:H1	1.66	0.43
1:S2:798:A:O2'	7:SH:111:LYS:O	2.37	0.43
1:S2:1109:C:C1'	13:SR:124:VAL:CG2	2.95	0.43
1:S2:1545:A:H4'	12:SQ:75:GLY:H	1.84	0.43
1:S2:1568:C:OP2	15:ST:98:SER:OG	2.34	0.43
5:SE:158:ASP:OD1	5:SE:159:THR:N	2.52	0.43
25:SJ:121:LYS:O	25:SJ:125:HIS:HB3	2.19	0.43
36:B:47:LEU:HD12	36:B:84:MET:HE1	2.01	0.43
41:G:190:HIS:CD2	41:G:192:LYS:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q:131:ARG:HH21	79:t:1578:U:H2'	1.83	0.43
60:Z:34:LEU:HD22	60:Z:38:LEU:HD22	2.00	0.43
64:d:8:LYS:HG3	64:d:9:LYS:HD3	2.00	0.43
66:f:82:VAL:HG13	66:f:114:ARG:HG2	2.01	0.43
68:h:97:ILE:HD11	79:t:4091:G:C5	2.53	0.43
79:t:742:G:N2	79:t:743:G:O6	2.52	0.43
80:u:15:G:N1	80:u:16:U:O2	2.51	0.43
1:S2:918:U:O2'	29:SW:56:HIS:O	2.33	0.43
1:S2:941:C:H2'	1:S2:942:G:C8	2.54	0.43
1:S2:1325:G:N2	1:S2:1504:U:O2	2.52	0.43
4:SD:133:GLY:O	4:SD:189:MET:N	2.42	0.43
12:SQ:90:LYS:HA	12:SQ:93:VAL:HB	2.00	0.43
35:A:24:LYS:HG2	35:A:49:ILE:HD12	2.00	0.43
36:B:57:VAL:HG22	36:B:73:VAL:HG12	2.01	0.43
36:B:165:HIS:HB2	36:B:178:ALA:HB1	2.01	0.43
41:G:176:THR:O	41:G:176:THR:OG1	2.33	0.43
42:H:94:ARG:HB2	42:H:114:LEU:HD23	2.00	0.43
42:H:222:LYS:O	42:H:224:THR:N	2.51	0.43
43:I:73:ARG:NH2	79:t:4124:C:O2	2.51	0.43
54:T:143:LYS:HA	54:T:146:HIS:HD1	1.84	0.43
54:T:164:LYS:CD	79:t:4833:G:C2	2.96	0.43
68:h:55:GLY:N	79:t:2662:C:O2'	2.47	0.43
73:m:43:HIS:CD2	73:m:45:ARG:H	2.37	0.43
79:t:166:G:H22	79:t:261:G:H1	1.65	0.43
79:t:654:G:H2'	79:t:655:A:C8	2.54	0.43
79:t:1228:C:H42	79:t:1247:C:N4	2.15	0.43
79:t:2444:C:H1'	79:t:3643:G:H1	1.84	0.43
1:S2:830:A:OP2	1:S2:846:G:N2	2.50	0.42
1:S2:1495:G:H1	21:Sd:24:CYS:CB	2.32	0.42
3:SB:186:ASN:O	3:SB:190:PRO:HD2	2.19	0.42
8:SI:84:ASN:HD22	8:SI:90:LEU:HB2	1.84	0.42
12:SQ:50:LYS:HA	12:SQ:53:GLU:HB2	2.01	0.42
19:Sa:22:ARG:NH1	28:SO:145:GLY:O	2.42	0.42
26:SM:31:LEU:HD22	26:SM:89:VAL:HA	2.01	0.42
27:SN:4:MET:HG2	27:SN:5:HIS:CD2	2.54	0.42
38:D:37:A:OP1	38:D:38:U:O2'	2.30	0.42
45:K:154:ARG:NH1	79:t:4376:A:H5''	2.34	0.42
48:N:58:THR:HG22	48:N:91:TRP:CZ3	2.54	0.42
52:R:7:HIS:CE1	79:t:1648:C:O5'	2.65	0.42
18:SX:7:LEU:HD23	18:SX:7:LEU:H	1.85	0.42
37:C:73:VAL:HB	37:C:78:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:109:ARG:HA	79:t:1324:U:H5'	2.02	0.42
41:G:270:TYR:OH	48:N:106:ASP:OD2	2.33	0.42
43:I:247:VAL:HA	43:I:250:ILE:HD12	2.01	0.42
46:L:136:ARG:NH2	46:L:161:GLU:OE2	2.52	0.42
76:p:22:LYS:HE2	76:p:22:LYS:HB2	1.85	0.42
79:t:1228:C:H2'	79:t:1229:G:C8	2.55	0.42
79:t:4973:G:O2'	79:t:4992:A:N6	2.47	0.42
7:SH:13:GLY:CA	7:SH:14:GLU:OE1	2.68	0.42
12:SQ:97:GLN:HB3	12:SQ:105:LYS:HD3	1.99	0.42
23:SC:94:ILE:HD11	23:SC:162:ILE:HD13	2.00	0.42
36:B:36:ASP:HA	36:B:37:PRO:HD3	1.85	0.42
36:B:47:LEU:HD11	36:B:181:MET:HB2	2.00	0.42
39:E:50:A:OP1	40:F:224:SER:OG	2.28	0.42
42:H:86:GLU:HA	42:H:87:PRO:HD3	1.83	0.42
49:O:50:ARG:HA	79:t:113:A:H1'	2.00	0.42
51:Q:138:PRO:HB2	51:Q:140:MET:HG3	2.01	0.42
51:Q:139:TYR:HE2	79:t:2400:G:H1'	1.84	0.42
56:V:28:PRO:O	56:V:32:GLY:N	2.53	0.42
59:Y:77:ILE:HD13	59:Y:77:ILE:HG21	1.81	0.42
76:p:61:LYS:HD3	76:p:87:ARG:HH12	1.84	0.42
1:S2:691:G:N2	1:S2:692:G:N3	2.67	0.42
2:SA:128:ARG:HB3	2:SA:153:PRO:HD2	2.01	0.42
2:SA:159:ILE:HD11	17:SV:34:MET:HE1	2.02	0.42
4:SD:27:ARG:HB2	9:SK:61:GLN:OE1	2.19	0.42
7:SH:53:VAL:HG11	7:SH:172:THR:HA	2.02	0.42
7:SH:146:VAL:HA	7:SH:152:ARG:HA	2.01	0.42
11:SP:17:TYR:HE1	11:SP:112:ILE:HG22	1.82	0.42
17:SV:17:CYS:HB2	17:SV:56:CYS:HB3	2.01	0.42
18:SX:61:GLN:N	18:SX:62:PRO:HD2	2.34	0.42
18:SX:132:ALA:HB1	18:SX:137:LYS:HB2	2.01	0.42
23:SC:196:ILE:HB	23:SC:223:TYR:HB2	2.02	0.42
28:SO:99:ALA:H	28:SO:133:THR:HB	1.85	0.42
30:SY:23:MET:SD	30:SY:23:MET:N	2.92	0.42
40:F:106:ALA:HB2	40:F:166:ALA:HA	2.01	0.42
40:F:122:GLN:NE2	40:F:126:THR:OG1	2.51	0.42
41:G:43:HIS:CD2	41:G:44:CYS:H	2.36	0.42
41:G:46:ARG:HH11	41:G:46:ARG:HD2	1.68	0.42
41:G:179:LEU:HB2	41:G:250:GLN:NE2	2.35	0.42
43:I:102:TYR:HH	43:I:208:ASN:H	1.62	0.42
43:I:156:VAL:HB	43:I:202:VAL:HG22	2.01	0.42
54:T:29:ARG:HB2	55:U:148:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:84:TYR:HA	54:T:124:ILE:HA	2.02	0.42
54:T:162:GLN:HG3	54:T:166:ARG:HG2	2.01	0.42
59:Y:80:PRO:HA	59:Y:98:PHE:HA	2.00	0.42
62:b:86:THR:OG1	62:b:87:ARG:N	2.50	0.42
66:f:75:ARG:HB2	66:f:95:TYR:CD1	2.54	0.42
78:r:22:LYS:HB3	78:r:23:GLN:H	1.65	0.42
79:t:4726:A:N6	79:t:4826:G:H22	2.15	0.42
1:S2:1031:A2M:HM'3	1:S2:1031:A2M:H1'	1.76	0.42
1:S2:1171:G:O2'	1:S2:1187:G:O6	2.28	0.42
1:S2:1174:U:H2'	1:S2:1175:G:C8	2.55	0.42
2:SA:166:LYS:HE3	2:SA:166:LYS:HB3	1.86	0.42
11:SP:17:TYR:CZ	11:SP:18:ARG:CZ	3.00	0.42
11:SP:17:TYR:HD2	11:SP:18:ARG:HB2	1.85	0.42
16:SU:79:ARG:H	21:Sd:54:LYS:NZ	2.17	0.42
27:SN:4:MET:SD	27:SN:124:ARG:NH1	2.93	0.42
38:D:90:C:H2'	38:D:91:A:C8	2.53	0.42
41:G:152:ILE:HD12	41:G:189:THR:HG21	2.01	0.42
52:R:64:SER:OG	52:R:89:ASP:OD2	2.28	0.42
55:U:13:TYR:OH	79:t:1772:U:OP2	2.28	0.42
61:a:41:ALA:HB2	61:a:77:TYR:HE1	1.84	0.42
79:t:1846:G:N2	79:t:1849:A:OP2	2.51	0.42
2:SA:77:ILE:HD11	2:SA:124:VAL:HG22	2.01	0.42
4:SD:5:ILE:H	4:SD:5:ILE:HG13	1.63	0.42
10:SL:22:ARG:CZ	10:SL:26:GLY:HA3	2.50	0.42
13:SR:38:ILE:HD12	13:SR:38:ILE:HA	1.84	0.42
16:SU:54:VAL:HG12	16:SU:88:LEU:HB3	2.02	0.42
19:Sa:29:CYS:SG	28:SO:146:ARG:NH1	2.92	0.42
21:Sd:19:ARG:NH1	21:Sd:32:ARG:HH11	2.17	0.42
36:B:83:PRO:HB3	36:B:206:PRO:HA	2.01	0.42
37:C:266:THR:OG1	37:C:267:TRP:N	2.51	0.42
49:O:63:ARG:HA	49:O:131:GLU:HA	2.00	0.42
52:R:162:HIS:HA	79:t:1479:A:H5'	2.01	0.42
53:S:159:ALA:O	53:S:162:ARG:NH1	2.53	0.42
54:T:93:MET:HG3	79:t:1933:G:H4'	2.02	0.42
62:b:7:LYS:HE3	62:b:11:LEU:HD22	2.02	0.42
62:b:115:GLY:HA3	79:t:1381:A:C8	2.54	0.42
66:f:84:GLU:OE1	78:r:20:ARG:NH2	2.52	0.42
79:t:1200:G:H2'	79:t:1201:G:C8	2.55	0.42
79:t:1336:G:O2'	79:t:1338:G:O2'	2.36	0.42
79:t:2652:G:H5''	79:t:2653:A:H3'	2.00	0.42
79:t:3660:G:O2'	79:t:3789:U:OP2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1222:G:H4'	1:S2:1676:U:H3	1.85	0.42
1:S2:1863:A:OP2	19:Sa:4:LYS:NZ	2.45	0.42
3:SB:89:GLU:HB3	3:SB:223:PHE:CE1	2.55	0.42
13:SR:17:ILE:HD11	13:SR:61:ILE:HD13	2.01	0.42
22:Sg:286:CYS:HA	22:Sg:302:TYR:HD1	1.84	0.42
43:I:73:ARG:NH1	79:t:4046:G:OP1	2.52	0.42
49:O:179:LYS:O	79:t:291:U:O2'	2.37	0.42
54:T:62:VAL:HG11	55:U:141:VAL:HG11	2.02	0.42
55:U:108:ARG:O	55:U:112:ASN:N	2.53	0.42
57:W:37:LEU:HD21	57:W:105:ILE:HD11	2.02	0.42
79:t:1658:C:H41	79:t:4340:A:H2'	1.84	0.42
79:t:3583:C:H1'	79:t:4974:A:C8	2.54	0.42
1:S2:190:G:N1	1:S2:208:G:N7	2.68	0.42
1:S2:208:G:H2'	1:S2:209:A:H8	1.85	0.42
1:S2:520:A:O2'	1:S2:825:A:N3	2.46	0.42
1:S2:527:C:OP1	25:SJ:122:SER:OG	2.32	0.42
1:S2:1587:G:OP1	1:S2:1587:G:N2	2.53	0.42
2:SA:76:VAL:HG23	2:SA:123:VAL:HG13	2.01	0.42
6:SF:39:ILE:HG22	6:SF:41:VAL:HG23	2.02	0.42
9:SK:77:GLN:HA	9:SK:80:ARG:HG2	2.01	0.42
38:D:142:U:P	49:O:38:ARG:HH22	2.43	0.42
41:G:167:GLN:HA	41:G:173:LEU:HA	2.02	0.42
47:M:87:HIS:CD2	47:M:89:LYS:H	2.38	0.42
50:P:179:LYS:HA	50:P:182:GLU:HG2	2.00	0.42
53:S:104:ARG:HB3	53:S:107:ARG:HH11	1.83	0.42
54:T:95:ARG:NH1	79:t:1932:G:O3'	2.53	0.42
67:g:58:VAL:HG13	67:g:64:PRO:HA	2.00	0.42
79:t:4228:G:H8	79:t:4228:G:H2'	1.69	0.42
1:S2:587:A:H5'	1:S2:592:C:H41	1.84	0.42
6:SF:35:LEU:HD22	6:SF:117:ILE:HD13	2.01	0.42
7:SH:15:LYS:N	7:SH:16:PRO:HD2	2.34	0.42
15:ST:113:VAL:HA	15:ST:123:LEU:HA	2.01	0.42
18:SX:46:HIS:HB3	18:SX:101:LEU:HD11	2.02	0.42
23:SC:116:THR:HG21	23:SC:121:ARG:HG2	2.00	0.42
24:SG:49:VAL:HG22	24:SG:115:LYS:HE3	2.02	0.42
35:A:115:CYS:HB3	35:A:165:VAL:HG12	2.02	0.42
37:C:52:TYR:HB2	37:C:111:TRP:HH2	1.85	0.42
37:C:113:ARG:HA	37:C:113:ARG:HD3	1.92	0.42
47:M:76:PHE:CE2	47:M:117:LEU:HD13	2.54	0.42
48:N:46:ARG:NH1	79:t:925:C:O5'	2.39	0.42
54:T:164:LYS:HD3	79:t:4833:G:C2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:V:40:GLU:HG3	56:V:63:ILE:HG21	2.02	0.42
65:e:79:ASN:HD22	79:t:4615:C:H5'	1.85	0.42
68:h:43:LYS:HD3	68:h:52:ARG:HH12	1.85	0.42
68:h:97:ILE:HD11	79:t:4091:G:N7	2.35	0.42
79:t:3770:A:N3	79:t:4468:C:O2'	2.49	0.42
1:S2:416:U:HO2'	1:S2:652:U:HO2'	1.65	0.42
1:S2:429:C:OP1	5:SE:10:LYS:NZ	2.36	0.42
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.18	0.42
1:S2:1233:G:N3	1:S2:1252:C:O2'	2.45	0.42
1:S2:1355:C:O3'	23:SC:238:LYS:NZ	2.53	0.42
1:S2:1401:A:N6	1:S2:1441:U:O2'	2.53	0.42
1:S2:1543:U:OP1	15:ST:62:ARG:NH1	2.52	0.42
3:SB:128:LYS:HA	3:SB:134:LEU:HA	2.02	0.42
42:H:32:ARG:HH22	79:t:950:G:H21	1.66	0.42
49:O:10:LEU:HB2	70:j:44:ILE:HD11	2.01	0.42
49:O:117:ASN:N	49:O:117:ASN:OD1	2.52	0.42
52:R:16:LYS:O	52:R:33:ARG:NH2	2.49	0.42
62:b:123:ILE:HG21	62:b:123:ILE:HD13	1.84	0.42
66:f:75:ARG:HD2	66:f:95:TYR:HE1	1.85	0.42
1:S2:913:A:N6	7:SH:99:ARG:O	2.53	0.41
2:SA:89:LYS:O	2:SA:93:ALA:N	2.53	0.41
5:SE:191:ARG:HD2	5:SE:218:PHE:CE1	2.55	0.41
12:SQ:112:LEU:HD22	12:SQ:119:LEU:HD22	2.01	0.41
22:Sg:31:ILE:HD13	22:Sg:299:PHE:CE2	2.55	0.41
37:C:316:LYS:NZ	79:t:1266:G:OP2	2.39	0.41
48:N:12:VAL:O	48:N:58:THR:OG1	2.26	0.41
51:Q:139:TYR:CD1	79:t:3830:G:H4'	2.55	0.41
55:U:8:ARG:NH2	55:U:52:MET:SD	2.74	0.41
55:U:11:THR:O	55:U:11:THR:OG1	2.28	0.41
65:e:50:ARG:NH2	79:t:2353:A:OP1	2.54	0.41
79:t:2722:A:H2'	79:t:2723:A:C8	2.55	0.41
79:t:3624:A:H61	79:t:3662:G:HO2'	1.60	0.41
79:t:3763:G:O6	79:t:3778:A:N6	2.53	0.41
81:v:48:C:H2'	81:v:59:U:H1'	2.02	0.41
1:S2:529:A:H62	1:S2:555:A:H62	1.67	0.41
1:S2:1497:G:C6	9:SK:62:PHE:CD1	3.09	0.41
4:SD:48:ILE:HB	4:SD:86:LEU:HD23	2.02	0.41
10:SL:120:VAL:HG22	10:SL:145:VAL:HG21	2.01	0.41
22:Sg:5:MET:HE2	22:Sg:270:LEU:HD21	2.02	0.41
22:Sg:70:VAL:HG22	22:Sg:111:VAL:HG23	2.02	0.41
38:D:60:G:OP1	59:Y:68:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L:35:ARG:HG3	46:L:123:ILE:HA	2.01	0.41
48:N:89:THR:HG23	48:N:92:ALA:H	1.85	0.41
48:N:123:ILE:O	48:N:127:VAL:N	2.42	0.41
50:P:58:LEU:HD22	50:P:74:ARG:HH21	1.84	0.41
66:f:38:PRO:HB2	66:f:43:ASN:ND2	2.35	0.41
71:k:13:ASN:OD1	71:k:13:ASN:N	2.51	0.41
74:n:94:MET:HG2	74:n:105:PRO:HA	2.02	0.41
75:o:1:MET:HE1	75:o:9:ARG:HH11	1.85	0.41
1:S2:1289:U:C5	34:Sf:97:LYS:HE2	2.55	0.41
2:SA:205:ARG:HE	2:SA:206:ASP:H	1.68	0.41
38:D:149:G:H21	43:I:64:GLN:NE2	2.18	0.41
40:F:41:LYS:HB3	40:F:41:LYS:HE3	1.85	0.41
47:M:127:PHE:HB2	69:i:118:LYS:HG3	2.02	0.41
69:i:122:LYS:HD2	69:i:122:LYS:HA	1.86	0.41
1:S2:1512:C:H5''	21:Sd:8:TRP:HZ3	1.86	0.41
1:S2:1720:U:HO2'	79:t:3767:U:HO2'	1.57	0.41
22:Sg:154:VAL:HG22	22:Sg:167:SER:HA	2.02	0.41
26:SM:99:ASN:OD1	26:SM:99:ASN:N	2.53	0.41
50:P:125:LYS:HE3	50:P:135:PHE:CD1	2.55	0.41
58:X:4:GLU:O	58:X:13:ILE:N	2.39	0.41
60:Z:11:ARG:HG3	79:t:225:C:H5''	2.01	0.41
60:Z:72:GLN:NE2	60:Z:74:TYR:HE1	2.19	0.41
62:b:89:ASN:O	62:b:92:LYS:HG2	2.20	0.41
77:q:41:PHE:CD2	77:q:62:LYS:HD2	2.55	0.41
79:t:301:A:N3	79:t:304:G:O2'	2.45	0.41
79:t:919:A:O2'	79:t:921:C:O4'	2.36	0.41
79:t:3681:G:H1	79:t:3683:A:H62	1.68	0.41
79:t:4251:U:O2'	79:t:4282:G:O2'	2.37	0.41
1:S2:145:G:H2'	1:S2:146:G:C8	2.55	0.41
1:S2:368:U:OP1	1:S2:369:C:O2'	2.28	0.41
1:S2:919:A:OP2	27:SN:64:ARG:NH2	2.48	0.41
2:SA:90:PHE:HD1	2:SA:179:ALA:HB2	1.84	0.41
5:SE:51:ARG:NH2	5:SE:109:PHE:O	2.54	0.41
7:SH:14:GLU:N	7:SH:14:GLU:CD	2.73	0.41
7:SH:51:ILE:H	7:SH:51:ILE:HG13	1.58	0.41
10:SL:60:CYS:SG	10:SL:114:SER:OG	2.65	0.41
10:SL:111:VAL:HG11	10:SL:128:VAL:HG11	2.02	0.41
11:SP:13:ARG:O	11:SP:14:LYS:HB2	2.20	0.41
20:Sc:21:THR:N	20:Sc:27:CYS:O	2.47	0.41
40:F:37:VAL:HG22	40:F:50:ARG:HD3	2.03	0.41
41:G:162:VAL:CB	41:G:175:VAL:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:178:SER:OG	42:H:179:LEU:N	2.53	0.41
43:I:106:THR:HG22	43:I:109:GLU:HG2	2.03	0.41
44:J:17:ASP:OD1	44:J:17:ASP:N	2.52	0.41
54:T:96:GLU:HB2	54:T:139:ARG:HG3	2.02	0.41
54:T:159:LEU:HG	79:t:1902:C:H1'	2.03	0.41
81:v:50:U:O2	81:v:65:G:N2	2.34	0.41
5:SE:183:VAL:HG13	5:SE:189:LEU:HA	2.02	0.41
6:SF:82:ASN:N	6:SF:82:ASN:OD1	2.53	0.41
12:SQ:146:ARG:NH2	81:v:34:C:OP2	2.50	0.41
16:SU:67:LYS:HE2	16:SU:78:ASP:HB3	2.03	0.41
30:SY:79:LEU:HD12	30:SY:82:ALA:HB3	2.02	0.41
30:SY:90:ARG:HG2	30:SY:93:ARG:HD2	2.01	0.41
37:C:12:SER:OG	37:C:13:GLU:N	2.53	0.41
37:C:29:LYS:HB2	37:C:267:TRP:HH2	1.85	0.41
39:E:99:G:N7	54:T:55:LYS:NZ	2.68	0.41
42:H:53:LYS:NZ	42:H:189:ASP:OD2	2.44	0.41
65:e:51:LYS:HA	65:e:54:MET:HG2	2.02	0.41
76:p:12:CYS:SG	76:p:19:GLN:NE2	2.83	0.41
79:t:1256:G:H2'	79:t:1257:A:C8	2.56	0.41
79:t:1523:C:O2'	79:t:2427:G:N3	2.46	0.41
79:t:1614:A:H1'	79:t:3612:U:H1'	2.03	0.41
79:t:1791:C:H2'	79:t:1792:G:C8	2.56	0.41
1:S2:874:G:H2'	1:S2:875:A:C8	2.56	0.41
9:SK:65:ARG:HD2	21:Sd:22:ARG:O	2.20	0.41
10:SL:17:PHE:CE2	10:SL:19:ASN:HB2	2.55	0.41
29:SW:15:ASN:HD21	29:SW:71:LYS:HG3	1.85	0.41
36:B:117:ARG:HA	36:B:117:ARG:HD2	1.88	0.41
36:B:292:LEU:HB3	36:B:293:ILE:H	1.68	0.41
61:a:51:ARG:HB2	61:a:65:ARG:HB3	2.02	0.41
63:c:18:ARG:HH11	63:c:18:ARG:HD2	1.76	0.41
79:t:729:C:H2'	79:t:730:G:C8	2.56	0.41
79:t:3725:G:N2	79:t:3742:C:O2	2.53	0.41
79:t:4072:C:O2	79:t:4077:G:N2	2.54	0.41
1:S2:38:A:O2'	25:SJ:5:ARG:NH2	2.54	0.41
1:S2:484:A2M:HM'2	1:S2:485:A:C4	2.55	0.41
1:S2:1332:A:H2	4:SD:180:GLY:HA2	1.86	0.41
1:S2:1481:G:H4'	21:Sd:54:LYS:HE3	2.01	0.41
7:SH:96:ALA:HB3	7:SH:98:ARG:HE	1.85	0.41
9:SK:59:LYS:HZ3	9:SK:70:TYR:HD2	1.67	0.41
9:SK:74:GLU:HA	9:SK:77:GLN:HG3	2.03	0.41
19:Sa:45:VAL:HG21	19:Sa:64:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Sa:49:ALA:HB2	28:SO:117:ARG:HD3	2.01	0.41
23:SC:144:SER:HB3	23:SC:150:ALA:HB2	2.02	0.41
36:B:369:ASP:N	36:B:369:ASP:OD1	2.53	0.41
38:D:3:A:H4'	51:Q:61:ARG:HD3	2.03	0.41
38:D:132:G:OP1	59:Y:108:GLN:NE2	2.54	0.41
41:G:150:LEU:HB2	41:G:162:VAL:HG23	2.03	0.41
45:K:46:PHE:HB2	45:K:139:ARG:NH1	2.36	0.41
52:R:10:ASP:C	79:t:2062:C:O2'	2.56	0.41
57:W:71:GLU:HG2	57:W:72:LEU:HD12	2.03	0.41
72:l:35:LYS:HE2	79:t:2675:A:H62	1.85	0.41
79:t:2375:A:H5''	79:t:2785:A:N6	2.36	0.41
79:t:2580:A:N6	79:t:2723:A:OP2	2.53	0.41
79:t:4248:C:H2'	79:t:4249:G:H8	1.86	0.41
1:S2:416:U:O4	1:S2:417:C:N4	2.53	0.41
1:S2:560:A:C6	25:SJ:165:TYR:HA	2.56	0.41
1:S2:1123:C:O2'	3:SB:148:ASN:OD1	2.28	0.41
1:S2:1497:G:N9	9:SK:62:PHE:CD2	2.89	0.41
2:SA:89:LYS:HE2	2:SA:201:LEU:HG	2.03	0.41
3:SB:171:ILE:HD12	3:SB:197:ILE:HG22	2.03	0.41
6:SF:87:LEU:HD11	12:SQ:78:VAL:HG22	2.03	0.41
9:SK:60:GLU:HB3	9:SK:69:TRP:NE1	2.36	0.41
10:SL:22:ARG:C	10:SL:23:VAL:CG1	2.91	0.41
12:SQ:68:ILE:H	12:SQ:68:ILE:HG13	1.74	0.41
14:SS:87:GLN:HA	14:SS:95:TYR:HD1	1.86	0.41
16:SU:35:VAL:HG21	16:SU:107:GLU:HG2	2.01	0.41
21:Sd:39:CYS:O	21:Sd:42:CYS:CA	2.69	0.41
22:Sg:17:TRP:N	22:Sg:36:ARG:HB3	2.35	0.41
25:SJ:136:ARG:HA	25:SJ:141:VAL:HA	2.02	0.41
29:SW:89:TRP:HE3	29:SW:93:LEU:HD21	1.86	0.41
30:SY:20:ARG:NH2	30:SY:74:MET:HE3	2.36	0.41
31:SZ:110:THR:OG1	31:SZ:111:ARG:N	2.54	0.41
34:Sf:89:LYS:HE3	34:Sf:89:LYS:HB3	1.95	0.41
36:B:117:ARG:NH1	36:B:179:HIS:HA	2.36	0.41
37:C:100:ARG:NH2	79:t:1503:C:OP1	2.42	0.41
37:C:183:VAL:HG11	37:C:226:GLY:HA3	2.02	0.41
38:D:9:A:H2'	38:D:10:G:H8	1.85	0.41
43:I:221:ALA:O	43:I:225:ASN:ND2	2.54	0.41
47:M:28:GLN:HG3	47:M:29:PRO:HD3	2.03	0.41
50:P:177:LEU:HD23	50:P:177:LEU:HA	1.90	0.41
51:Q:7:ASP:OD1	51:Q:7:ASP:N	2.54	0.41
52:R:72:LEU:HD13	52:R:72:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S:67:THR:O	53:S:71:ARG:N	2.53	0.41
53:S:105:LEU:HD23	53:S:138:LEU:HD12	2.01	0.41
55:U:115:LYS:HD3	55:U:126:VAL:HG21	2.03	0.41
59:Y:129:ARG:NH1	59:Y:131:ASP:HB2	2.36	0.41
61:a:46:ILE:HD12	61:a:68:ILE:HD11	2.02	0.41
62:b:86:THR:O	62:b:90:ALA:N	2.51	0.41
63:c:111:ARG:NH2	79:t:1248:G:O5'	2.54	0.41
74:n:100:TYR:OH	79:t:4387:G:OP1	2.37	0.41
78:r:99:LYS:HD3	78:r:99:LYS:HA	1.89	0.41
79:t:47:A:H5'	79:t:49:U:H1'	2.03	0.41
79:t:735:G:H2'	79:t:736:G:C8	2.56	0.41
79:t:944:G:N7	79:t:1267:G:O2'	2.51	0.41
79:t:1373:G:N2	79:t:1376:G:OP2	2.53	0.41
79:t:1398:G:H2'	79:t:1399:G:C8	2.56	0.41
79:t:1844:U:O2'	79:t:4182:A:N1	2.42	0.41
79:t:2586:C:H2'	79:t:2587:G:H8	1.86	0.41
81:v:12:C:H42	81:v:23:A:H61	1.67	0.41
1:S2:101:U:H5''	8:SI:19:LYS:HE2	2.02	0.41
1:S2:388:U:H2'	1:S2:389:A:C8	2.56	0.41
1:S2:1424:G:H2'	1:S2:1425:G:H8	1.86	0.41
21:Sd:24:CYS:O	21:Sd:25:SER:HB3	2.20	0.41
23:SC:187:ARG:HG2	23:SC:192:LEU:HB3	2.03	0.41
36:B:176:LYS:NZ	79:t:4945:C:OP1	2.46	0.41
39:E:11:A:O2'	39:E:13:A:OP2	2.34	0.41
42:H:126:ASN:HD22	42:H:126:ASN:HA	1.70	0.41
49:O:65:ARG:HD2	49:O:127:TYR:CD2	2.56	0.41
53:S:23:TRP:NE1	53:S:49:LEU:O	2.49	0.41
54:T:28:TYR:CE2	54:T:52:LYS:HG3	2.56	0.41
57:W:91:LYS:HD3	57:W:91:LYS:HA	1.92	0.41
61:a:17:ARG:NH1	79:t:2557:G:N7	2.69	0.41
68:h:29:ARG:NH2	79:t:2501:G:OP2	2.54	0.41
70:j:29:ARG:NH2	79:t:270:C:N3	2.58	0.41
72:l:27:LYS:HA	72:l:32:VAL:HG23	2.03	0.41
79:t:3590:G:O2'	79:t:3593:C:N4	2.54	0.41
79:t:3789:U:H6	79:t:3789:U:H2'	1.71	0.41
79:t:4108:G:H4'	79:t:4109:G:C6	2.56	0.41
79:t:4174:A:N6	79:t:4181:A:OP2	2.48	0.41
79:t:4832:A:H1'	79:t:4834:U:C2	2.56	0.41
1:S2:1232:U:H2'	1:S2:1233:G:C8	2.55	0.40
3:SB:185:VAL:O	3:SB:189:ILE:HD12	2.22	0.40
4:SD:74:GLN:HG3	4:SD:79:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:45:ILE:HA	5:SE:61:VAL:HG11	2.03	0.40
5:SE:246:LEU:HD23	5:SE:250:GLU:HG2	2.04	0.40
18:SX:108:LYS:HD2	18:SX:108:LYS:HA	1.88	0.40
23:SC:107:LEU:HD22	23:SC:209:VAL:HG23	2.03	0.40
28:SO:104:ARG:HB3	28:SO:105:THR:H	1.71	0.40
31:SZ:57:LYS:HE2	31:SZ:57:LYS:HB3	1.89	0.40
36:B:285:TYR:OH	36:B:334:LYS:HD3	2.21	0.40
40:F:211:LEU:HD23	40:F:211:LEU:HA	1.83	0.40
40:F:217:ASP:HA	40:F:220:LYS:HZ2	1.86	0.40
48:N:105:THR:OG1	48:N:106:ASP:N	2.53	0.40
79:t:1069:C:H2'	79:t:1070:A:H8	1.86	0.40
79:t:4199:C:O3'	79:t:4288:G:N2	2.54	0.40
79:t:4951:G:N2	79:t:5017:C:O2	2.54	0.40
1:S2:682:U:P	18:SX:8:ARG:HE	2.43	0.40
1:S2:1616:U:OP2	11:SP:43:ARG:NH2	2.50	0.40
11:SP:17:TYR:HD1	11:SP:112:ILE:HG21	1.82	0.40
12:SQ:1:MET:HA	12:SQ:2:PRO:HD3	1.87	0.40
22:Sg:288:SER:O	22:Sg:301:GLY:N	2.43	0.40
31:SZ:69:THR:HB	31:SZ:72:VAL:HG23	2.02	0.40
36:B:36:ASP:OD1	36:B:36:ASP:N	2.53	0.40
36:B:334:LYS:NZ	79:t:4637:U:OP1	2.53	0.40
37:C:337:ARG:NH2	41:G:58:SER:HA	2.35	0.40
41:G:179:LEU:HD11	41:G:183:ARG:NH1	2.35	0.40
43:I:103:ARG:HD3	43:I:195:HIS:NE2	2.36	0.40
45:K:150:GLU:OE2	45:K:153:ARG:NH2	2.54	0.40
49:O:71:ARG:HD2	49:O:94:PHE:HB2	2.03	0.40
62:b:103:VAL:HB	62:b:108:TYR:HB2	2.03	0.40
65:e:97:ASP:OD1	65:e:97:ASP:N	2.50	0.40
73:m:9:ILE:HD13	73:m:9:ILE:HA	1.93	0.40
79:t:216:G:H22	79:t:233:G:H1	1.69	0.40
79:t:1058:G:H1	79:t:1218:G:H22	1.69	0.40
79:t:2824:A:H61	79:t:3814:C:H42	1.69	0.40
1:S2:67:C:H4'	1:S2:68:A:N7	2.36	0.40
1:S2:202:G:N2	1:S2:202:G:OP2	2.54	0.40
1:S2:509:OMG:H1'	1:S2:509:OMG:HM23	1.68	0.40
3:SB:84:PHE:CD2	3:SB:103:MET:HB3	2.57	0.40
6:SF:30:ILE:HD13	6:SF:42:LYS:NZ	2.36	0.40
11:SP:44:ARG:NH1	11:SP:82:ASP:O	2.53	0.40
12:SQ:87:SER:O	12:SQ:91:ALA:N	2.54	0.40
22:Sg:20:GLN:NE2	22:Sg:69:VAL:O	2.55	0.40
30:SY:74:MET:HE2	30:SY:74:MET:HB2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:68:ARG:NH2	79:t:4054:G:N7	2.70	0.40
37:C:242:PRO:HB2	79:t:2276:G:H4'	2.04	0.40
41:G:286:LEU:HD22	41:G:288:PHE:CE2	2.57	0.40
42:H:223:LYS:NZ	79:t:1888:A:O2'	2.49	0.40
43:I:187:LYS:HE2	43:I:198:THR:HG21	2.02	0.40
43:I:244:PRO:HA	43:I:247:VAL:HG12	2.03	0.40
44:J:86:LEU:HD13	44:J:186:THR:HG21	2.03	0.40
52:R:161:SER:HB2	52:R:163:THR:OG1	2.21	0.40
76:p:37:GLY:O	81:v:75:C:N4	2.51	0.40
79:t:1060:C:H42	79:t:1217:G:H1	1.68	0.40
79:t:1397:C:H2'	79:t:1398:G:H8	1.85	0.40
1:S2:65:C:C4	24:SG:174:PRO:HG3	2.56	0.40
1:S2:208:G:H2'	1:S2:209:A:C8	2.56	0.40
1:S2:737:G:H2'	1:S2:738:C:H4'	2.03	0.40
1:S2:1497:G:C6	9:SK:62:PHE:CE1	3.09	0.40
1:S2:1497:G:N9	9:SK:62:PHE:CE2	2.88	0.40
2:SA:110:ASN:HB3	2:SA:113:GLN:HE22	1.86	0.40
5:SE:191:ARG:HH11	5:SE:245:ARG:HD2	1.85	0.40
8:SI:195:LEU:HG	8:SI:199:LEU:HD23	2.03	0.40
12:SQ:42:ILE:HD12	12:SQ:42:ILE:HA	1.95	0.40
18:SX:94:ILE:HG22	18:SX:125:VAL:HG21	2.03	0.40
21:Sd:16:GLN:N	21:Sd:19:ARG:HH21	2.20	0.40
22:Sg:99:ARG:HH22	22:Sg:134:THR:HB	1.86	0.40
23:SC:70:VAL:HG11	23:SC:93:ILE:HG13	2.02	0.40
25:SJ:101:LYS:HG3	25:SJ:103:GLU:H	1.86	0.40
29:SW:55:ASP:OD1	29:SW:56:HIS:N	2.53	0.40
35:A:60:LYS:HE2	35:A:73:THR:HG21	2.04	0.40
42:H:162:ILE:HD11	42:H:167:ILE:HG12	2.03	0.40
47:M:130:LYS:O	47:M:132:SER:N	2.54	0.40
50:P:173:GLN:HE21	50:P:177:LEU:HD11	1.87	0.40
51:Q:23:ARG:HA	51:Q:143:PRO:HB3	2.03	0.40
55:U:93:ILE:HA	55:U:93:ILE:HD12	1.88	0.40
67:g:81:SER:O	67:g:81:SER:OG	2.39	0.40
78:r:53:PRO:HD3	78:r:117:ILE:HD11	2.03	0.40
79:t:1648:C:O2'	79:t:1670:G:OP1	2.37	0.40
1:S2:57:U:OP1	1:S2:504:G:O2'	2.38	0.40
2:SA:18:PHE:HD1	2:SA:18:PHE:HA	1.79	0.40
3:SB:105:LEU:HD13	3:SB:213:ARG:HA	2.02	0.40
5:SE:100:ARG:HH22	5:SE:122:LYS:HA	1.87	0.40
14:SS:42:HIS:HD2	14:SS:52:LEU:HD21	1.86	0.40
18:SX:108:LYS:HE3	18:SX:108:LYS:HB3	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sg:21:ILE:HG21	22:Sg:299:PHE:HB3	2.04	0.40
22:Sg:212:LYS:HG3	22:Sg:235:ILE:HD12	2.04	0.40
25:SJ:41:ARG:HH11	25:SJ:41:ARG:HD3	1.72	0.40
27:SN:3:ARG:HG2	27:SN:6:ALA:HB3	2.03	0.40
50:P:179:LYS:HE3	79:t:4830:G:C8	2.57	0.40
57:W:84:GLN:NE2	57:W:86:LYS:HB3	2.37	0.40
63:c:111:ARG:NH1	79:t:1249:G:OP2	2.53	0.40
65:e:27:ILE:HA	65:e:27:ILE:HD13	1.90	0.40
76:p:28:LYS:O	79:t:4306:U:O2'	2.30	0.40
79:t:220:G:C8	79:t:240:A:H4'	2.57	0.40
79:t:388:G:N2	79:t:391:G:OP2	2.51	0.40
79:t:3754:A:H2	79:t:3761:U:H3	1.68	0.40
79:t:4601:G:H1	79:t:4622:G:H1	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	192 (88%)	26 (12%)	1 (0%)	24	57
3	SB	212/214 (99%)	191 (90%)	21 (10%)	0	100	100
4	SD	224/226 (99%)	194 (87%)	30 (13%)	0	100	100
5	SE	257/259 (99%)	241 (94%)	16 (6%)	0	100	100
6	SF	187/189 (99%)	171 (91%)	16 (9%)	0	100	100
7	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
8	SI	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
9	SK	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	12	44
10	SL	151/153 (99%)	135 (89%)	15 (10%)	1 (1%)	18	51
11	SP	125/127 (98%)	111 (89%)	14 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	SQ	144/146 (99%)	127 (88%)	15 (10%)	2 (1%)	9	38
13	SR	132/134 (98%)	119 (90%)	12 (9%)	1 (1%)	16	49
14	SS	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
15	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	18	51
16	SU	102/104 (98%)	93 (91%)	9 (9%)	0	100	100
17	SV	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
18	SX	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	12	44
20	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
21	Sd	53/55 (96%)	44 (83%)	9 (17%)	0	100	100
22	Sg	310/312 (99%)	255 (82%)	55 (18%)	0	100	100
23	SC	219/220 (100%)	201 (92%)	17 (8%)	1 (0%)	24	57
24	SG	235/237 (99%)	212 (90%)	23 (10%)	0	100	100
25	SJ	184/185 (100%)	168 (91%)	15 (8%)	1 (0%)	24	57
26	SM	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
27	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
28	SO	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
29	SW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
30	SY	130/131 (99%)	119 (92%)	10 (8%)	1 (1%)	16	49
31	SZ	71/73 (97%)	58 (82%)	13 (18%)	0	100	100
32	Sb	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
33	Se	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
34	Sf	65/67 (97%)	52 (80%)	13 (20%)	0	100	100
35	A	250/252 (99%)	222 (89%)	27 (11%)	1 (0%)	30	62
36	B	395/397 (100%)	355 (90%)	37 (9%)	3 (1%)	16	49
37	C	361/363 (99%)	326 (90%)	31 (9%)	4 (1%)	11	43
40	F	292/294 (99%)	257 (88%)	32 (11%)	3 (1%)	12	44
41	G	232/247 (94%)	194 (84%)	38 (16%)	0	100	100
42	H	223/225 (99%)	209 (94%)	13 (6%)	1 (0%)	30	62
43	I	232/234 (99%)	212 (91%)	20 (9%)	0	100	100
44	J	189/191 (99%)	170 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	K	204/211 (97%)	179 (88%)	24 (12%)	1 (0%)	24	57
46	L	167/169 (99%)	150 (90%)	16 (10%)	1 (1%)	21	54
47	M	203/205 (99%)	168 (83%)	31 (15%)	4 (2%)	6	32
48	N	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
49	O	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
50	P	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	57
51	Q	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
52	R	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
53	S	179/181 (99%)	171 (96%)	8 (4%)	0	100	100
54	T	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
55	U	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	9	39
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
57	W	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
58	X	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
59	Y	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
60	Z	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
61	a	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
62	b	145/147 (99%)	125 (86%)	19 (13%)	1 (1%)	18	51
63	c	94/121 (78%)	83 (88%)	11 (12%)	0	100	100
64	d	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
65	e	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
66	f	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	49
67	g	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
68	h	112/114 (98%)	101 (90%)	10 (9%)	1 (1%)	14	47
69	i	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	49
70	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	43
71	k	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
72	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
73	m	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
74	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	p	103/105 (98%)	93 (90%)	9 (9%)	1 (1%)	12	44
77	q	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
78	r	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	28
All	All	11195/11390 (98%)	10073 (90%)	1081 (10%)	41 (0%)	31	62

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	SK	63	ALA
10	SL	23	VAL
13	SR	129	LYS
15	ST	41	LYS
23	SC	78	LEU
55	U	19	PHE
62	b	95	THR
66	f	7	LEU
12	SQ	117	ARG
19	Sa	47	ALA
37	C	69	THR
40	F	10	LYS
47	M	64	VAL
68	h	47	GLY
70	j	35	LYS
2	SA	12	GLU
40	F	8	LYS
40	F	260	GLU
45	K	11	TYR
69	i	88	THR
78	r	23	GLN
35	A	251	THR
36	B	4	ARG
36	B	299	ILE
42	H	223	LYS
55	U	53	PRO
76	p	104	ILE
12	SQ	116	ASP
37	C	56	GLU
37	C	303	ARG
47	M	63	THR
78	r	21	ASN
78	r	22	LYS

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Mol	Chain	Res	Type
36	B	3	HIS
46	L	171	ASP
25	SJ	123	ILE
30	SY	95	GLY
37	C	70	GLY
47	M	153	PRO
50	P	185	VAL
47	M	47	ALA

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	
2	SA	183/183 (100%)	180 (98%)	3 (2%)	55	70
3	SB	195/195 (100%)	191 (98%)	4 (2%)	47	66
4	SD	189/189 (100%)	185 (98%)	4 (2%)	47	66
5	SE	222/222 (100%)	219 (99%)	3 (1%)	59	71
6	SF	159/159 (100%)	157 (99%)	2 (1%)	61	72
7	SH	166/169 (98%)	164 (99%)	2 (1%)	63	73
8	SI	177/177 (100%)	176 (99%)	1 (1%)	78	79
9	SK	89/89 (100%)	84 (94%)	5 (6%)	19	46
10	SL	137/137 (100%)	135 (98%)	2 (2%)	57	71
11	SP	113/113 (100%)	108 (96%)	5 (4%)	25	51
12	SQ	121/121 (100%)	118 (98%)	3 (2%)	42	63
13	SR	121/121 (100%)	120 (99%)	1 (1%)	73	77
14	SS	126/126 (100%)	125 (99%)	1 (1%)	73	77
15	ST	113/113 (100%)	111 (98%)	2 (2%)	51	69
16	SU	94/94 (100%)	94 (100%)	0	100	100
17	SV	66/66 (100%)	64 (97%)	2 (3%)	36	60
18	SX	113/113 (100%)	110 (97%)	3 (3%)	39	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Sa	89/89 (100%)	89 (100%)	0	100	100
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	43 (90%)	5 (10%)	7	27
22	Sg	271/271 (100%)	271 (100%)	0	100	100
23	SC	187/186 (100%)	186 (100%)	1 (0%)	81	80
24	SG	207/207 (100%)	206 (100%)	1 (0%)	81	80
25	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	73
26	SM	98/100 (98%)	98 (100%)	0	100	100
27	SN	130/130 (100%)	128 (98%)	2 (2%)	57	71
28	SO	107/107 (100%)	105 (98%)	2 (2%)	50	68
29	SW	112/112 (100%)	111 (99%)	1 (1%)	70	76
30	SY	114/113 (101%)	113 (99%)	1 (1%)	70	76
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	35	59
32	Sb	74/74 (100%)	73 (99%)	1 (1%)	59	71
33	Se	46/46 (100%)	45 (98%)	1 (2%)	45	65
34	Sf	60/60 (100%)	60 (100%)	0	100	100
35	A	194/194 (100%)	190 (98%)	4 (2%)	47	66
36	B	345/345 (100%)	339 (98%)	6 (2%)	53	70
37	C	302/302 (100%)	297 (98%)	5 (2%)	53	70
40	F	248/248 (100%)	248 (100%)	0	100	100
41	G	209/220 (95%)	205 (98%)	4 (2%)	50	68
42	H	194/194 (100%)	188 (97%)	6 (3%)	35	59
43	I	199/199 (100%)	197 (99%)	2 (1%)	68	75
44	J	170/170 (100%)	166 (98%)	4 (2%)	43	64
45	K	178/179 (99%)	175 (98%)	3 (2%)	53	70
46	L	142/142 (100%)	142 (100%)	0	100	100
47	M	171/171 (100%)	167 (98%)	4 (2%)	44	64
48	N	118/118 (100%)	116 (98%)	2 (2%)	53	70
49	O	171/171 (100%)	166 (97%)	5 (3%)	37	60
50	P	168/168 (100%)	166 (99%)	2 (1%)	63	73
51	Q	134/134 (100%)	130 (97%)	4 (3%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	R	164/164 (100%)	156 (95%)	8 (5%)	22	48
53	S	160/160 (100%)	160 (100%)	0	100	100
54	T	156/156 (100%)	151 (97%)	5 (3%)	34	59
55	U	138/138 (100%)	135 (98%)	3 (2%)	45	65
56	V	89/89 (100%)	88 (99%)	1 (1%)	65	74
57	W	100/100 (100%)	99 (99%)	1 (1%)	68	75
58	X	53/53 (100%)	52 (98%)	1 (2%)	50	68
59	Y	105/105 (100%)	102 (97%)	3 (3%)	37	60
60	Z	124/124 (100%)	120 (97%)	4 (3%)	34	59
61	a	117/117 (100%)	115 (98%)	2 (2%)	53	70
62	b	120/120 (100%)	116 (97%)	4 (3%)	33	58
63	c	82/101 (81%)	82 (100%)	0	100	100
64	d	88/88 (100%)	86 (98%)	2 (2%)	44	64
65	e	97/97 (100%)	95 (98%)	2 (2%)	47	66
66	f	115/115 (100%)	114 (99%)	1 (1%)	70	76
67	g	88/88 (100%)	85 (97%)	3 (3%)	32	57
68	h	98/98 (100%)	98 (100%)	0	100	100
69	i	109/109 (100%)	109 (100%)	0	100	100
70	j	83/83 (100%)	83 (100%)	0	100	100
71	k	71/71 (100%)	71 (100%)	0	100	100
72	l	64/64 (100%)	63 (98%)	1 (2%)	55	70
73	m	47/47 (100%)	47 (100%)	0	100	100
74	n	46/46 (100%)	46 (100%)	0	100	100
75	o	24/24 (100%)	24 (100%)	0	100	100
76	p	93/93 (100%)	90 (97%)	3 (3%)	34	59
77	q	74/74 (100%)	73 (99%)	1 (1%)	59	71
78	r	106/106 (100%)	104 (98%)	2 (2%)	50	68
All	All	9764/9797 (100%)	9604 (98%)	160 (2%)	54	70

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	29	ASN

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Mol	Chain	Res	Type
2	SA	82	THR
2	SA	89	LYS
3	SB	87	ILE
3	SB	166	LYS
3	SB	188	LEU
3	SB	189	ILE
4	SD	5	ILE
4	SD	66	ILE
4	SD	126	ILE
4	SD	210	ILE
5	SE	7	LYS
5	SE	90	ILE
5	SE	228	ILE
6	SF	68	ILE
6	SF	99	ILE
7	SH	51	ILE
7	SH	166	VAL
8	SI	60	LEU
9	SK	15	LEU
9	SK	40	VAL
9	SK	43	LEU
9	SK	58	VAL
9	SK	59	LYS
10	SL	40	ILE
10	SL	68	ILE
11	SP	13	ARG
11	SP	15	PHE
11	SP	79	HIS
11	SP	121	ILE
11	SP	127	LYS
12	SQ	22	VAL
12	SQ	111	ILE
12	SQ	125	ARG
13	SR	106	LEU
14	SS	3	LEU
15	ST	4	VAL
15	ST	131	LEU
17	SV	9	VAL
17	SV	21	ASN
18	SX	61	GLN
18	SX	112	VAL
18	SX	125	VAL

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Mol	Chain	Res	Type
21	Sd	22	ARG
21	Sd	26	ASN
21	Sd	40	ARG
21	Sd	42	CYS
21	Sd	53	ILE
23	SC	155	ILE
24	SG	111	LEU
25	SJ	138[A]	ARG
25	SJ	138[B]	ARG
27	SN	43	LYS
27	SN	46	THR
28	SO	76	LEU
28	SO	135	ILE
29	SW	103	VAL
30	SY	94	HIS
31	SZ	44	LEU
31	SZ	62	VAL
32	Sb	24	LEU
33	Se	6	LEU
35	A	20	VAL
35	A	45	VAL
35	A	101	VAL
35	A	225	ILE
36	B	67	VAL
36	B	85	VAL
36	B	144	LYS
36	B	258	HIS
36	B	295	ASP
36	B	337	VAL
37	C	150	LEU
37	C	193	LYS
37	C	199	ARG
37	C	209	ILE
37	C	278	ASN
41	G	50	LEU
41	G	125	LEU
41	G	176	THR
41	G	279	ASN
42	H	95	ILE
42	H	126	ASN
42	H	147	LEU
42	H	179	LEU

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Mol	Chain	Res	Type
42	H	185	ILE
42	H	191	ILE
43	I	45	ILE
43	I	128	VAL
44	J	42	ASN
44	J	63	ASN
44	J	103	VAL
44	J	105	ILE
45	K	26	VAL
45	K	87	ILE
45	K	200	ILE
47	M	125	ILE
47	M	144	LEU
47	M	157	VAL
47	M	169	ILE
48	N	31	ILE
48	N	45	VAL
49	O	18	VAL
49	O	64	ILE
49	O	115	VAL
49	O	133	ILE
49	O	183	THR
50	P	93	LYS
50	P	185	VAL
51	Q	24	VAL
51	Q	43	LYS
51	Q	127	ARG
51	Q	146	ILE
52	R	4	ASP
52	R	5	ILE
52	R	28	LEU
52	R	48	LEU
52	R	63	LEU
52	R	72	LEU
52	R	138	LEU
52	R	163	THR
54	T	68	PHE
54	T	70	LYS
54	T	124	ILE
54	T	158	VAL
54	T	162	GLN
55	U	68	THR

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Mol	Chain	Res	Type
55	U	75	VAL
55	U	143	THR
56	V	112	LEU
57	W	65	VAL
58	X	43	LYS
59	Y	52	LEU
59	Y	96	LEU
59	Y	119	ILE
60	Z	55	VAL
60	Z	79	VAL
60	Z	85	VAL
60	Z	104	VAL
61	a	10	VAL
61	a	13	VAL
62	b	63	LEU
62	b	87	ARG
62	b	94	LYS
62	b	122	VAL
64	d	35	LEU
64	d	77	ASN
65	e	93	ASN
65	e	109	VAL
66	f	85	LEU
67	g	33	VAL
67	g	59	THR
67	g	84	VAL
72	l	46	VAL
76	p	23	VAL
76	p	66	ILE
76	p	93	LEU
77	q	29	ILE
78	r	17	LEU
78	r	78	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	50	ASN
3	SB	40	ASN
3	SB	75	GLN
3	SB	92	GLN
3	SB	186	ASN

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Mol	Chain	Res	Type
3	SB	202	GLN
4	SD	226	GLN
5	SE	142	HIS
6	SF	79	HIS
6	SF	118	ASN
6	SF	148	ASN
7	SH	12	ASN
7	SH	39	GLN
7	SH	168	HIS
8	SI	35	ASN
8	SI	167	GLN
8	SI	168	GLN
8	SI	181	GLN
9	SK	61	GLN
10	SL	11	GLN
10	SL	18	GLN
10	SL	65	ASN
10	SL	83	GLN
10	SL	154	GLN
11	SP	35	GLN
13	SR	74	GLN
13	SR	83	ASN
13	SR	127	ASN
14	SS	135	HIS
15	ST	126	GLN
16	SU	100	GLN
17	SV	2	GLN
17	SV	21	ASN
17	SV	35	ASN
18	SX	16	HIS
18	SX	31	HIS
18	SX	61	GLN
19	Sa	72	HIS
20	Sc	24	GLN
21	Sd	26	ASN
22	Sg	14	HIS
22	Sg	20	GLN
22	Sg	117	ASN
22	Sg	162	ASN
22	Sg	222	ASN
22	Sg	285	GLN
23	SC	115	GLN

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Mol	Chain	Res	Type
23	SC	235	ASN
23	SC	267	GLN
24	SG	59	GLN
24	SG	110	ASN
24	SG	163	ASN
24	SG	186	GLN
24	SG	197	GLN
25	SJ	113	GLN
25	SJ	124	HIS
25	SJ	154	GLN
25	SJ	177	ASN
27	SN	5	HIS
27	SN	69	ASN
27	SN	105	ASN
28	SO	32	HIS
28	SO	79	GLN
29	SW	15	ASN
29	SW	16	ASN
29	SW	98	GLN
30	SY	2	ASN
32	Sb	65	GLN
33	Se	58	ASN
34	Sf	91	ASN
35	A	50	HIS
35	A	83	HIS
35	A	95	GLN
35	A	97	ASN
35	A	132	ASN
35	A	162	ASN
35	A	205	ASN
35	A	209	HIS
36	B	55	HIS
36	B	158	GLN
36	B	204	GLN
36	B	258	HIS
36	B	271	GLN
36	B	301	ASN
36	B	322	HIS
37	C	38	ASN
37	C	94	ASN
37	C	223	ASN
37	C	236	ASN

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Mol	Chain	Res	Type
37	C	278	ASN
37	C	347	HIS
40	F	122	GLN
40	F	198	HIS
40	F	202	GLN
41	G	190	HIS
41	G	191	GLN
41	G	211	HIS
41	G	250	GLN
41	G	279	ASN
42	H	24	ASN
42	H	80	ASN
42	H	126	ASN
42	H	131	ASN
42	H	151	ASN
42	H	226	HIS
43	I	206	GLN
43	I	225	ASN
44	J	42	ASN
44	J	63	ASN
44	J	78	GLN
44	J	106	GLN
44	J	108	ASN
44	J	116	ASN
45	K	14	ASN
45	K	86	HIS
45	K	130	HIS
45	K	163	GLN
45	K	213	HIS
46	L	42	GLN
46	L	71	HIS
46	L	112	HIS
47	M	87	HIS
48	N	33	GLN
48	N	44	GLN
48	N	48	GLN
48	N	66	HIS
48	N	70	GLN
48	N	120	ASN
49	O	87	HIS
49	O	199	GLN
50	P	14	HIS

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Mol	Chain	Res	Type
50	P	50	ASN
50	P	63	ASN
50	P	173	GLN
51	Q	10	ASN
51	Q	34	GLN
51	Q	80	GLN
51	Q	116	HIS
51	Q	133	HIS
52	R	160	HIS
53	S	130	ASN
54	T	122	HIS
54	T	162	GLN
54	T	163	HIS
55	U	22	HIS
55	U	49	GLN
55	U	131	GLN
57	W	77	HIS
57	W	101	ASN
59	Y	107	HIS
59	Y	111	GLN
60	Z	20	ASN
60	Z	61	HIS
60	Z	72	GLN
60	Z	96	HIS
62	b	25	HIS
62	b	28	HIS
64	d	51	ASN
64	d	77	ASN
65	e	34	HIS
65	e	79	ASN
65	e	93	ASN
66	f	43	ASN
67	g	55	ASN
67	g	56	ASN
70	j	26	HIS
70	j	92	ASN
71	k	57	ASN
71	k	66	HIS
73	m	4	HIS
73	m	43	HIS
74	n	104	HIS
76	p	19	GLN

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Mol	Chain	Res	Type
78	r	6	GLN
78	r	41	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1698/1714 (99%)	568 (33%)	31 (1%)
38	D	156/157 (99%)	38 (24%)	0
39	E	118/121 (97%)	19 (16%)	0
79	t	3593/3607 (99%)	880 (24%)	0
80	u	74/76 (97%)	28 (37%)	0
81	v	72/76 (94%)	28 (38%)	0
82	w	9/10 (90%)	2 (22%)	0
All	All	5720/5761 (99%)	1563 (27%)	31 (0%)

All (1563) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	9	U
1	S2	10	G
1	S2	11	A
1	S2	16	G
1	S2	17	C
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	36	U
1	S2	37	C
1	S2	38	A
1	S2	39	A
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	44	U
1	S2	46	A
1	S2	49	C
1	S2	54	A
1	S2	55	U
1	S2	56	G
1	S2	58	C

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Mol	Chain	Res	Type
1	S2	60	A
1	S2	61	A
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	69	C
1	S2	70	G
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	79	A
1	S2	80	G
1	S2	103	A
1	S2	112	U
1	S2	113	G
1	S2	115	U
1	S2	116	OMU
1	S2	119	PSU
1	S2	121	OMU
1	S2	125	C
1	S2	126	G
1	S2	130	G
1	S2	140	C
1	S2	142	C
1	S2	143	U
1	S2	147	A
1	S2	155	G
1	S2	159	A2M
1	S2	161	U
1	S2	162	C
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	176	U
1	S2	182	C
1	S2	183	G
1	S2	189	U
1	S2	191	A

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Mol	Chain	Res	Type
1	S2	192	C
1	S2	193	C
1	S2	194	C
1	S2	195	C
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	208	G
1	S2	209	A
1	S2	210	U
1	S2	215	G
1	S2	289	G
1	S2	293	C
1	S2	294	U
1	S2	295	C
1	S2	302	A
1	S2	305	U
1	S2	308	G
1	S2	310	C
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	328	U
1	S2	329	G
1	S2	332	G
1	S2	333	G
1	S2	338	G
1	S2	340	C
1	S2	347	G
1	S2	351	G
1	S2	360	A

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Mol	Chain	Res	Type
1	S2	363	A
1	S2	364	A
1	S2	367	U
1	S2	368	U
1	S2	369	C
1	S2	370	G
1	S2	373	G
1	S2	377	G
1	S2	379	C
1	S2	382	C
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	417	C
1	S2	418	A
1	S2	419	G
1	S2	429	C
1	S2	436	G
1	S2	438	G
1	S2	446	G
1	S2	447	A
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	467	G
1	S2	470	G
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	482	G
1	S2	485	A
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A

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Mol	Chain	Res	Type
1	S2	496	C
1	S2	502	C
1	S2	507	G
1	S2	516	A
1	S2	528	A
1	S2	531	A
1	S2	532	C
1	S2	535	G
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	544	G
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	548	C
1	S2	549	C
1	S2	553	U
1	S2	554	A
1	S2	555	A
1	S2	556	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	561	A
1	S2	564	A
1	S2	568	E3C
1	S2	578	C
1	S2	579	C
1	S2	583	C
1	S2	587	A
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	594	A
1	S2	603	C
1	S2	607	U

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Mol	Chain	Res	Type
1	S2	608	C
1	S2	614	C
1	S2	617	G
1	S2	621	C
1	S2	625	G
1	S2	626	G
1	S2	627	U
1	S2	628	A
1	S2	629	A
1	S2	631	U
1	S2	632	C
1	S2	634	A
1	S2	643	A
1	S2	655	A
1	S2	660	C
1	S2	662	G
1	S2	663	C
1	S2	664	A
1	S2	668	A2M
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	675	U
1	S2	681	U
1	S2	683	OMG
1	S2	689	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	736	C
1	S2	737	G
1	S2	738	C
1	S2	739	C

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Mol	Chain	Res	Type
1	S2	748	C
1	S2	749	U
1	S2	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	794	A
1	S2	797	C
1	S2	799	U
1	S2	804	U
1	S2	810	A
1	S2	811	A
1	S2	815	U
1	S2	821	G
1	S2	822	PSU
1	S2	823	PSU
1	S2	830	A
1	S2	831	G
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	856	C
1	S2	858	A
1	S2	859	G
1	S2	861	A
1	S2	865	A
1	S2	866	U
1	S2	867	G
1	S2	868	G
1	S2	871	U
1	S2	873	G

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Mol	Chain	Res	Type
1	S2	878	G
1	S2	883	U
1	S2	885	U
1	S2	886	A
1	S2	887	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	893	U
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	902	G
1	S2	903	A
1	S2	906	U
1	S2	913	A
1	S2	914	U
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	932	G
1	S2	933	G
1	S2	936	G
1	S2	966	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	973	C
1	S2	988	C
1	S2	989	C
1	S2	990	A
1	S2	992	A
1	S2	996	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1003	U
1	S2	1005	G
1	S2	1006	C

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Mol	Chain	Res	Type
1	S2	1007	C
1	S2	1016	U
1	S2	1017	U
1	S2	1021	U
1	S2	1023	A
1	S2	1026	C
1	S2	1027	A
1	S2	1028	A
1	S2	1033	G
1	S2	1049	A
1	S2	1055	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1064	C
1	S2	1083	A
1	S2	1085	C
1	S2	1088	U
1	S2	1089	G
1	S2	1109	C
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1117	C
1	S2	1119	A
1	S2	1121	G
1	S2	1123	C
1	S2	1133	A
1	S2	1135	C
1	S2	1138	C
1	S2	1144	A
1	S2	1145	A
1	S2	1146	C
1	S2	1149	A
1	S2	1154	U
1	S2	1155	U
1	S2	1158	G
1	S2	1159	G
1	S2	1166	G
1	S2	1195	A
1	S2	1197	G
1	S2	1207	G

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Mol	Chain	Res	Type
1	S2	1208	A
1	S2	1215	C
1	S2	1217	A
1	S2	1220	A
1	S2	1221	G
1	S2	1224	G
1	S2	1233	G
1	S2	1242	U
1	S2	1244	U
1	S2	1246	A
1	S2	1248	B8N
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1260	A
1	S2	1262	C
1	S2	1265	A
1	S2	1269	G
1	S2	1273	C
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1294	G
1	S2	1295	A
1	S2	1296	U
1	S2	1298	G
1	S2	1300	U
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1312	G
1	S2	1313	A
1	S2	1322	G
1	S2	1323	U
1	S2	1328	G
1	S2	1330	G

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Mol	Chain	Res	Type
1	S2	1331	C
1	S2	1333	U
1	S2	1340	U
1	S2	1341	C
1	S2	1348	G
1	S2	1354	G
1	S2	1355	C
1	S2	1364	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1375	G
1	S2	1376	A
1	S2	1378	A
1	S2	1382	A
1	S2	1396	A
1	S2	1397	U
1	S2	1402	A
1	S2	1403	C
1	S2	1404	U
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G
1	S2	1454	A
1	S2	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1470	C
1	S2	1477	U

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Mol	Chain	Res	Type
1	S2	1478	U
1	S2	1480	A
1	S2	1482	C
1	S2	1489	A
1	S2	1490	G
1	S2	1493	C
1	S2	1494	U
1	S2	1495	G
1	S2	1496	U
1	S2	1497	G
1	S2	1505	U
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1523	C
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C
1	S2	1535	U
1	S2	1536	G
1	S2	1543	U
1	S2	1544	C
1	S2	1545	A
1	S2	1548	G
1	S2	1552	G
1	S2	1553	C
1	S2	1556	A
1	S2	1557	C
1	S2	1558	C
1	S2	1560	U
1	S2	1566	G
1	S2	1568	C
1	S2	1570	G
1	S2	1573	G
1	S2	1578	U
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U

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Mol	Chain	Res	Type
1	S2	1586	U
1	S2	1588	A
1	S2	1594	A
1	S2	1598	G
1	S2	1599	U
1	S2	1600	G
1	S2	1601	A
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1634	A
1	S2	1638	G
1	S2	1639	G
1	S2	1647	A
1	S2	1648	G
1	S2	1654	G
1	S2	1661	A
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1671	G
1	S2	1675	A
1	S2	1676	U
1	S2	1680	G
1	S2	1682	C
1	S2	1683	C
1	S2	1686	G
1	S2	1688	C
1	S2	1693	G
1	S2	1695	A
1	S2	1698	C
1	S2	1699	A
1	S2	1702	G
1	S2	1703	OMC
1	S2	1720	U
1	S2	1721	U
1	S2	1722	G
1	S2	1726	G
1	S2	1728	U
1	S2	1729	U
1	S2	1744	G
1	S2	1749	G

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Mol	Chain	Res	Type
1	S2	1750	C
1	S2	1751	C
1	S2	1752	C
1	S2	1780	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1786	U
1	S2	1789	G
1	S2	1797	U
1	S2	1800	A
1	S2	1803	U
1	S2	1805	G
1	S2	1811	C
1	S2	1813	A
1	S2	1814	G
1	S2	1815	A
1	S2	1816	G
1	S2	1817	G
1	S2	1823	A
1	S2	1824	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	UR3
1	S2	1831	A
1	S2	1835	A
1	S2	1836	G
1	S2	1838	U
1	S2	1841	C
1	S2	1849	G
1	S2	1850	MA6
1	S2	1851	MA6
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1869	A
38	D	13	G

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Mol	Chain	Res	Type
38	D	23	C
38	D	32	C
38	D	34	U
38	D	35	C
38	D	37	A
38	D	59	A
38	D	63	U
38	D	72	A
38	D	80	A
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	87	G
38	D	94	G
38	D	95	A
38	D	101	C
38	D	103	A
38	D	105	C
38	D	107	C
38	D	109	C
38	D	110	U
38	D	111	U
38	D	116	C
38	D	120	G
38	D	121	G
38	D	122	G
38	D	123	U
38	D	124	U
38	D	125	C
38	D	126	C
38	D	127	U
38	D	128	C
38	D	129	C
38	D	130	C
38	D	148	A
38	D	150	C
39	E	7	G
39	E	14	C
39	E	22	A
39	E	23	A
39	E	25	G

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Mol	Chain	Res	Type
39	E	27	G
39	E	38	U
39	E	48	G
39	E	53	U
39	E	54	A
39	E	63	C
39	E	64	G
39	E	74	A
39	E	76	U
39	E	88	A
39	E	97	G
39	E	98	G
39	E	103	A
39	E	110	G
79	t	9	C
79	t	17	A
79	t	18	C
79	t	21	G
79	t	25	A
79	t	30	C
79	t	32	G
79	t	39	A
79	t	42	A
79	t	48	G
79	t	49	U
79	t	59	A
79	t	64	A
79	t	65	A
79	t	71	C
79	t	72	C
79	t	73	A
79	t	74	G
79	t	91	G
79	t	93	G
79	t	98	A
79	t	101	A
79	t	108	A
79	t	110	C
79	t	112	C
79	t	116	G
79	t	119	G
79	t	120	A

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Mol	Chain	Res	Type
79	t	121	A
79	t	131	C
79	t	132	G
79	t	134	G
79	t	135	G
79	t	137	G
79	t	138	C
79	t	143	G
79	t	144	A
79	t	148	G
79	t	149	U
79	t	156	C
79	t	157	G
79	t	158	G
79	t	169	C
79	t	173	G
79	t	181	U
79	t	182	C
79	t	183	G
79	t	184	U
79	t	185	G
79	t	196	G
79	t	197	U
79	t	205	A
79	t	206	U
79	t	212	C
79	t	213	C
79	t	214	C
79	t	215	A
79	t	221	U
79	t	226	G
79	t	227	G
79	t	228	U
79	t	229	G
79	t	230	U
79	t	233	G
79	t	234	G
79	t	235	C
79	t	236	C
79	t	237	G
79	t	242	C
79	t	250	G

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Mol	Chain	Res	Type
79	t	251	G
79	t	252	C
79	t	253	G
79	t	260	C
79	t	261	G
79	t	272	G
79	t	274	G
79	t	289	A
79	t	291	U
79	t	300	A
79	t	309	G
79	t	310	U
79	t	311	A
79	t	323	A
79	t	334	C
79	t	338	A
79	t	339	C
79	t	341	A
79	t	343	A
79	t	346	G
79	t	348	U
79	t	357	A
79	t	367	G
79	t	370	A
79	t	375	U
79	t	377	A
79	t	381	G
79	t	404	A
79	t	405	G
79	t	406	G
79	t	407	G
79	t	408	C
79	t	409	G
79	t	425	G
79	t	426	U
79	t	434	U
79	t	437	G
79	t	443	C
79	t	444	G
79	t	446	A
79	t	447	G
79	t	448	U

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Mol	Chain	Res	Type
79	t	449	C
79	t	451	G
79	t	456	G
79	t	458	G
79	t	463	C
79	t	465	A
79	t	473	G
79	t	474	C
79	t	479	C
79	t	481	G
79	t	482	G
79	t	483	C
79	t	486	U
79	t	487	G
79	t	489	C
79	t	492	C
79	t	493	G
79	t	494	G
79	t	495	C
79	t	497	C
79	t	498	G
79	t	504	U
79	t	507	U
79	t	508	U
79	t	509	C
79	t	511	C
79	t	512	G
79	t	514	C
79	t	516	C
79	t	633	U
79	t	634	C
79	t	635	G
79	t	636	G
79	t	641	G
79	t	645	C
79	t	647	U
79	t	648	C
79	t	649	C
79	t	650	C
79	t	654	G
79	t	658	G
79	t	661	G

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Mol	Chain	Res	Type
79	t	662	A
79	t	663	C
79	t	674	C
79	t	675	G
79	t	676	G
79	t	677	G
79	t	678	C
79	t	679	G
79	t	680	C
79	t	690	C
79	t	693	U
79	t	695	C
79	t	698	C
79	t	703	C
79	t	709	C
79	t	719	U
79	t	720	G
79	t	721	G
79	t	724	A
79	t	728	C
79	t	737	A
79	t	738	A
79	t	739	G
79	t	899	G
79	t	902	A
79	t	904	A
79	t	905	G
79	t	906	C
79	t	907	C
79	t	914	G
79	t	917	G
79	t	919	A
79	t	920	G
79	t	921	C
79	t	922	A
79	t	923	C
79	t	924	U
79	t	925	C
79	t	926	G
79	t	927	C
79	t	929	G
79	t	933	C

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Mol	Chain	Res	Type
79	t	944	G
79	t	947	A
79	t	948	G
79	t	949	C
79	t	950	G
79	t	952	G
79	t	953	A
79	t	954	C
79	t	957	G
79	t	958	U
79	t	959	C
79	t	976	U
79	t	1051	G
79	t	1055	C
79	t	1061	A
79	t	1065	C
79	t	1070	A
79	t	1083	U
79	t	1086	C
79	t	1087	C
79	t	1149	G
79	t	1150	C
79	t	1152	G
79	t	1156	G
79	t	1162	U
79	t	1165	C
79	t	1167	A
79	t	1174	C
79	t	1176	C
79	t	1179	G
79	t	1192	U
79	t	1193	C
79	t	1196	G
79	t	1197	C
79	t	1198	C
79	t	1199	C
79	t	1201	G
79	t	1220	C
79	t	1221	A
79	t	1222	C
79	t	1223	G
79	t	1224	C

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Mol	Chain	Res	Type
79	t	1225	G
79	t	1226	C
79	t	1228	C
79	t	1234	C
79	t	1236	G
79	t	1238	A
79	t	1240	G
79	t	1248	G
79	t	1249	G
79	t	1250	C
79	t	1251	G
79	t	1253	A
79	t	1258	G
79	t	1259	C
79	t	1268	U
79	t	1269	C
79	t	1271	G
79	t	1273	G
79	t	1277	A
79	t	1279	G
79	t	1285	U
79	t	1286	A
79	t	1301	C
79	t	1309	A
79	t	1322	U
79	t	1336	G
79	t	1337	A
79	t	1341	G
79	t	1342	G
79	t	1348	C
79	t	1350	C
79	t	1351	A
79	t	1353	G
79	t	1360	G
79	t	1361	C
79	t	1362	C
79	t	1364	U
79	t	1370	A
79	t	1380	A
79	t	1381	A
79	t	1389	G
79	t	1390	C

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Mol	Chain	Res	Type
79	t	1391	G
79	t	1392	C
79	t	1393	U
79	t	1394	C
79	t	1395	G
79	t	1401	C
79	t	1403	A
79	t	1404	G
79	t	1420	C
79	t	1421	U
79	t	1423	U
79	t	1424	C
79	t	1425	C
79	t	1426	A
79	t	1430	C
79	t	1431	G
79	t	1439	G
79	t	1463	C
79	t	1464	G
79	t	1465	C
79	t	1466	G
79	t	1467	C
79	t	1468	C
79	t	1473	A
79	t	1474	G
79	t	1480	G
79	t	1484	G
79	t	1485	A
79	t	1498	G
79	t	1500	A
79	t	1507	A
79	t	1516	A
79	t	1517	C
79	t	1525	G
79	t	1531	G
79	t	1542	A
79	t	1545	A
79	t	1548	C
79	t	1560	U
79	t	1564	U
79	t	1573	U
79	t	1578	U

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Mol	Chain	Res	Type
79	t	1583	A
79	t	1587	G
79	t	1595	A
79	t	1606	G
79	t	1607	G
79	t	1613	A
79	t	1614	A
79	t	1615	G
79	t	1616	A
79	t	1622	C
79	t	1623	G
79	t	1624	A
79	t	1636	G
79	t	1643	C
79	t	1652	G
79	t	1658	C
79	t	1659	U
79	t	1660	C
79	t	1663	G
79	t	1673	G
79	t	1679	G
79	t	1680	C
79	t	1700	C
79	t	1701	A
79	t	1702	C
79	t	1711	A
79	t	1716	G
79	t	1723	G
79	t	1728	A
79	t	1742	G
79	t	1746	G
79	t	1747	A
79	t	1748	A
79	t	1750	C
79	t	1751	G
79	t	1769	A
79	t	1776	A
79	t	1786	A
79	t	1788	G
79	t	1794	C
79	t	1797	G
79	t	1801	G

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Mol	Chain	Res	Type
79	t	1803	G
79	t	1804	U
79	t	1814	G
79	t	1816	G
79	t	1818	A
79	t	1823	G
79	t	1836	G
79	t	1840	C
79	t	1844	U
79	t	1850	G
79	t	1862	C
79	t	1863	U
79	t	1872	A
79	t	1873	A
79	t	1881	C
79	t	1887	U
79	t	1891	G
79	t	1896	C
79	t	1900	G
79	t	1902	C
79	t	1903	G
79	t	1906	G
79	t	1910	A
79	t	1912	C
79	t	1913	A
79	t	1916	C
79	t	1920	A
79	t	1921	G
79	t	1928	U
79	t	1929	G
79	t	1932	G
79	t	1933	G
79	t	1938	U
79	t	1939	A
79	t	1940	U
79	t	1941	A
79	t	1942	G
79	t	1943	A
79	t	1952	C
79	t	1956	G
79	t	1961	U
79	t	1963	G

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Mol	Chain	Res	Type
79	t	1964	A
79	t	1968	C
79	t	1972	A
79	t	1973	U
79	t	1978	U
79	t	1979	A
79	t	1980	A
79	t	1983	A
79	t	1984	G
79	t	1991	A
79	t	1994	A
79	t	2003	C
79	t	2007	A
79	t	2011	A
79	t	2021	A
79	t	2025	U
79	t	2027	G
79	t	2029	U
79	t	2036	G
79	t	2037	G
79	t	2043	C
79	t	2051	U
79	t	2065	C
79	t	2069	G
79	t	2070	U
79	t	2072	G
79	t	2073	A
79	t	2075	A
79	t	2077	U
79	t	2078	G
79	t	2081	C
79	t	2082	G
79	t	2087	C
79	t	2088	G
79	t	2090	C
79	t	2091	G
79	t	2092	G
79	t	2231	G
79	t	2232	A
79	t	2233	G
79	t	2234	C
79	t	2235	C

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Mol	Chain	Res	Type
79	t	2236	C
79	t	2237	C
79	t	2241	G
79	t	2242	A
79	t	2245	C
79	t	2246	U
79	t	2247	A
79	t	2264	A
79	t	2265	G
79	t	2268	C
79	t	2278	G
79	t	2279	A
79	t	2280	G
79	t	2282	C
79	t	2285	G
79	t	2292	A
79	t	2295	G
79	t	2321	G
79	t	2323	U
79	t	2325	C
79	t	2327	G
79	t	2330	C
79	t	2340	G
79	t	2343	G
79	t	2358	A
79	t	2374	A
79	t	2375	A
79	t	2391	A
79	t	2396	A
79	t	2400	G
79	t	2401	C
79	t	2404	U
79	t	2405	U
79	t	2416	C
79	t	2421	G
79	t	2426	U
79	t	2429	G
79	t	2431	G
79	t	2432	A
79	t	2442	G
79	t	2446	U
79	t	2447	U

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Mol	Chain	Res	Type
79	t	2449	C
79	t	2458	G
79	t	2467	C
79	t	2468	C
79	t	2469	U
79	t	2473	U
79	t	2482	G
79	t	2483	C
79	t	2484	C
79	t	2485	G
79	t	2490	A
79	t	2492	A
79	t	2499	C
79	t	2523	G
79	t	2524	U
79	t	2525	G
79	t	2526	G
79	t	2532	A
79	t	2533	U
79	t	2544	A
79	t	2562	C
79	t	2565	G
79	t	2566	A
79	t	2568	C
79	t	2580	A
79	t	2585	G
79	t	2606	C
79	t	2617	G
79	t	2618	U
79	t	2632	C
79	t	2640	U
79	t	2648	C
79	t	2652	G
79	t	2665	G
79	t	2666	U
79	t	2673	G
79	t	2675	A
79	t	2687	U
79	t	2689	C
79	t	2690	G
79	t	2691	G
79	t	2698	C

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Mol	Chain	Res	Type
79	t	2700	G
79	t	2705	G
79	t	2714	G
79	t	2719	U
79	t	2722	A
79	t	2723	A
79	t	2726	U
79	t	2733	G
79	t	2737	G
79	t	2741	G
79	t	2745	A
79	t	2748	U
79	t	2766	A
79	t	2767	U
79	t	2768	A
79	t	2769	U
79	t	2773	C
79	t	2775	G
79	t	2776	C
79	t	2778	G
79	t	2785	A
79	t	2793	C
79	t	2798	U
79	t	2805	U
79	t	2806	G
79	t	2809	G
79	t	2814	A
79	t	2817	G
79	t	2821	G
79	t	2824	A
79	t	2834	G
79	t	2835	C
79	t	2855	G
79	t	2858	A
79	t	2860	A
79	t	2863	G
79	t	2871	C
79	t	2879	U
79	t	2881	G
79	t	3570	A
79	t	3571	G
79	t	3572	C

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Mol	Chain	Res	Type
79	t	3573	C
79	t	3577	U
79	t	3587	U
79	t	3589	C
79	t	3591	G
79	t	3596	G
79	t	3597	G
79	t	3606	A
79	t	3612	U
79	t	3615	U
79	t	3616	U
79	t	3617	A
79	t	3619	A
79	t	3624	A
79	t	3633	A
79	t	3635	G
79	t	3644	C
79	t	3651	U
79	t	3661	U
79	t	3662	G
79	t	3663	A
79	t	3667	C
79	t	3683	A
79	t	3700	U
79	t	3707	A
79	t	3719	A
79	t	3722	G
79	t	3724	G
79	t	3725	G
79	t	3728	G
79	t	3730	A
79	t	3731	A
79	t	3733	U
79	t	3742	C
79	t	3744	U
79	t	3745	A
79	t	3748	G
79	t	3751	G
79	t	3754	A
79	t	3755	A
79	t	3759	C
79	t	3781	C

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Mol	Chain	Res	Type
79	t	3782	G
79	t	3783	C
79	t	3784	A
79	t	3785	U
79	t	3788	A
79	t	3789	U
79	t	3790	G
79	t	3795	A
79	t	3798	G
79	t	3799	A
79	t	3809	U
79	t	3810	G
79	t	3811	U
79	t	3822	U
79	t	3838	A
79	t	3847	A
79	t	3848	A
79	t	3849	C
79	t	3850	G
79	t	3851	G
79	t	3852	G
79	t	3860	G
79	t	3863	U
79	t	3865	A
79	t	3866	G
79	t	3868	G
79	t	3869	G
79	t	3872	A
79	t	3876	A
79	t	3877	A
79	t	3878	G
79	t	3879	A
79	t	3880	C
79	t	3886	U
79	t	3887	G
79	t	3894	A
79	t	3909	G
79	t	3917	G
79	t	3918	A
79	t	4046	G
79	t	4054	G
79	t	4062	G

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Mol	Chain	Res	Type
79	t	4064	G
79	t	4065	G
79	t	4069	G
79	t	4070	C
79	t	4071	C
79	t	4072	C
79	t	4074	A
79	t	4079	C
79	t	4080	U
79	t	4083	C
79	t	4084	G
79	t	4086	U
79	t	4088	C
79	t	4096	A
79	t	4101	C
79	t	4106	C
79	t	4107	C
79	t	4108	G
79	t	4109	G
79	t	4110	C
79	t	4111	C
79	t	4119	A
79	t	4124	C
79	t	4125	U
79	t	4126	C
79	t	4130	G
79	t	4132	A
79	t	4139	C
79	t	4145	G
79	t	4146	G
79	t	4153	G
79	t	4158	G
79	t	4165	A
79	t	4167	A
79	t	4174	A
79	t	4176	A
79	t	4187	G
79	t	4190	G
79	t	4191	U
79	t	4195	A
79	t	4205	C
79	t	4211	G

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Mol	Chain	Res	Type
79	t	4213	A
79	t	4216	G
79	t	4217	A
79	t	4228	G
79	t	4230	A
79	t	4234	G
79	t	4235	A
79	t	4242	A
79	t	4243	A
79	t	4253	G
79	t	4266	A
79	t	4267	G
79	t	4276	C
79	t	4291	G
79	t	4292	G
79	t	4294	C
79	t	4300	G
79	t	4301	A
79	t	4311	C
79	t	4316	U
79	t	4322	U
79	t	4326	G
79	t	4333	G
79	t	4334	U
79	t	4338	A
79	t	4339	G
79	t	4340	A
79	t	4341	A
79	t	4343	A
79	t	4344	G
79	t	4349	C
79	t	4353	G
79	t	4356	A
79	t	4358	A
79	t	4360	C
79	t	4367	G
79	t	4384	A
79	t	4388	C
79	t	4402	G
79	t	4406	C
79	t	4414	U
79	t	4426	A

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Mol	Chain	Res	Type
79	t	4428	C
79	t	4437	G
79	t	4453	G
79	t	4455	U
79	t	4460	U
79	t	4462	U
79	t	4464	C
79	t	4472	A
79	t	4474	U
79	t	4475	A
79	t	4480	A
79	t	4485	A
79	t	4486	G
79	t	4490	G
79	t	4501	U
79	t	4510	A
79	t	4511	G
79	t	4517	U
79	t	4522	C
79	t	4529	G
79	t	4531	U
79	t	4537	G
79	t	4551	A
79	t	4552	A
79	t	4561	A
79	t	4562	G
79	t	4570	G
79	t	4578	A
79	t	4595	G
79	t	4598	U
79	t	4599	G
79	t	4601	G
79	t	4614	G
79	t	4618	A
79	t	4619	U
79	t	4632	C
79	t	4640	G
79	t	4656	G
79	t	4657	C
79	t	4662	A
79	t	4671	U
79	t	4682	C

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Mol	Chain	Res	Type
79	t	4683	G
79	t	4684	G
79	t	4686	A
79	t	4692	C
79	t	4693	G
79	t	4694	G
79	t	4695	C
79	t	4696	A
79	t	4697	G
79	t	4703	C
79	t	4704	G
79	t	4706	A
79	t	4714	U
79	t	4715	U
79	t	4716	G
79	t	4718	C
79	t	4720	U
79	t	4722	G
79	t	4726	A
79	t	4732	U
79	t	4736	C
79	t	4737	G
79	t	4817	G
79	t	4818	G
79	t	4824	C
79	t	4827	U
79	t	4828	G
79	t	4830	G
79	t	4831	G
79	t	4832	A
79	t	4833	G
79	t	4834	U
79	t	4838	C
79	t	4840	U
79	t	4841	C
79	t	4847	G
79	t	4852	A
79	t	4853	C
79	t	4854	G
79	t	4855	G
79	t	4856	G
79	t	4858	C

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Mol	Chain	Res	Type
79	t	4859	G
79	t	4864	C
79	t	4865	G
79	t	4866	G
79	t	4867	A
79	t	4868	A
79	t	4870	G
79	t	4871	G
79	t	4872	C
79	t	4882	C
79	t	4883	U
79	t	4884	C
79	t	4885	G
79	t	4886	C
79	t	4892	A
79	t	4894	G
79	t	4895	C
79	t	4896	A
79	t	4898	C
79	t	4901	A
79	t	4902	C
79	t	4903	G
79	t	4909	G
79	t	4914	A
79	t	4921	G
79	t	4924	A
79	t	4933	G
79	t	4934	U
79	t	4936	G
79	t	4943	U
79	t	4946	U
79	t	4947	U
79	t	4949	U
79	t	4950	G
79	t	4957	G
79	t	4971	C
79	t	4972	A
79	t	4975	G
79	t	4981	C
79	t	4982	C
79	t	4984	U
79	t	4985	C

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Mol	Chain	Res	Type
79	t	4986	G
79	t	4999	G
79	t	5007	G
79	t	5008	C
79	t	5011	U
79	t	5012	C
79	t	5013	G
79	t	5015	C
79	t	5016	A
79	t	5020	G
79	t	5024	U
79	t	5028	C
80	u	4	C
80	u	7	A
80	u	8	U
80	u	11	C
80	u	17	C
80	u	18	G
80	u	19	G
80	u	20	U
80	u	21	A
80	u	22	G
80	u	23	A
80	u	25	C
80	u	38	A
80	u	46	G
80	u	47	U
80	u	48	C
80	u	52	G
80	u	56	C
80	u	59	U
80	u	60	U
80	u	61	C
80	u	62	C
80	u	64	A
80	u	69	G
80	u	71	G
80	u	72	C
80	u	74	C
80	u	76	A
81	v	2	G
81	v	8	U

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Mol	Chain	Res	Type
81	v	10	G
81	v	15	G
81	v	16	A
81	v	17	A
81	v	19	G
81	v	20	U
81	v	21	A
81	v	30	G
81	v	46	G
81	v	47	U
81	v	48	C
81	v	49	C
81	v	51	U
81	v	54	U
81	v	55	U
81	v	56	C
81	v	57	G
81	v	58	A
81	v	61	C
81	v	62	C
81	v	69	G
81	v	70	G
81	v	71	G
81	v	72	C
81	v	75	C
81	v	76	A
82	w	17	G
82	w	21	G

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	42	A
1	S2	53	C
1	S2	60	A
1	S2	79	A
1	S2	196	C
1	S2	205	G
1	S2	292	A
1	S2	304	C
1	S2	317	C
1	S2	386	C

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Mol	Chain	Res	Type
1	S2	417	C
1	S2	445	A
1	S2	536	A
1	S2	559	G
1	S2	563	G
1	S2	670	A
1	S2	814	5MU
1	S2	872	A
1	S2	1261	C
1	S2	1375	G
1	S2	1396	A
1	S2	1567	G
1	S2	1572	C
1	S2	1600	G
1	S2	1661	A
1	S2	1681	U
1	S2	1802	C
1	S2	1813	A
1	S2	1814	G
1	S2	1815	A
1	S2	1828	C

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

34 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	PSU	S2	1243	1	18,21,22	4.39	7 (38%)	21,30,33	1.96	4 (19%)
1	A2M	S2	1678	1	22,25,26	4.21	9 (40%)	30,36,39	2.83	13 (43%)
1	A2M	S2	159	1	22,25,26	4.12	9 (40%)	30,36,39	3.12	17 (56%)
1	MA6	S2	1851	1	23,26,27	1.56	5 (21%)	33,38,41	3.66	14 (42%)
1	OMG	S2	683	1	23,26,27	2.38	8 (34%)	32,38,41	2.14	10 (31%)
1	PSU	S2	612	1	18,21,22	4.25	8 (44%)	21,30,33	2.22	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	1081	1	18,21,22	4.30	8 (44%)	21,30,33	1.95	4 (19%)
1	MA6	S2	1850	1	23,26,27	1.53	5 (21%)	33,38,41	3.73	13 (39%)
1	OMG	S2	644	1	23,26,27	2.40	9 (39%)	32,38,41	2.23	10 (31%)
1	A2M	S2	166	1	22,25,26	4.12	9 (40%)	30,36,39	3.02	14 (46%)
1	5MU	S2	814	1	19,22,23	7.59	8 (42%)	27,32,35	3.61	11 (40%)
1	4AC	S2	1337	1	21,24,25	3.28	9 (42%)	28,34,37	1.25	3 (10%)
1	OMG	S2	509	1	23,26,27	2.38	7 (30%)	32,38,41	2.16	10 (31%)
1	OMC	S2	174	1	19,22,23	3.53	8 (42%)	25,31,34	0.92	1 (4%)
1	UR3	S2	1830	1	19,22,23	2.79	7 (36%)	26,32,35	3.04	9 (34%)
1	B8Q	S2	1219	1	18,22,23	4.74	7 (38%)	21,32,35	1.90	5 (23%)
1	6MZ	S2	1832	1	22,25,26	2.60	5 (22%)	29,36,39	2.39	9 (31%)
1	OMU	S2	116	1	19,22,23	3.16	6 (31%)	25,31,34	1.81	4 (16%)
1	OMU	S2	121	1	19,22,23	3.08	7 (36%)	25,31,34	2.00	6 (24%)
1	PSU	S2	822	1	18,21,22	4.38	8 (44%)	21,30,33	1.92	4 (19%)
1	A2M	S2	27	1	22,25,26	4.09	9 (40%)	30,36,39	3.04	14 (46%)
1	B8N	S2	1248	1	25,29,30	3.15	7 (28%)	28,42,45	2.12	7 (25%)
1	M7A	S2	1806	1	19,25,26	1.67	2 (10%)	25,37,40	3.74	8 (32%)
1	OMC	S2	1703	1	19,22,23	3.48	8 (42%)	25,31,34	0.61	0
1	A2M	S2	668	1	22,25,26	4.09	10 (45%)	30,36,39	3.14	14 (46%)
1	4AC	S2	1842	1	21,24,25	3.23	9 (42%)	28,34,37	1.12	3 (10%)
1	OMC	S2	1710	1	19,22,23	3.58	8 (42%)	25,31,34	0.65	0
1	5MC	S2	1374	1	19,22,23	3.64	8 (42%)	26,32,35	1.05	2 (7%)
1	A2M	S2	484	1	22,25,26	4.11	9 (40%)	30,36,39	3.01	12 (40%)
1	PSU	S2	823	1	18,21,22	4.49	8 (44%)	21,30,33	2.18	4 (19%)
1	PSU	S2	119	1	18,21,22	4.45	7 (38%)	21,30,33	2.10	5 (23%)
1	E3C	S2	568	1	19,23,24	3.59	7 (36%)	21,33,36	2.64	6 (28%)
1	OMC	S2	517	1	19,22,23	3.39	8 (42%)	25,31,34	0.86	1 (4%)
1	A2M	S2	1031	1	22,25,26	4.13	9 (40%)	30,36,39	3.05	15 (50%)

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
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	1678	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	MA6	S2	1851	1	-	4/11/29/30	0/3/3/3
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	612	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	2/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	5/11/29/30	0/3/3/3
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	6MZ	S2	1832	1	-	2/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	PSU	S2	822	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	A2M	S2	668	1	-	3/9/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	0/2/2/2
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.49	1.81	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C6-N1	16.54	1.66	1.38
1	S2	823	PSU	C6-C5	11.93	1.48	1.35
1	S2	814	5MU	C6-C5	-11.89	1.15	1.34
1	S2	1243	PSU	C6-C5	11.78	1.48	1.35
1	S2	1219	B8Q	C4-N3	11.32	1.65	1.48
1	S2	822	PSU	C6-C5	11.14	1.47	1.35
1	S2	1081	PSU	C6-C5	11.12	1.47	1.35
1	S2	119	PSU	C6-C5	11.08	1.47	1.35
1	S2	814	5MU	C4-N3	-11.03	1.18	1.38
1	S2	1219	B8Q	C6-C5	10.97	1.56	1.33
1	S2	612	PSU	C6-C5	10.74	1.47	1.35
1	S2	1678	A2M	C2'-C1'	-10.61	1.27	1.53
1	S2	484	A2M	C2'-C1'	-10.55	1.27	1.53
1	S2	668	A2M	C2'-C1'	-10.52	1.27	1.53
1	S2	1031	A2M	C2'-C1'	-10.52	1.27	1.53
1	S2	166	A2M	C2'-C1'	-10.50	1.27	1.53
1	S2	1678	A2M	C3'-C4'	-10.42	1.26	1.53
1	S2	27	A2M	C2'-C1'	-10.40	1.27	1.53
1	S2	1031	A2M	C3'-C4'	-10.27	1.26	1.53
1	S2	27	A2M	C3'-C4'	-10.22	1.27	1.53
1	S2	668	A2M	C3'-C4'	-10.18	1.27	1.53
1	S2	159	A2M	C2'-C1'	-10.13	1.28	1.53
1	S2	484	A2M	C3'-C4'	-10.05	1.27	1.53
1	S2	166	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	159	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	119	PSU	C2-N1	9.95	1.49	1.36
1	S2	822	PSU	C2-N1	9.29	1.48	1.36
1	S2	1219	B8Q	C2-N1	9.25	1.51	1.38
1	S2	612	PSU	C2-N1	9.21	1.48	1.36
1	S2	1081	PSU	C2-N1	9.06	1.48	1.36
1	S2	1243	PSU	C2-N1	9.05	1.48	1.36
1	S2	1832	6MZ	C6-N6	9.01	1.44	1.34
1	S2	1374	5MC	C6-C5	9.01	1.49	1.34
1	S2	823	PSU	C2-N1	8.97	1.48	1.36
1	S2	1703	OMC	C4-N4	8.44	1.54	1.33
1	S2	1710	OMC	C4-N4	8.41	1.54	1.33
1	S2	174	OMC	C4-N4	8.35	1.54	1.33
1	S2	116	OMU	C2-N1	8.26	1.51	1.38
1	S2	517	OMC	C4-N4	8.19	1.53	1.33
1	S2	568	E3C	C2-N3	8.16	1.47	1.37
1	S2	1248	B8N	C4-N3	-8.10	1.26	1.40
1	S2	1830	UR3	C2-N1	8.08	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	568	E3C	C6-C5	8.03	1.50	1.33
1	S2	121	OMU	C2-N1	7.99	1.51	1.38
1	S2	823	PSU	C2-N3	7.94	1.50	1.37
1	S2	568	E3C	C2-N1	7.88	1.49	1.38
1	S2	1842	4AC	C4-N3	7.83	1.45	1.32
1	S2	1337	4AC	C4-N3	7.39	1.45	1.32
1	S2	1248	B8N	C6-N1	7.39	1.54	1.36
1	S2	119	PSU	C2-N3	7.35	1.49	1.37
1	S2	1248	B8N	C4-C5	7.16	1.63	1.47
1	S2	822	PSU	C2-N3	6.96	1.48	1.37
1	S2	1243	PSU	C2-N3	6.93	1.48	1.37
1	S2	174	OMC	C2-N3	6.83	1.49	1.36
1	S2	1710	OMC	C2-N3	6.80	1.49	1.36
1	S2	612	PSU	C2-N3	6.78	1.48	1.37
1	S2	1703	OMC	C6-C5	6.63	1.50	1.35
1	S2	1710	OMC	C6-C5	6.59	1.50	1.35
1	S2	1703	OMC	C2-N3	6.57	1.49	1.36
1	S2	174	OMC	C6-C5	6.54	1.50	1.35
1	S2	116	OMU	C2-N3	6.53	1.49	1.38
1	S2	517	OMC	C6-C5	6.52	1.50	1.35
1	S2	644	OMG	C4-N3	6.51	1.49	1.34
1	S2	509	OMG	C4-N3	6.51	1.49	1.34
1	S2	1081	PSU	C2-N3	6.48	1.48	1.37
1	S2	1678	A2M	C6-N6	6.46	1.50	1.34
1	S2	121	OMU	C2-N3	6.43	1.49	1.38
1	S2	517	OMC	C2-N3	6.39	1.49	1.36
1	S2	159	A2M	O4'-C1'	6.31	1.56	1.42
1	S2	683	OMG	C4-N3	6.29	1.48	1.34
1	S2	1710	OMC	C4-N3	6.29	1.46	1.34
1	S2	166	A2M	O4'-C1'	6.27	1.56	1.42
1	S2	1374	5MC	C4-N3	6.25	1.44	1.34
1	S2	1374	5MC	C5-C4	6.17	1.48	1.44
1	S2	116	OMU	C6-C5	6.13	1.49	1.35
1	S2	159	A2M	C3'-C2'	6.08	1.66	1.53
1	S2	1337	4AC	C6-C5	6.05	1.49	1.35
1	S2	1678	A2M	O4'-C1'	6.01	1.55	1.42
1	S2	1842	4AC	C2-N3	6.00	1.48	1.36
1	S2	121	OMU	C6-C5	5.93	1.48	1.35
1	S2	27	A2M	O4'-C1'	5.93	1.55	1.42
1	S2	174	OMC	C4-N3	5.92	1.46	1.34
1	S2	1031	A2M	O4'-C1'	5.91	1.55	1.42
1	S2	1337	4AC	C2-N3	5.90	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1703	OMC	C4-N3	5.90	1.46	1.34
1	S2	484	A2M	C3'-C2'	5.75	1.65	1.53
1	S2	484	A2M	O4'-C1'	5.74	1.55	1.42
1	S2	668	A2M	C3'-C2'	5.73	1.65	1.53
1	S2	1842	4AC	C6-C5	5.63	1.48	1.35
1	S2	1374	5MC	C2-N3	5.63	1.47	1.36
1	S2	1678	A2M	C3'-C2'	5.57	1.65	1.53
1	S2	1248	B8N	C2-N1	5.55	1.55	1.39
1	S2	668	A2M	O4'-C1'	5.53	1.54	1.42
1	S2	159	A2M	C6-N6	5.48	1.48	1.34
1	S2	517	OMC	C4-N3	5.48	1.45	1.34
1	S2	27	A2M	C6-N6	5.48	1.48	1.34
1	S2	166	A2M	C6-N6	5.47	1.48	1.34
1	S2	1031	A2M	C3'-C2'	5.46	1.64	1.53
1	S2	1031	A2M	C6-N6	5.44	1.48	1.34
1	S2	668	A2M	C6-N6	5.43	1.48	1.34
1	S2	484	A2M	C6-N6	5.43	1.48	1.34
1	S2	1219	B8Q	C2-N3	-5.41	1.25	1.35
1	S2	509	OMG	C2-N3	5.40	1.46	1.33
1	S2	166	A2M	C3'-C2'	5.35	1.64	1.53
1	S2	1830	UR3	C6-C5	5.35	1.47	1.35
1	S2	1081	PSU	O2-C2	-5.26	1.12	1.23
1	S2	27	A2M	C3'-C2'	5.21	1.64	1.53
1	S2	644	OMG	C2-N3	5.20	1.45	1.33
1	S2	568	E3C	C4-N3	5.18	1.56	1.48
1	S2	612	PSU	O2-C2	-5.14	1.12	1.23
1	S2	814	5MU	C2-N3	5.10	1.46	1.38
1	S2	823	PSU	O2-C2	-5.01	1.12	1.23
1	S2	1081	PSU	O4-C4	-4.99	1.14	1.23
1	S2	166	A2M	O4'-C4'	4.97	1.56	1.45
1	S2	119	PSU	O4-C4	-4.95	1.14	1.23
1	S2	822	PSU	O2-C2	-4.92	1.12	1.23
1	S2	1243	PSU	O2-C2	-4.91	1.12	1.23
1	S2	159	A2M	O4'-C4'	4.91	1.55	1.45
1	S2	683	OMG	C2-N3	4.88	1.45	1.33
1	S2	822	PSU	O4-C4	-4.87	1.14	1.23
1	S2	1806	M7A	C6-N6	4.87	1.46	1.34
1	S2	116	OMU	C4-N3	4.83	1.46	1.38
1	S2	1830	UR3	C2-N3	4.81	1.48	1.39
1	S2	1248	B8N	C6-C5	4.80	1.41	1.35
1	S2	119	PSU	O2-C2	-4.78	1.13	1.23
1	S2	1337	4AC	C7-N4	4.76	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	612	PSU	O4-C4	-4.71	1.14	1.23
1	S2	1243	PSU	O4-C4	-4.69	1.14	1.23
1	S2	484	A2M	O4'-C4'	4.68	1.55	1.45
1	S2	683	OMG	C2-N2	4.68	1.45	1.34
1	S2	644	OMG	C2-N2	4.67	1.45	1.34
1	S2	1678	A2M	O4'-C4'	4.64	1.55	1.45
1	S2	1031	A2M	O4'-C4'	4.63	1.55	1.45
1	S2	1219	B8Q	C4-C5	-4.63	1.39	1.49
1	S2	1832	6MZ	C5-C4	-4.61	1.30	1.39
1	S2	27	A2M	O4'-C4'	4.55	1.55	1.45
1	S2	1337	4AC	C4-N4	4.46	1.46	1.39
1	S2	1842	4AC	C2-N1	4.45	1.49	1.40
1	S2	1842	4AC	C7-N4	4.45	1.46	1.37
1	S2	121	OMU	C4-N3	4.44	1.46	1.38
1	S2	174	OMC	C2-N1	4.37	1.49	1.40
1	S2	1374	5MC	C4-N4	4.29	1.45	1.34
1	S2	509	OMG	C2-N2	4.25	1.44	1.34
1	S2	668	A2M	O4'-C4'	4.23	1.54	1.45
1	S2	119	PSU	C6-N1	4.21	1.43	1.36
1	S2	1374	5MC	C6-N1	4.15	1.45	1.38
1	S2	1337	4AC	C2-N1	4.14	1.48	1.40
1	S2	1337	4AC	C5-C4	4.14	1.50	1.41
1	S2	1842	4AC	C4-N4	4.02	1.45	1.39
1	S2	822	PSU	C6-N1	4.01	1.42	1.36
1	S2	1710	OMC	C2-N1	3.96	1.48	1.40
1	S2	517	OMC	C2-N1	3.91	1.48	1.40
1	S2	1806	M7A	C5-N7	3.90	1.48	1.39
1	S2	1243	PSU	C6-N1	3.88	1.42	1.36
1	S2	814	5MU	C2-N1	3.85	1.44	1.38
1	S2	1081	PSU	C6-N1	3.85	1.42	1.36
1	S2	612	PSU	C6-N1	3.85	1.42	1.36
1	S2	1710	OMC	C6-N1	3.84	1.47	1.38
1	S2	1832	6MZ	C8-N9	-3.81	1.31	1.37
1	S2	1374	5MC	C2-N1	3.80	1.48	1.40
1	S2	823	PSU	C6-N1	3.78	1.42	1.36
1	S2	1337	4AC	C6-N1	3.77	1.47	1.38
1	S2	1842	4AC	C5-C4	3.67	1.49	1.41
1	S2	1832	6MZ	C5-N7	-3.67	1.32	1.39
1	S2	1851	MA6	C5-C4	-3.62	1.32	1.39
1	S2	1842	4AC	C6-N1	3.61	1.46	1.38
1	S2	1850	MA6	C5-C4	-3.58	1.32	1.39
1	S2	174	OMC	C6-N1	3.58	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1703	OMC	C6-N1	3.57	1.46	1.38
1	S2	823	PSU	C4-N3	3.48	1.45	1.38
1	S2	1703	OMC	C2-N1	3.46	1.47	1.40
1	S2	683	OMG	C5-N7	-3.44	1.32	1.39
1	S2	823	PSU	O4-C4	-3.41	1.17	1.23
1	S2	509	OMG	C5-N7	-3.39	1.32	1.39
1	S2	668	A2M	C5-C4	-3.30	1.33	1.39
1	S2	1851	MA6	C6-N6	3.29	1.45	1.36
1	S2	1850	MA6	C6-N6	3.28	1.45	1.36
1	S2	517	OMC	C6-N1	3.28	1.45	1.38
1	S2	1031	A2M	C5-C4	-3.26	1.33	1.39
1	S2	27	A2M	C5-C4	-3.23	1.33	1.39
1	S2	1374	5MC	O2-C2	-3.17	1.17	1.23
1	S2	1031	A2M	C5-N7	-3.12	1.33	1.39
1	S2	1851	MA6	C5-N7	-3.12	1.33	1.39
1	S2	484	A2M	C5-C4	-3.09	1.33	1.39
1	S2	27	A2M	C5-N7	-3.08	1.33	1.39
1	S2	166	A2M	C5-N7	-3.02	1.33	1.39
1	S2	568	E3C	C6-N1	3.02	1.45	1.38
1	S2	1219	B8Q	C31-N3	3.00	1.52	1.46
1	S2	1850	MA6	C5-N7	-2.97	1.33	1.39
1	S2	644	OMG	C5-N7	-2.96	1.33	1.39
1	S2	822	PSU	C4-N3	2.95	1.44	1.38
1	S2	159	A2M	C5-C4	-2.95	1.33	1.39
1	S2	1830	UR3	O2-C2	-2.92	1.17	1.22
1	S2	484	A2M	C5-N7	-2.89	1.33	1.39
1	S2	119	PSU	C4-N3	2.87	1.44	1.38
1	S2	668	A2M	C5-N7	-2.87	1.33	1.39
1	S2	1678	A2M	C5-N7	-2.86	1.33	1.39
1	S2	166	A2M	C5-C4	-2.85	1.34	1.39
1	S2	1219	B8Q	C6-N1	-2.85	1.31	1.38
1	S2	1243	PSU	C4-N3	2.85	1.44	1.38
1	S2	568	E3C	C31-N3	2.82	1.55	1.47
1	S2	644	OMG	O6-C6	-2.81	1.18	1.23
1	S2	1850	MA6	C8-N9	-2.79	1.32	1.37
1	S2	1081	PSU	O4'-C1'	-2.76	1.40	1.43
1	S2	683	OMG	O6-C6	-2.76	1.18	1.23
1	S2	612	PSU	C4-N3	2.75	1.44	1.38
1	S2	1830	UR3	C5-C4	2.75	1.50	1.43
1	S2	1830	UR3	C4-N3	2.72	1.46	1.40
1	S2	1851	MA6	C8-N9	-2.71	1.32	1.37
1	S2	159	A2M	C5-N7	-2.70	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1678	A2M	C8-N9	-2.68	1.33	1.37
1	S2	116	OMU	C6-N1	2.67	1.44	1.38
1	S2	509	OMG	O6-C6	-2.67	1.18	1.23
1	S2	1851	MA6	C4-N9	-2.64	1.32	1.37
1	S2	1031	A2M	C8-N9	-2.62	1.33	1.37
1	S2	121	OMU	C6-N1	2.61	1.44	1.38
1	S2	1081	PSU	C4-N3	2.58	1.43	1.38
1	S2	823	PSU	O4'-C1'	-2.56	1.40	1.43
1	S2	159	A2M	C8-N9	-2.53	1.33	1.37
1	S2	484	A2M	C8-N9	-2.48	1.33	1.37
1	S2	683	OMG	C4-N9	-2.47	1.31	1.38
1	S2	27	A2M	C8-N9	-2.45	1.33	1.37
1	S2	568	E3C	C4-C5	-2.44	1.44	1.49
1	S2	517	OMC	O2-C2	-2.43	1.19	1.23
1	S2	1703	OMC	O2-C2	-2.43	1.19	1.23
1	S2	1710	OMC	O2-C2	-2.43	1.19	1.23
1	S2	814	5MU	O4-C4	-2.42	1.19	1.23
1	S2	668	A2M	C8-N9	-2.40	1.33	1.37
1	S2	1337	4AC	O2-C2	-2.39	1.19	1.23
1	S2	822	PSU	O4'-C1'	-2.39	1.40	1.43
1	S2	644	OMG	C2-N1	2.35	1.43	1.37
1	S2	1678	A2M	C5-C4	-2.35	1.34	1.39
1	S2	1710	OMC	C5-C4	2.31	1.48	1.42
1	S2	644	OMG	C5-C6	2.29	1.53	1.44
1	S2	683	OMG	C2-N1	2.26	1.43	1.37
1	S2	509	OMG	C2-N1	2.26	1.43	1.37
1	S2	1830	UR3	C6-N1	2.25	1.43	1.38
1	S2	1850	MA6	C4-N9	-2.24	1.33	1.37
1	S2	509	OMG	C5-C6	2.23	1.52	1.44
1	S2	1248	B8N	O4-C4	-2.16	1.18	1.23
1	S2	814	5MU	O2-C2	-2.14	1.19	1.23
1	S2	1248	B8N	O4'-C1'	-2.13	1.40	1.43
1	S2	174	OMC	C5-C4	2.12	1.47	1.42
1	S2	644	OMG	C4-N9	-2.12	1.32	1.38
1	S2	174	OMC	O2-C2	-2.11	1.19	1.23
1	S2	1832	6MZ	C9-N6	2.11	1.48	1.45
1	S2	668	A2M	C4-N9	-2.11	1.33	1.37
1	S2	121	OMU	O4-C4	-2.10	1.20	1.24
1	S2	644	OMG	C6-N1	2.10	1.42	1.38
1	S2	166	A2M	C8-N9	-2.10	1.34	1.37
1	S2	116	OMU	O4-C4	-2.10	1.20	1.24
1	S2	1842	4AC	O2-C2	-2.08	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	121	OMU	C5-C4	2.07	1.48	1.43
1	S2	517	OMC	C5-C4	2.06	1.47	1.42
1	S2	1703	OMC	C5-C4	2.02	1.47	1.42
1	S2	683	OMG	C5-C6	2.02	1.52	1.44
1	S2	612	PSU	O4'-C1'	-2.02	1.41	1.43

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	N1-C6-N6	-13.26	100.69	116.86
1	S2	1850	MA6	N1-C6-N6	-12.61	101.50	116.86
1	S2	1806	M7A	C5-C6-N6	11.08	142.57	123.75
1	S2	814	5MU	C5-C4-N3	9.88	123.91	115.32
1	S2	1806	M7A	N6-C6-N1	-9.59	97.03	118.38
1	S2	1851	MA6	C5-C6-N6	9.19	139.87	125.33
1	S2	1850	MA6	C5-C6-N6	8.71	139.12	125.33
1	S2	814	5MU	C5-C6-N1	-8.41	114.18	123.31
1	S2	1830	UR3	C1'-N1-C2	8.03	130.18	117.04
1	S2	668	A2M	C4-N9-C1'	-7.59	108.88	126.63
1	S2	568	E3C	C1'-N1-C2	7.37	129.10	117.04
1	S2	814	5MU	C4-N3-C2	-7.30	117.77	127.34
1	S2	1031	A2M	C4-N9-C1'	-7.04	110.16	126.63
1	S2	166	A2M	C4-N9-C1'	-6.98	110.31	126.63
1	S2	484	A2M	C4-N9-C1'	-6.98	110.32	126.63
1	S2	166	A2M	C1'-N9-C8	6.96	142.55	127.09
1	S2	1806	M7A	N3-C4-N9	6.93	135.55	126.88
1	S2	668	A2M	C1'-N9-C8	6.85	142.29	127.09
1	S2	1830	UR3	O2-C2-N3	-6.81	111.92	121.33
1	S2	1830	UR3	C6-N1-C2	-6.75	116.28	121.80
1	S2	484	A2M	C1'-N9-C8	6.42	141.34	127.09
1	S2	1031	A2M	C1'-N9-C8	6.39	141.28	127.09
1	S2	27	A2M	C4-N9-C1'	-6.17	112.21	126.63
1	S2	1850	MA6	N1-C2-N3	-6.08	119.38	128.58
1	S2	1678	A2M	C4-N9-C1'	-6.06	112.46	126.63
1	S2	1850	MA6	C1'-N9-C8	-5.96	113.86	127.09
1	S2	484	A2M	N3-C2-N1	-5.95	119.58	128.58
1	S2	121	OMU	C4-N3-C2	-5.94	119.23	126.61
1	S2	159	A2M	N3-C2-N1	-5.93	119.60	128.58
1	S2	1031	A2M	N3-C2-N1	-5.92	119.63	128.58
1	S2	27	A2M	C1'-N9-C8	5.84	140.05	127.09
1	S2	1248	B8N	C1'-C5-C4	5.83	126.45	117.61
1	S2	159	A2M	C4-N9-C1'	-5.78	113.12	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	509	OMG	C5-C4-N3	-5.76	119.22	128.39
1	S2	1678	A2M	C1'-N9-C8	5.74	139.83	127.09
1	S2	27	A2M	N3-C2-N1	-5.74	119.90	128.58
1	S2	27	A2M	C5-C4-N3	-5.72	118.85	126.72
1	S2	159	A2M	C5-C4-N3	-5.70	118.87	126.72
1	S2	1832	6MZ	N1-C2-N3	-5.69	119.97	128.58
1	S2	668	A2M	N3-C2-N1	-5.65	120.03	128.58
1	S2	166	A2M	N3-C2-N1	-5.63	120.06	128.58
1	S2	1851	MA6	N1-C2-N3	-5.61	120.08	128.58
1	S2	1830	UR3	C4-N3-C2	-5.54	120.12	124.58
1	S2	1832	6MZ	C5-C4-N3	-5.53	119.10	126.72
1	S2	166	A2M	N6-C6-N1	-5.51	106.10	118.38
1	S2	159	A2M	N6-C6-N1	-5.40	106.35	118.38
1	S2	1806	M7A	N3-C2-N1	-5.38	120.44	128.58
1	S2	27	A2M	N6-C6-N1	-5.34	106.49	118.38
1	S2	668	A2M	N6-C6-N1	-5.33	106.50	118.38
1	S2	484	A2M	N6-C6-N1	-5.32	106.53	118.38
1	S2	568	E3C	O2-C2-N3	-5.31	115.31	122.10
1	S2	823	PSU	C6-N1-C2	-5.30	117.77	122.69
1	S2	612	PSU	C4-N3-C2	-5.23	119.17	126.37
1	S2	116	OMU	C4-N3-C2	-5.20	120.15	126.61
1	S2	119	PSU	C4-N3-C2	-5.19	119.22	126.37
1	S2	159	A2M	C1'-N9-C8	5.19	138.61	127.09
1	S2	644	OMG	C5-C4-N3	-5.17	120.17	128.39
1	S2	814	5MU	N3-C2-N1	5.13	121.57	114.89
1	S2	612	PSU	N1-C2-N3	5.09	120.54	115.17
1	S2	1850	MA6	N9-C8-N7	-5.07	106.74	113.94
1	S2	814	5MU	C5M-C5-C6	-5.02	116.06	122.85
1	S2	823	PSU	O2-C2-N1	-4.96	117.67	122.79
1	S2	121	OMU	N3-C2-N1	4.95	121.33	114.89
1	S2	683	OMG	C5-C4-N3	-4.94	120.53	128.39
1	S2	1832	6MZ	C4-C5-C6	4.93	120.88	116.78
1	S2	1219	B8Q	N3-C2-N1	4.92	124.02	117.16
1	S2	1678	A2M	C5-C4-N3	-4.91	119.95	126.72
1	S2	644	OMG	C1'-N9-C4	-4.90	112.00	126.49
1	S2	484	A2M	C5-C4-N3	-4.88	119.99	126.72
1	S2	166	A2M	C5-C4-N3	-4.84	120.06	126.72
1	S2	1678	A2M	N6-C6-N1	-4.74	107.82	118.38
1	S2	1081	PSU	C4-N3-C2	-4.74	119.84	126.37
1	S2	1248	B8N	C5-C4-N3	4.73	124.74	116.15
1	S2	1031	A2M	N6-C6-N1	-4.73	107.84	118.38
1	S2	1851	MA6	N9-C8-N7	-4.69	107.28	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1678	A2M	N3-C2-N1	-4.68	121.50	128.58
1	S2	1031	A2M	C5-C4-N3	-4.66	120.30	126.72
1	S2	668	A2M	N9-C8-N7	-4.65	107.34	113.94
1	S2	1850	MA6	C5-C4-N3	-4.65	120.31	126.72
1	S2	1243	PSU	C4-N3-C2	-4.65	119.97	126.37
1	S2	1219	B8Q	C31-N3-C4	4.63	122.78	114.76
1	S2	644	OMG	C2-N3-C4	4.60	120.22	112.30
1	S2	683	OMG	C2-N3-C4	4.57	120.17	112.30
1	S2	119	PSU	N1-C2-N3	4.56	119.98	115.17
1	S2	1031	A2M	N9-C8-N7	-4.54	107.49	113.94
1	S2	822	PSU	C4-N3-C2	-4.53	120.13	126.37
1	S2	683	OMG	C1'-N9-C4	-4.49	113.21	126.49
1	S2	1851	MA6	C5-C4-N3	-4.47	120.56	126.72
1	S2	1243	PSU	N1-C2-N3	4.46	119.87	115.17
1	S2	1081	PSU	N1-C2-N3	4.46	119.87	115.17
1	S2	822	PSU	N1-C2-N3	4.43	119.84	115.17
1	S2	823	PSU	N1-C2-N3	4.42	119.83	115.17
1	S2	1851	MA6	C1'-N9-C8	-4.37	117.40	127.09
1	S2	814	5MU	O4-C4-C5	-4.33	119.96	124.92
1	S2	668	A2M	C5-C4-N3	-4.31	120.78	126.72
1	S2	1678	A2M	C5-C6-N6	4.30	133.93	123.29
1	S2	644	OMG	C1'-N9-C8	4.27	138.86	126.73
1	S2	814	5MU	C6-C5-C4	4.23	121.50	118.02
1	S2	568	E3C	C6-N1-C2	-4.22	118.35	121.80
1	S2	166	A2M	C5-C6-N6	4.19	133.67	123.29
1	S2	27	A2M	N9-C8-N7	-4.17	108.02	113.94
1	S2	159	A2M	N9-C8-N7	-4.14	108.06	113.94
1	S2	484	A2M	N9-C8-N7	-4.14	108.07	113.94
1	S2	509	OMG	C2-N3-C4	4.11	119.37	112.30
1	S2	1850	MA6	C4-N9-C1'	4.10	136.23	126.63
1	S2	1850	MA6	C4-C5-C6	4.09	120.13	115.91
1	S2	509	OMG	C1'-N9-C4	-4.06	114.49	126.49
1	S2	1248	B8N	C4-N3-C2	-4.06	120.62	125.62
1	S2	668	A2M	C5-C6-N6	4.02	133.24	123.29
1	S2	1850	MA6	C4-N9-C8	3.97	109.90	105.74
1	S2	1830	UR3	C3U-N3-C4	3.96	123.35	117.87
1	S2	1678	A2M	N9-C8-N7	-3.92	108.37	113.94
1	S2	27	A2M	C5-C6-N6	3.91	132.97	123.29
1	S2	159	A2M	C5-C6-N6	3.91	132.97	123.29
1	S2	1851	MA6	C4-C5-C6	3.89	119.94	115.91
1	S2	1031	A2M	C5-C6-N6	3.89	132.91	123.29
1	S2	568	E3C	C1'-N1-C6	-3.88	112.49	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1806	M7A	C4-N9-C1'	-3.85	117.65	126.63
1	S2	509	OMG	N9-C4-N3	3.85	133.65	125.95
1	S2	683	OMG	C1'-N9-C8	3.85	137.66	126.73
1	S2	159	A2M	N3-C4-N9	3.82	133.67	127.17
1	S2	484	A2M	C5-C6-N6	3.81	132.71	123.29
1	S2	159	A2M	C2-N3-C4	3.76	121.01	111.83
1	S2	509	OMG	C2-N1-C6	-3.75	118.31	125.11
1	S2	1832	6MZ	N9-C8-N7	-3.72	108.66	113.94
1	S2	159	A2M	C2'-C1'-N9	-3.71	107.65	113.75
1	S2	568	E3C	C31-N3-C2	3.70	122.14	117.49
1	S2	27	A2M	C2-N3-C4	3.70	120.87	111.83
1	S2	612	PSU	C6-C5-C4	3.70	120.67	118.17
1	S2	116	OMU	C5-C4-N3	3.69	119.97	114.80
1	S2	1248	B8N	N3-C2-N1	3.67	121.20	116.72
1	S2	1850	MA6	C2-N1-C6	3.65	120.75	111.83
1	S2	116	OMU	N3-C2-N1	3.65	119.64	114.89
1	S2	1832	6MZ	N3-C4-N9	3.63	133.34	127.17
1	S2	823	PSU	C4-N3-C2	-3.62	121.38	126.37
1	S2	166	A2M	N9-C8-N7	-3.61	108.82	113.94
1	S2	509	OMG	C1'-N9-C8	3.60	136.97	126.73
1	S2	1806	M7A	C71-N7-C5	-3.60	108.44	123.44
1	S2	1219	B8Q	O2-C2-N3	-3.58	117.92	122.95
1	S2	1850	MA6	N3-C4-N9	3.53	133.18	127.17
1	S2	27	A2M	N3-C4-N9	3.52	133.15	127.17
1	S2	1830	UR3	C1'-N1-C6	-3.51	113.28	120.78
1	S2	484	A2M	C2-N3-C4	3.50	120.38	111.83
1	S2	1832	6MZ	C2-N3-C4	3.48	120.34	111.83
1	S2	612	PSU	C6-N1-C2	-3.47	119.47	122.69
1	S2	1851	MA6	C2-N1-C6	3.47	120.30	111.83
1	S2	1243	PSU	C6-N1-C2	-3.47	119.47	122.69
1	S2	814	5MU	C5M-C5-C4	3.42	122.43	118.78
1	S2	121	OMU	C5-C4-N3	3.39	119.55	114.80
1	S2	822	PSU	C6-N1-C2	-3.38	119.55	122.69
1	S2	1850	MA6	C2-N3-C4	3.36	120.04	111.83
1	S2	119	PSU	C6-C5-C4	3.36	120.44	118.17
1	S2	1081	PSU	C6-N1-C2	-3.35	119.58	122.69
1	S2	644	OMG	N9-C8-N7	-3.33	107.22	113.40
1	S2	644	OMG	N9-C4-N3	3.33	132.61	125.95
1	S2	166	A2M	C2-N3-C4	3.30	119.90	111.83
1	S2	568	E3C	C4-N3-C2	-3.29	116.08	122.00
1	S2	683	OMG	N9-C8-N7	-3.27	107.34	113.40
1	S2	1337	4AC	C6-C5-C4	3.26	120.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	683	OMG	N9-C4-N3	3.24	132.43	125.95
1	S2	1806	M7A	C2-N3-C4	3.23	119.72	111.83
1	S2	1851	MA6	C2-N3-C4	3.22	119.69	111.83
1	S2	644	OMG	C2-N1-C6	-3.19	119.33	125.11
1	S2	1031	A2M	C2-N3-C4	3.17	119.57	111.83
1	S2	116	OMU	O4-C4-C5	-3.16	119.71	125.16
1	S2	1243	PSU	O2-C2-N1	-3.16	119.53	122.79
1	S2	119	PSU	C6-N1-C2	-3.16	119.76	122.69
1	S2	159	A2M	O2'-C2'-C1'	3.14	114.95	108.99
1	S2	668	A2M	C2-N3-C4	3.12	119.45	111.83
1	S2	1031	A2M	C2'-C1'-N9	-3.12	108.62	113.75
1	S2	1678	A2M	C5-N7-C8	3.10	108.32	103.45
1	S2	1374	5MC	C5-C6-N1	-3.09	119.95	123.31
1	S2	484	A2M	N3-C4-N9	3.07	132.38	127.17
1	S2	1851	MA6	C4-N9-C1'	3.06	133.78	126.63
1	S2	27	A2M	C5-N7-C8	3.05	108.25	103.45
1	S2	1678	A2M	C4-C5-N7	-3.05	107.09	110.58
1	S2	1850	MA6	C5-N7-C8	3.02	108.19	103.45
1	S2	822	PSU	O2-C2-N1	-3.01	119.68	122.79
1	S2	1248	B8N	C31-N3-C4	3.01	121.44	117.18
1	S2	1678	A2M	C6-C5-C4	3.00	121.28	117.18
1	S2	1806	M7A	C5-C4-N3	-3.00	119.63	126.56
1	S2	1851	MA6	C5-N7-C8	2.99	108.14	103.45
1	S2	1031	A2M	C5-N7-C8	2.98	108.14	103.45
1	S2	1337	4AC	C5-C4-N3	-2.96	117.97	122.60
1	S2	509	OMG	N9-C8-N7	-2.95	107.94	113.40
1	S2	668	A2M	C3'-C2'-C1'	2.94	108.43	102.81
1	S2	668	A2M	C4-N9-C8	2.93	108.81	105.74
1	S2	1851	MA6	C4-N9-C8	2.93	108.81	105.74
1	S2	159	A2M	C5-N7-C8	2.91	108.03	103.45
1	S2	644	OMG	C5-C6-N1	2.88	120.58	113.25
1	S2	1678	A2M	C2-N3-C4	2.87	118.84	111.83
1	S2	612	PSU	O2-C2-N1	-2.84	119.86	122.79
1	S2	683	OMG	O6-C6-C5	-2.84	119.04	126.53
1	S2	1031	A2M	N3-C4-N9	2.83	131.99	127.17
1	S2	668	A2M	C5-N7-C8	2.81	107.87	103.45
1	S2	509	OMG	C5-C6-N1	2.81	120.40	113.25
1	S2	119	PSU	O2-C2-N1	-2.79	119.91	122.79
1	S2	814	5MU	O3'-C3'-C2'	2.75	120.63	111.82
1	S2	668	A2M	C2'-C3'-C4'	2.74	107.88	101.99
1	S2	683	OMG	C2-N1-C6	-2.72	120.17	125.11
1	S2	1031	A2M	C4-N9-C8	2.69	108.56	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1248	B8N	O4-C4-N3	-2.61	115.75	119.99
1	S2	1851	MA6	N3-C4-N9	2.59	131.58	127.17
1	S2	683	OMG	C5-C6-N1	2.59	119.84	113.25
1	S2	644	OMG	O6-C6-C5	-2.59	119.71	126.53
1	S2	668	A2M	N3-C4-N9	2.58	131.56	127.17
1	S2	484	A2M	C5-N7-C8	2.56	107.47	103.45
1	S2	166	A2M	N3-C4-N9	2.55	131.51	127.17
1	S2	509	OMG	O6-C6-C5	-2.55	119.79	126.53
1	S2	1678	A2M	N3-C4-N9	2.55	131.51	127.17
1	S2	121	OMU	O4-C4-C5	-2.55	120.76	125.16
1	S2	166	A2M	C5-N7-C8	2.52	107.40	103.45
1	S2	1678	A2M	C5-C4-N9	2.50	108.54	105.81
1	S2	484	A2M	C4-N9-C8	2.47	108.33	105.74
1	S2	1842	4AC	C6-C5-C4	2.46	119.96	117.00
1	S2	517	OMC	O2-C2-N3	-2.45	118.47	122.33
1	S2	1832	6MZ	C5-N7-C8	2.44	107.29	103.45
1	S2	166	A2M	C4'-O4'-C1'	-2.44	104.08	109.47
1	S2	1081	PSU	C6-C5-C4	2.42	119.81	118.17
1	S2	121	OMU	C6-N1-C2	-2.41	118.06	121.00
1	S2	1374	5MC	CM5-C5-C6	-2.41	119.58	122.85
1	S2	159	A2M	C4-N9-C8	2.40	108.26	105.74
1	S2	166	A2M	C5-C4-N9	2.40	108.43	105.81
1	S2	1832	6MZ	C9-N6-C6	-2.40	120.63	122.85
1	S2	1842	4AC	C5-C4-N3	-2.38	118.88	122.60
1	S2	1219	B8Q	C31-N3-C2	2.35	121.40	117.70
1	S2	1851	MA6	C4-C5-N7	-2.34	107.91	110.58
1	S2	27	A2M	C6-C5-C4	2.34	120.37	117.18
1	S2	1830	UR3	O4-C4-N3	2.31	122.47	119.66
1	S2	814	5MU	O2-C2-N1	-2.30	119.80	122.80
1	S2	1031	A2M	C6-C5-C4	2.30	120.32	117.18
1	S2	1830	UR3	C6-C5-C4	2.28	125.09	120.73
1	S2	27	A2M	C4-C5-N7	-2.25	108.01	110.58
1	S2	1337	4AC	O7-C7-CM7	-2.22	118.10	122.05
1	S2	1842	4AC	O7-C7-CM7	-2.21	118.11	122.05
1	S2	159	A2M	C2'-C3'-C4'	2.21	106.75	101.99
1	S2	174	OMC	O2-C2-N3	-2.21	118.84	122.33
1	S2	484	A2M	C3'-C2'-C1'	2.18	106.98	102.81
1	S2	1832	6MZ	C1'-N9-C8	-2.17	122.28	127.09
1	S2	121	OMU	O2-C2-N1	-2.17	119.97	122.80
1	S2	1031	A2M	C4-C5-N7	-2.17	108.10	110.58
1	S2	668	A2M	C2'-C1'-N9	-2.15	110.22	113.75
1	S2	27	A2M	C3'-C2'-C1'	2.13	106.88	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	612	PSU	O4'-C1'-C2'	2.12	108.09	105.15
1	S2	814	5MU	O4-C4-N3	-2.12	116.13	120.11
1	S2	683	OMG	N1-C2-N3	-2.12	119.45	123.32
1	S2	1219	B8Q	O2-C2-N1	-2.12	118.06	122.78
1	S2	644	OMG	C8-N7-C5	2.10	108.01	104.26
1	S2	159	A2M	C4-C5-N7	-2.09	108.20	110.58
1	S2	166	A2M	C4-C5-N7	-2.07	108.21	110.58
1	S2	159	A2M	C6-C5-C4	2.07	120.01	117.18
1	S2	166	A2M	C2'-C1'-N9	-2.07	110.35	113.75
1	S2	159	A2M	C5'-C4'-C3'	-2.07	107.77	115.21
1	S2	1248	B8N	O4'-C1'-C2'	2.04	107.97	105.15
1	S2	1830	UR3	C3'-C2'-C1'	2.03	105.31	101.46
1	S2	1031	A2M	C4'-O4'-C1'	-2.03	104.99	109.47
1	S2	509	OMG	C8-N7-C5	2.02	107.86	104.26
1	S2	27	A2M	C5-C4-N9	2.01	108.00	105.81

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2
1	S2	568	E3C	O4'-C1'-N1-C2
1	S2	568	E3C	O4'-C1'-N1-C6
1	S2	568	E3C	O4'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	822	PSU	C2'-C1'-C5-C4
1	S2	822	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C1'-N1-C6
1	S2	1830	UR3	O4'-C1'-N1-C2
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1850	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	1850	MA6	C5-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	119	PSU	O4'-C4'-C5'-O5'
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	822	PSU	C3'-C4'-C5'-O5'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	823	PSU	O4'-C4'-C5'-O5'
1	S2	1850	MA6	N1-C6-N6-C9
1	S2	1703	OMC	C3'-C4'-C5'-O5'
1	S2	823	PSU	C3'-C4'-C5'-O5'
1	S2	1248	B8N	O4'-C4'-C5'-O5'
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	119	PSU	C3'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C3'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	1806	M7A	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C2'-C1'-N9-C8
1	S2	1081	PSU	O4'-C4'-C5'-O5'
1	S2	174	OMC	C3'-C2'-O2'-CM2
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	612	PSU	O4'-C1'-C5-C4
1	S2	823	PSU	O4'-C1'-C5-C4
1	S2	1081	PSU	C4'-C5'-O5'-P
1	S2	1850	MA6	C5-C6-N6-C10
1	S2	1851	MA6	C5-C6-N6-C10
1	S2	1248	B8N	C32-C33-C34-O35
1	S2	121	OMU	C4'-C5'-O5'-P
1	S2	1248	B8N	C32-C33-C34-O36
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	612	PSU	O4'-C1'-C5-C6
1	S2	1248	B8N	C3'-C4'-C5'-O5'
1	S2	822	PSU	C2'-C1'-C5-C6

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	683	OMG	1	0
1	S2	814	5MU	1	0
1	S2	509	OMG	2	0
1	S2	1832	6MZ	1	0
1	S2	121	OMU	2	0
1	S2	484	A2M	1	0
1	S2	1031	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	MVM	t	5110	-	35,35,35	1.82	6 (17%)	44,49,49	3.14	15 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	MVM	t	5110	-	-	3/20/28/28	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	N4-N5	-6.18	1.31	1.38
86	t	5110	MVM	C5-N1	5.94	1.45	1.37
86	t	5110	MVM	C6-N1	2.40	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	C12-C5	2.26	1.53	1.50
86	t	5110	MVM	C7-C3	-2.01	1.48	1.53
86	t	5110	MVM	C15-N4	2.00	1.45	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5110	MVM	C15-N4-N5	10.16	128.40	119.25
86	t	5110	MVM	C15-N4-C22	-9.80	121.84	130.55
86	t	5110	MVM	N7-C22-N4	8.01	134.88	125.88
86	t	5110	MVM	C18-C22-N7	-5.04	120.25	127.18
86	t	5110	MVM	C6-N1-C5	-4.82	117.17	122.94
86	t	5110	MVM	C1-C9-N1	-4.15	105.75	116.16
86	t	5110	MVM	N3-C6-N1	3.80	120.42	116.35
86	t	5110	MVM	C21-N7-C22	3.39	122.73	115.05
86	t	5110	MVM	C7-C3-C9	3.02	116.55	110.81
86	t	5110	MVM	C19-C18-N6	2.99	134.39	130.50
86	t	5110	MVM	C8-N3-C6	2.78	121.35	115.05
86	t	5110	MVM	C3-C9-C1	-2.66	107.65	110.81
86	t	5110	MVM	C20-C21-N7	-2.21	119.92	123.42
86	t	5110	MVM	C6-N1-C9	2.15	121.60	118.40
86	t	5110	MVM	C12-C5-N1	2.14	121.19	118.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

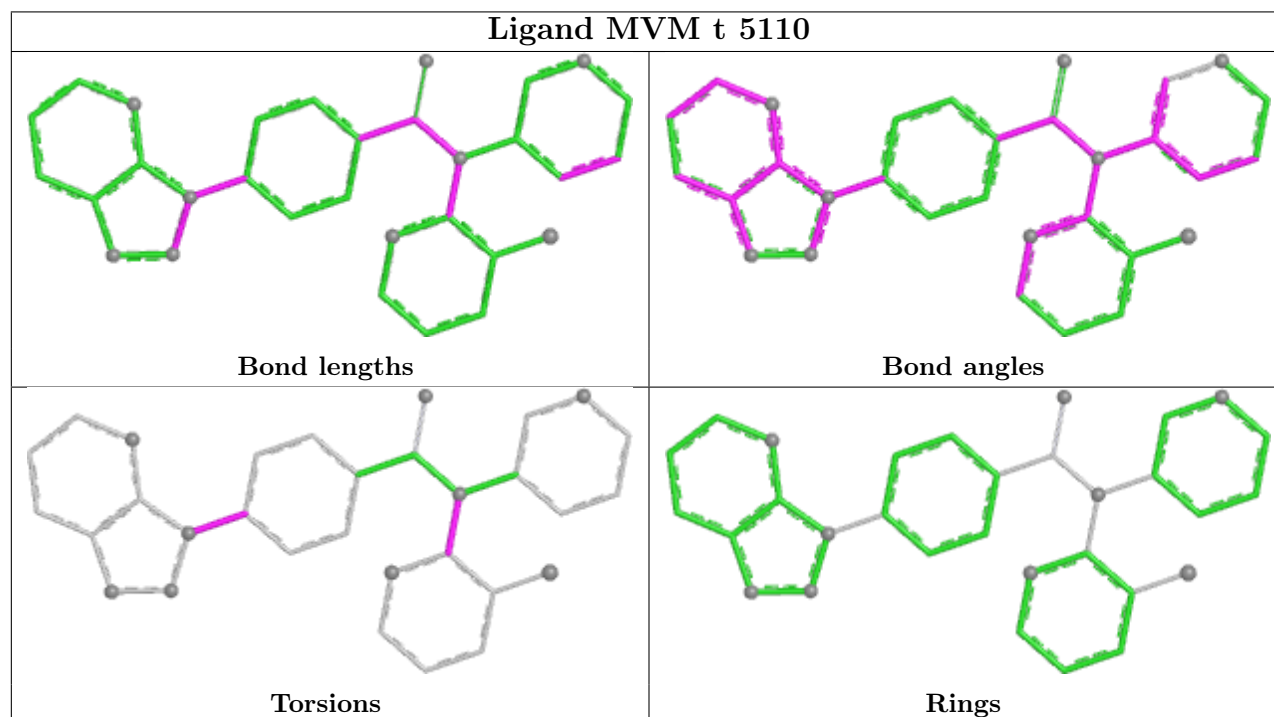
Mol	Chain	Res	Type	Atoms
86	t	5110	MVM	C16-C15-N4-C22
86	t	5110	MVM	C2-C6-N1-C5
86	t	5110	MVM	C14-C15-N4-C22

There are no ring outliers.

No monomer is involved in short contacts.

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	t	16
1	S2	5
81	v	4
63	c	1
80	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	25.98
1	t	750:G	O3'	890:C	P	20.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	3919:C	O3'	4035:G	P	18.39
1	t	517:C	O3'	629:G	P	17.30
1	t	1680:C	O3'	1699:C	P	16.29
1	t	4737:G	O3'	4815:C	P	15.93
1	S2	1752:C	O3'	1779:G	P	15.75
1	t	1089:A	O3'	1145:G	P	15.58
1	t	976:U	O3'	1047:G	P	15.45
1	t	1202:G	O3'	1216:G	P	15.13
1	t	2881:G	O3'	3569:C	P	14.86
1	t	2093:C	O3'	2228:C	P	14.28
1	t	1253:A	O3'	1256:G	P	13.38
1	S2	698:G	O3'	730:C	P	12.31
1	S2	739:C	O3'	746:C	P	11.72
1	c	119:CYS	C	120:ARG	N	7.10
1	S2	225:G	O3'	287:U	P	6.95
1	t	945:G	O3'	946:G	P	6.49
1	v	17:A	O3'	18:G	P	5.54
1	t	4734:C	O3'	4735:C	P	4.98
1	v	10:G	O3'	11:C	P	4.38
1	u	54:U	O3'	55:U	P	4.19
1	v	21:A	O3'	22:G	P	3.91
1	t	4817:G	O3'	4818:G	P	3.34
1	t	964:C	O3'	965:G	P	3.27
1	t	1938:U	O3'	1939:A	P	3.24
1	v	41:C	O3'	42:C	P	3.22

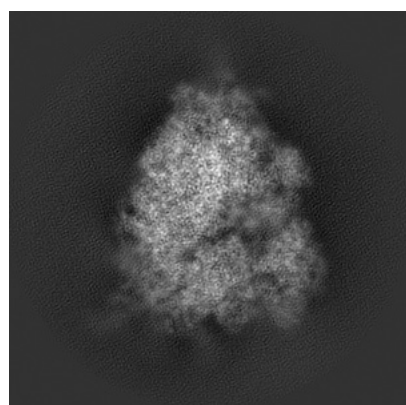
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0526. These allow visual inspection of the internal detail of the map and identification of artifacts.

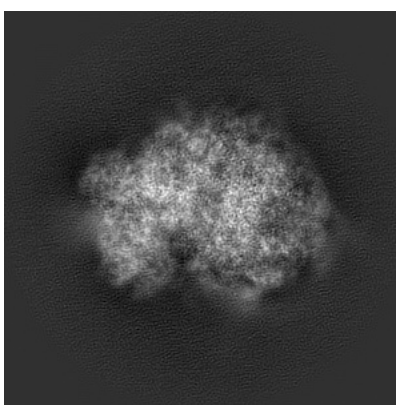
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

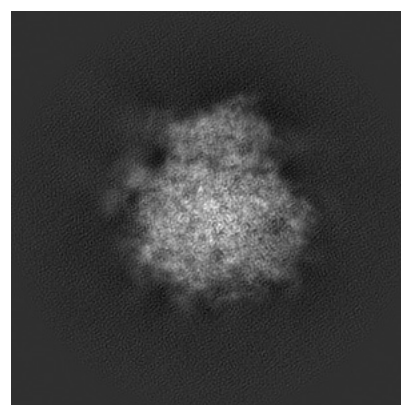
6.1.1 Primary map



X



Y

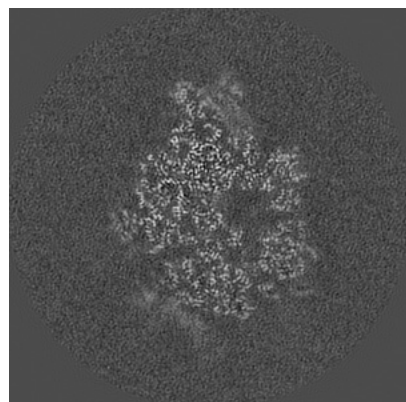


Z

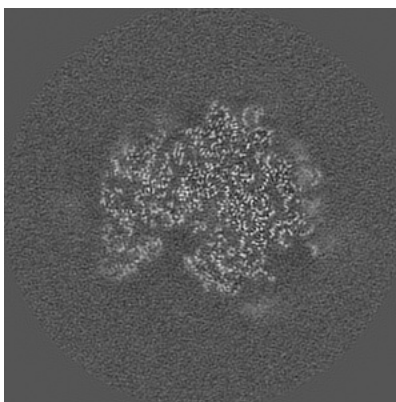
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

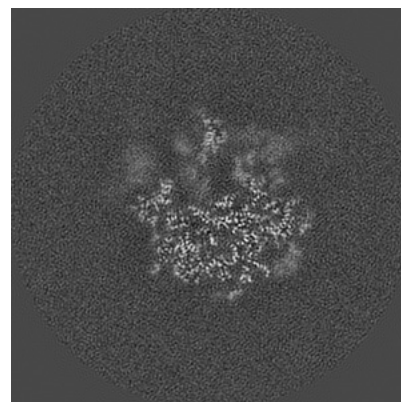
6.2.1 Primary map



X Index: 200



Y Index: 200

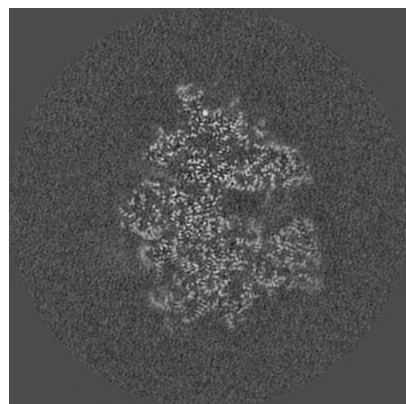


Z Index: 200

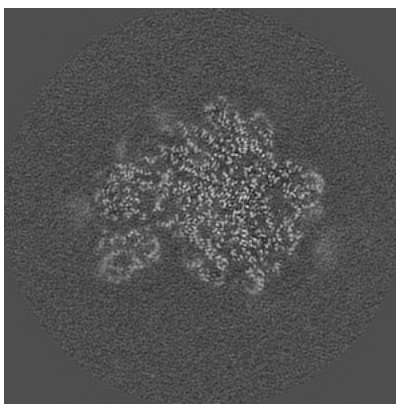
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

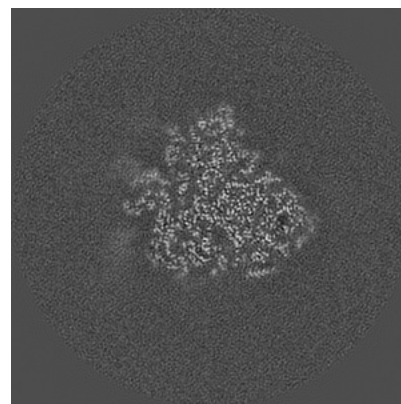
6.3.1 Primary map



X Index: 216



Y Index: 192

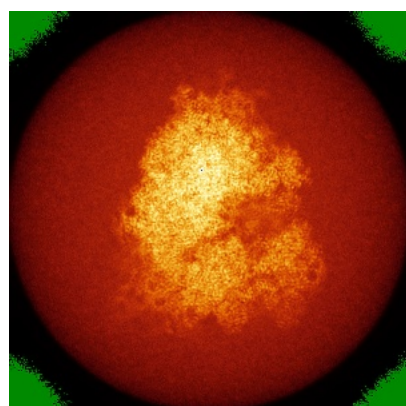


Z Index: 230

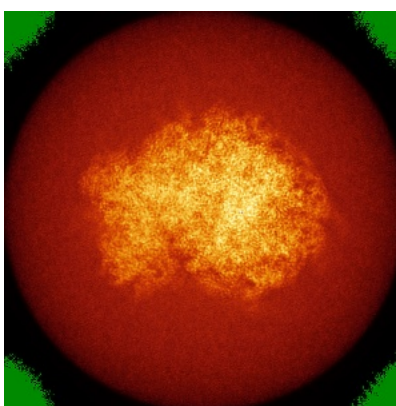
The images above show the largest variance slices of the map in three orthogonal directions.

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

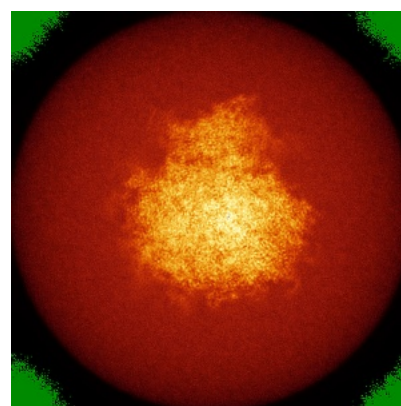
6.4.1 Primary map



X



Y

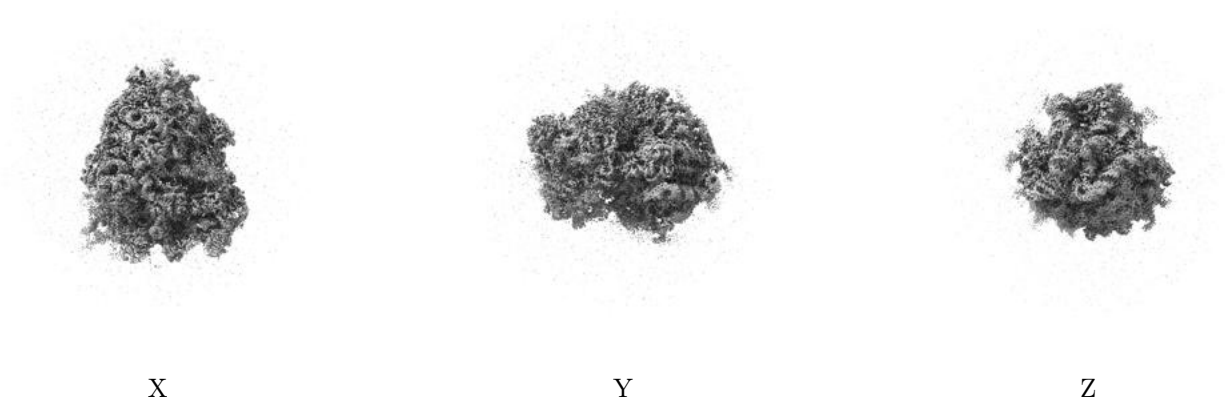


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

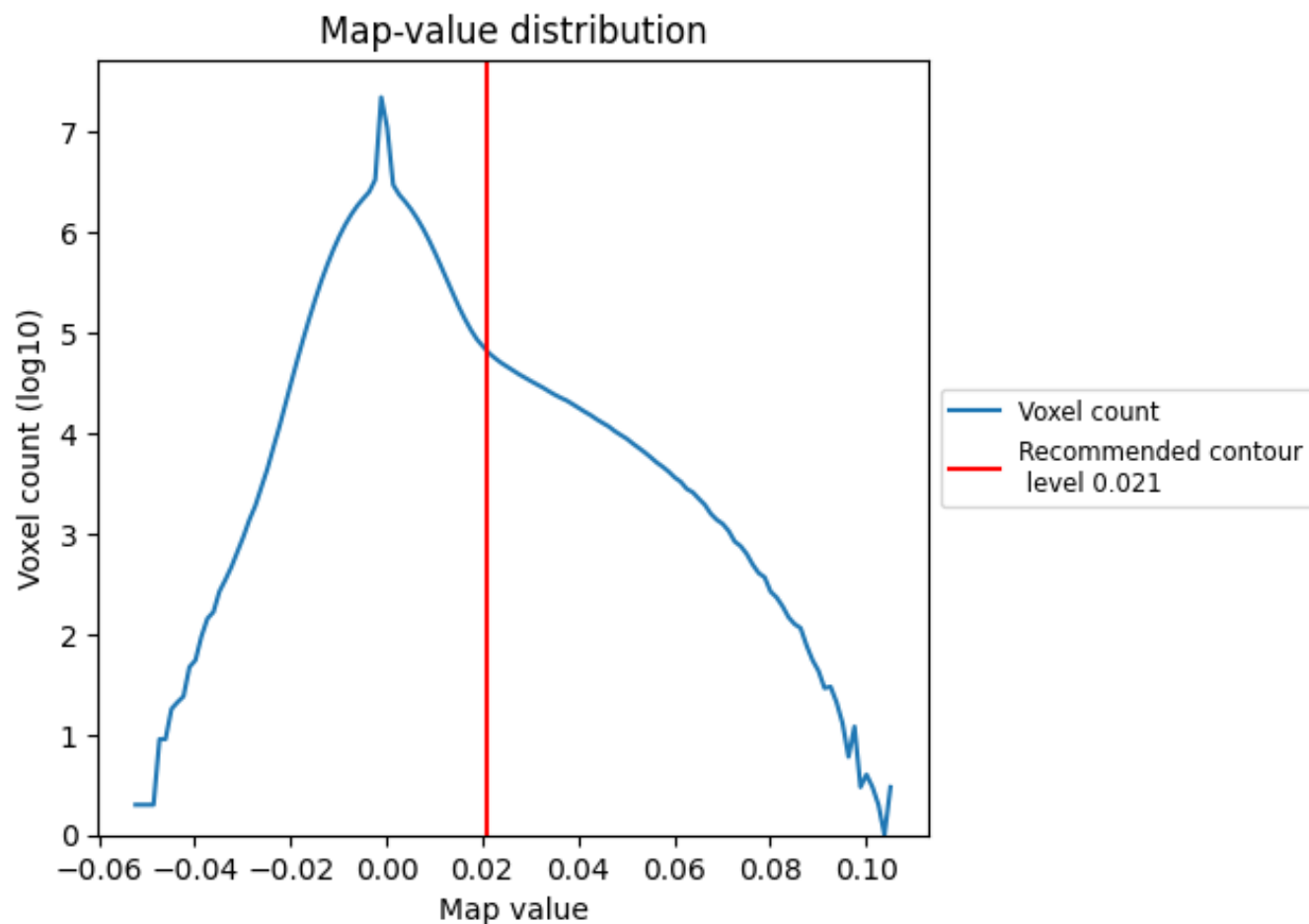
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

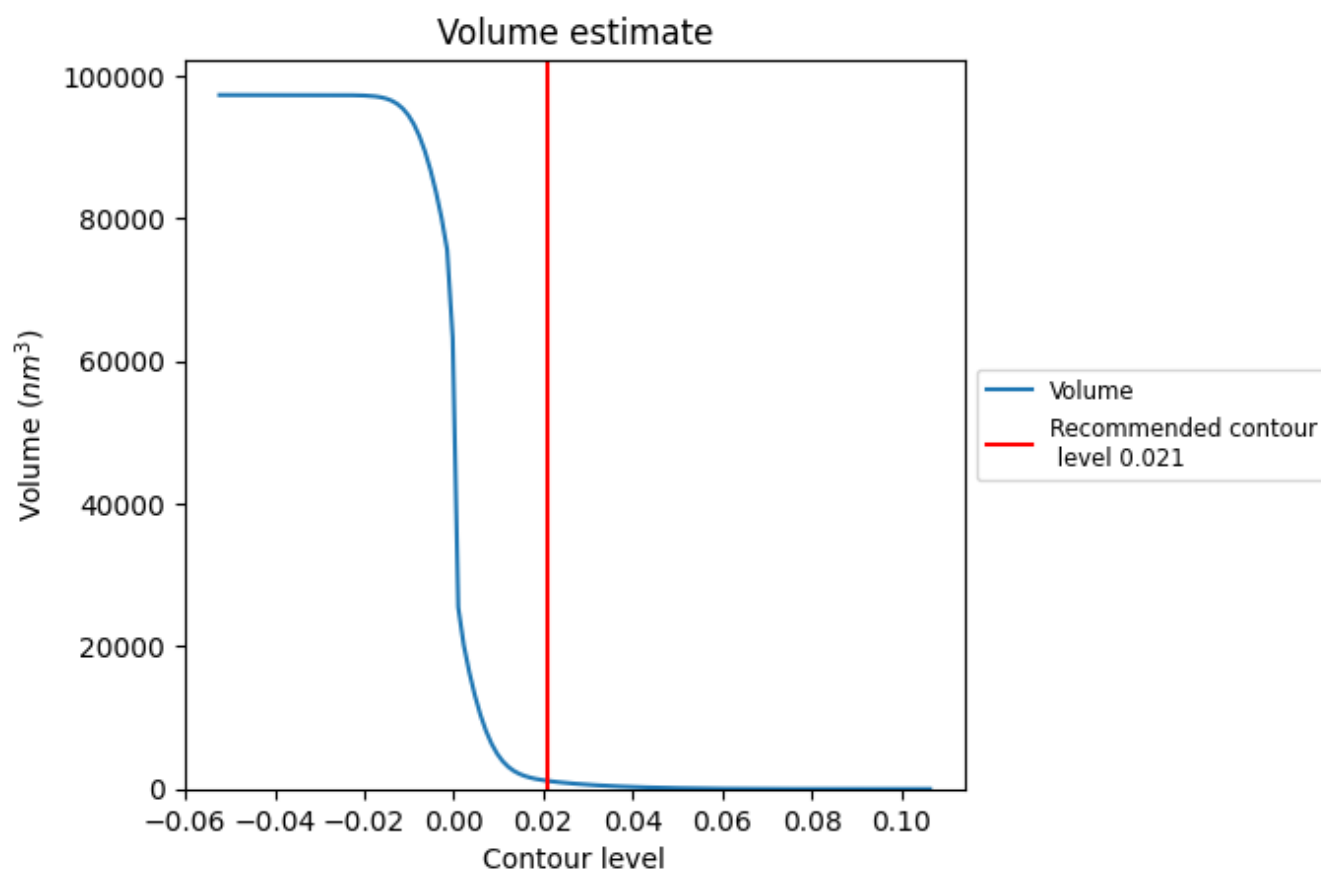
This section contains the results of statistical analysis of the map.

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.

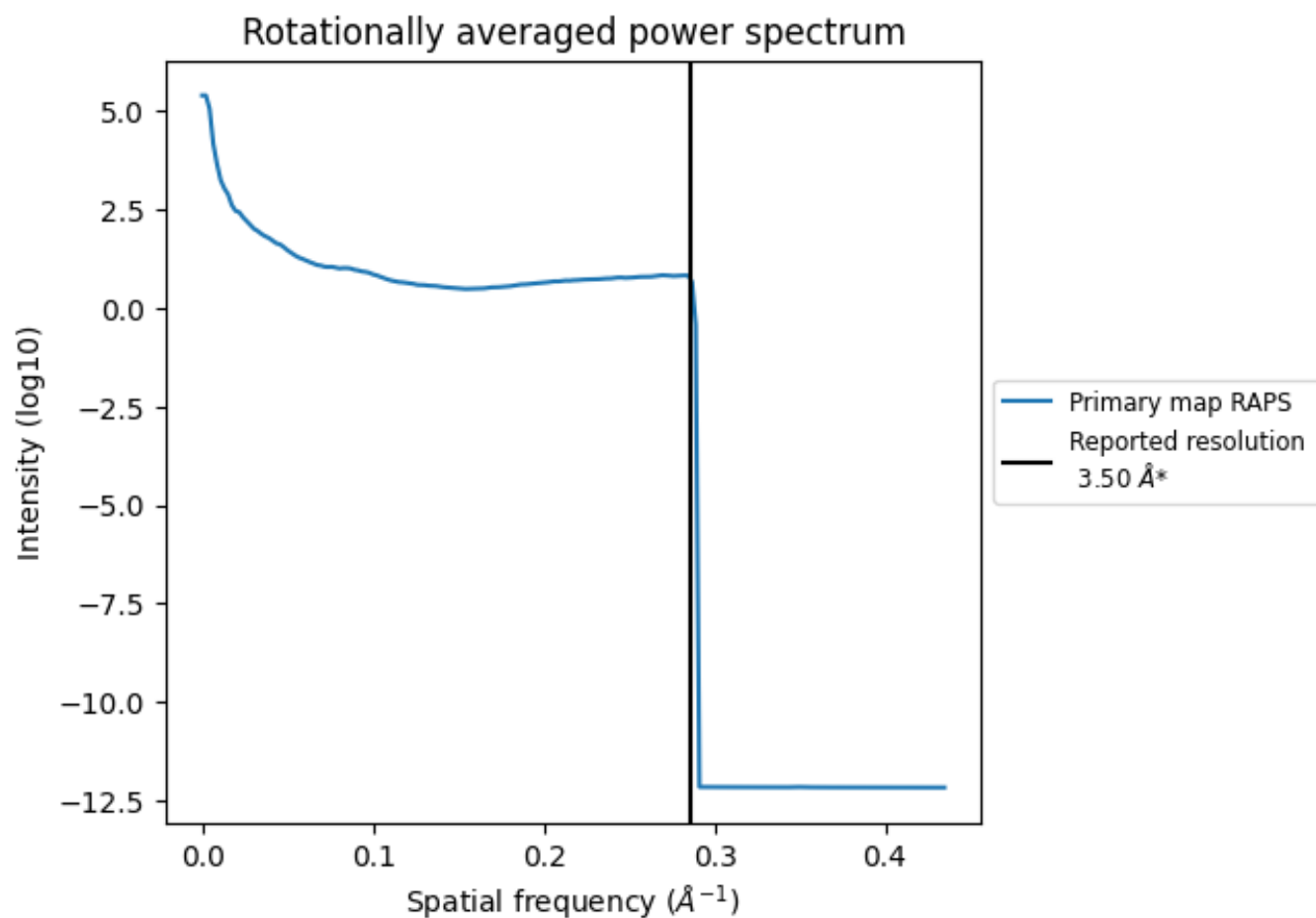
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm³; this corresponds to an approximate mass of 1022 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 ⓘ

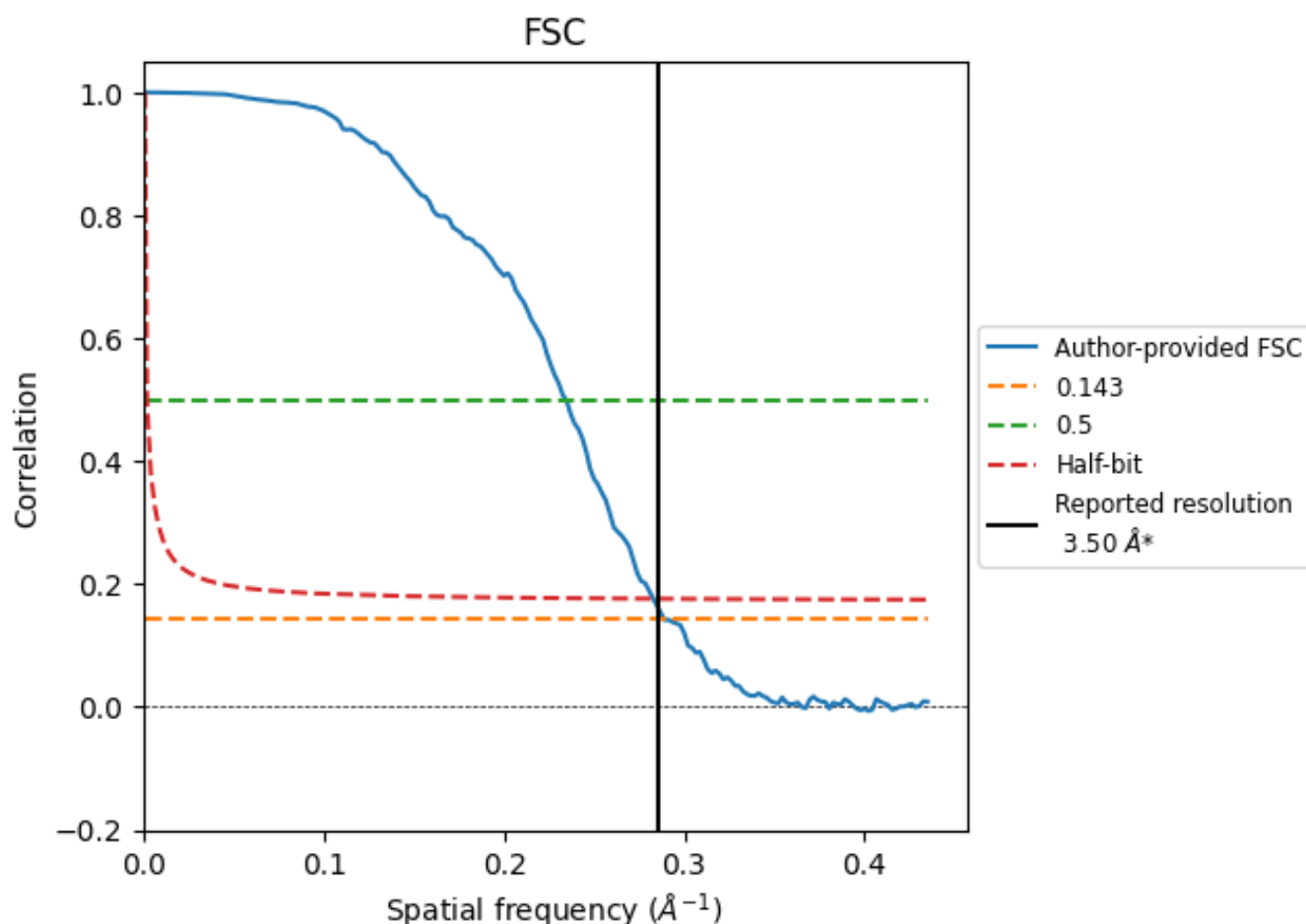


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

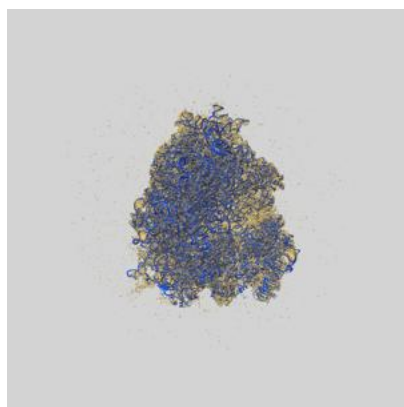
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	4.27	3.54
Unmasked-calculated*	-	-	-

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

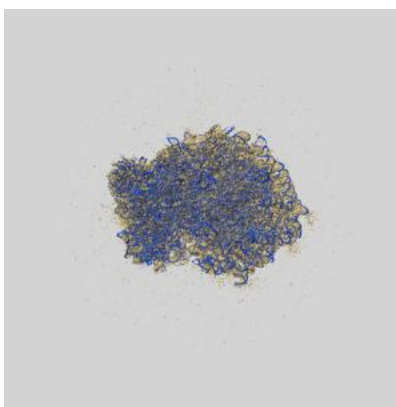
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0526 and PDB model 6OLI. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

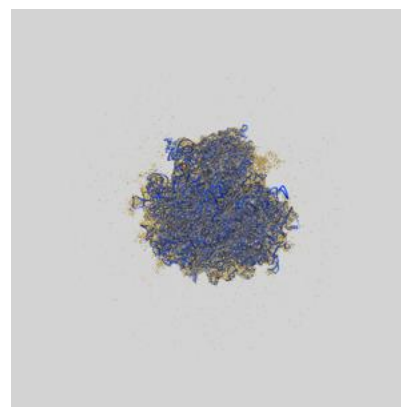
9.1 Map-model overlay [i](#)



X



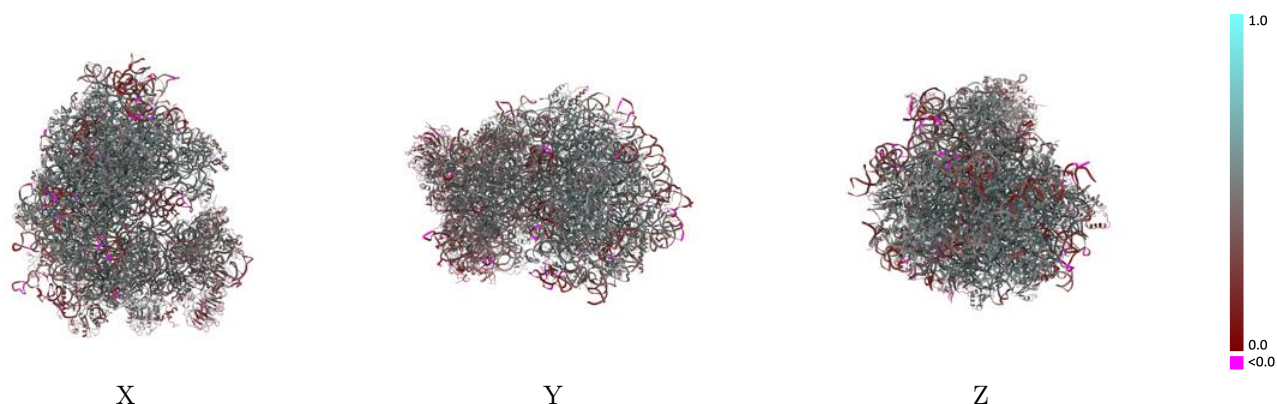
Y



Z

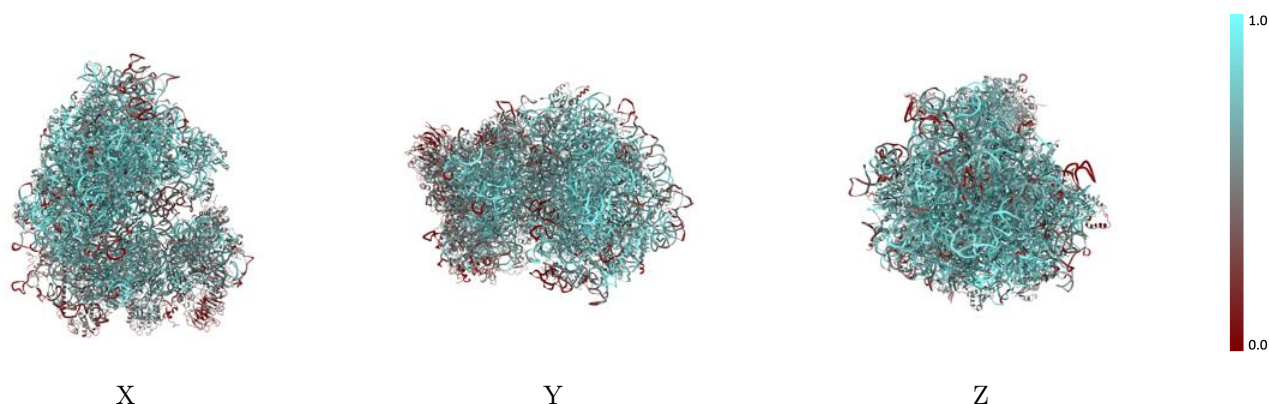
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



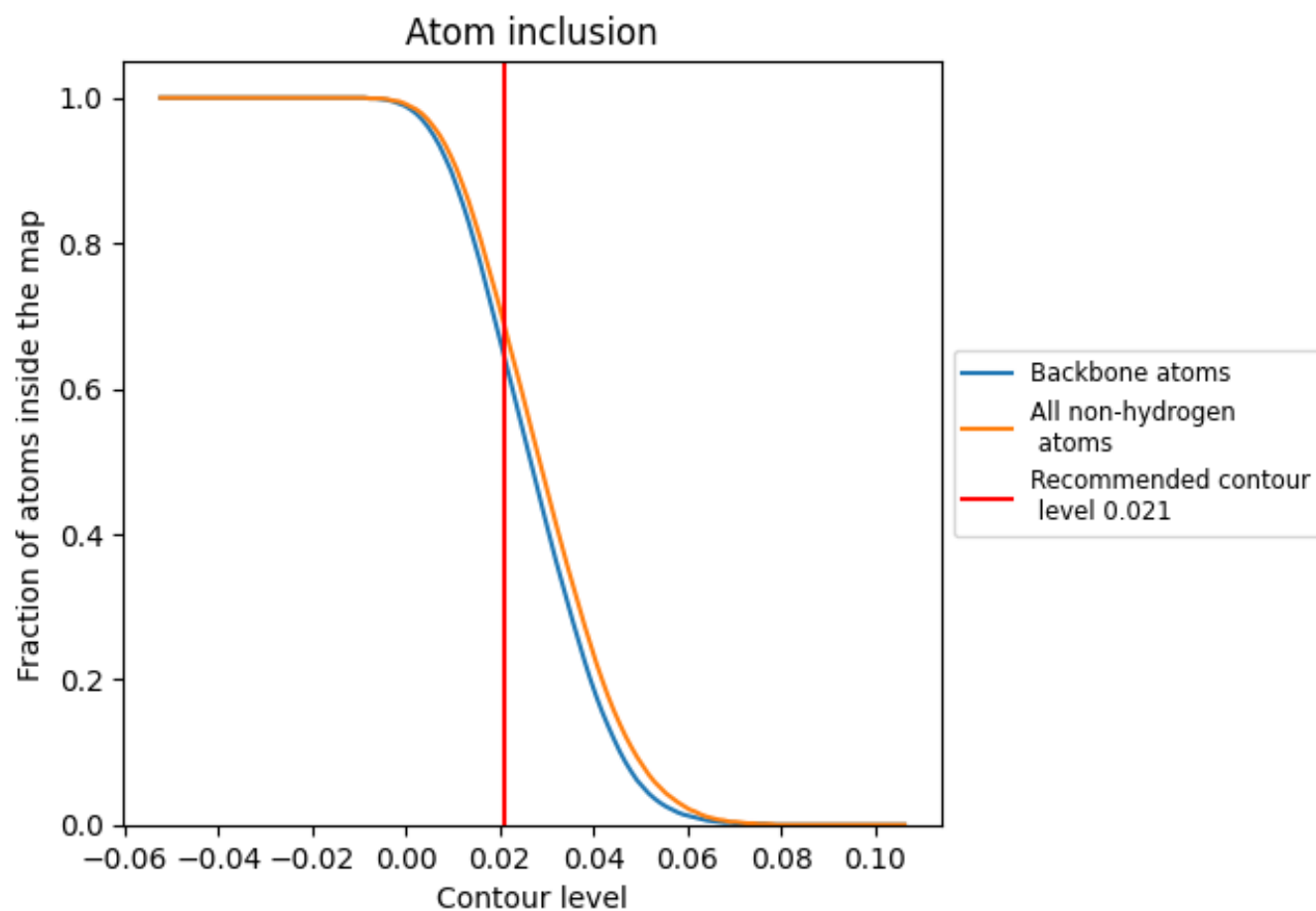
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 69% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.4460
A	 0.7050	 0.5190
B	 0.6990	 0.4940
C	 0.7380	 0.5140
D	 0.8160	 0.4720
E	 0.9000	 0.5080
F	 0.6510	 0.4550
G	 0.6160	 0.4300
H	 0.7230	 0.5050
I	 0.5910	 0.4390
J	 0.6140	 0.4570
K	 0.6690	 0.4830
L	 0.6210	 0.4500
M	 0.6650	 0.4670
N	 0.6720	 0.4870
O	 0.7600	 0.5300
P	 0.7080	 0.5010
Q	 0.7410	 0.5120
R	 0.7090	 0.5040
S	 0.6140	 0.4470
S2	 0.7340	 0.4290
SA	 0.4960	 0.4220
SB	 0.5460	 0.4450
SC	 0.5710	 0.4530
SD	 0.4250	 0.3930
SE	 0.4950	 0.4090
SF	 0.4650	 0.3900
SG	 0.3580	 0.3210
SH	 0.3740	 0.3560
SI	 0.4570	 0.3860
SJ	 0.5280	 0.3850
SK	 0.3960	 0.3550
SL	 0.5350	 0.4160
SM	 0.0890	 0.1970
SN	 0.5730	 0.4500



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Chain	Atom inclusion	Q-score
SO	 0.5630	 0.4530
SP	 0.5110	 0.4060
SQ	 0.4940	 0.4080
SR	 0.4050	 0.3720
SS	 0.5230	 0.3960
ST	 0.5300	 0.4170
SU	 0.3940	 0.3650
SV	 0.5250	 0.4280
SW	 0.6190	 0.4930
SX	 0.5890	 0.4600
SY	 0.4350	 0.3420
SZ	 0.4130	 0.3530
Sa	 0.6050	 0.4510
Sb	 0.4820	 0.4200
Sc	 0.3480	 0.3440
Sd	 0.6050	 0.4310
Se	 0.4530	 0.3850
Sf	 0.0810	 0.2030
Sg	 0.2720	 0.2970
T	 0.7280	 0.5090
U	 0.6790	 0.4890
V	 0.5590	 0.4190
W	 0.6740	 0.5070
X	 0.6970	 0.4850
Y	 0.6930	 0.5050
Z	 0.6960	 0.4900
a	 0.6450	 0.4660
b	 0.7440	 0.5230
c	 0.6150	 0.4490
d	 0.5820	 0.4390
e	 0.6950	 0.4720
f	 0.7520	 0.5240
g	 0.7540	 0.5210
h	 0.6810	 0.4820
i	 0.6800	 0.4830
j	 0.6500	 0.4650
k	 0.8050	 0.5360
l	 0.5460	 0.4340
m	 0.7230	 0.5010
n	 0.6930	 0.4800
o	 0.5640	 0.4820
p	 0.6660	 0.4870

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Chain	Atom inclusion	Q-score
q	 0.6820	 0.4990
r	 0.7620	 0.5120
t	 0.7940	 0.4590
u	 0.3360	 0.2860
v	 0.5480	 0.3300
w	 0.7650	 0.4830
y	 0.1290	 0.3260