



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 09:13 AM EDT

PDB ID : 6OLF / pdb_00006olf
EMDB ID : EMD-0599
Title : Human ribosome nascent chain complex (CDH1-RNC) stalled by a drug-like molecule with AA and PE tRNAs
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-16
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

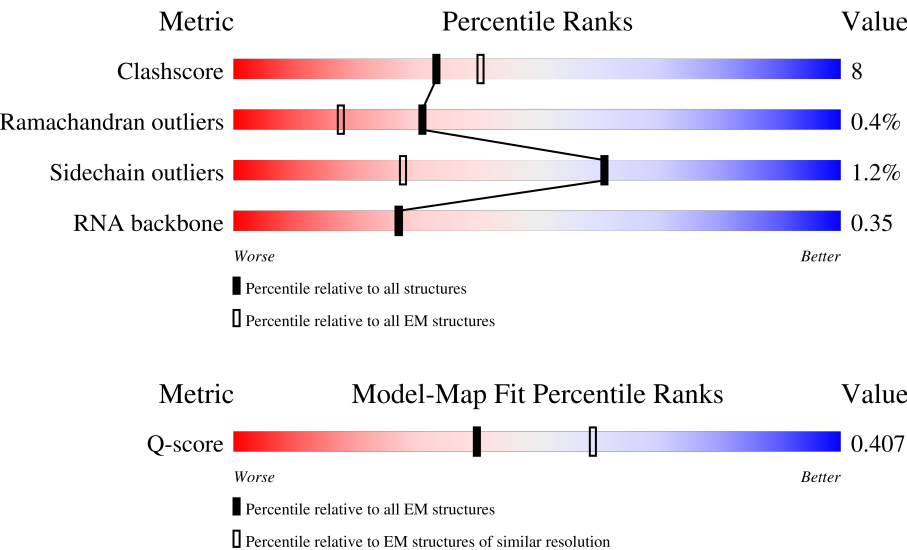
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	S2	1714	
2	SA	221	
3	SB	214	

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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	

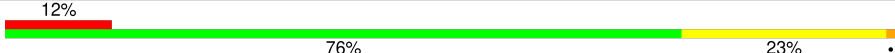
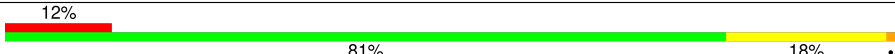
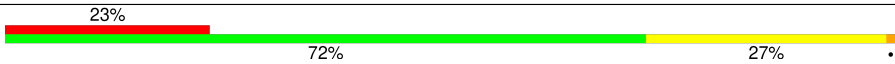
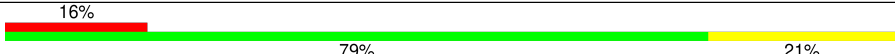
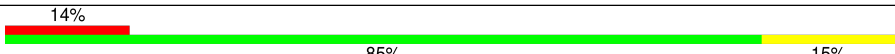
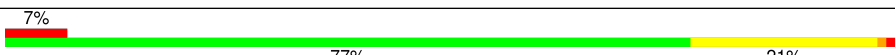
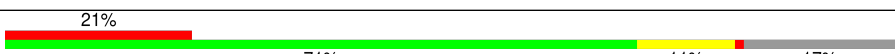
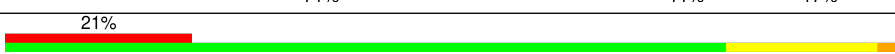
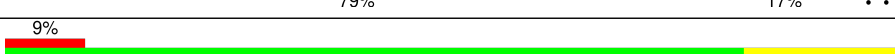
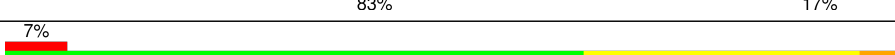
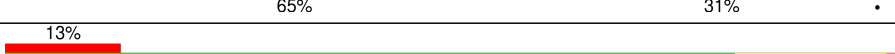
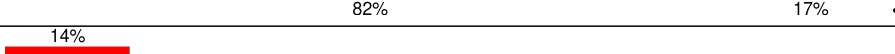
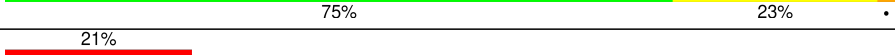
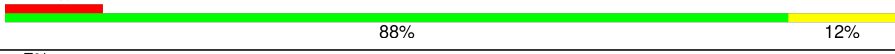
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Mol	Chain	Length	Quality of chain
29	SW	129	
30	SY	131	
31	SZ	73	
32	Sb	82	
33	Se	57	
34	Sf	67	
35	A	252	
36	B	397	
37	C	363	
38	D	157	
39	E	119	
40	F	294	
41	G	247	
42	H	225	
43	I	234	
44	J	191	
45	K	211	
46	L	169	
47	M	205	
48	N	139	
49	O	203	
50	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	121	
59	Y	117	
60	Z	134	
61	b	147	
62	c	121	
63	d	103	
64	e	106	
65	f	129	
66	g	109	
67	h	114	
68	i	122	
69	j	97	
70	k	84	
71	l	69	
72	m	50	
73	n	50	
74	o	25	
75	p	105	
76	q	91	
77	r	122	
78	t	3607	

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Mol	Chain	Length	Quality of chain
79	v	76	50% 39% 57%
80	w	10	10% 30% 60% 10%
81	y	39	95% 69% 28%
82	u	76	62% 36% 46% 17%
83	a	134	16% 81% 19%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215429 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	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- 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 L27a.

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

- Molecule 62 is a protein called 60S ribosomal protein L29.

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

- Molecule 63 is a protein called 60S ribosomal protein L30.

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

- Molecule 64 is a protein called 60S ribosomal protein L31.

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

- Molecule 65 is a protein called 60S ribosomal protein L32.

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

- Molecule 66 is a protein called 60S ribosomal protein L35a.

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

- Molecule 67 is a protein called 60S ribosomal protein L34.

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

- Molecule 68 is a protein called 60S ribosomal protein L35.

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

- Molecule 69 is a protein called 60S ribosomal protein L36.

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

- Molecule 70 is a protein called 60S ribosomal protein L37.

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

- Molecule 71 is a protein called 60S ribosomal protein L38.

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

- Molecule 72 is a protein called 60S ribosomal protein L39.

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

- Molecule 73 is a protein called 60S ribosomal protein L40.

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

- Molecule 74 is a protein called 60S ribosomal protein L41.

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

- Molecule 75 is a protein called 60S ribosomal protein L36a.

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

- Molecule 76 is a protein called 60S ribosomal protein L37a.

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

- Molecule 77 is a protein called 60S ribosomal protein L28.

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

- Molecule 78 is a RNA chain called 28S ribosomal RNA.

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

- Molecule 79 is a RNA chain called PE tRNA.

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

- Molecule 80 is a RNA chain called mRNA.

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

- Molecule 81 is a protein called Cadherin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	y	39	Total	C	N	O	0	0
			262	180	40	42		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	6	ALA	-	insertion	UNP P12830

- Molecule 82 is a RNA chain called AA tRNA.

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

- Molecule 83 is a protein called 60S ribosomal protein L27.

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

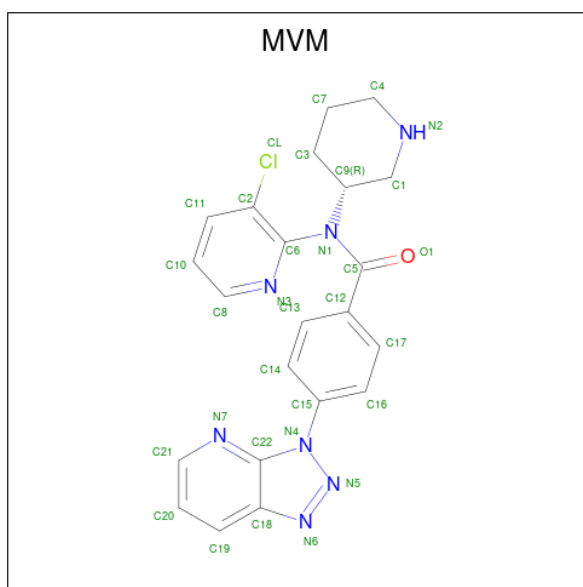
- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	S2	3	Total	Mg	0
			3	3	
85	D	6	Total	Mg	0
			6	6	
85	E	9	Total	Mg	0
			9	9	
85	b	2	Total	Mg	0
			2	2	
85	t	11	Total	Mg	0
			11	11	

- 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	C	Cl	N	O	0
			31	22	1	7	1	

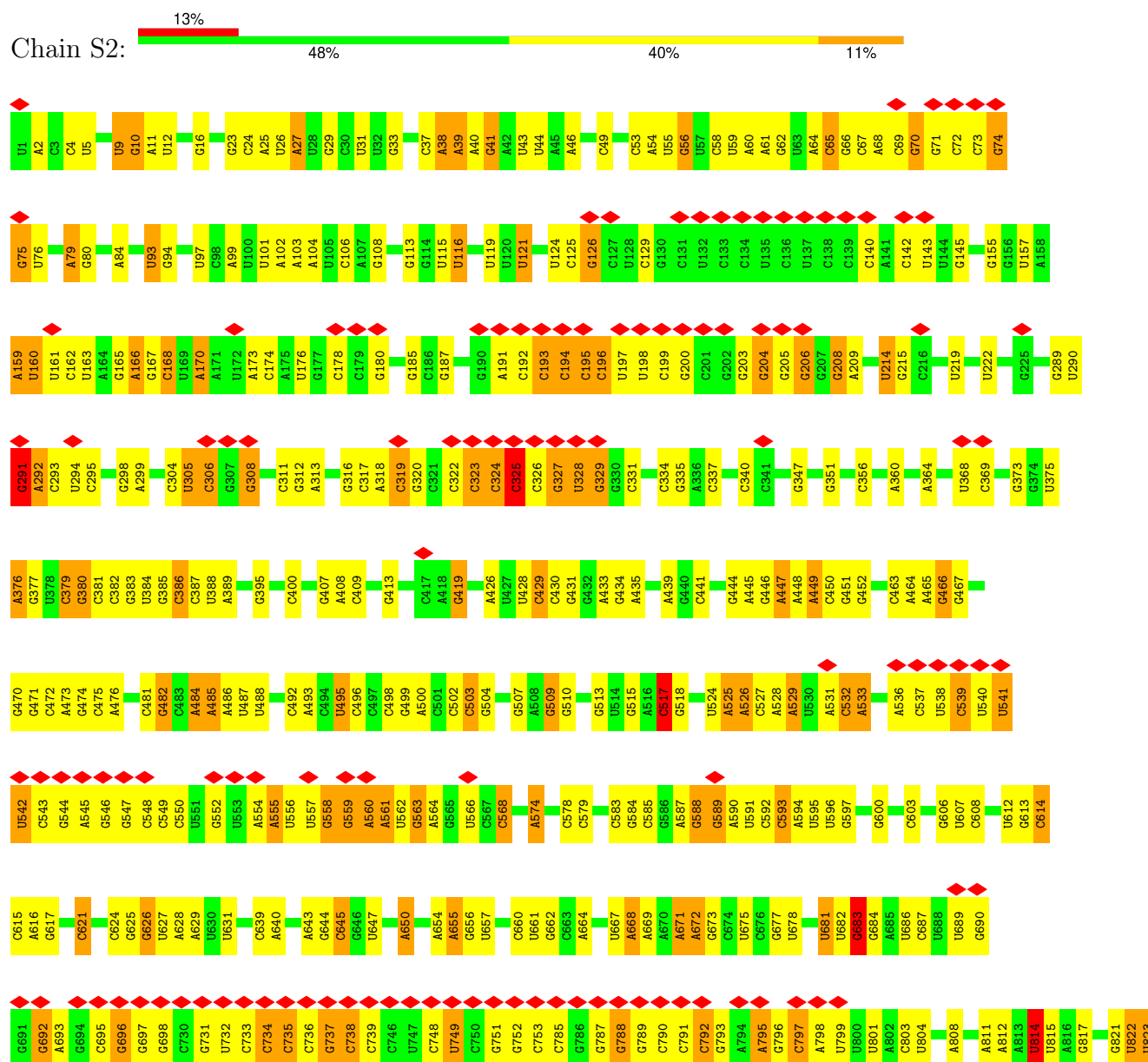
- Molecule 87 is water.

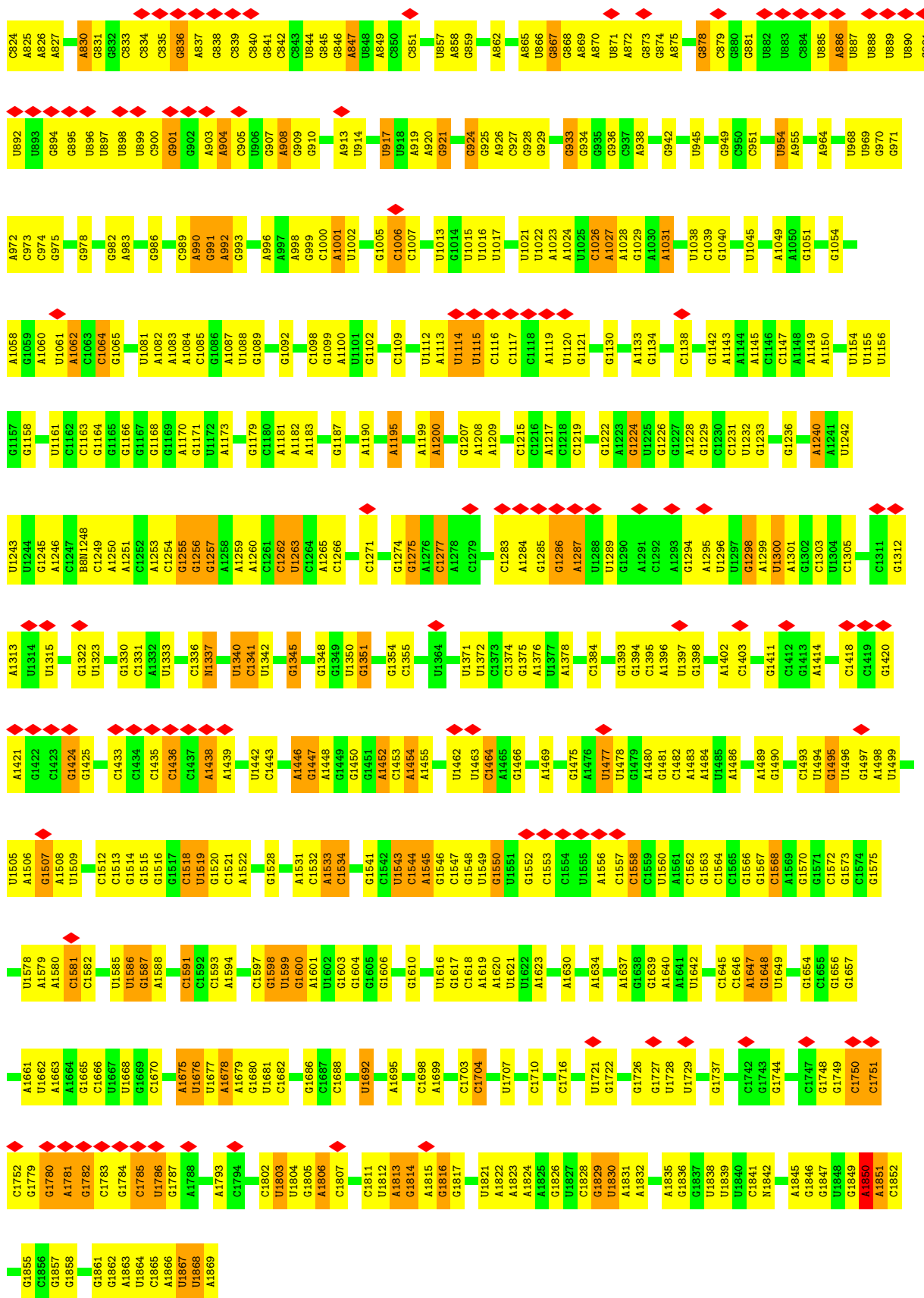
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total	O	0
			5	5	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SR	1	Total	O	0
			1	1	
87	SS	2	Total	O	0
			2	2	
87	SV	1	Total	O	0
			1	1	
87	SN	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

3 Residue-property plots

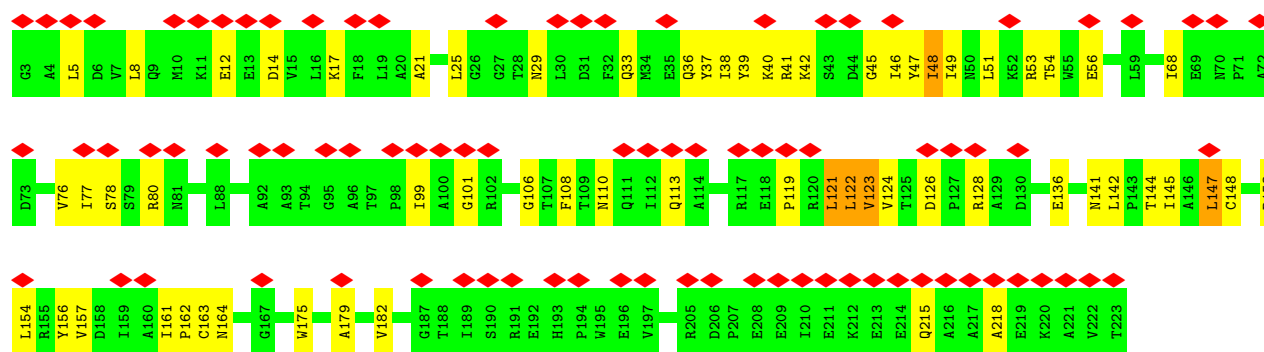
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



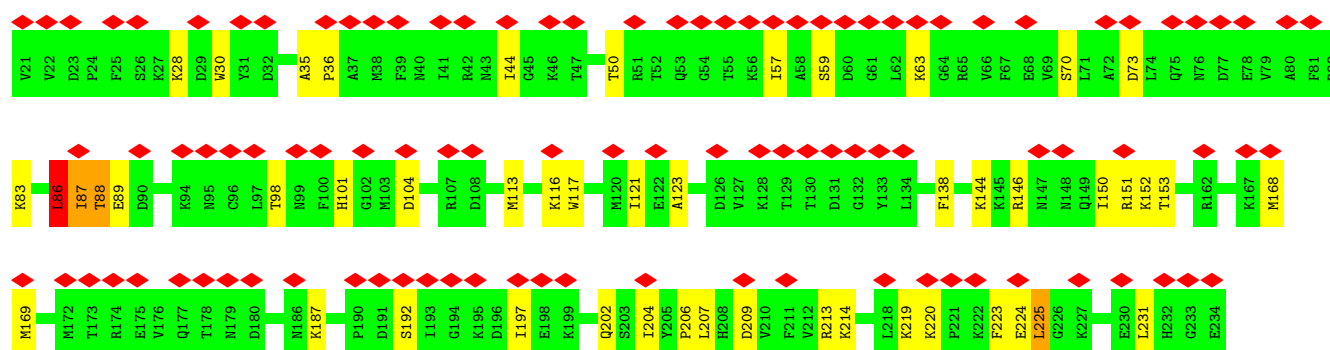


Chain SA: 



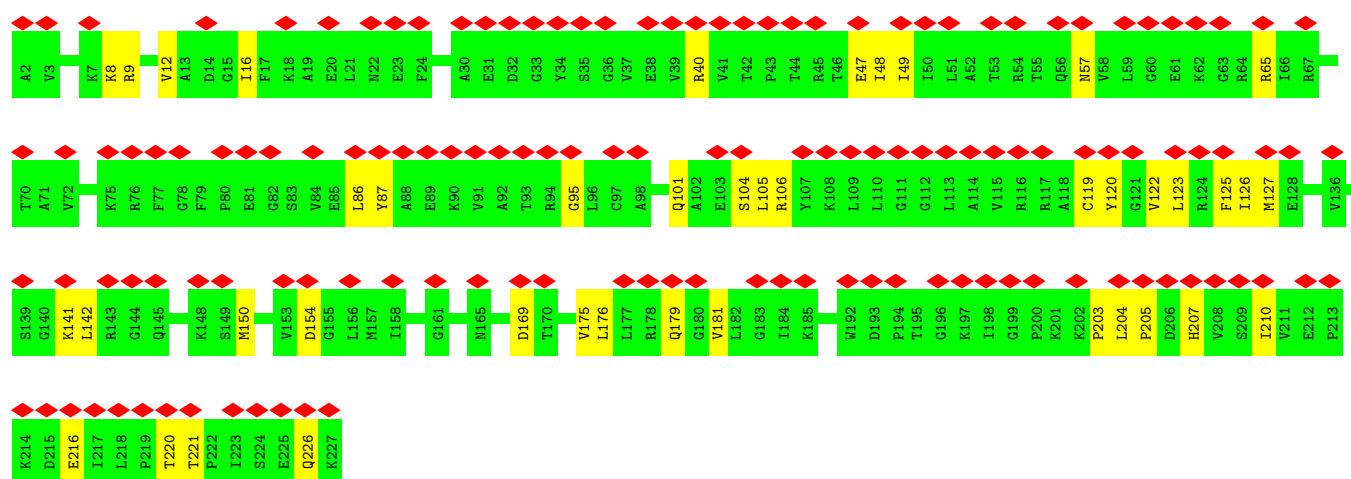
• Molecule 3: 40S ribosomal protein S3a

Chain SB: 



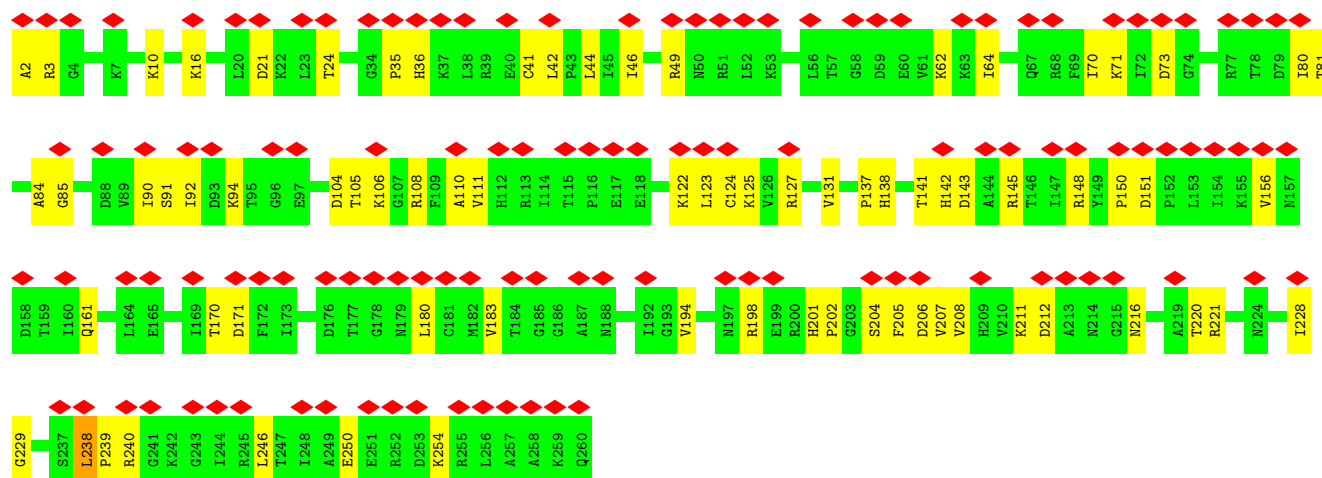
• Molecule 4: 40S ribosomal protein S3

Chain SD: 



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

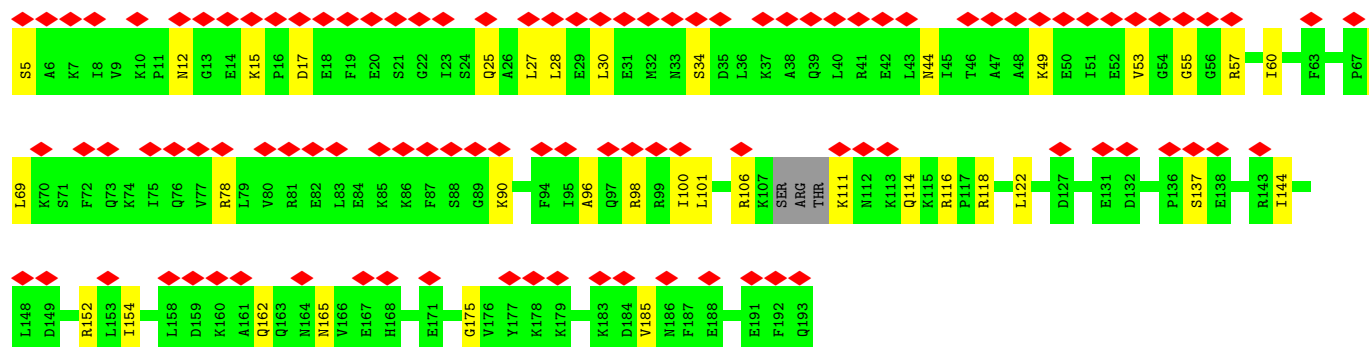
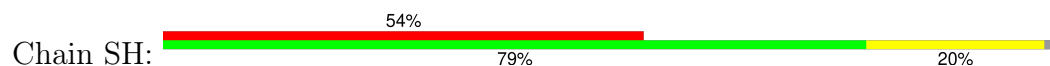
Chain SE: 



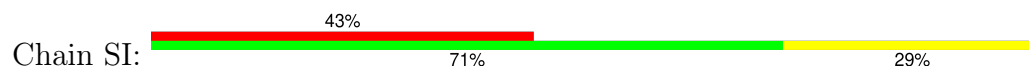
• Molecule 6: 40S ribosomal protein S5

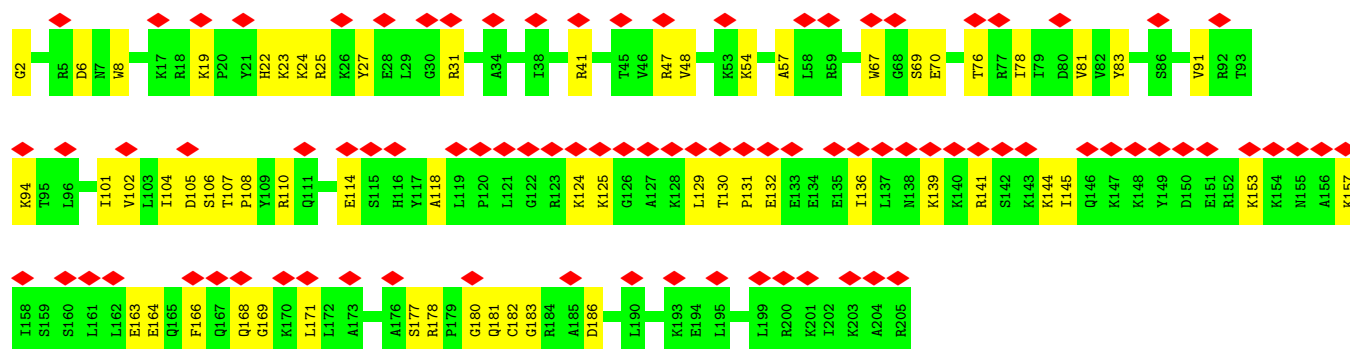


• Molecule 7: 40S ribosomal protein S7

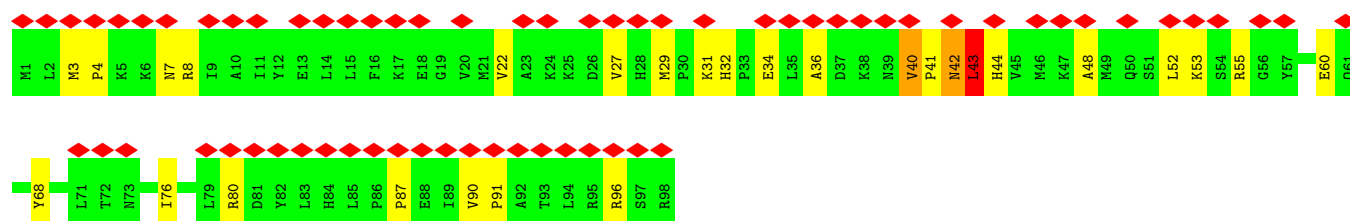
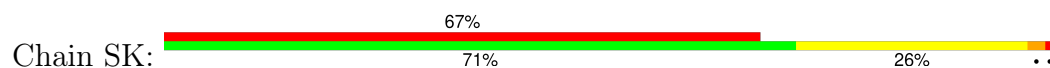


• Molecule 8: 40S ribosomal protein S8

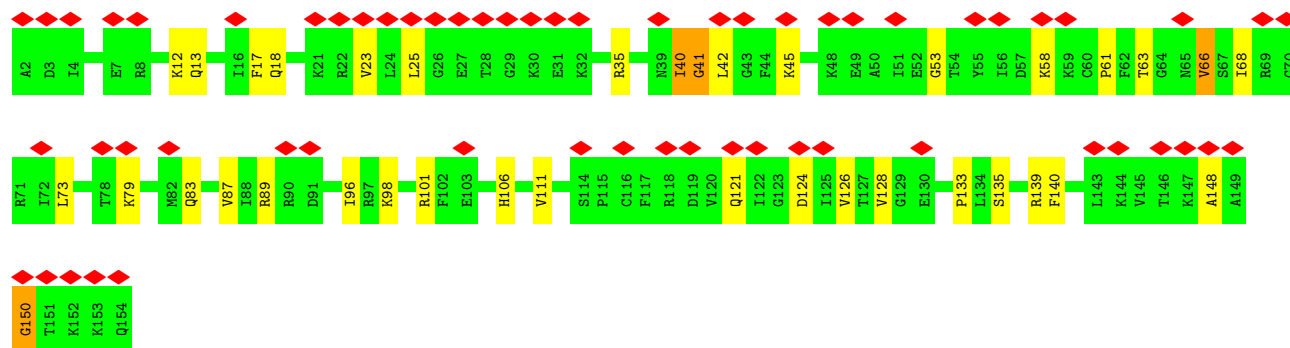
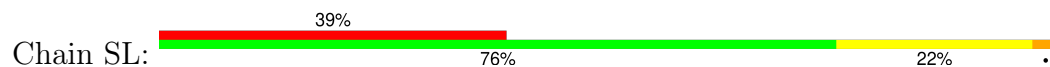




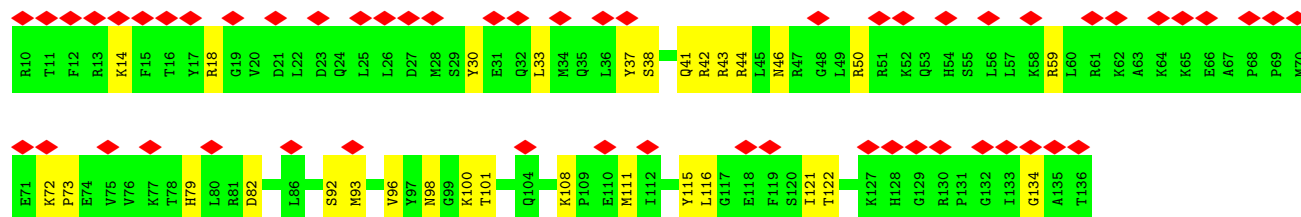
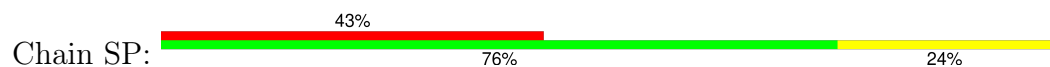
• Molecule 9: 40S ribosomal protein S10



• Molecule 10: 40S ribosomal protein S11

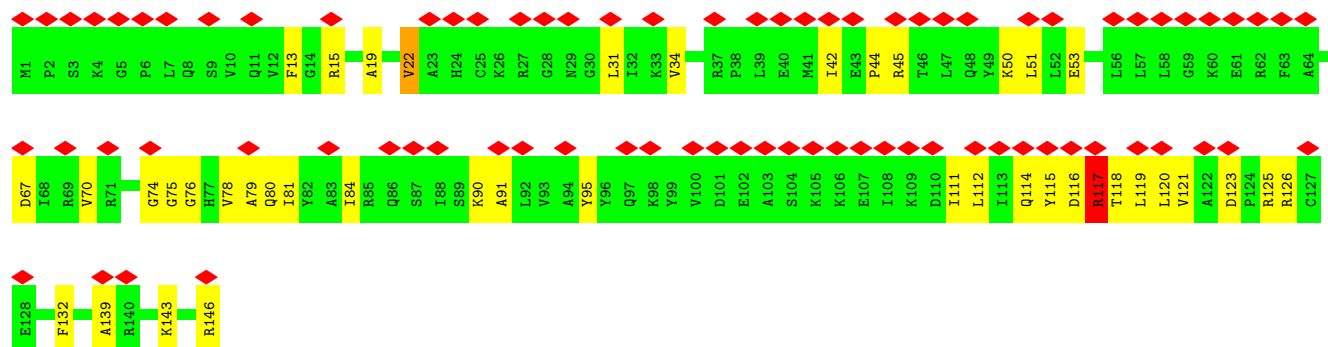


• Molecule 11: 40S ribosomal protein S15



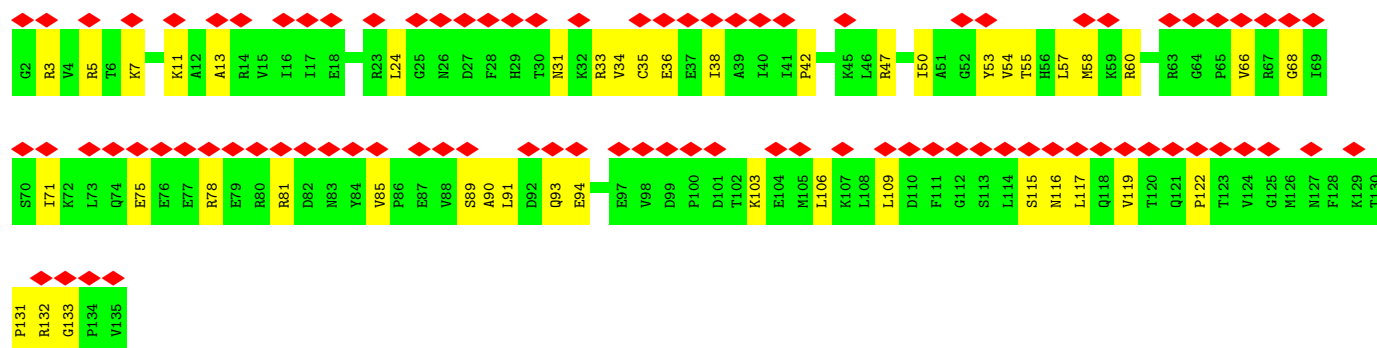
• Molecule 12: 40S ribosomal protein S16

Chain SQ: 



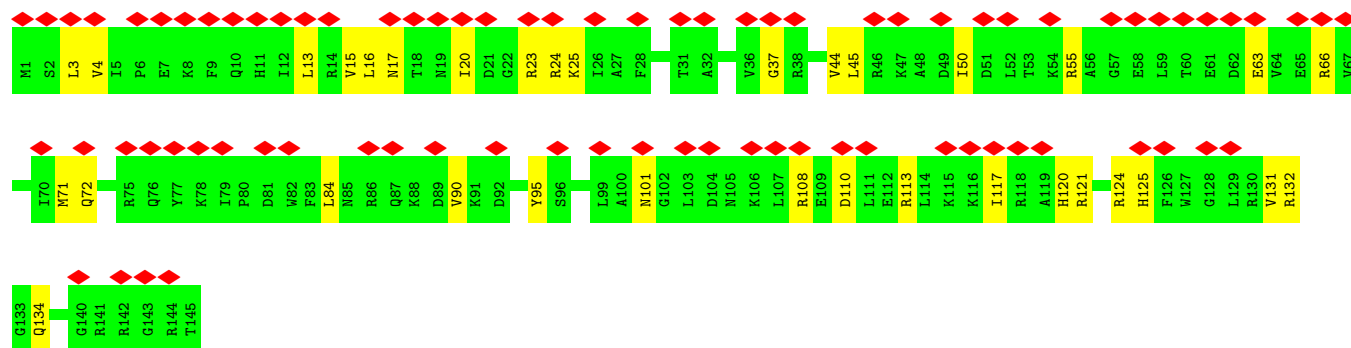
• Molecule 13: 40S ribosomal protein S17

Chain SR: 



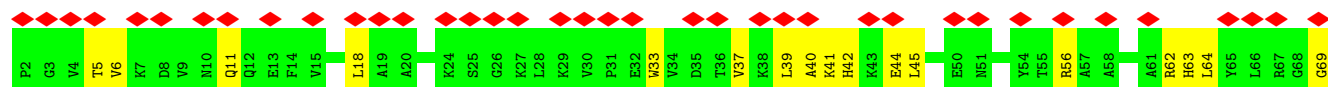
• Molecule 14: 40S ribosomal protein S18

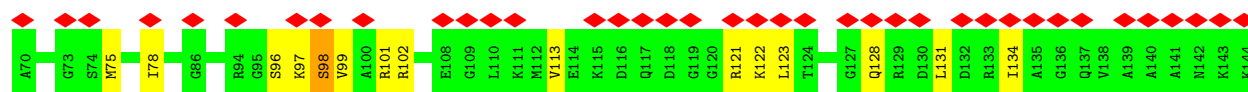
Chain SS: 



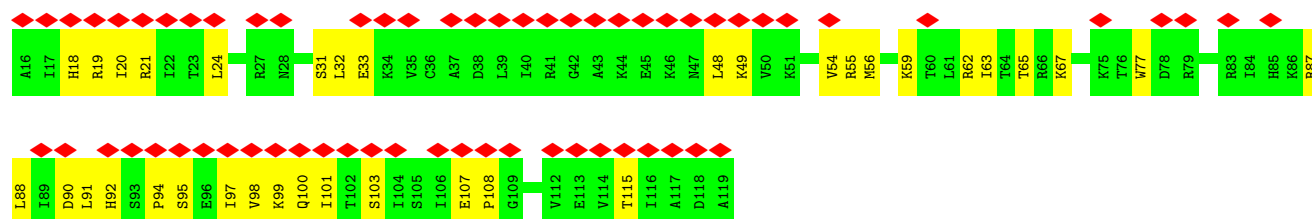
• Molecule 15: 40S ribosomal protein S19

Chain ST: 

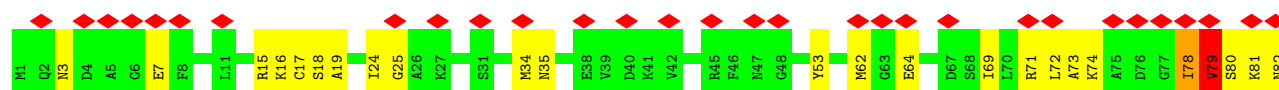
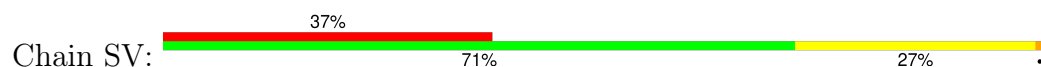




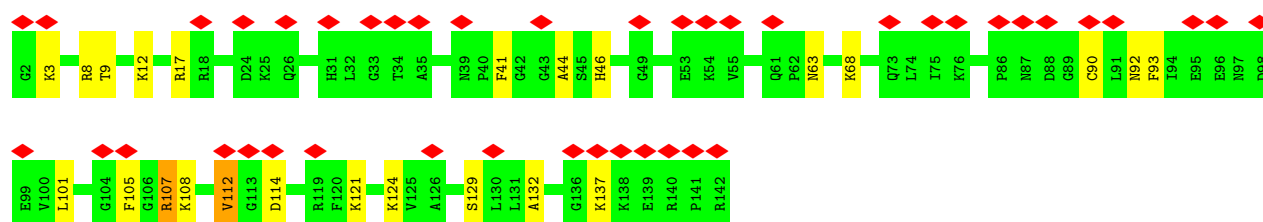
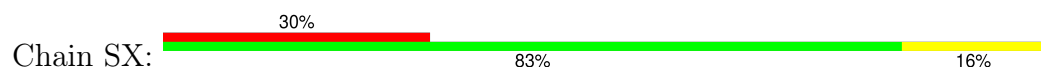
- Molecule 16: 40S ribosomal protein S20



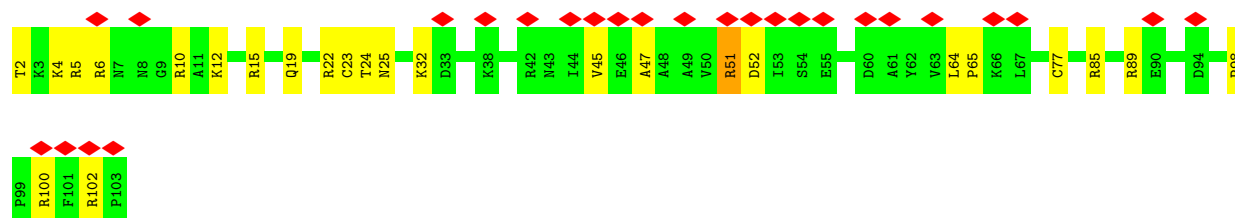
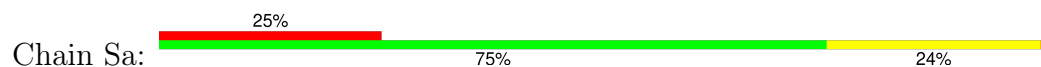
- Molecule 17: 40S ribosomal protein S21



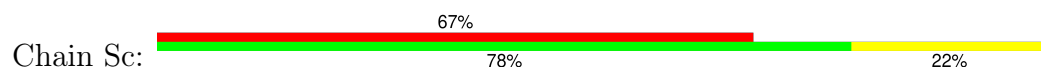
- Molecule 18: 40S ribosomal protein S23

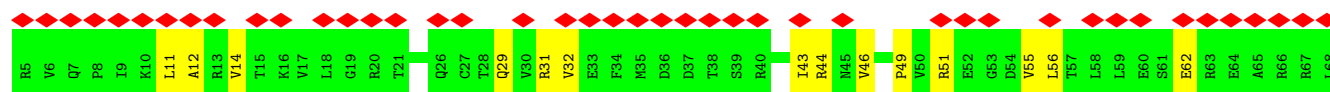


- Molecule 19: 40S ribosomal protein S26

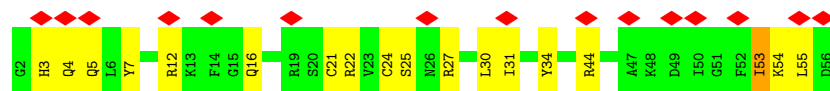


- Molecule 20: 40S ribosomal protein S28

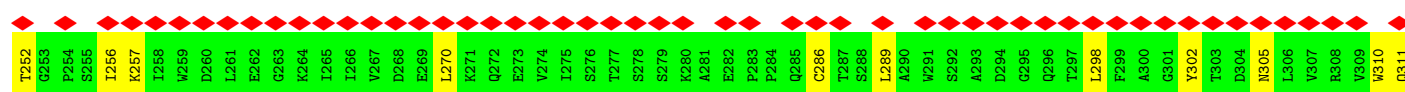
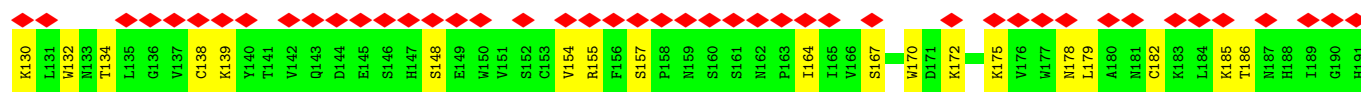
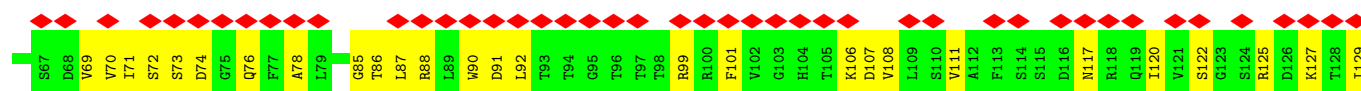
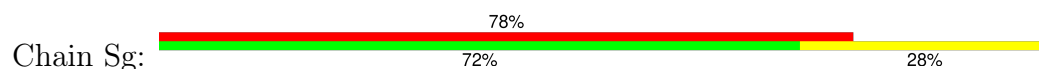




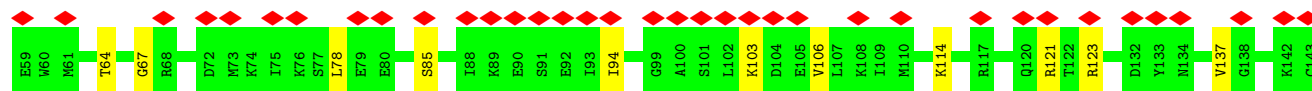
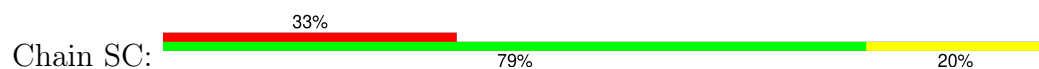
- Molecule 21: 40S ribosomal protein S29

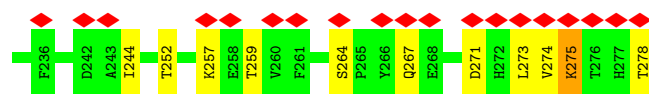


- Molecule 22: Receptor of activated protein C kinase 1

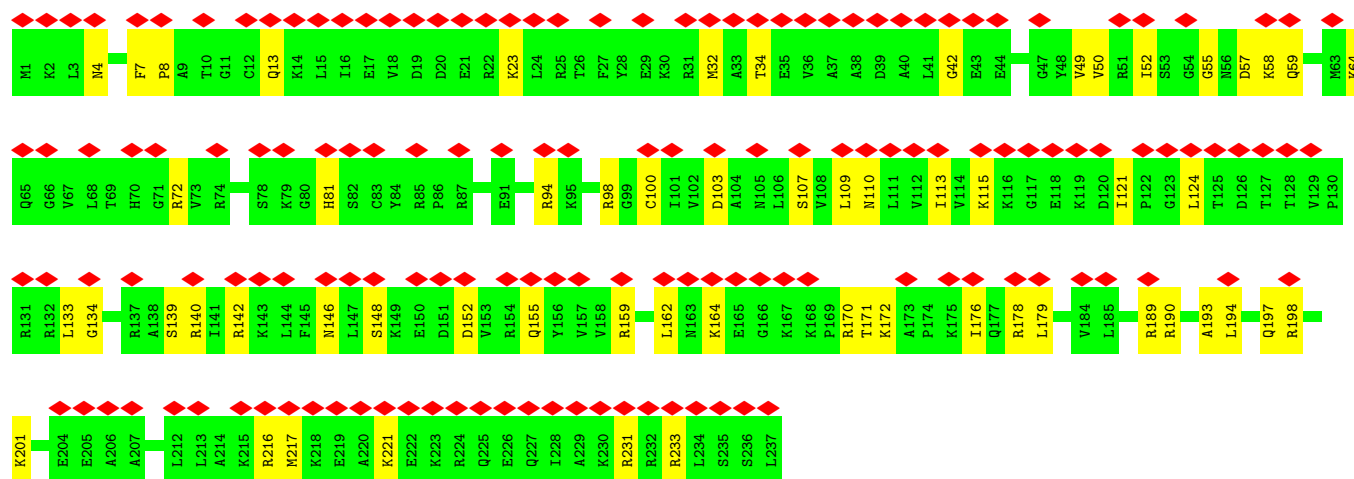
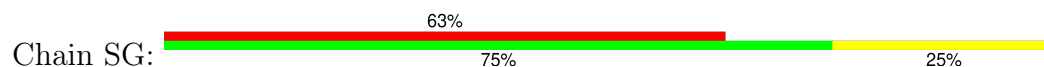


- Molecule 23: 40S ribosomal protein S2

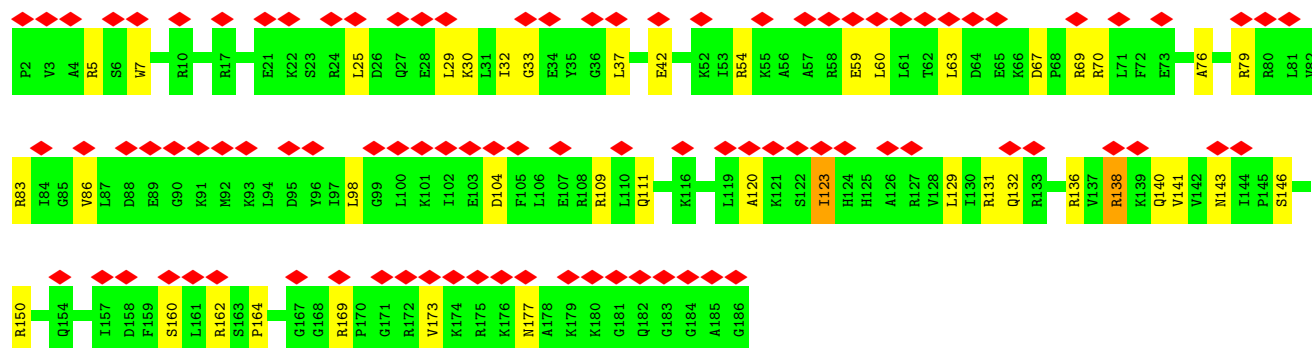
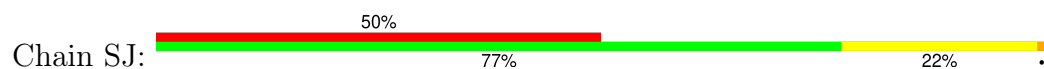




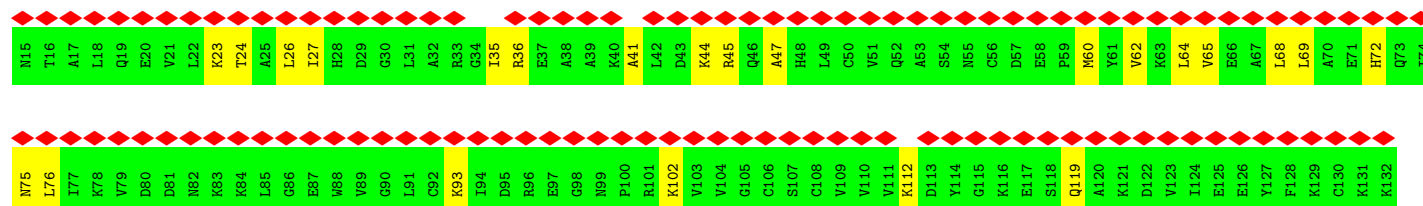
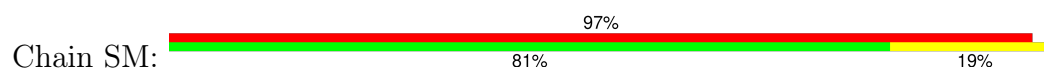
- Molecule 24: 40S ribosomal protein S6



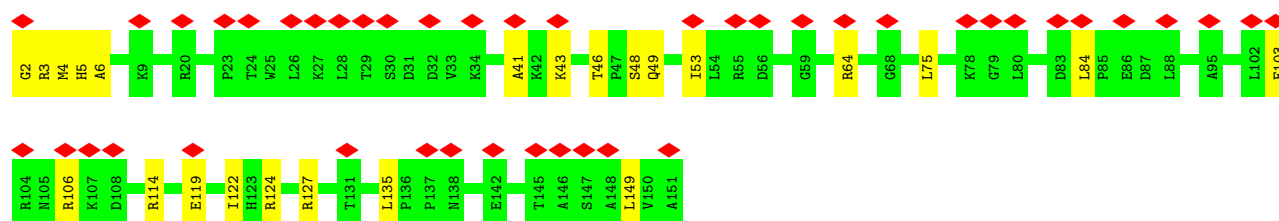
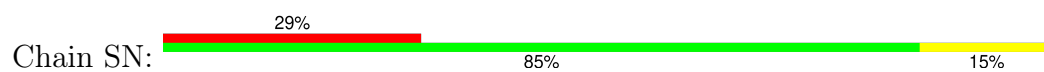
- Molecule 25: 40S ribosomal protein S9



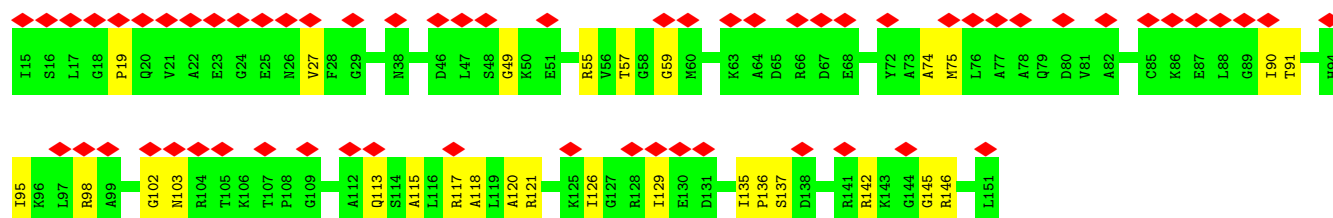
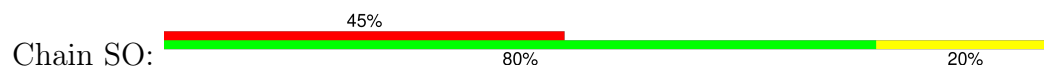
- Molecule 26: 40S ribosomal protein S12



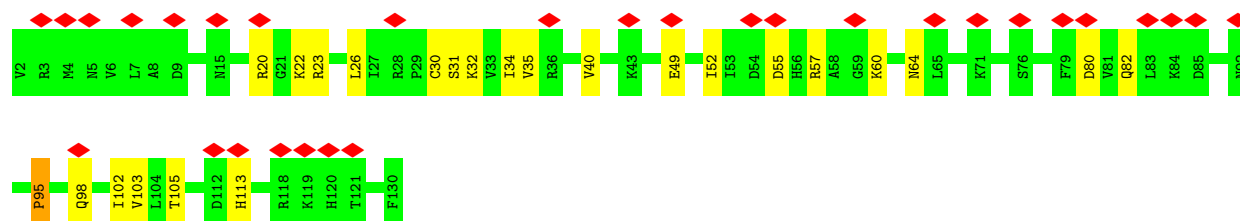
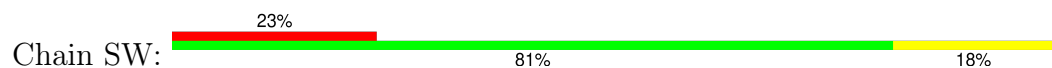
- Molecule 27: 40S ribosomal protein S13



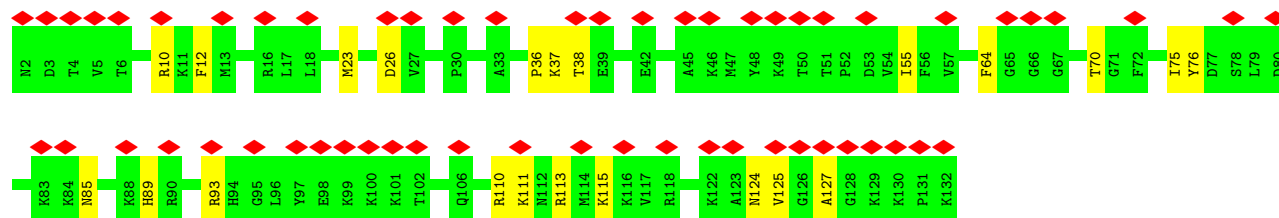
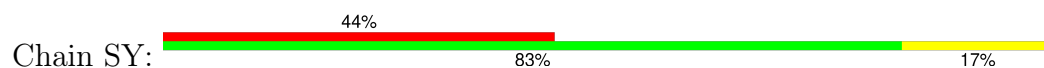
• Molecule 28: 40S ribosomal protein S14



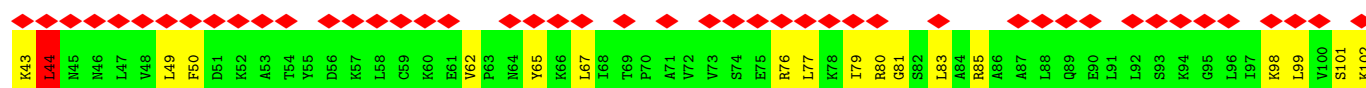
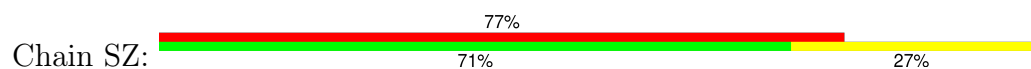
• Molecule 29: 40S ribosomal protein S15a

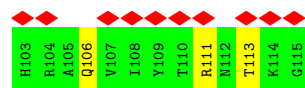


• Molecule 30: 40S ribosomal protein S24

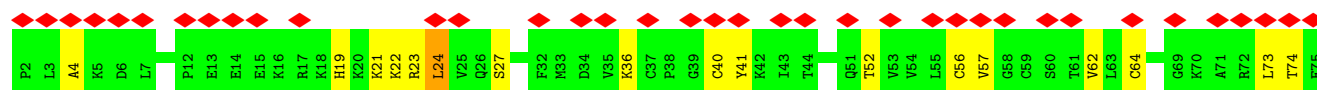
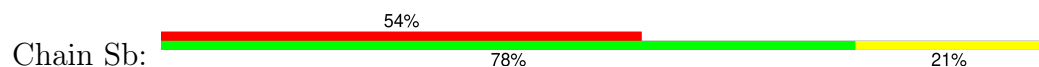


• Molecule 31: 40S ribosomal protein S25

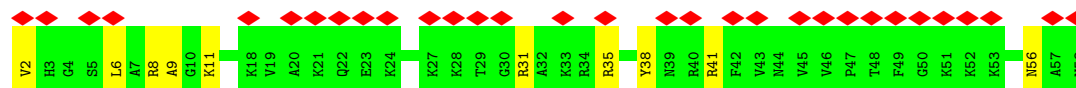
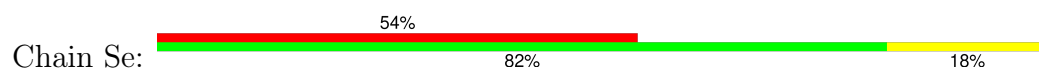




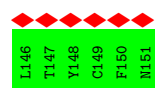
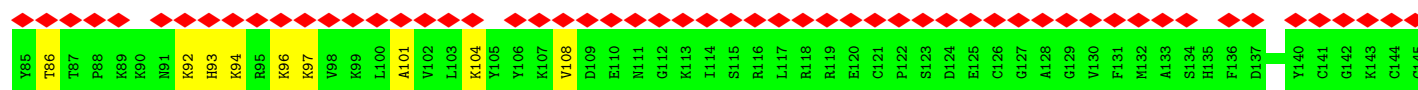
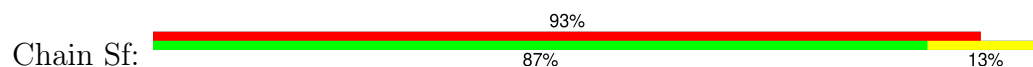
- Molecule 32: 40S ribosomal protein S27



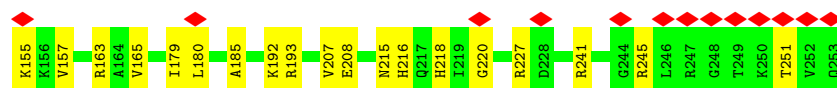
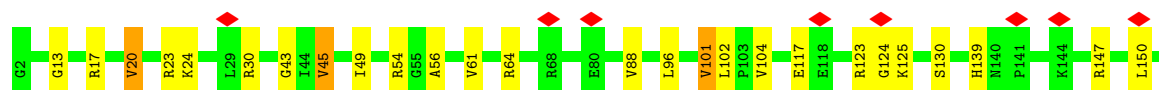
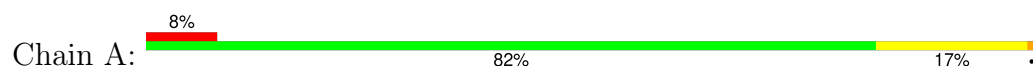
- Molecule 33: 40S ribosomal protein S30



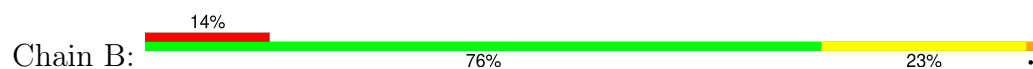
- Molecule 34: 40S ribosomal protein S27a

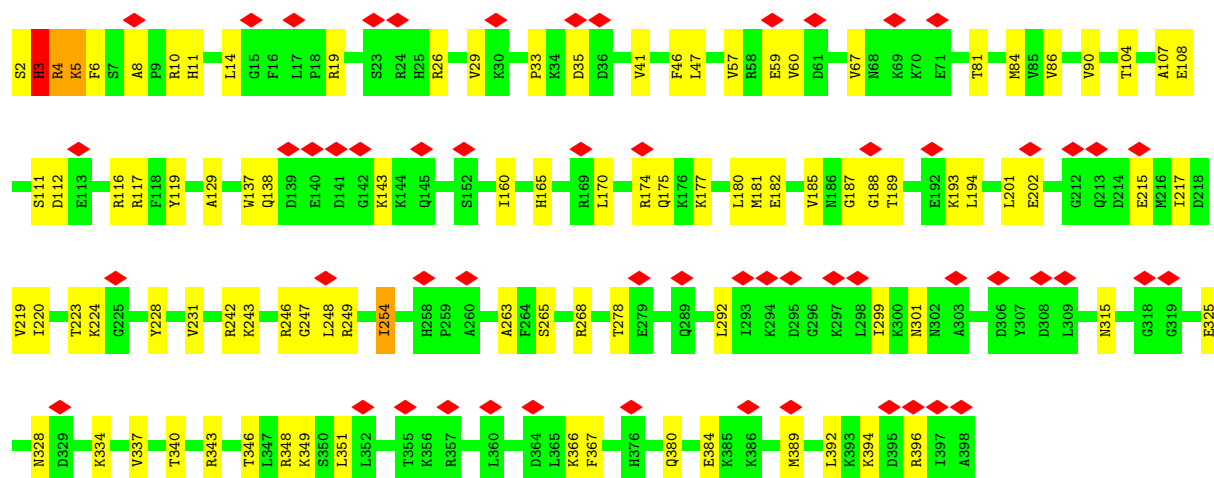


- Molecule 35: 60S ribosomal protein L8

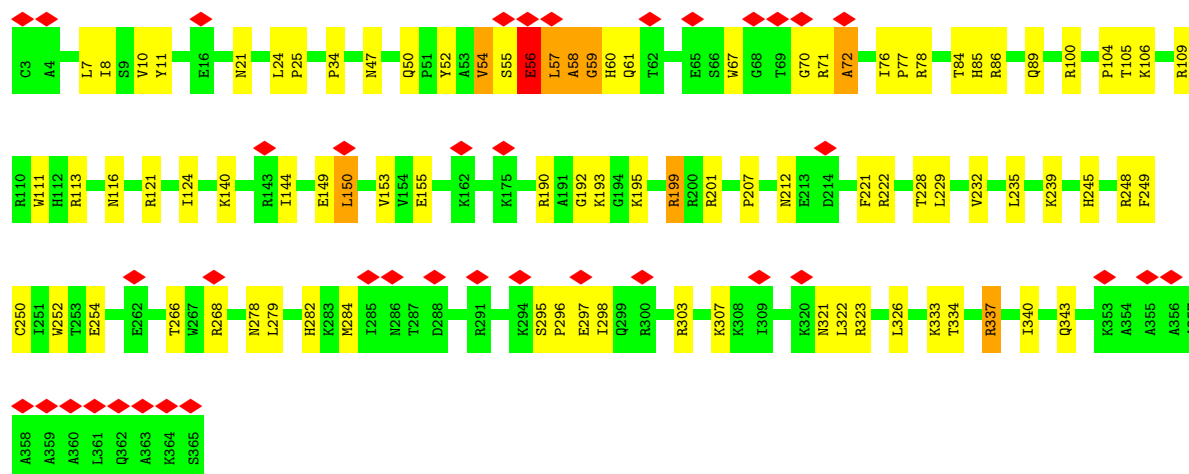
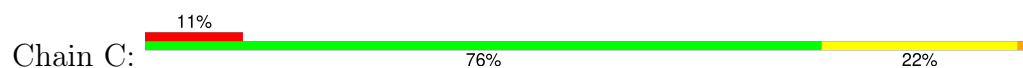


- Molecule 36: 60S ribosomal protein L3

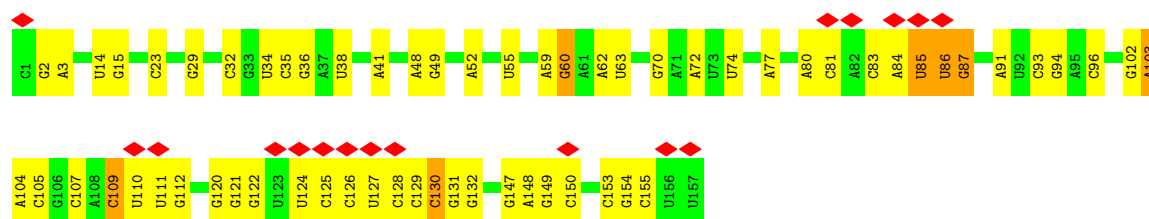




• Molecule 37: 60S ribosomal protein L4



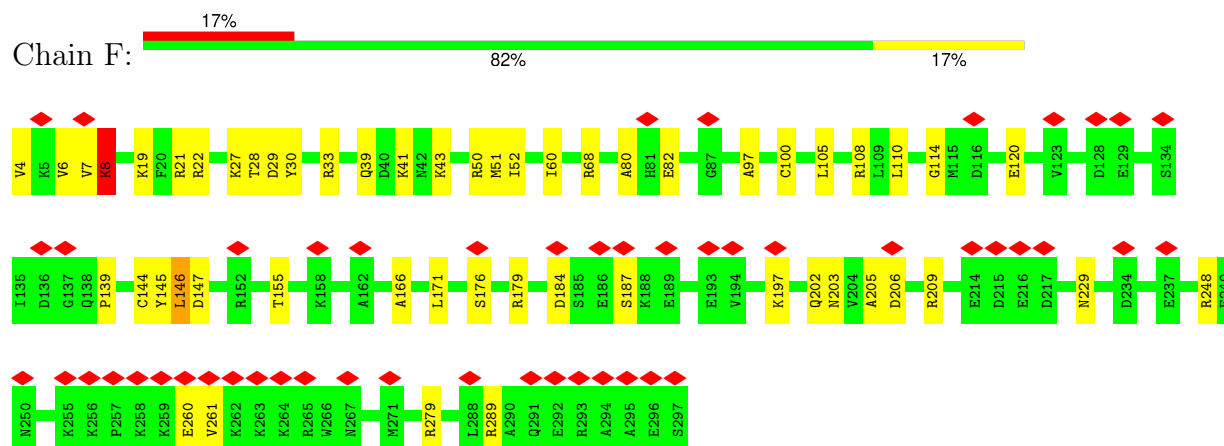
• Molecule 38: 5.8S ribosomal RNA



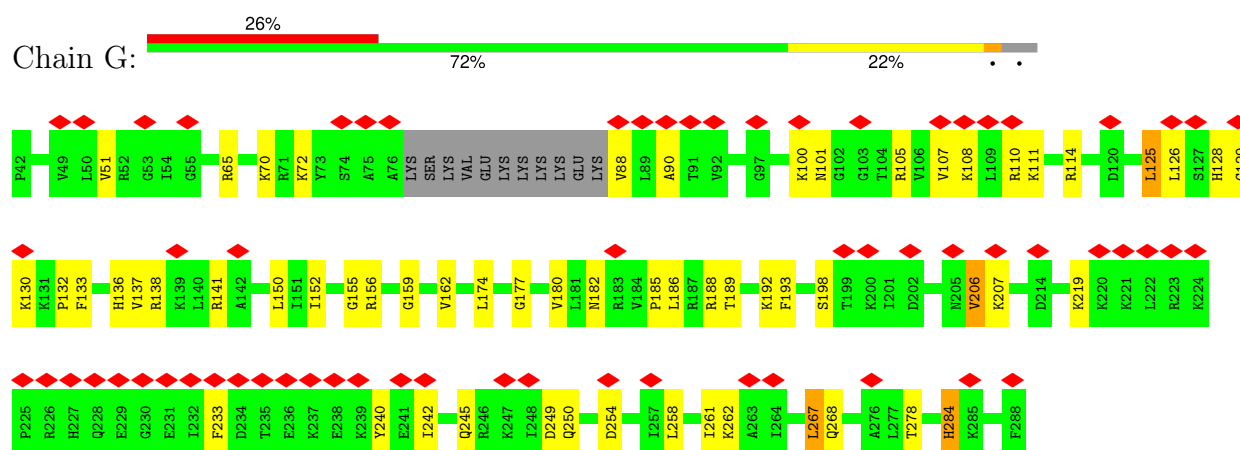
• Molecule 39: 5S ribosomal RNA



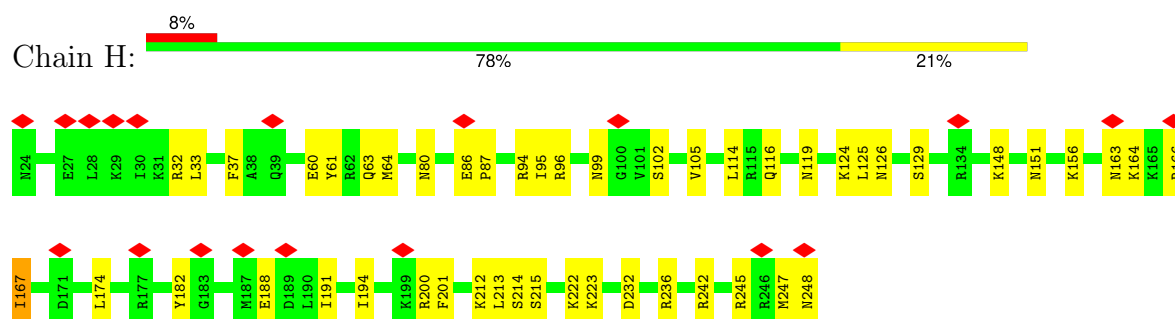
- Molecule 40: 60S ribosomal protein L5



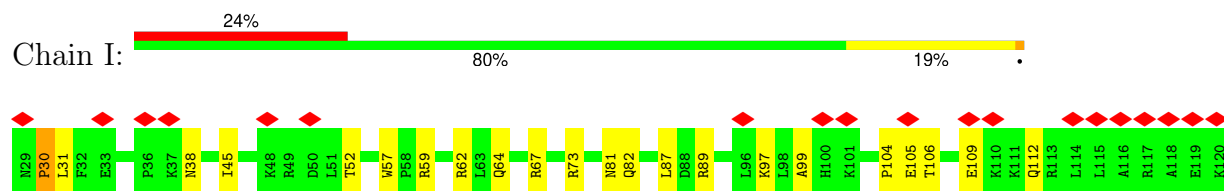
- Molecule 41: 60S ribosomal protein L6

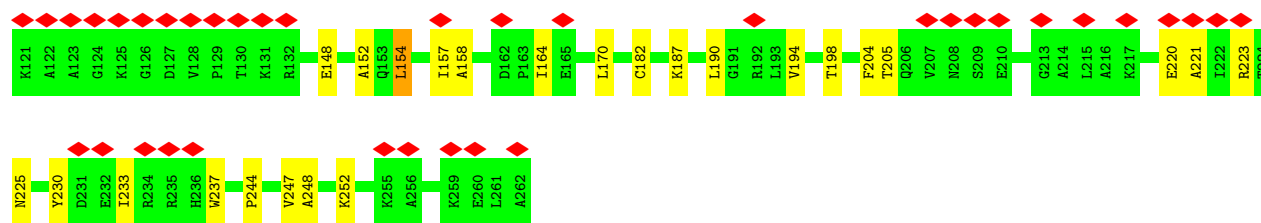


- Molecule 42: 60S ribosomal protein L7

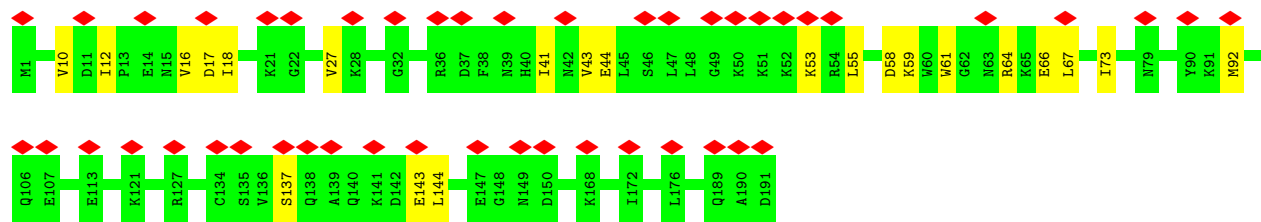
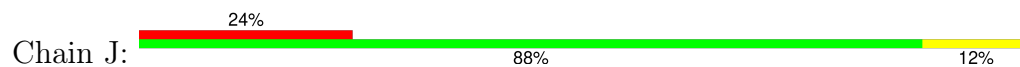


- Molecule 43: 60S ribosomal protein L7a

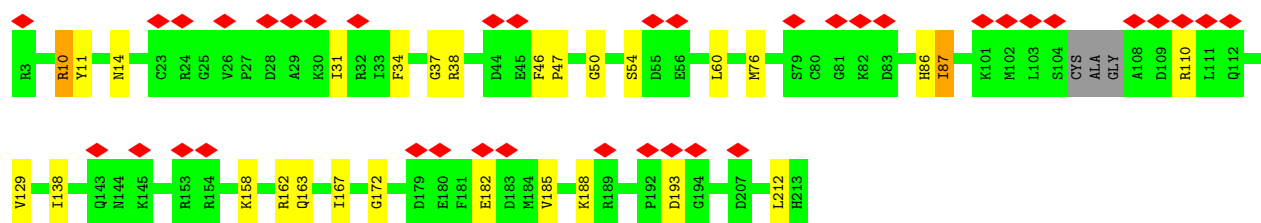
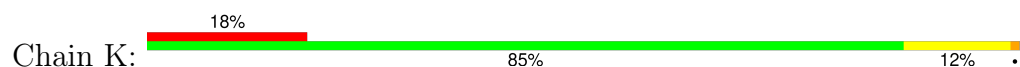




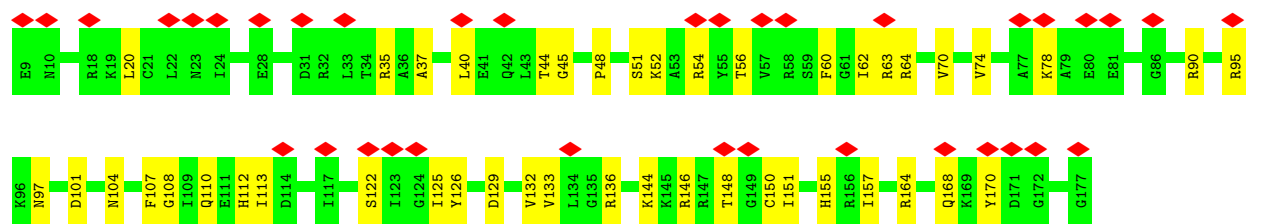
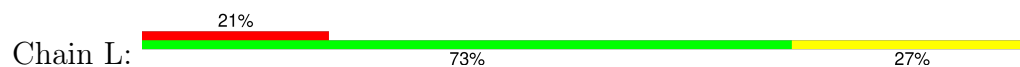
• Molecule 44: 60S ribosomal protein L9



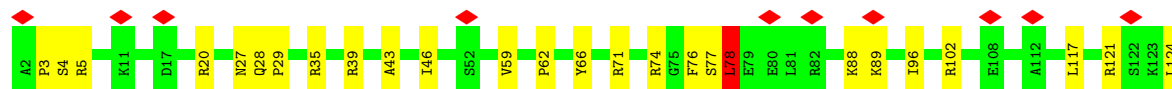
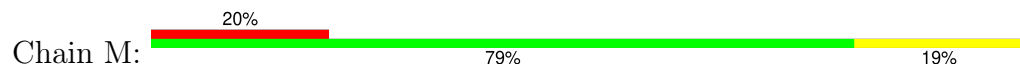
• Molecule 45: 60S ribosomal protein L10

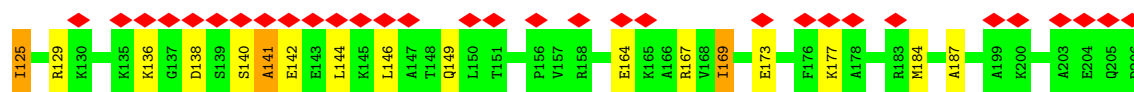


• Molecule 46: 60S ribosomal protein L11

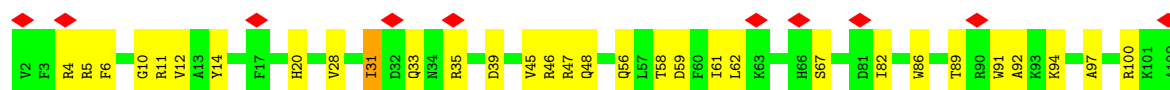
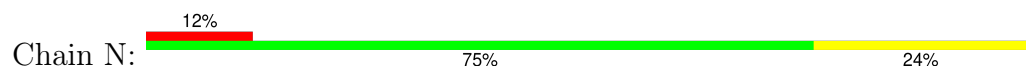


• Molecule 47: 60S ribosomal protein L13

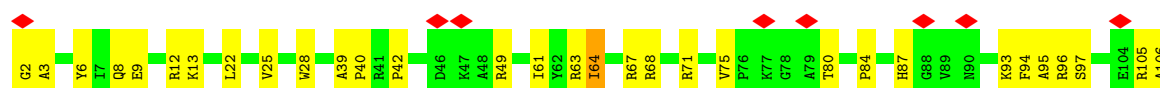
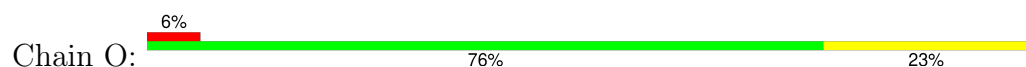




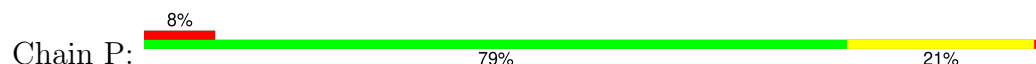
- Molecule 48: 60S ribosomal protein L14



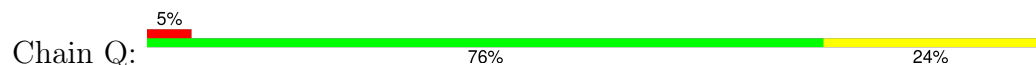
- Molecule 49: 60S ribosomal protein L15



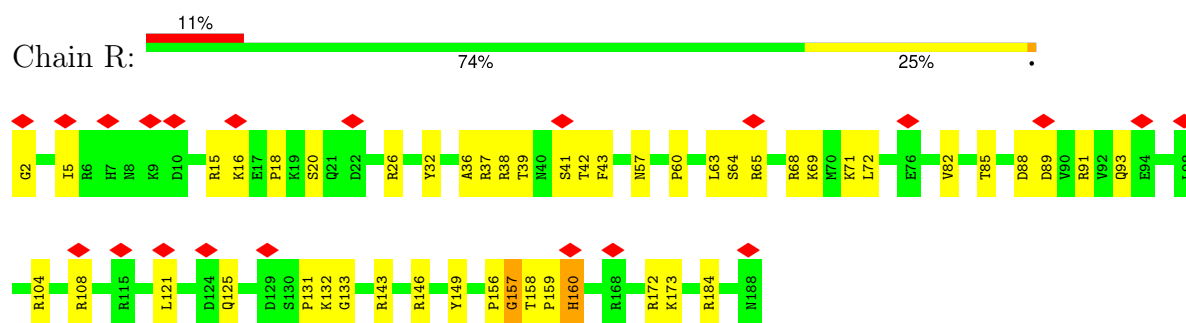
- Molecule 50: 60S ribosomal protein L13a



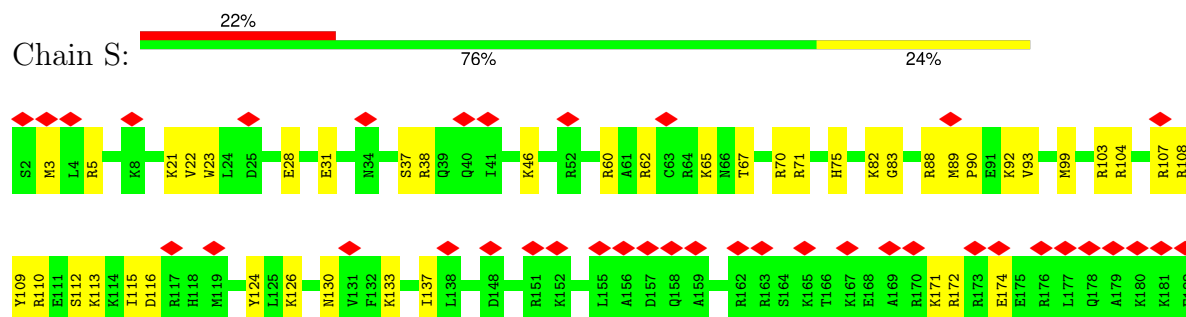
- Molecule 51: 60S ribosomal protein L17



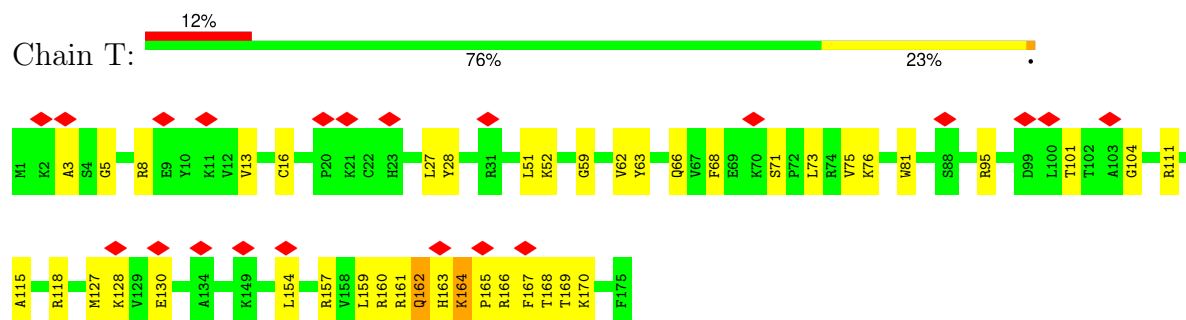
- Molecule 52: 60S ribosomal protein L18



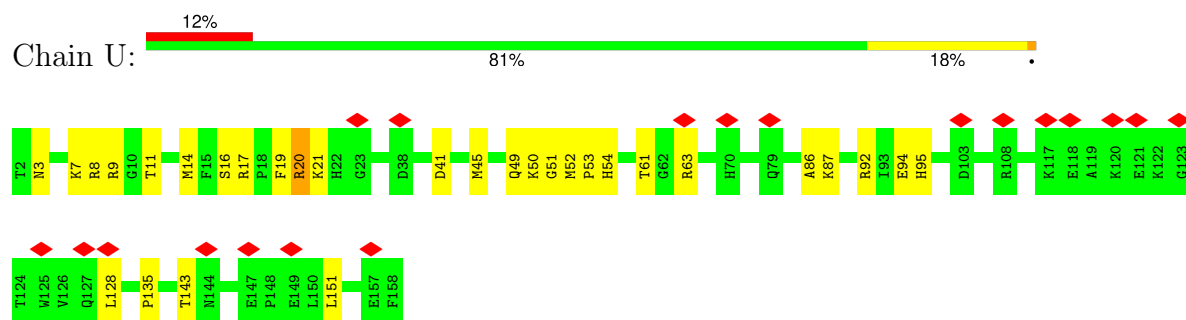
• Molecule 53: 60S ribosomal protein L19



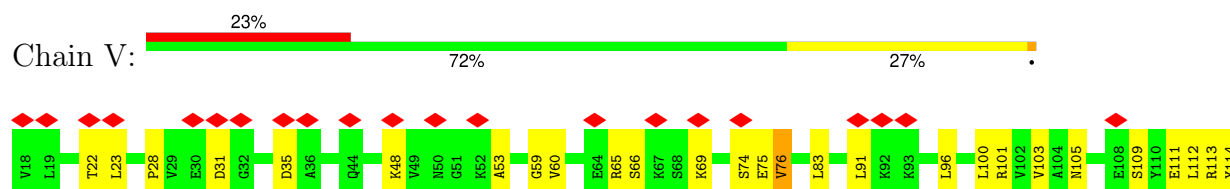
• Molecule 54: 60S ribosomal protein L18a



• Molecule 55: 60S ribosomal protein L21

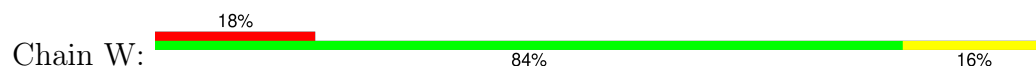


• Molecule 56: 60S ribosomal protein L22

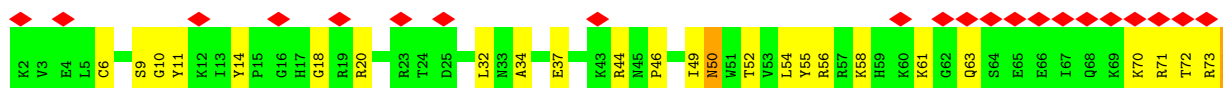




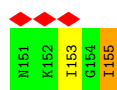
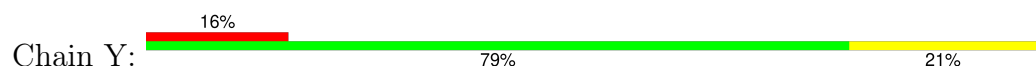
- Molecule 57: 60S ribosomal protein L23



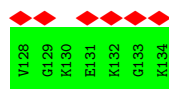
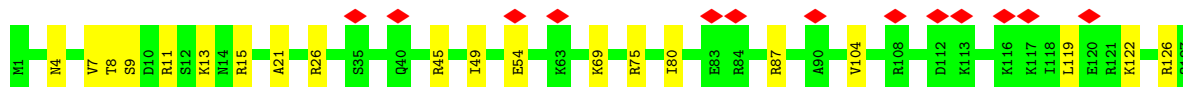
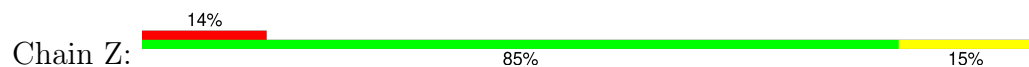
- Molecule 58: 60S ribosomal protein L24



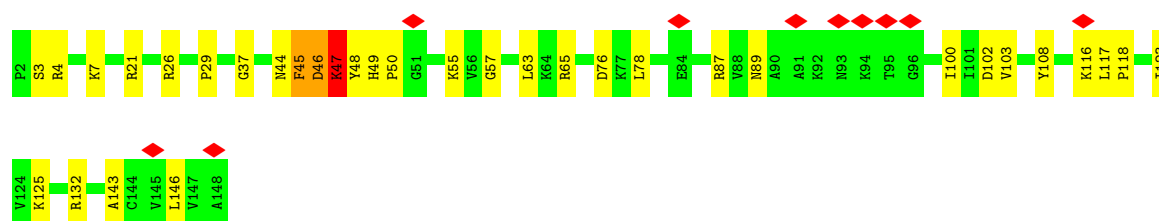
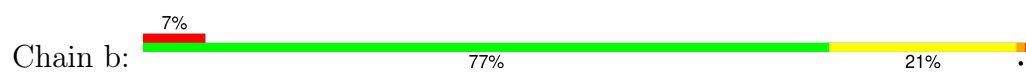
- Molecule 59: 60S ribosomal protein L23a



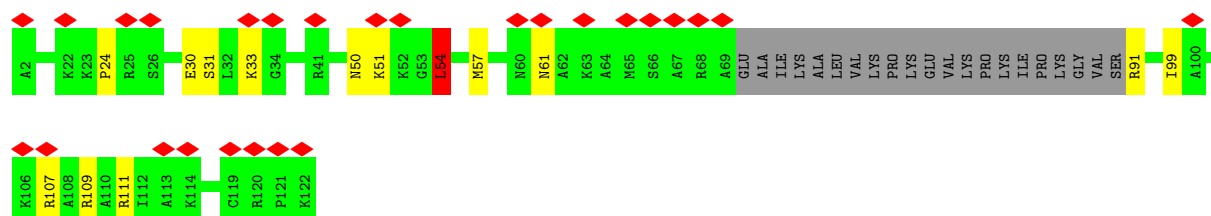
- Molecule 60: 60S ribosomal protein L26



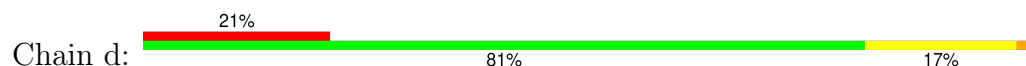
- Molecule 61: 60S ribosomal protein L27a



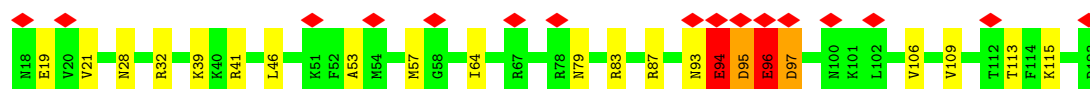
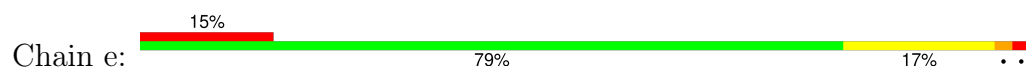
- Molecule 62: 60S ribosomal protein L29



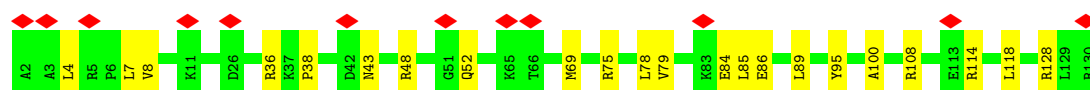
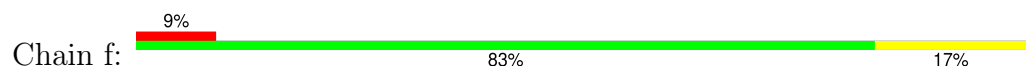
- Molecule 63: 60S ribosomal protein L30



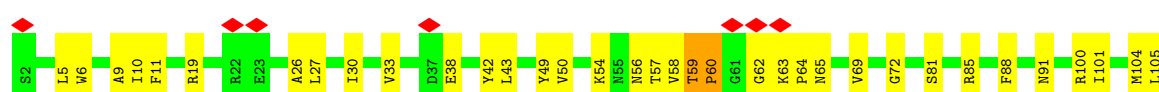
- Molecule 64: 60S ribosomal protein L31

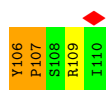


- Molecule 65: 60S ribosomal protein L32

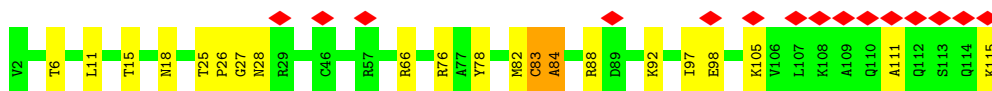
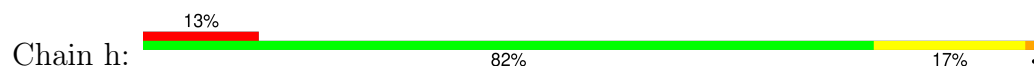


- Molecule 66: 60S ribosomal protein L35a

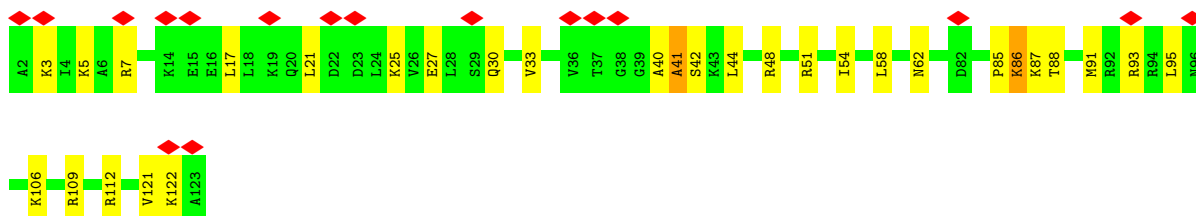




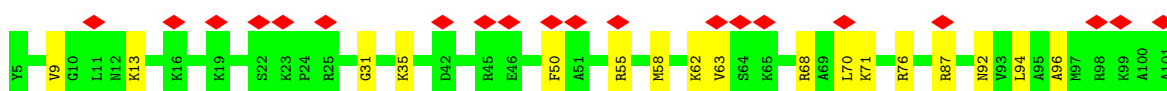
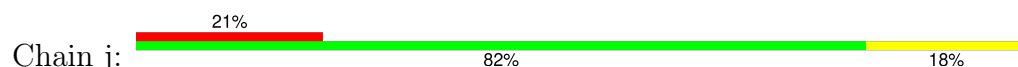
- Molecule 67: 60S ribosomal protein L34



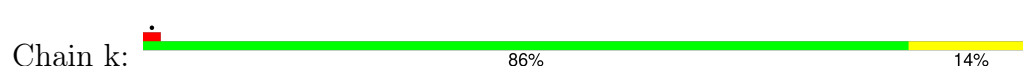
- Molecule 68: 60S ribosomal protein L35



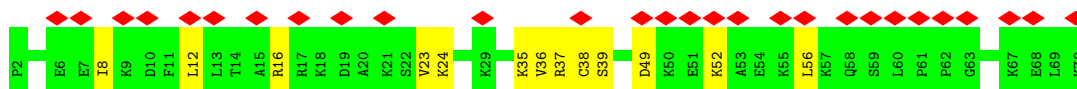
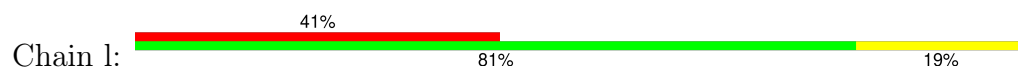
- Molecule 69: 60S ribosomal protein L36



- Molecule 70: 60S ribosomal protein L37



- Molecule 71: 60S ribosomal protein L38



- Molecule 72: 60S ribosomal protein L39

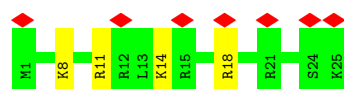
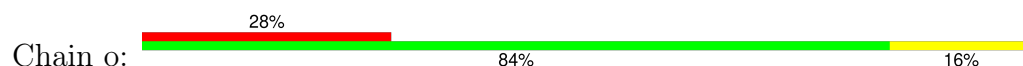




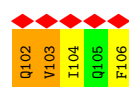
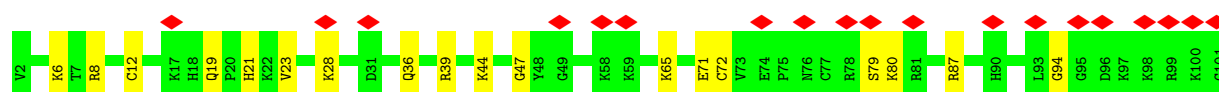
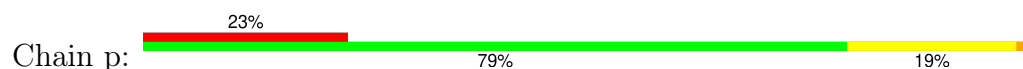
- Molecule 73: 60S ribosomal protein L40



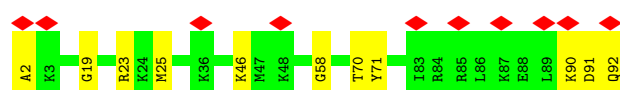
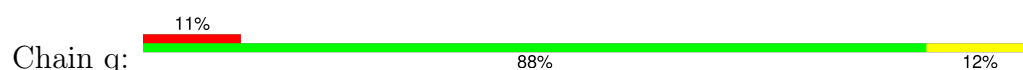
- Molecule 74: 60S ribosomal protein L41



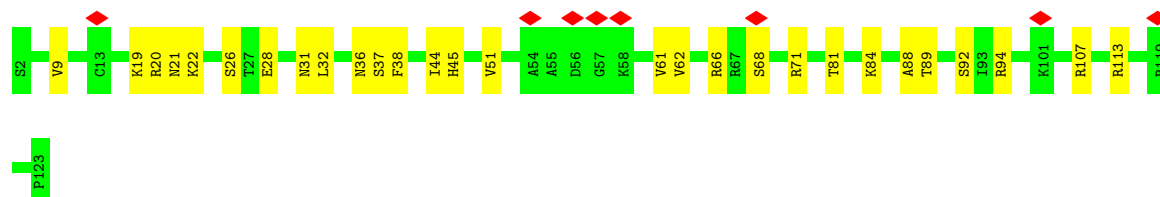
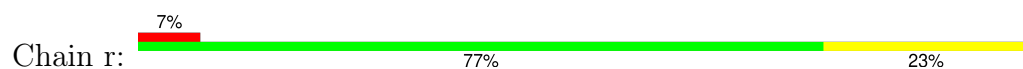
- Molecule 75: 60S ribosomal protein L36a



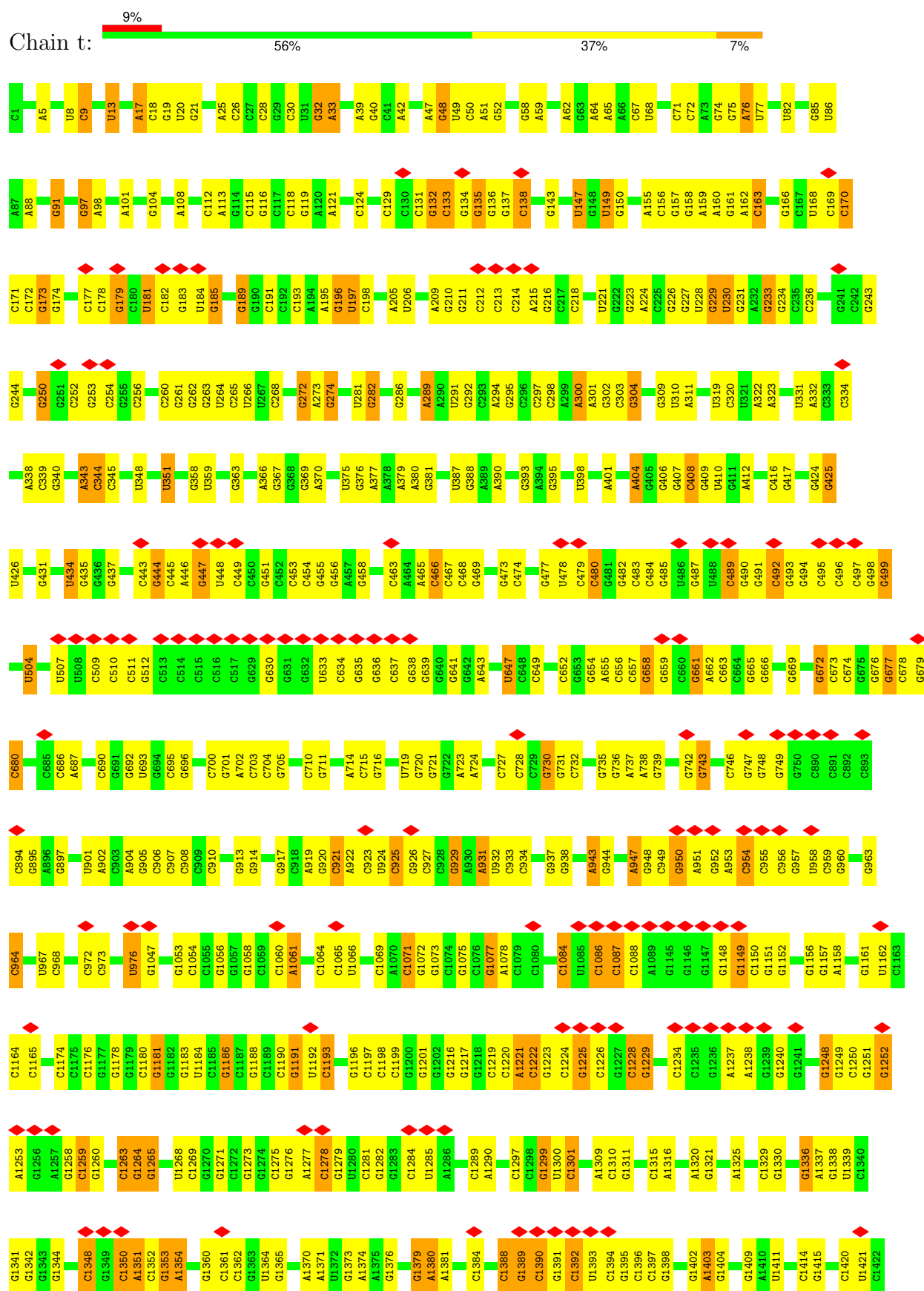
- Molecule 76: 60S ribosomal protein L37a

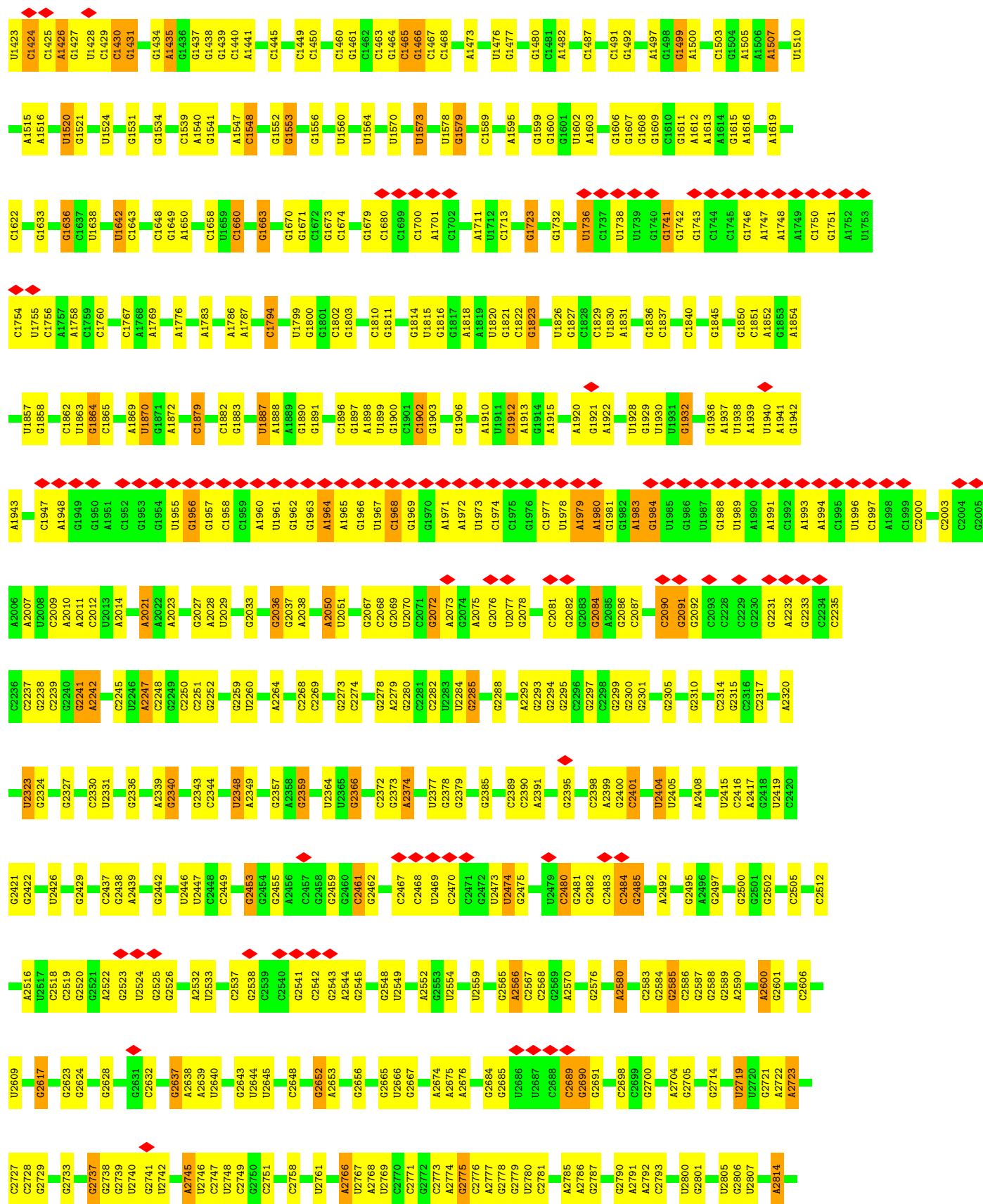


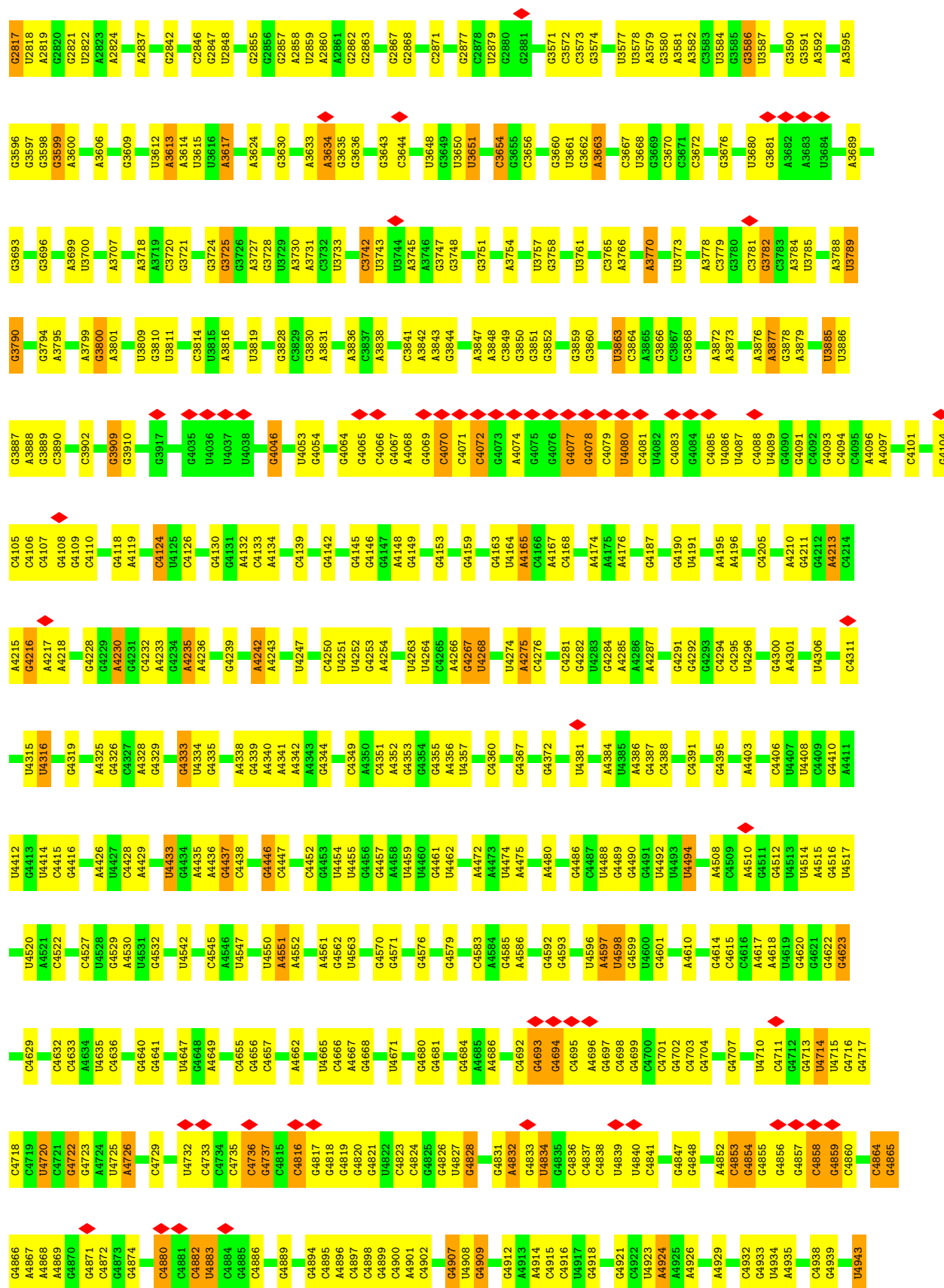
- Molecule 77: 60S ribosomal protein L28

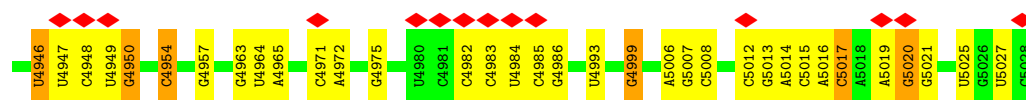


- Molecule 78: 28S ribosomal RNA

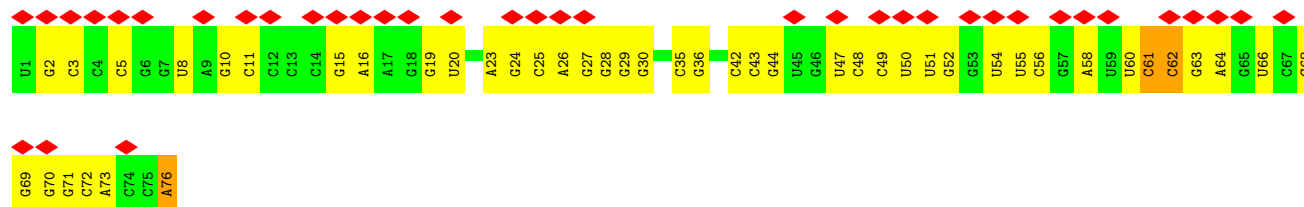
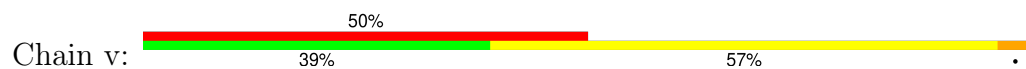




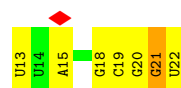




• Molecule 79: PE tRNA



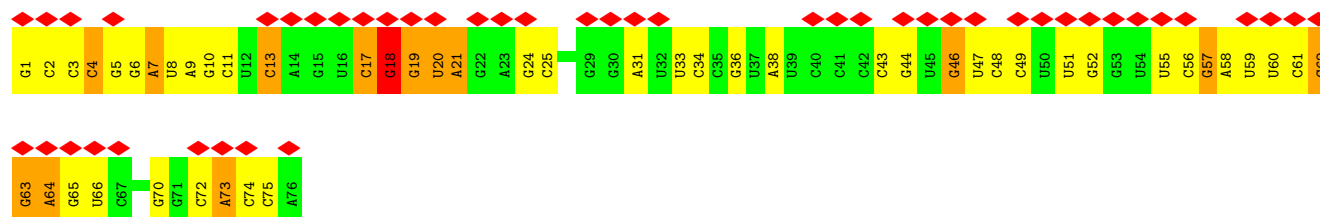
• Molecule 80: mRNA



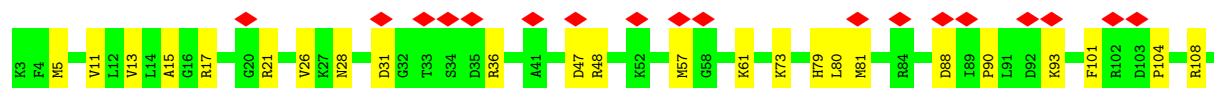
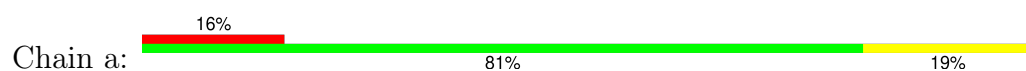
• Molecule 81: Cadherin-1



• Molecule 82: AA tRNA



• Molecule 83: 60S ribosomal protein L27





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10350	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 ($e^-/\text{\AA}^2$)	50	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	0.096	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	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: MG, MA6, UR3, A2M, 5MU, M7A, ZN, 5MC, B8Q, 6MZ, OMC, MVM, 4AC, OMU, B8N, PSU, OMG, E3C

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	0.83	13/39959 (0.0%)	0.46	1/62253 (0.0%)
2	SA	0.36	0/1778	0.70	0/2416
3	SB	0.33	0/1765	0.59	0/2362
4	SD	0.33	0/1785	0.71	0/2404
5	SE	0.32	0/2101	0.67	3/2828 (0.1%)
6	SF	0.32	0/1516	0.67	0/2037
7	SH	0.36	1/1519 (0.1%)	0.70	0/2033
8	SI	0.33	0/1702	0.72	2/2271 (0.1%)
9	SK	0.36	0/851	0.93	3/1147 (0.3%)
10	SL	1.85	2/1268 (0.2%)	0.90	7/1696 (0.4%)
11	SP	0.33	0/1065	0.71	0/1423
12	SQ	0.36	0/1177	0.77	1/1575 (0.1%)
13	SR	0.32	0/1097	0.73	0/1474
14	SS	0.32	0/1216	0.67	0/1628
15	ST	0.30	0/1131	0.66	0/1515
16	SU	0.30	0/831	0.75	0/1115
17	SV	0.43	0/631	0.80	3/844 (0.4%)
18	SX	0.40	0/1116	0.75	0/1490
19	Sa	0.40	0/836	0.71	0/1121
20	Sc	0.34	0/508	0.73	0/680
21	Sd	0.42	0/470	0.83	0/623
22	Sg	0.29	0/2486	0.71	0/3384
23	SC	0.41	0/1755	0.75	0/2371
24	SG	0.29	0/1946	0.68	0/2590
25	SJ	0.33	0/1561	0.77	0/2083
26	SM	0.27	0/922	0.67	0/1238
27	SN	0.33	0/1232	0.60	0/1656
28	SO	0.35	0/1037	0.69	0/1391
29	SW	0.40	0/1051	0.72	1/1406 (0.1%)
30	SY	0.30	0/1094	0.57	0/1452
31	SZ	0.34	0/585	0.86	2/785 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.30	0/653	0.63	0/876
33	Se	0.28	0/458	0.70	0/604
34	Sf	0.32	0/560	0.82	1/745 (0.1%)
35	A	0.46	0/1968	0.69	0/2639
36	B	0.42	0/3270	0.75	2/4377 (0.0%)
37	C	0.46	0/2942	0.77	4/3951 (0.1%)
38	D	0.42	0/3726	0.44	0/5804
39	E	0.40	0/2839	0.40	0/4425
40	F	0.38	0/2437	0.71	1/3262 (0.0%)
41	G	0.40	0/1942	0.80	5/2606 (0.2%)
42	H	0.49	0/1905	0.80	3/2539 (0.1%)
43	I	0.41	0/1913	0.71	0/2576
44	J	0.38	0/1545	0.70	0/2077
45	K	0.39	0/1730	0.69	1/2311 (0.0%)
46	L	0.36	0/1376	0.70	2/1841 (0.1%)
47	M	0.44	0/1688	0.86	2/2260 (0.1%)
48	N	0.40	0/1161	0.66	0/1554
49	O	0.51	0/1746	0.73	0/2338
50	P	0.44	0/1638	0.70	1/2191 (0.0%)
51	Q	0.43	0/1268	0.65	1/1701 (0.1%)
52	R	0.45	0/1537	0.75	0/2052
53	S	0.44	0/1533	0.77	0/2025
54	T	0.45	0/1488	0.72	3/1997 (0.2%)
55	U	0.42	0/1312	0.73	0/1753
56	V	0.37	0/822	0.87	3/1103 (0.3%)
57	W	0.41	0/983	0.61	0/1319
58	X	3.42	1/1004 (0.1%)	0.93	3/1332 (0.2%)
59	Y	0.40	0/975	0.63	0/1312
60	Z	0.42	0/1132	0.70	0/1504
61	b	0.49	0/1191	0.72	0/1591
62	c	0.40	0/826	0.80	0/1088
63	d	0.44	0/812	0.77	2/1089 (0.2%)
64	e	0.42	0/894	0.83	2/1204 (0.2%)
65	f	0.45	0/1082	0.71	0/1443
66	g	0.49	0/895	0.90	5/1198 (0.4%)
67	h	0.44	0/916	0.82	3/1220 (0.2%)
68	i	0.40	0/1023	0.83	3/1351 (0.2%)
69	j	0.35	0/805	0.73	0/1065
70	k	0.45	0/703	0.75	0/929
71	l	0.32	0/575	0.63	0/761
72	m	0.41	0/454	0.75	0/599
73	n	0.38	0/417	0.72	0/553
74	o	0.40	0/241	0.82	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	p	0.39	0/877	0.77	1/1156 (0.1%)
76	q	0.45	0/718	0.79	2/953 (0.2%)
77	r	0.49	0/995	0.83	0/1334
78	t	0.43	0/86502	0.47	3/134927 (0.0%)
79	v	0.28	0/1802	0.51	1/2797 (0.0%)
80	w	0.35	0/235	0.58	0/365
81	y	0.41	0/263	1.07	1/359 (0.3%)
82	u	0.28	0/1800	0.54	1/2804 (0.0%)
83	a	0.40	0/1126	0.72	0/1502
All	All	0.57	17/230694 (0.0%)	0.58	79/338958 (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
11	SP	0	1
15	ST	0	1
16	SU	0	1
56	V	0	1
62	c	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	X	119	LYS	CD-CE	107.75	4.75	1.52
1	S2	291	G	N9-C4	69.64	2.77	1.38
1	S2	291	G	N7-C5	68.78	2.76	1.39
1	S2	291	G	N9-C8	64.67	2.67	1.37
1	S2	291	G	C8-N7	64.22	2.59	1.30
10	SL	41	GLY	CA-C	63.88	2.24	1.52
1	S2	291	G	C5-C4	56.34	2.51	1.38
1	S2	325	C	C2-N3	18.58	1.73	1.35
1	S2	325	C	N1-C2	17.92	1.75	1.40
1	S2	325	C	N3-C4	17.67	1.69	1.33
1	S2	325	C	N1-C6	17.10	1.71	1.37
1	S2	325	C	C4-C5	14.14	1.71	1.43
1	S2	325	C	C5-C6	13.32	1.60	1.34
10	SL	41	GLY	C-N	7.46	1.44	1.33
7	SH	15	LYS	C-N	5.95	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	484	A2M	O3'-P	5.59	1.61	1.56
1	S2	1678	A2M	O3'-P	5.04	1.61	1.56

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	SL	41	GLY	O-C-N	-20.06	99.45	123.12
58	X	50	ASN	N-CA-C	13.20	125.75	111.36
9	SK	40	VAL	CA-C-N	12.39	132.45	120.31
9	SK	40	VAL	C-N-CA	12.39	132.45	120.31
64	e	94	GLU	N-CA-C	12.36	120.62	108.75
68	i	86	LYS	N-CA-C	11.88	124.31	111.36
29	SW	40	VAL	N-CA-C	-10.85	103.40	113.71
37	C	56	GLU	N-CA-C	10.23	122.02	111.07
67	h	83	CYS	N-CA-C	10.03	122.21	111.28
17	SV	79	VAL	N-CA-C	9.19	128.45	109.34
56	V	76	VAL	CA-C-N	-8.39	111.09	119.90
56	V	76	VAL	C-N-CA	-8.39	111.09	119.90
10	SL	41	GLY	N-CA-C	8.36	127.18	112.64
42	H	164	LYS	N-CA-C	-8.32	98.92	108.49
66	g	106	TYR	CA-C-N	7.95	129.77	119.84
66	g	106	TYR	C-N-CA	7.95	129.77	119.84
63	d	9	LYS	N-CA-C	7.79	122.14	111.71
8	SI	130	THR	N-CA-C	7.77	126.99	109.81
58	X	72	THR	N-CA-C	7.39	120.97	109.52
64	e	96	GLU	N-CA-C	-7.24	103.49	112.47
40	F	8	LYS	N-CA-C	7.01	119.58	111.02
66	g	59	THR	CA-C-N	6.92	128.49	119.84
66	g	59	THR	C-N-CA	6.92	128.49	119.84
76	q	91	ASP	CA-C-N	6.71	133.77	121.70
76	q	91	ASP	C-N-CA	6.71	133.77	121.70
9	SK	43	LEU	N-CA-C	6.59	118.46	111.28
36	B	3	HIS	N-CA-C	-6.49	96.97	110.80
8	SI	131	PRO	N-CA-C	6.47	122.72	113.47
37	C	58	ALA	N-CA-C	6.31	118.16	111.28
47	M	141	ALA	CA-C-N	-6.26	113.26	122.78
47	M	141	ALA	C-N-CA	-6.26	113.26	122.78
78	t	3595	A	C2'-C3'-O3'	6.25	118.87	109.50
56	V	59	GLY	N-CA-C	6.18	115.84	110.21
42	H	163	ASN	CA-C-N	6.18	130.88	120.81
42	H	163	ASN	C-N-CA	6.18	130.88	120.81
82	u	18	G	P-O3'-C3'	6.15	129.42	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	SE	64	ILE	N-CA-C	-6.14	106.82	112.96
10	SL	41	GLY	CA-C-N	6.03	130.94	122.08
10	SL	41	GLY	C-N-CA	6.03	130.94	122.08
5	SE	156	VAL	CA-C-N	6.02	132.50	123.05
5	SE	156	VAL	C-N-CA	6.02	132.50	123.05
12	SQ	78	VAL	N-CA-C	-5.94	107.02	112.96
68	i	85	PRO	CA-C-N	5.94	128.72	120.29
68	i	85	PRO	C-N-CA	5.94	128.72	120.29
41	G	206	VAL	CA-C-N	5.92	132.85	121.54
41	G	206	VAL	C-N-CA	5.92	132.85	121.54
34	Sf	92	LYS	N-CA-C	5.85	118.75	110.50
41	G	233	PHE	CA-C-N	5.81	136.44	126.32
41	G	233	PHE	C-N-CA	5.81	136.44	126.32
63	d	11	LEU	N-CA-C	-5.62	106.24	114.39
10	SL	150	GLY	CA-C-N	5.61	132.25	121.54
10	SL	150	GLY	C-N-CA	5.61	132.25	121.54
78	t	3595	A	P-O3'-C3'	5.61	128.61	120.20
66	g	106	TYR	C-N-CD	-5.57	102.17	125.00
54	T	27	LEU	CA-CB-CG	5.54	135.69	116.30
17	SV	78	ILE	CA-C-N	5.51	131.88	121.97
17	SV	78	ILE	C-N-CA	5.51	131.88	121.97
78	t	4946	U	P-O3'-C3'	5.46	128.38	120.20
81	y	19	ILE	N-CA-C	-5.43	98.05	109.34
10	SL	41	GLY	CA-C-O	5.33	131.35	122.56
79	v	61	C	C2-N1-C1'	5.31	134.74	118.80
54	T	162	GLN	CA-C-N	5.30	127.38	120.28
54	T	162	GLN	C-N-CA	5.30	127.38	120.28
67	h	27	GLY	CA-C-N	5.27	131.60	121.54
67	h	27	GLY	C-N-CA	5.27	131.60	121.54
50	P	187	LYS	N-CA-C	-5.25	108.14	114.75
1	S2	291	G	C6-N1-C2	5.18	140.64	125.10
41	G	284	HIS	N-CA-C	-5.18	106.06	114.09
36	B	4	ARG	N-CA-C	5.14	117.62	111.71
51	Q	6	LEU	CA-CB-CG	5.12	134.22	116.30
45	K	10	ARG	N-CA-C	-5.11	99.91	110.80
58	X	119	LYS	CG-CD-CE	5.11	123.06	111.30
31	SZ	44	LEU	CA-C-N	5.10	131.29	121.54
31	SZ	44	LEU	C-N-CA	5.10	131.29	121.54
37	C	150	LEU	CA-C-N	-5.08	113.49	119.84
37	C	150	LEU	C-N-CA	-5.08	113.49	119.84
75	p	103	VAL	N-CA-C	-5.08	100.57	107.99
46	L	170	TYR	CA-C-N	5.07	131.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	L	170	TYR	C-N-CA	5.07	131.22	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	SP	14	LYS	Peptide
15	ST	98	SER	Peptide
16	SU	95	SER	Peptide
56	V	74	SER	Mainchain
62	c	54	LEU	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	18403	399	0
2	SA	1741	0	1745	69	0
3	SB	1738	0	1809	48	0
4	SD	1757	0	1853	32	0
5	SE	2059	0	2164	48	0
6	SF	1495	0	1549	41	0
7	SH	1497	0	1590	24	0
8	SI	1673	0	1756	42	0
9	SK	827	0	854	46	0
10	SL	1247	0	1323	43	0
11	SP	1045	0	1095	22	0
12	SQ	1158	0	1232	40	0
13	SR	1082	0	1137	31	0
14	SS	1198	0	1261	26	0
15	ST	1112	0	1146	21	0
16	SU	821	0	883	23	0
17	SV	625	0	628	33	0
18	SX	1098	0	1167	25	0
19	Sa	821	0	871	21	0
20	Sc	506	0	536	13	0
21	Sd	459	0	450	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Sg	2429	0	2386	50	0
23	SC	1715	0	1804	53	0
24	SG	1923	0	2089	43	0
25	SJ	1533	0	1653	29	0
26	SM	912	0	930	16	0
27	SN	1208	0	1294	17	0
28	SO	1024	0	1050	21	0
29	SW	1034	0	1080	18	0
30	SY	1073	0	1155	14	0
31	SZ	579	0	639	12	0
32	Sb	640	0	665	11	0
33	Se	452	0	498	10	0
34	Sf	548	0	552	11	0
35	A	1930	0	2030	28	0
36	B	3202	0	3343	75	0
37	C	2888	0	3063	98	0
38	D	3337	0	1692	34	0
39	E	2541	0	1285	16	0
40	F	2392	0	2425	38	0
41	G	1904	0	2055	65	0
42	H	1870	0	1996	36	0
43	I	1880	0	2018	32	0
44	J	1526	0	1605	19	0
45	K	1692	0	1744	16	0
46	L	1353	0	1386	31	0
47	M	1657	0	1764	42	0
48	N	1138	0	1204	32	0
49	O	1701	0	1749	39	0
50	P	1606	0	1745	29	0
51	Q	1242	0	1269	27	0
52	R	1513	0	1628	39	0
53	S	1517	0	1670	39	0
54	T	1449	0	1493	42	0
55	U	1284	0	1352	45	0
56	V	808	0	831	21	0
57	W	969	0	1031	14	0
58	X	989	0	1039	57	0
59	Y	958	0	1029	17	0
60	Z	1115	0	1205	15	0
61	b	1162	0	1213	46	0
62	c	814	0	880	11	0
63	d	801	0	845	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	e	879	0	924	23	0
65	f	1064	0	1160	19	0
66	g	876	0	911	95	0
67	h	906	0	1002	17	0
68	i	1015	0	1148	22	0
69	j	794	0	870	10	0
70	k	689	0	717	8	0
71	l	569	0	637	7	0
72	m	444	0	483	11	0
73	n	411	0	443	14	0
74	o	240	0	289	3	0
75	p	863	0	930	20	0
76	q	708	0	758	7	0
77	r	980	0	1041	21	0
78	t	77332	0	39076	700	0
79	v	1618	0	826	6	0
80	w	213	0	109	6	0
81	y	262	0	290	29	0
82	u	1613	0	821	15	0
83	a	1103	0	1179	16	0
84	S2	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sf	1	0	0	0	0
84	k	1	0	0	0	0
84	p	1	0	0	0	0
84	q	1	0	0	0	0
85	D	6	0	0	0	0
85	E	9	0	0	0	0
85	S2	3	0	0	0	0
85	b	2	0	0	0	0
85	t	11	0	0	0	0
86	t	31	0	0	1	0
87	S2	5	0	0	1	0
87	SN	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	2	0	0	0	0
87	SV	1	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	0	0
All	All	215429	0	159450	2725	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 8.

All (2725) 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)
1:S2:814:5MU:C4	1:S2:814:5MU:C5	1.81	1.67
1:S2:325:C:C4	1:S2:325:C:N3	1.69	1.59
66:g:58:VAL:CG1	66:g:64:PRO:HA	1.22	1.58
1:S2:325:C:C6	1:S2:325:C:N1	1.71	1.58
66:g:54:LYS:CE	78:t:437:G:H5''	1.23	1.57
1:S2:325:C:N3	1:S2:325:C:C2	1.72	1.56
1:S2:325:C:N1	1:S2:325:C:C2	1.76	1.50
55:U:19:PHE:CE2	55:U:20:ARG:HB2	1.45	1.48
55:U:19:PHE:CD2	55:U:20:ARG:HB2	1.50	1.44
66:g:54:LYS:HE2	78:t:437:G:C5'	0.99	1.43
66:g:58:VAL:HG13	66:g:64:PRO:CA	1.46	1.43
66:g:59:THR:HG21	78:t:4902:C:C5	1.55	1.41
54:T:160:ARG:HD3	54:T:163:HIS:CD2	1.57	1.39
23:SC:274:VAL:CG1	23:SC:278:THR:OG1	1.69	1.37
17:SV:53:TYR:CE1	17:SV:72:LEU:CD1	2.06	1.37
66:g:106:TYR:CB	66:g:107:PRO:HD2	1.47	1.36
66:g:59:THR:CG2	66:g:60:PRO:HD3	1.55	1.36
66:g:56:ASN:OD1	66:g:65:ASN:N	1.66	1.28
9:SK:27:VAL:O	9:SK:43:LEU:HD11	1.20	1.27
23:SC:274:VAL:HG13	23:SC:278:THR:CB	1.65	1.27
66:g:54:LYS:CE	78:t:437:G:C5'	1.92	1.26
66:g:106:TYR:HB3	66:g:107:PRO:CD	1.64	1.26
37:C:58:ALA:O	37:C:60:HIS:N	1.68	1.25
66:g:54:LYS:HE2	78:t:437:G:C4'	1.41	1.25
66:g:58:VAL:HG11	66:g:63:LYS:O	1.39	1.23
66:g:59:THR:CG2	78:t:4902:C:C4	2.22	1.21
23:SC:274:VAL:HG13	23:SC:278:THR:CG2	1.71	1.21
54:T:160:ARG:HD3	54:T:163:HIS:CG	1.76	1.20
66:g:59:THR:HG23	66:g:60:PRO:CD	1.71	1.20
9:SK:29:MET:O	9:SK:42:ASN:OD1	1.63	1.17
41:G:128:HIS:NE2	78:t:1265:G:C6	2.12	1.17
36:B:215:GLU:OE1	36:B:217:ILE:HG23	1.41	1.16
37:C:70:GLY:O	78:t:3877:A:P	2.03	1.16
41:G:128:HIS:NE2	78:t:1265:G:O6	1.80	1.15
52:R:158:THR:OG1	52:R:159:PRO:HD2	1.44	1.14
54:T:160:ARG:CD	54:T:163:HIS:CD2	2.30	1.14
55:U:19:PHE:CD2	55:U:20:ARG:CB	2.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:g:59:THR:HG22	78:t:4902:C:C4	1.83	1.13
66:g:56:ASN:OD1	66:g:65:ASN:CA	1.97	1.12
41:G:128:HIS:NE2	78:t:1265:G:N7	1.96	1.12
41:G:128:HIS:NE2	78:t:1265:G:C5	2.17	1.12
56:V:60:VAL:HB	56:V:75:GLU:OE1	1.49	1.12
23:SC:274:VAL:HG12	23:SC:278:THR:OG1	1.41	1.12
34:Sf:94:LYS:HE2	34:Sf:94:LYS:HA	1.23	1.11
44:J:61:TRP:CZ3	48:N:33:GLN:NE2	2.19	1.11
17:SV:53:TYR:CE1	17:SV:72:LEU:HD11	1.79	1.10
37:C:70:GLY:O	78:t:3876:A:O3'	1.69	1.10
41:G:128:HIS:CD2	78:t:1265:G:C6	2.40	1.10
66:g:59:THR:CG2	78:t:4902:C:C5	2.33	1.10
10:SL:41:GLY:CA	10:SL:41:GLY:C	2.24	1.10
64:e:94:GLU:O	64:e:97:ASP:HB3	1.50	1.09
17:SV:53:TYR:CE1	17:SV:72:LEU:HD13	1.81	1.09
3:SB:86:LEU:HD23	3:SB:98:THR:CB	1.82	1.09
66:g:104:MET:HG2	66:g:106:TYR:CE2	1.88	1.09
66:g:58:VAL:CG1	66:g:64:PRO:CA	2.14	1.07
44:J:61:TRP:HZ3	48:N:33:GLN:NE2	1.48	1.07
2:SA:122:LEU:HD23	2:SA:144:THR:HG22	1.37	1.06
37:C:67:TRP:NE1	37:C:78:ARG:HG3	1.69	1.06
2:SA:40:LYS:O	2:SA:48:ILE:CD1	2.04	1.05
37:C:85:HIS:CD2	81:y:20:LEU:CD2	2.40	1.05
37:C:85:HIS:CD2	81:y:20:LEU:HD21	1.93	1.04
9:SK:27:VAL:HB	9:SK:43:LEU:HD12	1.36	1.03
37:C:84:THR:O	81:y:20:LEU:HD11	1.58	1.03
2:SA:40:LYS:H	2:SA:48:ILE:HD11	1.22	1.03
2:SA:56:GLU:HB2	17:SV:79:VAL:HG11	1.36	1.03
37:C:85:HIS:HA	81:y:20:LEU:HD21	1.41	1.03
41:G:128:HIS:CE1	78:t:1265:G:O6	2.11	1.03
9:SK:29:MET:N	9:SK:42:ASN:HD21	1.55	1.02
55:U:19:PHE:CE2	55:U:20:ARG:CB	2.41	1.02
9:SK:27:VAL:C	9:SK:43:LEU:HD11	1.85	1.02
61:b:37:GLY:CA	61:b:45:PHE:CD2	2.41	1.02
37:C:70:GLY:O	78:t:3877:A:OP1	1.75	1.02
9:SK:29:MET:HB3	9:SK:42:ASN:ND2	1.75	1.01
41:G:133:PHE:HA	41:G:136:HIS:CE1	1.93	1.01
44:J:61:TRP:CH2	48:N:33:GLN:HB2	1.95	1.01
54:T:164:LYS:HB3	54:T:165:PRO:CD	1.91	1.01
58:X:46:PRO:O	58:X:49:ILE:HG12	1.61	1.01
9:SK:43:LEU:HD22	9:SK:43:LEU:H	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SK:27:VAL:O	9:SK:43:LEU:CD1	2.08	1.00
9:SK:29:MET:O	9:SK:42:ASN:CG	2.03	1.00
66:g:54:LYS:CD	78:t:437:G:H5''	1.91	1.00
3:SB:86:LEU:HD23	3:SB:98:THR:CG2	1.91	0.99
23:SC:274:VAL:HG13	23:SC:278:THR:OG1	1.36	0.99
1:S2:291:G:C4	1:S2:291:G:C5	2.51	0.99
61:b:37:GLY:HA3	61:b:45:PHE:CE2	1.97	0.98
66:g:104:MET:HB3	66:g:106:TYR:CD2	1.99	0.98
66:g:56:ASN:OD1	66:g:65:ASN:C	2.06	0.98
1:S2:291:G:C4	10:SL:41:GLY:HA2	1.99	0.97
66:g:5:LEU:O	66:g:105:LEU:HD23	1.64	0.97
41:G:125:LEU:CD2	78:t:947:A:C5	2.47	0.97
3:SB:87:ILE:CD1	3:SB:220:LYS:NZ	2.28	0.97
47:M:77:SER:O	47:M:78:LEU:CB	2.13	0.96
66:g:104:MET:CB	66:g:106:TYR:HD2	1.77	0.96
2:SA:40:LYS:H	2:SA:48:ILE:CD1	1.77	0.96
23:SC:274:VAL:HG13	23:SC:278:THR:HG21	1.44	0.96
3:SB:86:LEU:HD23	3:SB:98:THR:HG21	1.46	0.96
41:G:128:HIS:CD2	78:t:1265:G:C5	2.54	0.96
2:SA:40:LYS:O	2:SA:48:ILE:HD12	1.66	0.95
61:b:37:GLY:HA3	61:b:45:PHE:CD2	2.00	0.95
66:g:58:VAL:HG21	66:g:62:GLY:O	1.67	0.95
64:e:94:GLU:O	64:e:97:ASP:CB	2.15	0.95
12:SQ:116:ASP:OD1	12:SQ:118:THR:CG2	2.15	0.94
37:C:70:GLY:C	78:t:3877:A:OP1	2.11	0.94
66:g:104:MET:HG2	66:g:106:TYR:HE2	1.28	0.93
66:g:58:VAL:HG11	66:g:64:PRO:HA	1.50	0.93
66:g:54:LYS:CE	78:t:437:G:C4'	2.13	0.93
81:y:22:ILE:HG12	81:y:24:GLY:H	1.34	0.92
36:B:215:GLU:OE1	36:B:217:ILE:CG2	2.16	0.92
61:b:37:GLY:HA2	61:b:45:PHE:CD2	2.05	0.92
66:g:54:LYS:CE	78:t:437:G:H4'	1.99	0.92
41:G:133:PHE:HA	41:G:136:HIS:HE1	1.29	0.91
55:U:19:PHE:HE2	55:U:20:ARG:HB2	1.29	0.91
55:U:19:PHE:HE2	55:U:20:ARG:HD3	1.34	0.91
1:S2:291:G:C8	10:SL:41:GLY:C	2.49	0.90
9:SK:29:MET:H	9:SK:42:ASN:HD21	0.94	0.90
66:g:54:LYS:HE3	78:t:437:G:H5''	1.53	0.90
2:SA:40:LYS:O	2:SA:48:ILE:HD11	1.72	0.90
37:C:71:ARG:HH12	81:y:26:ILE:HA	1.34	0.90
55:U:19:PHE:HD2	55:U:20:ARG:CB	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:58:ALA:C	37:C:60:HIS:H	1.80	0.89
9:SK:27:VAL:HB	9:SK:43:LEU:CD1	2.03	0.89
12:SQ:117:ARG:O	12:SQ:121:VAL:CG2	2.19	0.89
3:SB:87:ILE:HD13	3:SB:220:LYS:HZ1	1.38	0.89
44:J:61:TRP:HH2	48:N:33:GLN:HB2	1.33	0.88
1:S2:291:G:C5	10:SL:41:GLY:C	2.51	0.88
12:SQ:116:ASP:OD1	12:SQ:118:THR:HG22	1.74	0.88
56:V:75:GLU:OE1	56:V:75:GLU:N	2.08	0.87
61:b:46:ASP:O	61:b:48:TYR:N	2.06	0.87
3:SB:87:ILE:CD1	3:SB:220:LYS:HZ1	1.84	0.87
61:b:37:GLY:CA	61:b:45:PHE:HD2	1.83	0.87
12:SQ:116:ASP:CG	12:SQ:118:THR:HG22	2.00	0.87
78:t:1069:C:H42	78:t:1193:C:H42	1.23	0.87
1:S2:1782:G:O6	58:X:73:ARG:HD2	1.75	0.87
3:SB:87:ILE:HG12	3:SB:101:HIS:HB2	1.56	0.87
3:SB:87:ILE:HD12	3:SB:220:LYS:HZ3	1.39	0.87
17:SV:53:TYR:CD1	17:SV:72:LEU:HD11	2.10	0.87
66:g:56:ASN:OD1	66:g:65:ASN:O	1.93	0.86
2:SA:77:ILE:HG12	2:SA:122:LEU:CD1	2.06	0.86
67:h:83:CYS:O	67:h:84:ALA:CB	2.21	0.86
17:SV:53:TYR:HE1	17:SV:72:LEU:HD13	1.35	0.86
66:g:59:THR:HG21	78:t:4902:C:C4	1.96	0.86
9:SK:29:MET:H	9:SK:42:ASN:ND2	1.74	0.86
55:U:19:PHE:CD2	55:U:20:ARG:N	2.43	0.86
47:M:77:SER:O	47:M:78:LEU:HB2	1.74	0.85
66:g:104:MET:HB3	66:g:106:TYR:HD2	1.37	0.85
66:g:104:MET:CB	66:g:106:TYR:CD2	2.57	0.85
66:g:59:THR:HB	78:t:4902:C:N4	1.90	0.85
1:S2:291:G:C8	10:SL:41:GLY:CA	2.59	0.85
64:e:94:GLU:O	64:e:97:ASP:CA	2.25	0.84
41:G:128:HIS:CD2	78:t:1265:G:O6	2.28	0.84
56:V:60:VAL:HB	56:V:75:GLU:CD	2.02	0.84
56:V:60:VAL:HG21	56:V:76:VAL:HG23	1.58	0.84
54:T:160:ARG:HG2	54:T:163:HIS:HB3	1.58	0.84
1:S2:291:G:C4	10:SL:41:GLY:CA	2.60	0.84
12:SQ:116:ASP:CG	12:SQ:118:THR:CG2	2.51	0.84
2:SA:121:LEU:HD21	2:SA:145:ILE:CD1	2.06	0.84
37:C:70:GLY:HA3	78:t:3877:A:H5''	1.60	0.83
47:M:76:PHE:CE2	47:M:96:ILE:CG2	2.62	0.83
1:S2:291:G:C4	10:SL:41:GLY:C	2.57	0.83
58:X:54:LEU:O	58:X:58:LYS:HG2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:67:TRP:HE1	37:C:78:ARG:HG3	1.43	0.83
37:C:85:HIS:HD2	81:y:20:LEU:CD2	1.88	0.83
1:S2:291:G:C5	10:SL:41:GLY:CA	2.63	0.82
3:SB:86:LEU:HD23	3:SB:98:THR:HB	1.59	0.82
4:SD:123:LEU:O	4:SD:127:MET:HG2	1.80	0.82
12:SQ:117:ARG:O	12:SQ:121:VAL:HG22	1.80	0.82
2:SA:40:LYS:N	2:SA:48:ILE:HD11	1.92	0.81
37:C:85:HIS:CD2	81:y:20:LEU:HD23	2.14	0.81
34:Sf:94:LYS:HA	34:Sf:94:LYS:CE	2.09	0.81
48:N:31:ILE:HD11	48:N:35:ARG:HB2	1.62	0.81
78:t:4707:G:H22	78:t:4912:G:H1	1.29	0.81
12:SQ:116:ASP:OD2	12:SQ:118:THR:HG23	1.81	0.80
9:SK:29:MET:CB	9:SK:42:ASN:ND2	2.43	0.80
1:S2:291:G:N9	10:SL:41:GLY:CA	2.45	0.79
17:SV:53:TYR:CD1	17:SV:72:LEU:CD1	2.66	0.79
51:Q:136:ILE:HB	81:y:21:GLY:O	1.82	0.79
1:S2:291:G:N9	10:SL:41:GLY:HA3	1.98	0.79
1:S2:291:G:N7	10:SL:41:GLY:N	2.30	0.79
12:SQ:116:ASP:C	12:SQ:118:THR:H	1.91	0.79
37:C:70:GLY:HA3	78:t:3877:A:C5'	2.13	0.79
3:SB:225:LEU:O	3:SB:225:LEU:HD13	1.82	0.79
3:SB:86:LEU:CD2	3:SB:98:THR:CB	2.61	0.78
41:G:125:LEU:HD21	78:t:947:A:C5	2.17	0.78
1:S2:1782:G:C6	58:X:73:ARG:HD2	2.19	0.78
9:SK:41:PRO:HG2	9:SK:44:HIS:HD2	1.46	0.78
54:T:164:LYS:HB3	54:T:165:PRO:HD2	1.63	0.78
22:Sg:226:HIS:HE2	22:Sg:229:THR:HG1	1.31	0.78
9:SK:29:MET:CA	9:SK:42:ASN:HD21	1.96	0.77
37:C:85:HIS:CA	81:y:20:LEU:HD21	2.15	0.77
41:G:125:LEU:CD2	78:t:947:A:C6	2.67	0.77
41:G:125:LEU:HD22	78:t:947:A:C6	2.19	0.77
67:h:83:CYS:O	67:h:84:ALA:HB3	1.83	0.77
44:J:61:TRP:HZ3	48:N:33:GLN:HE21	0.78	0.77
55:U:19:PHE:CE2	55:U:20:ARG:HD3	2.19	0.77
53:S:113:LYS:HE3	53:S:113:LYS:HA	1.66	0.77
66:g:54:LYS:HE2	78:t:437:G:H4'	1.59	0.77
2:SA:56:GLU:HB2	17:SV:79:VAL:CG1	2.12	0.77
17:SV:53:TYR:CZ	17:SV:72:LEU:CD1	2.68	0.77
66:g:54:LYS:CG	78:t:437:G:H5''	2.14	0.77
66:g:59:THR:HG22	78:t:4902:C:N3	2.00	0.77
66:g:104:MET:CG	66:g:106:TYR:CE2	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:b:46:ASP:C	61:b:48:TYR:H	1.93	0.76
64:e:96:GLU:O	64:e:97:ASP:O	2.03	0.76
1:S2:291:G:N7	10:SL:41:GLY:CA	2.49	0.75
61:b:37:GLY:CA	61:b:45:PHE:CE2	2.65	0.75
2:SA:123:VAL:HG21	2:SA:175:TRP:CH2	2.21	0.75
55:U:19:PHE:O	55:U:21:LYS:N	2.19	0.75
75:p:104:ILE:HD12	75:p:104:ILE:O	1.86	0.75
52:R:157:GLY:HA3	61:b:47:LYS:HA	1.69	0.74
78:t:465:A:H62	78:t:677:G:H21	1.34	0.74
41:G:125:LEU:HD23	78:t:947:A:N7	2.02	0.74
9:SK:27:VAL:CA	9:SK:43:LEU:CD1	2.66	0.74
51:Q:136:ILE:CB	81:y:21:GLY:O	2.36	0.74
47:M:77:SER:O	47:M:78:LEU:HB3	1.88	0.73
3:SB:86:LEU:CD2	3:SB:98:THR:HG21	2.18	0.73
2:SA:48:ILE:HD12	2:SA:48:ILE:N	2.03	0.73
37:C:84:THR:C	81:y:20:LEU:HD11	2.12	0.73
66:g:58:VAL:HG11	66:g:63:LYS:C	2.13	0.73
1:S2:291:G:N7	10:SL:41:GLY:C	2.46	0.73
23:SC:271:ASP:O	23:SC:275:LYS:HB2	1.89	0.72
1:S2:992:A:N7	19:Sa:15:ARG:NH2	2.37	0.72
54:T:160:ARG:CD	54:T:163:HIS:CG	2.62	0.72
61:b:37:GLY:HA3	61:b:45:PHE:HE2	1.55	0.72
78:t:197:U:H5	78:t:210:G:H1	1.38	0.72
78:t:703:C:H42	78:t:943:A:H61	1.37	0.72
1:S2:291:G:N9	10:SL:41:GLY:C	2.47	0.72
9:SK:27:VAL:CB	9:SK:43:LEU:HD12	2.18	0.72
1:S2:325:C:C2	1:S2:325:C:C1'	2.71	0.72
9:SK:41:PRO:HG2	9:SK:44:HIS:CD2	2.23	0.72
12:SQ:116:ASP:OD2	12:SQ:118:THR:CG2	2.38	0.72
19:Sa:10:ARG:HH12	19:Sa:12:LYS:HE3	1.55	0.72
47:M:136:LYS:NZ	47:M:138:ASP:O	2.22	0.72
66:g:104:MET:HG2	66:g:106:TYR:CD2	2.25	0.72
2:SA:123:VAL:CG2	2:SA:175:TRP:HH2	2.02	0.71
58:X:49:ILE:HD11	58:X:52:THR:HG21	1.70	0.71
66:g:5:LEU:O	66:g:105:LEU:CD2	2.37	0.71
78:t:3663:A:H62	78:t:3794:G:H21	1.37	0.71
23:SC:274:VAL:CG1	23:SC:278:THR:HG21	2.20	0.71
66:g:106:TYR:HB3	66:g:107:PRO:HD2	0.74	0.71
36:B:215:GLU:OE2	36:B:349:LYS:HG2	1.90	0.71
11:SP:44:ARG:HH22	11:SP:82:ASP:HB3	1.54	0.71
56:V:101:ARG:HG2	56:V:115:PHE:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:291:G:C8	1:S2:291:G:N7	2.59	0.71
54:T:160:ARG:HD2	54:T:163:HIS:CD2	2.25	0.71
58:X:46:PRO:O	58:X:49:ILE:CG1	2.38	0.71
58:X:49:ILE:HG13	58:X:52:THR:CG2	2.21	0.71
2:SA:56:GLU:CB	17:SV:79:VAL:HG11	2.20	0.70
37:C:54:VAL:HB	37:C:105:THR:O	1.91	0.70
66:g:59:THR:HG23	66:g:60:PRO:HD3	0.76	0.70
47:M:125:ILE:HD13	47:M:140:SER:HB3	1.71	0.70
66:g:59:THR:CG2	66:g:60:PRO:CD	2.49	0.70
37:C:55:SER:O	37:C:104:PRO:HB2	1.92	0.70
23:SC:274:VAL:CG1	23:SC:278:THR:CG2	2.63	0.70
54:T:164:LYS:HB3	54:T:165:PRO:HD3	1.72	0.70
55:U:16:SER:OG	78:t:4239:G:OP1	2.10	0.69
56:V:23:LEU:HD11	56:V:83:LEU:HD13	1.75	0.69
80:w:21:G:H1	82:u:34:C:H42	1.40	0.69
58:X:50:ASN:OD1	78:t:4964:U:C4	2.45	0.69
78:t:4710:U:H3	78:t:4909:G:H1	1.40	0.69
9:SK:43:LEU:H	9:SK:43:LEU:CD2	2.04	0.69
37:C:199:ARG:HH12	78:t:343:A:H4'	1.56	0.69
14:SS:3:LEU:HD12	14:SS:4:VAL:HG23	1.74	0.69
9:SK:29:MET:O	9:SK:42:ASN:ND2	2.26	0.69
14:SS:16:LEU:HD21	14:SS:72:GLN:HE22	1.58	0.69
12:SQ:116:ASP:O	12:SQ:118:THR:N	2.25	0.69
78:t:32:G:H1'	78:t:51:A:H61	1.57	0.69
78:t:4315:U:H5'	78:t:4316:U:H5'	1.74	0.69
9:SK:29:MET:CA	9:SK:42:ASN:ND2	2.56	0.68
49:O:39:ALA:HB2	49:O:63:ARG:HE	1.58	0.68
1:S2:561:A:N3	25:SJ:132:GLN:NE2	2.41	0.68
1:S2:1001:A:N7	19:Sa:19:GLN:NE2	2.42	0.68
66:g:58:VAL:HG11	66:g:64:PRO:CA	2.10	0.68
2:SA:122:LEU:CD2	2:SA:144:THR:HG22	2.21	0.68
9:SK:43:LEU:HD22	9:SK:43:LEU:N	2.05	0.68
48:N:31:ILE:HG22	54:T:75:VAL:CG1	2.24	0.68
66:g:106:TYR:CB	66:g:107:PRO:CD	2.38	0.67
1:S2:291:G:C8	10:SL:41:GLY:HA3	2.28	0.67
9:SK:27:VAL:CB	9:SK:43:LEU:CD1	2.70	0.67
72:m:45:ARG:HH21	78:t:2775:G:H5'	1.58	0.67
1:S2:291:G:N9	10:SL:42:LEU:N	2.43	0.67
17:SV:53:TYR:CZ	17:SV:72:LEU:HD11	2.26	0.67
1:S2:41:G:H1	1:S2:481:C:H42	1.41	0.67
1:S2:681:U:O2'	18:SX:8:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:51:HIS:O	12:SQ:50:LYS:NZ	2.25	0.67
56:V:23:LEU:HD21	56:V:83:LEU:HB3	1.74	0.67
58:X:73:ARG:O	58:X:74:ARG:HB2	1.93	0.67
66:g:33:VAL:HG23	66:g:38:GLU:HG3	1.77	0.67
2:SA:76:VAL:HG23	2:SA:123:VAL:HG13	1.75	0.67
3:SB:36:PRO:HB3	3:SB:231:LEU:HB3	1.77	0.67
12:SQ:117:ARG:O	12:SQ:121:VAL:HG21	1.94	0.67
8:SI:132:GLU:OE1	8:SI:132:GLU:N	2.28	0.67
23:SC:275:LYS:NZ	23:SC:275:LYS:HB3	2.10	0.67
83:a:15:ALA:HB3	83:a:79:HIS:HD2	1.60	0.67
1:S2:529:A:N6	1:S2:555:A:N7	2.43	0.67
5:SE:104:ASP:HB3	5:SE:110:ALA:HB2	1.77	0.67
58:X:18:GLY:HA2	58:X:32:LEU:HA	1.75	0.67
69:j:31:GLY:HA2	78:t:302:G:H21	1.59	0.67
8:SI:114:GLU:HB3	8:SI:136:ILE:HD13	1.77	0.67
41:G:245:GLN:NE2	41:G:249:ASP:OD2	2.28	0.67
52:R:65:ARG:NH2	78:t:1441:A:OP1	2.28	0.67
1:S2:1341:C:N4	1:S2:1486:A:N1	2.43	0.66
4:SD:49:ILE:HG22	4:SD:87:TYR:HB2	1.77	0.66
58:X:61:LYS:HB2	58:X:63:GLN:HE21	1.59	0.66
1:S2:1464:C:H4'	13:SR:60:ARG:HH22	1.59	0.66
36:B:246:ARG:NH2	78:t:4520:U:OP2	2.28	0.66
2:SA:77:ILE:HG22	2:SA:99:ILE:HB	1.77	0.66
38:D:85:U:H2'	38:D:86:U:H2'	1.77	0.66
47:M:76:PHE:CE2	47:M:96:ILE:HG23	2.30	0.66
53:S:103:ARG:NH1	53:S:124:TYR:OH	2.28	0.66
78:t:2689:C:H5'	78:t:2690:G:H5''	1.76	0.66
54:T:160:ARG:HG2	54:T:163:HIS:CB	2.26	0.66
79:v:55:U:H2'	79:v:56:C:H2'	1.77	0.66
1:S2:429:C:OP1	5:SE:10:LYS:NZ	2.28	0.66
66:g:104:MET:CG	66:g:106:TYR:HE2	2.04	0.66
2:SA:123:VAL:CG2	2:SA:175:TRP:CH2	2.78	0.66
4:SD:95:GLY:HA3	4:SD:125:PHE:CE2	2.30	0.66
7:SH:144:ILE:HD13	7:SH:154:ILE:HG13	1.77	0.66
78:t:484:C:O2	78:t:658:G:N2	2.29	0.66
7:SH:154:ILE:HB	7:SH:185:VAL:HG12	1.78	0.66
9:SK:29:MET:N	9:SK:42:ASN:ND2	2.38	0.66
41:G:126:LEU:CD1	78:t:958:U:H5'	2.25	0.66
2:SA:37:TYR:O	2:SA:49:ILE:HG23	1.95	0.65
53:S:67:THR:HA	53:S:70:ARG:HG2	1.78	0.65
78:t:4514:U:H2'	78:t:4515:A:H8	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:19:PHE:HE2	55:U:20:ARG:CD	2.06	0.65
56:V:28:PRO:HG3	56:V:100:LEU:HD21	1.78	0.65
78:t:2401:C:HO2'	78:t:3828:G:HO2'	1.44	0.65
1:S2:874:G:H21	7:SH:114:GLN:HE22	1.44	0.65
34:Sf:94:LYS:HE2	34:Sf:94:LYS:CA	2.12	0.65
53:S:99:MET:HG2	53:S:103:ARG:HE	1.62	0.65
1:S2:1748:G:H1	1:S2:1786:U:H3	1.45	0.65
4:SD:40:ARG:HH21	4:SD:47:GLU:HG2	1.62	0.65
28:SO:103:ASN:HD21	28:SO:142:ARG:HA	1.60	0.65
1:S2:325:C:N4	1:S2:329:G:O2'	2.29	0.65
4:SD:40:ARG:HG3	16:SU:108:PRO:HG3	1.76	0.65
61:b:26:ARG:NH2	78:t:1638:U:OP2	2.30	0.65
61:b:7:LYS:NZ	78:t:2264:A:OP2	2.30	0.65
66:g:54:LYS:CD	78:t:437:G:C5'	2.65	0.65
29:SW:55:ASP:OD2	29:SW:57:ARG:NH1	2.25	0.65
5:SE:71:LYS:HB2	5:SE:91:SER:HB2	1.79	0.65
9:SK:29:MET:HB3	9:SK:42:ASN:HD22	1.60	0.65
37:C:71:ARG:O	37:C:72:ALA:HB2	1.96	0.65
54:T:164:LYS:CB	54:T:165:PRO:CD	2.70	0.65
58:X:70:LYS:HD3	58:X:71:ARG:HG2	1.78	0.65
63:d:8:LYS:HG3	63:d:9:LYS:HD3	1.79	0.65
53:S:104:ARG:HH12	78:t:2877:G:H5''	1.61	0.65
41:G:261:ILE:HG23	41:G:267:LEU:HD12	1.79	0.64
78:t:2372:C:OP2	78:t:2373:G:N2	2.30	0.64
26:SM:68:LEU:O	26:SM:72:HIS:ND1	2.26	0.64
58:X:49:ILE:HD12	58:X:52:THR:HB	1.78	0.64
35:A:216:HIS:HB2	35:A:218:HIS:HD2	1.63	0.64
2:SA:77:ILE:HG12	2:SA:122:LEU:HD12	1.79	0.64
7:SH:12:ASN:ND2	7:SH:17:ASP:OD1	2.30	0.64
55:U:8:ARG:NH1	78:t:4295:C:O2'	2.30	0.64
61:b:47:LYS:HG2	61:b:48:TYR:CD2	2.32	0.64
26:SM:47:ALA:HA	26:SM:112:LYS:HA	1.79	0.64
2:SA:121:LEU:HD21	2:SA:145:ILE:HD13	1.79	0.64
5:SE:207:VAL:HA	5:SE:221:ARG:HA	1.80	0.64
49:O:179:LYS:NZ	78:t:292:G:OP1	2.31	0.64
58:X:49:ILE:HG13	58:X:52:THR:HG22	1.79	0.64
1:S2:291:G:H1'	5:SE:202:PRO:HB3	1.80	0.64
61:b:47:LYS:HD3	61:b:48:TYR:CE2	2.32	0.64
1:S2:325:C:C6	1:S2:325:C:C1'	2.76	0.64
2:SA:33:GLN:NE2	17:SV:64:GLU:OE1	2.30	0.64
5:SE:73:ASP:OD2	5:SE:145:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q:80:GLN:NE2	78:t:3863:U:O2'	2.31	0.64
5:SE:41:CYS:SG	5:SE:42:LEU:N	2.70	0.63
38:D:86:U:H4'	38:D:87:G:H2'	1.79	0.63
62:c:57:MET:HE2	78:t:1794:C:H5'	1.80	0.63
78:t:1534:G:O2'	78:t:1556:G:N2	2.29	0.63
66:g:104:MET:CG	66:g:106:TYR:CD2	2.82	0.63
78:t:443:C:N4	78:t:444:G:N7	2.46	0.63
40:F:4:VAL:N	78:t:1760:C:HO2'	1.96	0.63
67:h:78:TYR:HB3	67:h:82:MET:HG3	1.81	0.63
5:SE:35:PRO:HB2	5:SE:143:ASP:HB2	1.80	0.63
47:M:76:PHE:CZ	47:M:117:LEU:HD13	2.33	0.63
14:SS:23:ARG:O	31:SZ:80:ARG:NH1	2.31	0.63
22:Sg:87:LEU:HB2	22:Sg:101:PHE:HB2	1.81	0.63
53:S:133:LYS:H	53:S:137:ILE:HD11	1.64	0.63
56:V:105:ASN:ND2	56:V:111:GLU:OE1	2.32	0.63
58:X:49:ILE:CD1	58:X:52:THR:HG21	2.28	0.63
78:t:161:G:H1	78:t:266:U:H3	1.44	0.63
1:S2:1812:U:O4	1:S2:1813:A:N6	2.31	0.63
17:SV:16:LYS:NZ	23:SC:257:LYS:O	2.32	0.63
37:C:85:HIS:HA	81:y:20:LEU:CD2	2.21	0.63
1:S2:291:G:N7	10:SL:41:GLY:O	2.32	0.63
1:S2:683:OMG:N1	1:S2:1022:U:OP2	2.29	0.63
25:SJ:37:LEU:HD23	25:SJ:42:GLU:HG3	1.80	0.63
34:Sf:93:HIS:HE1	34:Sf:96:LYS:HD2	1.63	0.63
43:I:73:ARG:NH2	78:t:4124:C:O2	2.31	0.63
66:g:58:VAL:HG13	66:g:64:PRO:C	2.21	0.63
2:SA:40:LYS:C	2:SA:48:ILE:HD11	2.24	0.63
36:B:5:LYS:O	36:B:6:PHE:CG	2.51	0.63
36:B:108:GLU:OE2	36:B:138:GLN:NE2	2.32	0.63
1:S2:936:G:O6	63:d:8:LYS:NZ	2.30	0.62
22:Sg:256:ILE:HB	22:Sg:270:LEU:HB2	1.79	0.62
54:T:28:TYR:OH	54:T:52:LYS:NZ	2.33	0.62
66:g:59:THR:CB	78:t:4902:C:N4	2.62	0.62
83:a:104:PRO:O	83:a:108:ARG:NH1	2.32	0.62
1:S2:1040:G:H5''	76:q:25:MET:HE2	1.81	0.62
39:E:110:G:O6	40:F:21:ARG:NH1	2.32	0.62
3:SB:57:ILE:HD12	3:SB:59:SER:H	1.64	0.62
12:SQ:116:ASP:CG	12:SQ:118:THR:HG23	2.23	0.62
24:SG:139:SER:HA	24:SG:142:ARG:HB3	1.81	0.62
37:C:85:HIS:CG	81:y:20:LEU:HD21	2.32	0.62
51:Q:136:ILE:HG13	81:y:21:GLY:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:u:1:G:N2	82:u:73:A:N7	2.47	0.62
38:D:52:A:H4'	72:m:19:GLN:HA	1.81	0.62
61:b:89:ASN:ND2	78:t:504:U:O2'	2.32	0.62
19:Sa:51:ARG:NH1	19:Sa:52:ASP:OD1	2.30	0.62
37:C:54:VAL:HG21	37:C:105:THR:C	2.24	0.62
60:Z:8:THR:O	78:t:223:G:N2	2.33	0.62
77:r:84:LYS:NZ	78:t:672:G:OP1	2.30	0.62
78:t:174:G:H1	78:t:254:C:H41	1.47	0.62
2:SA:41:ARG:HA	2:SA:47:TYR:CD1	2.34	0.62
66:g:105:LEU:HD22	66:g:105:LEU:N	2.15	0.62
26:SM:35:ILE:HD12	26:SM:36:ARG:HG3	1.81	0.62
77:r:107:ARG:NH2	78:t:2242:A:OP1	2.32	0.62
1:S2:812:A:H5'	5:SE:16:LYS:HD3	1.81	0.62
32:Sb:36:LYS:HB3	32:Sb:78:SER:HB3	1.82	0.62
43:I:230:TYR:HA	43:I:233:ILE:HG22	1.82	0.62
64:e:96:GLU:OE1	64:e:96:GLU:HA	1.97	0.62
78:t:4853:C:N4	78:t:4854:G:N3	2.48	0.62
1:S2:291:G:C8	1:S2:291:G:N9	2.67	0.62
1:S2:509:OMG:H2'	1:S2:510:G:C8	2.35	0.62
1:S2:526:A:H61	1:S2:558:G:H22	1.47	0.62
1:S2:928:G:H1	1:S2:1013:U:H3	1.47	0.62
9:SK:27:VAL:CA	9:SK:43:LEU:HD11	2.28	0.62
37:C:56:GLU:H	37:C:56:GLU:CD	2.08	0.62
61:b:65:ARG:NH2	78:t:86:U:O2'	2.32	0.62
78:t:162:A:H61	78:t:265:C:H42	1.47	0.62
78:t:474:C:N3	78:t:669:G:N2	2.48	0.62
3:SB:86:LEU:CD2	3:SB:98:THR:OG1	2.47	0.61
10:SL:12:LYS:HB2	10:SL:18:GLN:HE22	1.64	0.61
14:SS:25:LYS:HA	14:SS:55:ARG:HA	1.82	0.61
36:B:174:ARG:NH2	78:t:4943:U:O2	2.32	0.61
41:G:125:LEU:HD22	78:t:947:A:N6	2.14	0.61
78:t:2586:C:H2'	78:t:2587:G:H8	1.64	0.61
1:S2:1678:A2M:N6	6:SF:57:ALA:O	2.32	0.61
1:S2:1704:C:N4	80:w:18:G:OP1	2.30	0.61
7:SH:144:ILE:HD11	7:SH:152:ARG:HB2	1.82	0.61
12:SQ:19:ALA:HB2	12:SQ:75:GLY:HA3	1.82	0.61
38:D:87:G:OP2	68:i:5:LYS:NZ	2.31	0.61
41:G:128:HIS:CD2	78:t:1265:G:N7	2.64	0.61
58:X:44:ARG:HE	78:t:3586:G:H1'	1.64	0.61
17:SV:74:LYS:O	17:SV:81:LYS:HD2	2.01	0.61
36:B:223:THR:O	36:B:343:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:4647:U:O4	78:t:4668:G:N2	2.33	0.61
1:S2:165:G:H2'	1:S2:166:A2M:H8	1.82	0.61
47:M:76:PHE:HE2	47:M:96:ILE:HG23	1.64	0.61
55:U:51:GLY:HA3	55:U:92:ARG:HG3	1.81	0.61
78:t:133:C:N4	78:t:135:G:N3	2.47	0.61
78:t:1086:C:N3	78:t:1178:G:O2'	2.33	0.61
1:S2:495:U:OP1	5:SE:49:ARG:NH1	2.33	0.61
10:SL:13:GLN:NE2	10:SL:63:THR:OG1	2.33	0.61
49:O:22:LEU:HA	49:O:25:VAL:HG12	1.83	0.61
1:S2:926:A:H61	1:S2:1015:U:H3	1.47	0.61
1:S2:1587:G:H2'	15:ST:78:ILE:HG22	1.83	0.61
42:H:94:ARG:HB2	42:H:114:LEU:HD23	1.82	0.61
42:H:232:ASP:HB2	42:H:236:ARG:HH22	1.65	0.61
60:Z:126:ARG:NH1	78:t:193:C:OP1	2.33	0.61
67:h:98:GLU:OE2	78:t:4091:G:N2	2.31	0.61
78:t:1955:U:N3	78:t:1983:A:N7	2.49	0.61
3:SB:86:LEU:HD21	3:SB:98:THR:OG1	2.00	0.61
12:SQ:116:ASP:C	12:SQ:118:THR:N	2.59	0.61
54:T:159:LEU:O	54:T:161:ARG:NH1	2.34	0.61
1:S2:1060:A:O2'	1:S2:1062:A:N7	2.32	0.61
1:S2:1305:C:OP1	34:Sf:96:LYS:NZ	2.32	0.61
6:SF:195:GLU:OE1	6:SF:198:ARG:NH2	2.32	0.61
19:Sa:23:CYS:SG	19:Sa:24:THR:N	2.74	0.61
41:G:125:LEU:HD23	41:G:125:LEU:O	2.01	0.61
48:N:47:ARG:HD3	54:T:73:LEU:HD13	1.80	0.61
78:t:198:C:H42	78:t:209:A:H61	1.46	0.61
1:S2:325:C:C2	58:X:119:LYS:CE	2.84	0.61
8:SI:48:VAL:HG11	8:SI:54:LYS:HE3	1.82	0.61
12:SQ:76:GLY:H	12:SQ:79:ALA:HB3	1.65	0.61
13:SR:94:GLU:OE1	13:SR:116:ASN:ND2	2.34	0.61
41:G:136:HIS:CD2	78:t:702:A:H1'	2.36	0.61
1:S2:325:C:C2	58:X:119:LYS:CD	2.84	0.61
51:Q:136:ILE:CG1	81:y:21:GLY:O	2.48	0.61
1:S2:886:A:H61	1:S2:901:G:H1	1.46	0.60
8:SI:67:TRP:NE1	8:SI:70:GLU:OE1	2.33	0.60
10:SL:124:ASP:HA	10:SL:148:ALA:HB3	1.83	0.60
29:SW:102:ILE:HG13	29:SW:113:HIS:HB3	1.83	0.60
36:B:10:ARG:NH1	36:B:11:HIS:O	2.34	0.60
58:X:73:ARG:O	58:X:74:ARG:CB	2.49	0.60
3:SB:88:THR:HG22	3:SB:88:THR:O	2.00	0.60
28:SO:57:THR:HG22	28:SO:59:GLY:H	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:c:50:ASN:HA	62:c:54:LEU:HD21	1.84	0.60
78:t:463:C:N4	78:t:680:C:O2	2.34	0.60
1:S2:692:G:N7	1:S2:734:C:N4	2.44	0.60
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	1.83	0.60
42:H:223:LYS:HD2	78:t:1888:A:H4'	1.81	0.60
54:T:101:THR:HG23	54:T:104:GLY:H	1.66	0.60
64:e:95:ASP:C	64:e:97:ASP:N	2.57	0.60
78:t:510:C:O2	78:t:639:G:N2	2.26	0.60
78:t:4381:U:OP1	78:t:4437:G:N2	2.32	0.60
81:y:19:ILE:HG12	81:y:19:ILE:O	2.01	0.60
1:S2:974:C:H2'	1:S2:975:G:H8	1.66	0.60
23:SC:274:VAL:HG22	23:SC:278:THR:HG21	1.82	0.60
17:SV:19:ALA:O	29:SW:23:ARG:NH2	2.34	0.60
31:SZ:99:LEU:HD11	31:SZ:102:LYS:HB2	1.82	0.60
41:G:126:LEU:HD13	78:t:958:U:H5'	1.82	0.60
48:N:31:ILE:HG22	54:T:75:VAL:HG11	1.82	0.60
51:Q:118:GLN:NE2	51:Q:147:GLU:OE1	2.32	0.60
78:t:445:C:N4	78:t:1278:C:N3	2.49	0.60
70:k:19:CYS:SG	70:k:20:ARG:N	2.75	0.60
78:t:490:G:N2	78:t:652:C:O2	2.34	0.60
58:X:54:LEU:O	58:X:58:LYS:CG	2.48	0.60
1:S2:844:U:OP1	5:SE:240:ARG:NH2	2.34	0.60
11:SP:30:TYR:HA	11:SP:33:LEU:HB2	1.84	0.60
15:ST:11:GLN:OE1	15:ST:62:ARG:NH2	2.35	0.60
35:A:123:ARG:NH1	78:t:4053:U:OP1	2.34	0.60
78:t:1977:C:H42	78:t:1980:A:H3'	1.67	0.60
81:y:16:ILE:HG13	81:y:17:PRO:HD3	1.84	0.60
2:SA:76:VAL:HG23	2:SA:123:VAL:CG1	2.31	0.60
6:SF:140:ASP:HB2	20:Sc:46:VAL:HG12	1.84	0.60
9:SK:42:ASN:OD1	9:SK:42:ASN:N	2.31	0.60
15:ST:37:VAL:HG22	15:ST:39:LEU:H	1.66	0.60
47:M:149:GLN:NE2	68:i:121:VAL:O	2.35	0.60
65:f:128:ARG:NH2	78:t:2285:G:OP1	2.35	0.60
75:p:39:ARG:NH1	78:t:289:A:OP2	2.35	0.60
1:S2:145:G:N7	24:SG:178:ARG:NH2	2.50	0.60
1:S2:990:A:OP1	3:SB:116:LYS:NZ	2.34	0.60
5:SE:92:ILE:HG22	5:SE:94:LYS:H	1.67	0.60
37:C:71:ARG:O	37:C:72:ALA:CB	2.50	0.60
50:P:90:HIS:O	50:P:96:GLN:NE2	2.35	0.60
62:c:51:LYS:NZ	78:t:1384:C:OP1	2.35	0.60
1:S2:1546:G:N2	1:S2:1670:C:O2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1692:U:O3'	19:Sa:89:ARG:NH1	2.34	0.59
5:SE:137:PRO:HG2	5:SE:150:PRO:HD2	1.84	0.59
8:SI:8:TRP:HZ2	8:SI:24:LYS:HB3	1.66	0.59
55:U:87:LYS:HZ3	78:t:4267:G:H22	1.50	0.59
1:S2:322:C:O2'	1:S2:324:C:N4	2.34	0.59
1:S2:1262:C:O2'	21:Sd:12:ARG:NH1	2.35	0.59
55:U:63:ARG:NH2	62:c:30:GLU:OE2	2.35	0.59
68:i:109:ARG:HA	68:i:112:ARG:HG2	1.84	0.59
1:S2:1199:A:OP1	19:Sa:2:THR:N	2.35	0.59
2:SA:110:ASN:HB3	2:SA:113:GLN:HE22	1.66	0.59
3:SB:59:SER:HB3	3:SB:63:LYS:HE2	1.84	0.59
37:C:303:ARG:NH2	78:t:2067:G:OP1	2.36	0.59
78:t:1071:C:H42	78:t:1190:C:H42	1.51	0.59
78:t:1956:G:N2	78:t:1964:A:OP1	2.35	0.59
1:S2:291:G:C4	10:SL:42:LEU:N	2.69	0.59
2:SA:123:VAL:HG22	2:SA:175:TRP:HH2	1.66	0.59
2:SA:147:LEU:HA	2:SA:161:ILE:HB	1.82	0.59
30:SY:110:ARG:HH22	30:SY:127:ALA:H	1.50	0.59
73:n:99:CYS:HB3	73:n:115:CYS:HB3	1.84	0.59
78:t:274:G:N2	78:t:300:A:OP2	2.35	0.59
48:N:28:VAL:HG12	48:N:67:SER:HA	1.85	0.59
52:R:39:THR:O	52:R:132:LYS:NZ	2.34	0.59
78:t:2245:C:O2	78:t:2247:A:N6	2.36	0.59
1:S2:1147:C:OP1	19:Sa:6:ARG:NH1	2.35	0.59
1:S2:1751:C:N4	1:S2:1782:G:OP2	2.36	0.59
37:C:50:GLN:OE1	78:t:1354:A:N6	2.36	0.59
38:D:86:U:O2'	68:i:5:LYS:NZ	2.36	0.59
52:R:38:ARG:NH1	78:t:2068:C:OP2	2.35	0.59
61:b:116:LYS:NZ	78:t:1403:A:OP2	2.35	0.59
82:u:17:C:H5'	82:u:18:G:H4'	1.85	0.59
82:u:62:C:N4	82:u:63:G:O6	2.36	0.59
1:S2:613:G:N2	1:S2:626:G:OP1	2.32	0.59
1:S2:1256:G:N2	21:Sd:30:LEU:O	2.35	0.59
19:Sa:45:VAL:HG21	19:Sa:64:LEU:HD22	1.84	0.59
68:i:27:GLU:HA	68:i:30:GLN:HG2	1.84	0.59
72:m:27:ILE:O	72:m:33:ASN:ND2	2.36	0.59
16:SU:18:HIS:HD2	16:SU:94:PRO:HA	1.68	0.59
37:C:71:ARG:NH1	81:y:26:ILE:HA	2.13	0.59
46:L:64:ARG:O	75:p:103:VAL:HG23	2.02	0.59
53:S:103:ARG:NH1	78:t:2645:U:OP2	2.36	0.59
60:Z:13:LYS:NZ	78:t:340:G:OP2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:e:87:ARG:HH21	64:e:109:VAL:HG11	1.68	0.59
75:p:103:VAL:O	75:p:103:VAL:HG13	2.02	0.59
81:y:22:ILE:HG12	81:y:24:GLY:N	2.12	0.59
83:a:5:MET:O	83:a:28:ASN:ND2	2.35	0.59
1:S2:1751:C:H5''	58:X:76:VAL:HB	1.85	0.59
8:SI:69:SER:OG	8:SI:70:GLU:OE1	2.20	0.59
37:C:323:ARG:HA	37:C:326:LEU:HB2	1.85	0.59
47:M:125:ILE:HD13	47:M:140:SER:CB	2.32	0.59
78:t:4284:G:N2	78:t:4287:A:OP2	2.35	0.59
81:y:22:ILE:HG12	81:y:23:LEU:N	2.18	0.59
1:S2:444:G:N1	1:S2:447:A:OP2	2.36	0.59
16:SU:63:ILE:HD11	21:Sd:31:ILE:HD13	1.85	0.59
1:S2:798:A:O2'	7:SH:111:LYS:O	2.21	0.58
1:S2:919:A:OP2	27:SN:64:ARG:NH2	2.36	0.58
36:B:224:LYS:HD3	36:B:340:THR:HG22	1.83	0.58
43:I:81:ASN:ND2	43:I:237:TRP:O	2.36	0.58
66:g:58:VAL:CG1	66:g:63:LYS:O	2.32	0.58
77:r:94:ARG:NH2	78:t:2241:G:OP1	2.36	0.58
13:SR:13:ALA:HB2	13:SR:50:ILE:HG23	1.86	0.58
47:M:77:SER:OG	47:M:102:ARG:HD3	2.04	0.58
78:t:1390:C:OP1	78:t:1392:C:N4	2.36	0.58
83:a:88:ASP:HB3	83:a:121:ARG:HH12	1.69	0.58
1:S2:1289:U:OP2	34:Sf:97:LYS:NZ	2.33	0.58
22:Sg:8:ARG:NH1	22:Sg:311:GLN:OE1	2.36	0.58
48:N:11:ARG:HE	48:N:61:ILE:HG22	1.69	0.58
49:O:49:ARG:NH1	78:t:149:U:OP2	2.37	0.58
1:S2:419:G:N2	1:S2:661:U:O2	2.37	0.58
1:S2:539:C:N4	1:S2:542:U:OP2	2.36	0.58
1:S2:1513:C:OP2	21:Sd:12:ARG:NH2	2.37	0.58
1:S2:1610:G:OP1	14:SS:121:ARG:NH2	2.36	0.58
3:SB:150:ILE:HG23	13:SR:131:PRO:HA	1.86	0.58
47:M:35:ARG:NH2	78:t:331:U:OP1	2.36	0.58
49:O:97:SER:HB3	78:t:294:A:H5''	1.86	0.58
53:S:99:MET:SD	53:S:103:ARG:NH2	2.71	0.58
1:S2:1299:A:OP1	11:SP:59:ARG:NH1	2.36	0.58
13:SR:103:LYS:HD2	13:SR:119:VAL:HG11	1.84	0.58
38:D:70:G:O2'	38:D:87:G:N2	2.36	0.58
56:V:75:GLU:CD	56:V:75:GLU:H	2.07	0.58
78:t:376:G:H4'	78:t:401:A:H61	1.68	0.58
18:SX:63:ASN:ND2	18:SX:114:ASP:OD2	2.37	0.58
29:SW:20:ARG:HG2	29:SW:22:LYS:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:k:9:GLY:HA3	78:t:2779:G:H1'	1.84	0.58
78:t:2378:G:O2'	78:t:2801:G:O2'	2.22	0.58
1:S2:1113:A:H4'	3:SB:202:GLN:HE22	1.67	0.58
23:SC:274:VAL:HG12	23:SC:274:VAL:O	2.03	0.58
42:H:194:ILE:HG13	42:H:201:PHE:HE1	1.69	0.58
59:Y:107:HIS:O	59:Y:111:GLN:NE2	2.36	0.58
1:S2:74:G:H21	1:S2:75:G:H22	1.52	0.58
35:A:13:GLY:O	35:A:17:ARG:NH1	2.37	0.58
43:I:157:ILE:HD12	43:I:170:LEU:HD22	1.85	0.58
49:O:181:HIS:NE2	78:t:286:G:O6	2.37	0.58
52:R:172:ARG:HD2	61:b:57:GLY:HA3	1.85	0.58
58:X:49:ILE:CG1	58:X:52:THR:HG21	2.34	0.58
78:t:485:G:O6	78:t:655:A:N6	2.37	0.58
8:SI:141:ARG:HD2	8:SI:145:ILE:HG21	1.84	0.58
37:C:7:LEU:HB3	37:C:21:ASN:HB3	1.86	0.58
37:C:250:CYS:SG	37:C:252:TRP:NE1	2.75	0.58
40:F:50:ARG:NH1	40:F:147:ASP:OD2	2.35	0.58
44:J:59:LYS:HE2	44:J:66:GLU:HB3	1.85	0.58
51:Q:127:ARG:NH1	78:t:2399:A:OP2	2.37	0.58
66:g:19:ARG:NH2	78:t:1870:U:OP1	2.37	0.58
78:t:3612:U:OP2	78:t:3617:A:N6	2.37	0.58
1:S2:509:OMG:H2'	1:S2:510:G:H8	1.68	0.58
1:S2:626:G:O6	80:w:20:G:N2	2.37	0.58
2:SA:48:ILE:HD12	2:SA:48:ILE:H	1.67	0.58
10:SL:35:ARG:NH1	10:SL:53:GLY:O	2.36	0.58
22:Sg:154:VAL:O	22:Sg:155:ARG:NH1	2.35	0.58
36:B:2:SER:O	36:B:3:HIS:O	2.22	0.58
1:S2:1597:C:OP2	31:SZ:85:ARG:NH2	2.34	0.57
7:SH:5:SER:N	7:SH:25:GLN:OE1	2.37	0.57
61:b:45:PHE:O	61:b:49:HIS:HB2	2.03	0.57
67:h:111:ALA:O	67:h:115:LYS:NZ	2.35	0.57
1:S2:165:G:OP2	1:S2:165:G:N2	2.37	0.57
1:S2:482:G:H21	1:S2:484:A2M:H8	1.69	0.57
1:S2:1156:U:O4	23:SC:194:ARG:NH1	2.37	0.57
1:S2:1782:G:O6	58:X:73:ARG:CD	2.50	0.57
6:SF:100:ILE:HD11	6:SF:177:LEU:HD21	1.85	0.57
6:SF:118:ASN:ND2	6:SF:181:ALA:O	2.36	0.57
9:SK:53:LYS:HD3	9:SK:60:GLU:HG2	1.87	0.57
35:A:96:LEU:H	76:q:92:GLN:HE22	1.51	0.57
36:B:247:GLY:HA2	78:t:2817:G:H5'	1.84	0.57
41:G:132:PRO:O	41:G:136:HIS:CE1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:j:50:PHE:O	69:j:55:ARG:NH1	2.37	0.57
78:t:1061:A:H2	78:t:1216:G:H1	1.51	0.57
78:t:1579:G:N2	86:t:5112:MVM:O1	2.36	0.57
23:SC:274:VAL:HA	23:SC:278:THR:HG23	1.86	0.57
37:C:106:LYS:NZ	78:t:1499:G:O6	2.37	0.57
41:G:177:GLY:HA3	41:G:182:ASN:HD22	1.69	0.57
50:P:118:MET:HG2	54:T:169:THR:HG22	1.85	0.57
75:p:104:ILE:HD12	75:p:104:ILE:C	2.29	0.57
1:S2:656:G:N3	23:SC:227:ARG:NH2	2.52	0.57
1:S2:1543:U:OP2	15:ST:62:ARG:NH1	2.35	0.57
5:SE:122:LYS:NZ	5:SE:143:ASP:OD2	2.37	0.57
23:SC:274:VAL:O	23:SC:278:THR:OG1	2.22	0.57
35:A:208:GLU:OE2	78:t:1611:G:N2	2.32	0.57
42:H:126:ASN:HB3	42:H:129:SER:H	1.69	0.57
52:R:158:THR:CB	52:R:159:PRO:HD2	2.33	0.57
53:S:28:GLU:HB3	53:S:31:GLU:HB3	1.86	0.57
78:t:4333:G:N2	79:v:76:A:O2'	2.38	0.57
1:S2:678:U:OP2	1:S2:1026:C:N4	2.35	0.57
2:SA:42:LYS:HD3	2:SA:46:ILE:HB	1.85	0.57
3:SB:121:ILE:HD11	3:SB:207:LEU:HD21	1.86	0.57
5:SE:44:LEU:HD11	5:SE:70:ILE:HG21	1.86	0.57
8:SI:124:LYS:HG2	8:SI:125:LYS:HG2	1.86	0.57
31:SZ:49:LEU:H	31:SZ:83:LEU:HD22	1.69	0.57
70:k:12:ARG:NH2	78:t:1599:G:O3'	2.37	0.57
1:S2:1277:C:H5'	9:SK:55:ARG:HD3	1.85	0.57
16:SU:20:ILE:HD11	16:SU:91:LEU:HD12	1.86	0.57
16:SU:99:LYS:NZ	16:SU:103:SER:OG	2.37	0.57
32:Sb:56:CYS:SG	32:Sb:57:VAL:N	2.78	0.57
37:C:78:ARG:NH2	78:t:2331:U:OP1	2.37	0.57
41:G:125:LEU:CD2	78:t:947:A:N7	2.65	0.57
46:L:90:ARG:NH2	46:L:108:GLY:O	2.37	0.57
52:R:63:LEU:HB2	52:R:88:ASP:HA	1.87	0.57
75:p:12:CYS:SG	75:p:19:GLN:NE2	2.77	0.57
78:t:1380:A:HO2'	78:t:1449:C:HO2'	1.49	0.57
78:t:2766:A:H2	78:t:2780:U:H3	1.52	0.57
78:t:3624:A:N6	78:t:3662:G:O2'	2.37	0.57
79:v:60:U:OP1	79:v:62:C:N4	2.37	0.57
82:u:9:A:OP2	82:u:13:C:N4	2.35	0.57
1:S2:29:G:H5'	18:SX:124:LYS:HD2	1.85	0.57
36:B:3:HIS:O	36:B:3:HIS:ND1	2.37	0.57
36:B:220:ILE:HG12	36:B:278:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:g:58:VAL:CG2	66:g:62:GLY:O	2.46	0.57
78:t:1741:G:H1	78:t:1755:U:H3	1.52	0.57
78:t:1851:C:H2'	78:t:1852:A:H8	1.70	0.57
78:t:4489:G:N2	78:t:4489:G:OP2	2.35	0.57
78:t:4865:G:N2	78:t:4872:C:O2	2.32	0.57
82:u:64:A:H2'	82:u:65:G:H8	1.69	0.57
1:S2:566:U:H3	1:S2:584:G:H1	1.52	0.57
4:SD:205:PRO:HA	13:SR:42:PRO:HG2	1.87	0.57
18:SX:92:ASN:ND2	33:Se:9:ALA:O	2.37	0.57
46:L:35:ARG:NH1	46:L:122:SER:O	2.38	0.57
60:Z:9:SER:HA	78:t:223:G:H21	1.70	0.57
77:r:26:SER:HB2	77:r:36:ASN:HB3	1.87	0.57
78:t:727:C:H42	78:t:914:G:H1	1.50	0.57
78:t:2455:G:H1	78:t:2480:C:H42	1.53	0.57
78:t:4163:G:O2'	78:t:4165:A:N6	2.38	0.57
14:SS:15:VAL:HG12	14:SS:16:LEU:HD12	1.87	0.57
22:Sg:5:MET:HB3	22:Sg:310:TRP:HB3	1.87	0.57
22:Sg:199:THR:HG21	22:Sg:240:CYS:HA	1.87	0.57
50:P:173:GLN:OE1	50:P:176:ARG:NH1	2.38	0.57
53:S:3:MET:HG3	53:S:5:ARG:H	1.69	0.57
71:l:37:ARG:NH1	78:t:2516:A:OP2	2.37	0.57
78:t:196:G:N2	78:t:206:U:OP1	2.37	0.57
78:t:4351:C:H2'	78:t:4352:A:H8	1.68	0.57
1:S2:1240:A:N6	11:SP:122:THR:O	2.37	0.57
5:SE:180:LEU:HB3	5:SE:229:GLY:HA3	1.86	0.57
22:Sg:32:LEU:HB3	22:Sg:42:MET:HG2	1.86	0.57
41:G:108:LYS:HD2	41:G:111:LYS:HG2	1.87	0.57
46:L:150:CYS:SG	46:L:151:ILE:N	2.78	0.57
49:O:93:LYS:NZ	78:t:281:U:O2	2.38	0.57
55:U:19:PHE:CD2	55:U:20:ARG:CA	2.88	0.57
63:d:32:LYS:HA	63:d:35:LEU:HB2	1.87	0.57
78:t:4713:G:N2	78:t:4907:G:O6	2.36	0.57
6:SF:140:ASP:OD2	20:Sc:44:ARG:NH1	2.37	0.56
9:SK:27:VAL:HA	9:SK:43:LEU:CD1	2.35	0.56
13:SR:89:SER:O	13:SR:93:GLN:NE2	2.38	0.56
27:SN:46:THR:HG22	27:SN:49:GLN:HG2	1.86	0.56
36:B:60:VAL:HG11	36:B:67:VAL:HG12	1.86	0.56
40:F:60:ILE:HG22	40:F:80:ALA:HB2	1.87	0.56
53:S:21:LYS:NZ	78:t:2800:U:OP1	2.38	0.56
62:c:57:MET:O	62:c:61:ASN:ND2	2.38	0.56
66:g:10:ILE:HA	66:g:100:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:n:122:ARG:NH2	78:t:4435:A:O2'	2.38	0.56
4:SD:101:GLN:O	4:SD:105:LEU:N	2.34	0.56
8:SI:78:ILE:HA	8:SI:104:ILE:HG22	1.87	0.56
9:SK:4:PRO:HG2	9:SK:7:ASN:HB2	1.86	0.56
35:A:117:GLU:HG2	35:A:124:GLY:H	1.70	0.56
39:E:83:A:O2'	39:E:85:G:OP1	2.23	0.56
49:O:49:ARG:NH2	78:t:150:G:OP2	2.38	0.56
53:S:113:LYS:HE3	53:S:113:LYS:CA	2.29	0.56
73:n:96:CYS:SG	73:n:97:ARG:N	2.78	0.56
2:SA:36:GLN:O	2:SA:53:ARG:NH1	2.39	0.56
6:SF:170:ALA:HB3	31:SZ:106:GLN:HE21	1.69	0.56
20:Sc:14:VAL:HG12	20:Sc:32:VAL:HG12	1.86	0.56
22:Sg:236:ILE:HG22	22:Sg:252:THR:HA	1.86	0.56
36:B:19:ARG:NH2	78:t:4585:G:OP1	2.38	0.56
36:B:35:ASP:OD2	36:B:193:LYS:NZ	2.37	0.56
37:C:85:HIS:HD2	81:y:20:LEU:HD21	1.47	0.56
42:H:166:ARG:HH22	42:H:212:LYS:HD3	1.71	0.56
46:L:40:LEU:HD22	46:L:48:PRO:HG3	1.87	0.56
72:m:2:SER:N	78:t:2385:G:N7	2.53	0.56
78:t:704:C:H2'	78:t:705:G:H8	1.70	0.56
1:S2:830:A:OP2	1:S2:846:G:N2	2.39	0.56
2:SA:77:ILE:HG13	2:SA:123:VAL:O	2.06	0.56
3:SB:113:MET:HE3	3:SB:209:ASP:HB3	1.86	0.56
26:SM:69:LEU:HD21	26:SM:76:LEU:HD23	1.87	0.56
30:SY:55:ILE:HG13	30:SY:75:ILE:HG12	1.87	0.56
42:H:167:ILE:HD13	42:H:174:LEU:HD23	1.87	0.56
44:J:61:TRP:CZ3	48:N:33:GLN:HB2	2.38	0.56
45:K:14:ASN:ND2	78:t:1845:G:OP2	2.38	0.56
53:S:60:ARG:NH1	78:t:2787:G:O2'	2.39	0.56
61:b:103:VAL:HB	61:b:108:TYR:HB2	1.87	0.56
67:h:6:THR:HG22	78:t:2379:G:H21	1.70	0.56
78:t:2790:G:N1	78:t:2793:C:OP2	2.37	0.56
1:S2:334:C:H41	24:SG:190:ARG:HH12	1.53	0.56
17:SV:35:ASN:ND2	23:SC:267:GLN:OE1	2.39	0.56
28:SO:120:ALA:HB2	28:SO:126:ILE:HD11	1.87	0.56
35:A:192:LYS:HB3	35:A:193:ARG:HE	1.69	0.56
37:C:61:GLN:NE2	78:t:351:U:O2'	2.38	0.56
40:F:166:ALA:HB1	40:F:171:LEU:HD12	1.87	0.56
46:L:64:ARG:O	75:p:103:VAL:CG2	2.54	0.56
78:t:133:C:H41	78:t:135:G:H1'	1.70	0.56
78:t:3634:A:N6	78:t:4130:G:O2'	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:524:U:H5''	1:S2:525:A:H4'	1.88	0.56
1:S2:526:A:OP1	33:Se:31:ARG:NH2	2.39	0.56
49:O:105:ARG:NH1	78:t:2438:G:N7	2.53	0.56
66:g:6:TRP:HA	66:g:105:LEU:CD2	2.35	0.56
1:S2:124:U:OP1	5:SE:148:ARG:NH1	2.39	0.56
1:S2:667:U:O4	1:S2:1143:A:N6	2.39	0.56
4:SD:105:LEU:HD22	4:SD:122:VAL:HG11	1.86	0.56
8:SI:76:THR:OG1	8:SI:105:ASP:OD1	2.23	0.56
23:SC:182:CYS:HB2	29:SW:95:PRO:HB2	1.87	0.56
35:A:130:SER:HG	78:t:3654:C:HO2'	1.53	0.56
40:F:7:VAL:HG22	78:t:1760:C:H5''	1.87	0.56
51:Q:4:TYR:HE2	51:Q:16:LYS:HB2	1.70	0.56
53:S:130:ASN:ND2	78:t:1553:G:O2'	2.39	0.56
66:g:100:ARG:NH2	78:t:4714:U:O5'	2.38	0.56
73:n:93:LYS:HD3	73:n:102:ARG:HB3	1.87	0.56
77:r:88:ALA:O	77:r:92:SER:N	2.39	0.56
35:A:179:ILE:HG21	35:A:185:ALA:HB2	1.88	0.56
52:R:93:GLN:OE1	61:b:87:ARG:NH2	2.38	0.56
56:V:105:ASN:OD1	56:V:109:SER:OG	2.23	0.56
62:c:99:ILE:O	62:c:109:ARG:NH1	2.39	0.56
63:d:12:GLU:O	63:d:16:SER:OG	2.20	0.56
78:t:1161:G:N2	78:t:1164:C:OP1	2.39	0.56
13:SR:36:GLU:OE1	13:SR:47:ARG:NH1	2.39	0.56
20:Sc:62:GLU:HG2	28:SO:121:ARG:HG3	1.87	0.56
72:m:40:LYS:NZ	78:t:359:U:O2'	2.38	0.56
73:n:115:CYS:SG	73:n:116:GLY:N	2.79	0.56
78:t:4698:C:H2'	78:t:4699:G:H8	1.70	0.56
1:S2:1647:A:N6	1:S2:1677:U:O4	2.39	0.56
2:SA:141:ASN:ND2	23:SC:85:SER:O	2.39	0.56
6:SF:138:ALA:O	6:SF:204:ARG:NH2	2.39	0.56
12:SQ:50:LYS:HA	12:SQ:53:GLU:HB2	1.87	0.56
17:SV:73:ALA:HB1	17:SV:78:ILE:HB	1.86	0.56
22:Sg:73:SER:HB2	22:Sg:117:ASN:HD21	1.71	0.56
66:g:100:ARG:HH21	78:t:4713:G:H3'	1.70	0.56
1:S2:801:U:O4	7:SH:106:ARG:NH2	2.39	0.55
1:S2:996:A:OP1	27:SN:114:ARG:NH1	2.39	0.55
1:S2:1548:G:H5'	16:SU:62:ARG:HH21	1.71	0.55
1:S2:1737:G:OP1	24:SG:94:ARG:NH2	2.40	0.55
8:SI:106:SER:OG	8:SI:110:ARG:NH2	2.40	0.55
35:A:125:LYS:NZ	78:t:3651:U:O4	2.38	0.55
42:H:232:ASP:O	42:H:236:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:g:54:LYS:HG2	78:t:437:G:C5'	2.36	0.55
66:g:59:THR:HG21	78:t:4902:C:C6	2.31	0.55
69:j:76:ARG:NH2	78:t:298:C:O3'	2.39	0.55
78:t:4717:G:N2	78:t:4836:C:N3	2.54	0.55
1:S2:65:C:H4'	24:SG:172:LYS:HE2	1.88	0.55
1:S2:444:G:OP2	8:SI:47:ARG:NH1	2.39	0.55
1:S2:1024:A:OP2	27:SN:124:ARG:NH2	2.38	0.55
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.70	0.55
1:S2:1648:G:H5''	12:SQ:125:ARG:HB2	1.87	0.55
13:SR:35:CYS:HA	13:SR:38:ILE:HG22	1.88	0.55
22:Sg:223:GLU:HG2	22:Sg:225:LYS:H	1.72	0.55
27:SN:84:LEU:HD11	27:SN:149:LEU:HD23	1.87	0.55
36:B:10:ARG:NH2	36:B:265:SER:O	2.39	0.55
51:Q:95:LEU:HD21	51:Q:114:ILE:HD11	1.89	0.55
66:g:5:LEU:C	66:g:105:LEU:CD2	2.80	0.55
1:S2:975:G:OP1	28:SO:98:ARG:NH1	2.37	0.55
37:C:207:PRO:O	37:C:248:ARG:NH2	2.38	0.55
58:X:49:ILE:CD1	58:X:52:THR:HB	2.35	0.55
58:X:86:SER:HB2	58:X:89:ASP:HB2	1.89	0.55
66:g:58:VAL:CG1	66:g:64:PRO:C	2.78	0.55
78:t:1964:A:H4'	78:t:1965:A:H5'	1.88	0.55
78:t:4726:A:H61	78:t:4826:G:H22	1.54	0.55
78:t:4729:C:H42	78:t:4823:C:H42	1.55	0.55
83:a:26:VAL:O	83:a:93:LYS:NZ	2.39	0.55
1:S2:439:A:OP2	8:SI:23:LYS:NZ	2.39	0.55
1:S2:925:G:N2	27:SN:48:SER:OG	2.39	0.55
1:S2:1533:A:O2'	6:SF:81:ARG:NH2	2.36	0.55
46:L:110:GLN:HG3	78:t:4213:A:H1'	1.88	0.55
48:N:89:THR:HG23	48:N:92:ALA:H	1.71	0.55
78:t:1056:G:H1	78:t:1221:A:H2	1.55	0.55
1:S2:56:G:OP1	30:SY:111:LYS:NZ	2.40	0.55
1:S2:1610:G:O2'	14:SS:110:ASP:OD2	2.22	0.55
3:SB:87:ILE:HD12	3:SB:220:LYS:NZ	2.02	0.55
24:SG:217:MET:O	24:SG:221:LYS:NZ	2.35	0.55
38:D:132:G:OP1	59:Y:108:GLN:NE2	2.40	0.55
38:D:149:G:H21	43:I:64:GLN:HE22	1.53	0.55
75:p:65:LYS:HE3	75:p:87:ARG:HH21	1.71	0.55
78:t:26:C:O2'	78:t:332:A:N3	2.39	0.55
1:S2:834:C:H2'	1:S2:836:G:H1	1.71	0.55
2:SA:106:GLY:O	2:SA:113:GLN:NE2	2.39	0.55
38:D:3:A:N6	78:t:424:G:O6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:D:155:C:OP2	43:I:89:ARG:NH1	2.40	0.55
45:K:110:ARG:NH1	78:t:4403:A:OP2	2.40	0.55
64:e:94:GLU:O	64:e:97:ASP:HA	2.07	0.55
71:l:12:LEU:HB3	71:l:16:ARG:HH22	1.70	0.55
73:n:124:LYS:O	73:n:126:LYS:NZ	2.33	0.55
1:S2:909:G:OP1	53:S:172:ARG:NH2	2.29	0.55
1:S2:1512:C:O2'	21:Sd:7:TYR:O	2.24	0.55
4:SD:106:ARG:HG3	4:SD:175:VAL:HG22	1.88	0.55
5:SE:183:VAL:HG21	5:SE:220:THR:HG21	1.89	0.55
9:SK:80:ARG:HH11	9:SK:87:PRO:HA	1.72	0.55
37:C:149:GLU:OE2	77:r:71:ARG:NH1	2.39	0.55
39:E:27:G:OP1	46:L:146:ARG:NH2	2.40	0.55
40:F:19:LYS:NZ	78:t:4242:A:OP2	2.38	0.55
50:P:26:GLN:HG3	54:T:167:PHE:HZ	1.71	0.55
67:h:66:ARG:HD3	78:t:2518:C:H5''	1.88	0.55
1:S2:38:A:O3'	25:SJ:5:ARG:NH1	2.40	0.55
1:S2:56:G:OP2	30:SY:115:LYS:NZ	2.39	0.55
1:S2:660:C:O2'	10:SL:101:ARG:NH1	2.31	0.55
1:S2:929:G:N2	1:S2:1013:U:O2	2.39	0.55
1:S2:1236:G:H4'	11:SP:134:GLY:H	1.71	0.55
4:SD:216:GLU:OE2	22:Sg:172:LYS:NZ	2.40	0.55
13:SR:60:ARG:HE	13:SR:66:VAL:HG11	1.70	0.55
24:SG:189:ARG:O	24:SG:193:ALA:N	2.40	0.55
28:SO:74:ALA:HB1	28:SO:115:ALA:HB2	1.89	0.55
37:C:334:THR:HA	37:C:337:ARG:HD3	1.88	0.55
42:H:80:ASN:HD22	55:U:143:THR:H	1.55	0.55
52:R:39:THR:HG23	52:R:41:SER:H	1.69	0.55
67:h:11:LEU:O	67:h:18:ASN:ND2	2.39	0.55
78:t:4070:C:OP2	78:t:4072:C:N4	2.39	0.55
78:t:4562:G:O2'	78:t:4571:G:O6	2.24	0.55
10:SL:40:ILE:HG21	10:SL:68:ILE:HG23	1.88	0.55
10:SL:111:VAL:HG12	10:SL:140:PHE:HB2	1.88	0.55
41:G:262:LYS:NZ	41:G:268:GLN:OE1	2.40	0.55
61:b:26:ARG:HH12	78:t:1638:U:H5	1.53	0.55
78:t:4733:C:N4	78:t:4820:G:O6	2.39	0.55
82:u:19:G:O4'	82:u:57:G:N2	2.39	0.55
2:SA:128:ARG:HB3	2:SA:153:PRO:HD2	1.88	0.55
23:SC:176:LYS:O	23:SC:200[B]:ARG:NH1	2.40	0.55
54:T:71:SER:O	54:T:76:LYS:NZ	2.39	0.55
67:h:76:ARG:HG2	83:a:17:ARG:H	1.71	0.55
82:u:18:G:HO2'	82:u:57:G:H1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:449:A:O3'	5:SE:3:ARG:NH1	2.40	0.54
1:S2:1112:U:O2'	3:SB:146:ARG:NH2	2.40	0.54
27:SN:53:ILE:HG22	32:Sb:52:THR:HG21	1.89	0.54
30:SY:12:PHE:HD1	30:SY:23:MET:HB3	1.72	0.54
37:C:67:TRP:CE2	37:C:78:ARG:HG3	2.41	0.54
41:G:88:VAL:N	78:t:2238:G:O6	2.40	0.54
53:S:109:TYR:HA	53:S:112:SER:OG	2.07	0.54
63:d:31:TYR:OH	63:d:59:GLU:OE2	2.26	0.54
5:SE:127:ARG:NH2	5:SE:142:HIS:O	2.40	0.54
9:SK:31:LYS:HE3	9:SK:36:ALA:HA	1.89	0.54
36:B:57:VAL:HB	36:B:367:PHE:HB3	1.90	0.54
37:C:222:ARG:NH1	78:t:221:U:OP1	2.40	0.54
40:F:29:ASP:OD1	40:F:29:ASP:N	2.39	0.54
69:j:58:MET:O	69:j:62:LYS:NZ	2.32	0.54
74:o:11:ARG:HA	74:o:14:LYS:HG2	1.89	0.54
15:ST:97:LYS:O	15:ST:101:ARG:N	2.39	0.54
32:Sb:19:HIS:CD2	32:Sb:21:LYS:H	2.25	0.54
37:C:84:THR:O	81:y:20:LEU:CD1	2.47	0.54
44:J:18:ILE:HG12	44:J:27:VAL:HG22	1.89	0.54
52:R:2:GLY:N	78:t:1879:C:OP1	2.41	0.54
78:t:1084:C:N3	78:t:1178:G:N2	2.55	0.54
5:SE:161:GLN:HB3	5:SE:171:ASP:H	1.73	0.54
6:SF:85:LYS:HB3	6:SF:88:MET:HG2	1.88	0.54
14:SS:132:ARG:HB2	14:SS:134:GLN:HE22	1.71	0.54
35:A:207:VAL:HG23	35:A:208:GLU:HG3	1.88	0.54
48:N:5:ARG:NH1	48:N:59:ASP:OD1	2.39	0.54
52:R:172:ARG:NH2	78:t:88:A:OP1	2.40	0.54
1:S2:503:C:OP1	5:SE:62:LYS:NZ	2.41	0.54
1:S2:1568:C:OP2	15:ST:98:SER:OG	2.24	0.54
1:S2:1617:G:N1	1:S2:1620:A:OP2	2.37	0.54
2:SA:68:ILE:HD11	2:SA:121:LEU:HD12	1.90	0.54
22:Sg:19:THR:HG22	22:Sg:36:ARG:HH11	1.73	0.54
24:SG:146:ASN:O	58:X:86:SER:OG	2.25	0.54
41:G:72:LYS:NZ	78:t:1222:C:O2'	2.40	0.54
42:H:188:GLU:OE2	78:t:931:A:N6	2.40	0.54
43:I:187:LYS:HE2	43:I:198:THR:HG21	1.90	0.54
51:Q:67:VAL:HG22	51:Q:82:ARG:HH21	1.71	0.54
53:S:5:ARG:NH2	78:t:2364:U:OP1	2.40	0.54
53:S:88:ARG:O	78:t:2704:A:N6	2.41	0.54
67:h:83:CYS:O	67:h:84:ALA:HB2	2.08	0.54
78:t:1077:G:H1	78:t:1184:U:H3	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:2643:G:H4'	78:t:2656:G:H4'	1.90	0.54
80:w:19:C:H2'	80:w:20:G:H8	1.72	0.54
1:S2:696:G:N2	1:S2:735:C:OP2	2.39	0.54
1:S2:1100:A:O3'	13:SR:132:ARG:NH1	2.40	0.54
11:SP:72:LYS:HZ1	11:SP:93:MET:HE2	1.73	0.54
29:SW:26:LEU:HD11	29:SW:60:LYS:HB3	1.90	0.54
37:C:282:HIS:ND1	37:C:284:MET:O	2.39	0.54
42:H:33:LEU:O	42:H:37:PHE:N	2.41	0.54
78:t:730:G:H2'	78:t:731:G:H8	1.72	0.54
1:S2:26:U:H2'	1:S2:27:A2M:H8	1.89	0.54
1:S2:1249:C:O3'	12:SQ:143:LYS:NZ	2.40	0.54
1:S2:1562:C:H2'	1:S2:1563:G:H8	1.73	0.54
1:S2:1782:G:C6	58:X:73:ARG:CD	2.89	0.54
12:SQ:115:TYR:C	12:SQ:115:TYR:CD2	2.86	0.54
22:Sg:4:GLN:NE2	22:Sg:5:MET:O	2.39	0.54
37:C:54:VAL:CB	37:C:105:THR:C	2.81	0.54
52:R:85:THR:HG22	52:R:104:ARG:HB3	1.90	0.54
78:t:149:U:O2'	78:t:150:G:N2	2.41	0.54
78:t:4077:G:O6	78:t:4078:G:N2	2.41	0.54
78:t:4819:G:H2'	78:t:4820:G:H8	1.73	0.54
78:t:4929:A:H2	78:t:5020:G:H1	1.54	0.54
1:S2:1300:U:O2'	21:Sd:5:GLN:NE2	2.40	0.54
4:SD:142:LEU:HD13	4:SD:150:MET:HE3	1.90	0.54
18:SX:46:HIS:HB3	18:SX:101:LEU:HD11	1.90	0.54
19:Sa:4:LYS:HG2	19:Sa:5:ARG:HG3	1.90	0.54
22:Sg:251:ALA:HB2	22:Sg:289:LEU:HD22	1.90	0.54
43:I:104:PRO:HG2	43:I:194:VAL:HG23	1.90	0.54
47:M:71:ARG:NH2	78:t:74:G:O3'	2.40	0.54
78:t:4232:C:H5''	78:t:4233:A:H5''	1.90	0.54
1:S2:1618:C:H4'	11:SP:50:ARG:HH22	1.71	0.54
2:SA:49:ILE:HD13	2:SA:162:PRO:O	2.08	0.54
4:SD:95:GLY:HA3	4:SD:125:PHE:HE2	1.69	0.54
10:SL:135:SER:O	10:SL:139:ARG:NH1	2.40	0.54
13:SR:5:ARG:HH21	13:SR:53:TYR:HD1	1.55	0.54
18:SX:90:CYS:HA	18:SX:93:PHE:HD2	1.73	0.54
22:Sg:120:ILE:O	22:Sg:132:TRP:N	2.40	0.54
25:SJ:140:GLN:NE2	30:SY:64:PHE:O	2.41	0.54
26:SM:64:LEU:HD22	34:Sf:104:LYS:HD2	1.88	0.54
31:SZ:98:LYS:HE2	31:SZ:113:THR:HG23	1.89	0.54
41:G:129:GLY:O	41:G:130:LYS:C	2.51	0.54
78:t:1060:C:H42	78:t:1217:G:H22	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Se:8:ARG:HB2	33:Se:11:LYS:HB2	1.90	0.54
35:A:104:VAL:O	35:A:139:HIS:NE2	2.38	0.54
40:F:82:GLU:OE2	40:F:108:ARG:NH2	2.41	0.54
40:F:176:SER:HB3	78:t:4285:A:H4'	1.90	0.54
46:L:90:ARG:NH2	46:L:107:PHE:O	2.39	0.54
1:S2:441:C:OP1	8:SI:2:GLY:N	2.41	0.53
24:SG:146:ASN:HA	58:X:83:THR:HA	1.91	0.53
49:O:195:ARG:NH2	78:t:98:A:O3'	2.40	0.53
51:Q:50:ASP:HB3	51:Q:55:LYS:HB2	1.89	0.53
55:U:92:ARG:HB2	55:U:95:HIS:HD2	1.73	0.53
56:V:48:LYS:NZ	78:t:2609:U:OP1	2.36	0.53
78:t:2417:A:O2'	78:t:2419:U:OP2	2.27	0.53
78:t:2580:A:N6	78:t:2723:A:OP2	2.41	0.53
1:S2:1064:C:H2'	1:S2:1065:G:H8	1.73	0.53
5:SE:80:ILE:HG13	5:SE:81:THR:HG23	1.90	0.53
55:U:19:PHE:CD2	55:U:19:PHE:C	2.86	0.53
60:Z:87:ARG:NH2	78:t:398:U:O3'	2.40	0.53
61:b:46:ASP:C	61:b:48:TYR:N	2.57	0.53
78:t:637:C:H2'	78:t:638:G:H8	1.74	0.53
78:t:1339:U:O2'	78:t:1487:C:O2	2.27	0.53
9:SK:76:ILE:HG23	9:SK:91:PRO:HG2	1.89	0.53
36:B:5:LYS:O	36:B:6:PHE:CD2	2.62	0.53
38:D:29:G:H5''	47:M:27:ASN:HB3	1.90	0.53
48:N:106:ASP:OD1	48:N:109:ARG:NH1	2.41	0.53
49:O:67:ARG:NH2	78:t:2437:C:OP1	2.38	0.53
53:S:92:LYS:NZ	78:t:2585:G:O3'	2.38	0.53
78:t:2719:U:O2'	78:t:2721:G:N2	2.41	0.53
1:S2:291:G:C5	1:S2:291:G:N7	2.76	0.53
1:S2:616:A:OP1	18:SX:68:LYS:NZ	2.41	0.53
6:SF:61:PHE:HB3	20:Sc:51:ARG:HH21	1.74	0.53
24:SG:194:LEU:HD13	24:SG:197:GLN:HE21	1.73	0.53
71:l:38:CYS:SG	71:l:39:SER:N	2.79	0.53
73:n:95:ILE:HG21	78:t:4435:A:H4'	1.90	0.53
1:S2:291:G:C4	1:S2:291:G:N9	2.77	0.53
1:S2:1161:U:OP1	18:SX:12:LYS:NZ	2.41	0.53
1:S2:1224:G:H1	1:S2:1642:U:H3	1.57	0.53
1:S2:1866:A:H61	19:Sa:85:ARG:H	1.57	0.53
6:SF:20:PHE:O	6:SF:22:LYS:NZ	2.42	0.53
37:C:85:HIS:O	37:C:89:GLN:NE2	2.41	0.53
38:D:93:C:OP1	70:k:76:HIS:NE2	2.28	0.53
41:G:136:HIS:HD2	78:t:702:A:H1'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:I:57:TRP:O	43:I:62:ARG:NH1	2.42	0.53
54:T:170:LYS:HE2	78:t:4828:G:C5	2.43	0.53
55:U:3:ASN:O	55:U:9:ARG:NH1	2.41	0.53
60:Z:21:ALA:O	60:Z:26:ARG:NH2	2.41	0.53
66:g:43:LEU:O	66:g:109:ARG:NH2	2.41	0.53
78:t:112:C:H2'	78:t:113:A:H8	1.74	0.53
1:S2:1114:U:OP2	1:S2:1115:U:O2'	2.25	0.53
1:S2:1803:U:OP1	57:W:35:LYS:NZ	2.39	0.53
25:SJ:136:ARG:HA	25:SJ:141:VAL:HA	1.90	0.53
31:SZ:76:ARG:HE	31:SZ:77:LEU:HD12	1.72	0.53
45:K:162:ARG:NH2	78:t:2014:A:OP1	2.42	0.53
53:S:107:ARG:NH2	78:t:2645:U:OP1	2.42	0.53
56:V:103:VAL:HG23	56:V:111:GLU:HB3	1.90	0.53
58:X:49:ILE:CD1	58:X:52:THR:CG2	2.86	0.53
66:g:56:ASN:HA	66:g:65:ASN:O	2.08	0.53
1:S2:196:C:N3	1:S2:204:G:N1	2.56	0.53
1:S2:797:C:O2	1:S2:798:A:N6	2.39	0.53
51:Q:61:ARG:NH2	51:Q:76:TRP:O	2.42	0.53
78:t:1642:U:HO2'	78:t:2324:G:HO2'	1.55	0.53
78:t:2519:C:H2'	78:t:2520:G:H8	1.74	0.53
23:SC:275:LYS:HB3	23:SC:275:LYS:HZ3	1.72	0.53
37:C:54:VAL:HB	37:C:105:THR:C	2.34	0.53
48:N:6:PHE:O	48:N:11:ARG:NH1	2.41	0.53
76:q:2:ALA:N	78:t:1552:G:O6	2.42	0.53
78:t:1060:C:H42	78:t:1217:G:H1	1.57	0.53
81:y:22:ILE:CG1	81:y:24:GLY:H	2.13	0.53
1:S2:379:C:O2	8:SI:31:ARG:NE	2.40	0.53
5:SE:212:ASP:OD1	5:SE:216:ASN:N	2.41	0.53
14:SS:63:GLU:OE1	14:SS:66:ARG:NH2	2.41	0.53
78:t:231:G:O2'	78:t:233:G:OP1	2.25	0.53
78:t:3782:G:O2'	78:t:3785:U:OP2	2.27	0.53
1:S2:788:G:O6	24:SG:233:ARG:NH2	2.41	0.53
1:S2:1173:A:O2'	1:S2:1716:C:O2'	2.24	0.53
3:SB:219:LYS:HE2	76:q:90:LYS:HA	1.90	0.53
18:SX:8:ARG:HH22	18:SX:9:THR:HB	1.74	0.53
35:A:147:ARG:HD3	35:A:155:LYS:HD3	1.91	0.53
41:G:180:VAL:HG21	41:G:258:LEU:HD21	1.91	0.53
41:G:206:VAL:HG13	41:G:207:LYS:H	1.73	0.53
49:O:113:LEU:HB3	49:O:134:LEU:HD12	1.90	0.53
68:i:93:ARG:NH2	78:t:19:G:OP2	2.41	0.53
78:t:4545:C:O2'	78:t:4680:G:N2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:486:A:H1'	1:S2:513:G:H22	1.74	0.52
1:S2:1443:C:H5''	12:SQ:15:ARG:HH21	1.74	0.52
2:SA:80:ARG:NH2	2:SA:126:ASP:OD2	2.41	0.52
7:SH:101:LEU:O	7:SH:116:ARG:NH1	2.42	0.52
16:SU:65:THR:HG22	16:SU:67:LYS:H	1.74	0.52
17:SV:69:ILE:HA	17:SV:72:LEU:HG	1.92	0.52
29:SW:30:CYS:SG	29:SW:31:SER:N	2.82	0.52
32:Sb:23:ARG:NH1	32:Sb:27:SER:OG	2.42	0.52
36:B:5:LYS:NZ	36:B:5:LYS:HB3	2.24	0.52
52:R:108:ARG:NH1	78:t:1338:G:OP1	2.41	0.52
64:e:94:GLU:O	64:e:97:ASP:N	2.41	0.52
78:t:104:G:HO2'	78:t:1344:G:HO2'	1.45	0.52
1:S2:106:C:OP1	1:S2:431:G:O2'	2.25	0.52
1:S2:532:C:N3	1:S2:552:G:N1	2.58	0.52
10:SL:23:VAL:HG23	10:SL:25:LEU:H	1.72	0.52
14:SS:90:VAL:HG11	14:SS:113:ARG:HH22	1.74	0.52
17:SV:74:LYS:O	17:SV:81:LYS:CD	2.57	0.52
48:N:46:ARG:NH1	78:t:925:C:O5'	2.39	0.52
63:d:103:ASP:OD1	63:d:103:ASP:N	2.42	0.52
66:g:27:LEU:HA	66:g:85:ARG:HA	1.91	0.52
70:k:18:LEU:HA	70:k:25:LYS:HA	1.90	0.52
71:l:8:ILE:HG23	71:l:56:LEU:HD12	1.90	0.52
19:Sa:22:ARG:NH1	28:SO:145:GLY:O	2.33	0.52
38:D:36:G:N2	78:t:20:U:OP2	2.41	0.52
48:N:10:GLY:O	48:N:62:LEU:N	2.39	0.52
49:O:3:ALA:HA	49:O:6:TYR:HD2	1.74	0.52
53:S:108:ARG:O	53:S:112:SER:N	2.42	0.52
55:U:19:PHE:C	55:U:21:LYS:N	2.65	0.52
78:t:2484:C:O2'	78:t:2485:G:N2	2.43	0.52
1:S2:1143:A:H5'	23:SC:190:SER:HB3	1.90	0.52
1:S2:1179:G:N2	1:S2:1182:A:OP2	2.43	0.52
2:SA:163:CYS:SG	2:SA:164:ASN:N	2.77	0.52
3:SB:138:PHE:HD2	3:SB:214:LYS:HB3	1.74	0.52
26:SM:24:THR:HG21	26:SM:119:GLN:HB3	1.91	0.52
54:T:160:ARG:NH2	78:t:1902:C:N3	2.49	0.52
58:X:49:ILE:HD11	58:X:52:THR:CG2	2.40	0.52
65:f:79:VAL:HG21	65:f:85:LEU:HD23	1.92	0.52
78:t:485:G:N2	78:t:656:C:O2	2.42	0.52
1:S2:1436:C:O2'	1:S2:1438:A:OP2	2.28	0.52
16:SU:33:GLU:OE2	16:SU:87:ARG:NH1	2.37	0.52
22:Sg:85:GLY:HA2	22:Sg:108:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:367:PHE:HZ	36:B:380:GLN:HE22	1.57	0.52
37:C:212:ASN:HB3	37:C:232:VAL:HG12	1.92	0.52
37:C:295:SER:OG	37:C:297:GLU:OE1	2.27	0.52
38:D:36:G:O2'	38:D:103:A:N1	2.39	0.52
52:R:72:LEU:HG	78:t:1439:G:H5'	1.91	0.52
52:R:158:THR:OG1	78:t:4268:U:OP1	2.20	0.52
71:l:23:VAL:HG22	71:l:36:VAL:HG22	1.91	0.52
78:t:3584:U:HO2'	78:t:4993:U:HO2'	1.55	0.52
1:S2:560:A:H2'	25:SJ:164:PRO:HB3	1.91	0.52
1:S2:1549:U:H2'	1:S2:1550:G:H8	1.75	0.52
13:SR:115:SER:HB3	13:SR:117:LEU:HD23	1.90	0.52
29:SW:30:CYS:HA	29:SW:34:ILE:HD11	1.92	0.52
36:B:175:GLN:HG3	78:t:4943:U:H4'	1.92	0.52
52:R:18:PRO:O	52:R:26:ARG:NH2	2.43	0.52
58:X:11:TYR:OH	78:t:4999:G:N2	2.43	0.52
67:h:66:ARG:NH2	78:t:2497:G:OP1	2.39	0.52
78:t:33:A:OP2	78:t:48:G:N2	2.43	0.52
78:t:1979:A:N3	78:t:2000:C:O2'	2.37	0.52
1:S2:10:G:H21	23:SC:114:LYS:HA	1.75	0.52
1:S2:1846:G:O6	74:o:8:LYS:NZ	2.42	0.52
8:SI:157:LYS:HE2	10:SL:23:VAL:HB	1.90	0.52
16:SU:31:SER:OG	16:SU:107:GLU:OE2	2.27	0.52
23:SC:64:THR:HG23	23:SC:67:GLY:H	1.74	0.52
26:SM:60:MET:O	26:SM:64:LEU:N	2.41	0.52
47:M:76:PHE:HE2	47:M:96:ILE:CG2	2.16	0.52
68:i:48:ARG:HA	68:i:51:ARG:HG2	1.91	0.52
1:S2:533:A:H61	1:S2:550:C:H42	1.58	0.52
1:S2:1518:C:H5'	1:S2:1519:U:H5'	1.92	0.52
2:SA:41:ARG:HD3	2:SA:45:GLY:HA2	1.91	0.52
4:SD:8:LYS:HE3	16:SU:59:LYS:HD3	1.90	0.52
10:SL:121:GLN:NE2	10:SL:148:ALA:O	2.42	0.52
13:SR:7:LYS:O	13:SR:11:LYS:N	2.41	0.52
17:SV:80:SER:OG	17:SV:82:ASN:OD1	2.27	0.52
47:M:76:PHE:CD2	47:M:96:ILE:HG22	2.44	0.52
47:M:96:ILE:HD13	47:M:117:LEU:HD11	1.92	0.52
47:M:177:LYS:HD2	61:b:146:LEU:H	1.72	0.52
53:S:82:LYS:O	78:t:2842:G:O2'	2.27	0.52
58:X:49:ILE:HG13	58:X:52:THR:HG21	1.92	0.52
58:X:50:ASN:HB3	78:t:4963:G:O2'	2.10	0.52
77:r:19:LYS:NZ	78:t:2317:C:OP1	2.43	0.52
77:r:61:VAL:HG12	77:r:81:THR:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:51:A:N3	78:t:1510:U:O2'	2.42	0.52
78:t:455:G:H22	78:t:687:A:H2	1.58	0.52
1:S2:559:G:OP2	25:SJ:177:ASN:ND2	2.42	0.52
1:S2:792:C:O2'	1:S2:793:G:O4'	2.28	0.52
1:S2:1271:C:O2'	21:Sd:3:HIS:NE2	2.39	0.52
16:SU:21:ARG:H	16:SU:115:THR:HB	1.75	0.52
16:SU:54:VAL:HG12	16:SU:88:LEU:HB3	1.91	0.52
37:C:333:LYS:NZ	78:t:964:C:OP1	2.43	0.52
49:O:155:VAL:O	49:O:162:ARG:NH2	2.43	0.52
53:S:113:LYS:HA	53:S:113:LYS:CE	2.30	0.52
55:U:86:ALA:HB2	62:c:24:PRO:HG3	1.92	0.52
58:X:49:ILE:CG1	58:X:52:THR:CG2	2.88	0.52
64:e:64:ILE:HG22	64:e:106:VAL:HB	1.91	0.52
66:g:54:LYS:HG2	78:t:437:G:H5''	1.92	0.52
78:t:181:U:O2'	78:t:185:G:O5'	2.27	0.52
78:t:1415:G:O2'	78:t:1434:G:O6	2.23	0.52
78:t:4622:G:H2'	78:t:4623:G:H8	1.75	0.52
11:SP:73:PRO:HG2	11:SP:92:SER:HA	1.91	0.52
24:SG:98:ARG:NH2	24:SG:103:ASP:OD2	2.42	0.52
42:H:148:LYS:HD3	42:H:245:ARG:HH21	1.75	0.52
42:H:151:ASN:HA	42:H:191:ILE:HD11	1.92	0.52
45:K:37:GLY:HA3	45:K:86:HIS:HA	1.91	0.52
53:S:22:VAL:HG13	53:S:23:TRP:HB2	1.92	0.52
54:T:81:TRP:HB3	54:T:127:MET:HE3	1.90	0.52
66:g:49:TYR:HD1	66:g:101:ILE:HG22	1.73	0.52
66:g:81:SER:N	78:t:1899:U:OP1	2.42	0.52
78:t:469:G:H1	78:t:673:C:H42	1.56	0.52
78:t:1636:G:N2	78:t:1660:C:OP1	2.43	0.52
23:SC:274:VAL:CG1	23:SC:278:THR:HG1	2.10	0.51
36:B:26:ARG:NH1	36:B:180:LEU:O	2.36	0.51
41:G:133:PHE:CA	41:G:136:HIS:CE1	2.82	0.51
66:g:58:VAL:HG13	66:g:64:PRO:HA	0.55	0.51
78:t:2554:U:OP1	83:a:48:ARG:NH2	2.43	0.51
3:SB:87:ILE:CD1	3:SB:220:LYS:HZ3	1.99	0.51
23:SC:148:ALA:HA	23:SC:151:ILE:HG22	1.93	0.51
24:SG:159:ARG:HH21	24:SG:171:THR:HG23	1.75	0.51
36:B:47:LEU:HD12	36:B:84:MET:HE1	1.93	0.51
37:C:34:PRO:HG3	77:r:9:VAL:HG22	1.93	0.51
41:G:114:ARG:NH2	78:t:453:C:OP2	2.39	0.51
42:H:95:ILE:HD12	42:H:96:ARG:HG2	1.91	0.51
57:W:123:LYS:HB2	57:W:140:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:d:43:ALA:HA	63:d:97:ILE:HG22	1.91	0.51
78:t:715:C:H2'	78:t:716:G:H8	1.74	0.51
1:S2:463:C:O2'	1:S2:466:G:O6	2.28	0.51
6:SF:127:ARG:H	6:SF:135:ARG:HD3	1.74	0.51
12:SQ:146:ARG:NH2	79:v:35:C:OP2	2.43	0.51
23:SC:273:LEU:O	23:SC:273:LEU:HD23	2.10	0.51
37:C:221:PHE:HB2	37:C:229:LEU:HD11	1.91	0.51
51:Q:119:VAL:HG22	51:Q:146:ILE:HG22	1.92	0.51
66:g:57:THR:OG1	78:t:1281:C:OP1	2.17	0.51
78:t:477:G:N3	78:t:666:G:N2	2.59	0.51
78:t:1977:C:N4	78:t:1981:G:OP2	2.44	0.51
4:SD:40:ARG:HH22	4:SD:49:ILE:HG23	1.75	0.51
7:SH:55:GLY:H	7:SH:57:ARG:HH11	1.58	0.51
61:b:46:ASP:OD1	61:b:46:ASP:N	2.28	0.51
77:r:68:SER:OG	78:t:663:C:OP1	2.28	0.51
1:S2:862:A:N3	29:SW:105:THR:OG1	2.39	0.51
5:SE:21:ASP:OD2	5:SE:24:THR:N	2.43	0.51
43:I:59:ARG:HH22	78:t:2449:C:H1'	1.76	0.51
46:L:144:LYS:O	46:L:148:THR:OG1	2.29	0.51
52:R:160:HIS:CD2	52:R:160:HIS:N	2.75	0.51
78:t:2378:G:HO2'	78:t:2801:G:HO2'	1.56	0.51
8:SI:91:VAL:O	8:SI:94:LYS:NZ	2.41	0.51
41:G:126:LEU:HD11	78:t:958:U:H5'	1.91	0.51
49:O:2:GLY:N	78:t:115:C:OP1	2.43	0.51
51:Q:15:CYS:SG	51:Q:16:LYS:N	2.83	0.51
58:X:97:LYS:HG2	58:X:99:GLU:H	1.75	0.51
78:t:1649:G:N1	78:t:2260:U:OP2	2.39	0.51
78:t:2474:U:H2'	78:t:2475:G:H8	1.74	0.51
8:SI:178:ARG:HH21	8:SI:181:GLN:HG2	1.76	0.51
11:SP:108:LYS:HG2	11:SP:111:MET:HE3	1.93	0.51
36:B:5:LYS:NZ	36:B:5:LYS:CB	2.73	0.51
43:I:152:ALA:HA	43:I:205:THR:HG22	1.92	0.51
47:M:184:MET:HA	47:M:187:ALA:HB3	1.93	0.51
66:g:5:LEU:C	66:g:105:LEU:HD23	2.35	0.51
78:t:2339:A:H61	78:t:3831:A:H5''	1.75	0.51
78:t:4924:A:H61	78:t:5025:U:H3	1.59	0.51
1:S2:660:C:OP1	18:SX:17:ARG:NH1	2.44	0.51
14:SS:120:HIS:HE1	14:SS:124:ARG:HH11	1.59	0.51
47:M:39:ARG:O	47:M:43:ALA:N	2.40	0.51
59:Y:129:ARG:HH12	59:Y:133:GLU:HB2	1.75	0.51
66:g:59:THR:CB	78:t:4902:C:C4	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:358:G:O2'	78:t:369:G:O6	2.28	0.51
1:S2:1163:C:H2'	1:S2:1164:G:H8	1.76	0.51
3:SB:152:LYS:HD3	13:SR:133:GLY:HA3	1.91	0.51
14:SS:13:LEU:HD22	14:SS:20:ILE:HD11	1.92	0.51
49:O:178:HIS:ND1	78:t:68:U:OP1	2.31	0.51
60:Z:15:ARG:NH1	78:t:226:G:OP1	2.44	0.51
67:h:88:ARG:HG2	67:h:92:LYS:HE2	1.92	0.51
69:j:9:VAL:HG23	69:j:13:LYS:HE2	1.93	0.51
77:r:66:ARG:NH1	78:t:473:G:OP1	2.44	0.51
78:t:489:C:H2'	78:t:490:G:H8	1.75	0.51
78:t:1072:G:H2'	78:t:1073:G:H8	1.76	0.51
78:t:2576:G:H1	78:t:2727:C:H5	1.57	0.51
1:S2:325:C:C4	58:X:119:LYS:CD	2.94	0.51
1:S2:1454:A:N6	1:S2:1477:U:OP2	2.44	0.51
25:SJ:59:GLU:OE2	25:SJ:69:ARG:NH2	2.36	0.51
35:A:193:ARG:NH2	78:t:3656:C:OP1	2.43	0.51
36:B:59:GLU:HB2	36:B:366:LYS:HD2	1.93	0.51
38:D:149:G:N2	78:t:8:U:O2	2.44	0.51
41:G:250:GLN:O	41:G:254:ASP:N	2.37	0.51
44:J:10:VAL:HB	44:J:55:LEU:HB3	1.92	0.51
46:L:95:ARG:HH12	46:L:97:ASN:HD21	1.58	0.51
50:P:15:LEU:HD21	50:P:129:LEU:HD11	1.92	0.51
78:t:132:G:N2	78:t:135:G:O6	2.44	0.51
78:t:2617:G:H1	78:t:2676:A:H61	1.59	0.51
82:u:3:C:O2'	82:u:4:C:O4'	2.29	0.51
1:S2:1829:G:H1'	1:S2:1850:MA6:H2	1.94	0.50
40:F:279:ARG:NH2	78:t:1161:G:OP1	2.42	0.50
48:N:31:ILE:HD11	48:N:35:ARG:CB	2.38	0.50
78:t:723:A:H61	78:t:921:C:H42	1.59	0.50
78:t:1830:U:O2'	78:t:1831:A:O4'	2.29	0.50
78:t:2359:G:N2	78:t:2404:U:OP1	2.42	0.50
78:t:2737:G:H21	78:t:2745:A:H2	1.59	0.50
1:S2:1286:G:H8	34:Sf:101:ALA:HA	1.75	0.50
24:SG:152:ASP:OD2	24:SG:155:GLN:NE2	2.45	0.50
30:SY:110:ARG:NH2	30:SY:125:VAL:O	2.43	0.50
35:A:101:VAL:HA	35:A:165:VAL:HA	1.92	0.50
46:L:104:ASN:HD22	46:L:133:VAL:HG12	1.76	0.50
55:U:7:LYS:O	78:t:4296:U:O2'	2.25	0.50
58:X:106:GLU:HG2	58:X:109:ILE:HD12	1.92	0.50
64:e:79:ASN:ND2	78:t:4615:C:OP1	2.45	0.50
78:t:658:G:O2'	78:t:662:A:N6	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:976:U:N3	78:t:1047:G:O6	2.43	0.50
78:t:1800:G:O2'	78:t:1802:C:OP2	2.27	0.50
78:t:4819:G:H2'	78:t:4820:G:C8	2.46	0.50
6:SF:130:ARG:NH2	80:w:13:U:OP1	2.43	0.50
24:SG:4:ASN:HB3	24:SG:110:ASN:HA	1.93	0.50
31:SZ:98:LYS:NZ	31:SZ:111:ARG:O	2.44	0.50
36:B:29:VAL:HG22	36:B:220:ILE:HD12	1.93	0.50
36:B:111:SER:OG	36:B:112:ASP:N	2.44	0.50
37:C:192:GLY:O	37:C:195:LYS:NZ	2.42	0.50
38:D:60:G:OP1	59:Y:68:ARG:NH2	2.44	0.50
41:G:101:ASN:OD1	41:G:105:ARG:NH2	2.44	0.50
55:U:45:MET:HE3	55:U:94:GLU:HB3	1.92	0.50
65:f:69:MET:SD	65:f:75:ARG:NE	2.78	0.50
78:t:1947:C:H2'	78:t:1948:A:H8	1.75	0.50
2:SA:179:ALA:HA	2:SA:182:VAL:HG12	1.93	0.50
6:SF:70:GLU:OE2	6:SF:74:ASN:ND2	2.39	0.50
8:SI:164:GLU:OE2	8:SI:168:GLN:NE2	2.45	0.50
24:SG:55:GLY:HA3	24:SG:109:LEU:HA	1.93	0.50
38:D:102:G:OP1	38:D:109:C:N4	2.43	0.50
49:O:71:ARG:HD2	49:O:94:PHE:HB2	1.93	0.50
50:P:133:ARG:NH1	78:t:2036:G:OP2	2.40	0.50
51:Q:69:ARG:HE	78:t:4939:G:H1'	1.76	0.50
54:T:8:ARG:HH21	78:t:926:G:H1	1.59	0.50
1:S2:306:C:OP2	8:SI:41:ARG:NH1	2.44	0.50
1:S2:1395:C:H42	1:S2:1450:G:H1	1.57	0.50
3:SB:87:ILE:HD13	3:SB:220:LYS:NZ	2.06	0.50
8:SI:81:VAL:HG22	8:SI:102:VAL:HG23	1.93	0.50
14:SS:108:ARG:HH22	46:L:113:ILE:HG21	1.75	0.50
22:Sg:286:CYS:HA	22:Sg:302:TYR:HD1	1.76	0.50
40:F:197:LYS:HB3	40:F:202:GLN:HG2	1.94	0.50
64:e:28:ASN:HB3	64:e:83:ARG:HE	1.76	0.50
77:r:32:LEU:O	77:r:113:ARG:NH2	2.45	0.50
78:t:480:C:H42	78:t:665:G:H1	1.59	0.50
1:S2:1039:C:H2'	1:S2:1040:G:H8	1.76	0.50
7:SH:137:SER:HB3	7:SH:162:GLN:HB3	1.94	0.50
8:SI:107:THR:HG23	8:SI:108:PRO:HD3	1.93	0.50
36:B:384:GLU:OE2	58:X:14:TYR:OH	2.28	0.50
36:B:392:LEU:HD22	36:B:394:LYS:HD3	1.93	0.50
38:D:112:G:OP1	78:t:2758:C:O2'	2.23	0.50
22:Sg:76:GLN:NE2	22:Sg:91:ASP:OD1	2.45	0.50
38:D:153:C:H2'	38:D:154:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:63:C:H5'	39:E:64:G:H5''	1.94	0.50
61:b:102:ASP:HB3	61:b:125:LYS:HB2	1.93	0.50
64:e:95:ASP:C	64:e:97:ASP:H	2.19	0.50
78:t:492:C:O2'	78:t:495:C:N4	2.45	0.50
4:SD:48:ILE:HB	4:SD:86:LEU:HD23	1.94	0.50
15:ST:44:GLU:HG2	15:ST:45:LEU:HD12	1.93	0.50
22:Sg:170:TRP:HA	22:Sg:194:TYR:HB2	1.94	0.50
37:C:84:THR:HG23	37:C:86:ARG:H	1.77	0.50
53:S:126:LYS:NZ	78:t:1541:G:OP1	2.45	0.50
54:T:3:ALA:O	54:T:111:ARG:NH2	2.40	0.50
64:e:113:THR:HG22	64:e:115:LYS:H	1.76	0.50
78:t:2072:G:O2'	78:t:2241:G:N2	2.44	0.50
1:S2:678:U:OP1	27:SN:127:ARG:NH1	2.45	0.50
1:S2:1495:G:H22	21:Sd:24:CYS:H	1.60	0.50
4:SD:57:ASN:O	4:SD:65:ARG:NH1	2.43	0.50
11:SP:111:MET:HE2	14:SS:117:ILE:HB	1.94	0.50
24:SG:148:SER:HA	58:X:84:GLY:HA2	1.94	0.50
24:SG:176:ILE:HG21	24:SG:179:LEU:HD22	1.93	0.50
25:SJ:60:LEU:HD23	25:SJ:63:LEU:HD12	1.94	0.50
26:SM:45:ARG:HH12	26:SM:72:HIS:CD2	2.30	0.50
32:Sb:40:CYS:SG	32:Sb:41:TYR:N	2.83	0.50
49:O:115:VAL:HA	49:O:134:LEU:HD13	1.92	0.50
78:t:1409:G:N2	78:t:1440:C:OP2	2.34	0.50
78:t:1424:C:H42	78:t:2084:G:H22	1.57	0.50
78:t:1862:C:H5'	78:t:2260:U:H1'	1.93	0.50
2:SA:148:CYS:N	2:SA:161:ILE:O	2.45	0.49
3:SB:86:LEU:CD2	3:SB:98:THR:HB	2.34	0.49
14:SS:17:ASN:ND2	14:SS:101:ASN:OD1	2.38	0.49
42:H:32:ARG:HH22	78:t:950:G:H21	1.60	0.49
45:K:182:GLU:HA	45:K:185:VAL:HG12	1.94	0.49
55:U:92:ARG:NH1	78:t:4275:A:OP1	2.45	0.49
75:p:36:GLN:HB3	78:t:4325:A:H5''	1.93	0.49
78:t:477:G:N1	78:t:665:G:O6	2.39	0.49
2:SA:108:PHE:HB2	2:SA:136:GLU:HG2	1.93	0.49
6:SF:28:VAL:HG12	6:SF:110:GLN:HB2	1.94	0.49
35:A:220:GLY:O	78:t:3720:C:O2'	2.30	0.49
47:M:3:PRO:HB2	61:b:44:ASN:ND2	2.25	0.49
55:U:41:ASP:HA	55:U:61:THR:HA	1.93	0.49
66:g:59:THR:CG2	78:t:4902:C:N4	2.67	0.49
69:j:70:LEU:HB2	69:j:87:ARG:HG3	1.94	0.49
78:t:410:U:O2'	78:t:2288:G:N2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:466:C:H42	78:t:676:G:H1	1.58	0.49
1:S2:430:C:H2'	1:S2:431:G:H8	1.78	0.49
1:S2:1226:G:H21	1:S2:1640:A:H62	1.59	0.49
23:SC:106:VAL:HG11	23:SC:151:ILE:HD11	1.94	0.49
25:SJ:5:ARG:HD3	25:SJ:7:TRP:H	1.77	0.49
28:SO:102:GLY:HA2	28:SO:136:PRO:HD3	1.93	0.49
56:V:35:ASP:OD1	56:V:35:ASP:N	2.45	0.49
58:X:6:CYS:SG	58:X:10:GLY:N	2.85	0.49
61:b:47:LYS:CG	61:b:48:TYR:CD2	2.95	0.49
69:j:92:ASN:O	69:j:96:ALA:N	2.45	0.49
73:n:124:LYS:NZ	78:t:4435:A:OP1	2.41	0.49
78:t:485:G:N2	78:t:657:C:N3	2.59	0.49
78:t:954:C:O2'	78:t:956:C:OP2	2.29	0.49
1:S2:325:C:C4	58:X:119:LYS:CE	2.95	0.49
8:SI:177:SER:OG	8:SI:182:CYS:SG	2.70	0.49
20:Sc:14:VAL:HA	20:Sc:32:VAL:HA	1.94	0.49
22:Sg:24:THR:HG22	22:Sg:71:ILE:HG21	1.93	0.49
22:Sg:76:GLN:HE21	22:Sg:92:LEU:HB2	1.76	0.49
47:M:141:ALA:O	47:M:142:GLU:C	2.50	0.49
53:S:116:ASP:OD1	53:S:116:ASP:N	2.45	0.49
55:U:19:PHE:CG	55:U:20:ARG:N	2.81	0.49
72:m:5:LYS:NZ	78:t:2761:U:OP1	2.44	0.49
78:t:2068:C:H5''	78:t:2069:G:H3'	1.94	0.49
1:S2:193:C:O2'	1:S2:195:C:N4	2.38	0.49
1:S2:386:C:O2	8:SI:31:ARG:NH2	2.43	0.49
37:C:58:ALA:O	37:C:59:GLY:C	2.41	0.49
37:C:323:ARG:NH2	78:t:1263:C:O2'	2.35	0.49
37:C:343:GLN:HE22	78:t:934:C:H1'	1.77	0.49
38:D:86:U:H3	68:i:7:ARG:HB3	1.76	0.49
40:F:203:ASN:HA	40:F:206:ASP:HB2	1.94	0.49
47:M:74:ARG:NH1	78:t:76:A:OP2	2.46	0.49
54:T:13:VAL:HG22	54:T:63:TYR:HB3	1.94	0.49
63:d:77:ASN:HD22	63:d:78:ASN:H	1.61	0.49
66:g:9:ALA:HA	66:g:30:ILE:HA	1.94	0.49
1:S2:194:C:OP2	1:S2:196:C:N4	2.45	0.49
1:S2:975:G:O2'	28:SO:49:GLY:O	2.30	0.49
1:S2:1610:G:N7	14:SS:132:ARG:NH2	2.60	0.49
7:SH:25:GLN:HA	7:SH:28:LEU:HD12	1.93	0.49
9:SK:44:HIS:O	9:SK:48:ALA:N	2.43	0.49
14:SS:108:ARG:HH12	46:L:125:ILE:HD11	1.78	0.49
22:Sg:16:GLY:N	22:Sg:305:ASN:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sg:72:SER:OG	22:Sg:74:ASP:OD1	2.28	0.49
24:SG:34:THR:H	24:SG:52:ILE:HG22	1.78	0.49
28:SO:27:VAL:HG13	28:SO:90:ILE:HD12	1.95	0.49
36:B:189:THR:O	36:B:193:LYS:N	2.41	0.49
43:I:109:GLU:HA	43:I:112:GLN:HG2	1.94	0.49
45:K:87:ILE:HB	45:K:138:ILE:HG22	1.94	0.49
61:b:123:ILE:HG22	61:b:143:ALA:HB3	1.94	0.49
72:m:36:ARG:HG3	72:m:37:TYR:HD1	1.78	0.49
73:n:114:LYS:NZ	78:t:4447:C:O2'	2.39	0.49
78:t:2537:C:N4	78:t:2538:G:O6	2.45	0.49
1:S2:219:U:O2'	8:SI:186:ASP:OD2	2.31	0.49
1:S2:539:C:H5	1:S2:541:U:H5''	1.77	0.49
1:S2:682:U:P	18:SX:8:ARG:HE	2.36	0.49
1:S2:804:U:H5''	29:SW:82:GLN:HG2	1.95	0.49
1:S2:1142:G:OP2	23:SC:187:ARG:NH2	2.45	0.49
4:SD:119:CYS:SG	4:SD:120:TYR:N	2.85	0.49
6:SF:127:ARG:HG2	6:SF:136:ARG:HD3	1.93	0.49
9:SK:90:VAL:HG23	9:SK:96:ARG:HH12	1.78	0.49
21:Sd:25:SER:OG	21:Sd:27:ARG:NH1	2.46	0.49
36:B:117:ARG:NH2	78:t:4542:U:OP1	2.46	0.49
44:J:44:GLU:N	78:t:4725:U:O2	2.45	0.49
48:N:39:ASP:OD2	48:N:47:ARG:NH1	2.45	0.49
60:Z:54:GLU:HA	60:Z:69:LYS:HA	1.93	0.49
78:t:2009:C:H2'	78:t:2010:A:H8	1.77	0.49
1:S2:1255:G:O6	1:S2:1257:G:N2	2.46	0.49
6:SF:124:ASP:N	6:SF:124:ASP:OD1	2.45	0.49
12:SQ:42:ILE:HG23	12:SQ:44:PRO:HD2	1.95	0.49
25:SJ:111:GLN:NE2	25:SJ:123:ILE:O	2.46	0.49
37:C:24:LEU:HD12	37:C:25:PRO:HD2	1.95	0.49
41:G:174:LEU:HD21	41:G:186:LEU:HD12	1.93	0.49
49:O:189:ARG:NH1	78:t:28:C:OP2	2.46	0.49
50:P:171:LYS:NZ	78:t:4720:U:OP2	2.37	0.49
54:T:162:GLN:HE21	78:t:1900:G:H4'	1.77	0.49
56:V:31:ASP:OD2	56:V:114:TYR:OH	2.29	0.49
58:X:34:ALA:HA	58:X:37:GLU:HB3	1.95	0.49
78:t:178:C:N4	78:t:179:G:O6	2.46	0.49
78:t:2422:G:OP2	78:t:2495:G:N2	2.45	0.49
83:a:11:VAL:HG11	83:a:80:LEU:HD23	1.94	0.49
1:S2:846:G:OP2	5:SE:108:ARG:NH2	2.45	0.49
1:S2:1454:A:H2'	13:SR:3:ARG:HG3	1.94	0.49
1:S2:1616:U:OP2	11:SP:43:ARG:NH2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SX:124:LYS:HG2	18:SX:129:SER:HA	1.95	0.49
44:J:137:SER:HB3	44:J:143:GLU:HB3	1.93	0.49
45:K:188:LYS:HD2	45:K:212:LEU:HD13	1.95	0.49
47:M:76:PHE:CD2	47:M:96:ILE:CG2	2.96	0.49
51:Q:120:ASN:N	51:Q:120:ASN:OD1	2.45	0.49
51:Q:122:ALA:HB3	51:Q:143:PRO:HG2	1.94	0.49
69:j:62:LYS:HE3	69:j:94:LEU:HD21	1.94	0.49
75:p:72:CYS:HB3	75:p:79:SER:H	1.77	0.49
78:t:193:C:O2	78:t:218:C:O2'	2.24	0.49
78:t:3909:G:N2	78:t:4133:C:OP2	2.46	0.49
78:t:4436:A:OP2	78:t:4438:C:N4	2.46	0.49
4:SD:95:GLY:CA	4:SD:125:PHE:HE2	2.24	0.49
7:SH:100:ILE:HD12	7:SH:122:LEU:HA	1.95	0.49
16:SU:98:VAL:HA	16:SU:101:ILE:HD12	1.94	0.49
24:SG:58:LYS:HD3	24:SG:107:SER:HB2	1.94	0.49
24:SG:64:LYS:HZ3	24:SG:81:HIS:HB3	1.77	0.49
36:B:165:HIS:HB3	36:B:180:LEU:HD12	1.94	0.49
38:D:87:G:OP2	68:i:3:LYS:NZ	2.32	0.49
65:f:78:LEU:O	77:r:20:ARG:NH1	2.45	0.49
78:t:85:G:O2'	78:t:97:G:O6	2.30	0.49
78:t:1281:C:H2'	78:t:1282:G:H8	1.78	0.49
78:t:1869:A:N6	78:t:3844:G:O2'	2.46	0.49
78:t:3765:C:H2'	78:t:3766:A:C8	2.46	0.49
78:t:4684:G:OP2	78:t:4684:G:N2	2.45	0.49
78:t:4693:G:H1'	78:t:4694:G:H2'	1.94	0.49
1:S2:69:C:OP2	24:SG:164:LYS:NZ	2.45	0.48
1:S2:737:G:H2'	1:S2:738:C:H4'	1.94	0.48
2:SA:77:ILE:CG1	2:SA:122:LEU:HD12	2.43	0.48
6:SF:123:GLU:OE1	6:SF:204:ARG:NH1	2.46	0.48
11:SP:38:SER:OG	11:SP:41:GLN:OE1	2.29	0.48
16:SU:21:ARG:NH2	16:SU:90:ASP:OD1	2.45	0.48
22:Sg:30:MET:HA	22:Sg:45:LEU:HD23	1.95	0.48
25:SJ:67:ASP:OD2	25:SJ:70:ARG:N	2.46	0.48
29:SW:49:GLU:HB2	29:SW:64:ASN:HD22	1.78	0.48
39:E:34:C:O2	40:F:203:ASN:ND2	2.43	0.48
41:G:100:LYS:HB2	78:t:677:G:H4'	1.95	0.48
41:G:110:ARG:NH2	78:t:955:C:O4'	2.46	0.48
78:t:1072:G:H2'	78:t:1073:G:C8	2.48	0.48
1:S2:65:C:N4	24:SG:134:GLY:O	2.45	0.48
1:S2:101:U:H5''	8:SI:19:LYS:HE2	1.95	0.48
1:S2:482:G:N2	1:S2:484:A2M:H8	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1006:C:H4'	63:d:11:LEU:HB2	1.95	0.48
9:SK:32:HIS:CE1	9:SK:34:GLU:HB2	2.48	0.48
22:Sg:34:ALA:HB2	22:Sg:69:VAL:HG12	1.95	0.48
22:Sg:78:ALA:O	22:Sg:90:TRP:N	2.46	0.48
22:Sg:86:THR:HG21	22:Sg:88:ARG:HH21	1.78	0.48
22:Sg:107:ASP:N	22:Sg:107:ASP:OD1	2.46	0.48
37:C:201:ARG:NH1	78:t:224:A:OP2	2.46	0.48
57:W:89:ARG:HD3	78:t:4635:U:H5'	1.95	0.48
58:X:49:ILE:CD1	58:X:52:THR:CB	2.91	0.48
78:t:1275:C:H3'	78:t:1276:G:H21	1.77	0.48
78:t:1465:C:O2	78:t:1466:G:N1	2.46	0.48
78:t:2824:A:H61	78:t:3814:C:H42	1.62	0.48
1:S2:749:U:O4	1:S2:795:A:O2'	2.31	0.48
5:SE:201:HIS:N	5:SE:206:ASP:OD1	2.40	0.48
13:SR:31:ASN:HD22	13:SR:55:THR:HG22	1.78	0.48
23:SC:187:ARG:HG2	23:SC:192:LEU:HB3	1.95	0.48
24:SG:142:ARG:HA	58:X:83:THR:HG21	1.95	0.48
39:E:6:C:H4'	40:F:52:ILE:HD13	1.94	0.48
48:N:12:VAL:O	48:N:58:THR:OG1	2.27	0.48
50:P:23:VAL:HG13	50:P:33:VAL:HG11	1.95	0.48
64:e:97:ASP:N	64:e:97:ASP:OD1	2.44	0.48
65:f:100:ALA:O	65:f:108:ARG:NH2	2.46	0.48
78:t:82:U:HO2'	78:t:1365:G:HO2'	1.60	0.48
78:t:363:G:N2	78:t:366:A:OP2	2.43	0.48
1:S2:867:G:H1	10:SL:150:GLY:H	1.61	0.48
1:S2:885:U:O2	1:S2:886:A:N6	2.46	0.48
2:SA:76:VAL:HA	2:SA:123:VAL:HG13	1.95	0.48
8:SI:57:ALA:H	8:SI:180:GLY:HA2	1.78	0.48
11:SP:96:VAL:HG11	11:SP:116:LEU:HB3	1.95	0.48
12:SQ:123:ASP:O	12:SQ:126:ARG:NH2	2.40	0.48
34:Sf:93:HIS:CE1	34:Sf:96:LYS:HD2	2.45	0.48
35:A:241:ARG:NH1	78:t:3630:G:OP1	2.37	0.48
57:W:15:ARG:NH1	57:W:16:ILE:O	2.46	0.48
68:i:21:LEU:HD11	68:i:58:LEU:HG	1.95	0.48
78:t:732:C:H42	78:t:910:C:H42	1.61	0.48
78:t:959:C:H2'	78:t:960:G:H8	1.78	0.48
78:t:1507:A:O2'	78:t:3887:G:O2'	2.31	0.48
81:y:22:ILE:CG1	81:y:23:LEU:N	2.77	0.48
1:S2:1857:G:O5'	28:SO:146:ARG:NH1	2.46	0.48
1:S2:1868:U:N3	19:Sa:98:PRO:O	2.46	0.48
22:Sg:252:THR:HG21	22:Sg:257:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O:162:ARG:O	78:t:28:C:O2'	2.30	0.48
62:c:107:ARG:O	62:c:111:ARG:NH1	2.47	0.48
64:e:41:ARG:NH2	78:t:4598:U:OP1	2.46	0.48
78:t:181:U:H1'	78:t:250:G:H22	1.79	0.48
81:y:18:ALA:C	81:y:20:LEU:N	2.72	0.48
1:S2:97:U:O2	1:S2:434:G:N2	2.47	0.48
1:S2:126:G:H21	1:S2:180:G:H21	1.61	0.48
1:S2:1495:G:H1	21:Sd:24:CYS:HG	1.62	0.48
1:S2:1779:G:H2'	1:S2:1780:G:C8	2.48	0.48
3:SB:138:PHE:O	3:SB:213:ARG:N	2.43	0.48
41:G:137:VAL:HG22	41:G:138:ARG:N	2.29	0.48
42:H:182:TYR:HB3	42:H:200:ARG:HG3	1.96	0.48
46:L:112:HIS:CD2	46:L:126:TYR:H	2.32	0.48
50:P:47:PHE:HE1	50:P:141:LEU:HB3	1.77	0.48
60:Z:11:ARG:NH2	78:t:226:G:OP1	2.46	0.48
66:g:58:VAL:HG23	66:g:58:VAL:O	2.14	0.48
77:r:37:SER:OG	77:r:38:PHE:N	2.46	0.48
78:t:425:G:C8	78:t:3859:G:H2'	2.49	0.48
79:v:28:G:H1	79:v:42:C:H42	1.61	0.48
1:S2:38:A:O2'	25:SJ:5:ARG:NH2	2.44	0.48
1:S2:145:G:OP2	24:SG:178:ARG:NH1	2.47	0.48
1:S2:686:U:O2	1:S2:917:U:N3	2.46	0.48
17:SV:3:ASN:OD1	17:SV:7:GLU:N	2.45	0.48
25:SJ:54:ARG:NH2	25:SJ:98:LEU:O	2.44	0.48
39:E:112:U:H2'	39:E:113:G:H8	1.79	0.48
47:M:167:ARG:NH1	47:M:173:GLU:OE2	2.40	0.48
49:O:96:ARG:NH2	78:t:2439:A:O2'	2.45	0.48
50:P:10:ASP:HB3	50:P:119:VAL:HG12	1.94	0.48
78:t:189:G:H1	78:t:244:G:H22	1.62	0.48
78:t:3819:U:O2'	78:t:4596:U:O4	2.32	0.48
1:S2:39:A:H3'	1:S2:40:A:H8	1.79	0.48
1:S2:160:U:O2'	1:S2:162:C:OP2	2.29	0.48
1:S2:1727:G:N2	1:S2:1807:C:O2	2.47	0.48
37:C:54:VAL:CG2	37:C:105:THR:C	2.87	0.48
43:I:30:PRO:HB2	43:I:31:LEU:HD23	1.94	0.48
47:M:59:VAL:HG13	78:t:74:G:H5'	1.96	0.48
51:Q:66:GLY:HA2	78:t:3864:C:H5''	1.96	0.48
55:U:19:PHE:O	55:U:20:ARG:C	2.56	0.48
55:U:19:PHE:C	55:U:21:LYS:H	2.21	0.48
75:p:28:LYS:O	78:t:4306:U:O2'	2.30	0.48
1:S2:945:U:O2	1:S2:982:G:N2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1678:A2M:H2'	1:S2:1679:A:C2	2.49	0.48
1:S2:1748:G:H22	1:S2:1786:U:H3	1.60	0.48
20:Sc:29:GLN:HE21	20:Sc:43:ILE:HD11	1.79	0.48
26:SM:23:LYS:HD2	26:SM:26:LEU:HD12	1.96	0.48
36:B:165:HIS:HB3	36:B:180:LEU:HA	1.96	0.48
53:S:37:SER:OG	53:S:38:ARG:N	2.45	0.48
55:U:52:MET:HB3	55:U:95:HIS:CE1	2.49	0.48
61:b:21:ARG:NH1	78:t:1301:C:OP2	2.47	0.48
64:e:32:ARG:NH2	78:t:4954:C:OP1	2.47	0.48
78:t:1058:G:N2	78:t:1219:C:O2	2.47	0.48
1:S2:677:G:N2	1:S2:678:U:O4	2.47	0.48
1:S2:1171:G:O2'	1:S2:1187:G:O6	2.31	0.48
1:S2:1507:G:N1	34:Sf:86:THR:O	2.47	0.48
1:S2:1821:U:H2'	1:S2:1822:A:H8	1.79	0.48
17:SV:62:MET:HE2	29:SW:20:ARG:HH11	1.79	0.48
40:F:206:ASP:HA	40:F:209:ARG:HB2	1.95	0.48
44:J:41:ILE:HG23	44:J:43:VAL:HG12	1.95	0.48
45:K:38:ARG:HD3	45:K:46:PHE:HZ	1.79	0.48
49:O:68:ARG:NH2	78:t:297:C:OP2	2.47	0.48
50:P:65:ASN:ND2	78:t:4527:C:OP1	2.45	0.48
66:g:104:MET:HB2	66:g:106:TYR:HD2	1.71	0.48
78:t:1078:A:H2	78:t:1183:G:H22	1.61	0.48
79:v:26:A:H2	79:v:44:G:H22	1.62	0.48
1:S2:1232:U:H2'	1:S2:1233:G:H8	1.79	0.47
6:SF:35:LEU:HD22	6:SF:117:ILE:HD13	1.94	0.47
14:SS:125:HIS:CE1	14:SS:131:VAL:HG21	2.49	0.47
41:G:152:ILE:HD12	41:G:189:THR:HG21	1.96	0.47
43:I:248:ALA:O	43:I:252:LYS:N	2.44	0.47
49:O:9:GLU:OE2	49:O:13:LYS:NZ	2.46	0.47
55:U:19:PHE:HE2	55:U:20:ARG:CG	2.27	0.47
59:Y:150:ALA:HB1	59:Y:155:ILE:HD12	1.96	0.47
65:f:75:ARG:HD3	77:r:22:LYS:HZ1	1.79	0.47
70:k:36:LYS:HA	70:k:45:ARG:HH21	1.79	0.47
78:t:735:G:H2'	78:t:736:G:C8	2.49	0.47
78:t:3581:A:H2'	78:t:3582:A:H8	1.79	0.47
1:S2:208:G:O6	8:SI:144:LYS:NZ	2.40	0.47
1:S2:615:C:HO2'	33:Se:8:ARG:HE	1.59	0.47
9:SK:27:VAL:HA	9:SK:43:LEU:HD13	1.95	0.47
11:SP:18:ARG:HH12	11:SP:37:TYR:HA	1.78	0.47
23:SC:137:VAL:HG21	23:SC:244:ILE:HD12	1.96	0.47
38:D:150:C:N4	43:I:52:THR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:F:146:LEU:HD12	78:t:4285:A:H2	1.79	0.47
50:P:54:TYR:OH	50:P:73:PHE:O	2.32	0.47
53:S:67:THR:O	53:S:71:ARG:N	2.47	0.47
59:Y:80:PRO:HG3	68:i:33:VAL:HG13	1.96	0.47
61:b:21:ARG:NH2	78:t:1300:U:OP1	2.48	0.47
78:t:132:G:O6	78:t:136:G:N2	2.46	0.47
78:t:2314:C:H2'	78:t:2315:G:H8	1.78	0.47
1:S2:954:U:H2'	1:S2:955:A:H8	1.80	0.47
1:S2:1130:G:OP2	1:S2:1130:G:N2	2.42	0.47
23:SC:183:LYS:HG2	29:SW:95:PRO:HA	1.97	0.47
36:B:174:ARG:NH2	78:t:4932:C:O2'	2.47	0.47
40:F:155:THR:HG22	40:F:179:ARG:HD3	1.97	0.47
41:G:284:HIS:ND1	66:g:42:TYR:OH	2.41	0.47
49:O:8:GLN:NE2	78:t:272:G:OP1	2.46	0.47
55:U:19:PHE:HD2	55:U:20:ARG:HB3	1.72	0.47
74:o:14:LYS:O	74:o:18:ARG:NH1	2.47	0.47
78:t:2586:C:H2'	78:t:2587:G:C8	2.47	0.47
78:t:4530:A:O2'	78:t:4939:G:N7	2.47	0.47
78:t:4856:G:H1	78:t:4880:C:H42	1.62	0.47
1:S2:587:A:O2'	1:S2:588:G:N2	2.47	0.47
1:S2:1114:U:H3'	1:S2:1115:U:H2'	1.95	0.47
1:S2:1115:U:OP1	1:S2:1116:C:N4	2.48	0.47
1:S2:1275:G:OP1	1:S2:1506:A:N6	2.47	0.47
13:SR:106:LEU:HA	13:SR:109:LEU:HB3	1.96	0.47
25:SJ:173:VAL:O	25:SJ:177:ASN:ND2	2.47	0.47
37:C:278:ASN:HD22	37:C:279:LEU:H	1.62	0.47
43:I:221:ALA:O	43:I:225:ASN:ND2	2.47	0.47
48:N:31:ILE:HG22	54:T:75:VAL:HG13	1.95	0.47
75:p:71:GLU:HG2	75:p:80:LYS:HG2	1.95	0.47
1:S2:323:C:H2'	1:S2:327:G:H22	1.79	0.47
1:S2:328:U:O2	58:X:119:LYS:NZ	2.41	0.47
1:S2:672:A:N6	1:S2:1027:A:OP1	2.44	0.47
1:S2:803:C:O2'	29:SW:80:ASP:OD1	2.28	0.47
1:S2:847:A:OP1	5:SE:108:ARG:NH1	2.47	0.47
1:S2:1645:C:H5'	12:SQ:139:ALA:HA	1.96	0.47
2:SA:144:THR:OG1	2:SA:156:TYR:O	2.31	0.47
5:SE:204:SER:OG	5:SE:205:PHE:N	2.48	0.47
20:Sc:12:ALA:N	20:Sc:56:LEU:O	2.47	0.47
22:Sg:157:SER:HB3	22:Sg:164:ILE:H	1.79	0.47
47:M:88:LYS:HG3	47:M:89:LYS:HG3	1.96	0.47
78:t:404:A:O2'	78:t:408:C:O2'	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:1228:C:H2'	78:t:1229:G:C8	2.49	0.47
78:t:1671:G:N2	78:t:1829:C:O2	2.47	0.47
78:t:2617:G:N2	78:t:2676:A:N1	2.63	0.47
82:u:18:G:HO2'	82:u:57:G:N2	2.12	0.47
1:S2:924:G:OP1	27:SN:3:ARG:NE	2.33	0.47
1:S2:1145:A:O2'	1:S2:1200:A:OP1	2.32	0.47
3:SB:35:ALA:HB2	3:SB:44:ILE:HD11	1.97	0.47
23:SC:196:ILE:HB	23:SC:223:TYR:HB2	1.96	0.47
27:SN:3:ARG:HG2	27:SN:6:ALA:HB3	1.96	0.47
36:B:220:ILE:HD11	36:B:348:ARG:HE	1.79	0.47
37:C:326:LEU:HD21	37:C:333:LYS:HD3	1.96	0.47
41:G:219:LYS:NZ	78:t:1275:C:OP1	2.31	0.47
66:g:105:LEU:CD2	66:g:105:LEU:N	2.77	0.47
78:t:499:G:H1	78:t:647:U:H3	1.62	0.47
78:t:746:C:H2'	78:t:747:G:C8	2.50	0.47
78:t:1430:C:H2'	78:t:1431:G:C4	2.50	0.47
78:t:4429:A:O2'	78:t:4472:A:N3	2.42	0.47
1:S2:298:G:H2'	1:S2:299:A:H8	1.80	0.47
1:S2:1564:C:OP1	15:ST:121:ARG:NH1	2.48	0.47
3:SB:168:MET:HG2	3:SB:197:ILE:HD12	1.97	0.47
5:SE:123:LEU:HD22	5:SE:228:ILE:HG22	1.97	0.47
9:SK:32:HIS:HE1	9:SK:34:GLU:HB2	1.79	0.47
11:SP:42:ARG:O	11:SP:46:ASN:N	2.47	0.47
12:SQ:31:LEU:HB3	12:SQ:67:ASP:HA	1.95	0.47
29:SW:32:LYS:HA	29:SW:35:VAL:HG22	1.96	0.47
31:SZ:65:TYR:OH	31:SZ:76:ARG:NH2	2.47	0.47
38:D:15:G:N1	78:t:412:A:OP2	2.38	0.47
43:I:67:ARG:HB3	49:O:28:TRP:HZ3	1.79	0.47
43:I:73:ARG:NH1	78:t:4046:G:OP1	2.47	0.47
46:L:74:VAL:HG13	46:L:78:LYS:HE2	1.96	0.47
47:M:129:ARG:NH1	78:t:171:C:OP1	2.47	0.47
50:P:184:ASN:O	50:P:187:LYS:NZ	2.28	0.47
65:f:38:PRO:HB2	65:f:43:ASN:HD21	1.78	0.47
68:i:93:ARG:NH1	78:t:19:G:OP1	2.48	0.47
77:r:28:GLU:HB2	77:r:31:ASN:HB2	1.97	0.47
78:t:1180:C:N4	78:t:1181:G:O6	2.48	0.47
78:t:1310:C:H2'	78:t:1311:G:C8	2.49	0.47
78:t:2567:C:OP1	78:t:2747:C:O2'	2.28	0.47
1:S2:291:G:C5	10:SL:41:GLY:HA2	2.47	0.47
1:S2:1544:C:O2'	12:SQ:80:GLN:NE2	2.48	0.47
1:S2:1550:G:O2'	1:S2:1558:C:O2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:144:LYS:HB3	3:SB:206:PRO:HB2	1.96	0.47
5:SE:46:ILE:HA	5:SE:49:ARG:HG3	1.97	0.47
10:SL:79:LYS:HB3	10:SL:87:VAL:HB	1.96	0.47
37:C:321:ASN:ND2	78:t:1265:G:OP1	2.48	0.47
42:H:156:LYS:HD3	42:H:248:ASN:HD21	1.80	0.47
46:L:60:PHE:HB2	46:L:62:ILE:HG22	1.97	0.47
66:g:91:ASN:O	78:t:434:U:O2'	2.29	0.47
78:t:1539:C:H2'	78:t:1540:A:H8	1.79	0.47
78:t:2461:C:H2'	78:t:2462:G:C8	2.49	0.47
78:t:2589:G:H2'	78:t:2590:A:H8	1.80	0.47
78:t:2728:C:H2'	78:t:2729:G:H8	1.80	0.47
78:t:4190:G:HO2'	78:t:4335:G:H1	1.62	0.47
1:S2:989:C:O2	19:Sa:32:LYS:NZ	2.48	0.47
1:S2:1499:U:H5''	4:SD:176:LEU:HD21	1.97	0.47
1:S2:1845:A:H2'	1:S2:1846:G:H8	1.79	0.47
17:SV:78:ILE:CG2	17:SV:79:VAL:HG23	2.45	0.47
46:L:37:ALA:HB2	46:L:70:VAL:HG11	1.95	0.47
52:R:20:SER:O	52:R:26:ARG:NH2	2.48	0.47
75:p:44:LYS:NZ	78:t:91:G:OP1	2.40	0.47
78:t:301:A:N3	78:t:304:G:O2'	2.45	0.47
78:t:894:C:N4	78:t:895:G:O6	2.48	0.47
78:t:1329:C:H2'	78:t:1330:G:C8	2.50	0.47
1:S2:833:C:H41	30:SY:10:ARG:HD3	1.81	0.47
1:S2:1515:G:H2'	1:S2:1516:G:H8	1.80	0.47
1:S2:1528:G:O2'	1:S2:1666:C:OP1	2.25	0.47
1:S2:1533:A:OP1	6:SF:164:ARG:NH1	2.41	0.47
1:S2:1675:A:OP1	6:SF:86:LYS:NZ	2.35	0.47
17:SV:78:ILE:HG22	17:SV:79:VAL:HG23	1.96	0.47
23:SC:166:ARG:NH1	23:SC:252:THR:OG1	2.42	0.47
23:SC:273:LEU:HD22	23:SC:274:VAL:HG23	1.96	0.47
45:K:50:GLY:HA2	45:K:167:ILE:HA	1.97	0.47
52:R:71:LYS:NZ	78:t:1402:G:OP1	2.38	0.47
61:b:132:ARG:NH2	78:t:1450:C:OP1	2.40	0.47
64:e:53:ALA:O	64:e:57:MET:N	2.44	0.47
78:t:2297:G:N2	78:t:2300:G:OP2	2.38	0.47
78:t:3757:U:OP1	78:t:4512:G:O2'	2.29	0.47
78:t:4735:C:O2'	78:t:4736:C:O2	2.32	0.47
1:S2:1051:G:OP1	1:S2:1847:G:O2'	2.32	0.46
1:S2:1226:G:N1	1:S2:1639:G:OP2	2.47	0.46
1:S2:1345:G:OP1	1:S2:1688:C:O2'	2.33	0.46
2:SA:40:LYS:CA	2:SA:48:ILE:HD11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:25:THR:OG1	6:SF:41:VAL:O	2.28	0.46
8:SI:118:ALA:O	8:SI:153:LYS:NZ	2.48	0.46
11:SP:108:LYS:HD3	14:SS:117:ILE:HG22	1.96	0.46
14:SS:44:VAL:HG11	14:SS:71:MET:HE2	1.96	0.46
14:SS:108:ARG:NH2	46:L:113:ILE:HD13	2.30	0.46
37:C:199:ARG:NH2	78:t:344:C:OP1	2.48	0.46
47:M:76:PHE:CE2	47:M:96:ILE:HG22	2.45	0.46
64:e:19:GLU:HB3	64:e:21:VAL:HG13	1.96	0.46
65:f:52:GLN:O	78:t:431:G:O2'	2.26	0.46
78:t:2566:A:H5'	78:t:2749:C:H5'	1.96	0.46
78:t:3668:U:O2	78:t:3790:G:N2	2.49	0.46
78:t:4737:G:N7	78:t:4816:C:N4	2.62	0.46
1:S2:498:C:N4	1:S2:499:G:O6	2.48	0.46
1:S2:614:C:H5'	1:S2:626:G:H1'	1.98	0.46
12:SQ:51:LEU:HB2	12:SQ:84:ILE:HD11	1.98	0.46
19:Sa:25:ASN:HD21	19:Sa:77:CYS:HB3	1.81	0.46
36:B:10:ARG:HH21	36:B:14:LEU:HD21	1.80	0.46
37:C:298:ILE:HD13	52:R:131:PRO:HG3	1.96	0.46
38:D:153:C:H2'	38:D:154:G:C8	2.50	0.46
61:b:29:PRO:HB2	78:t:1663:G:H5'	1.97	0.46
67:h:25:THR:HG22	78:t:2500:G:H5''	1.97	0.46
73:n:79:GLU:O	73:n:83:ARG:N	2.36	0.46
73:n:80:PRO:HA	73:n:83:ARG:HB3	1.97	0.46
78:t:1148:G:H2'	78:t:1149:G:H8	1.80	0.46
81:y:19:ILE:O	81:y:19:ILE:HG23	2.15	0.46
1:S2:606:G:H5''	33:Se:56:ASN:HB3	1.97	0.46
1:S2:904:A:N1	87:S2:2001:HOH:O	2.36	0.46
4:SD:127:MET:HE2	4:SD:154:ASP:OD2	2.15	0.46
7:SH:69:LEU:HD13	7:SH:96:ALA:HB2	1.97	0.46
11:SP:18:ARG:HH12	11:SP:37:TYR:HD1	1.63	0.46
17:SV:53:TYR:CE1	17:SV:72:LEU:HD12	2.32	0.46
17:SV:53:TYR:CD1	17:SV:72:LEU:HD13	2.39	0.46
36:B:389:MET:HE2	36:B:392:LEU:HG	1.98	0.46
37:C:54:VAL:CB	37:C:105:THR:O	2.62	0.46
39:E:8:G:O6	40:F:21:ARG:NH2	2.39	0.46
39:E:103:A:O2'	78:t:1723:G:O6	2.27	0.46
48:N:14:TYR:N	48:N:56:GLN:O	2.47	0.46
60:Z:49:ILE:HD13	60:Z:80:ILE:HG21	1.96	0.46
65:f:79:VAL:HB	65:f:84:GLU:HG3	1.97	0.46
75:p:6:LYS:HE2	75:p:94:GLY:HA3	1.97	0.46
75:p:102:GLN:HE21	75:p:102:GLN:HB3	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:1524:U:O2	78:t:1600:G:N2	2.48	0.46
2:SA:77:ILE:CG1	2:SA:122:LEU:CD1	2.87	0.46
5:SE:198:ARG:HA	5:SE:208:VAL:HG12	1.98	0.46
6:SF:28:VAL:HG11	6:SF:109:LEU:HB2	1.97	0.46
7:SH:44:ASN:OD1	7:SH:68:GLN:NE2	2.48	0.46
15:ST:64:LEU:HD23	15:ST:123:LEU:HB3	1.97	0.46
16:SU:24:LEU:HD13	16:SU:32:LEU:HB2	1.97	0.46
40:F:22:ARG:HD2	40:F:27:LYS:HB2	1.97	0.46
40:F:289:ARG:NH2	78:t:1164:C:OP2	2.48	0.46
49:O:8:GLN:NE2	78:t:273:A:OP2	2.47	0.46
78:t:40:G:N3	78:t:3885:U:N3	2.61	0.46
78:t:1310:C:H2'	78:t:1311:G:H8	1.80	0.46
78:t:1424:C:H42	78:t:2084:G:N2	2.13	0.46
1:S2:383:G:O2'	10:SL:133:PRO:O	2.28	0.46
8:SI:139:LYS:HB2	8:SI:141:ARG:HE	1.80	0.46
18:SX:41:PHE:HB3	18:SX:44:ALA:HB3	1.96	0.46
22:Sg:178:ASN:HB3	22:Sg:185:LYS:HD2	1.97	0.46
30:SY:26:ASP:HA	30:SY:70:THR:HA	1.98	0.46
37:C:322:LEU:O	78:t:1264:G:O2'	2.31	0.46
46:L:108:GLY:HA2	46:L:129:ASP:HA	1.97	0.46
47:M:4:SER:OG	47:M:5:ARG:N	2.46	0.46
50:P:166:ILE:O	50:P:170:LYS:NZ	2.42	0.46
55:U:49:GLN:HA	55:U:52:MET:HE3	1.98	0.46
77:r:84:LYS:HB2	77:r:89:THR:HB	1.96	0.46
83:a:90:PRO:HB2	83:a:117:LYS:HB3	1.96	0.46
1:S2:124:U:OP1	24:SG:201:LYS:NZ	2.49	0.46
1:S2:1340:U:OP2	1:S2:1341:C:O2'	2.29	0.46
5:SE:161:GLN:N	5:SE:171:ASP:O	2.45	0.46
7:SH:27:LEU:HA	7:SH:30:LEU:HD22	1.98	0.46
8:SI:6:ASP:OD2	8:SI:8:TRP:NE1	2.48	0.46
17:SV:17:CYS:SG	17:SV:18:SER:N	2.88	0.46
30:SY:36:PRO:HB2	30:SY:38:THR:HG22	1.98	0.46
35:A:54:ARG:HG2	35:A:56:ALA:H	1.81	0.46
41:G:152:ILE:O	41:G:159:GLY:N	2.48	0.46
42:H:214:SER:OG	42:H:215:SER:N	2.49	0.46
49:O:12:ARG:NE	78:t:273:A:N7	2.64	0.46
78:t:1539:C:H2'	78:t:1540:A:C8	2.51	0.46
78:t:2637:G:N2	78:t:2637:G:OP2	2.49	0.46
81:y:18:ALA:C	81:y:20:LEU:H	2.23	0.46
82:u:64:A:H2'	82:u:65:G:C8	2.50	0.46
7:SH:144:ILE:HG23	29:SW:52:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SK:41:PRO:CG	9:SK:44:HIS:HD2	2.22	0.46
22:Sg:167:SER:OG	22:Sg:175:LYS:O	2.33	0.46
23:SC:273:LEU:HD23	23:SC:273:LEU:C	2.40	0.46
26:SM:23:LYS:HA	26:SM:26:LEU:HD12	1.97	0.46
31:SZ:43:LYS:HG3	31:SZ:44:LEU:HD22	1.98	0.46
43:I:105:GLU:HG3	43:I:109:GLU:HG3	1.98	0.46
59:Y:113:VAL:HG12	59:Y:119:ILE:HD11	1.97	0.46
61:b:3:SER:OG	78:t:2323:U:O4	2.33	0.46
66:g:5:LEU:C	66:g:105:LEU:HD21	2.41	0.46
78:t:1547:A:C5	78:t:1548:C:H1'	2.50	0.46
78:t:2390:C:H2'	78:t:2391:A:C8	2.51	0.46
78:t:3636:G:H1	78:t:3648:U:H3	1.63	0.46
78:t:4722:G:H2'	78:t:4723:G:H8	1.80	0.46
1:S2:1532:C:OP1	1:S2:1604:G:O2'	2.33	0.46
8:SI:106:SER:HB3	8:SI:171:LEU:HD13	1.98	0.46
18:SX:105:PHE:CE2	18:SX:112:VAL:HG22	2.51	0.46
36:B:160:ILE:HG21	36:B:194:LEU:HD12	1.98	0.46
36:B:181:MET:HG2	36:B:182:GLU:H	1.80	0.46
39:E:92:C:H2'	39:E:93:G:C8	2.51	0.46
40:F:205:ALA:O	40:F:209:ARG:N	2.47	0.46
45:K:158:LYS:NZ	78:t:4391:C:N3	2.62	0.46
49:O:143:ARG:NH1	68:i:95:LEU:HA	2.31	0.46
57:W:69:LYS:HB2	57:W:72:LEU:HD13	1.97	0.46
59:Y:47:ARG:NH2	78:t:2453:G:O4'	2.48	0.46
68:i:86:LYS:O	68:i:86:LYS:HD2	2.16	0.46
78:t:1912:C:N4	78:t:2021:A:N3	2.64	0.46
2:SA:21:ALA:HB2	13:SR:91:LEU:HD11	1.97	0.46
6:SF:39:ILE:HD11	6:SF:116:ILE:HG21	1.97	0.46
23:SC:169:TYR:OH	23:SC:175:GLY:O	2.29	0.46
36:B:2:SER:C	36:B:3:HIS:O	2.59	0.46
36:B:107:ALA:HA	36:B:201:LEU:HD13	1.98	0.46
41:G:70:LYS:NZ	78:t:1054:C:O2'	2.37	0.46
43:I:148:GLU:OE1	49:O:6:TYR:OH	2.34	0.46
46:L:51:SER:OG	46:L:52:LYS:N	2.49	0.46
46:L:56:THR:OG1	46:L:64:ARG:N	2.49	0.46
78:t:434:U:H2'	78:t:435:G:H8	1.79	0.46
78:t:746:C:H2'	78:t:747:G:H8	1.81	0.46
4:SD:9:ARG:HA	4:SD:12:VAL:HG22	1.98	0.46
4:SD:101:GLN:HA	4:SD:104:SER:HB3	1.98	0.46
14:SS:84:LEU:HD22	14:SS:95:TYR:HB3	1.98	0.46
22:Sg:138:CYS:SG	22:Sg:139:LYS:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:D:130:C:H2'	38:D:131:G:H8	1.80	0.46
40:F:6:VAL:HG23	40:F:8:LYS:HE3	1.96	0.46
49:O:42:PRO:HG3	49:O:61:ILE:HG13	1.97	0.46
49:O:84:PRO:HA	49:O:87:HIS:CD2	2.51	0.46
50:P:26:GLN:HG3	54:T:167:PHE:CZ	2.50	0.46
50:P:77:SER:HB3	50:P:106:ASP:HB2	1.98	0.46
52:R:32:TYR:O	52:R:36:ALA:N	2.48	0.46
59:Y:150:ALA:HA	59:Y:153:ILE:HG13	1.96	0.46
78:t:967:U:H2'	78:t:968:C:H6	1.81	0.46
78:t:3581:A:H2'	78:t:3582:A:C8	2.50	0.46
1:S2:678:U:H5''	27:SN:127:ARG:HH12	1.81	0.45
1:S2:942:G:N2	28:SO:137:SER:O	2.50	0.45
2:SA:25:LEU:O	2:SA:164:ASN:ND2	2.49	0.45
13:SR:24:LEU:HD11	13:SR:34:VAL:HG11	1.97	0.45
20:Sc:62:GLU:HA	28:SO:117:ARG:HH22	1.81	0.45
32:Sb:62:VAL:HG13	32:Sb:74:THR:HG21	1.97	0.45
36:B:47:LEU:HD23	36:B:346:THR:HG22	1.97	0.45
37:C:76:ILE:HD12	37:C:77:PRO:HD2	1.97	0.45
66:g:6:TRP:HA	66:g:105:LEU:HD21	1.97	0.45
73:n:82:LEU:O	73:n:86:ALA:N	2.45	0.45
1:S2:687:C:N3	7:SH:118:ARG:NH1	2.62	0.45
1:S2:1814:G:H2'	1:S2:1816:G:H5''	1.98	0.45
2:SA:51:LEU:HA	2:SA:54:THR:HG22	1.98	0.45
3:SB:225:LEU:CB	78:t:4080:U:H1'	2.45	0.45
9:SK:52:LEU:HD22	9:SK:55:ARG:HH21	1.80	0.45
22:Sg:157:SER:HB3	22:Sg:164:ILE:HG22	1.98	0.45
25:SJ:32:ILE:HD12	25:SJ:37:LEU:HB2	1.98	0.45
31:SZ:101:SER:OG	31:SZ:102:LYS:N	2.49	0.45
37:C:56:GLU:HB2	37:C:57:LEU:CD2	2.47	0.45
42:H:116:GLN:HB2	42:H:119:ASN:HD21	1.80	0.45
44:J:64:ARG:NH2	78:t:4655:C:OP1	2.48	0.45
49:O:40:PRO:HG3	78:t:8:U:H5'	1.98	0.45
49:O:84:PRO:HA	49:O:87:HIS:HD2	1.80	0.45
50:P:36:VAL:HG12	50:P:108:ILE:HG12	1.99	0.45
53:S:38:ARG:N	78:t:2505:C:OP2	2.43	0.45
54:T:128:LYS:NZ	54:T:130:GLU:OE2	2.49	0.45
71:l:24:LYS:HB2	71:l:35:LYS:HB2	1.97	0.45
78:t:1086:C:H5''	78:t:1087:C:H5	1.80	0.45
78:t:1348:C:O2'	78:t:1350:C:OP2	2.32	0.45
78:t:1742:G:H2'	78:t:1743:G:H8	1.79	0.45
78:t:2251:C:H2'	78:t:2252:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:3841:C:H2'	78:t:3842:A:C8	2.51	0.45
78:t:3888:A:H2'	78:t:3889:G:H8	1.82	0.45
1:S2:16:G:H21	1:S2:1195:A:H62	1.64	0.45
1:S2:681:U:O3'	18:SX:8:ARG:NE	2.41	0.45
1:S2:933:G:H21	1:S2:1000:C:H3'	1.81	0.45
4:SD:204:LEU:HD12	4:SD:205:PRO:HD2	1.98	0.45
12:SQ:116:ASP:OD2	12:SQ:119:LEU:HD12	2.16	0.45
13:SR:66:VAL:O	13:SR:68:GLY:N	2.49	0.45
20:Sc:11:LEU:HD12	20:Sc:55:VAL:HG11	1.99	0.45
25:SJ:138[A]:ARG:H	25:SJ:138[A]:ARG:HG3	1.41	0.45
26:SM:93:LYS:HG3	26:SM:102:LYS:H	1.80	0.45
36:B:334:LYS:NZ	78:t:4636:C:O3'	2.48	0.45
65:f:75:ARG:HB2	65:f:95:TYR:HD1	1.81	0.45
78:t:1962:G:O6	78:t:1969:G:N2	2.49	0.45
78:t:4698:C:H2'	78:t:4699:G:C8	2.50	0.45
1:S2:170:A:OP2	24:SG:140:ARG:NH1	2.50	0.45
3:SB:89:GLU:HB3	3:SB:223:PHE:HE1	1.81	0.45
5:SE:246:LEU:HD23	5:SE:250:GLU:HG2	1.97	0.45
36:B:5:LYS:HB3	36:B:5:LYS:HZ3	1.80	0.45
36:B:35:ASP:OD1	36:B:35:ASP:N	2.48	0.45
53:S:171:LYS:HA	53:S:174:GLU:HG3	1.98	0.45
54:T:13:VAL:HG23	54:T:62:VAL:HG23	1.98	0.45
58:X:6:CYS:HG	58:X:9:SER:HG	1.57	0.45
78:t:1414:C:H42	78:t:1435:A:H61	1.64	0.45
78:t:1810:C:H2'	78:t:1811:G:C8	2.52	0.45
78:t:3725:G:N2	78:t:3742:C:O2	2.50	0.45
1:S2:503:C:H3'	1:S2:504:G:H8	1.82	0.45
1:S2:562:U:H2'	1:S2:563:G:C8	2.52	0.45
26:SM:41:ALA:HA	26:SM:44:LYS:HD3	1.98	0.45
37:C:190:ARG:NH1	78:t:2274:C:OP1	2.50	0.45
40:F:28:THR:O	78:t:4242:A:N6	2.38	0.45
42:H:80:ASN:HA	55:U:143:THR:HG22	1.99	0.45
47:M:76:PHE:CE1	47:M:117:LEU:HD13	2.52	0.45
52:R:57:ASN:OD1	52:R:143:ARG:NH1	2.49	0.45
52:R:184:ARG:NH1	61:b:55:LYS:O	2.50	0.45
54:T:162:GLN:CG	54:T:166:ARG:HH12	2.29	0.45
61:b:4:ARG:NH2	78:t:2320:A:OP2	2.49	0.45
64:e:39:LYS:NZ	78:t:2348:U:O2	2.49	0.45
65:f:108:ARG:NH1	78:t:2305:G:OP1	2.50	0.45
77:r:44:ILE:HG13	77:r:45:HIS:CD2	2.52	0.45
78:t:159:A:H61	78:t:268:C:H42	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:2269:C:HO2'	78:t:2301:G:HO2'	1.63	0.45
83:a:73:LYS:HA	83:a:101:PHE:HZ	1.81	0.45
1:S2:381:C:H41	8:SI:27:TYR:HB2	1.82	0.45
1:S2:475:C:H2'	1:S2:476:A:H8	1.80	0.45
30:SY:76:TYR:OH	30:SY:85:ASN:O	2.34	0.45
36:B:315:ASN:ND2	36:B:325:GLU:OE2	2.49	0.45
37:C:228:THR:HG21	37:C:239:LYS:HD2	1.99	0.45
44:J:17:ASP:N	44:J:17:ASP:OD1	2.49	0.45
45:K:54:SER:HA	45:K:163:GLN:HG3	1.97	0.45
56:V:22:THR:HG23	56:V:69:LYS:HG3	1.98	0.45
57:W:66:LYS:NZ	78:t:3770:A:OP1	2.43	0.45
61:b:117:LEU:HD12	61:b:118:PRO:HD2	1.97	0.45
65:f:89:LEU:HD13	65:f:118:LEU:HD22	1.97	0.45
78:t:2600:A:H2'	78:t:2601:G:H8	1.81	0.45
1:S2:1549:U:OP2	4:SD:8:LYS:NZ	2.50	0.45
1:S2:1630:A:H5''	14:SS:37:GLY:H	1.80	0.45
2:SA:14:ASP:HA	2:SA:17:LYS:HZ1	1.82	0.45
13:SR:90:ALA:HA	13:SR:93:GLN:HE22	1.82	0.45
17:SV:15:ARG:HH21	17:SV:24:ILE:HG21	1.81	0.45
27:SN:41:ALA:HB1	27:SN:75:LEU:HD11	1.99	0.45
75:p:36:GLN:N	78:t:4325:A:OP1	2.48	0.45
77:r:26:SER:OG	77:r:28:GLU:OE2	2.34	0.45
78:t:75:G:N2	78:t:320:C:OP1	2.44	0.45
78:t:1820:U:H2'	78:t:1821:G:H8	1.81	0.45
78:t:1964:A:H62	78:t:1968:C:H5	1.65	0.45
78:t:2390:C:HO2'	78:t:2505:C:HO2'	1.61	0.45
1:S2:380:G:N1	1:S2:383:G:OP2	2.49	0.45
1:S2:785:C:O3'	24:SG:231:ARG:NH2	2.47	0.45
6:SF:59:LYS:HB3	6:SF:62:ARG:HH12	1.82	0.45
7:SH:162:GLN:NE2	7:SH:165:ASN:OD1	2.49	0.45
15:ST:40:ALA:O	15:ST:42:HIS:N	2.50	0.45
16:SU:49:LYS:HG3	16:SU:92:HIS:CE1	2.51	0.45
17:SV:25:GLY:O	23:SC:85:SER:OG	2.35	0.45
21:Sd:21:CYS:SG	21:Sd:22:ARG:N	2.89	0.45
41:G:133:PHE:CA	41:G:136:HIS:HE1	2.13	0.45
47:M:121:ARG:HD2	47:M:124:LEU:HD23	1.99	0.45
52:R:42:THR:HB	78:t:1411:U:H5''	1.98	0.45
1:S2:305:U:OP1	1:S2:308:G:O2'	2.34	0.45
1:S2:596:U:O2'	1:S2:645:C:O2	2.31	0.45
4:SD:16:ILE:HD13	21:Sd:22:ARG:HH11	1.82	0.45
5:SE:36:HIS:CG	5:SE:85:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:144:LEU:HD23	20:Sc:49:PRO:HG2	1.99	0.45
7:SH:34:SER:HB2	7:SH:78:ARG:HD3	1.99	0.45
24:SG:57:ASP:OD2	24:SG:72:ARG:NH2	2.47	0.45
35:A:207:VAL:HG12	78:t:3890:C:H4'	1.98	0.45
36:B:231:VAL:HG22	36:B:268:ARG:HA	1.99	0.45
56:V:91:LEU:HD22	56:V:96:LEU:HB2	1.98	0.45
57:W:24:ALA:HB3	57:W:39:ILE:HD12	1.98	0.45
1:S2:185:G:O6	1:S2:214:U:N3	2.50	0.45
1:S2:466:G:H8	24:SG:59:GLN:HE22	1.64	0.45
1:S2:482:G:N3	1:S2:484:A2M:H8	2.32	0.45
1:S2:656:G:OP2	1:S2:662:G:N2	2.50	0.45
10:SL:96:ILE:HG22	10:SL:98:LYS:H	1.82	0.45
36:B:263:ALA:HA	50:P:64:THR:HA	1.98	0.45
51:Q:23:ARG:NH2	78:t:2398:C:OP1	2.38	0.45
56:V:48:LYS:HE2	56:V:53:ALA:HB2	1.97	0.45
78:t:742:G:N2	78:t:743:G:N7	2.55	0.45
78:t:4666:C:H2'	78:t:4667:A:C8	2.51	0.45
1:S2:1452:A:O2'	1:S2:1475:G:N2	2.50	0.44
1:S2:1598:G:H1'	1:S2:1599:U:H5	1.81	0.44
3:SB:28:LYS:HA	3:SB:50:THR:HA	1.98	0.44
11:SP:100:LYS:HG2	11:SP:101:THR:HG23	1.98	0.44
13:SR:60:ARG:HG2	13:SR:66:VAL:HG21	1.99	0.44
23:SC:94:ILE:HD11	23:SC:162:ILE:HD13	1.99	0.44
43:I:87:LEU:HD11	43:I:182:CYS:HB2	1.98	0.44
49:O:64:ILE:HG21	49:O:106:ALA:HB2	1.99	0.44
78:t:637:C:H2'	78:t:638:G:C8	2.52	0.44
78:t:2623:G:H2'	78:t:2624:G:H8	1.82	0.44
5:SE:151:ASP:OD1	24:SG:216:ARG:NE	2.50	0.44
6:SF:50:PRO:HG3	6:SF:69:VAL:HG12	1.98	0.44
23:SC:274:VAL:CG1	23:SC:278:THR:CB	2.51	0.44
24:SG:32:MET:HB2	24:SG:100:CYS:HB2	1.99	0.44
41:G:278:THR:OG1	78:t:4839:U:O4	2.27	0.44
43:I:38:ASN:OD1	78:t:4085:C:N4	2.51	0.44
46:L:101:ASP:N	78:t:4210:A:O2'	2.47	0.44
54:T:160:ARG:HD3	54:T:163:HIS:NE2	2.19	0.44
78:t:3660:G:O2'	78:t:3789:U:OP2	2.30	0.44
1:S2:1821:U:H2'	1:S2:1822:A:C8	2.52	0.44
3:SB:70:SER:OG	3:SB:73:ASP:OD1	2.34	0.44
5:SE:246:LEU:HD22	5:SE:254:LYS:HE2	1.99	0.44
6:SF:87:LEU:HA	6:SF:90:VAL:HG12	1.99	0.44
8:SI:76:THR:HG21	8:SI:104:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SI:132:GLU:C	8:SI:132:GLU:CD	2.85	0.44
9:SK:22:VAL:HG13	9:SK:68:TYR:HE1	1.82	0.44
15:ST:18:LEU:HD12	15:ST:134:ILE:HD11	1.99	0.44
27:SN:103:GLU:OE1	27:SN:106:ARG:NH2	2.49	0.44
36:B:3:HIS:O	36:B:3:HIS:CG	2.70	0.44
40:F:41:LYS:HE3	40:F:41:LYS:HB3	1.81	0.44
42:H:116:GLN:OE1	42:H:212:LYS:NZ	2.51	0.44
45:K:47:PRO:O	45:K:172:GLY:N	2.41	0.44
46:L:164:ARG:O	46:L:168:GLN:N	2.47	0.44
57:W:61:VAL:O	57:W:79:ALA:N	2.47	0.44
58:X:49:ILE:O	58:X:55:TYR:HB2	2.16	0.44
66:g:58:VAL:HG21	66:g:63:LYS:C	2.42	0.44
68:i:88:THR:HG23	68:i:91:MET:H	1.83	0.44
78:t:2542:C:H2'	78:t:2543:G:C8	2.51	0.44
78:t:2559:U:H5'	83:a:36:ARG:HH12	1.81	0.44
78:t:2652:G:H5''	78:t:2653:A:H3'	2.00	0.44
1:S2:874:G:H2'	1:S2:875:A:H8	1.83	0.44
4:SD:203:PRO:HB2	4:SD:207:HIS:CE1	2.53	0.44
12:SQ:91:ALA:O	12:SQ:95:TYR:N	2.48	0.44
14:SS:45:LEU:HB3	14:SS:50:ILE:HD11	2.00	0.44
16:SU:18:HIS:CD2	16:SU:94:PRO:HA	2.50	0.44
36:B:315:ASN:HD22	36:B:325:GLU:HG2	1.83	0.44
39:E:75:G:H22	39:E:99:G:H2'	1.82	0.44
43:I:164:ILE:HG23	49:O:22:LEU:HD13	1.99	0.44
43:I:244:PRO:HA	43:I:247:VAL:HG12	2.00	0.44
46:L:136:ARG:NH1	46:L:155:HIS:O	2.50	0.44
52:R:156:PRO:HG2	61:b:48:TYR:HA	1.99	0.44
65:f:48:ARG:O	78:t:1864:G:O2'	2.34	0.44
66:g:72:GLY:HA3	66:g:88:PHE:CD1	2.53	0.44
68:i:17:LEU:O	68:i:21:LEU:N	2.46	0.44
78:t:147:U:H5''	78:t:149:U:H5'	1.98	0.44
78:t:704:C:H2'	78:t:705:G:C8	2.51	0.44
78:t:1540:A:H2'	78:t:1541:G:H8	1.83	0.44
82:u:7:A:H61	82:u:66:U:H3	1.65	0.44
1:S2:290:U:N3	1:S2:292:A:O3'	2.50	0.44
1:S2:878:G:H22	1:S2:908:A:H2	1.66	0.44
1:S2:1121:G:O2'	3:SB:204:ILE:O	2.29	0.44
1:S2:1163:C:H2'	1:S2:1164:G:C8	2.53	0.44
1:S2:1544:C:H4'	12:SQ:80:GLN:HE22	1.82	0.44
1:S2:1549:U:OP1	21:Sd:34:TYR:OH	2.34	0.44
1:S2:1785:C:C4	58:X:73:ARG:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:225:LEU:HB3	78:t:4080:U:H1'	1.99	0.44
8:SI:57:ALA:HB2	8:SI:183:GLY:HA2	1.99	0.44
40:F:144:CYS:SG	40:F:145:TYR:N	2.90	0.44
41:G:188:ARG:NH2	78:t:4899:G:OP2	2.41	0.44
46:L:112:HIS:HD2	46:L:126:TYR:H	1.66	0.44
50:P:121:PRO:HD3	54:T:168:THR:HG22	2.00	0.44
78:t:434:U:H2'	78:t:435:G:C8	2.52	0.44
78:t:1857:U:H2'	78:t:1858:G:H8	1.82	0.44
78:t:2590:A:H5'	78:t:2667:G:H4'	1.99	0.44
78:t:4205:C:O2'	78:t:4230:A:N3	2.43	0.44
1:S2:166:A2M:H1'	24:SG:13:GLN:OE1	2.17	0.44
1:S2:325:C:N3	58:X:119:LYS:CD	2.80	0.44
8:SI:83:TYR:HB3	8:SI:101:ILE:HB	2.00	0.44
16:SU:97:ILE:HB	16:SU:100:GLN:HE21	1.82	0.44
22:Sg:289:LEU:HD12	22:Sg:298:LEU:HD21	2.00	0.44
37:C:56:GLU:CD	37:C:56:GLU:N	2.72	0.44
37:C:266:THR:HG23	37:C:268:ARG:H	1.82	0.44
38:D:130:C:H2'	38:D:131:G:C8	2.53	0.44
53:S:46:LYS:NZ	78:t:2685:G:O6	2.45	0.44
53:S:93:VAL:HG11	78:t:2704:A:H1'	1.99	0.44
78:t:467:C:H2'	78:t:468:C:C6	2.53	0.44
78:t:1373:G:N2	78:t:1376:G:OP2	2.50	0.44
78:t:1981:G:OP2	78:t:1981:G:N2	2.50	0.44
78:t:2461:C:H2'	78:t:2462:G:H8	1.83	0.44
78:t:3592:A:O2'	78:t:4620:G:O2'	2.29	0.44
78:t:4722:G:H2'	78:t:4723:G:C8	2.52	0.44
1:S2:166:A2M:HM'2	1:S2:167:G:H5'	1.99	0.44
1:S2:621:C:H5'	18:SX:107:ARG:HH22	1.82	0.44
1:S2:788:G:O2'	1:S2:789:G:O4'	2.36	0.44
1:S2:1143:A:OP2	23:SC:187:ARG:NH1	2.51	0.44
1:S2:1591:C:H5'	6:SF:85:LYS:HE3	2.00	0.44
1:S2:1656:G:H1	1:S2:1668:U:H3	1.66	0.44
15:ST:33:TRP:HE1	15:ST:102:ARG:NH2	2.16	0.44
18:SX:107:ARG:HG3	18:SX:112:VAL:HG12	2.00	0.44
18:SX:132:ALA:HB1	18:SX:137:LYS:HB2	1.99	0.44
25:SJ:83:ARG:HE	25:SJ:150:ARG:HD3	1.83	0.44
25:SJ:136:ARG:HD3	25:SJ:160:SER:HA	2.00	0.44
41:G:155:GLY:HA2	78:t:4900:C:H5''	1.99	0.44
43:I:82:GLN:HG2	43:I:233:ILE:HG12	1.98	0.44
46:L:44:THR:OG1	46:L:45:GLY:N	2.50	0.44
56:V:60:VAL:HG21	56:V:76:VAL:CG2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:W:65:VAL:HG21	57:W:72:LEU:HB3	2.00	0.44
61:b:100:ILE:HA	61:b:123:ILE:HG13	1.98	0.44
1:S2:650:A:OP2	18:SX:108:LYS:NZ	2.51	0.44
1:S2:1545:A:H4'	12:SQ:74:GLY:HA2	1.99	0.44
1:S2:1750:C:O2'	58:X:74:ARG:NH1	2.50	0.44
17:SV:71:ARG:HD3	32:Sb:4:ALA:HB1	1.99	0.44
21:Sd:53:ILE:H	21:Sd:53:ILE:HG13	1.53	0.44
54:T:5:GLY:O	54:T:111:ARG:NH2	2.51	0.44
61:b:45:PHE:HD1	61:b:45:PHE:HA	1.61	0.44
76:q:19:GLY:O	76:q:23:ARG:NE	2.47	0.44
78:t:301:A:H2'	78:t:302:G:C8	2.53	0.44
82:u:9:A:O4'	82:u:46:G:N2	2.50	0.44
1:S2:325:C:N3	58:X:119:LYS:CE	2.81	0.44
1:S2:1513:C:H2'	1:S2:1514:G:C8	2.53	0.44
2:SA:46:ILE:O	2:SA:47:TYR:HD1	2.01	0.44
11:SP:98:ASN:OD1	11:SP:101:THR:N	2.42	0.44
13:SR:54:VAL:O	13:SR:58:MET:N	2.51	0.44
25:SJ:29:LEU:HD21	33:Se:41:ARG:HD2	2.00	0.44
26:SM:62:VAL:HA	26:SM:65:VAL:HG12	2.00	0.44
36:B:46:PHE:HE2	36:B:81:THR:HB	1.82	0.44
39:E:7:G:O5'	40:F:33:ARG:NH1	2.51	0.44
52:R:43:PHE:CD2	52:R:133:GLY:HA3	2.52	0.44
54:T:66:GLN:HG2	54:T:68:PHE:HD1	1.83	0.44
55:U:17:ARG:HD2	55:U:17:ARG:N	2.33	0.44
78:t:483:C:O2'	78:t:661:G:N2	2.51	0.44
78:t:1259:C:H2'	78:t:1260:G:C8	2.52	0.44
1:S2:591:U:H4'	1:S2:592:C:H3'	2.00	0.43
1:S2:1084:A:OP1	1:S2:1858:G:O2'	2.35	0.43
6:SF:49:LEU:HD21	12:SQ:50:LYS:HG3	1.99	0.43
6:SF:61:PHE:O	20:Sc:51:ARG:NH2	2.51	0.43
22:Sg:99:ARG:HH22	22:Sg:134:THR:HB	1.83	0.43
23:SC:103:LYS:HZ3	23:SC:216:MET:HG3	1.82	0.43
41:G:198:SER:HG	48:N:105:THR:HG1	1.63	0.43
47:M:125:ILE:CD1	47:M:140:SER:HB3	2.44	0.43
50:P:137:TYR:HB2	50:P:140:ARG:HG3	2.00	0.43
51:Q:10:ASN:HD21	51:Q:13:LYS:HE2	1.82	0.43
52:R:91:ARG:HG3	61:b:76:ASP:HB3	1.99	0.43
60:Z:26:ARG:HD3	60:Z:75:ARG:O	2.18	0.43
67:h:26:PRO:HD2	78:t:2500:G:H4'	2.00	0.43
78:t:229:G:H21	78:t:230:U:H2'	1.83	0.43
78:t:1476:U:H2'	78:t:1477:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:168:C:O2'	24:SG:133:LEU:O	2.29	0.43
1:S2:1676:U:O2'	1:S2:1677:U:O4'	2.34	0.43
3:SB:187:LYS:HG3	3:SB:192:SER:HB3	2.00	0.43
5:SE:41:CYS:SG	5:SE:84:ALA:N	2.91	0.43
8:SI:163:GLU:HA	8:SI:166:PHE:HD2	1.82	0.43
22:Sg:63:SER:OG	22:Sg:64:HIS:N	2.51	0.43
24:SG:49:VAL:HG22	24:SG:115:LYS:HE3	2.00	0.43
28:SO:95:ILE:HB	28:SO:129:ILE:HA	1.99	0.43
34:Sf:94:LYS:CE	34:Sf:94:LYS:CA	2.85	0.43
37:C:11:TYR:N	37:C:153:VAL:O	2.50	0.43
40:F:229:ASN:OD1	40:F:229:ASN:N	2.51	0.43
42:H:156:LYS:HD3	42:H:248:ASN:ND2	2.34	0.43
47:M:164:GLU:HB2	61:b:100:ILE:HD13	1.99	0.43
62:c:91:ARG:HG3	78:t:1248:G:H1	1.83	0.43
78:t:216:G:H1	78:t:233:G:H1	1.66	0.43
78:t:4281:C:H2'	78:t:4282:G:C8	2.53	0.43
1:S2:93:U:OP1	5:SE:2:ALA:N	2.51	0.43
1:S2:671:A:OP1	1:S2:1163:C:O2'	2.35	0.43
1:S2:1275:G:N2	1:S2:1506:A:OP2	2.38	0.43
1:S2:1298:G:H1'	11:SP:79:HIS:HB2	2.00	0.43
2:SA:29:ASN:OD1	2:SA:29:ASN:N	2.50	0.43
22:Sg:5:MET:HG3	22:Sg:312:VAL:HG22	2.00	0.43
35:A:43:GLY:O	35:A:88:VAL:N	2.37	0.43
36:B:254:ILE:H	36:B:254:ILE:HG13	1.65	0.43
38:D:41:A:N6	38:D:102:G:O2'	2.51	0.43
38:D:102:G:OP2	38:D:104:A:O2'	2.36	0.43
41:G:90:ALA:HB3	41:G:107:VAL:HG12	2.00	0.43
50:P:54:TYR:HE2	50:P:145:VAL:HG11	1.83	0.43
61:b:100:ILE:HG22	61:b:123:ILE:HD11	2.00	0.43
75:p:104:ILE:HD12	75:p:106:PHE:N	2.34	0.43
78:t:4933:G:O2'	78:t:4935:A:N6	2.45	0.43
1:S2:515:G:O2'	1:S2:517:OMC:OP2	2.33	0.43
1:S2:1102:G:OP1	3:SB:151:ARG:NH1	2.52	0.43
1:S2:1336:C:H4'	21:Sd:44:ARG:HH12	1.83	0.43
2:SA:77:ILE:HD11	2:SA:124:VAL:HG22	1.99	0.43
32:Sb:64:CYS:HB3	32:Sb:73:LEU:HD23	1.99	0.43
36:B:242:ARG:HA	36:B:248:LEU:HD11	1.99	0.43
38:D:55:U:H3	38:D:62:A:H2	1.64	0.43
42:H:167:ILE:H	42:H:167:ILE:HG13	1.66	0.43
43:I:99:ALA:HB2	43:I:204:PHE:HZ	1.83	0.43
43:I:220:GLU:HA	43:I:223:ARG:HG2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:X:56:ARG:O	58:X:63:GLN:NE2	2.52	0.43
64:e:93:ASN:HD22	64:e:94:GLU:H	1.66	0.43
78:t:166:G:H22	78:t:261:G:H1	1.66	0.43
78:t:920:G:N2	78:t:925:C:O2'	2.46	0.43
78:t:1157:G:H2'	78:t:1158:A:C8	2.54	0.43
78:t:1225:G:N7	78:t:1252:G:O2'	2.41	0.43
1:S2:482:G:N2	1:S2:485:A:OP2	2.42	0.43
1:S2:589:G:H2'	1:S2:591:U:H5	1.84	0.43
1:S2:591:U:O2	1:S2:593:C:N4	2.52	0.43
1:S2:639:C:H2'	1:S2:640:A:H8	1.84	0.43
1:S2:1424:G:H2'	1:S2:1425:G:H8	1.83	0.43
4:SD:169:ASP:OD1	4:SD:169:ASP:N	2.52	0.43
5:SE:105:THR:HG23	5:SE:106:LYS:HG3	2.01	0.43
5:SE:138:HIS:CD2	5:SE:148:ARG:HG2	2.53	0.43
7:SH:60:ILE:HG23	7:SH:90:LYS:HD2	1.99	0.43
9:SK:29:MET:C	9:SK:42:ASN:ND2	2.76	0.43
18:SX:9:THR:O	18:SX:12:LYS:N	2.50	0.43
22:Sg:195:LEU:HA	22:Sg:211:GLY:HA3	2.00	0.43
23:SC:211:LYS:HG2	23:SC:215:MET:HE2	1.99	0.43
36:B:315:ASN:OD1	36:B:315:ASN:N	2.51	0.43
42:H:86:GLU:HG3	55:U:135:PRO:HB2	2.00	0.43
51:Q:101:ASN:OD1	78:t:393:G:N2	2.51	0.43
78:t:730:G:H2'	78:t:731:G:C8	2.52	0.43
11:SP:41:GLN:HG3	11:SP:115:TYR:HE1	1.84	0.43
26:SM:75:ASN:OD1	26:SM:75:ASN:N	2.45	0.43
35:A:64:ARG:HE	43:I:45:ILE:HD11	1.83	0.43
36:B:33:PRO:HA	36:B:351:LEU:HG	2.00	0.43
36:B:228:TYR:O	78:t:2814:A:O2'	2.35	0.43
37:C:71:ARG:NH1	81:y:25:GLY:O	2.52	0.43
40:F:39:GLN:HE21	40:F:43:LYS:HD2	1.82	0.43
43:I:154:LEU:HB3	43:I:204:PHE:HB2	2.00	0.43
45:K:193:ASP:N	45:K:193:ASP:OD1	2.51	0.43
46:L:56:THR:HG23	46:L:63:ARG:HA	2.01	0.43
48:N:28:VAL:HG11	48:N:47:ARG:HH22	1.83	0.43
59:Y:79:PHE:HB2	59:Y:99:ILE:HB	2.00	0.43
63:d:103:ASP:HB3	63:d:106:ARG:HH21	1.83	0.43
78:t:1865:C:O2'	78:t:2050:A:O2'	2.36	0.43
78:t:4494:U:OP2	78:t:4516:G:N2	2.38	0.43
1:S2:104:A:H62	1:S2:356:C:H5	1.66	0.43
1:S2:1350:U:O2'	2:SA:110:ASN:OD1	2.32	0.43
1:S2:1447:G:H2'	1:S2:1448:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:17:LYS:HG2	13:SR:91:LEU:HB3	2.00	0.43
2:SA:41:ARG:HA	2:SA:47:TYR:HD1	1.83	0.43
4:SD:141:LYS:HZ3	4:SD:179:GLN:HB2	1.83	0.43
6:SF:59:LYS:H	6:SF:62:ARG:HH22	1.65	0.43
10:SL:45:LYS:HE3	10:SL:45:LYS:HB3	1.90	0.43
12:SQ:112:LEU:HD22	12:SQ:119:LEU:HD22	2.00	0.43
36:B:243:LYS:NZ	78:t:1573:U:OP2	2.37	0.43
37:C:326:LEU:HD23	78:t:963:G:H4'	1.99	0.43
37:C:340:ILE:HD13	41:G:51:VAL:HG21	2.00	0.43
38:D:60:G:O6	68:i:62:ASN:ND2	2.49	0.43
47:M:3:PRO:C	61:b:44:ASN:HD21	2.27	0.43
47:M:28:GLN:HG3	47:M:29:PRO:HD3	2.00	0.43
51:Q:52:THR:HG22	51:Q:85:LYS:HA	2.00	0.43
59:Y:127:LEU:HD11	78:t:2415:U:H3'	2.01	0.43
64:e:96:GLU:O	64:e:97:ASP:C	2.61	0.43
68:i:25:LYS:HG2	68:i:54:ILE:HD11	2.00	0.43
68:i:41:ALA:HA	68:i:44:LEU:HD13	1.99	0.43
78:t:477:G:N2	78:t:478:U:O4	2.51	0.43
78:t:1520:U:O2'	78:t:1611:G:OP1	2.35	0.43
78:t:4328:A:N6	78:t:4329:G:O6	2.52	0.43
78:t:4950:G:H1	78:t:5017:C:H42	1.67	0.43
1:S2:319:C:H2'	1:S2:320:G:H8	1.84	0.43
1:S2:795:A:H2'	1:S2:796:G:H8	1.83	0.43
1:S2:927:C:H2'	1:S2:928:G:H8	1.84	0.43
1:S2:1534:C:H41	1:S2:1600:G:H1	1.66	0.43
1:S2:1782:G:H21	58:X:75:ALA:HB3	1.82	0.43
3:SB:104:ASP:N	3:SB:104:ASP:OD1	2.48	0.43
4:SD:125:PHE:HD2	4:SD:126:ILE:HD12	1.84	0.43
7:SH:96:ALA:HB3	7:SH:98:ARG:HH21	1.84	0.43
12:SQ:132:PHE:HB2	16:SU:77:TRP:HB2	1.99	0.43
22:Sg:122:SER:OG	22:Sg:132:TRP:NE1	2.48	0.43
23:SC:146:GLU:HB3	23:SC:149:THR:HG22	2.00	0.43
38:D:48:A:N7	38:D:62:A:N6	2.66	0.43
40:F:110:LEU:O	40:F:114:GLY:N	2.52	0.43
49:O:185:GLY:H	49:O:191:ALA:HB2	1.83	0.43
52:R:156:PRO:O	61:b:50:PRO:HG3	2.18	0.43
53:S:110:ARG:NH1	78:t:2643:G:OP1	2.52	0.43
59:Y:119:ILE:HD13	59:Y:140:LEU:HD22	1.99	0.43
66:g:58:VAL:CB	66:g:64:PRO:HA	2.25	0.43
78:t:1397:C:H2'	78:t:1398:G:C8	2.54	0.43
1:S2:639:C:H2'	1:S2:640:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1350:U:H2'	1:S2:1351:G:C8	2.54	0.43
5:SE:238:LEU:HD22	5:SE:239:PRO:HD2	2.00	0.43
6:SF:188:TYR:HA	6:SF:191:LYS:HG2	2.00	0.43
14:SS:120:HIS:CE1	14:SS:124:ARG:HH11	2.37	0.43
25:SJ:30:LYS:HA	33:Se:38:TYR:HE1	1.84	0.43
35:A:20:VAL:HG13	35:A:23:ARG:HD2	2.01	0.43
36:B:219:VAL:HG11	36:B:337:VAL:HG13	2.00	0.43
38:D:147:G:H1	78:t:9:C:H42	1.67	0.43
46:L:110:GLN:NE2	78:t:4213:A:O2'	2.51	0.43
48:N:97:ALA:HB1	50:P:198:THR:HG23	2.01	0.43
49:O:161:MET:N	49:O:161:MET:SD	2.91	0.43
56:V:103:VAL:HG21	56:V:113:ARG:NH1	2.33	0.43
78:t:445:C:H5''	78:t:447:G:H8	1.83	0.43
78:t:972:C:H2'	78:t:973:C:C6	2.54	0.43
1:S2:433:A:OP1	8:SI:25:ARG:NH1	2.47	0.43
1:S2:1679:A:C2	6:SF:60:ARG:HB3	2.54	0.43
6:SF:30:ILE:HG21	6:SF:36:GLN:HA	2.00	0.43
9:SK:40:VAL:HA	9:SK:41:PRO:HD3	1.85	0.43
18:SX:114:ASP:N	18:SX:114:ASP:OD1	2.52	0.43
22:Sg:40:ILE:HB	22:Sg:59:LEU:HB2	2.01	0.43
25:SJ:131:ARG:HA	25:SJ:143:ASN:HB2	2.00	0.43
39:E:85:G:P	42:H:222:LYS:HZ1	2.42	0.43
42:H:86:GLU:HA	42:H:87:PRO:HD3	1.88	0.43
50:P:18:ARG:HH11	50:P:128:ARG:HH11	1.67	0.43
51:Q:94:MET:O	51:Q:98:ALA:N	2.52	0.43
70:k:48:ASN:ND2	78:t:52:G:OP2	2.36	0.43
78:t:700:C:H2'	78:t:701:G:C8	2.54	0.43
78:t:1650:A:OP2	78:t:2259:G:N2	2.49	0.43
78:t:2791:A:N6	78:t:2792:A:N1	2.66	0.43
1:S2:1549:U:H2'	1:S2:1550:G:C8	2.52	0.42
25:SJ:109:ARG:HE	25:SJ:146:SER:HA	1.84	0.42
27:SN:119:GLU:HA	27:SN:122:ILE:HD12	2.01	0.42
37:C:56:GLU:HB2	37:C:57:LEU:HD23	1.99	0.42
37:C:307:LYS:NZ	78:t:2070:U:OP2	2.43	0.42
52:R:37:ARG:H	52:R:37:ARG:HG3	1.71	0.42
60:Z:4:ASN:HB3	60:Z:7:VAL:HG12	2.00	0.42
78:t:1315:C:H2'	78:t:1316:A:C8	2.54	0.42
78:t:2541:G:O2'	78:t:2544:A:N6	2.52	0.42
78:t:3696:G:N2	78:t:3699:A:OP2	2.42	0.42
1:S2:9:U:N3	1:S2:12:U:OP2	2.52	0.42
1:S2:84:A:H4'	30:SY:124:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:844:U:H2'	1:S2:845:G:H8	1.84	0.42
13:SR:55:THR:HA	13:SR:58:MET:HB2	2.01	0.42
23:SC:274:VAL:HG12	23:SC:278:THR:HG1	1.68	0.42
30:SY:37:LYS:NZ	30:SY:93:ARG:HE	2.17	0.42
36:B:41:VAL:HA	36:B:187:GLY:HA2	2.01	0.42
36:B:170:LEU:O	36:B:328:ASN:ND2	2.45	0.42
37:C:207:PRO:HB3	37:C:249:PHE:CD2	2.54	0.42
47:M:20:ARG:HH22	78:t:50:C:H5''	1.83	0.42
48:N:20:HIS:CD2	48:N:48:GLN:HE22	2.37	0.42
50:P:65:ASN:OD1	50:P:65:ASN:N	2.52	0.42
51:Q:60:PHE:O	51:Q:78:TRP:NE1	2.52	0.42
78:t:2293:G:H2'	78:t:2294:G:H8	1.83	0.42
82:u:20:U:H2'	82:u:21:A:H4'	2.01	0.42
1:S2:808:A:H2'	5:SE:221:ARG:HH11	1.84	0.42
9:SK:3:MET:HG3	9:SK:8:ARG:HG3	2.00	0.42
15:ST:96:SER:HB3	15:ST:99:VAL:HG12	2.02	0.42
22:Sg:179:LEU:HA	22:Sg:182:CYS:HA	2.01	0.42
23:SC:221:ASP:N	23:SC:221:ASP:OD1	2.52	0.42
32:Sb:24:LEU:HD22	32:Sb:24:LEU:HA	1.90	0.42
40:F:43:LYS:HE3	78:t:1799:U:H4'	2.01	0.42
42:H:232:ASP:OD1	42:H:232:ASP:N	2.51	0.42
44:J:92:MET:HG3	44:J:144:LEU:HB3	2.01	0.42
45:K:76:MET:HE1	45:K:138:ILE:HD13	2.00	0.42
50:P:168:TYR:OH	78:t:4729:C:OP1	2.29	0.42
78:t:1826:U:H2'	78:t:1827:G:H8	1.84	0.42
78:t:1966:G:N3	78:t:1984:G:O2'	2.53	0.42
78:t:2552:A:H62	78:t:2740:U:H3	1.68	0.42
78:t:3680:U:N3	78:t:3681:G:O6	2.51	0.42
78:t:4597:A:H8	78:t:5006:A:H61	1.67	0.42
78:t:4864:C:H1'	78:t:4865:G:H5'	2.01	0.42
2:SA:48:ILE:CD1	2:SA:48:ILE:C	2.92	0.42
5:SE:202:PRO:HB2	10:SL:42:LEU:HG	2.01	0.42
8:SI:23:LYS:O	8:SI:25:ARG:NH2	2.53	0.42
24:SG:7:PHE:HA	24:SG:8:PRO:HD3	1.92	0.42
25:SJ:33:GLY:HA3	33:Se:38:TYR:CG	2.55	0.42
38:D:52:A:N6	72:m:27:ILE:HD13	2.34	0.42
59:Y:60:TYR:OH	78:t:17:A:OP2	2.30	0.42
66:g:54:LYS:CG	78:t:437:G:C5'	2.86	0.42
76:q:46:LYS:HE3	76:q:58:GLY:HA3	2.00	0.42
78:t:2589:G:H2'	78:t:2590:A:C8	2.53	0.42
83:a:21:ARG:NH1	83:a:47:ASP:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:655:A:H4'	1:S2:656:G:H3'	2.00	0.42
1:S2:1541:G:OP1	15:ST:56:ARG:NE	2.35	0.42
8:SI:110:ARG:HH22	8:SI:169:GLY:HA2	1.84	0.42
15:ST:69:GLY:H	15:ST:122:LYS:HG2	1.83	0.42
25:SJ:25:LEU:O	25:SJ:29:LEU:N	2.52	0.42
36:B:174:ARG:HH22	78:t:4932:C:H1'	1.84	0.42
37:C:10:VAL:HA	37:C:153:VAL:HG23	2.01	0.42
42:H:124:LYS:HE3	42:H:201:PHE:HD2	1.84	0.42
52:R:121:LEU:HA	52:R:125:GLN:HE21	1.84	0.42
78:t:172:C:H2'	78:t:173:G:C8	2.54	0.42
78:t:950:G:N7	78:t:951:A:N6	2.67	0.42
83:a:57:MET:HA	83:a:61:LYS:HE3	2.02	0.42
1:S2:921:G:C2	32:Sb:22:LYS:HG2	2.54	0.42
1:S2:1263:U:O2	21:Sd:16:GLN:NE2	2.47	0.42
1:S2:1438:A:H2'	1:S2:1439:A:C8	2.54	0.42
1:S2:1562:C:H2'	1:S2:1563:G:C8	2.52	0.42
1:S2:1603:G:H22	14:SS:24:ARG:HD3	1.83	0.42
2:SA:42:LYS:HE3	13:SR:122:PRO:HG3	2.01	0.42
6:SF:171:GLU:O	6:SF:175:ASP:N	2.47	0.42
7:SH:53:VAL:HG12	7:SH:175:GLY:HA3	2.01	0.42
23:SC:274:VAL:CG2	23:SC:278:THR:HG21	2.46	0.42
36:B:41:VAL:HG22	36:B:188:GLY:H	1.85	0.42
36:B:185:VAL:HG12	36:B:187:GLY:H	1.85	0.42
40:F:120:GLU:O	40:F:248:ARG:NH2	2.52	0.42
41:G:70:LYS:NZ	78:t:1054:C:O2	2.43	0.42
41:G:240:TYR:CD2	41:G:242:ILE:HG22	2.55	0.42
42:H:242:ARG:NH2	78:t:929:G:OP2	2.52	0.42
44:J:12:ILE:HD12	44:J:53:LYS:HB3	2.00	0.42
47:M:146:LEU:HD21	68:i:122:LYS:HG3	2.01	0.42
50:P:116:LYS:NZ	78:t:4720:U:OP1	2.51	0.42
52:R:15:ARG:HD3	78:t:1673:G:OP1	2.20	0.42
57:W:84:GLN:NE2	57:W:86:LYS:HB3	2.34	0.42
78:t:2588:G:H2'	78:t:2589:G:H8	1.84	0.42
78:t:3800:G:H2'	78:t:3801:A:H8	1.84	0.42
1:S2:964:A:N3	1:S2:1054:G:O2'	2.49	0.42
13:SR:71:ILE:O	13:SR:75:GLU:N	2.48	0.42
19:Sa:64:LEU:HA	19:Sa:65:PRO:HD3	1.91	0.42
20:Sc:31:ARG:HE	20:Sc:43:ILE:HD13	1.84	0.42
24:SG:121:ILE:HB	24:SG:124:LEU:HB3	2.01	0.42
39:E:8:G:OP2	40:F:30:TYR:OH	2.28	0.42
52:R:146:ARG:HD3	52:R:149:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:154:LEU:HD12	54:T:157:ARG:HD3	2.02	0.42
62:c:33:LYS:HE2	62:c:33:LYS:HB3	1.83	0.42
72:m:27:ILE:HG13	72:m:30:LYS:HD3	2.02	0.42
75:p:47:GLY:HA2	78:t:282:G:H5'	2.01	0.42
78:t:1388:C:H2'	78:t:1389:G:C8	2.55	0.42
78:t:1602:U:H2'	78:t:1603:A:H8	1.83	0.42
78:t:1736:U:H3	78:t:1758:A:H61	1.67	0.42
78:t:1822:C:H2'	78:t:1823:G:H4'	2.01	0.42
78:t:4551:A:N6	78:t:4583:C:O2'	2.47	0.42
1:S2:1199:A:H2'	1:S2:1200:A:C8	2.55	0.42
2:SA:38:ILE:CD1	2:SA:48:ILE:O	2.68	0.42
9:SK:41:PRO:CG	9:SK:44:HIS:CD2	2.98	0.42
15:ST:113:VAL:HA	15:ST:123:LEU:HA	2.01	0.42
16:SU:19:ARG:HH22	16:SU:49:LYS:HZ1	1.66	0.42
17:SV:15:ARG:HA	23:SC:259:THR:HG21	2.01	0.42
19:Sa:100:ARG:HH21	19:Sa:102:ARG:HH21	1.68	0.42
22:Sg:122:SER:N	22:Sg:130:LYS:O	2.50	0.42
23:SC:192:LEU:HG	23:SC:227:ARG:HB3	2.01	0.42
24:SG:162:LEU:HD13	24:SG:162:LEU:HA	1.87	0.42
52:R:121:LEU:HD23	52:R:125:GLN:HG3	2.01	0.42
54:T:16:CYS:HA	54:T:59:GLY:HA2	2.02	0.42
57:W:69:LYS:HA	57:W:70:PRO:HD3	1.92	0.42
65:f:43:ASN:ND2	78:t:1299:G:OP1	2.52	0.42
72:m:43:HIS:HD2	72:m:46:ARG:HG3	1.84	0.42
78:t:262:G:H2'	78:t:263:G:H8	1.84	0.42
5:SE:124:CYS:HB3	5:SE:141:THR:HB	2.02	0.42
19:Sa:10:ARG:HH11	19:Sa:10:ARG:HD3	1.67	0.42
25:SJ:86:VAL:HG23	25:SJ:104:ASP:HB3	2.02	0.42
28:SO:27:VAL:N	28:SO:91:THR:OG1	2.53	0.42
29:SW:57:ARG:H	29:SW:57:ARG:HD2	1.85	0.42
35:A:227:ARG:HH22	78:t:3630:G:H4'	1.85	0.42
36:B:86:VAL:O	36:B:202:GLU:N	2.50	0.42
40:F:184:ASP:HB3	40:F:187:SER:HB3	2.02	0.42
41:G:150:LEU:HB2	41:G:162:VAL:HG23	2.02	0.42
55:U:50:LYS:NZ	78:t:4274:U:OP1	2.42	0.42
66:g:11:PHE:HE1	66:g:26:ALA:HB1	1.83	0.42
78:t:715:C:H2'	78:t:716:G:C8	2.52	0.42
78:t:1148:G:H2'	78:t:1149:G:C8	2.53	0.42
78:t:1426:A:O2'	78:t:1427:G:O4'	2.31	0.42
78:t:2090:C:N4	78:t:2091:G:O6	2.53	0.42
78:t:2374:A:O2'	78:t:2786:A:OP2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:4562:G:H1'	78:t:4563:U:H5	1.85	0.42
83:a:81:MET:HE3	83:a:81:MET:HB3	1.93	0.42
1:S2:376:A:OP2	10:SL:58:LYS:NZ	2.43	0.42
6:SF:177:LEU:O	6:SF:181:ALA:N	2.52	0.42
10:SL:126:VAL:HG12	10:SL:128:VAL:HG23	2.01	0.42
16:SU:56:MET:HB3	16:SU:56:MET:HE3	1.83	0.42
19:Sa:45:VAL:O	28:SO:113:GLN:NE2	2.53	0.42
24:SG:23:LYS:HD2	24:SG:42:GLY:H	1.85	0.42
35:A:45:VAL:HB	35:A:61:VAL:HG22	2.02	0.42
41:G:193:PHE:CE1	66:g:107:PRO:HD3	2.55	0.42
43:I:158:ALA:HB2	43:I:190:LEU:HD21	2.02	0.42
47:M:169:ILE:H	47:M:169:ILE:HG13	1.58	0.42
49:O:144:ARG:NH1	78:t:124:C:OP1	2.53	0.42
57:W:94:VAL:HG21	58:X:20:ARG:CZ	2.50	0.42
59:Y:139:ARG:NH1	78:t:2512:C:OP1	2.52	0.42
63:d:16:SER:HA	63:d:19:GLN:HG3	2.01	0.42
67:h:97:ILE:HD11	78:t:4091:G:C5	2.54	0.42
78:t:191:C:O2	78:t:243:G:N2	2.53	0.42
78:t:454:C:H2'	78:t:455:G:C8	2.55	0.42
78:t:4429:A:H61	78:t:4452:C:H42	1.68	0.42
1:S2:27:A2M:HM'3	1:S2:27:A2M:H1'	1.74	0.41
1:S2:624:C:N4	18:SX:63:ASN:OD1	2.40	0.41
1:S2:1337:4AC:O5'	1:S2:1337:4AC:H6	2.20	0.41
3:SB:123:ALA:HB1	3:SB:169:MET:HE2	2.02	0.41
18:SX:3:LYS:HE3	18:SX:3:LYS:HB2	1.90	0.41
23:SC:264:SER:H	23:SC:267:GLN:HE21	1.68	0.41
36:B:292:LEU:HD12	36:B:299:ILE:HD11	2.02	0.41
37:C:121:ARG:HA	37:C:124:ILE:HG22	2.01	0.41
40:F:139:PRO:HB3	78:t:1802:C:H5'	2.01	0.41
41:G:141:ARG:HH12	41:G:192:LYS:HA	1.85	0.41
44:J:41:ILE:HD13	44:J:73:ILE:HD11	2.02	0.41
44:J:64:ARG:HA	44:J:67:LEU:HB2	2.01	0.41
47:M:62:PRO:HG3	78:t:74:G:H1'	2.02	0.41
48:N:91:TRP:HA	48:N:94:LYS:HE2	2.02	0.41
54:T:115:ALA:O	54:T:118:ARG:NH1	2.53	0.41
1:S2:1092:G:OP1	27:SN:2:GLY:N	2.53	0.41
2:SA:39:TYR:HB3	2:SA:48:ILE:HD13	2.02	0.41
3:SB:117:TRP:CD1	3:SB:153:THR:HG22	2.55	0.41
10:SL:61:PRO:HA	10:SL:66:VAL:HG13	2.01	0.41
15:ST:40:ALA:O	15:ST:42:HIS:ND1	2.53	0.41
28:SO:75:MET:HG2	28:SO:118:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:160:ILE:HD11	36:B:193:LYS:HG2	2.02	0.41
39:E:11:A:O2'	39:E:13:A:OP2	2.35	0.41
42:H:151:ASN:ND2	78:t:931:A:N1	2.67	0.41
52:R:173:LYS:HE2	52:R:173:LYS:HB3	1.85	0.41
55:U:87:LYS:HZ3	78:t:4267:G:N2	2.16	0.41
56:V:65:ARG:HG2	56:V:66:SER:O	2.19	0.41
66:g:59:THR:CG2	78:t:4902:C:C6	2.95	0.41
77:r:51:VAL:HG12	77:r:62:VAL:HG22	2.00	0.41
78:t:1648:C:O2'	78:t:1670:G:OP1	2.37	0.41
78:t:2390:C:O2'	78:t:2505:C:O2'	2.33	0.41
78:t:3724:G:N2	78:t:3743:U:O2	2.54	0.41
1:S2:1337:4AC:OP1	21:Sd:44:ARG:NH2	2.52	0.41
2:SA:5:LEU:HD23	2:SA:8:LEU:HD12	2.02	0.41
2:SA:154:LEU:HD22	2:SA:157:VAL:HG21	2.02	0.41
13:SR:78:ARG:HE	13:SR:81:ARG:HH21	1.68	0.41
22:Sg:220:ASP:OD1	22:Sg:221:LEU:N	2.53	0.41
23:SC:169:TYR:O	29:SW:98:GLN:NE2	2.43	0.41
27:SN:4:MET:HG2	27:SN:5:HIS:CD2	2.55	0.41
37:C:113:ARG:HD3	37:C:113:ARG:HA	1.84	0.41
40:F:51:MET:HE3	40:F:51:MET:HB2	1.89	0.41
40:F:97:ALA:HA	40:F:100:CYS:HB3	2.01	0.41
42:H:125:LEU:HD23	42:H:125:LEU:HA	1.92	0.41
44:J:58:ASP:OD1	44:J:58:ASP:N	2.53	0.41
48:N:82:ILE:O	48:N:86:TRP:N	2.44	0.41
60:Z:45:ARG:NH2	78:t:234:G:OP2	2.53	0.41
78:t:686:C:H2'	78:t:687:A:H8	1.84	0.41
78:t:1075:G:H22	78:t:1186:G:H22	1.68	0.41
78:t:2398:C:H5	78:t:2408:A:H1'	1.85	0.41
6:SF:44:LYS:NZ	12:SQ:114:GLN:O	2.41	0.41
10:SL:89:ARG:HE	10:SL:106:HIS:CD2	2.39	0.41
27:SN:135:LEU:HD23	27:SN:135:LEU:HA	1.90	0.41
31:SZ:79:ILE:HD12	31:SZ:81:GLY:H	1.86	0.41
35:A:30:ARG:O	35:A:163:ARG:NH2	2.54	0.41
37:C:116:ASN:OD1	37:C:116:ASN:N	2.53	0.41
39:E:38:U:N3	39:E:41:G:OP2	2.39	0.41
42:H:99:ASN:OD1	42:H:99:ASN:N	2.53	0.41
53:S:75:HIS:ND1	78:t:2868:G:OP1	2.53	0.41
55:U:54:HIS:CD2	78:t:4263:U:H4'	2.56	0.41
58:X:49:ILE:HD11	58:X:52:THR:CB	2.50	0.41
63:d:96:ILE:H	63:d:96:ILE:HG13	1.68	0.41
66:g:50:VAL:HG22	66:g:69:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:t:1491:C:H2'	78:t:1492:G:C8	2.55	0.41
78:t:4235:A:H2'	78:t:4236:A:C8	2.55	0.41
78:t:4701:C:H2'	78:t:4702:G:H8	1.85	0.41
1:S2:433:A:H5''	8:SI:22:HIS:HB3	2.02	0.41
1:S2:991:G:C6	1:S2:1134:G:H4'	2.55	0.41
3:SB:30:TRP:CE2	28:SO:19:PRO:HD3	2.55	0.41
4:SD:220:THR:OG1	4:SD:221:THR:N	2.53	0.41
15:ST:39:LEU:HA	15:ST:39:LEU:HD23	1.76	0.41
36:B:108:GLU:HA	36:B:137:TRP:CD1	2.55	0.41
36:B:119:TYR:OH	36:B:129:ALA:N	2.53	0.41
37:C:8:ILE:HG23	37:C:149:GLU:HG2	2.02	0.41
48:N:100:ARG:HA	48:N:103:LYS:HE3	2.03	0.41
58:X:109:ILE:HG23	58:X:113:LYS:HE3	2.00	0.41
61:b:102:ASP:OD1	61:b:102:ASP:N	2.49	0.41
69:j:62:LYS:HG3	69:j:63:VAL:HG13	2.02	0.41
78:t:62:A:N3	78:t:77:U:O2'	2.45	0.41
78:t:748:G:H2'	78:t:749:G:C8	2.55	0.41
78:t:1289:C:H2'	78:t:1290:A:C8	2.55	0.41
78:t:1619:A:OP1	78:t:1622:C:N4	2.51	0.41
83:a:31:ASP:OD1	83:a:31:ASP:N	2.53	0.41
1:S2:222:U:H5''	10:SL:17:PHE:CG	2.54	0.41
1:S2:527:C:OP1	33:Se:35:ARG:NH2	2.54	0.41
1:S2:934:G:OP2	1:S2:993:G:N2	2.52	0.41
1:S2:1446:A:N3	16:SU:55:ARG:HG3	2.34	0.41
18:SX:8:ARG:NH2	18:SX:9:THR:HB	2.34	0.41
26:SM:35:ILE:H	26:SM:35:ILE:HG13	1.74	0.41
36:B:8:ALA:HB2	57:W:49:LEU:HD12	2.02	0.41
43:I:97:LYS:HE2	43:I:97:LYS:HB3	1.93	0.41
50:P:46:ASN:N	50:P:46:ASN:OD1	2.53	0.41
50:P:118:MET:SD	54:T:167:PHE:O	2.79	0.41
60:Z:122:LYS:HG2	78:t:191:C:H4'	2.02	0.41
78:t:159:A:H2'	78:t:160:A:C8	2.55	0.41
78:t:294:A:H2'	78:t:295:G:H8	1.85	0.41
78:t:1088:C:O2	78:t:1148:G:N2	2.53	0.41
78:t:1351:A:OP2	78:t:1353:G:O2'	2.39	0.41
78:t:2340:G:O2'	78:t:3830:G:O6	2.31	0.41
78:t:2847:G:N2	78:t:2862:G:O6	2.53	0.41
1:S2:325:C:C4	1:S2:325:C:C2	3.01	0.41
1:S2:954:U:O2	28:SO:55:ARG:NH2	2.53	0.41
4:SD:40:ARG:NH2	4:SD:49:ILE:HG23	2.35	0.41
5:SE:194:VAL:N	5:SE:211:LYS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SQ:34:VAL:HG12	12:SQ:70:VAL:HB	2.02	0.41
19:Sa:89:ARG:HA	19:Sa:89:ARG:HD3	1.94	0.41
22:Sg:127:LYS:HE2	22:Sg:148:SER:HA	2.01	0.41
25:SJ:120:ALA:HB2	25:SJ:129:LEU:HD12	2.03	0.41
41:G:284:HIS:HD1	66:g:42:TYR:HH	1.55	0.41
42:H:60:GLU:HA	42:H:63:GLN:HG2	2.03	0.41
43:I:106:THR:HG22	43:I:109:GLU:HG2	2.02	0.41
52:R:60:PRO:HG3	78:t:1336:G:H22	1.85	0.41
78:t:416:C:H2'	78:t:417:G:H8	1.86	0.41
78:t:1437:G:H2'	78:t:1438:G:C8	2.55	0.41
78:t:1460:C:H2'	78:t:1461:G:C8	2.55	0.41
78:t:1820:U:H2'	78:t:1821:G:C8	2.55	0.41
78:t:1887:U:H2'	78:t:1888:A:H8	1.86	0.41
78:t:1956:G:H1'	78:t:1965:A:H5''	2.02	0.41
78:t:4148:A:H2'	78:t:4149:G:C8	2.56	0.41
78:t:4351:C:H2'	78:t:4352:A:C8	2.53	0.41
78:t:4818:G:H2'	78:t:4819:G:C8	2.56	0.41
1:S2:373:G:H21	10:SL:83:GLN:NE2	2.19	0.41
1:S2:574:A:H4'	30:SY:89:HIS:HB2	2.03	0.41
1:S2:1593:C:H2'	1:S2:1594:A:H8	1.85	0.41
16:SU:48:LEU:HB3	16:SU:92:HIS:HE1	1.86	0.41
33:Se:2:VAL:O	33:Se:8:ARG:NH2	2.53	0.41
35:A:215:ASN:ND2	78:t:4508:A:N7	2.69	0.41
37:C:47:ASN:OD1	37:C:113:ARG:N	2.43	0.41
37:C:54:VAL:HG21	37:C:106:LYS:N	2.36	0.41
37:C:70:GLY:HA3	78:t:3877:A:H5'	1.95	0.41
38:D:14:U:H5''	51:Q:123:PRO:HD3	2.03	0.41
46:L:54:ARG:HA	46:L:64:ARG:HG3	2.02	0.41
51:Q:18:ARG:HB3	78:t:393:G:H4'	2.02	0.41
55:U:19:PHE:O	55:U:21:LYS:HB2	2.21	0.41
55:U:87:LYS:HE3	55:U:87:LYS:HB3	1.85	0.41
59:Y:141:ALA:HB3	59:Y:144:TYR:HD2	1.85	0.41
65:f:36:ARG:NH2	78:t:2301:G:OP1	2.53	0.41
65:f:79:VAL:HA	77:r:20:ARG:HH12	1.85	0.41
68:i:106:LYS:NZ	78:t:112:C:OP2	2.50	0.41
75:p:8:ARG:HH22	78:t:4254:A:HO2'	1.67	0.41
78:t:1329:C:H2'	78:t:1330:G:H8	1.85	0.41
78:t:2818:U:O4	78:t:2819:A:N6	2.54	0.41
78:t:3579:A:H2'	78:t:3580:G:H8	1.86	0.41
78:t:4832:A:H1'	78:t:4834:U:N3	2.35	0.41
1:S2:325:C:N1	58:X:119:LYS:CE	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1115:U:H5''	1:S2:1116:C:C4	2.56	0.41
1:S2:1414:A:O2'	15:ST:128:GLN:NE2	2.54	0.41
7:SH:49:LYS:HD3	7:SH:49:LYS:HA	1.94	0.41
13:SR:57:LEU:HG	13:SR:60:ARG:HD3	2.03	0.41
15:ST:5:THR:OG1	15:ST:6:VAL:N	2.53	0.41
18:SX:105:PHE:HD1	18:SX:121:LYS:HB3	1.85	0.41
22:Sg:70:VAL:HG22	22:Sg:111:VAL:HG23	2.03	0.41
24:SG:50:VAL:HG12	24:SG:113:ILE:HA	2.03	0.41
24:SG:58:LYS:HA	24:SG:107:SER:HB2	2.03	0.41
36:B:249:ARG:NH1	78:t:3816:A:OP2	2.37	0.41
37:C:124:ILE:HD11	37:C:235:LEU:HB2	2.02	0.41
41:G:156:ARG:NH2	78:t:4898:C:OP1	2.39	0.41
46:L:20:LEU:HD13	46:L:132:VAL:HG22	2.02	0.41
49:O:75:VAL:HG21	49:O:80:THR:HA	2.02	0.41
51:Q:139:TYR:HD1	51:Q:139:TYR:HA	1.74	0.41
53:S:65:LYS:HE2	53:S:65:LYS:HB3	1.85	0.41
57:W:35:LYS:HA	57:W:35:LYS:HD2	1.85	0.41
69:j:68:ARG:NH1	78:t:3693:G:OP1	2.54	0.41
70:k:3:LYS:N	78:t:3613:A:O2'	2.54	0.41
71:l:49:ASP:HB2	71:l:52:LYS:HB2	2.03	0.41
73:n:97:ARG:NH1	73:n:121:LEU:O	2.53	0.41
78:t:137:G:N3	78:t:138:C:N4	2.69	0.41
78:t:163:C:H42	78:t:264:U:H3	1.69	0.41
78:t:189:G:H22	78:t:244:G:H22	1.67	0.41
78:t:1071:C:O2	78:t:1191:G:N2	2.54	0.41
78:t:3578:U:H2'	78:t:3579:A:C8	2.56	0.41
78:t:3598:G:H2'	78:t:3599:G:H8	1.86	0.41
78:t:3843:A:H2'	78:t:3844:G:C8	2.55	0.41
78:t:4216:G:O2'	78:t:4218:A:N1	2.41	0.41
78:t:4416:G:H1	78:t:4488:U:H3	1.69	0.41
1:S2:70:G:H22	1:S2:79:A:H3'	1.86	0.41
1:S2:1581:C:H5'	1:S2:1582:C:H5	1.86	0.41
1:S2:1780:G:H3'	1:S2:1781:A:H4'	2.03	0.41
12:SQ:13:PHE:HA	12:SQ:22:VAL:HA	2.02	0.41
17:SV:34:MET:HE3	17:SV:34:MET:HB2	1.95	0.41
21:Sd:54:LYS:HG3	21:Sd:55:LEU:H	1.86	0.41
25:SJ:162:ARG:HH22	25:SJ:169:ARG:HB3	1.86	0.41
28:SO:27:VAL:O	28:SO:91:THR:OG1	2.37	0.41
36:B:4:ARG:HH12	36:B:8:ALA:HB3	1.86	0.41
36:B:90:VAL:HG22	36:B:104:THR:HG22	2.01	0.41
37:C:54:VAL:CG2	37:C:105:THR:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:140:LYS:NZ	37:C:245:HIS:O	2.45	0.41
40:F:68:ARG:HA	40:F:68:ARG:HD3	1.80	0.41
63:d:47:ILE:HD12	63:d:94:LEU:HD11	2.02	0.41
65:f:7:LEU:HB3	65:f:8:VAL:H	1.57	0.41
73:n:100:TYR:OH	78:t:4387:G:OP1	2.38	0.41
78:t:67:C:N4	78:t:319:U:O2'	2.54	0.41
78:t:387:U:H2'	78:t:388:G:C8	2.56	0.41
78:t:1071:C:H2'	78:t:1072:G:C8	2.56	0.41
78:t:4882:C:H2'	78:t:4883:U:C2	2.55	0.41
82:u:7:A:N6	82:u:66:U:H3	2.19	0.41
1:S2:193:C:H2'	1:S2:206:G:H1	1.86	0.40
1:S2:509:OMG:HM23	1:S2:509:OMG:H1'	1.69	0.40
1:S2:1098:C:H2'	1:S2:1099:G:C8	2.56	0.40
1:S2:1867:U:C2	19:Sa:98:PRO:HG2	2.56	0.40
2:SA:215:GLN:HA	2:SA:218:ALA:HB3	2.03	0.40
4:SD:226:GLN:HG3	22:Sg:186:THR:HG22	2.03	0.40
12:SQ:90:LYS:HB3	12:SQ:120:LEU:HB2	2.02	0.40
24:SG:198:ARG:HA	24:SG:201:LYS:HB3	2.03	0.40
37:C:155:GLU:HA	37:C:254:GLU:HG3	2.03	0.40
42:H:102:SER:HB2	42:H:105:VAL:HG12	2.04	0.40
48:N:31:ILE:H	48:N:31:ILE:HG13	1.76	0.40
52:R:64:SER:OG	52:R:89:ASP:OD2	2.31	0.40
52:R:68:ARG:HH21	52:R:69:LYS:NZ	2.19	0.40
53:S:62:ARG:NH2	78:t:4610:A:OP1	2.49	0.40
54:T:51:LEU:HD12	55:U:151:LEU:HD13	2.03	0.40
67:h:15:THR:OG1	67:h:18:ASN:N	2.45	0.40
68:i:40:ALA:O	68:i:42:SER:N	2.55	0.40
72:m:23:ILE:H	72:m:23:ILE:HG13	1.69	0.40
78:t:489:C:H2'	78:t:490:G:C8	2.55	0.40
78:t:710:C:H2'	78:t:711:G:C8	2.57	0.40
1:S2:70:G:O6	24:SG:170:ARG:NH1	2.55	0.40
1:S2:533:A:H61	1:S2:550:C:N4	2.18	0.40
1:S2:1287:A:C8	26:SM:35:ILE:HD11	2.56	0.40
5:SE:161:GLN:HG2	5:SE:170:THR:HB	2.03	0.40
11:SP:72:LYS:HA	11:SP:73:PRO:HD3	1.95	0.40
25:SJ:76:ALA:HA	25:SJ:79:ARG:HG3	2.03	0.40
37:C:295:SER:HA	37:C:296:PRO:HD3	1.96	0.40
41:G:125:LEU:HD21	78:t:947:A:C4	2.53	0.40
41:G:207:LYS:HD3	41:G:207:LYS:HA	1.83	0.40
52:R:16:LYS:HD2	52:R:16:LYS:HA	1.92	0.40
53:S:23:TRP:CE3	78:t:2366:G:H5'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:11:THR:HA	55:U:14:MET:HG2	2.04	0.40
62:c:31:SER:HB3	78:t:1445:C:H5'	2.01	0.40
64:e:46:LEU:HD23	64:e:64:ILE:HD11	2.03	0.40
65:f:4:LEU:HD23	65:f:4:LEU:HA	1.93	0.40
65:f:86:GLU:OE2	65:f:114:ARG:NH2	2.55	0.40
78:t:1826:U:H2'	78:t:1827:G:C8	2.56	0.40
78:t:3902:C:H1'	78:t:4142:G:H22	1.85	0.40
78:t:4433:U:H3	78:t:4446:G:H1	1.67	0.40
83:a:15:ALA:HB3	83:a:79:HIS:CD2	2.48	0.40
1:S2:31:U:H4'	1:S2:595:U:H4'	2.04	0.40
1:S2:388:U:H2'	1:S2:389:A:C8	2.55	0.40
1:S2:942:G:H21	28:SO:137:SER:HB2	1.85	0.40
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.56	0.40
1:S2:1547:C:N4	1:S2:1586:U:O4	2.52	0.40
2:SA:78:SER:O	2:SA:101:GLY:N	2.53	0.40
6:SF:103:LEU:HD22	6:SF:178:ILE:HD11	2.02	0.40
10:SL:73:LEU:HD12	10:SL:140:PHE:HE2	1.86	0.40
13:SR:33:ARG:HG3	22:Sg:125:ARG:NH2	2.37	0.40
37:C:100:ARG:NH2	78:t:1503:C:OP1	2.55	0.40
37:C:109:ARG:HD2	37:C:111:TRP:CH2	2.55	0.40
37:C:326:LEU:HD21	37:C:333:LYS:HB2	2.03	0.40
45:K:31:ILE:HD12	45:K:34:PHE:HE1	1.86	0.40
53:S:83:GLY:N	78:t:2791:A:OP1	2.48	0.40
59:Y:56:ARG:HE	78:t:13:U:H1'	1.87	0.40
60:Z:119:LEU:HD23	60:Z:119:LEU:HA	1.92	0.40
67:h:105:LYS:HE2	67:h:105:LYS:HB3	1.84	0.40
78:t:1371:A:N7	78:t:1379:G:N2	2.70	0.40
78:t:1403:A:C5	78:t:1482:A:H4'	2.56	0.40
1:S2:825:A:H2'	1:S2:826:A:C8	2.56	0.40
17:SV:53:TYR:CZ	17:SV:72:LEU:HD12	2.53	0.40
22:Sg:106:LYS:HD3	22:Sg:130:LYS:HG3	2.02	0.40
35:A:24:LYS:HG3	35:A:49:ILE:HD12	2.03	0.40
36:B:116:ARG:HG2	36:B:177:LYS:HG2	2.04	0.40
37:C:52:TYR:HB3	37:C:111:TRP:CH2	2.57	0.40
41:G:65:ARG:NH1	78:t:1053:G:OP2	2.38	0.40
42:H:61:TYR:HA	42:H:64:MET:HG2	2.03	0.40
45:K:60:LEU:HD13	45:K:129:VAL:HG21	2.03	0.40
48:N:4:ARG:HG3	48:N:5:ARG:HD3	2.04	0.40
53:S:89:MET:HA	53:S:90:PRO:HD3	1.90	0.40
54:T:95:ARG:HH22	78:t:1932:G:HO2'	1.62	0.40
55:U:87:LYS:NZ	78:t:4267:G:H22	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Y:43:SER:HA	59:Y:44:PRO:HD3	1.91	0.40
75:p:8:ARG:O	75:p:21:HIS:N	2.55	0.40
78:t:159:A:H2'	78:t:160:A:H8	1.87	0.40
78:t:169:C:H4'	78:t:170:C:H5'	2.04	0.40
78:t:466:C:N4	78:t:676:G:H1	2.19	0.40
78:t:710:C:H2'	78:t:711:G:H8	1.86	0.40
78:t:735:G:H2'	78:t:736:G:H8	1.85	0.40
78:t:4858:C:H2'	78:t:4859:G:H4'	2.03	0.40
80:w:20:G:H2'	80:w:21:G:C8	2.56	0.40
1:S2:1394:G:H5'	12:SQ:126:ARG:HG3	2.03	0.40
2:SA:80:ARG:HH11	2:SA:80:ARG:HD3	1.77	0.40
3:SB:83:LYS:HG3	3:SB:104:ASP:OD1	2.21	0.40
5:SE:125:LYS:HB3	5:SE:142:HIS:HB2	2.03	0.40
15:ST:63:HIS:HB3	15:ST:75:MET:HE1	2.04	0.40
23:SC:121:ARG:HB3	23:SC:123:ARG:NH2	2.36	0.40
35:A:245:ARG:HB2	78:t:3718:A:C8	2.56	0.40
42:H:213:LEU:HB3	42:H:247:MET:HB3	2.04	0.40
47:M:66:TYR:OH	78:t:1365:G:OP1	2.31	0.40
50:P:194:GLU:O	50:P:199:HIS:N	2.55	0.40
66:g:54:LYS:HG2	78:t:437:G:H5'	2.02	0.40
66:g:104:MET:C	66:g:105:LEU:HD22	2.46	0.40
76:q:70:THR:OG1	76:q:71:TYR:N	2.52	0.40
78:t:4726:A:N6	78:t:4826:G:H22	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	SA	219/221 (99%)	185 (84%)	33 (15%)	1 (0%)	24 59
3	SB	212/214 (99%)	183 (86%)	28 (13%)	1 (0%)	24 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SD	224/226 (99%)	191 (85%)	33 (15%)	0	100	100
5	SE	257/259 (99%)	223 (87%)	34 (13%)	0	100	100
6	SF	187/189 (99%)	161 (86%)	26 (14%)	0	100	100
7	SH	182/189 (96%)	159 (87%)	23 (13%)	0	100	100
8	SI	202/204 (99%)	171 (85%)	31 (15%)	0	100	100
9	SK	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
10	SL	151/153 (99%)	134 (89%)	17 (11%)	0	100	100
11	SP	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
12	SQ	144/146 (99%)	123 (85%)	19 (13%)	2 (1%)	9	38
13	SR	132/134 (98%)	107 (81%)	25 (19%)	0	100	100
14	SS	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
15	ST	141/143 (99%)	127 (90%)	13 (9%)	1 (1%)	18	53
16	SU	102/104 (98%)	91 (89%)	11 (11%)	0	100	100
17	SV	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	9	40
18	SX	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
19	Sa	100/102 (98%)	84 (84%)	15 (15%)	1 (1%)	12	45
20	Sc	62/64 (97%)	48 (77%)	14 (23%)	0	100	100
21	Sd	53/55 (96%)	39 (74%)	13 (24%)	1 (2%)	6	33
22	Sg	310/312 (99%)	245 (79%)	65 (21%)	0	100	100
23	SC	219/220 (100%)	191 (87%)	27 (12%)	1 (0%)	24	59
24	SG	235/237 (99%)	207 (88%)	28 (12%)	0	100	100
25	SJ	184/185 (100%)	163 (89%)	20 (11%)	1 (0%)	24	59
26	SM	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
27	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
28	SO	135/137 (98%)	116 (86%)	19 (14%)	0	100	100
29	SW	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	50
30	SY	130/131 (99%)	118 (91%)	12 (9%)	0	100	100
31	SZ	71/73 (97%)	58 (82%)	12 (17%)	1 (1%)	9	38
32	Sb	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
33	Se	55/57 (96%)	45 (82%)	10 (18%)	0	100	100
34	Sf	65/67 (97%)	51 (78%)	14 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	A	250/252 (99%)	219 (88%)	30 (12%)	1 (0%)	30	64
36	B	395/397 (100%)	342 (87%)	52 (13%)	1 (0%)	36	69
37	C	361/363 (99%)	326 (90%)	32 (9%)	3 (1%)	16	50
40	F	292/294 (99%)	253 (87%)	38 (13%)	1 (0%)	36	69
41	G	232/247 (94%)	188 (81%)	43 (18%)	1 (0%)	30	64
42	H	223/225 (99%)	202 (91%)	21 (9%)	0	100	100
43	I	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	30	64
44	J	189/191 (99%)	162 (86%)	27 (14%)	0	100	100
45	K	204/211 (97%)	183 (90%)	19 (9%)	2 (1%)	12	45
46	L	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
47	M	203/205 (99%)	166 (82%)	36 (18%)	1 (0%)	24	59
48	N	137/139 (99%)	122 (89%)	15 (11%)	0	100	100
49	O	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	24	59
50	P	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
51	Q	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
52	R	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	24	59
53	S	179/181 (99%)	164 (92%)	15 (8%)	0	100	100
54	T	173/175 (99%)	153 (88%)	19 (11%)	1 (1%)	21	55
55	U	155/157 (99%)	130 (84%)	23 (15%)	2 (1%)	9	40
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
57	W	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
58	X	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	16	50
59	Y	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
60	Z	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
61	b	145/147 (99%)	124 (86%)	20 (14%)	1 (1%)	18	53
62	c	94/121 (78%)	82 (87%)	12 (13%)	0	100	100
63	d	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
64	e	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	6	33
65	f	127/129 (98%)	111 (87%)	16 (13%)	0	100	100
66	g	107/109 (98%)	93 (87%)	12 (11%)	2 (2%)	6	33
67	h	112/114 (98%)	98 (88%)	12 (11%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	i	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	35
69	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	43
70	k	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
71	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
72	m	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
73	n	48/50 (96%)	39 (81%)	9 (19%)	0	100	100
74	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
75	p	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
76	q	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
77	r	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16	50
81	y	37/39 (95%)	18 (49%)	19 (51%)	0	100	100
83	a	132/134 (98%)	113 (86%)	19 (14%)	0	100	100
All	All	11292/11489 (98%)	9844 (87%)	1408 (12%)	40 (0%)	31	64

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	SB	86	LEU
12	SQ	117	ARG
17	SV	79	VAL
23	SC	78	LEU
37	C	59	GLY
37	C	72	ALA
55	U	20	ARG
58	X	74	ARG
64	e	97	ASP
66	g	107	PRO
68	i	87	LYS
15	ST	41	LYS
21	Sd	4	GLN
40	F	260	GLU
47	M	78	LEU
61	b	47	LYS
67	h	84	ALA
68	i	41	ALA
2	SA	12	GLU
19	Sa	47	ALA
35	A	251	THR

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Mol	Chain	Res	Type
37	C	57	LEU
49	O	95	ALA
52	R	157	GLY
64	e	95	ASP
36	B	3	HIS
45	K	11	TYR
54	T	164	LYS
55	U	53	PRO
77	r	21	ASN
12	SQ	45	ARG
31	SZ	50	PHE
45	K	10	ARG
66	g	60	PRO
67	h	28	ASN
69	j	35	LYS
29	SW	95	PRO
41	G	185	PRO
25	SJ	123	ILE
43	I	30	PRO

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%)	178 (97%)	5 (3%)	39	60
3	SB	195/195 (100%)	190 (97%)	5 (3%)	40	60
4	SD	189/189 (100%)	187 (99%)	2 (1%)	65	74
5	SE	222/222 (100%)	218 (98%)	4 (2%)	51	67
6	SF	159/159 (100%)	156 (98%)	3 (2%)	50	66
7	SH	166/169 (98%)	166 (100%)	0	100	100
8	SI	177/177 (100%)	176 (99%)	1 (1%)	78	80
9	SK	89/89 (100%)	87 (98%)	2 (2%)	45	64
10	SL	137/137 (100%)	135 (98%)	2 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	SP	113/113 (100%)	112 (99%)	1 (1%)	70	75
12	SQ	121/121 (100%)	117 (97%)	4 (3%)	33	56
13	SR	121/121 (100%)	120 (99%)	1 (1%)	73	77
14	SS	126/126 (100%)	126 (100%)	0	100	100
15	ST	113/113 (100%)	112 (99%)	1 (1%)	70	75
16	SU	94/94 (100%)	94 (100%)	0	100	100
17	SV	66/66 (100%)	65 (98%)	1 (2%)	57	70
18	SX	113/113 (100%)	111 (98%)	2 (2%)	51	67
19	Sa	89/89 (100%)	88 (99%)	1 (1%)	65	74
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	47 (98%)	1 (2%)	47	65
22	Sg	271/271 (100%)	270 (100%)	1 (0%)	84	83
23	SC	187/186 (100%)	183 (98%)	4 (2%)	47	65
24	SG	207/207 (100%)	207 (100%)	0	100	100
25	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	72
26	SM	98/100 (98%)	97 (99%)	1 (1%)	68	75
27	SN	130/130 (100%)	129 (99%)	1 (1%)	73	77
28	SO	107/107 (100%)	106 (99%)	1 (1%)	70	75
29	SW	112/112 (100%)	111 (99%)	1 (1%)	70	75
30	SY	114/113 (101%)	112 (98%)	2 (2%)	51	67
31	SZ	64/64 (100%)	61 (95%)	3 (5%)	23	48
32	Sb	74/74 (100%)	73 (99%)	1 (1%)	59	71
33	Se	46/46 (100%)	45 (98%)	1 (2%)	45	64
34	Sf	60/60 (100%)	59 (98%)	1 (2%)	53	68
35	A	194/194 (100%)	187 (96%)	7 (4%)	31	54
36	B	345/345 (100%)	340 (99%)	5 (1%)	59	71
37	C	302/302 (100%)	295 (98%)	7 (2%)	44	63
40	F	248/248 (100%)	244 (98%)	4 (2%)	55	69
41	G	209/220 (95%)	207 (99%)	2 (1%)	68	75
42	H	194/194 (100%)	193 (100%)	1 (0%)	81	82
43	I	199/199 (100%)	198 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	J	170/170 (100%)	169 (99%)	1 (1%)	78	80
45	K	178/179 (99%)	177 (99%)	1 (1%)	78	80
46	L	142/142 (100%)	141 (99%)	1 (1%)	76	78
47	M	171/171 (100%)	166 (97%)	5 (3%)	37	58
48	N	118/118 (100%)	116 (98%)	2 (2%)	53	68
49	O	171/171 (100%)	168 (98%)	3 (2%)	51	67
50	P	168/168 (100%)	166 (99%)	2 (1%)	63	72
51	Q	134/134 (100%)	133 (99%)	1 (1%)	76	78
52	R	164/164 (100%)	161 (98%)	3 (2%)	51	67
53	S	160/160 (100%)	159 (99%)	1 (1%)	78	80
54	T	156/156 (100%)	156 (100%)	0	100	100
55	U	138/138 (100%)	137 (99%)	1 (1%)	76	78
56	V	89/89 (100%)	88 (99%)	1 (1%)	65	74
57	W	100/100 (100%)	99 (99%)	1 (1%)	68	75
58	X	100/100 (100%)	100 (100%)	0	100	100
59	Y	105/105 (100%)	103 (98%)	2 (2%)	50	66
60	Z	124/124 (100%)	123 (99%)	1 (1%)	73	77
61	b	120/120 (100%)	115 (96%)	5 (4%)	26	50
62	c	82/101 (81%)	81 (99%)	1 (1%)	63	72
63	d	88/88 (100%)	86 (98%)	2 (2%)	44	63
64	e	97/97 (100%)	95 (98%)	2 (2%)	47	65
65	f	115/115 (100%)	115 (100%)	0	100	100
66	g	88/88 (100%)	88 (100%)	0	100	100
67	h	98/98 (100%)	98 (100%)	0	100	100
68	i	109/109 (100%)	109 (100%)	0	100	100
69	j	83/83 (100%)	82 (99%)	1 (1%)	63	72
70	k	71/71 (100%)	70 (99%)	1 (1%)	59	71
71	l	64/64 (100%)	64 (100%)	0	100	100
72	m	47/47 (100%)	47 (100%)	0	100	100
73	n	46/46 (100%)	46 (100%)	0	100	100
74	o	24/24 (100%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	p	93/93 (100%)	91 (98%)	2 (2%)	45	64
76	q	74/74 (100%)	74 (100%)	0	100	100
77	r	106/106 (100%)	106 (100%)	0	100	100
81	y	23/29 (79%)	21 (91%)	2 (9%)	9	33
83	a	117/117 (100%)	116 (99%)	1 (1%)	70	75
All	All	9834/9873 (100%)	9709 (99%)	125 (1%)	61	71

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	48	ILE
2	SA	121	LEU
2	SA	122	LEU
2	SA	123	VAL
2	SA	147	LEU
3	SB	86	LEU
3	SB	87	ILE
3	SB	88	THR
3	SB	224	GLU
3	SB	225	LEU
4	SD	181	VAL
4	SD	210	ILE
5	SE	90	ILE
5	SE	111	VAL
5	SE	131	VAL
5	SE	238	LEU
6	SF	41	VAL
6	SF	87	LEU
6	SF	99	ILE
8	SI	129	LEU
9	SK	42	ASN
9	SK	43	LEU
10	SL	40	ILE
10	SL	66	VAL
11	SP	121	ILE
12	SQ	22	VAL
12	SQ	81	ILE
12	SQ	111	ILE
12	SQ	117	ARG
13	SR	85	VAL

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Mol	Chain	Res	Type
15	ST	131	LEU
17	SV	79	VAL
18	SX	107	ARG
18	SX	112	VAL
19	Sa	51	ARG
21	Sd	53	ILE
22	Sg	129	ILE
23	SC	155	ILE
23	SC	200[A]	ARG
23	SC	200[B]	ARG
23	SC	275	LYS
25	SJ	138[A]	ARG
25	SJ	138[B]	ARG
26	SM	27	ILE
27	SN	43	LYS
28	SO	135	ILE
29	SW	103	VAL
30	SY	113[A]	ARG
30	SY	113[B]	ARG
31	SZ	44	LEU
31	SZ	62	VAL
31	SZ	67	LEU
32	Sb	24	LEU
33	Se	6	LEU
34	Sf	108	VAL
35	A	20	VAL
35	A	45	VAL
35	A	101	VAL
35	A	102	LEU
35	A	150	LEU
35	A	157	VAL
35	A	180	LEU
36	B	5	LYS
36	B	143	LYS
36	B	254	ILE
36	B	301	ASN
36	B	396	ARG
37	C	54	VAL
37	C	56	GLU
37	C	144	ILE
37	C	150	LEU
37	C	193	LYS

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Mol	Chain	Res	Type
37	C	199	ARG
37	C	337	ARG
40	F	8	LYS
40	F	105	LEU
40	F	146	LEU
40	F	261	VAL
41	G	125	LEU
41	G	267	LEU
42	H	167	ILE
43	I	154	LEU
44	J	16	VAL
45	K	87	ILE
46	L	157	ILE
47	M	46	ILE
47	M	78	LEU
47	M	125	ILE
47	M	144	LEU
47	M	169	ILE
48	N	31	ILE
48	N	45	VAL
49	O	64	ILE
49	O	133	ILE
49	O	183	THR
50	P	187	LYS
50	P	188	LYS
51	Q	139	TYR
52	R	5	ILE
52	R	82	VAL
52	R	160	HIS
53	S	115	ILE
55	U	128	LEU
56	V	112	LEU
57	W	132	ILE
59	Y	96	LEU
59	Y	155	ILE
60	Z	104	VAL
61	b	45	PHE
61	b	46	ASP
61	b	47	LYS
61	b	63	LEU
61	b	78	LEU
62	c	54	LEU

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Mol	Chain	Res	Type
63	d	91	VAL
63	d	96	ILE
64	e	94	GLU
64	e	96	GLU
69	j	71	LYS
70	k	82	THR
75	p	23	VAL
75	p	102	GLN
81	y	19	ILE
81	y	35	LEU
83	a	13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	9	GLN
2	SA	50	ASN
3	SB	92	GLN
3	SB	160	GLN
3	SB	177	GLN
3	SB	186	ASN
3	SB	202	GLN
4	SD	145	GLN
4	SD	159	HIS
5	SE	112	HIS
5	SE	138	HIS
5	SE	216	ASN
5	SE	224	ASN
6	SF	137	GLN
6	SF	179	ASN
7	SH	25	GLN
7	SH	73	GLN
7	SH	76	GLN
7	SH	114	GLN
7	SH	168	HIS
8	SI	168	GLN
9	SK	28	HIS
9	SK	32	HIS
9	SK	42	ASN
9	SK	44	HIS
10	SL	18	GLN
10	SL	65	ASN

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Mol	Chain	Res	Type
10	SL	83	GLN
10	SL	94	HIS
10	SL	106	HIS
12	SQ	48	GLN
12	SQ	80	GLN
12	SQ	142	GLN
13	SR	31	ASN
13	SR	74	GLN
13	SR	83	ASN
13	SR	93	GLN
14	SS	11	HIS
14	SS	42	HIS
14	SS	72	GLN
14	SS	97	GLN
14	SS	120	HIS
14	SS	134	GLN
15	ST	12	GLN
15	ST	51	ASN
16	SU	18	HIS
16	SU	100	GLN
17	SV	2	GLN
17	SV	21	ASN
17	SV	29	HIS
17	SV	35	ASN
18	SX	87	ASN
18	SX	110	HIS
19	Sa	72	HIS
19	Sa	86	ASN
20	Sc	7	GLN
20	Sc	29	GLN
21	Sd	5	GLN
21	Sd	26	ASN
22	Sg	64	HIS
22	Sg	117	ASN
22	Sg	162	ASN
22	Sg	222	ASN
23	SC	178	HIS
23	SC	267	GLN
24	SG	59	GLN
24	SG	65	GLN
24	SG	163	ASN
24	SG	197	GLN

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Mol	Chain	Res	Type
24	SG	227	GLN
25	SJ	111	GLN
25	SJ	125	HIS
25	SJ	177	ASN
27	SN	5	HIS
28	SO	103	ASN
29	SW	16	ASN
30	SY	2	ASN
31	SZ	89	GLN
31	SZ	106	GLN
32	Sb	19	HIS
33	Se	3	HIS
33	Se	39	ASN
35	A	22	HIS
35	A	97	ASN
35	A	132	ASN
35	A	140	ASN
35	A	218	HIS
36	B	11	HIS
36	B	121	ASN
36	B	158	GLN
36	B	167	GLN
36	B	175	GLN
36	B	179	HIS
36	B	213	GLN
36	B	245	HIS
36	B	276	HIS
36	B	301	ASN
36	B	380	GLN
37	C	38	ASN
37	C	61	GLN
37	C	85	HIS
37	C	223	ASN
37	C	236	ASN
37	C	278	ASN
40	F	63	GLN
40	F	191	ASN
40	F	198	HIS
41	G	167	GLN
41	G	182	ASN
41	G	250	GLN
41	G	279	ASN

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Mol	Chain	Res	Type
42	H	24	ASN
42	H	80	ASN
42	H	119	ASN
42	H	226	HIS
43	I	64	GLN
43	I	206	GLN
43	I	225	ASN
44	J	42	ASN
44	J	63	ASN
44	J	108	ASN
44	J	116	ASN
45	K	130	HIS
45	K	213	HIS
46	L	10	ASN
46	L	112	HIS
47	M	115	GLN
48	N	44	GLN
48	N	48	GLN
48	N	56	GLN
48	N	120	ASN
49	O	87	HIS
49	O	109	HIS
49	O	201	HIS
50	P	50	ASN
50	P	63	ASN
51	Q	80	GLN
51	Q	133	HIS
52	R	160	HIS
53	S	121	HIS
53	S	130	ASN
54	T	50	GLN
54	T	162	GLN
55	U	22	HIS
55	U	49	GLN
55	U	69	GLN
55	U	79	GLN
55	U	95	HIS
55	U	98	HIS
57	W	77	HIS
57	W	101	ASN
57	W	135	ASN
58	X	63	GLN

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Mol	Chain	Res	Type
59	Y	73	HIS
59	Y	108	GLN
60	Z	61	HIS
60	Z	96	HIS
61	b	25	HIS
61	b	40	HIS
61	b	44	ASN
61	b	60	HIS
61	b	66	ASN
61	b	89	ASN
61	b	120	GLN
62	c	12	GLN
62	c	17	HIS
62	c	19	ASN
62	c	58	GLN
63	d	77	ASN
64	e	93	ASN
64	e	100	ASN
65	f	43	ASN
65	f	107	ASN
66	g	55	ASN
66	g	78	HIS
68	i	20	GLN
69	j	26	HIS
70	k	66	HIS
72	m	43	HIS
75	p	102	GLN
76	q	34	HIS
76	q	56	HIS
76	q	92	GLN
77	r	12	ASN
77	r	41	ASN
77	r	45	HIS
77	r	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1698/1714 (99%)	619 (36%)	26 (1%)
38	D	156/157 (99%)	40 (25%)	0
39	E	118/119 (99%)	20 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
78	t	3592/3607 (99%)	1002 (27%)	0
79	v	73/76 (96%)	38 (52%)	0
80	w	9/10 (90%)	3 (33%)	0
82	u	75/76 (98%)	43 (57%)	0
All	All	5721/5759 (99%)	1765 (30%)	26 (0%)

All (1765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	5	U
1	S2	9	U
1	S2	10	G
1	S2	11	A
1	S2	23	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	37	C
1	S2	38	A
1	S2	39	A
1	S2	41	G
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
1	S2	59	U
1	S2	60	A
1	S2	61	A
1	S2	62	G
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	71	G

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Mol	Chain	Res	Type
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	75	G
1	S2	76	U
1	S2	79	A
1	S2	80	G
1	S2	93	U
1	S2	94	G
1	S2	99	A
1	S2	102	A
1	S2	103	A
1	S2	108	G
1	S2	113	G
1	S2	115	U
1	S2	116	OMU
1	S2	121	OMU
1	S2	125	C
1	S2	126	G
1	S2	129	C
1	S2	140	C
1	S2	142	C
1	S2	143	U
1	S2	155	G
1	S2	157	U
1	S2	159	A2M
1	S2	160	U
1	S2	161	U
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	176	U
1	S2	178	C
1	S2	187	G
1	S2	191	A
1	S2	192	C
1	S2	193	C
1	S2	194	C
1	S2	195	C
1	S2	196	C
1	S2	197	U

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Mol	Chain	Res	Type
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	214	U
1	S2	215	G
1	S2	289	G
1	S2	291	G
1	S2	292	A
1	S2	293	C
1	S2	294	U
1	S2	295	C
1	S2	305	U
1	S2	306	C
1	S2	308	G
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	319	C
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	331	C
1	S2	335	G
1	S2	337	C
1	S2	340	C
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	364	A
1	S2	368	U
1	S2	369	C

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Mol	Chain	Res	Type
1	S2	375	U
1	S2	376	A
1	S2	377	G
1	S2	379	C
1	S2	380	G
1	S2	382	C
1	S2	384	U
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	395	G
1	S2	400	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	419	G
1	S2	426	A
1	S2	428	U
1	S2	429	C
1	S2	435	A
1	S2	446	G
1	S2	447	A
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	451	G
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	466	G
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

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Mol	Chain	Res	Type
1	S2	493	A
1	S2	495	U
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	503	C
1	S2	507	G
1	S2	517	OMC
1	S2	518	G
1	S2	525	A
1	S2	526	A
1	S2	528	A
1	S2	529	A
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	537	C
1	S2	538	U
1	S2	539	C
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	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	574	A
1	S2	578	C
1	S2	579	C

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Mol	Chain	Res	Type
1	S2	583	C
1	S2	585	C
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	593	C
1	S2	594	A
1	S2	597	G
1	S2	600	G
1	S2	603	C
1	S2	607	U
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	643	A
1	S2	645	C
1	S2	647	U
1	S2	650	A
1	S2	654	A
1	S2	655	A
1	S2	657	U
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	684	G
1	S2	689	U
1	S2	690	G
1	S2	692	G
1	S2	693	A

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Mol	Chain	Res	Type
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	735	C
1	S2	736	C
1	S2	737	G
1	S2	738	C
1	S2	739	C
1	S2	748	C
1	S2	749	U
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	787	G
1	S2	788	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	795	A
1	S2	797	C
1	S2	799	U
1	S2	811	A
1	S2	815	U
1	S2	817	G
1	S2	821	G
1	S2	822	PSU
1	S2	823	PSU
1	S2	824	C
1	S2	827	A
1	S2	830	A
1	S2	831	G
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	840	C

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Mol	Chain	Res	Type
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	849	A
1	S2	851	C
1	S2	857	U
1	S2	858	A
1	S2	859	G
1	S2	865	A
1	S2	866	U
1	S2	867	G
1	S2	868	G
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	872	A
1	S2	873	G
1	S2	878	G
1	S2	879	C
1	S2	881	G
1	S2	886	A
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	894	G
1	S2	895	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	905	C
1	S2	907	G
1	S2	908	A
1	S2	910	G
1	S2	913	A

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Mol	Chain	Res	Type
1	S2	914	U
1	S2	917	U
1	S2	920	A
1	S2	921	G
1	S2	924	G
1	S2	933	G
1	S2	938	A
1	S2	949	G
1	S2	951	C
1	S2	954	U
1	S2	968	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	972	A
1	S2	973	C
1	S2	978	G
1	S2	983	A
1	S2	986	G
1	S2	990	A
1	S2	991	G
1	S2	992	A
1	S2	998	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1005	G
1	S2	1006	C
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	1029	G
1	S2	1031	A2M
1	S2	1038	U
1	S2	1045	U
1	S2	1049	A
1	S2	1058	A

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Mol	Chain	Res	Type
1	S2	1061	U
1	S2	1062	A
1	S2	1064	C
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1087	A
1	S2	1088	U
1	S2	1089	G
1	S2	1109	C
1	S2	1114	U
1	S2	1115	U
1	S2	1117	C
1	S2	1119	A
1	S2	1120	U
1	S2	1133	A
1	S2	1138	C
1	S2	1149	A
1	S2	1150	A
1	S2	1154	U
1	S2	1155	U
1	S2	1158	G
1	S2	1166	G
1	S2	1168	G
1	S2	1170	A
1	S2	1181	A
1	S2	1183	A
1	S2	1190	A
1	S2	1195	A
1	S2	1200	A
1	S2	1207	G
1	S2	1208	A
1	S2	1209	A
1	S2	1215	C
1	S2	1217	A
1	S2	1222	G
1	S2	1224	G
1	S2	1231	C
1	S2	1240	A
1	S2	1242	U
1	S2	1245	G
1	S2	1246	A

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Mol	Chain	Res	Type
1	S2	1250	A
1	S2	1251	A
1	S2	1253	A
1	S2	1254	C
1	S2	1255	G
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1260	A
1	S2	1262	C
1	S2	1263	U
1	S2	1265	A
1	S2	1266	C
1	S2	1274	G
1	S2	1275	G
1	S2	1277	C
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	1303	C
1	S2	1312	G
1	S2	1313	A
1	S2	1315	U
1	S2	1322	G
1	S2	1323	U
1	S2	1330	G
1	S2	1331	C
1	S2	1333	U
1	S2	1340	U
1	S2	1341	C
1	S2	1342	U
1	S2	1345	G
1	S2	1348	G
1	S2	1351	G

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Mol	Chain	Res	Type
1	S2	1354	G
1	S2	1355	C
1	S2	1371	U
1	S2	1372	U
1	S2	1376	A
1	S2	1378	A
1	S2	1384	C
1	S2	1393	G
1	S2	1396	A
1	S2	1397	U
1	S2	1398	G
1	S2	1402	A
1	S2	1403	C
1	S2	1411	G
1	S2	1418	C
1	S2	1420	G
1	S2	1421	A
1	S2	1424	G
1	S2	1433	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G
1	S2	1452	A
1	S2	1453	C
1	S2	1454	A
1	S2	1455	A
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1469	A
1	S2	1477	U
1	S2	1478	U
1	S2	1480	A
1	S2	1481	G
1	S2	1482	C
1	S2	1483	A
1	S2	1484	A
1	S2	1489	A

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Mol	Chain	Res	Type
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	1498	A
1	S2	1505	U
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1518	C
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C
1	S2	1543	U
1	S2	1544	C
1	S2	1545	A
1	S2	1550	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	1572	C
1	S2	1573	G
1	S2	1575	G
1	S2	1578	U
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A

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Mol	Chain	Res	Type
1	S2	1591	C
1	S2	1598	G
1	S2	1599	U
1	S2	1601	A
1	S2	1606	G
1	S2	1619	A
1	S2	1621	U
1	S2	1623	A
1	S2	1634	A
1	S2	1637	A
1	S2	1646	C
1	S2	1647	A
1	S2	1648	G
1	S2	1649	U
1	S2	1654	G
1	S2	1657	G
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1675	A
1	S2	1676	U
1	S2	1680	G
1	S2	1682	C
1	S2	1686	G
1	S2	1692	U
1	S2	1695	A
1	S2	1698	C
1	S2	1699	A
1	S2	1704	C
1	S2	1707	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	1750	C
1	S2	1751	C
1	S2	1752	C
1	S2	1780	G
1	S2	1781	A
1	S2	1782	G

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Mol	Chain	Res	Type
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1786	U
1	S2	1787	G
1	S2	1793	A
1	S2	1803	U
1	S2	1804	U
1	S2	1805	G
1	S2	1806	M7A
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	1839	U
1	S2	1841	C
1	S2	1849	G
1	S2	1850	MA6
1	S2	1851	MA6
1	S2	1852	C
1	S2	1855	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1867	U
1	S2	1868	U
1	S2	1869	A
38	D	2	G
38	D	23	C

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Mol	Chain	Res	Type
38	D	32	C
38	D	34	U
38	D	35	C
38	D	38	U
38	D	49	G
38	D	59	A
38	D	60	G
38	D	63	U
38	D	72	A
38	D	74	U
38	D	77	A
38	D	80	A
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	86	U
38	D	87	G
38	D	91	A
38	D	94	G
38	D	96	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	120	G
38	D	121	G
38	D	122	G
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
39	E	7	G
39	E	11	A
39	E	22	A
39	E	23	A

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Mol	Chain	Res	Type
39	E	24	C
39	E	27	G
39	E	31	G
39	E	33	U
39	E	53	U
39	E	54	A
39	E	64	G
39	E	74	A
39	E	85	G
39	E	88	A
39	E	89	G
39	E	91	C
39	E	97	G
39	E	98	G
39	E	109	U
39	E	110	G
78	t	5	A
78	t	9	C
78	t	13	U
78	t	17	A
78	t	18	C
78	t	21	G
78	t	25	A
78	t	30	C
78	t	32	G
78	t	33	A
78	t	39	A
78	t	42	A
78	t	47	A
78	t	48	G
78	t	49	U
78	t	58	G
78	t	59	A
78	t	64	A
78	t	65	A
78	t	71	C
78	t	72	C
78	t	76	A
78	t	91	G
78	t	97	G
78	t	101	A
78	t	108	A

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Mol	Chain	Res	Type
78	t	116	G
78	t	118	C
78	t	119	G
78	t	121	A
78	t	129	C
78	t	131	C
78	t	132	G
78	t	133	C
78	t	134	G
78	t	135	G
78	t	138	C
78	t	143	G
78	t	147	U
78	t	149	U
78	t	155	A
78	t	156	C
78	t	157	G
78	t	158	G
78	t	163	C
78	t	168	U
78	t	170	C
78	t	173	G
78	t	177	C
78	t	179	G
78	t	181	U
78	t	182	C
78	t	183	G
78	t	184	U
78	t	185	G
78	t	189	G
78	t	195	A
78	t	196	G
78	t	197	U
78	t	205	A
78	t	211	G
78	t	212	C
78	t	213	C
78	t	214	C
78	t	215	A
78	t	227	G
78	t	228	U
78	t	229	G

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Mol	Chain	Res	Type
78	t	230	U
78	t	233	G
78	t	236	C
78	t	250	G
78	t	252	C
78	t	253	G
78	t	256	C
78	t	260	C
78	t	272	G
78	t	274	G
78	t	282	G
78	t	289	A
78	t	291	U
78	t	300	A
78	t	303	C
78	t	304	G
78	t	309	G
78	t	310	U
78	t	311	A
78	t	322	A
78	t	323	A
78	t	334	C
78	t	338	A
78	t	339	C
78	t	343	A
78	t	344	C
78	t	345	C
78	t	348	U
78	t	351	U
78	t	367	G
78	t	370	A
78	t	375	U
78	t	377	A
78	t	379	A
78	t	380	A
78	t	381	G
78	t	390	A
78	t	395	G
78	t	404	A
78	t	406	G
78	t	407	G
78	t	408	C

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Mol	Chain	Res	Type
78	t	409	G
78	t	425	G
78	t	426	U
78	t	434	U
78	t	444	G
78	t	446	A
78	t	447	G
78	t	448	U
78	t	449	C
78	t	451	G
78	t	456	G
78	t	458	G
78	t	466	C
78	t	479	C
78	t	480	C
78	t	482	G
78	t	487	G
78	t	489	C
78	t	491	G
78	t	492	C
78	t	493	G
78	t	494	G
78	t	496	C
78	t	497	C
78	t	498	G
78	t	499	G
78	t	504	U
78	t	507	U
78	t	509	C
78	t	511	C
78	t	512	G
78	t	630	G
78	t	633	U
78	t	634	C
78	t	635	G
78	t	636	G
78	t	641	G
78	t	643	A
78	t	647	U
78	t	649	C
78	t	654	G
78	t	658	G

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Mol	Chain	Res	Type
78	t	659	G
78	t	661	G
78	t	672	G
78	t	674	C
78	t	677	G
78	t	678	C
78	t	679	G
78	t	680	C
78	t	690	C
78	t	692	G
78	t	693	U
78	t	695	C
78	t	696	G
78	t	714	A
78	t	719	U
78	t	720	G
78	t	721	G
78	t	724	A
78	t	728	C
78	t	730	G
78	t	737	A
78	t	738	A
78	t	739	G
78	t	743	G
78	t	897	G
78	t	901	U
78	t	902	A
78	t	904	A
78	t	905	G
78	t	906	C
78	t	907	C
78	t	908	C
78	t	913	G
78	t	917	G
78	t	919	A
78	t	921	C
78	t	922	A
78	t	923	C
78	t	924	U
78	t	925	C
78	t	927	C
78	t	929	G

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Mol	Chain	Res	Type
78	t	931	A
78	t	932	U
78	t	933	C
78	t	937	G
78	t	938	G
78	t	943	A
78	t	944	G
78	t	947	A
78	t	948	G
78	t	949	C
78	t	950	G
78	t	952	G
78	t	953	A
78	t	954	C
78	t	957	G
78	t	964	C
78	t	976	U
78	t	1061	A
78	t	1064	C
78	t	1065	C
78	t	1066	U
78	t	1071	C
78	t	1077	G
78	t	1084	C
78	t	1086	C
78	t	1087	C
78	t	1149	G
78	t	1150	C
78	t	1151	G
78	t	1152	G
78	t	1156	G
78	t	1162	U
78	t	1165	C
78	t	1174	C
78	t	1176	C
78	t	1181	G
78	t	1186	G
78	t	1188	G
78	t	1191	G
78	t	1192	U
78	t	1193	C
78	t	1196	G

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Mol	Chain	Res	Type
78	t	1197	C
78	t	1198	C
78	t	1199	C
78	t	1201	G
78	t	1220	C
78	t	1221	A
78	t	1222	C
78	t	1223	G
78	t	1224	C
78	t	1225	G
78	t	1226	C
78	t	1228	C
78	t	1229	G
78	t	1234	C
78	t	1237	A
78	t	1238	A
78	t	1240	G
78	t	1248	G
78	t	1249	G
78	t	1250	C
78	t	1251	G
78	t	1252	G
78	t	1253	A
78	t	1258	G
78	t	1259	C
78	t	1263	C
78	t	1264	G
78	t	1265	G
78	t	1268	U
78	t	1269	C
78	t	1271	G
78	t	1273	G
78	t	1277	A
78	t	1278	C
78	t	1279	G
78	t	1284	C
78	t	1285	U
78	t	1297	C
78	t	1299	G
78	t	1301	C
78	t	1309	A
78	t	1320	A

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Mol	Chain	Res	Type
78	t	1321	G
78	t	1325	A
78	t	1336	G
78	t	1337	A
78	t	1341	G
78	t	1342	G
78	t	1348	C
78	t	1350	C
78	t	1351	A
78	t	1352	C
78	t	1353	G
78	t	1354	A
78	t	1360	G
78	t	1361	C
78	t	1362	C
78	t	1364	U
78	t	1370	A
78	t	1374	A
78	t	1379	G
78	t	1380	A
78	t	1381	A
78	t	1388	C
78	t	1389	G
78	t	1390	C
78	t	1391	G
78	t	1392	C
78	t	1393	U
78	t	1394	C
78	t	1395	G
78	t	1396	C
78	t	1403	A
78	t	1404	G
78	t	1420	C
78	t	1421	U
78	t	1423	U
78	t	1424	C
78	t	1425	C
78	t	1426	A
78	t	1428	U
78	t	1429	C
78	t	1430	C
78	t	1431	G

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Mol	Chain	Res	Type
78	t	1435	A
78	t	1463	C
78	t	1464	G
78	t	1465	C
78	t	1466	G
78	t	1467	C
78	t	1468	C
78	t	1473	A
78	t	1480	G
78	t	1497	A
78	t	1499	G
78	t	1500	A
78	t	1505	A
78	t	1507	A
78	t	1515	A
78	t	1516	A
78	t	1520	U
78	t	1521	G
78	t	1531	G
78	t	1548	C
78	t	1553	G
78	t	1560	U
78	t	1564	U
78	t	1570	U
78	t	1573	U
78	t	1578	U
78	t	1579	G
78	t	1589	C
78	t	1595	A
78	t	1606	G
78	t	1607	G
78	t	1608	G
78	t	1609	G
78	t	1612	A
78	t	1613	A
78	t	1615	G
78	t	1616	A
78	t	1633	G
78	t	1636	G
78	t	1642	U
78	t	1643	C
78	t	1658	C

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Mol	Chain	Res	Type
78	t	1660	C
78	t	1663	G
78	t	1674	C
78	t	1679	G
78	t	1680	C
78	t	1700	C
78	t	1701	A
78	t	1711	A
78	t	1713	C
78	t	1723	G
78	t	1732	G
78	t	1736	U
78	t	1738	U
78	t	1741	G
78	t	1746	G
78	t	1747	A
78	t	1748	A
78	t	1750	C
78	t	1751	G
78	t	1754	C
78	t	1756	C
78	t	1767	C
78	t	1769	A
78	t	1776	A
78	t	1783	A
78	t	1786	A
78	t	1787	A
78	t	1794	C
78	t	1803	G
78	t	1814	G
78	t	1815	U
78	t	1816	G
78	t	1818	A
78	t	1823	G
78	t	1836	G
78	t	1837	C
78	t	1840	C
78	t	1850	G
78	t	1854	A
78	t	1863	U
78	t	1864	G
78	t	1870	U

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Mol	Chain	Res	Type
78	t	1872	A
78	t	1879	C
78	t	1882	C
78	t	1883	G
78	t	1887	U
78	t	1890	G
78	t	1891	G
78	t	1896	C
78	t	1897	G
78	t	1898	A
78	t	1902	C
78	t	1903	G
78	t	1906	G
78	t	1910	A
78	t	1912	C
78	t	1913	A
78	t	1915	A
78	t	1920	A
78	t	1921	G
78	t	1922	A
78	t	1928	U
78	t	1929	G
78	t	1930	U
78	t	1932	G
78	t	1936	G
78	t	1937	A
78	t	1938	U
78	t	1939	A
78	t	1940	U
78	t	1941	A
78	t	1942	G
78	t	1943	A
78	t	1956	G
78	t	1957	G
78	t	1958	C
78	t	1960	A
78	t	1961	U
78	t	1963	G
78	t	1964	A
78	t	1967	U
78	t	1968	C
78	t	1971	A

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Mol	Chain	Res	Type
78	t	1972	A
78	t	1973	U
78	t	1974	C
78	t	1978	U
78	t	1979	A
78	t	1980	A
78	t	1983	A
78	t	1984	G
78	t	1988	G
78	t	1989	U
78	t	1991	A
78	t	1993	A
78	t	1994	A
78	t	1996	U
78	t	1997	C
78	t	2003	C
78	t	2007	A
78	t	2011	A
78	t	2012	C
78	t	2021	A
78	t	2023	A
78	t	2027	G
78	t	2028	A
78	t	2029	U
78	t	2033	G
78	t	2036	G
78	t	2037	G
78	t	2038	A
78	t	2050	A
78	t	2051	U
78	t	2072	G
78	t	2073	A
78	t	2075	A
78	t	2076	G
78	t	2077	U
78	t	2078	G
78	t	2081	C
78	t	2082	G
78	t	2084	G
78	t	2086	G
78	t	2087	C
78	t	2090	C

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Mol	Chain	Res	Type
78	t	2091	G
78	t	2092	G
78	t	2231	G
78	t	2232	A
78	t	2233	G
78	t	2235	C
78	t	2237	C
78	t	2239	C
78	t	2241	G
78	t	2242	A
78	t	2247	A
78	t	2248	C
78	t	2250	C
78	t	2268	C
78	t	2273	G
78	t	2278	G
78	t	2279	A
78	t	2280	G
78	t	2282	C
78	t	2284	U
78	t	2285	G
78	t	2292	A
78	t	2295	G
78	t	2299	G
78	t	2310	G
78	t	2323	U
78	t	2327	G
78	t	2330	C
78	t	2336	G
78	t	2340	G
78	t	2343	G
78	t	2344	C
78	t	2348	U
78	t	2349	A
78	t	2357	G
78	t	2359	G
78	t	2366	G
78	t	2374	A
78	t	2377	U
78	t	2389	C
78	t	2395	G
78	t	2400	G

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Mol	Chain	Res	Type
78	t	2401	C
78	t	2404	U
78	t	2405	U
78	t	2416	C
78	t	2421	G
78	t	2426	U
78	t	2429	G
78	t	2442	G
78	t	2446	U
78	t	2447	U
78	t	2453	G
78	t	2459	G
78	t	2461	C
78	t	2467	C
78	t	2468	C
78	t	2469	U
78	t	2470	C
78	t	2473	U
78	t	2474	U
78	t	2480	C
78	t	2481	G
78	t	2482	G
78	t	2483	C
78	t	2484	C
78	t	2485	G
78	t	2492	A
78	t	2502	G
78	t	2522	A
78	t	2523	G
78	t	2524	U
78	t	2525	G
78	t	2526	G
78	t	2532	A
78	t	2533	U
78	t	2545	G
78	t	2548	G
78	t	2549	U
78	t	2565	G
78	t	2566	A
78	t	2568	C
78	t	2570	A
78	t	2580	A

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Mol	Chain	Res	Type
78	t	2583	C
78	t	2584	G
78	t	2585	G
78	t	2600	A
78	t	2606	C
78	t	2617	G
78	t	2628	G
78	t	2632	C
78	t	2637	G
78	t	2638	A
78	t	2639	A
78	t	2640	U
78	t	2644	U
78	t	2648	C
78	t	2652	G
78	t	2665	G
78	t	2666	U
78	t	2674	A
78	t	2675	A
78	t	2684	G
78	t	2689	C
78	t	2690	G
78	t	2691	G
78	t	2698	C
78	t	2700	G
78	t	2705	G
78	t	2714	G
78	t	2719	U
78	t	2722	A
78	t	2723	A
78	t	2733	G
78	t	2737	G
78	t	2738	G
78	t	2739	G
78	t	2741	G
78	t	2742	U
78	t	2745	A
78	t	2746	U
78	t	2748	U
78	t	2751	C
78	t	2766	A
78	t	2767	U

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Mol	Chain	Res	Type
78	t	2768	A
78	t	2769	U
78	t	2771	C
78	t	2773	C
78	t	2774	A
78	t	2775	G
78	t	2776	C
78	t	2777	A
78	t	2778	G
78	t	2781	C
78	t	2785	A
78	t	2805	U
78	t	2806	G
78	t	2807	U
78	t	2814	A
78	t	2817	G
78	t	2821	G
78	t	2822	U
78	t	2837	A
78	t	2846	C
78	t	2848	U
78	t	2855	G
78	t	2857	G
78	t	2858	A
78	t	2859	U
78	t	2860	A
78	t	2863	G
78	t	2867	G
78	t	2871	C
78	t	2879	U
78	t	3571	G
78	t	3572	C
78	t	3573	C
78	t	3574	G
78	t	3577	U
78	t	3586	G
78	t	3587	U
78	t	3590	G
78	t	3591	G
78	t	3596	G
78	t	3597	G
78	t	3599	G

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Mol	Chain	Res	Type
78	t	3600	A
78	t	3606	A
78	t	3609	G
78	t	3613	A
78	t	3614	A
78	t	3615	U
78	t	3617	A
78	t	3633	A
78	t	3634	A
78	t	3635	G
78	t	3643	G
78	t	3644	C
78	t	3650	U
78	t	3651	U
78	t	3654	C
78	t	3661	U
78	t	3663	A
78	t	3667	C
78	t	3670	C
78	t	3672	C
78	t	3676	G
78	t	3689	A
78	t	3700	U
78	t	3707	A
78	t	3721	G
78	t	3725	G
78	t	3727	A
78	t	3728	G
78	t	3730	A
78	t	3731	A
78	t	3733	U
78	t	3742	C
78	t	3745	A
78	t	3747	G
78	t	3748	G
78	t	3751	G
78	t	3754	A
78	t	3758	G
78	t	3761	U
78	t	3770	A
78	t	3773	U
78	t	3778	A

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Mol	Chain	Res	Type
78	t	3779	C
78	t	3781	C
78	t	3782	G
78	t	3784	A
78	t	3788	A
78	t	3789	U
78	t	3790	G
78	t	3795	A
78	t	3799	A
78	t	3800	G
78	t	3809	U
78	t	3810	G
78	t	3811	U
78	t	3836	A
78	t	3838	A
78	t	3847	A
78	t	3848	A
78	t	3849	C
78	t	3850	G
78	t	3851	G
78	t	3852	G
78	t	3860	G
78	t	3863	U
78	t	3866	G
78	t	3868	G
78	t	3872	A
78	t	3873	A
78	t	3877	A
78	t	3878	G
78	t	3879	A
78	t	3885	U
78	t	3886	U
78	t	3909	G
78	t	3910	G
78	t	4046	G
78	t	4054	G
78	t	4064	G
78	t	4065	G
78	t	4066	C
78	t	4067	G
78	t	4068	A
78	t	4069	G

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Mol	Chain	Res	Type
78	t	4070	C
78	t	4071	C
78	t	4072	C
78	t	4074	A
78	t	4077	G
78	t	4078	G
78	t	4079	C
78	t	4080	U
78	t	4081	C
78	t	4083	C
78	t	4086	U
78	t	4087	U
78	t	4088	C
78	t	4089	U
78	t	4093	G
78	t	4094	C
78	t	4096	A
78	t	4097	A
78	t	4101	C
78	t	4104	G
78	t	4105	C
78	t	4106	C
78	t	4107	C
78	t	4108	G
78	t	4109	G
78	t	4110	C
78	t	4118	G
78	t	4119	A
78	t	4124	C
78	t	4126	C
78	t	4132	A
78	t	4134	A
78	t	4139	C
78	t	4145	G
78	t	4146	G
78	t	4153	G
78	t	4159	G
78	t	4164	U
78	t	4165	A
78	t	4167	A
78	t	4168	C
78	t	4174	A

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Mol	Chain	Res	Type
78	t	4176	A
78	t	4187	G
78	t	4191	U
78	t	4195	A
78	t	4196	A
78	t	4211	G
78	t	4213	A
78	t	4215	A
78	t	4216	G
78	t	4217	A
78	t	4228	G
78	t	4230	A
78	t	4235	A
78	t	4242	A
78	t	4243	A
78	t	4247	U
78	t	4250	C
78	t	4251	U
78	t	4252	U
78	t	4253	G
78	t	4264	U
78	t	4266	A
78	t	4267	G
78	t	4268	U
78	t	4275	A
78	t	4276	C
78	t	4291	G
78	t	4292	G
78	t	4294	C
78	t	4300	G
78	t	4301	A
78	t	4311	C
78	t	4316	U
78	t	4319	G
78	t	4326	G
78	t	4333	G
78	t	4334	U
78	t	4338	A
78	t	4339	G
78	t	4340	A
78	t	4341	A
78	t	4342	A

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Mol	Chain	Res	Type
78	t	4344	G
78	t	4349	C
78	t	4353	G
78	t	4355	G
78	t	4356	A
78	t	4357	U
78	t	4360	C
78	t	4367	G
78	t	4372	G
78	t	4384	A
78	t	4386	A
78	t	4388	C
78	t	4395	G
78	t	4406	C
78	t	4408	U
78	t	4410	G
78	t	4412	U
78	t	4414	U
78	t	4415	C
78	t	4426	A
78	t	4428	C
78	t	4433	U
78	t	4437	G
78	t	4446	G
78	t	4454	U
78	t	4455	U
78	t	4457	G
78	t	4459	U
78	t	4461	G
78	t	4462	U
78	t	4474	U
78	t	4475	A
78	t	4480	A
78	t	4486	G
78	t	4490	G
78	t	4492	U
78	t	4494	U
78	t	4510	A
78	t	4517	U
78	t	4522	C
78	t	4529	G
78	t	4532	G

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Mol	Chain	Res	Type
78	t	4547	U
78	t	4550	U
78	t	4551	A
78	t	4552	A
78	t	4561	A
78	t	4570	G
78	t	4576	G
78	t	4579	G
78	t	4586	A
78	t	4592	G
78	t	4593	G
78	t	4597	A
78	t	4598	U
78	t	4599	G
78	t	4601	G
78	t	4614	G
78	t	4617	A
78	t	4618	A
78	t	4623	G
78	t	4629	C
78	t	4632	C
78	t	4633	C
78	t	4640	G
78	t	4641	G
78	t	4649	A
78	t	4656	G
78	t	4657	C
78	t	4662	A
78	t	4665	U
78	t	4671	U
78	t	4681	G
78	t	4686	A
78	t	4692	C
78	t	4693	G
78	t	4694	G
78	t	4695	C
78	t	4696	A
78	t	4697	G
78	t	4703	C
78	t	4704	G
78	t	4711	C
78	t	4714	U

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Mol	Chain	Res	Type
78	t	4715	U
78	t	4716	G
78	t	4718	C
78	t	4720	U
78	t	4722	G
78	t	4726	A
78	t	4732	U
78	t	4736	C
78	t	4737	G
78	t	4816	C
78	t	4817	G
78	t	4821	G
78	t	4824	C
78	t	4827	U
78	t	4828	G
78	t	4831	G
78	t	4832	A
78	t	4833	G
78	t	4834	U
78	t	4837	C
78	t	4838	C
78	t	4840	U
78	t	4841	C
78	t	4847	G
78	t	4848	G
78	t	4852	A
78	t	4853	C
78	t	4854	G
78	t	4855	G
78	t	4857	G
78	t	4858	C
78	t	4859	G
78	t	4860	C
78	t	4864	C
78	t	4865	G
78	t	4866	G
78	t	4867	A
78	t	4868	A
78	t	4869	A
78	t	4871	G
78	t	4874	G
78	t	4880	C

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Mol	Chain	Res	Type
78	t	4882	C
78	t	4883	U
78	t	4886	C
78	t	4889	G
78	t	4894	G
78	t	4895	C
78	t	4896	A
78	t	4897	C
78	t	4901	A
78	t	4907	G
78	t	4908	U
78	t	4909	G
78	t	4914	A
78	t	4915	C
78	t	4916	C
78	t	4918	G
78	t	4921	G
78	t	4923	U
78	t	4924	A
78	t	4926	A
78	t	4934	U
78	t	4938	C
78	t	4943	U
78	t	4946	U
78	t	4947	U
78	t	4948	C
78	t	4949	U
78	t	4950	G
78	t	4954	C
78	t	4957	G
78	t	4965	A
78	t	4971	C
78	t	4972	A
78	t	4975	G
78	t	4982	C
78	t	4983	C
78	t	4984	U
78	t	4985	C
78	t	4986	G
78	t	4999	G
78	t	5007	G
78	t	5008	C

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Mol	Chain	Res	Type
78	t	5012	C
78	t	5013	G
78	t	5014	A
78	t	5015	C
78	t	5016	A
78	t	5017	C
78	t	5019	A
78	t	5020	G
78	t	5021	G
78	t	5027	U
79	v	2	G
79	v	3	C
79	v	5	C
79	v	8	U
79	v	10	G
79	v	11	C
79	v	15	G
79	v	16	A
79	v	19	G
79	v	20	U
79	v	23	A
79	v	24	G
79	v	25	C
79	v	27	G
79	v	29	G
79	v	30	G
79	v	36	G
79	v	43	C
79	v	47	U
79	v	48	C
79	v	49	C
79	v	50	U
79	v	51	U
79	v	52	G
79	v	54	U
79	v	58	A
79	v	61	C
79	v	62	C
79	v	63	G
79	v	64	A
79	v	66	U
79	v	68	C

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Mol	Chain	Res	Type
79	v	69	G
79	v	70	G
79	v	71	G
79	v	72	C
79	v	73	A
79	v	76	A
80	w	15	A
80	w	21	G
80	w	22	U
82	u	2	C
82	u	4	C
82	u	5	G
82	u	6	G
82	u	7	A
82	u	8	U
82	u	10	G
82	u	11	C
82	u	13	C
82	u	17	C
82	u	18	G
82	u	19	G
82	u	20	U
82	u	21	A
82	u	24	G
82	u	25	C
82	u	31	A
82	u	33	U
82	u	36	G
82	u	38	A
82	u	43	C
82	u	44	G
82	u	46	G
82	u	47	U
82	u	48	C
82	u	49	C
82	u	51	U
82	u	52	G
82	u	55	U
82	u	56	C
82	u	57	G
82	u	58	A
82	u	59	U

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Mol	Chain	Res	Type
82	u	60	U
82	u	61	C
82	u	62	C
82	u	63	G
82	u	64	A
82	u	70	G
82	u	72	C
82	u	73	A
82	u	74	C
82	u	75	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	53	C
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	445	A
1	S2	536	A
1	S2	559	G
1	S2	563	G
1	S2	814	5MU
1	S2	823	PSU
1	S2	872	A
1	S2	1375	G
1	S2	1556	A
1	S2	1567	G
1	S2	1572	C
1	S2	1600	G
1	S2	1661	A
1	S2	1681	U
1	S2	1749	G
1	S2	1802	C
1	S2	1813	A
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	1081	1	18,21,22	4.37	8 (44%)	21,30,33	1.99	5 (23%)
1	4AC	S2	1842	85,1	21,24,25	3.32	9 (42%)	28,34,37	1.26	5 (17%)
1	OMC	S2	174	1	19,22,23	3.59	8 (42%)	25,31,34	0.80	0
1	OMC	S2	517	1	19,22,23	3.54	8 (42%)	25,31,34	0.85	1 (4%)
1	A2M	S2	668	1	22,25,26	4.12	10 (45%)	30,36,39	3.30	15 (50%)
1	PSU	S2	823	1	18,21,22	4.43	8 (44%)	21,30,33	2.14	5 (23%)
1	A2M	S2	1678	1	22,25,26	4.19	9 (40%)	30,36,39	2.85	13 (43%)
1	6MZ	S2	1832	1	22,25,26	2.59	7 (31%)	29,36,39	2.19	9 (31%)
1	OMU	S2	116	1	19,22,23	3.16	6 (31%)	25,31,34	1.88	5 (20%)
1	A2M	S2	1031	1	22,25,26	4.07	9 (40%)	30,36,39	3.03	15 (50%)
1	4AC	S2	1337	1	21,24,25	3.36	9 (42%)	28,34,37	1.28	4 (14%)
1	5MU	S2	814	1	19,22,23	7.62	8 (42%)	27,32,35	3.52	11 (40%)
1	OMG	S2	683	1	23,26,27	2.44	7 (30%)	32,38,41	2.05	9 (28%)
1	MA6	S2	1850	1	23,26,27	1.48	5 (21%)	33,38,41	3.60	13 (39%)
1	PSU	S2	612	1	18,21,22	4.42	8 (44%)	21,30,33	2.12	6 (28%)
1	OMC	S2	1710	1	19,22,23	3.57	8 (42%)	25,31,34	0.73	0
1	B8N	S2	1248	1	25,29,30	3.11	6 (24%)	28,42,45	2.17	9 (32%)
1	OMG	S2	644	1	23,26,27	2.45	8 (34%)	32,38,41	2.07	9 (28%)
1	OMC	S2	1703	1	19,22,23	3.49	8 (42%)	25,31,34	0.80	1 (4%)
1	MA6	S2	1851	1	23,26,27	1.49	5 (21%)	33,38,41	3.42	13 (39%)
1	OMU	S2	121	1	19,22,23	3.10	7 (36%)	25,31,34	1.99	5 (20%)
1	B8Q	S2	1219	1	18,22,23	4.80	7 (38%)	21,32,35	1.76	5 (23%)
1	PSU	S2	1243	1	18,21,22	4.40	8 (44%)	21,30,33	1.76	4 (19%)
1	UR3	S2	1830	1	19,22,23	2.61	6 (31%)	26,32,35	2.82	8 (30%)
1	A2M	S2	166	1	22,25,26	4.16	9 (40%)	30,36,39	2.86	13 (43%)
1	OMG	S2	509	1	23,26,27	2.43	8 (34%)	32,38,41	2.12	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	822	1	18,21,22	4.44	8 (44%)	21,30,33	1.96	4 (19%)
1	E3C	S2	568	1	19,23,24	3.56	7 (36%)	21,33,36	2.73	6 (28%)
1	M7A	S2	1806	1	19,25,26	1.66	2 (10%)	25,37,40	3.69	8 (32%)
1	A2M	S2	27	1	22,25,26	4.13	9 (40%)	30,36,39	2.94	11 (36%)
1	A2M	S2	484	1	22,25,26	4.10	9 (40%)	30,36,39	2.92	14 (46%)
1	A2M	S2	159	1	22,25,26	4.10	9 (40%)	30,36,39	3.18	16 (53%)
1	5MC	S2	1374	1	19,22,23	3.70	8 (42%)	26,32,35	1.11	4 (15%)
1	PSU	S2	119	1	18,21,22	4.54	7 (38%)	21,30,33	1.94	4 (19%)

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	1081	1	-	2/7/25/26	0/2/2/2
1	4AC	S2	1842	85,1	-	0/11/29/30	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	2/9/27/28	0/2/2/2
1	A2M	S2	668	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	0/9/27/28	0/3/3/3
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	A2M	S2	1031	1	-	3/9/27/28	0/3/3/3
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	MA6	S2	1850	1	-	5/11/29/30	0/3/3/3
1	PSU	S2	612	1	-	1/7/25/26	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	0/16/34/35	0/2/2/2
1	OMG	S2	644	1	-	2/9/27/28	0/3/3/3
1	OMC	S2	1703	1	-	1/9/27/28	0/2/2/2
1	MA6	S2	1851	1	-	4/11/29/30	0/3/3/3
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
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	UR3	S2	1830	1	-	7/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	4/9/27/28	0/3/3/3
1	5MC	S2	1374	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	1/7/25/26	0/2/2/2

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.51	1.81	1.44
1	S2	814	5MU	C6-N1	16.74	1.66	1.38
1	S2	119	PSU	C6-C5	11.92	1.48	1.35
1	S2	814	5MU	C6-C5	-11.87	1.15	1.34
1	S2	1243	PSU	C6-C5	11.69	1.48	1.35
1	S2	1219	B8Q	C4-N3	11.60	1.66	1.48
1	S2	823	PSU	C6-C5	11.52	1.48	1.35
1	S2	822	PSU	C6-C5	11.32	1.47	1.35
1	S2	1219	B8Q	C6-C5	11.10	1.56	1.33
1	S2	814	5MU	C4-N3	-11.09	1.18	1.38
1	S2	1081	PSU	C6-C5	11.07	1.47	1.35
1	S2	612	PSU	C6-C5	11.03	1.47	1.35
1	S2	166	A2M	C2'-C1'	-10.68	1.26	1.53
1	S2	1678	A2M	C2'-C1'	-10.68	1.26	1.53
1	S2	668	A2M	C2'-C1'	-10.63	1.26	1.53
1	S2	1031	A2M	C2'-C1'	-10.49	1.27	1.53
1	S2	27	A2M	C2'-C1'	-10.48	1.27	1.53
1	S2	668	A2M	C3'-C4'	-10.38	1.26	1.53
1	S2	27	A2M	C3'-C4'	-10.29	1.26	1.53
1	S2	159	A2M	C2'-C1'	-10.27	1.27	1.53
1	S2	166	A2M	C3'-C4'	-10.19	1.27	1.53
1	S2	484	A2M	C2'-C1'	-10.15	1.28	1.53
1	S2	1678	A2M	C3'-C4'	-10.10	1.27	1.53
1	S2	484	A2M	C3'-C4'	-10.03	1.27	1.53
1	S2	1031	A2M	C3'-C4'	-10.01	1.27	1.53
1	S2	159	A2M	C3'-C4'	-9.85	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1219	B8Q	C2-N1	9.71	1.51	1.38
1	S2	119	PSU	C2-N1	9.67	1.49	1.36
1	S2	612	PSU	C2-N1	9.48	1.49	1.36
1	S2	822	PSU	C2-N1	9.42	1.48	1.36
1	S2	1081	PSU	C2-N1	9.35	1.48	1.36
1	S2	1832	6MZ	C6-N6	9.32	1.44	1.34
1	S2	823	PSU	C2-N1	9.16	1.48	1.36
1	S2	1243	PSU	C2-N1	9.09	1.48	1.36
1	S2	1374	5MC	C6-C5	9.04	1.49	1.34
1	S2	1703	OMC	C4-N4	8.54	1.54	1.33
1	S2	174	OMC	C4-N4	8.38	1.54	1.33
1	S2	1710	OMC	C4-N4	8.37	1.54	1.33
1	S2	517	OMC	C4-N4	8.32	1.54	1.33
1	S2	116	OMU	C2-N1	8.28	1.51	1.38
1	S2	1842	4AC	C4-N3	8.11	1.46	1.32
1	S2	1248	B8N	C4-N3	-8.09	1.26	1.40
1	S2	568	E3C	C6-C5	7.96	1.49	1.33
1	S2	568	E3C	C2-N3	7.95	1.47	1.37
1	S2	568	E3C	C2-N1	7.89	1.49	1.38
1	S2	1337	4AC	C4-N3	7.81	1.45	1.32
1	S2	1830	UR3	C2-N1	7.80	1.49	1.38
1	S2	612	PSU	C2-N3	7.60	1.50	1.37
1	S2	121	OMU	C2-N1	7.57	1.50	1.38
1	S2	823	PSU	C2-N3	7.52	1.49	1.37
1	S2	1248	B8N	C6-N1	7.35	1.54	1.36
1	S2	119	PSU	C2-N3	7.25	1.49	1.37
1	S2	174	OMC	C2-N3	6.98	1.50	1.36
1	S2	1081	PSU	C2-N3	6.94	1.48	1.37
1	S2	1243	PSU	C2-N3	6.89	1.48	1.37
1	S2	517	OMC	C6-C5	6.84	1.50	1.35
1	S2	822	PSU	C2-N3	6.81	1.48	1.37
1	S2	1248	B8N	C4-C5	6.81	1.63	1.47
1	S2	1710	OMC	C2-N3	6.77	1.49	1.36
1	S2	174	OMC	C6-C5	6.77	1.50	1.35
1	S2	121	OMU	C2-N3	6.73	1.49	1.38
1	S2	1710	OMC	C6-C5	6.66	1.50	1.35
1	S2	517	OMC	C2-N3	6.65	1.49	1.36
1	S2	509	OMG	C4-N3	6.63	1.49	1.34
1	S2	644	OMG	C4-N3	6.55	1.49	1.34
1	S2	116	OMU	C2-N3	6.53	1.49	1.38
1	S2	1703	OMC	C6-C5	6.52	1.50	1.35
1	S2	1703	OMC	C2-N3	6.51	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1374	5MC	C5-C4	6.46	1.49	1.44
1	S2	1842	4AC	C2-N3	6.37	1.49	1.36
1	S2	683	OMG	C4-N3	6.35	1.48	1.34
1	S2	1374	5MC	C4-N3	6.28	1.44	1.34
1	S2	1337	4AC	C2-N3	6.26	1.48	1.36
1	S2	1710	OMC	C4-N3	6.25	1.46	1.34
1	S2	166	A2M	O4'-C1'	6.25	1.56	1.42
1	S2	174	OMC	C4-N3	6.11	1.46	1.34
1	S2	116	OMU	C6-C5	6.05	1.49	1.35
1	S2	1678	A2M	C3'-C2'	6.02	1.66	1.53
1	S2	159	A2M	O4'-C1'	6.00	1.55	1.42
1	S2	121	OMU	C6-C5	5.99	1.49	1.35
1	S2	484	A2M	C3'-C2'	5.98	1.66	1.53
1	S2	159	A2M	C3'-C2'	5.95	1.66	1.53
1	S2	1678	A2M	C6-N6	5.94	1.49	1.34
1	S2	1374	5MC	C2-N3	5.92	1.48	1.36
1	S2	484	A2M	O4'-C1'	5.91	1.55	1.42
1	S2	27	A2M	O4'-C1'	5.89	1.55	1.42
1	S2	1703	OMC	C4-N3	5.89	1.46	1.34
1	S2	1678	A2M	O4'-C1'	5.87	1.55	1.42
1	S2	517	OMC	C4-N3	5.82	1.46	1.34
1	S2	1337	4AC	C6-C5	5.79	1.48	1.35
1	S2	1248	B8N	C2-N1	5.75	1.56	1.39
1	S2	668	A2M	C3'-C2'	5.73	1.65	1.53
1	S2	1031	A2M	O4'-C1'	5.70	1.55	1.42
1	S2	644	OMG	C2-N3	5.55	1.46	1.33
1	S2	27	A2M	C3'-C2'	5.55	1.65	1.53
1	S2	166	A2M	C6-N6	5.52	1.48	1.34
1	S2	1031	A2M	C6-N6	5.49	1.48	1.34
1	S2	159	A2M	C6-N6	5.49	1.48	1.34
1	S2	509	OMG	C2-N3	5.48	1.46	1.33
1	S2	1842	4AC	C6-C5	5.48	1.47	1.35
1	S2	27	A2M	C6-N6	5.45	1.48	1.34
1	S2	668	A2M	O4'-C1'	5.45	1.54	1.42
1	S2	683	OMG	C2-N3	5.42	1.46	1.33
1	S2	668	A2M	C6-N6	5.32	1.47	1.34
1	S2	166	A2M	C3'-C2'	5.32	1.64	1.53
1	S2	1031	A2M	C3'-C2'	5.29	1.64	1.53
1	S2	814	5MU	C2-N3	5.26	1.47	1.38
1	S2	484	A2M	C6-N6	5.24	1.47	1.34
1	S2	823	PSU	O2-C2	-5.17	1.12	1.23
1	S2	822	PSU	O2-C2	-5.16	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	568	E3C	C4-N3	5.10	1.56	1.48
1	S2	1081	PSU	O2-C2	-5.06	1.12	1.23
1	S2	1243	PSU	O2-C2	-5.02	1.12	1.23
1	S2	121	OMU	C4-N3	4.97	1.47	1.38
1	S2	1219	B8Q	C2-N3	-4.94	1.26	1.35
1	S2	1081	PSU	O4-C4	-4.91	1.14	1.23
1	S2	612	PSU	O4-C4	-4.87	1.14	1.23
1	S2	166	A2M	O4'-C4'	4.86	1.55	1.45
1	S2	1337	4AC	C2-N1	4.86	1.50	1.40
1	S2	1678	A2M	O4'-C4'	4.85	1.55	1.45
1	S2	822	PSU	O4-C4	-4.84	1.14	1.23
1	S2	1806	M7A	C6-N6	4.82	1.46	1.34
1	S2	119	PSU	O2-C2	-4.81	1.13	1.23
1	S2	683	OMG	C2-N2	4.81	1.45	1.34
1	S2	612	PSU	O2-C2	-4.77	1.13	1.23
1	S2	116	OMU	C4-N3	4.77	1.46	1.38
1	S2	1243	PSU	O4-C4	-4.76	1.14	1.23
1	S2	1842	4AC	C7-N4	4.76	1.46	1.37
1	S2	27	A2M	O4'-C4'	4.74	1.55	1.45
1	S2	119	PSU	O4-C4	-4.73	1.14	1.23
1	S2	159	A2M	O4'-C4'	4.73	1.55	1.45
1	S2	1337	4AC	C7-N4	4.71	1.46	1.37
1	S2	1031	A2M	O4'-C4'	4.69	1.55	1.45
1	S2	1248	B8N	C6-C5	4.65	1.41	1.35
1	S2	484	A2M	O4'-C4'	4.62	1.55	1.45
1	S2	644	OMG	C2-N2	4.60	1.44	1.34
1	S2	509	OMG	C2-N2	4.57	1.44	1.34
1	S2	1842	4AC	C2-N1	4.53	1.49	1.40
1	S2	1219	B8Q	C4-C5	-4.46	1.39	1.49
1	S2	1830	UR3	C6-C5	4.43	1.45	1.35
1	S2	1337	4AC	C4-N4	4.41	1.46	1.39
1	S2	1832	6MZ	C5-C4	-4.35	1.31	1.39
1	S2	1830	UR3	C2-N3	4.33	1.47	1.39
1	S2	1374	5MC	C4-N4	4.30	1.45	1.34
1	S2	119	PSU	C6-N1	4.25	1.43	1.36
1	S2	822	PSU	C6-N1	4.24	1.43	1.36
1	S2	174	OMC	C2-N1	4.24	1.49	1.40
1	S2	1081	PSU	C6-N1	4.17	1.43	1.36
1	S2	1374	5MC	C6-N1	4.14	1.45	1.38
1	S2	668	A2M	O4'-C4'	4.08	1.54	1.45
1	S2	1374	5MC	C2-N1	4.08	1.48	1.40
1	S2	1710	OMC	C2-N1	4.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	612	PSU	C6-N1	4.02	1.42	1.36
1	S2	517	OMC	C2-N1	4.02	1.48	1.40
1	S2	1842	4AC	C4-N4	4.01	1.45	1.39
1	S2	1243	PSU	C6-N1	3.88	1.42	1.36
1	S2	1337	4AC	C6-N1	3.84	1.47	1.38
1	S2	517	OMC	C6-N1	3.83	1.47	1.38
1	S2	1337	4AC	C5-C4	3.82	1.49	1.41
1	S2	823	PSU	C6-N1	3.81	1.42	1.36
1	S2	1806	M7A	C5-N7	3.77	1.48	1.39
1	S2	1703	OMC	C6-N1	3.75	1.47	1.38
1	S2	174	OMC	C6-N1	3.73	1.47	1.38
1	S2	1842	4AC	C5-C4	3.72	1.49	1.41
1	S2	1710	OMC	C6-N1	3.71	1.46	1.38
1	S2	1842	4AC	C6-N1	3.56	1.46	1.38
1	S2	1832	6MZ	C8-N9	-3.49	1.31	1.37
1	S2	823	PSU	O4-C4	-3.48	1.17	1.23
1	S2	668	A2M	C5-C4	-3.47	1.32	1.39
1	S2	814	5MU	C2-N1	3.45	1.43	1.38
1	S2	823	PSU	C4-N3	3.44	1.45	1.38
1	S2	1850	MA6	C5-C4	-3.38	1.33	1.39
1	S2	484	A2M	C5-N7	-3.37	1.32	1.39
1	S2	683	OMG	C5-N7	-3.36	1.32	1.39
1	S2	1703	OMC	C2-N1	3.31	1.47	1.40
1	S2	1851	MA6	C5-C4	-3.29	1.33	1.39
1	S2	1832	6MZ	C5-N7	-3.26	1.33	1.39
1	S2	166	A2M	C5-N7	-3.24	1.33	1.39
1	S2	1851	MA6	C6-N6	3.23	1.45	1.36
1	S2	1851	MA6	C5-N7	-3.17	1.33	1.39
1	S2	1031	A2M	C5-C4	-3.17	1.33	1.39
1	S2	509	OMG	C5-N7	-3.14	1.32	1.39
1	S2	119	PSU	C4-N3	3.12	1.44	1.38
1	S2	1031	A2M	C5-N7	-3.11	1.33	1.39
1	S2	159	A2M	C5-C4	-3.08	1.33	1.39
1	S2	27	A2M	C5-N7	-3.07	1.33	1.39
1	S2	644	OMG	C5-N7	-3.06	1.32	1.39
1	S2	612	PSU	C4-N3	3.05	1.44	1.38
1	S2	1830	UR3	O2-C2	-3.04	1.16	1.22
1	S2	27	A2M	C5-C4	-3.04	1.33	1.39
1	S2	1850	MA6	C6-N6	3.02	1.45	1.36
1	S2	159	A2M	C5-N7	-3.01	1.33	1.39
1	S2	1219	B8Q	C31-N3	3.00	1.52	1.46
1	S2	668	A2M	C5-N7	-2.97	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	568	E3C	C6-N1	2.96	1.45	1.38
1	S2	166	A2M	C5-C4	-2.94	1.33	1.39
1	S2	484	A2M	C5-C4	-2.92	1.33	1.39
1	S2	823	PSU	O4'-C1'	-2.90	1.39	1.43
1	S2	568	E3C	C31-N3	2.90	1.55	1.47
1	S2	822	PSU	C4-N3	2.89	1.44	1.38
1	S2	1678	A2M	C5-N7	-2.86	1.33	1.39
1	S2	1081	PSU	C4-N3	2.85	1.44	1.38
1	S2	1243	PSU	C4-N3	2.83	1.44	1.38
1	S2	612	PSU	O4'-C1'	-2.79	1.40	1.43
1	S2	484	A2M	C8-N9	-2.79	1.32	1.37
1	S2	1678	A2M	C5-C4	-2.78	1.34	1.39
1	S2	1850	MA6	C5-N7	-2.78	1.34	1.39
1	S2	644	OMG	C2-N1	2.74	1.44	1.37
1	S2	822	PSU	O4'-C1'	-2.74	1.40	1.43
1	S2	116	OMU	C6-N1	2.71	1.44	1.38
1	S2	683	OMG	O6-C6	-2.71	1.18	1.23
1	S2	1374	5MC	O2-C2	-2.70	1.18	1.23
1	S2	1703	OMC	O2-C2	-2.64	1.18	1.23
1	S2	644	OMG	O6-C6	-2.63	1.18	1.23
1	S2	1850	MA6	C4-N9	-2.63	1.32	1.37
1	S2	1678	A2M	C8-N9	-2.60	1.33	1.37
1	S2	1830	UR3	C6-N1	2.59	1.44	1.38
1	S2	568	E3C	C4-C5	-2.58	1.44	1.49
1	S2	683	OMG	C4-N9	-2.58	1.31	1.38
1	S2	1850	MA6	C8-N9	-2.54	1.33	1.37
1	S2	121	OMU	C6-N1	2.53	1.44	1.38
1	S2	509	OMG	C2-N1	2.52	1.43	1.37
1	S2	509	OMG	O6-C6	-2.51	1.18	1.23
1	S2	644	OMG	C5-C6	2.51	1.53	1.44
1	S2	27	A2M	C8-N9	-2.48	1.33	1.37
1	S2	509	OMG	C5-C6	2.45	1.53	1.44
1	S2	1219	B8Q	C6-N1	-2.44	1.32	1.38
1	S2	517	OMC	O2-C2	-2.43	1.19	1.23
1	S2	668	A2M	C8-N9	-2.43	1.33	1.37
1	S2	1248	B8N	O4-C4	-2.41	1.18	1.23
1	S2	1031	A2M	C8-N9	-2.41	1.33	1.37
1	S2	159	A2M	C8-N9	-2.39	1.33	1.37
1	S2	1851	MA6	C4-N9	-2.37	1.32	1.37
1	S2	814	5MU	O2-C2	-2.36	1.18	1.23
1	S2	814	5MU	O4-C4	-2.35	1.19	1.23
1	S2	683	OMG	C2-N1	2.32	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	166	A2M	C8-N9	-2.31	1.33	1.37
1	S2	1832	6MZ	C9-N6	2.31	1.48	1.45
1	S2	517	OMC	C5-C4	2.30	1.48	1.42
1	S2	644	OMG	C6-N1	2.29	1.43	1.38
1	S2	1337	4AC	O2-C2	-2.28	1.19	1.23
1	S2	1851	MA6	C5-C6	-2.26	1.35	1.41
1	S2	1830	UR3	C4-N3	2.24	1.45	1.40
1	S2	116	OMU	O4-C4	-2.23	1.20	1.24
1	S2	174	OMC	O2-C2	-2.23	1.19	1.23
1	S2	1710	OMC	C5-C4	2.19	1.48	1.42
1	S2	1710	OMC	O2-C2	-2.19	1.19	1.23
1	S2	1842	4AC	O2-C2	-2.18	1.19	1.23
1	S2	668	A2M	C4-N9	-2.18	1.33	1.37
1	S2	1703	OMC	C5-C4	2.18	1.48	1.42
1	S2	1081	PSU	O4'-C1'	-2.17	1.40	1.43
1	S2	509	OMG	C6-N1	2.16	1.42	1.38
1	S2	174	OMC	C5-C4	2.13	1.47	1.42
1	S2	121	OMU	O4-C4	-2.11	1.20	1.24
1	S2	1832	6MZ	C6-N1	-2.09	1.31	1.35
1	S2	121	OMU	C5-C4	2.05	1.48	1.43
1	S2	1243	PSU	O4'-C1'	-2.04	1.41	1.43
1	S2	1832	6MZ	C4-N9	-2.01	1.33	1.37

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1850	MA6	N1-C6-N6	-12.78	101.28	116.86
1	S2	1851	MA6	N1-C6-N6	-12.31	101.85	116.86
1	S2	1806	M7A	C5-C6-N6	10.92	142.30	123.75
1	S2	1806	M7A	N6-C6-N1	-9.32	97.62	118.38
1	S2	814	5MU	C5-C4-N3	9.19	123.31	115.32
1	S2	1851	MA6	C5-C6-N6	8.80	139.25	125.33
1	S2	1850	MA6	C5-C6-N6	8.79	139.25	125.33
1	S2	1830	UR3	C4-N3-C2	-8.22	117.97	124.58
1	S2	814	5MU	C5-C6-N1	-8.02	114.60	123.31
1	S2	668	A2M	C4-N9-C1'	-7.83	108.31	126.63
1	S2	668	A2M	C1'-N9-C8	7.78	144.37	127.09
1	S2	568	E3C	C1'-N1-C2	7.32	129.02	117.04
1	S2	814	5MU	C4-N3-C2	-7.03	118.12	127.34
1	S2	159	A2M	C4-N9-C1'	-6.54	111.34	126.63
1	S2	1830	UR3	C1'-N1-C2	6.45	127.61	117.04
1	S2	1031	A2M	C4-N9-C1'	-6.36	111.77	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1806	M7A	N3-C4-N9	6.28	134.74	126.88
1	S2	484	A2M	C4-N9-C1'	-6.13	112.29	126.63
1	S2	27	A2M	C4-N9-C1'	-6.09	112.38	126.63
1	S2	1031	A2M	C1'-N9-C8	6.08	140.58	127.09
1	S2	484	A2M	C1'-N9-C8	6.06	140.54	127.09
1	S2	668	A2M	N3-C2-N1	-6.03	119.45	128.58
1	S2	159	A2M	C1'-N9-C8	6.00	140.42	127.09
1	S2	1851	MA6	N1-C2-N3	-5.99	119.52	128.58
1	S2	121	OMU	C4-N3-C2	-5.94	119.23	126.61
1	S2	1678	A2M	C4-N9-C1'	-5.92	112.79	126.63
1	S2	668	A2M	N6-C6-N1	-5.85	105.35	118.38
1	S2	166	A2M	C4-N9-C1'	-5.85	112.96	126.63
1	S2	27	A2M	C1'-N9-C8	5.83	140.03	127.09
1	S2	509	OMG	C5-C4-N3	-5.71	119.30	128.39
1	S2	1031	A2M	N3-C2-N1	-5.69	119.96	128.58
1	S2	159	A2M	N3-C2-N1	-5.69	119.96	128.58
1	S2	166	A2M	N3-C2-N1	-5.69	119.97	128.58
1	S2	166	A2M	C1'-N9-C8	5.68	139.70	127.09
1	S2	27	A2M	N3-C2-N1	-5.65	120.03	128.58
1	S2	484	A2M	N3-C2-N1	-5.59	120.12	128.58
1	S2	1806	M7A	N3-C2-N1	-5.56	120.17	128.58
1	S2	159	A2M	C2'-C1'-N9	-5.54	104.63	113.75
1	S2	27	A2M	N6-C6-N1	-5.53	106.07	118.38
1	S2	27	A2M	C5-C4-N3	-5.51	119.13	126.72
1	S2	814	5MU	N3-C2-N1	5.48	122.03	114.89
1	S2	1678	A2M	N3-C2-N1	-5.48	120.29	128.58
1	S2	568	E3C	O2-C2-N3	-5.46	115.11	122.10
1	S2	484	A2M	N6-C6-N1	-5.43	106.28	118.38
1	S2	644	OMG	C5-C4-N3	-5.43	119.75	128.39
1	S2	1678	A2M	C5-C4-N3	-5.43	119.25	126.72
1	S2	1850	MA6	C1'-N9-C8	-5.38	115.15	127.09
1	S2	1031	A2M	C5-C4-N3	-5.36	119.34	126.72
1	S2	1850	MA6	N1-C2-N3	-5.35	120.48	128.58
1	S2	1248	B8N	C5-C4-N3	5.31	125.80	116.15
1	S2	166	A2M	C5-C4-N3	-5.26	119.47	126.72
1	S2	1832	6MZ	N1-C2-N3	-5.26	120.61	128.58
1	S2	116	OMU	C4-N3-C2	-5.24	120.10	126.61
1	S2	1031	A2M	N6-C6-N1	-5.18	106.85	118.38
1	S2	1081	PSU	C4-N3-C2	-5.17	119.25	126.37
1	S2	814	5MU	C5M-C5-C6	-5.15	115.88	122.85
1	S2	1678	A2M	C1'-N9-C8	5.14	138.51	127.09
1	S2	1830	UR3	O2-C2-N3	-5.12	114.26	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	484	A2M	C5-C4-N3	-5.11	119.67	126.72
1	S2	1248	B8N	C4-N3-C2	-5.03	119.43	125.62
1	S2	1832	6MZ	C5-C4-N3	-5.01	119.81	126.72
1	S2	159	A2M	C5-C4-N3	-4.98	119.86	126.72
1	S2	1850	MA6	N9-C8-N7	-4.96	106.90	113.94
1	S2	822	PSU	C4-N3-C2	-4.93	119.58	126.37
1	S2	1219	B8Q	N3-C2-N1	4.93	124.02	117.16
1	S2	166	A2M	N6-C6-N1	-4.89	107.47	118.38
1	S2	159	A2M	N6-C6-N1	-4.86	107.56	118.38
1	S2	119	PSU	C4-N3-C2	-4.84	119.71	126.37
1	S2	683	OMG	C5-C4-N3	-4.75	120.83	128.39
1	S2	668	A2M	C5-C4-N3	-4.68	120.27	126.72
1	S2	612	PSU	C4-N3-C2	-4.68	119.92	126.37
1	S2	822	PSU	N1-C2-N3	4.66	120.08	115.17
1	S2	568	E3C	C6-N1-C2	-4.61	118.03	121.80
1	S2	823	PSU	N1-C2-N3	4.60	120.02	115.17
1	S2	1081	PSU	N1-C2-N3	4.45	119.86	115.17
1	S2	823	PSU	C4-N3-C2	-4.40	120.31	126.37
1	S2	509	OMG	C2-N3-C4	4.39	119.86	112.30
1	S2	1806	M7A	C4-N9-C1'	-4.37	116.45	126.63
1	S2	823	PSU	O2-C2-N1	-4.36	118.30	122.79
1	S2	683	OMG	C1'-N9-C4	-4.35	113.63	126.49
1	S2	612	PSU	N1-C2-N3	4.35	119.75	115.17
1	S2	119	PSU	N1-C2-N3	4.35	119.75	115.17
1	S2	1830	UR3	C6-N1-C2	-4.33	118.26	121.80
1	S2	814	5MU	C6-C5-C4	4.31	121.57	118.02
1	S2	823	PSU	C6-N1-C2	-4.30	118.70	122.69
1	S2	116	OMU	N3-C2-N1	4.29	120.47	114.89
1	S2	121	OMU	N3-C2-N1	4.26	120.44	114.89
1	S2	644	OMG	C2-N3-C4	4.26	119.63	112.30
1	S2	668	A2M	C5-C6-N6	4.24	133.78	123.29
1	S2	568	E3C	C31-N3-C2	4.24	122.81	117.49
1	S2	1678	A2M	N9-C8-N7	-4.22	107.95	113.94
1	S2	683	OMG	C2-N3-C4	4.21	119.56	112.30
1	S2	1678	A2M	N6-C6-N1	-4.16	109.11	118.38
1	S2	1031	A2M	N9-C8-N7	-4.14	108.06	113.94
1	S2	484	A2M	C5-C6-N6	4.14	133.53	123.29
1	S2	159	A2M	N9-C8-N7	-4.13	108.08	113.94
1	S2	1832	6MZ	N9-C8-N7	-4.13	108.08	113.94
1	S2	1243	PSU	C4-N3-C2	-4.11	120.71	126.37
1	S2	1851	MA6	N9-C8-N7	-4.07	108.16	113.94
1	S2	27	A2M	C5-C6-N6	4.01	133.22	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	668	A2M	N9-C8-N7	-4.00	108.27	113.94
1	S2	1832	6MZ	C4-C5-C6	3.99	120.09	116.78
1	S2	1031	A2M	C5-C6-N6	3.98	133.15	123.29
1	S2	1243	PSU	N1-C2-N3	3.98	119.37	115.17
1	S2	644	OMG	C1'-N9-C4	-3.97	114.77	126.49
1	S2	1678	A2M	N3-C4-N9	3.95	133.89	127.17
1	S2	1851	MA6	C5-C4-N3	-3.94	121.30	126.72
1	S2	159	A2M	O2'-C2'-C1'	3.92	116.43	108.99
1	S2	1850	MA6	C5-C4-N3	-3.92	121.32	126.72
1	S2	509	OMG	C1'-N9-C4	-3.92	114.91	126.49
1	S2	1851	MA6	C2-N1-C6	3.92	121.40	111.83
1	S2	814	5MU	O4-C4-C5	-3.90	120.45	124.92
1	S2	612	PSU	C6-C5-C4	3.89	120.80	118.17
1	S2	1830	UR3	C3U-N3-C4	3.85	123.20	117.87
1	S2	1248	B8N	N3-C2-N1	3.84	121.41	116.72
1	S2	1219	B8Q	C31-N3-C4	3.81	121.35	114.76
1	S2	1851	MA6	C4-C5-C6	3.81	119.84	115.91
1	S2	166	A2M	C5-C6-N6	3.80	132.70	123.29
1	S2	1850	MA6	C4-N9-C8	3.80	109.73	105.74
1	S2	27	A2M	N9-C8-N7	-3.76	108.59	113.94
1	S2	1248	B8N	C31-N3-C4	3.76	122.51	117.18
1	S2	509	OMG	N9-C4-N3	3.72	133.40	125.95
1	S2	1851	MA6	C1'-N9-C8	-3.71	118.87	127.09
1	S2	1806	M7A	C71-N7-C5	-3.71	107.99	123.44
1	S2	1850	MA6	C4-C5-C6	3.67	119.70	115.91
1	S2	1374	5MC	C5-C6-N1	-3.67	119.33	123.31
1	S2	568	E3C	C1'-N1-C6	-3.66	112.95	120.78
1	S2	568	E3C	C4-N3-C2	-3.66	115.41	122.00
1	S2	121	OMU	C5-C4-N3	3.66	119.92	114.80
1	S2	1243	PSU	C6-N1-C2	-3.64	119.31	122.69
1	S2	159	A2M	C5-C6-N6	3.63	132.28	123.29
1	S2	1850	MA6	C4-N9-C1'	3.63	135.12	126.63
1	S2	612	PSU	O2-C2-N1	-3.59	119.09	122.79
1	S2	814	5MU	O2-C2-N1	-3.57	118.15	122.80
1	S2	683	OMG	N9-C4-N3	3.56	133.07	125.95
1	S2	27	A2M	C2-N3-C4	3.55	120.51	111.83
1	S2	644	OMG	C1'-N9-C8	3.55	136.83	126.73
1	S2	166	A2M	N9-C8-N7	-3.55	108.90	113.94
1	S2	668	A2M	C2-N3-C4	3.54	120.49	111.83
1	S2	814	5MU	C5M-C5-C4	3.52	122.54	118.78
1	S2	1031	A2M	C2-N3-C4	3.50	120.38	111.83
1	S2	683	OMG	C1'-N9-C8	3.50	136.67	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	116	OMU	C5-C4-N3	3.49	119.69	114.80
1	S2	644	OMG	N9-C4-N3	3.47	132.89	125.95
1	S2	121	OMU	O4-C4-C5	-3.45	119.21	125.16
1	S2	509	OMG	C1'-N9-C8	3.44	136.51	126.73
1	S2	1248	B8N	C1'-C5-C4	3.44	122.83	117.61
1	S2	644	OMG	C2-N1-C6	-3.44	118.87	125.11
1	S2	509	OMG	C2-N1-C6	-3.44	118.87	125.11
1	S2	27	A2M	N3-C4-N9	3.43	133.00	127.17
1	S2	1850	MA6	C2-N1-C6	3.43	120.20	111.83
1	S2	484	A2M	N9-C8-N7	-3.38	109.14	113.94
1	S2	1678	A2M	C2-N3-C4	3.36	120.04	111.83
1	S2	484	A2M	C2-N3-C4	3.35	120.02	111.83
1	S2	166	A2M	C2-N3-C4	3.34	119.99	111.83
1	S2	612	PSU	C6-N1-C2	-3.32	119.61	122.69
1	S2	1832	6MZ	C2-N3-C4	3.32	119.95	111.83
1	S2	166	A2M	N3-C4-N9	3.32	132.82	127.17
1	S2	119	PSU	C6-N1-C2	-3.30	119.63	122.69
1	S2	159	A2M	C2-N3-C4	3.29	119.88	111.83
1	S2	116	OMU	O4-C4-C5	-3.26	119.53	125.16
1	S2	166	A2M	O4'-C1'-C2'	-3.25	101.00	106.59
1	S2	1806	M7A	C2-N3-C4	3.22	119.70	111.83
1	S2	159	A2M	N3-C4-N9	3.21	132.63	127.17
1	S2	1678	A2M	C5-C6-N6	3.21	131.22	123.29
1	S2	822	PSU	C6-N1-C2	-3.20	119.72	122.69
1	S2	1219	B8Q	O2-C2-N3	-3.14	118.54	122.95
1	S2	683	OMG	N9-C8-N7	-3.13	107.60	113.40
1	S2	1830	UR3	C1'-N1-C6	-3.12	114.11	120.78
1	S2	668	A2M	C5-C4-N9	3.10	109.19	105.81
1	S2	1842	4AC	C6-C5-C4	3.08	120.71	117.00
1	S2	1031	A2M	N3-C4-N9	3.08	132.40	127.17
1	S2	119	PSU	O2-C2-N1	-3.01	119.69	122.79
1	S2	509	OMG	N9-C8-N7	-3.01	107.83	113.40
1	S2	668	A2M	C3'-C2'-C1'	2.97	108.49	102.81
1	S2	1851	MA6	C2-N3-C4	2.96	119.06	111.83
1	S2	1832	6MZ	C5-N7-C8	2.96	108.10	103.45
1	S2	484	A2M	N3-C4-N9	2.96	132.19	127.17
1	S2	1031	A2M	C5-N7-C8	2.94	108.08	103.45
1	S2	1248	B8N	O4-C4-C5	-2.88	117.59	122.58
1	S2	1806	M7A	C5-C4-N3	-2.88	119.91	126.56
1	S2	484	A2M	C4'-O4'-C1'	-2.87	103.13	109.47
1	S2	1850	MA6	C2-N3-C4	2.87	118.83	111.83
1	S2	668	A2M	C4'-O4'-C1'	-2.87	103.14	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1337	4AC	C5-C4-N3	-2.86	118.12	122.60
1	S2	1842	4AC	O7-C7-CM7	-2.85	116.98	122.05
1	S2	683	OMG	C2-N1-C6	-2.85	119.94	125.11
1	S2	1243	PSU	O2-C2-N1	-2.85	119.85	122.79
1	S2	644	OMG	N9-C8-N7	-2.85	108.12	113.40
1	S2	1678	A2M	C6-C5-C4	2.84	121.05	117.18
1	S2	1678	A2M	C5-N7-C8	2.84	107.91	103.45
1	S2	1081	PSU	C6-N1-C2	-2.81	120.08	122.69
1	S2	1678	A2M	C4-N9-C8	2.80	108.68	105.74
1	S2	822	PSU	O2-C2-N1	-2.80	119.90	122.79
1	S2	1851	MA6	C4-N9-C1'	2.79	133.17	126.63
1	S2	1850	MA6	C5-N7-C8	2.78	107.82	103.45
1	S2	121	OMU	O2-C2-N1	-2.78	119.18	122.80
1	S2	116	OMU	C6-N1-C2	-2.78	117.62	121.00
1	S2	683	OMG	C5-C6-N1	2.75	120.24	113.25
1	S2	1832	6MZ	C5-C4-N9	2.74	108.79	105.81
1	S2	1031	A2M	O4'-C1'-C2'	-2.73	101.88	106.59
1	S2	1832	6MZ	C4-C5-N7	-2.73	107.46	110.58
1	S2	1081	PSU	O2-C2-N1	-2.70	120.01	122.79
1	S2	509	OMG	C5-C6-N1	2.66	120.02	113.25
1	S2	1830	UR3	C5-C4-N3	2.66	118.54	115.04
1	S2	683	OMG	O6-C6-C5	-2.65	119.53	126.53
1	S2	644	OMG	C5-C6-N1	2.65	120.01	113.25
1	S2	159	A2M	C5-N7-C8	2.65	107.61	103.45
1	S2	1337	4AC	C6-C5-C4	2.65	120.19	117.00
1	S2	823	PSU	C6-C5-C4	2.61	119.94	118.17
1	S2	1850	MA6	N3-C4-N9	2.61	131.61	127.17
1	S2	27	A2M	C5-N7-C8	2.60	107.53	103.45
1	S2	814	5MU	O3'-C3'-C2'	2.58	120.10	111.82
1	S2	1248	B8N	O2-C2-N3	-2.58	118.51	121.98
1	S2	1678	A2M	C3'-C2'-C1'	2.56	107.70	102.81
1	S2	668	A2M	C5-N7-C8	2.55	107.45	103.45
1	S2	1842	4AC	N4-C4-N3	2.54	118.00	113.87
1	S2	1337	4AC	O7-C7-CM7	-2.53	117.55	122.05
1	S2	1851	MA6	C5-N7-C8	2.52	107.42	103.45
1	S2	1830	UR3	O4-C4-N3	2.52	122.72	119.66
1	S2	644	OMG	O6-C6-C5	-2.51	119.91	126.53
1	S2	166	A2M	C6-C5-C4	2.50	120.60	117.18
1	S2	1219	B8Q	C31-N3-C2	2.49	121.62	117.70
1	S2	1832	6MZ	N3-C4-N9	2.48	131.38	127.17
1	S2	166	A2M	C5-N7-C8	2.47	107.33	103.45
1	S2	1031	A2M	C6-C5-C4	2.46	120.54	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	668	A2M	C4-C5-N7	-2.45	107.78	110.58
1	S2	1337	4AC	N4-C4-N3	2.41	117.78	113.87
1	S2	1219	B8Q	O2-C2-N1	-2.40	117.44	122.78
1	S2	484	A2M	C5-N7-C8	2.37	107.18	103.45
1	S2	509	OMG	O6-C6-C5	-2.37	120.27	126.53
1	S2	159	A2M	C4-N9-C8	2.36	108.22	105.74
1	S2	166	A2M	C4'-O4'-C1'	-2.36	104.26	109.47
1	S2	1081	PSU	C6-C5-C4	2.32	119.74	118.17
1	S2	1031	A2M	C4'-O4'-C1'	-2.31	104.36	109.47
1	S2	1031	A2M	C4-C5-N7	-2.30	107.95	110.58
1	S2	1842	4AC	C5-C4-N3	-2.28	119.03	122.60
1	S2	1851	MA6	N3-C4-N9	2.27	131.03	127.17
1	S2	612	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	S2	1031	A2M	C5-C4-N9	2.25	108.26	105.81
1	S2	159	A2M	C2'-C3'-C4'	2.24	106.81	101.99
1	S2	159	A2M	CM'-O2'-C2'	2.22	120.17	114.47
1	S2	484	A2M	C2'-C1'-N9	-2.20	110.13	113.75
1	S2	159	A2M	C6-C5-C4	2.19	120.17	117.18
1	S2	484	A2M	C6-C5-C4	2.19	120.17	117.18
1	S2	1248	B8N	O36-C34-O35	-2.19	119.10	124.08
1	S2	509	OMG	C8-N7-C5	2.19	108.16	104.26
1	S2	27	A2M	C6-C5-C4	2.19	120.17	117.18
1	S2	668	A2M	C5'-C4'-C3'	-2.19	107.34	115.21
1	S2	1374	5MC	CM5-C5-C6	-2.18	119.90	122.85
1	S2	484	A2M	C5-C4-N9	2.13	108.13	105.81
1	S2	1851	MA6	C4-N9-C8	2.11	107.96	105.74
1	S2	1248	B8N	O4-C4-N3	-2.08	116.60	119.99
1	S2	814	5MU	O4-C4-N3	-2.06	116.24	120.11
1	S2	668	A2M	C2'-C3'-C4'	2.05	106.41	101.99
1	S2	517	OMC	O2-C2-N3	-2.05	119.10	122.33
1	S2	1703	OMC	C1'-N1-C6	2.04	125.13	120.78
1	S2	1842	4AC	O7-C7-N4	2.03	125.10	121.90
1	S2	1374	5MC	C5-C4-N3	-2.03	119.67	121.75
1	S2	1374	5MC	O2-C2-N3	-2.00	119.17	122.33

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
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	644	OMG	C1'-C2'-O2'-CM2
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	822	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C1'-C2'-O2'-CM'
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'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	1850	MA6	C5-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	568	E3C	O4'-C4'-C5'-O5'
1	S2	517	OMC	O4'-C4'-C5'-O5'
1	S2	823	PSU	O4'-C4'-C5'-O5'
1	S2	1031	A2M	C3'-C4'-C5'-O5'
1	S2	1850	MA6	N1-C6-N6-C9
1	S2	1830	UR3	C2'-C1'-N1-C6
1	S2	823	PSU	C3'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	517	OMC	C3'-C4'-C5'-O5'
1	S2	822	PSU	C3'-C4'-C5'-O5'
1	S2	1031	A2M	O4'-C4'-C5'-O5'
1	S2	1806	M7A	C3'-C4'-C5'-O5'
1	S2	1806	M7A	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C5-C6-N6-C10
1	S2	121	OMU	C4'-C5'-O5'-P
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	484	A2M	O4'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	1830	UR3	C2'-C1'-N1-C2
1	S2	1806	M7A	C2'-C1'-N9-C8
1	S2	1081	PSU	C3'-C4'-C5'-O5'
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	119	PSU	O4'-C1'-C5-C4
1	S2	823	PSU	O4'-C1'-C5-C4
1	S2	1830	UR3	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	1081	PSU	O4'-C4'-C5'-O5'
1	S2	1850	MA6	C5-C6-N6-C10
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	612	PSU	O4'-C4'-C5'-O5'
1	S2	1374	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	517	OMC	1	0
1	S2	1678	A2M	2	0
1	S2	1337	4AC	2	0
1	S2	814	5MU	1	0
1	S2	683	OMG	1	0
1	S2	1850	MA6	1	0
1	S2	166	A2M	3	0
1	S2	509	OMG	3	0
1	S2	27	A2M	2	0
1	S2	484	A2M	3	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	5112	-	35,35,35	1.94	4 (11%)	44,49,49	2.75	17 (38%)

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	5112	-	-	2/20/28/28	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5112	MVM	N4-N5	-7.18	1.30	1.38
86	t	5112	MVM	C5-N1	6.27	1.46	1.37
86	t	5112	MVM	C6-N1	2.55	1.45	1.39
86	t	5112	MVM	C12-C5	2.42	1.54	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5112	MVM	N7-C22-N4	7.39	134.19	125.88
86	t	5112	MVM	C15-N4-C22	-7.26	124.10	130.55
86	t	5112	MVM	C15-N4-N5	6.39	125.01	119.25
86	t	5112	MVM	C7-C3-C9	4.54	119.43	110.81
86	t	5112	MVM	C18-C22-N7	-4.37	121.18	127.18
86	t	5112	MVM	C6-N1-C5	-4.30	117.79	122.94
86	t	5112	MVM	C19-C18-N6	4.04	135.76	130.50
86	t	5112	MVM	N3-C6-N1	3.80	120.41	116.35
86	t	5112	MVM	C1-C9-N1	-3.67	106.93	116.16
86	t	5112	MVM	C21-N7-C22	3.34	122.60	115.05
86	t	5112	MVM	C12-C5-N1	3.33	122.78	118.36
86	t	5112	MVM	C8-N3-C6	2.99	121.82	115.05
86	t	5112	MVM	C11-C2-C6	2.51	120.84	118.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5112	MVM	C6-N1-C9	2.45	122.05	118.40
86	t	5112	MVM	C2-C6-N3	-2.24	119.51	123.00
86	t	5112	MVM	C20-C21-N7	-2.23	119.88	123.42
86	t	5112	MVM	C3-C9-C1	2.03	113.23	110.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

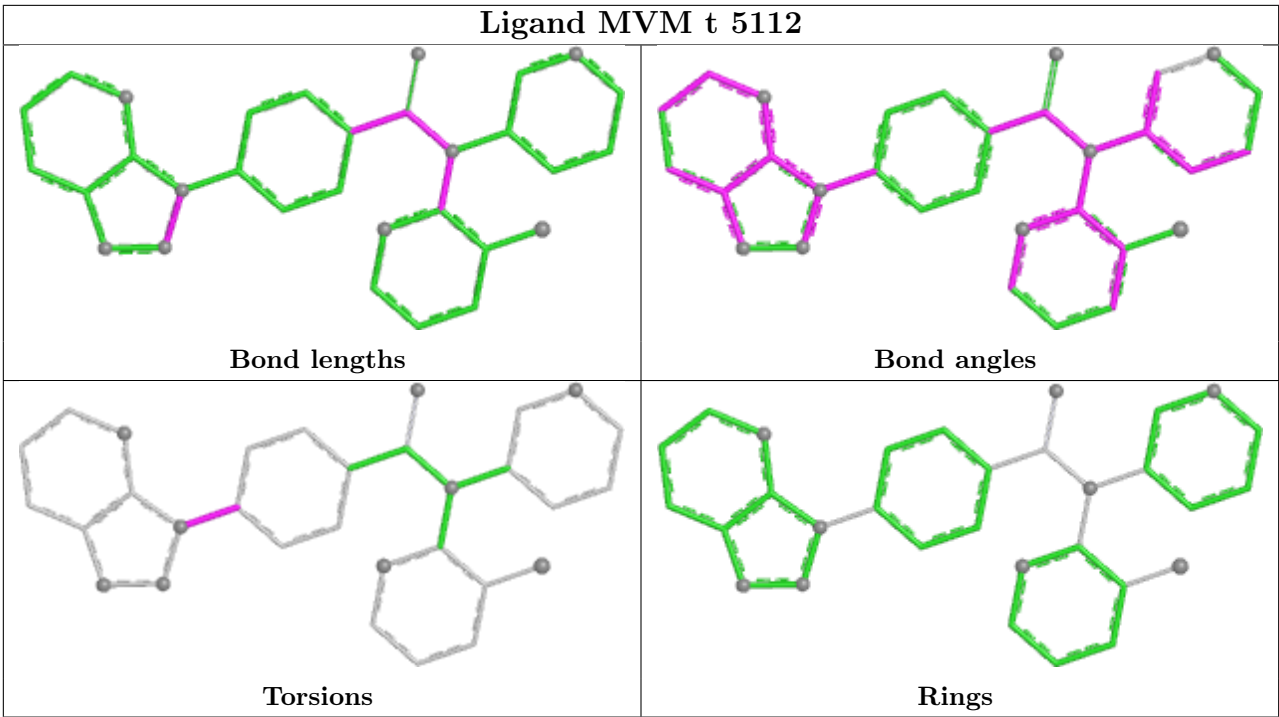
Mol	Chain	Res	Type	Atoms
86	t	5112	MVM	C16-C15-N4-C22
86	t	5112	MVM	C14-C15-N4-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	t	5112	MVM	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
78	t	16
1	S2	5
79	v	4
62	c	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	26.21
1	t	750:G	O3'	890:C	P	19.49
1	t	3919:C	O3'	4035:G	P	17.88
1	t	1680:C	O3'	1699:C	P	17.58
1	t	517:C	O3'	629:G	P	17.45
1	t	2881:G	O3'	3569:C	P	16.05
1	S2	1752:C	O3'	1779:G	P	15.45

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	976:U	O3'	1047:G	P	15.43
1	t	1202:G	O3'	1216:G	P	15.43
1	t	4737:G	O3'	4815:C	P	15.07
1	t	2093:C	O3'	2228:C	P	14.74
1	t	1089:A	O3'	1145:G	P	14.43
1	t	1253:A	O3'	1256:G	P	13.75
1	S2	739:C	O3'	746:C	P	13.39
1	S2	698:G	O3'	730:C	P	12.80
1	S2	225:G	O3'	287:U	P	7.22
1	c	119:CYS	C	120:ARG	N	6.78
1	t	945:G	O3'	946:G	P	6.36
1	t	4734:C	O3'	4735:C	P	4.98
1	v	17:A	O3'	18:G	P	4.55
1	v	21:A	O3'	22:G	P	4.01
1	t	4817:G	O3'	4818:G	P	3.97
1	v	10:G	O3'	11:C	P	3.35
1	t	964:C	O3'	965:G	P	3.31
1	t	1938:U	O3'	1939:A	P	3.27
1	v	41:C	O3'	42:C	P	3.14

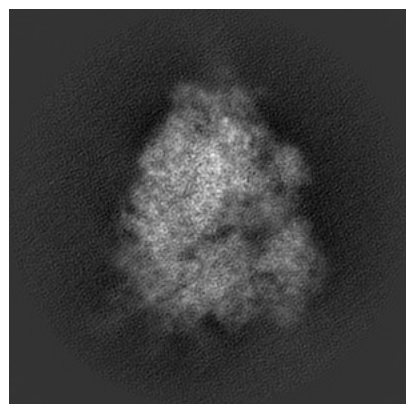
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0599. These allow visual inspection of the internal detail of the map and identification of artifacts.

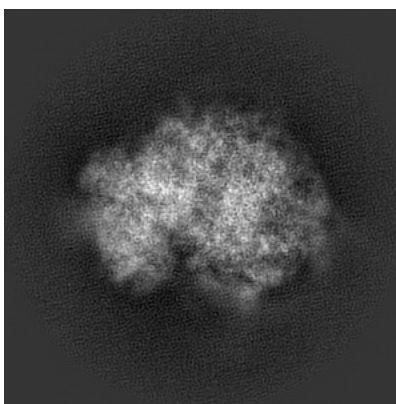
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

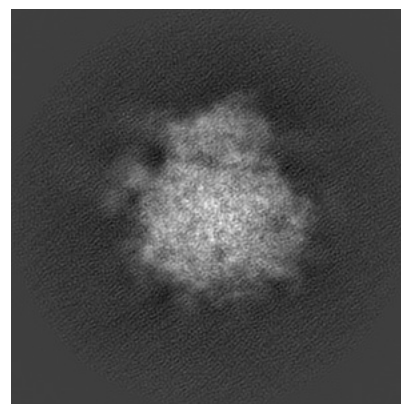
6.1.1 Primary map



X

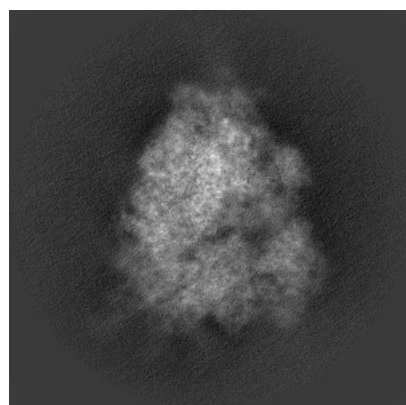


Y

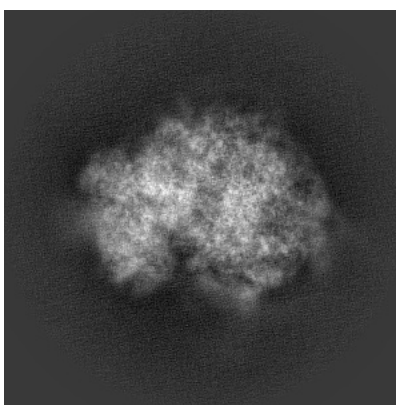


Z

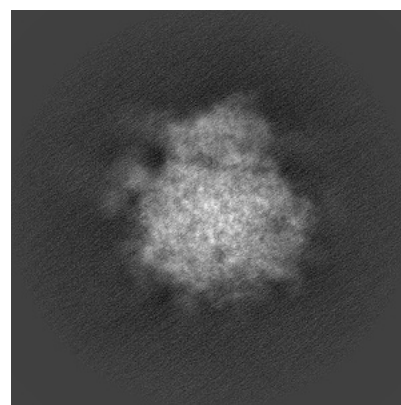
6.1.2 Raw map



X



Y

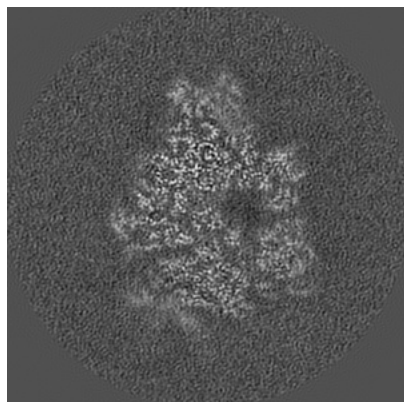


Z

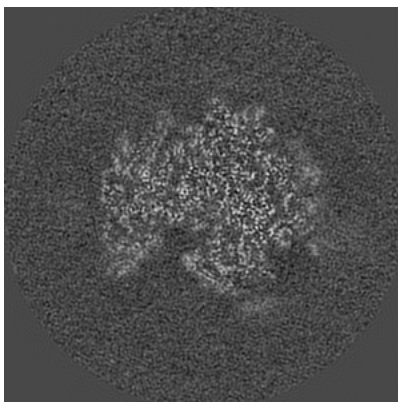
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

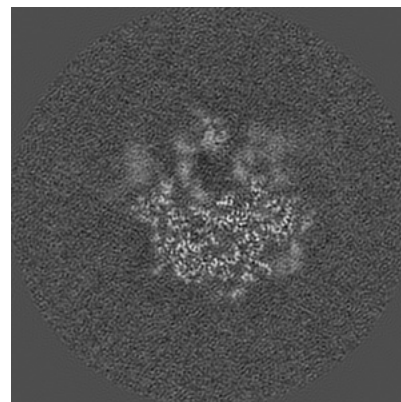
6.2.1 Primary map



X Index: 200

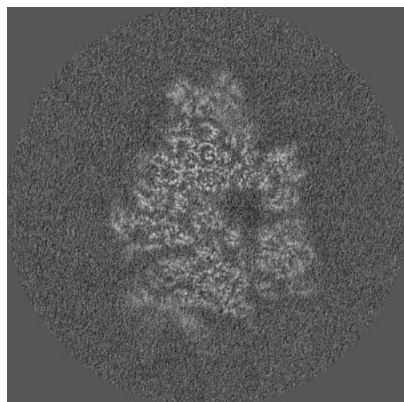


Y Index: 200

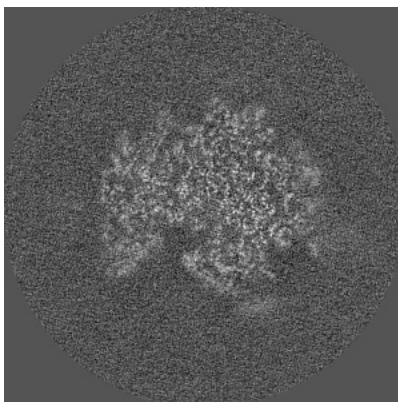


Z Index: 200

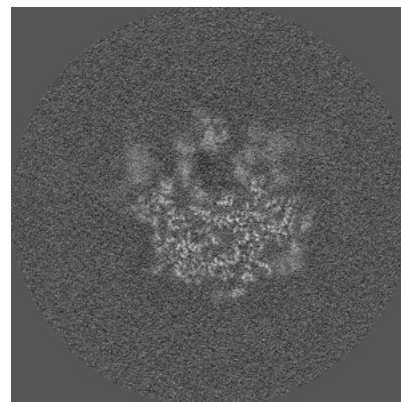
6.2.2 Raw map



X Index: 200



Y Index: 200

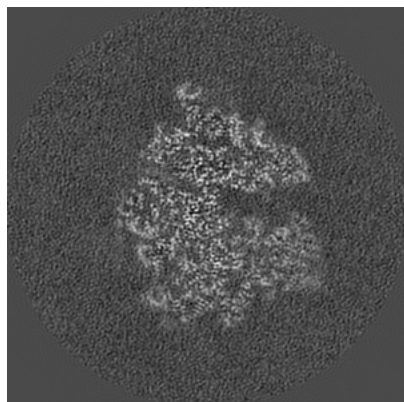


Z Index: 200

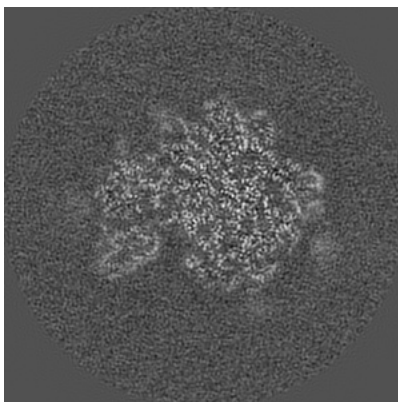
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

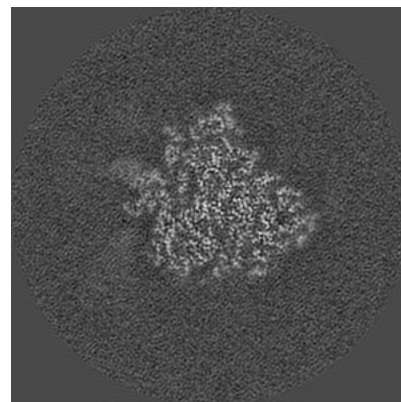
6.3.1 Primary map



X Index: 218

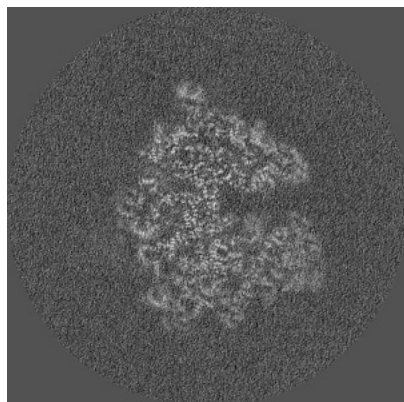


Y Index: 193

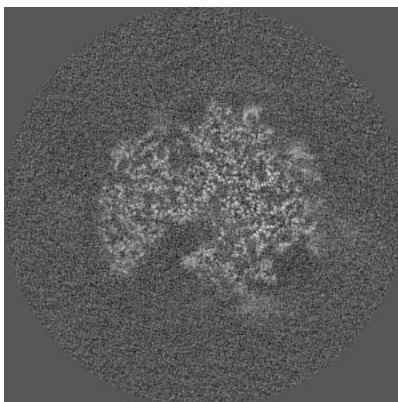


Z Index: 229

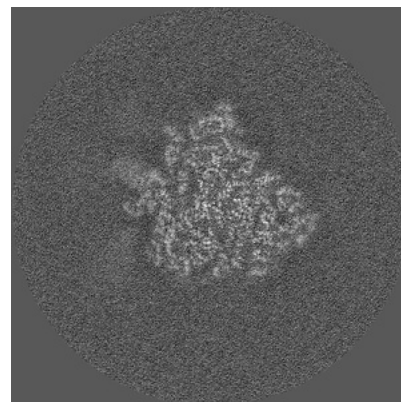
6.3.2 Raw map



X Index: 219



Y Index: 204

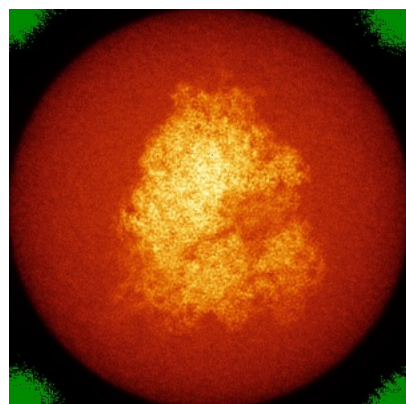


Z Index: 229

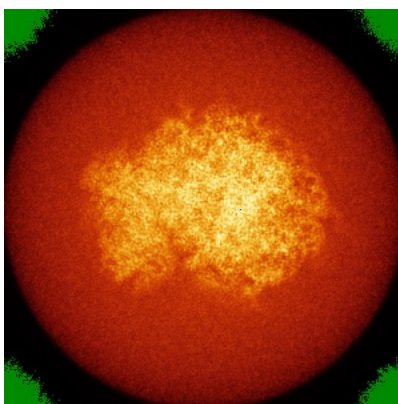
The images above show the largest variance slices of the map in three orthogonal directions.

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

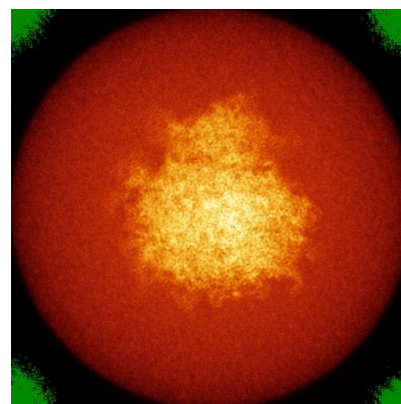
6.4.1 Primary map



X

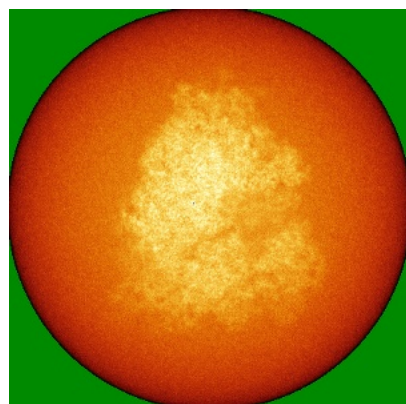


Y

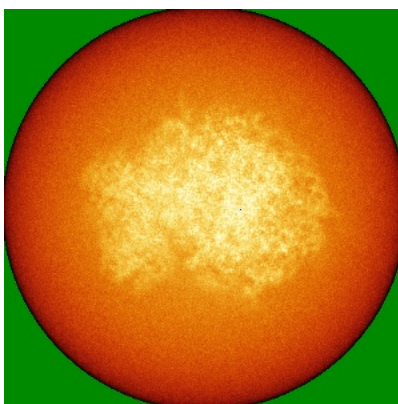


Z

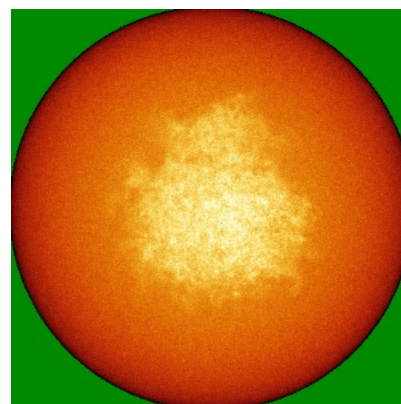
6.4.2 Raw map



X



Y

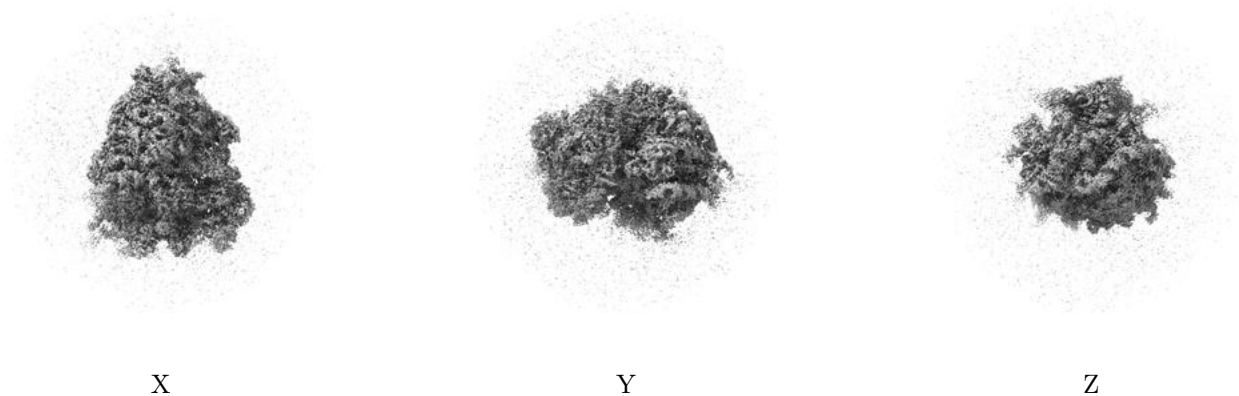


Z

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

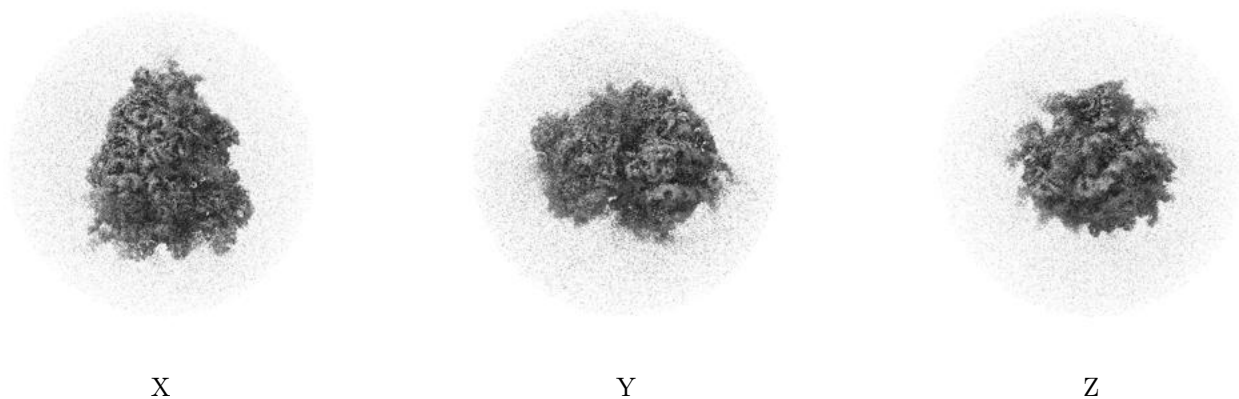
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

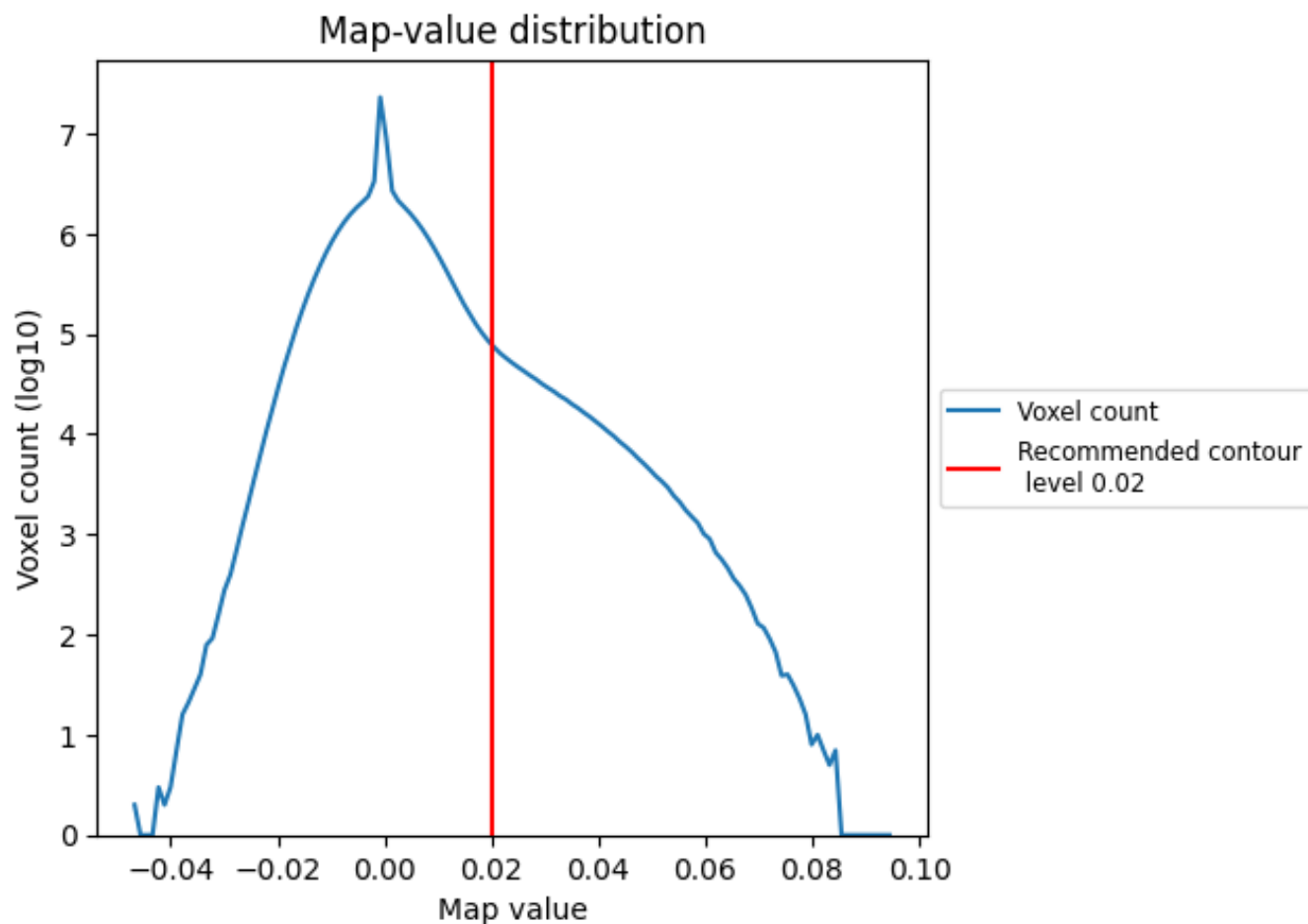
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

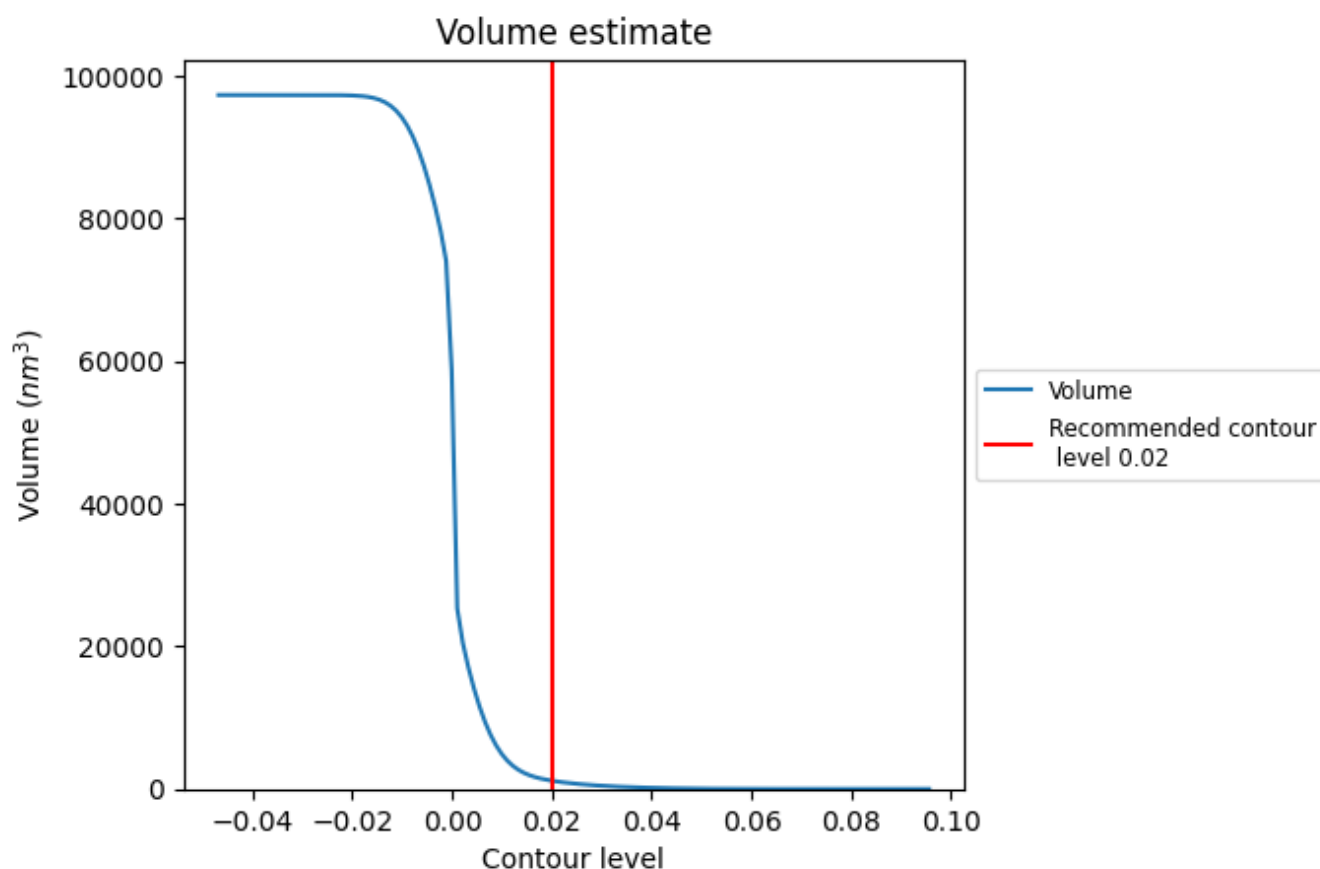
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

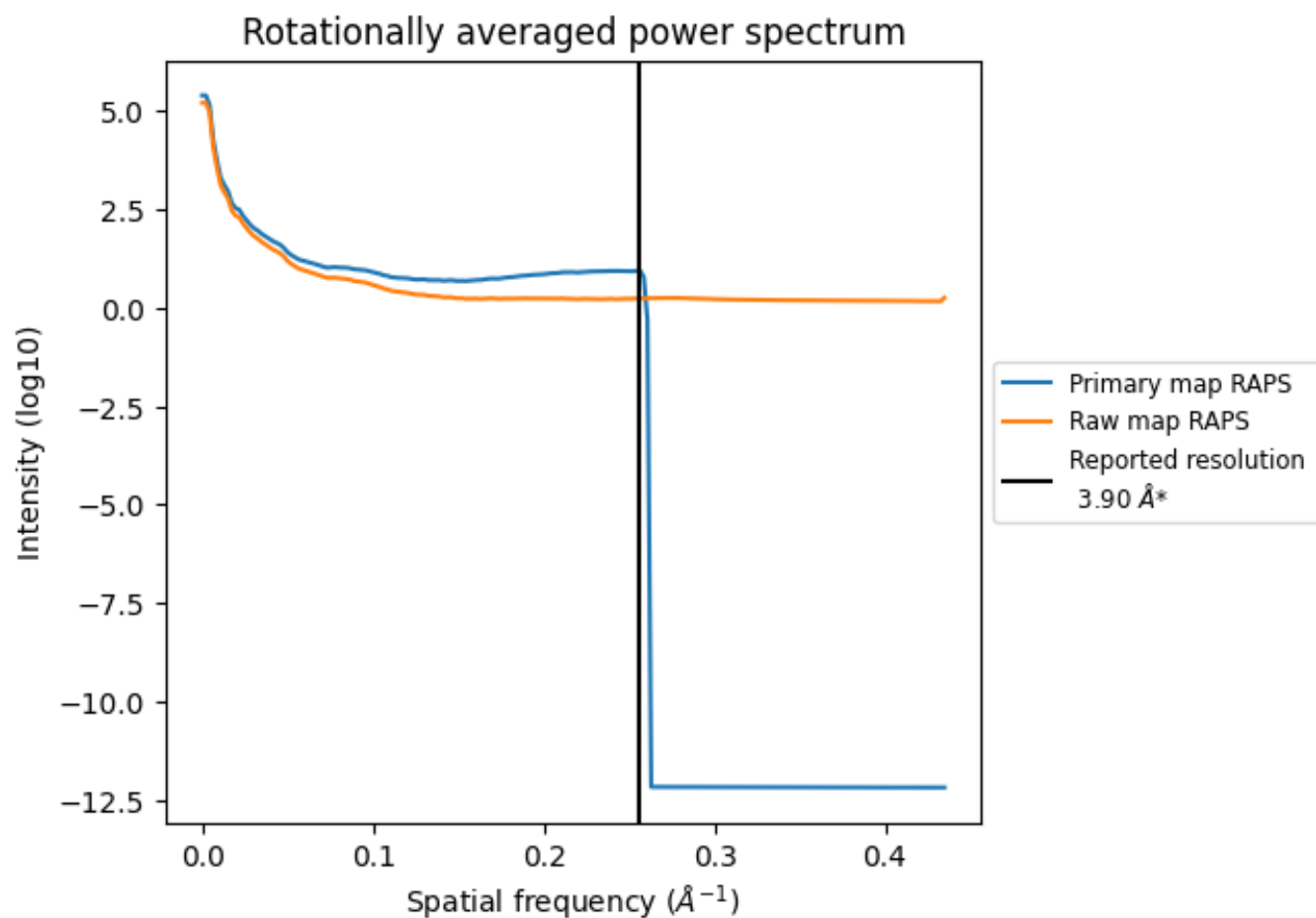
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1153 nm³; this corresponds to an approximate mass of 1042 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 ⓘ

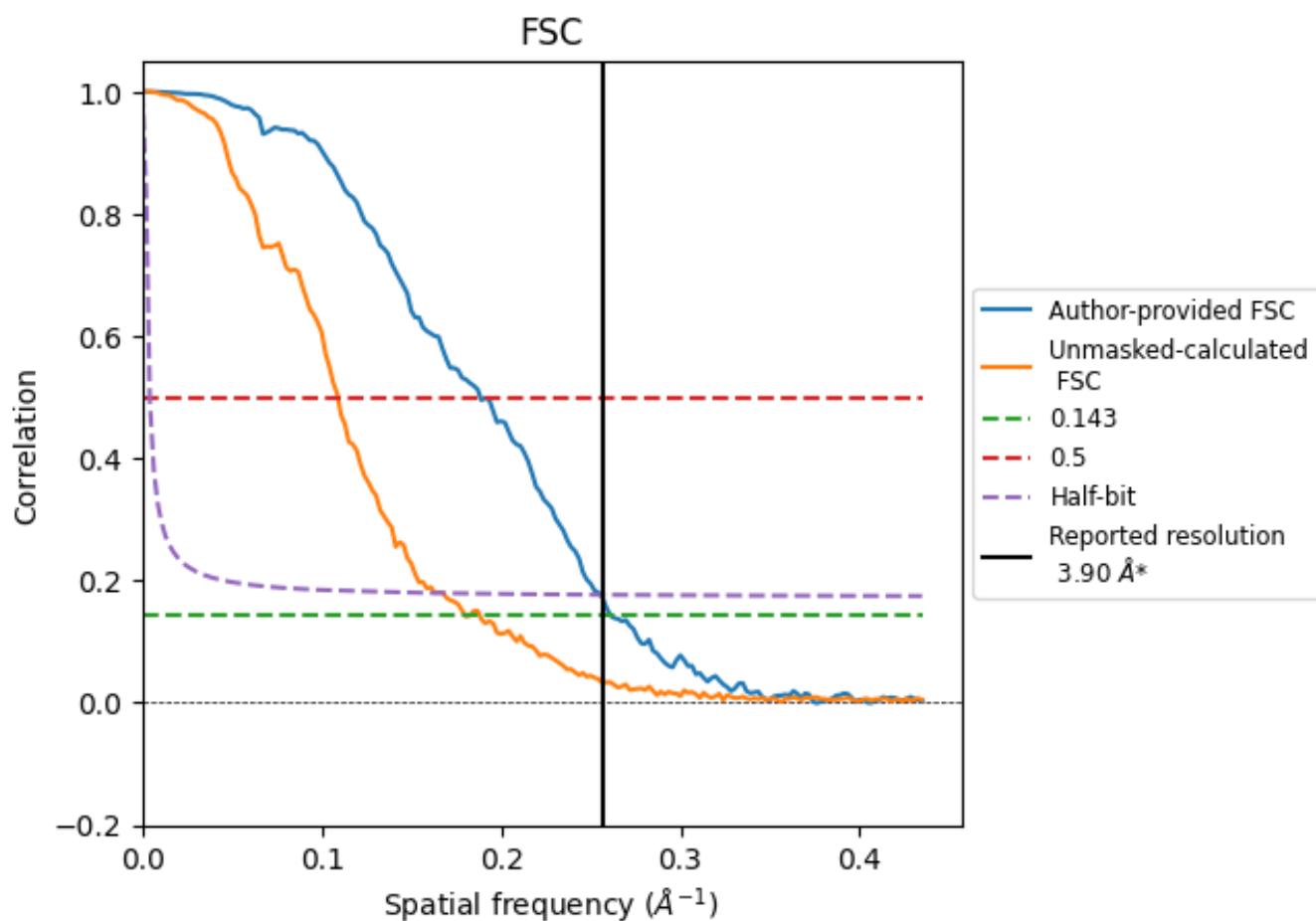


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates

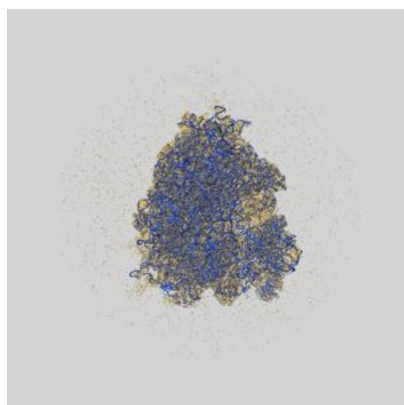
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	5.31	3.92
Unmasked-calculated*	5.56	9.17	5.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.56 differs from the reported value 3.9 by more than 10 %

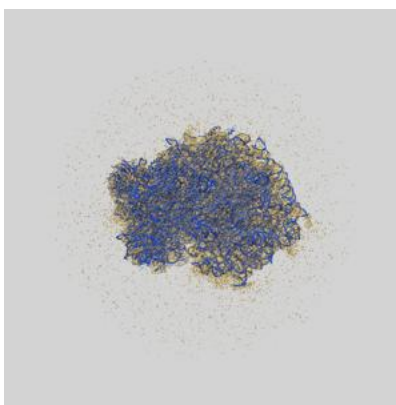
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0599 and PDB model 6OLF. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

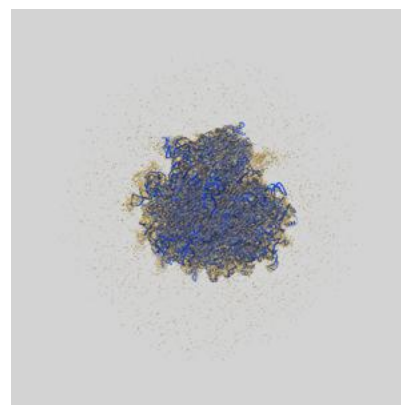
9.1 Map-model overlay [i](#)



X



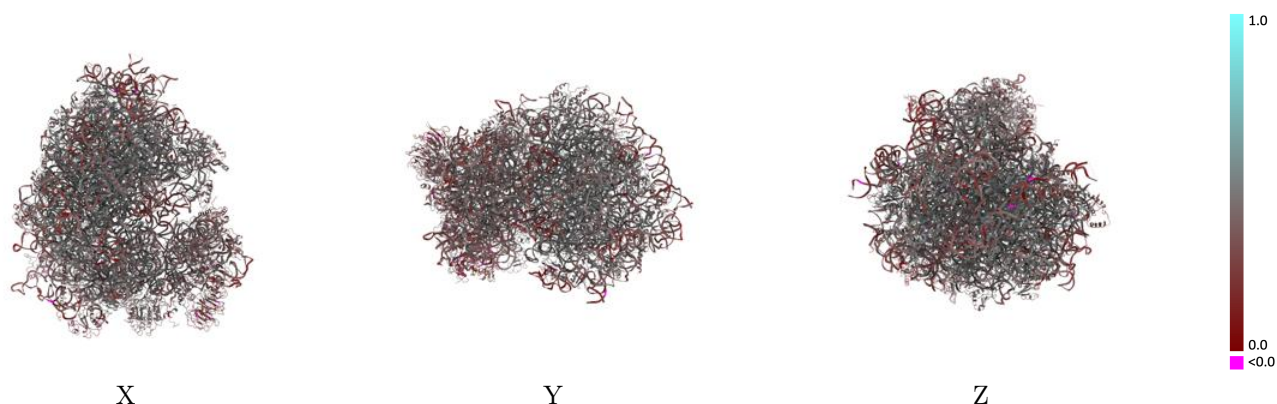
Y



Z

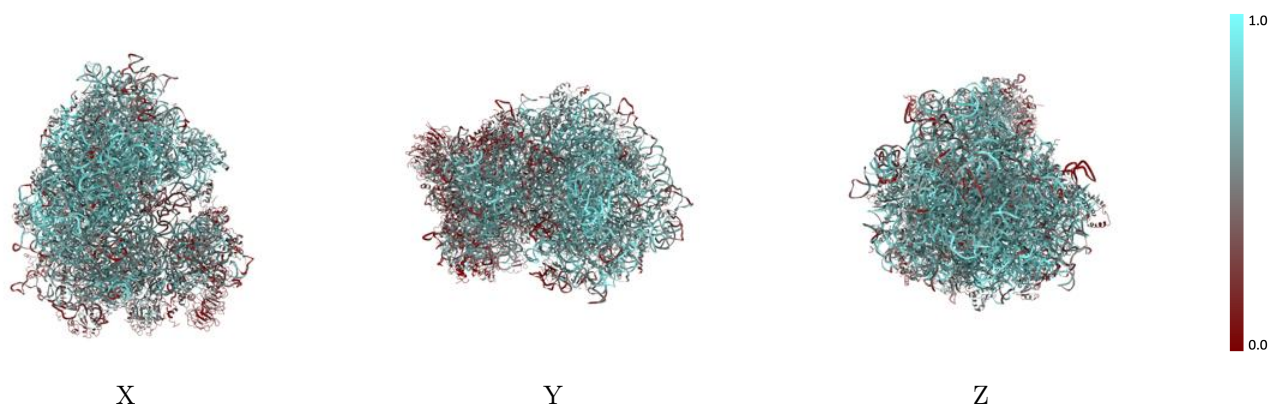
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



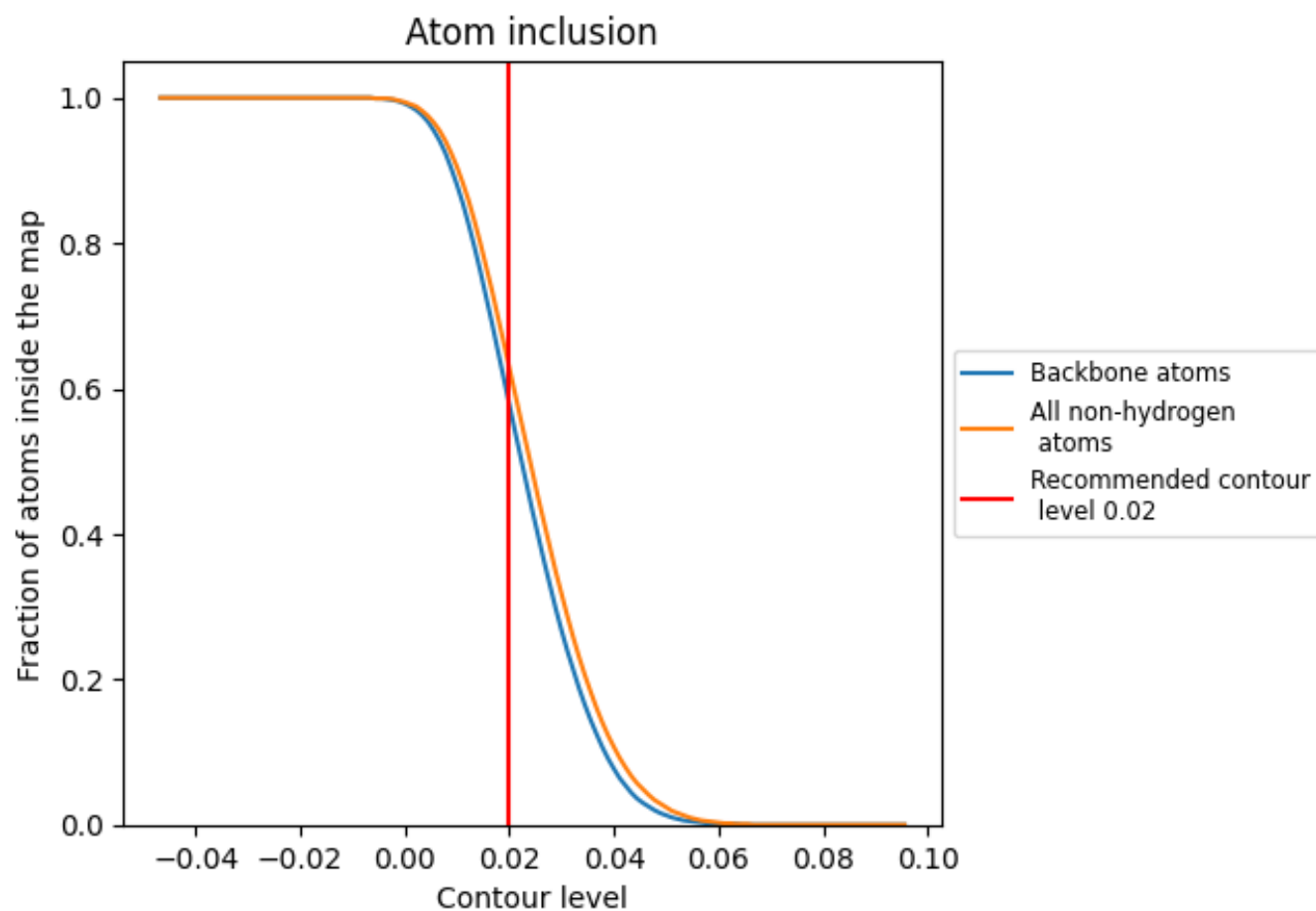
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.6280	 0.4070
A	 0.6380	 0.4810
B	 0.6080	 0.4550
C	 0.6370	 0.4590
D	 0.7640	 0.4230
E	 0.8510	 0.4420
F	 0.5970	 0.4180
G	 0.5380	 0.4070
H	 0.6460	 0.4600
I	 0.5590	 0.4220
J	 0.5330	 0.4310
K	 0.6050	 0.4520
L	 0.5520	 0.4140
M	 0.5970	 0.4250
N	 0.6120	 0.4410
O	 0.6910	 0.4830
P	 0.6420	 0.4600
Q	 0.6500	 0.4620
R	 0.6260	 0.4660
S	 0.5680	 0.4280
S2	 0.6710	 0.3900
SA	 0.4590	 0.4080
SB	 0.4140	 0.3990
SC	 0.5060	 0.4180
SD	 0.3400	 0.3550
SE	 0.4150	 0.3680
SF	 0.3310	 0.3550
SG	 0.3350	 0.3370
SH	 0.3600	 0.3410
SI	 0.4260	 0.3780
SJ	 0.4290	 0.3710
SK	 0.3130	 0.3370
SL	 0.4600	 0.3950
SM	 0.1020	 0.2340
SN	 0.5070	 0.4250



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Chain	Atom inclusion	Q-score
SO	 0.4350	 0.4040
SP	 0.4300	 0.3590
SQ	 0.3810	 0.3640
SR	 0.3360	 0.3670
SS	 0.3860	 0.3620
ST	 0.3960	 0.3630
SU	 0.3390	 0.3470
SV	 0.4780	 0.3850
SW	 0.5470	 0.4430
SX	 0.5070	 0.4150
SY	 0.4090	 0.3570
SZ	 0.2830	 0.3230
Sa	 0.5310	 0.4160
Sb	 0.3840	 0.3790
Sc	 0.2720	 0.3370
Sd	 0.5350	 0.4090
Se	 0.3750	 0.3740
Sf	 0.1440	 0.2410
Sg	 0.2310	 0.3030
T	 0.6180	 0.4550
U	 0.6070	 0.4540
V	 0.5380	 0.3890
W	 0.5790	 0.4650
X	 0.3400	 0.3120
Y	 0.6050	 0.4440
Z	 0.6170	 0.4420
a	 0.5960	 0.4350
b	 0.6670	 0.4700
c	 0.5580	 0.4300
d	 0.5620	 0.4200
e	 0.5940	 0.4400
f	 0.6510	 0.4670
g	 0.6890	 0.4790
h	 0.6100	 0.4630
i	 0.5890	 0.4170
j	 0.5840	 0.4220
k	 0.7280	 0.4870
l	 0.4880	 0.3950
m	 0.6150	 0.4560
n	 0.6020	 0.4420
o	 0.5570	 0.4410
p	 0.5440	 0.4490

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Chain	Atom inclusion	Q-score
q	 0.6270	 0.4670
r	 0.6620	 0.4560
t	 0.7560	 0.4140
u	 0.3390	 0.2500
v	 0.4060	 0.3060
w	 0.5920	 0.4150
y	 0.1150	 0.2570