



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 07:26 AM EDT

PDB ID : 6OM0 / pdb_00006om0
EMDB ID : EMD-0596
Title : Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like molecule with AP and PE tRNAs
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-17
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

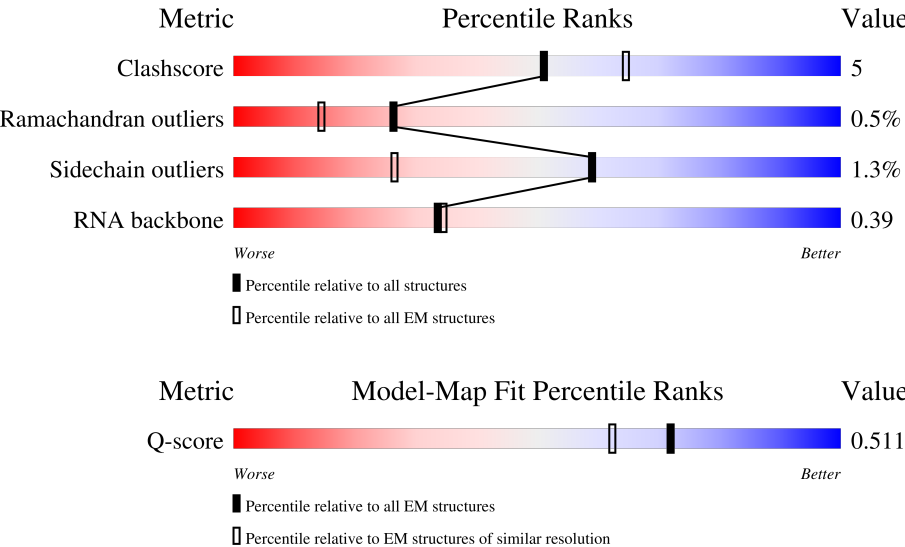
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14000 (2.58 - 3.58)

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	9% 57% 35% 7%
2	SA	221	13% 72% 26%
3	SB	214	5% 84% 15%

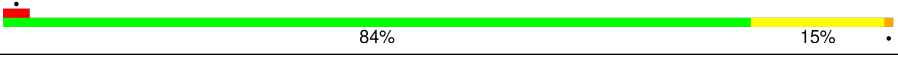
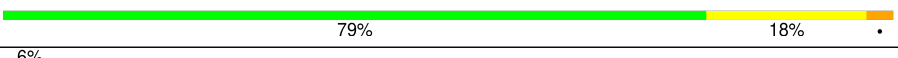
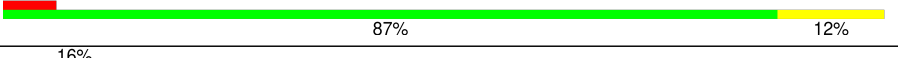
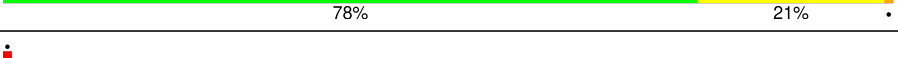
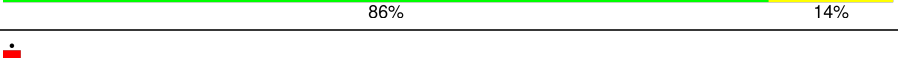
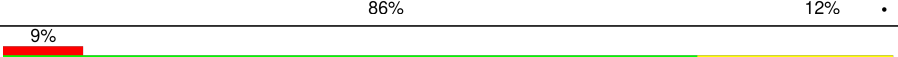
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Mol	Chain	Length	Quality of chain
4	SD	226	
5	SE	259	
6	SF	189	
7	SH	189	
8	SI	204	
9	SK	98	
10	SL	153	
11	SP	127	
12	SQ	146	
13	SR	134	
14	SS	145	
15	ST	143	
16	SU	104	
17	SV	82	
18	SX	141	
19	Sa	102	
20	Sc	64	
21	Sd	55	
22	Sg	312	
23	SC	220	
24	SG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

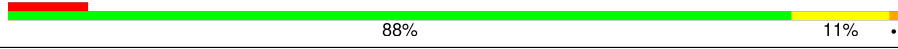
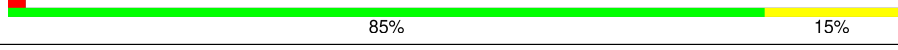
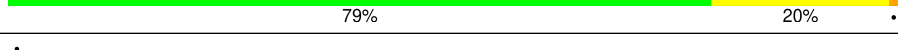
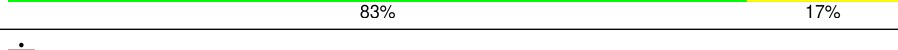
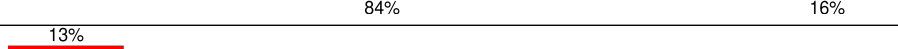
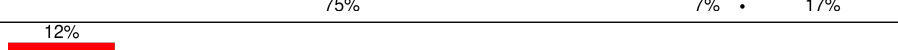
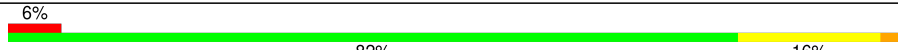
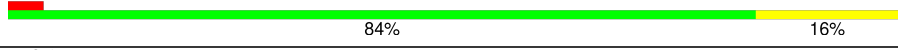
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Mol	Chain	Length	Quality of chain
29	SW	129	
30	SY	131	
31	SZ	73	
32	Sb	82	
33	Se	57	
34	Sf	67	
35	A	252	
36	B	397	
37	C	363	
38	D	157	
39	E	119	
40	F	294	
41	G	247	
42	H	225	
43	I	234	
44	J	191	
45	K	211	
46	L	169	
47	M	205	
48	N	139	
49	O	203	
50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

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Mol	Chain	Length	Quality of chain
79	t	3607	7% 65% 30% 5%
80	u	76	20% 51% 45%
81	v	76	11% 49% 37% 14%
82	w	10	60% 40%
83	y	26	15% 35% 88% 42% 8%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 214893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a RNA chain called tRNA.

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

- Molecule 81 is a RNA chain called tRNA.

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

- Molecule 82 is a RNA chain called mRNA.

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

- Molecule 83 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	y	26	Total	C	N	O	0	0
			204	138	32	34		

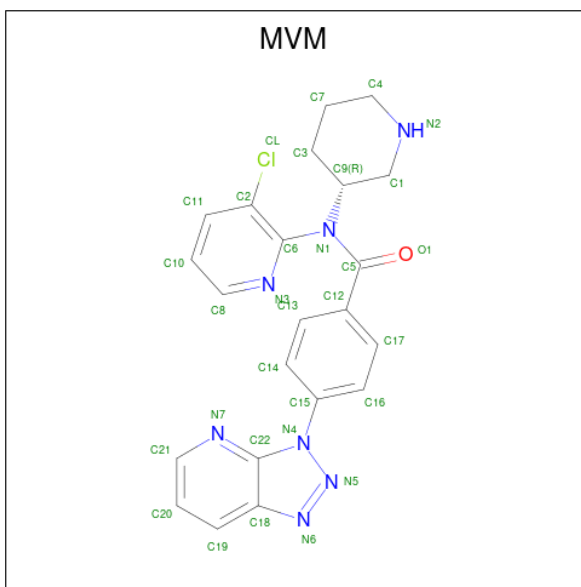
- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

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



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

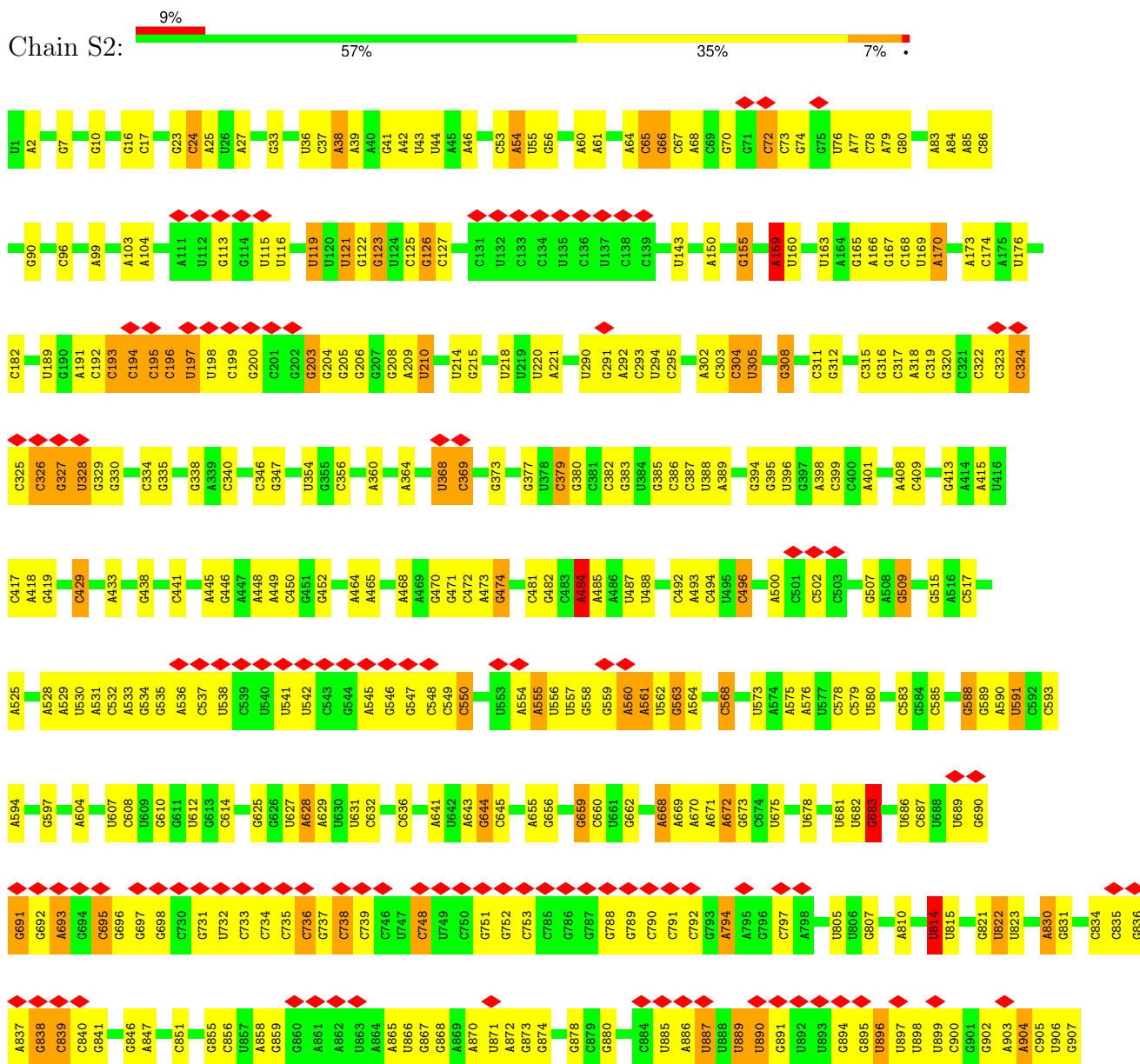
- Molecule 87 is water.

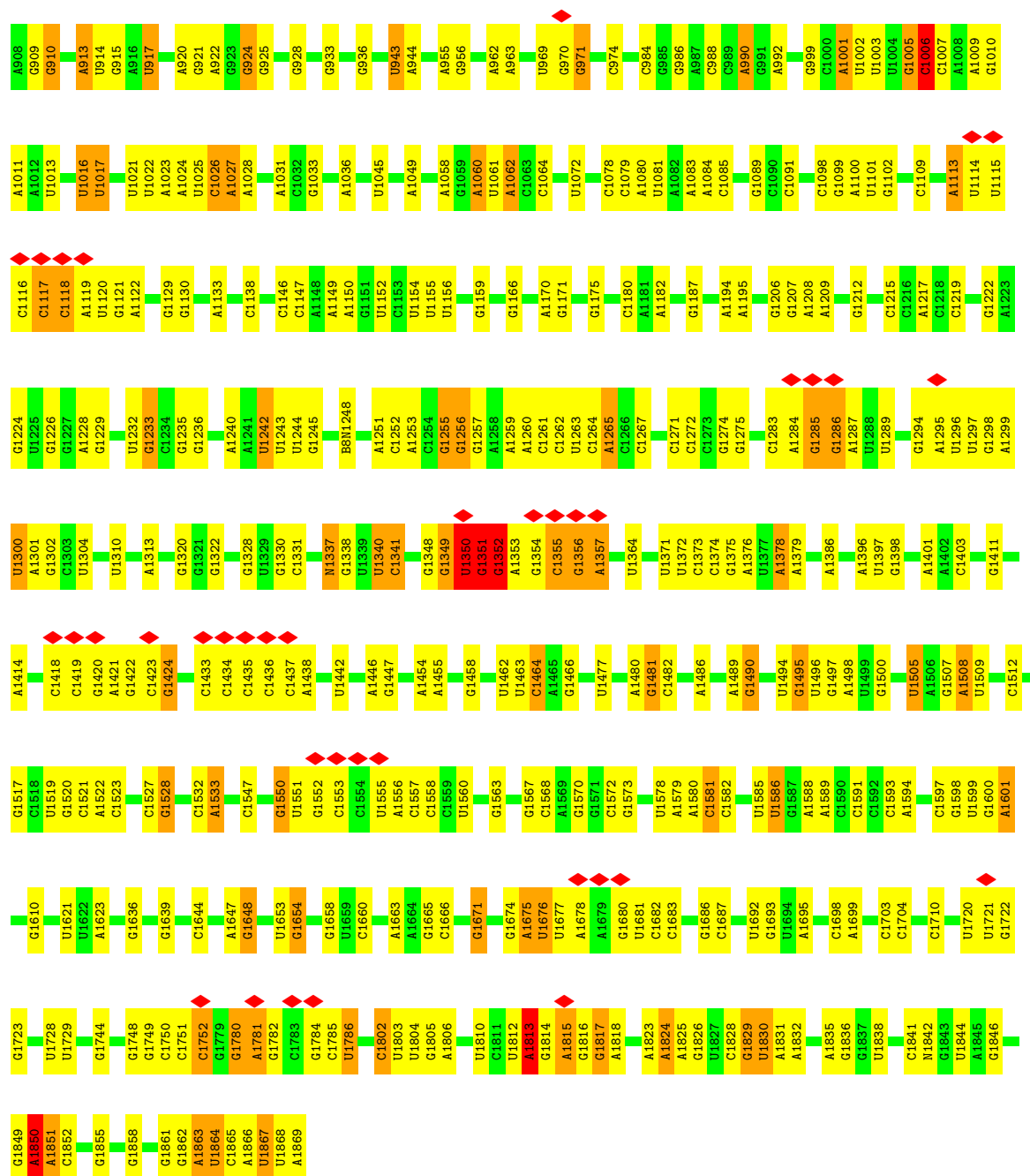
Mol	Chain	Residues	Atoms		AltConf
87	S2	6	Total	O	0
			6	6	
87	SA	1	Total	O	0
			1	1	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SS	1	Total	O	0
			1	1	
87	SC	1	Total	O	0
			1	1	
87	SN	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

3 Residue-property plots

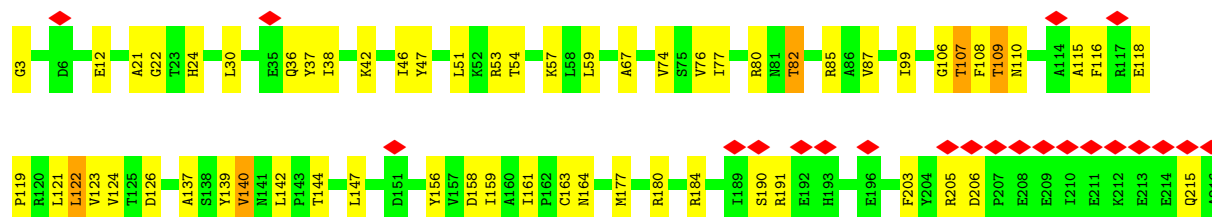
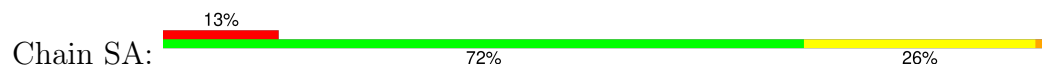
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



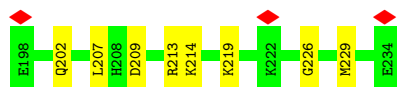
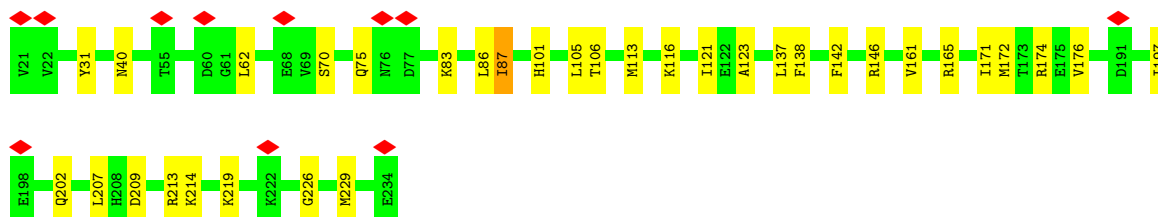
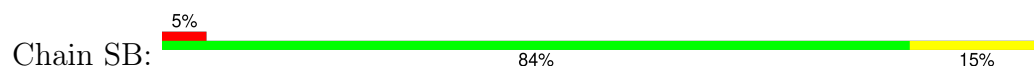


• Molecule 2: 40S ribosomal protein SA

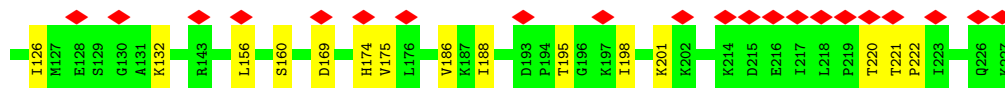
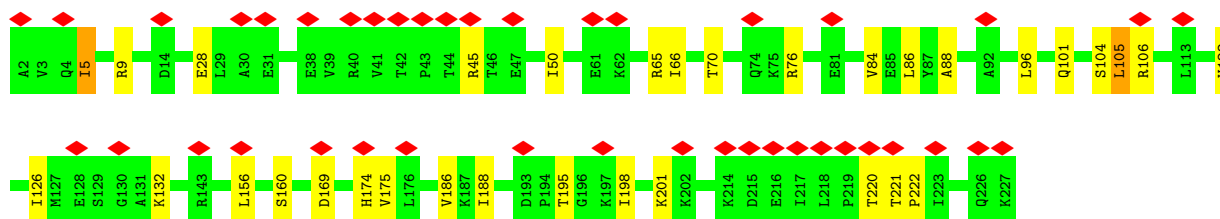
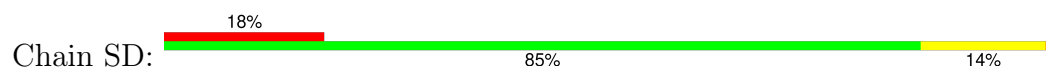




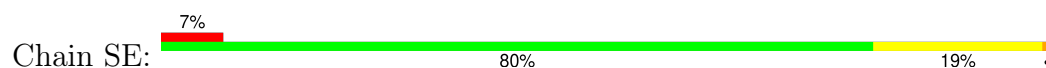
- Molecule 3: 40S ribosomal protein S3a



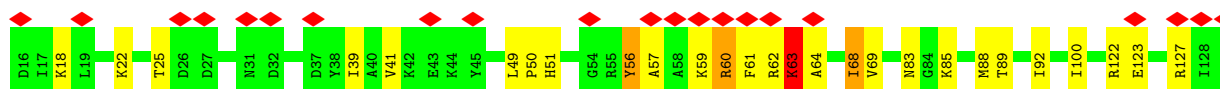
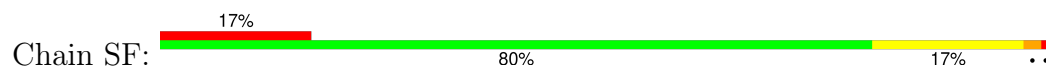
- Molecule 4: 40S ribosomal protein S3



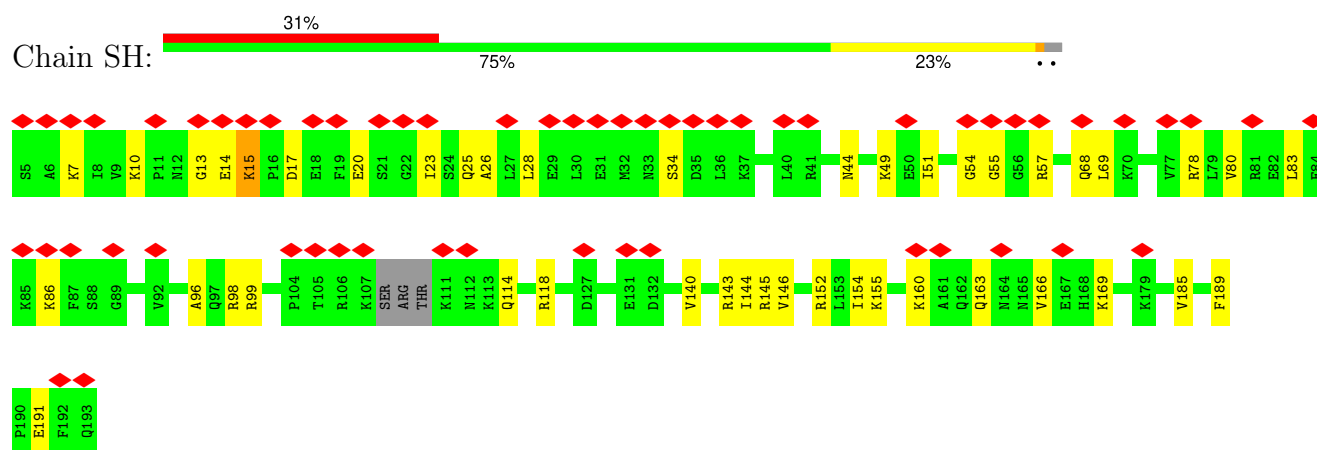
- Molecule 5: 40S ribosomal protein S4, X isoform



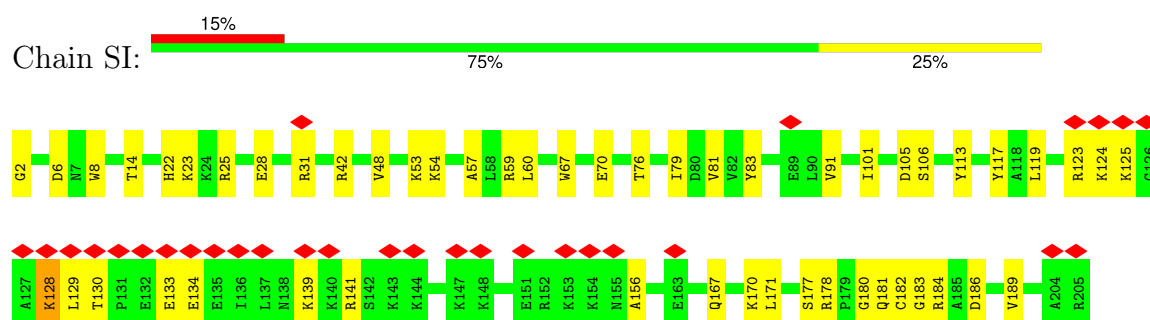
- Molecule 6: 40S ribosomal protein S5



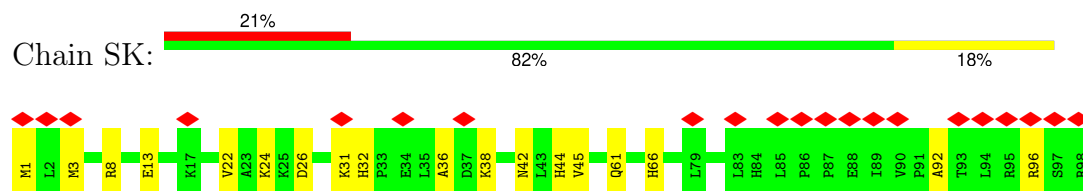
- Molecule 7: 40S ribosomal protein S7



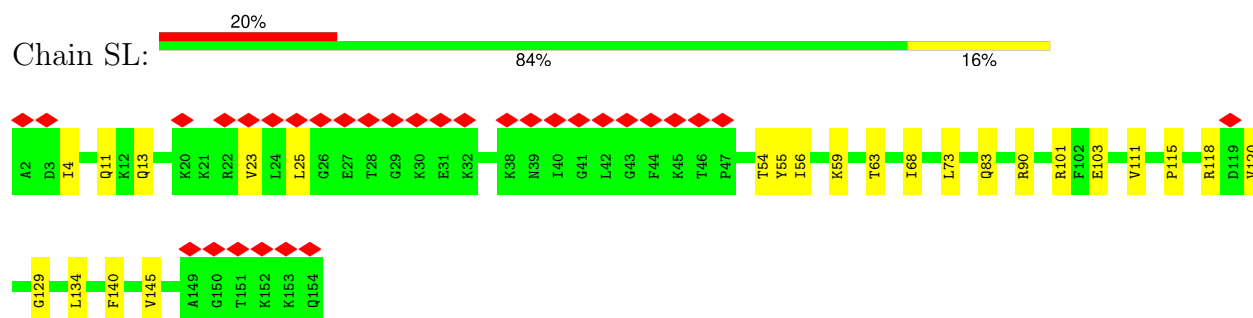
• Molecule 8: 40S ribosomal protein S8



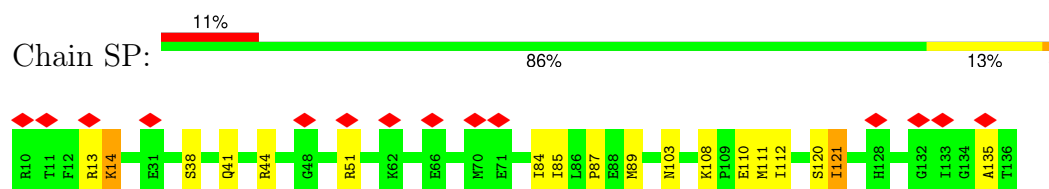
• Molecule 9: 40S ribosomal protein S10



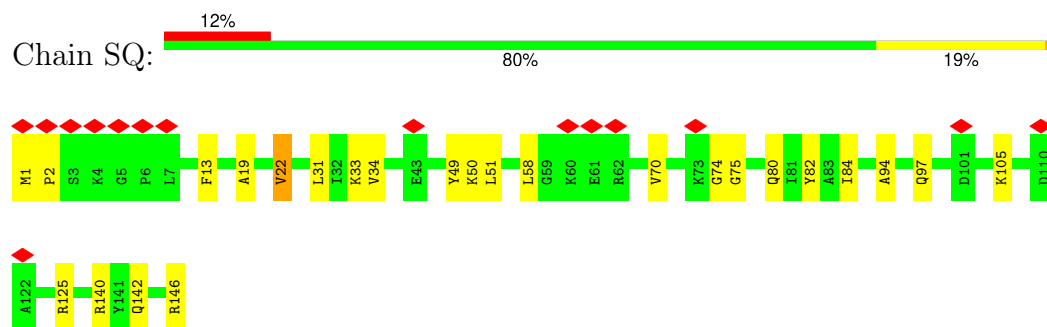
• Molecule 10: 40S ribosomal protein S11



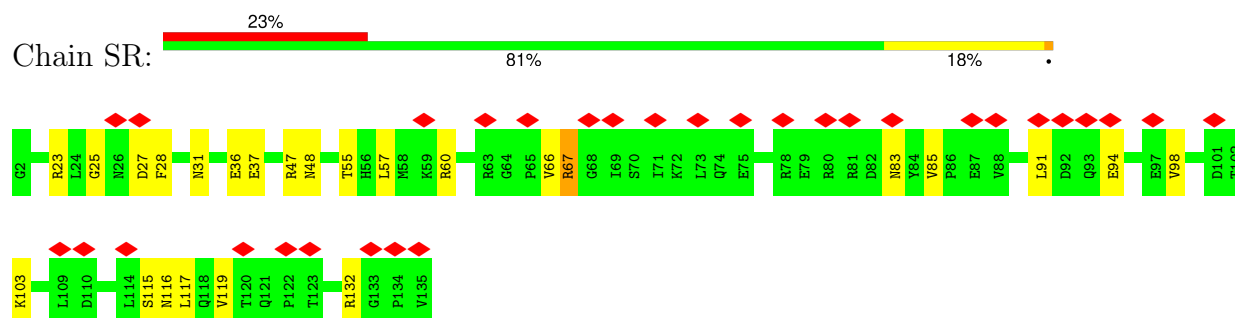
• Molecule 11: 40S ribosomal protein S15



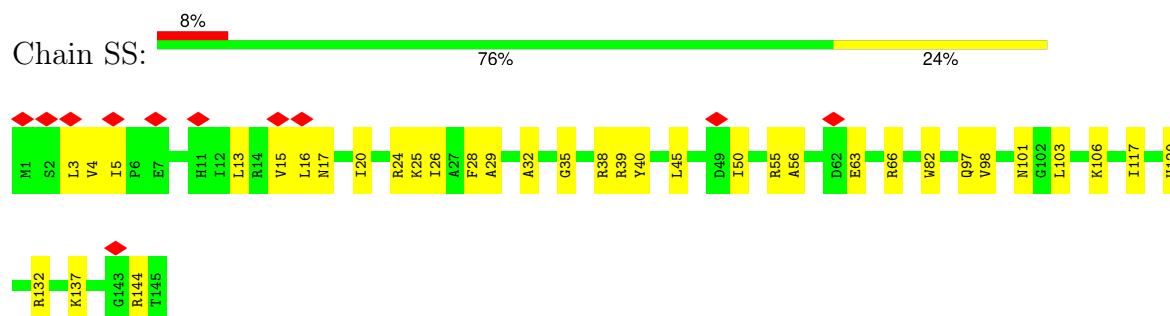
- Molecule 12: 40S ribosomal protein S16



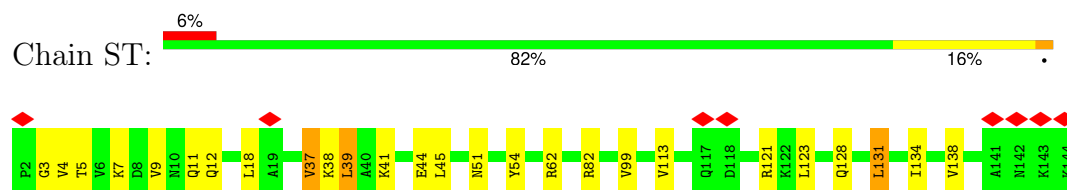
- Molecule 13: 40S ribosomal protein S17



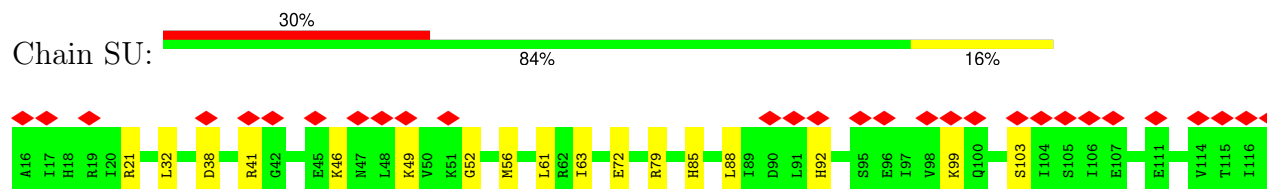
- Molecule 14: 40S ribosomal protein S18



- Molecule 15: 40S ribosomal protein S19

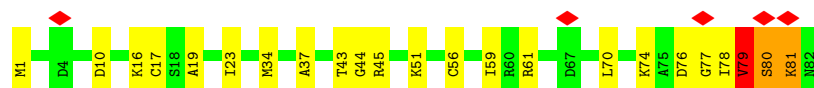
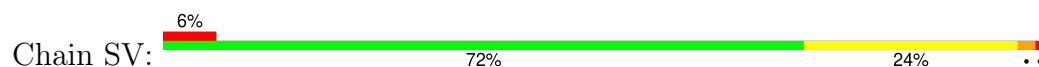


- Molecule 16: 40S ribosomal protein S20

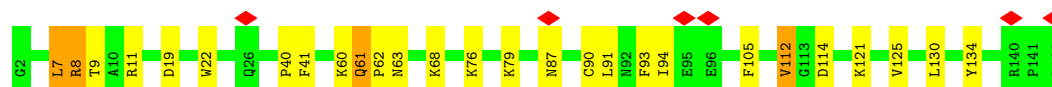
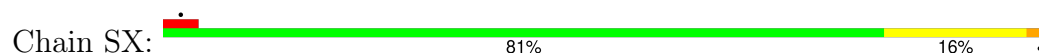




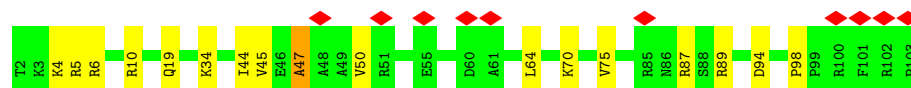
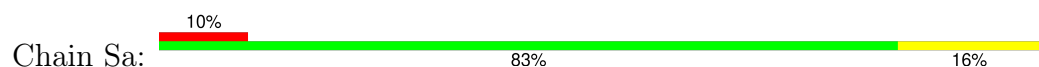
- Molecule 17: 40S ribosomal protein S21



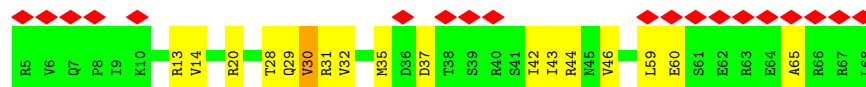
- Molecule 18: 40S ribosomal protein S23



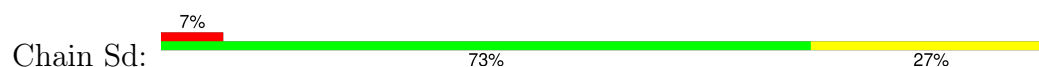
- Molecule 19: 40S ribosomal protein S26



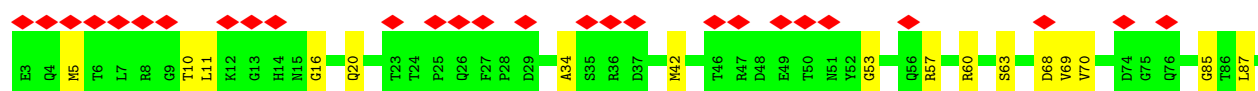
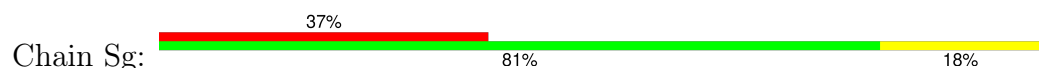
- Molecule 20: 40S ribosomal protein S28

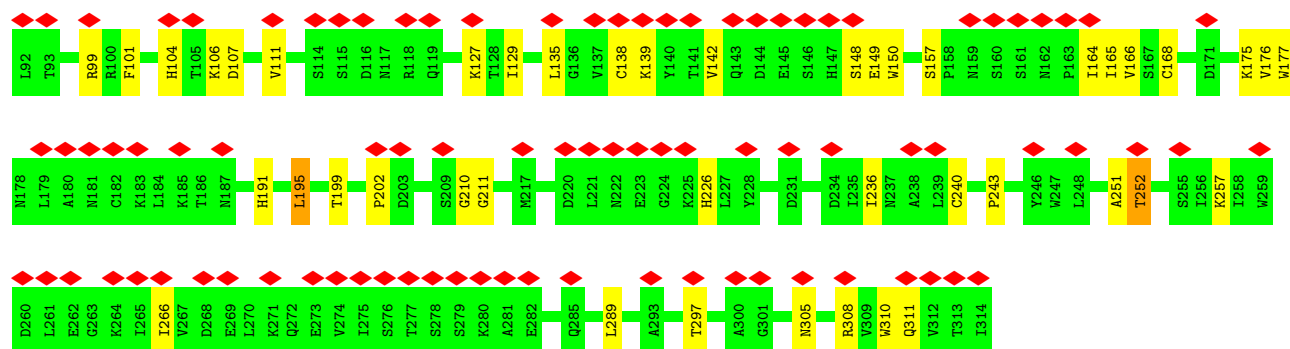


- Molecule 21: 40S ribosomal protein S29

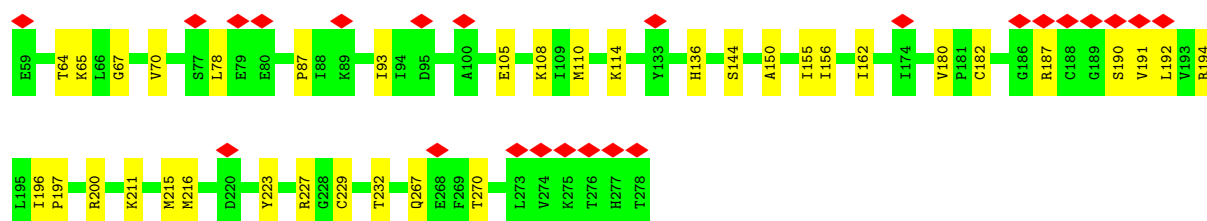
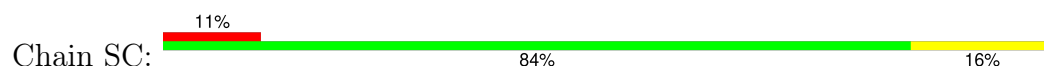


- Molecule 22: Receptor of activated protein C kinase 1

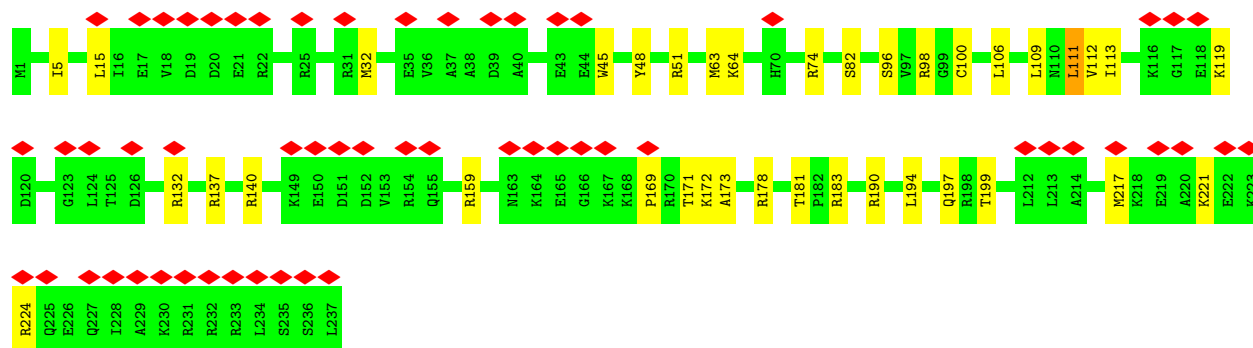
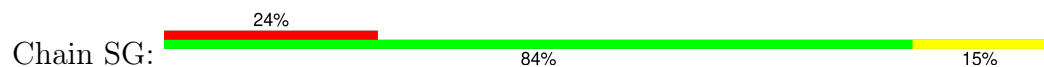




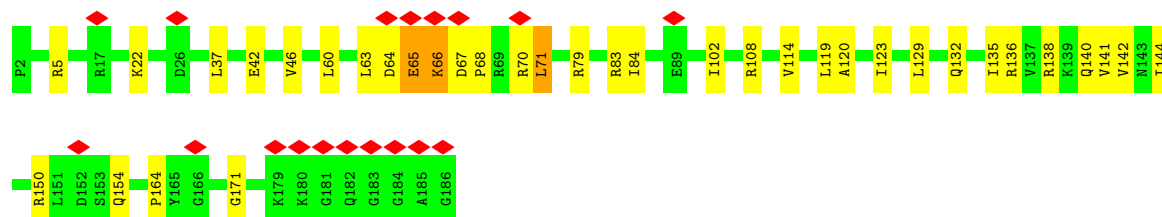
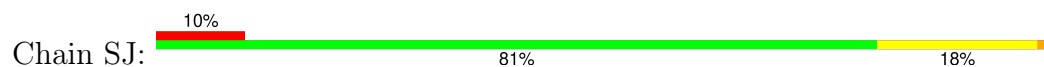
• Molecule 23: 40S ribosomal protein S2



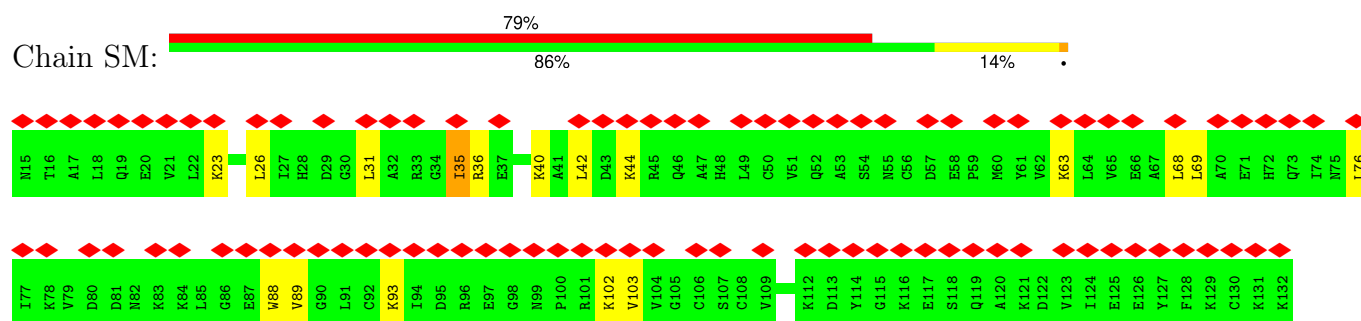
• Molecule 24: 40S ribosomal protein S6



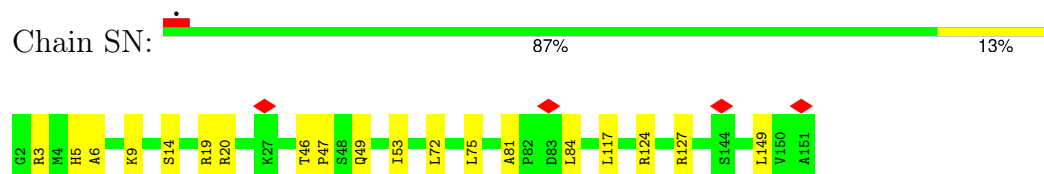
• Molecule 25: 40S ribosomal protein S9



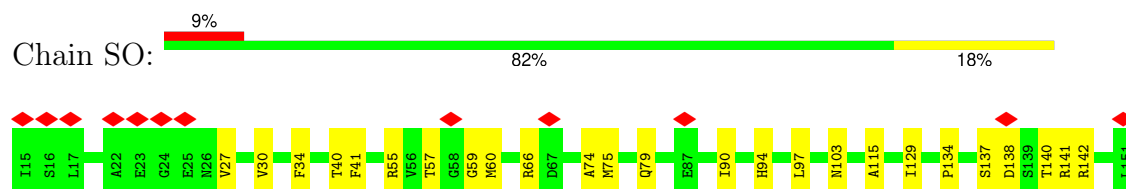
• Molecule 26: 40S ribosomal protein S12



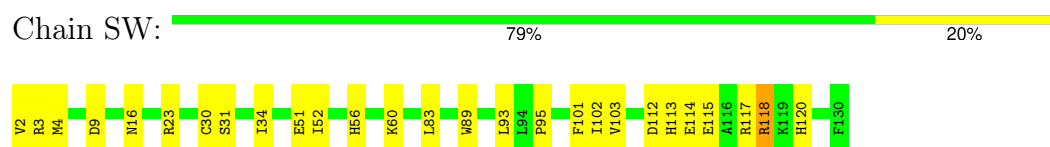
• Molecule 27: 40S ribosomal protein S13



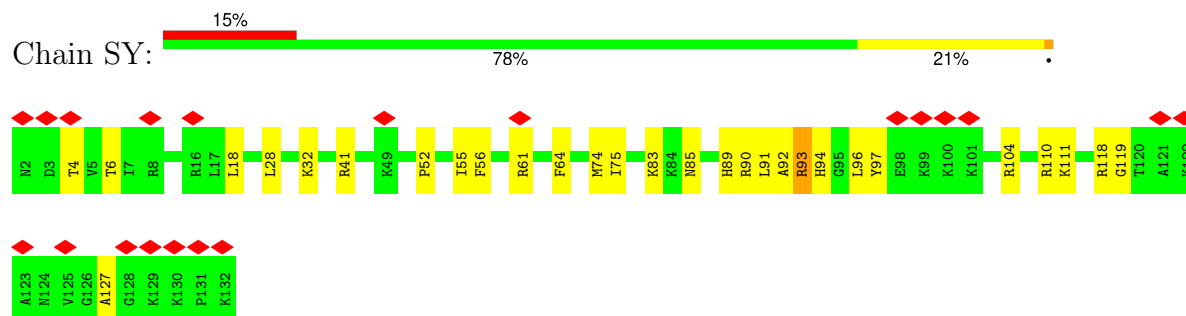
• Molecule 28: 40S ribosomal protein S14



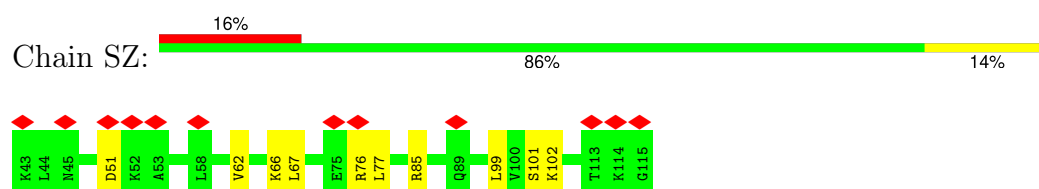
• Molecule 29: 40S ribosomal protein S15a



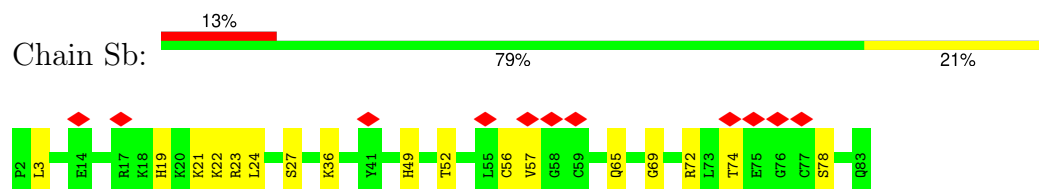
• Molecule 30: 40S ribosomal protein S24



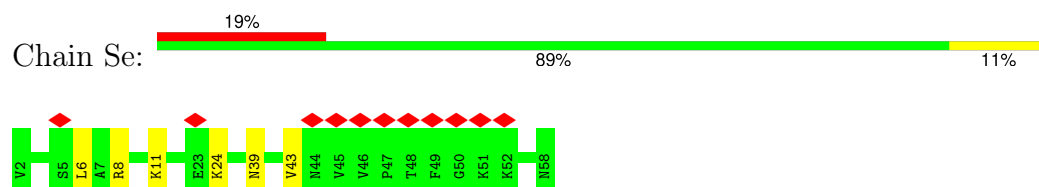
• Molecule 31: 40S ribosomal protein S25



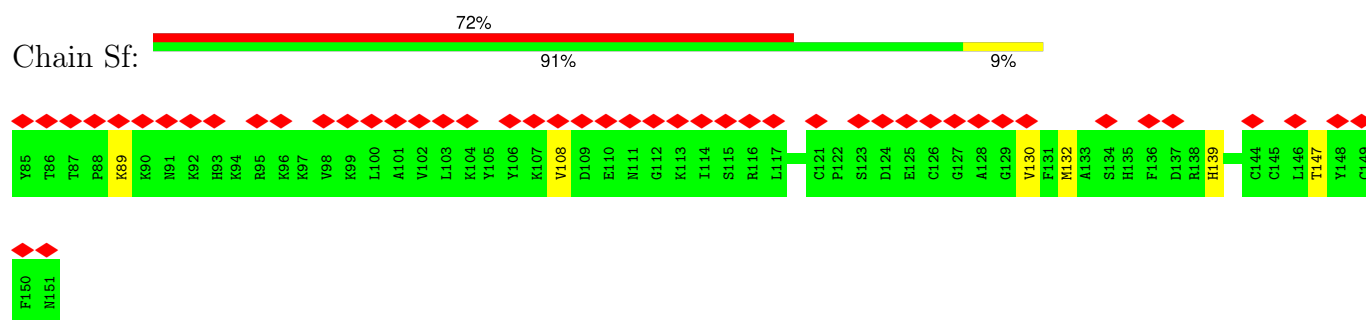
- Molecule 32: 40S ribosomal protein S27



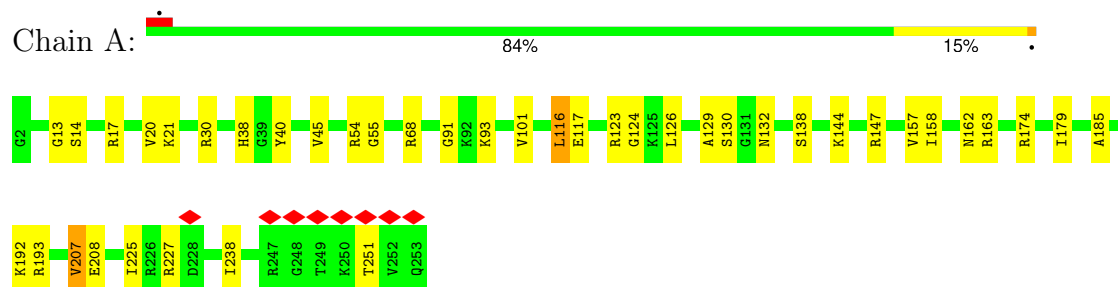
- Molecule 33: 40S ribosomal protein S30



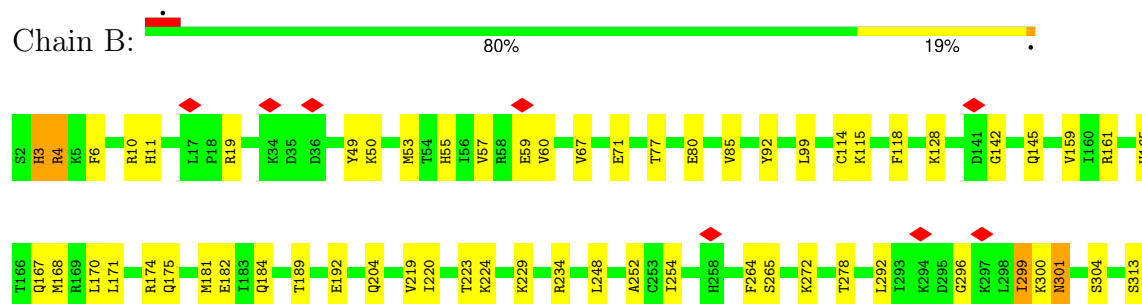
- Molecule 34: 40S ribosomal protein S27a

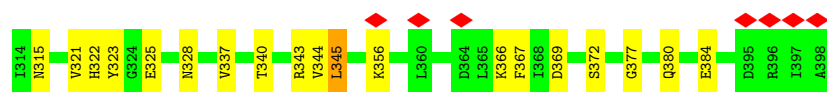


- Molecule 35: 60S ribosomal protein L8

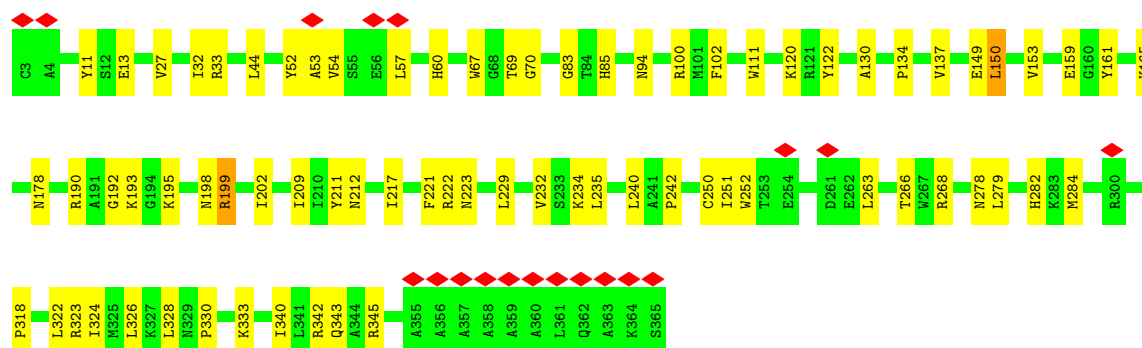
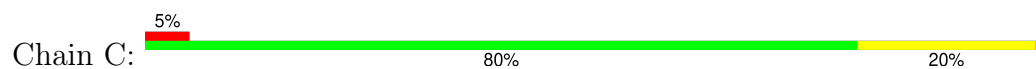


- Molecule 36: 60S ribosomal protein L3

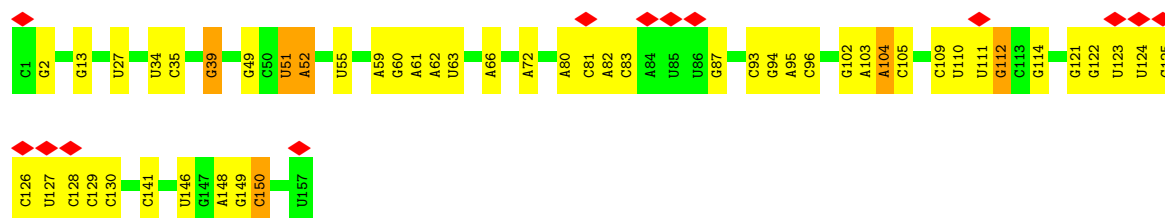




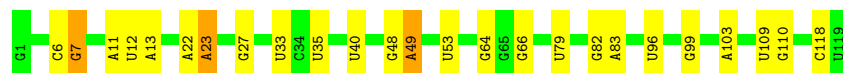
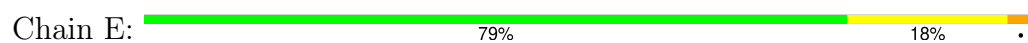
- Molecule 37: 60S ribosomal protein L4



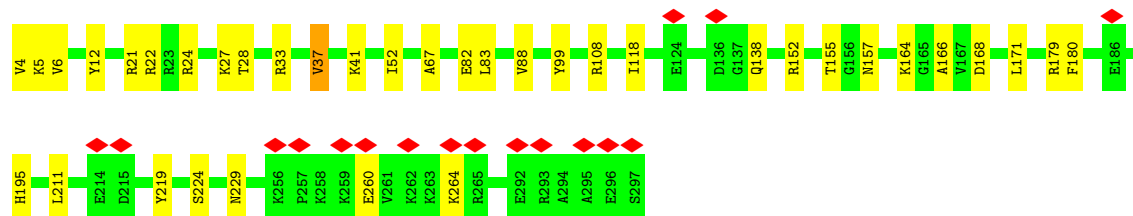
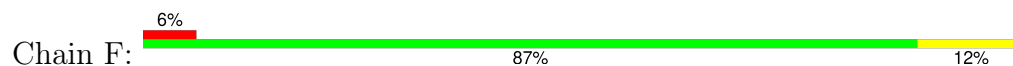
- Molecule 38: 5.8S ribosomal RNA



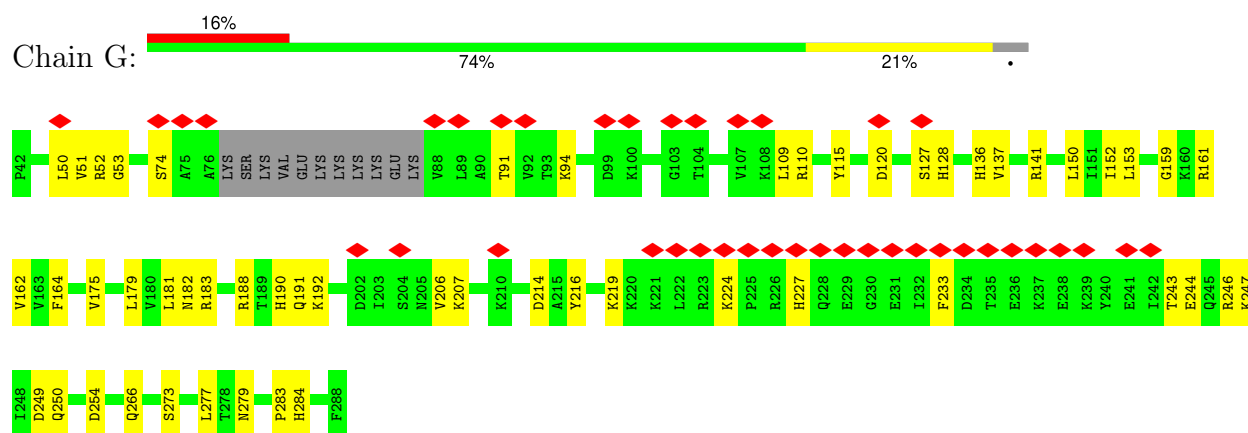
- Molecule 39: 5S ribosomal RNA



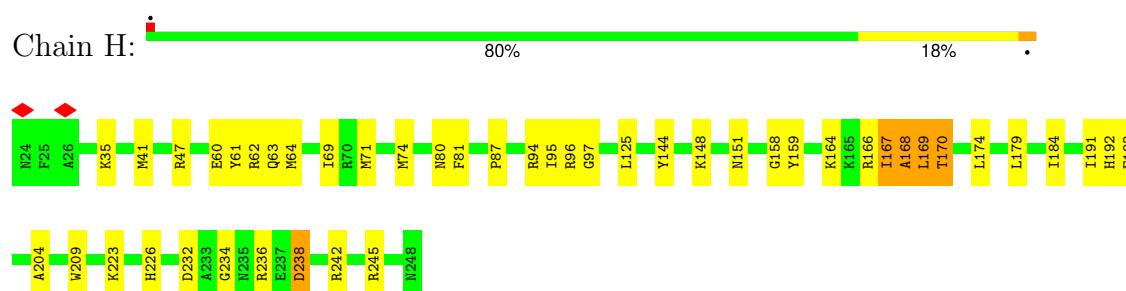
- Molecule 40: 60S ribosomal protein L5



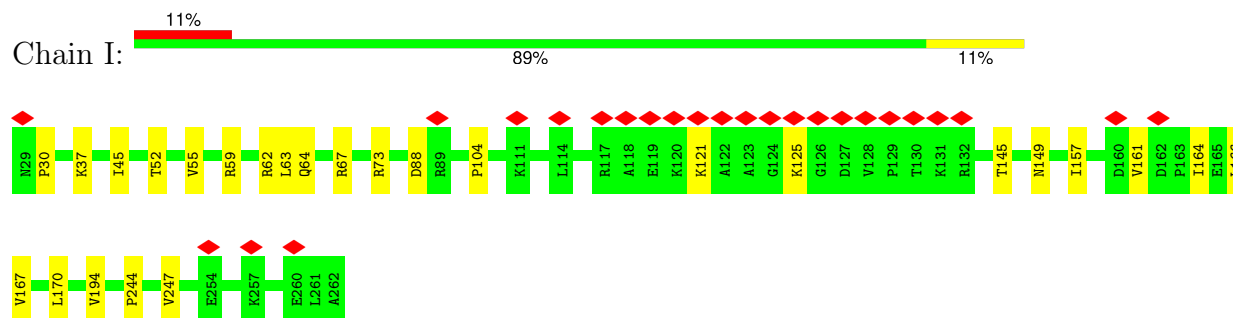
- Molecule 41: 60S ribosomal protein L6



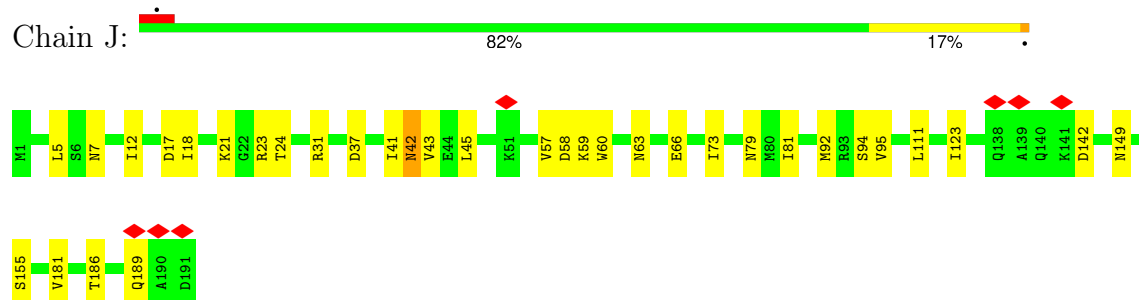
- Molecule 42: 60S ribosomal protein L7



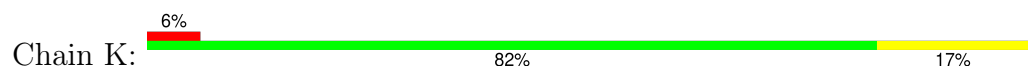
- Molecule 43: 60S ribosomal protein L7a

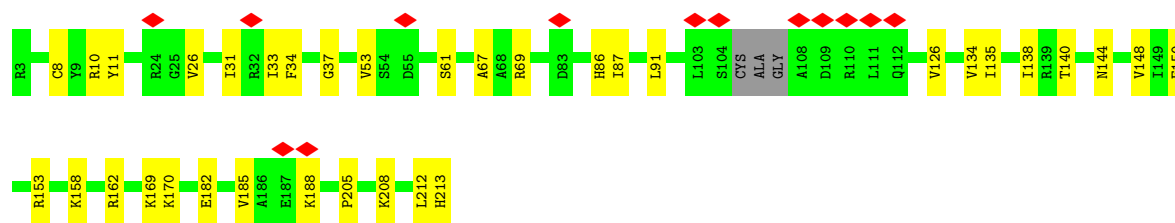


- Molecule 44: 60S ribosomal protein L9

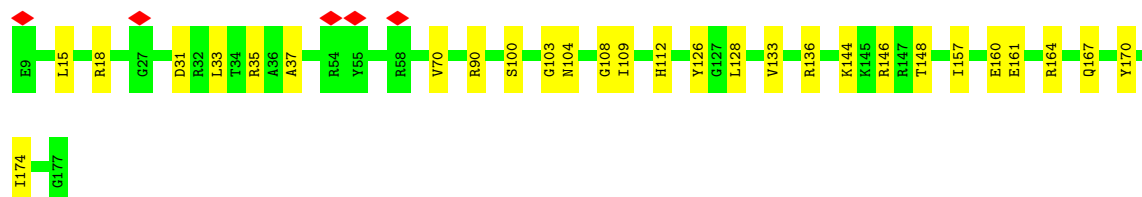
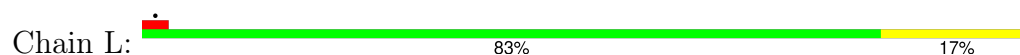


- Molecule 45: 60S ribosomal protein L10

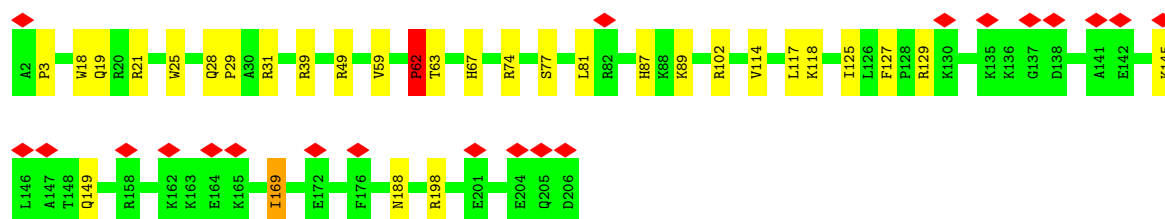
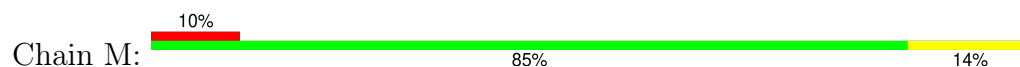




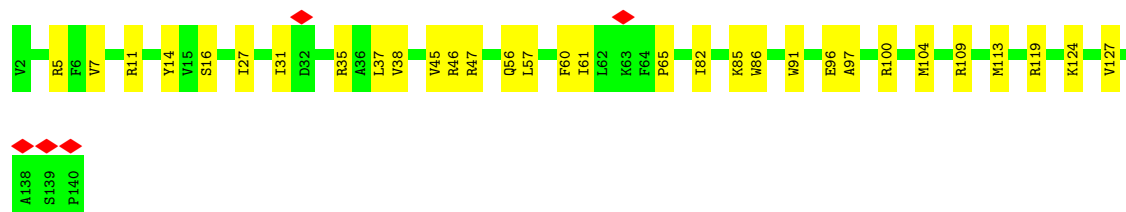
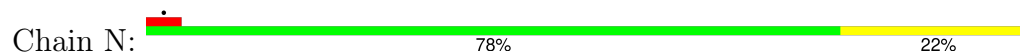
- Molecule 46: 60S ribosomal protein L11



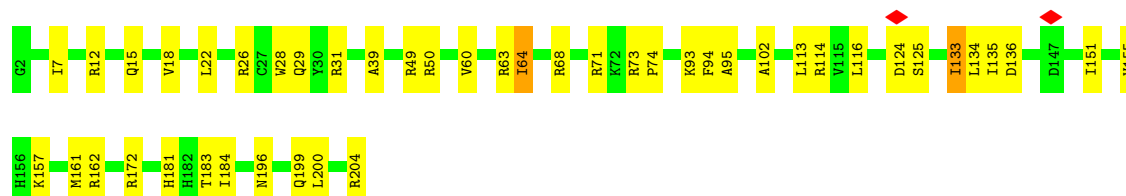
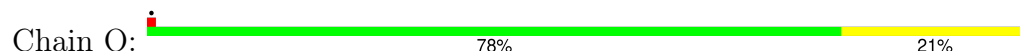
- Molecule 47: 60S ribosomal protein L13



- Molecule 48: 60S ribosomal protein L14

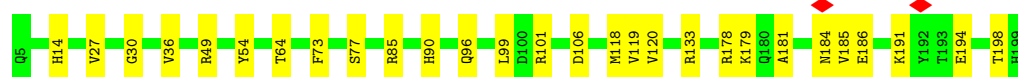


- Molecule 49: 60S ribosomal protein L15



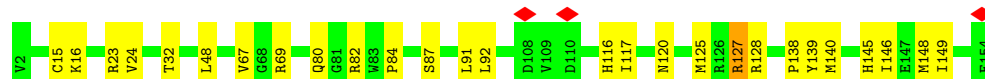
- Molecule 50: 60S ribosomal protein L13a

Chain P:  86% 14%



- Molecule 51: 60S ribosomal protein L17

Chain Q:  82% 17%



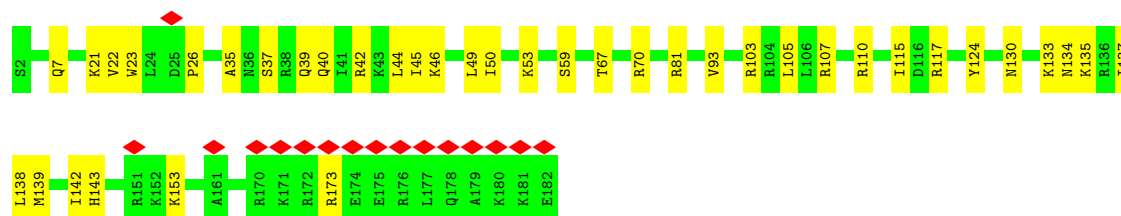
- Molecule 52: 60S ribosomal protein L18

Chain R:  86% 12%



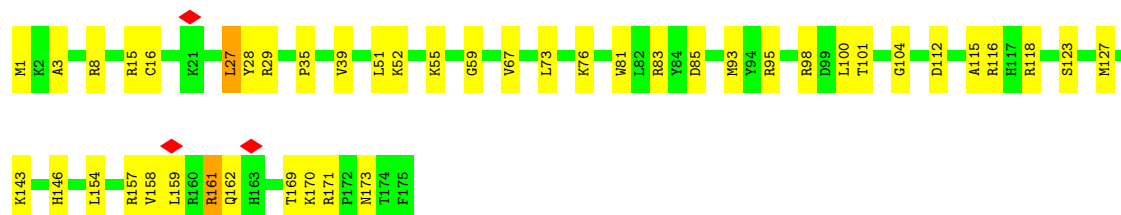
- Molecule 53: 60S ribosomal protein L19

Chain S:  9% 78% 22%



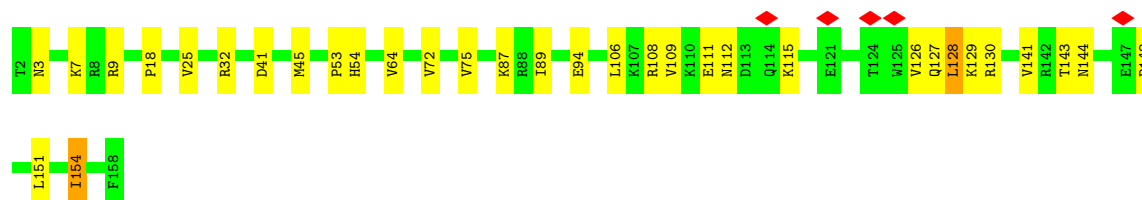
- Molecule 54: 60S ribosomal protein L18a

Chain T:  75% 24%

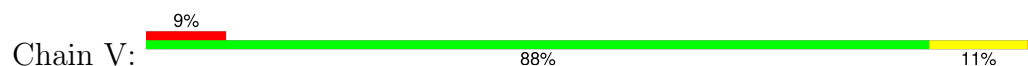


- Molecule 55: 60S ribosomal protein L21

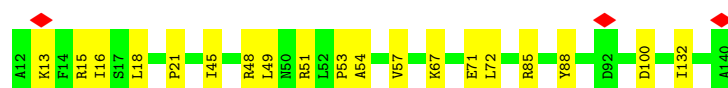
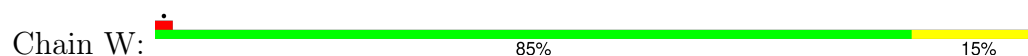
Chain U:  79% 20%



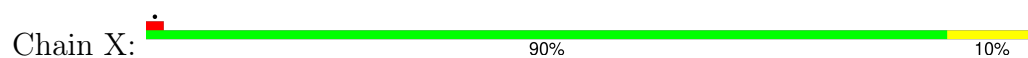
- Molecule 56: 60S ribosomal protein L22



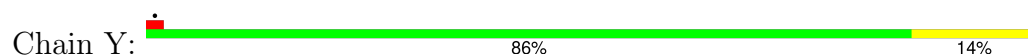
- Molecule 57: 60S ribosomal protein L23



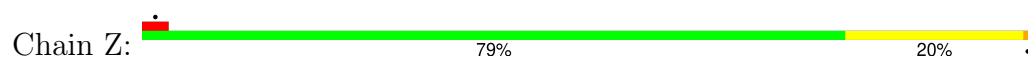
- Molecule 58: 60S ribosomal protein L24



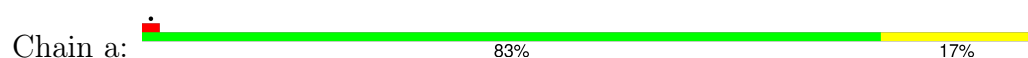
- Molecule 59: 60S ribosomal protein L23a



- Molecule 60: 60S ribosomal protein L26

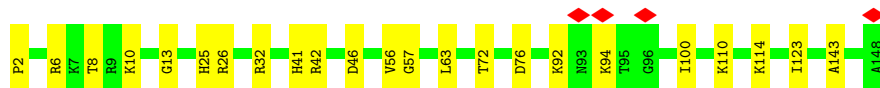
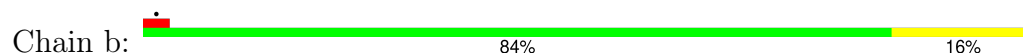


- Molecule 61: 60S ribosomal protein L27

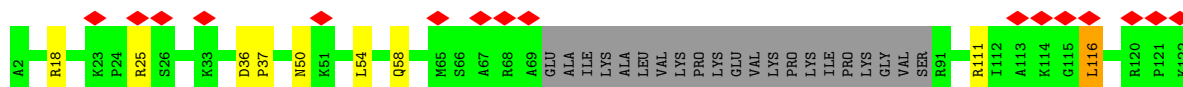




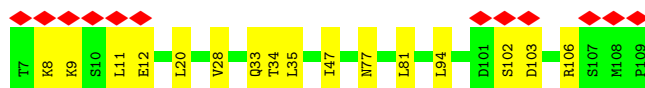
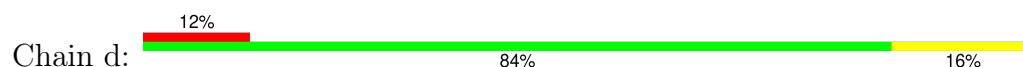
- Molecule 62: 60S ribosomal protein L27a



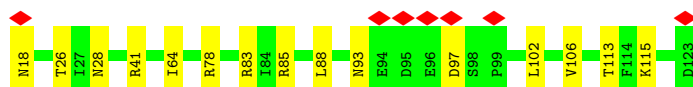
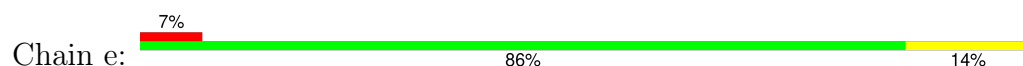
- Molecule 63: 60S ribosomal protein L29



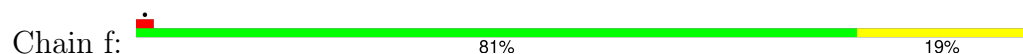
- Molecule 64: 60S ribosomal protein L30



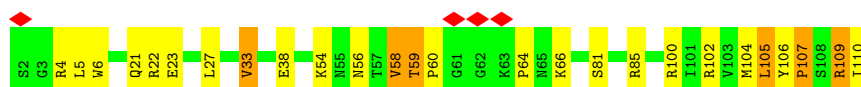
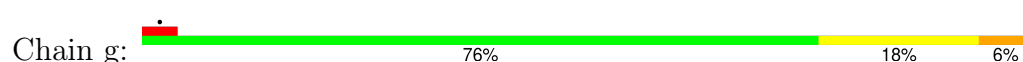
- Molecule 65: 60S ribosomal protein L31



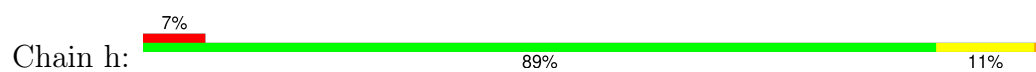
- Molecule 66: 60S ribosomal protein L32



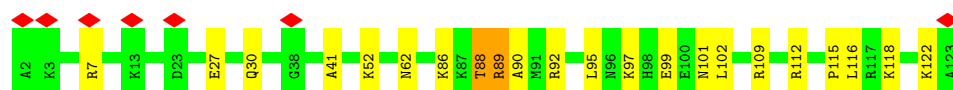
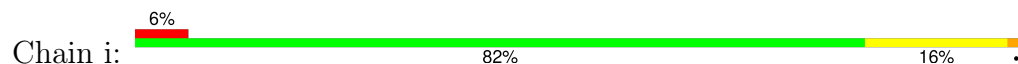
- Molecule 67: 60S ribosomal protein L35a



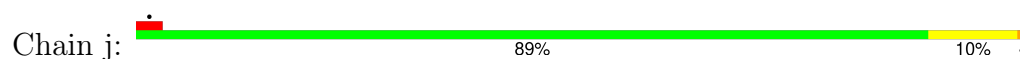
- Molecule 68: 60S ribosomal protein L34



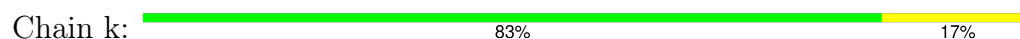
- Molecule 69: 60S ribosomal protein L35



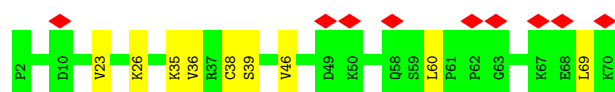
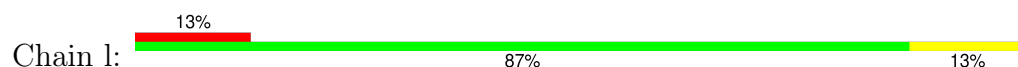
- Molecule 70: 60S ribosomal protein L36



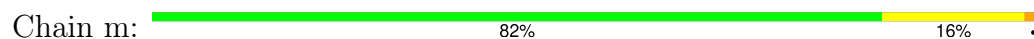
- Molecule 71: 60S ribosomal protein L37



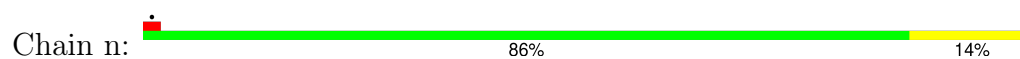
- Molecule 72: 60S ribosomal protein L38



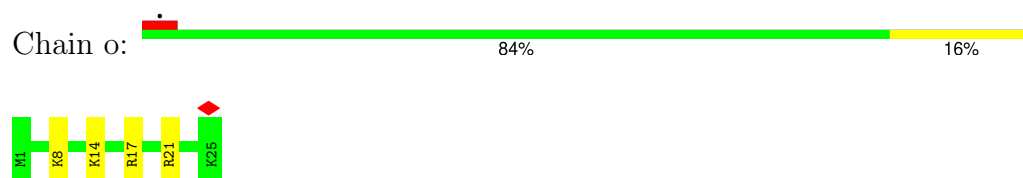
- Molecule 73: 60S ribosomal protein L39



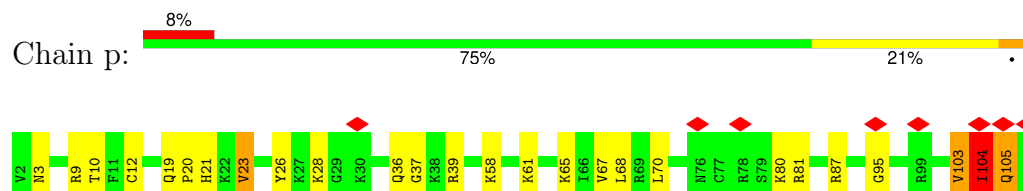
- Molecule 74: 60S ribosomal protein L40



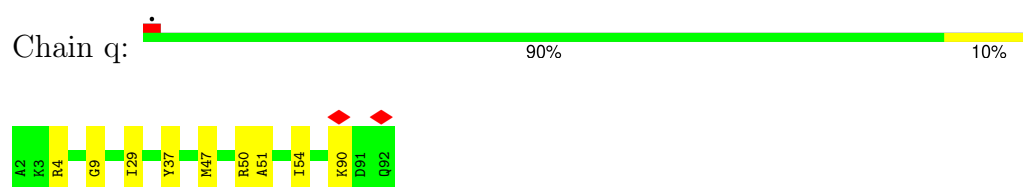
- Molecule 75: 60S ribosomal protein L41



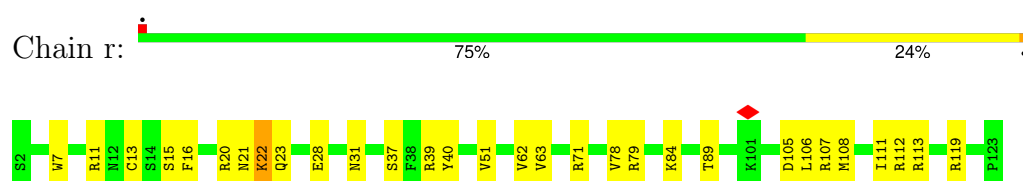
- Molecule 76: 60S ribosomal protein L36a



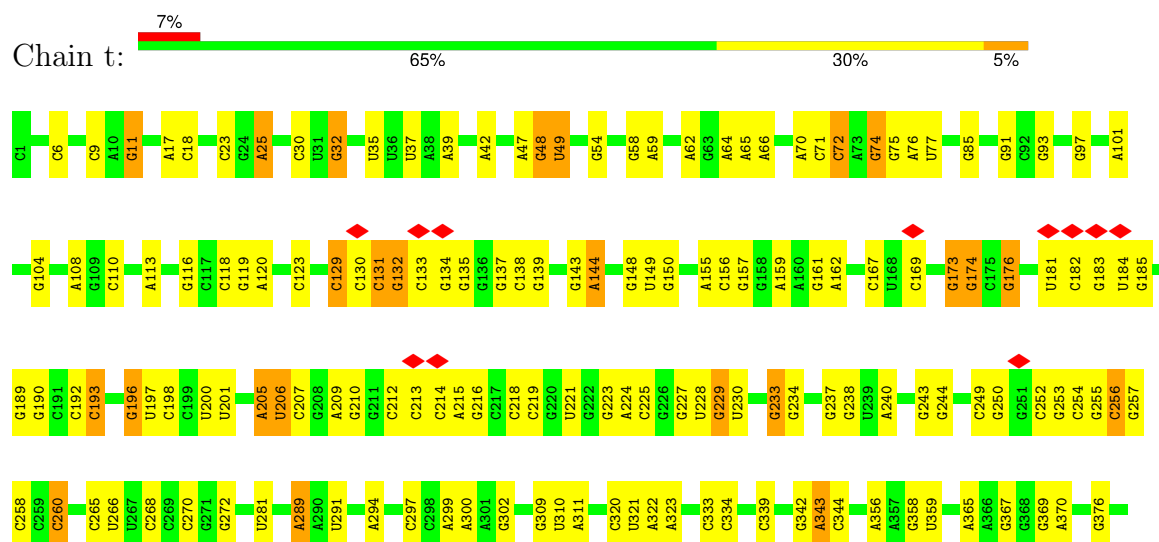
- Molecule 77: 60S ribosomal protein L37a

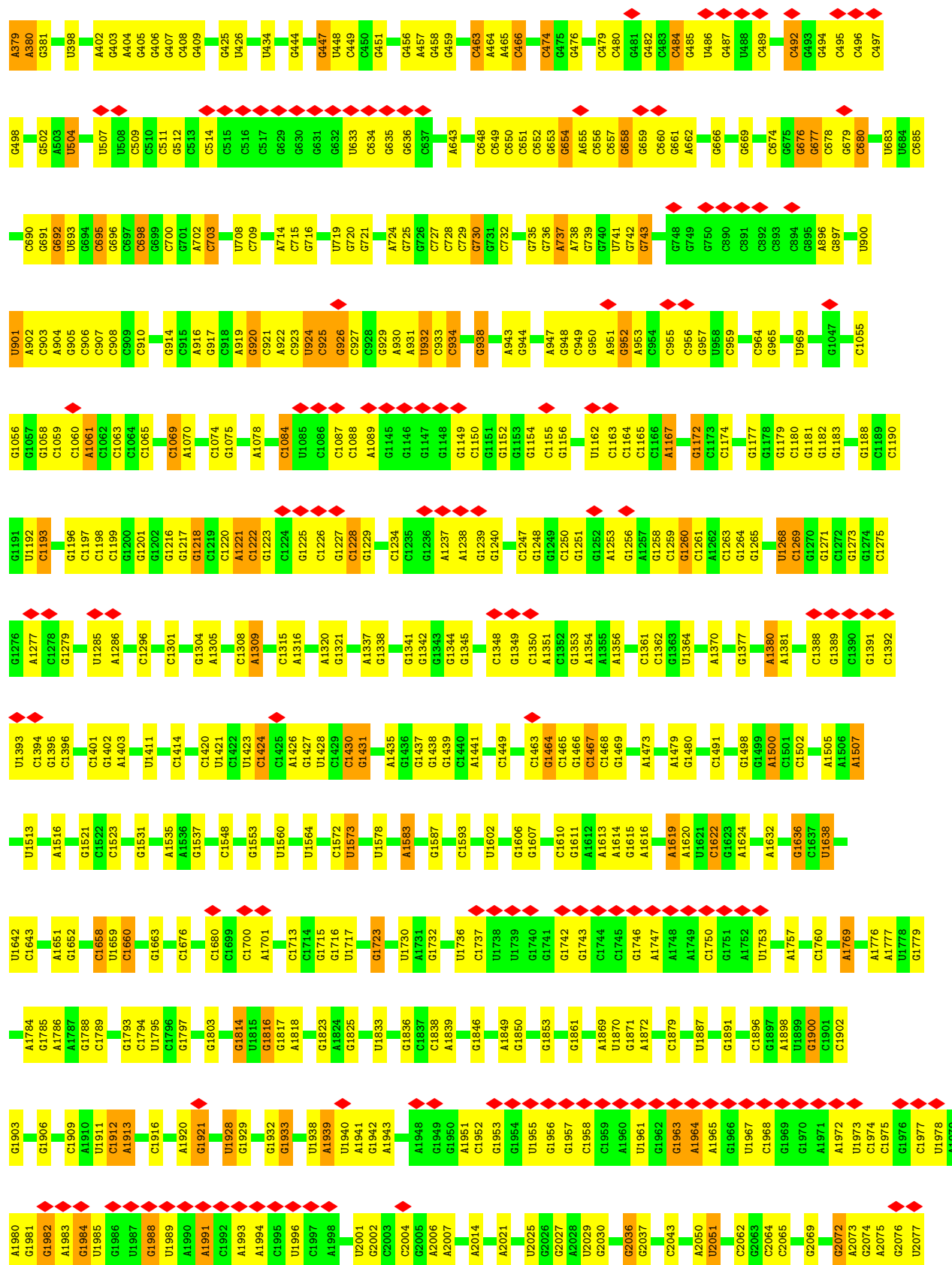


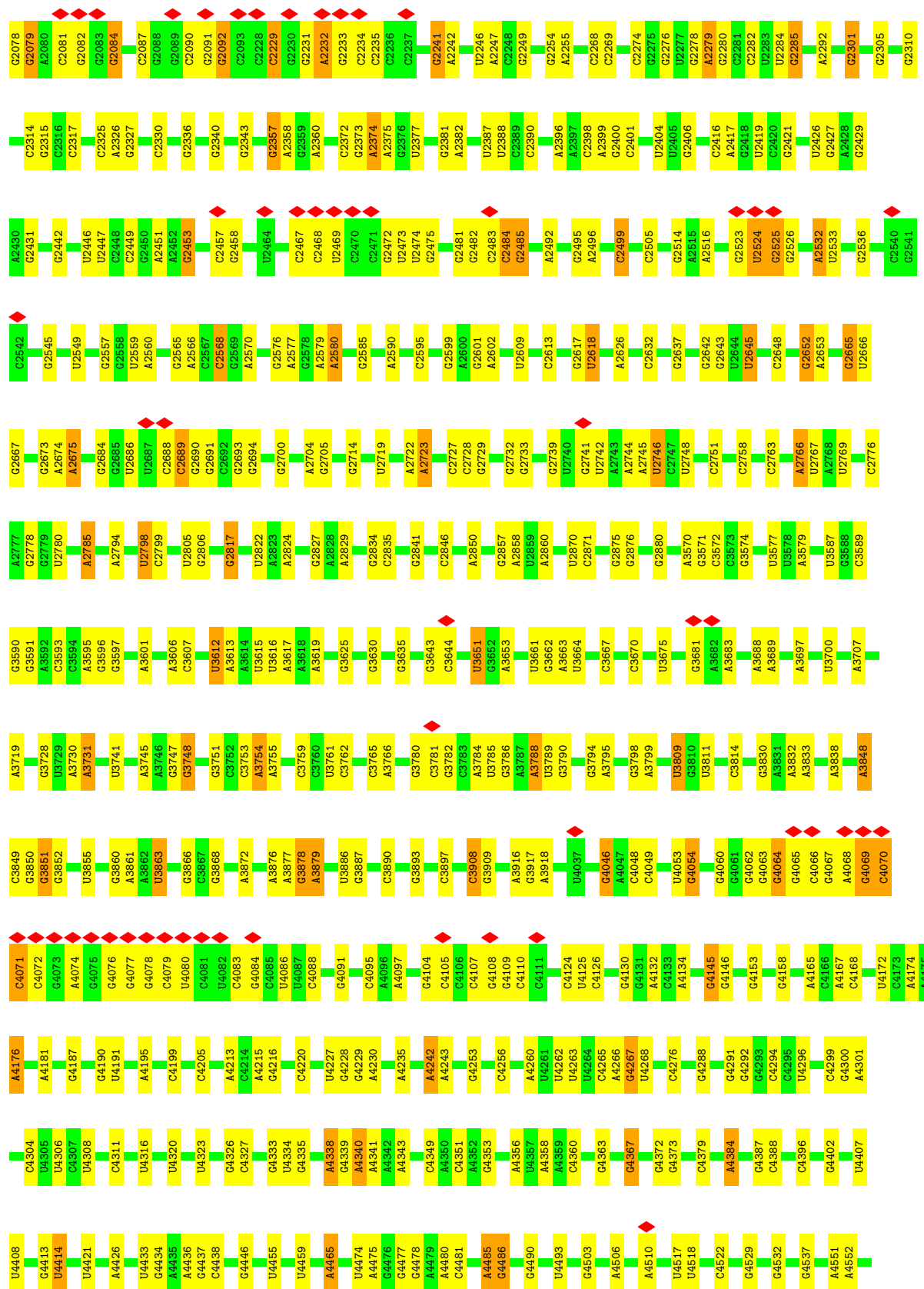
- Molecule 78: 60S ribosomal protein L28

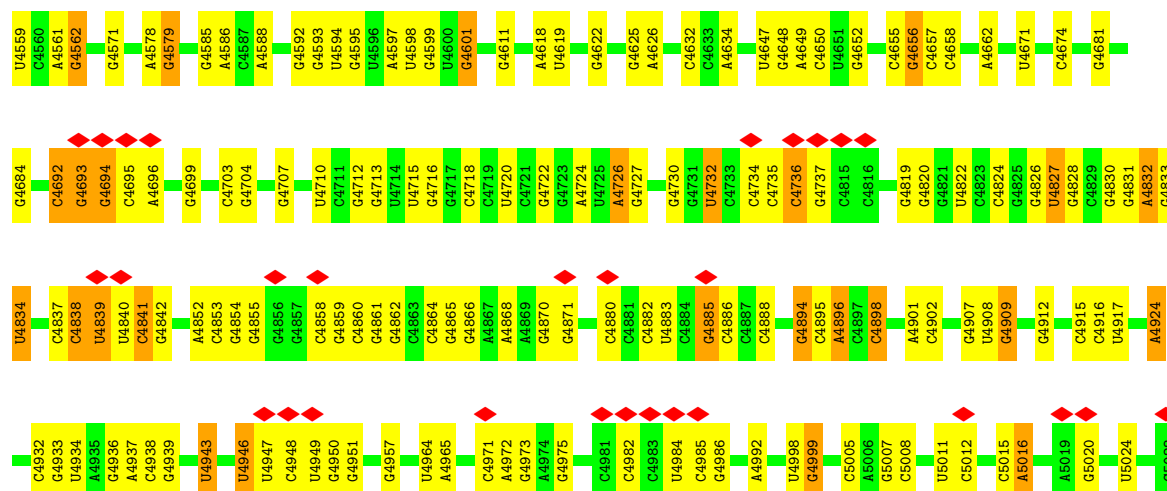


- Molecule 79: 28S ribosomal RNA

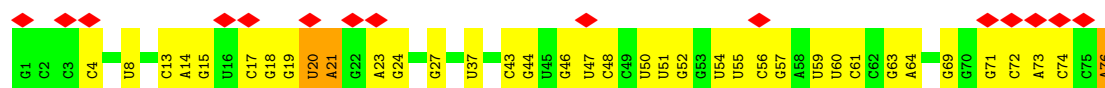




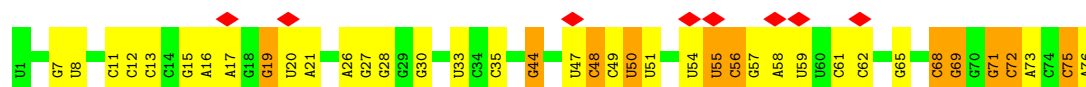




• Molecule 80: tRNA



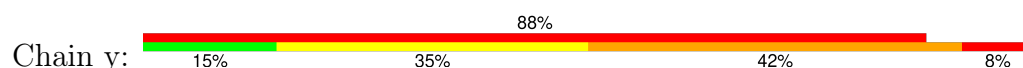
• Molecule 81: tRNA



• Molecule 82: mRNA



• Molecule 83: Proprotein convertase subtilisin/kexin type 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43666	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	0.178	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	524.60004, 524.60004, 524.60004	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E3C, 6MZ, MVM, M7A, 5MU, MG, UR3, OMU, A2M, 4AC, OMG, ZN, PSU, OMC, B8Q, 5MC, MA6, B8N

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	0.33	1/39949 (0.0%)	0.45	16/62213 (0.0%)
2	SA	0.35	0/1778	0.76	5/2416 (0.2%)
3	SB	0.30	0/1765	0.60	1/2362 (0.0%)
4	SD	0.30	0/1785	0.70	0/2404
5	SE	0.29	0/2099	0.62	0/2822
6	SF	0.40	0/1514	0.85	5/2031 (0.2%)
7	SH	0.30	0/1518	0.70	1/2029 (0.0%)
8	SI	0.29	0/1702	0.64	0/2271
9	SK	0.32	0/851	0.68	0/1147
10	SL	0.31	0/1266	0.62	0/1690
11	SP	0.31	0/1065	0.68	0/1423
12	SQ	0.34	0/1177	0.76	0/1575
13	SR	0.31	0/1097	0.74	0/1474
14	SS	0.29	0/1216	0.67	1/1628 (0.1%)
15	ST	0.29	0/1131	0.69	1/1515 (0.1%)
16	SU	0.31	0/831	0.73	2/1115 (0.2%)
17	SV	0.35	0/631	0.76	2/844 (0.2%)
18	SX	0.37	0/1116	0.75	2/1490 (0.1%)
19	Sa	0.42	0/836	0.72	0/1121
20	Sc	0.32	0/508	0.78	1/680 (0.1%)
21	Sd	0.37	0/470	0.81	0/623
22	Sg	0.26	0/2486	0.67	0/3384
23	SC	0.36	0/1753	0.72	0/2365
24	SG	0.25	0/1946	0.64	0/2590
25	SJ	0.70	3/1561 (0.2%)	0.91	5/2083 (0.2%)
26	SM	0.23	0/922	0.61	0/1238
27	SN	0.29	0/1232	0.56	0/1656
28	SO	0.32	0/1037	0.73	0/1391
29	SW	0.35	0/1051	0.68	1/1406 (0.1%)
30	SY	0.28	0/1094	0.64	1/1452 (0.1%)
31	SZ	0.34	0/585	0.81	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.27	0/653	0.58	0/876
33	Se	0.26	0/458	0.61	0/604
34	Sf	0.24	0/560	0.70	0/745
35	A	0.39	0/1968	0.67	0/2639
36	B	0.37	0/3270	0.73	0/4377
37	C	0.39	0/2942	0.70	1/3951 (0.0%)
38	D	0.34	0/3726	0.40	0/5804
39	E	0.33	0/2839	0.41	0/4425
40	F	0.34	0/2437	0.69	0/3262
41	G	0.37	1/1942 (0.1%)	0.81	2/2606 (0.1%)
42	H	0.41	0/1905	0.77	2/2539 (0.1%)
43	I	0.35	0/1913	0.68	0/2576
44	J	0.33	0/1545	0.67	0/2077
45	K	0.34	0/1730	0.66	3/2311 (0.1%)
46	L	0.32	0/1376	0.67	2/1841 (0.1%)
47	M	0.39	0/1688	0.80	2/2260 (0.1%)
48	N	0.34	0/1161	0.64	0/1554
49	O	0.43	0/1746	0.74	0/2338
50	P	0.39	0/1638	0.66	0/2191
51	Q	0.38	0/1268	0.66	0/1701
52	R	0.40	0/1537	0.75	0/2052
53	S	0.38	0/1533	0.71	0/2025
54	T	0.38	0/1488	0.68	3/1997 (0.2%)
55	U	0.39	0/1312	0.67	0/1753
56	V	0.28	0/822	0.63	1/1103 (0.1%)
57	W	0.34	0/983	0.56	0/1319
58	X	0.39	0/524	0.68	2/698 (0.3%)
59	Y	0.33	0/975	0.62	0/1312
60	Z	0.38	0/1132	0.68	0/1504
61	a	0.33	0/1126	0.67	0/1502
62	b	0.40	0/1191	0.80	2/1591 (0.1%)
63	c	0.32	0/826	0.73	0/1088
64	d	0.38	0/812	0.66	0/1089
65	e	0.37	0/894	0.70	0/1204
66	f	0.39	0/1082	0.71	0/1443
67	g	0.41	0/895	0.74	0/1198
68	h	0.38	0/916	0.78	1/1220 (0.1%)
69	i	0.33	0/1023	0.72	0/1351
70	j	0.32	0/805	0.69	0/1065
71	k	0.37	0/703	0.65	0/929
72	l	0.30	0/575	0.60	0/761
73	m	0.36	0/454	0.73	0/599
74	n	0.34	0/417	0.67	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	o	0.37	0/241	0.73	0/305
76	p	0.41	0/877	0.81	3/1156 (0.3%)
77	q	0.36	0/718	0.69	0/953
78	r	0.44	0/995	0.83	1/1334 (0.1%)
79	t	0.35	0/86502	0.42	2/134927 (0.0%)
80	u	0.23	0/1799	0.45	0/2800
81	v	0.25	0/1802	0.46	1/2797 (0.0%)
82	w	0.31	0/235	0.63	1/365 (0.3%)
83	y	0.72	2/210 (1.0%)	2.46	6/289 (2.1%)
All	All	0.35	7/230141 (0.0%)	0.55	79/338182 (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
1	S2	0	1
11	SP	0	1
13	SR	0	1
36	B	0	1
40	F	0	1
47	M	0	1
64	d	0	1
76	p	0	2
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	SJ	66	LYS	C-N	19.58	1.55	1.33
25	SJ	67	ASP	N-CA	7.20	1.52	1.46
83	y	16	PRO	C-O	6.46	1.32	1.24
83	y	16	PRO	CA-C	6.44	1.61	1.52
41	G	224	LYS	C-N	6.37	1.39	1.33
1	S2	1678	A2M	O3'-P	6.01	1.62	1.56
25	SJ	66	LYS	N-CA	5.49	1.53	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	y	15	GLY	CA-C-N	26.49	152.95	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	y	15	GLY	C-N-CA	26.49	152.95	119.84
6	SF	56	TYR	CA-CB-CG	12.99	137.28	113.90
6	SF	63	LYS	CA-CB-CG	8.74	131.58	114.10
20	Sc	30	VAL	N-CA-C	8.68	123.57	113.42
1	S2	1350	U	O3'-P-O5'	8.09	116.13	104.00
30	SY	93	ARG	N-CA-C	-7.75	102.84	111.28
18	SX	7	LEU	CA-C-N	7.61	136.08	121.54
18	SX	7	LEU	C-N-CA	7.61	136.08	121.54
7	SH	15	LYS	N-CA-C	7.53	123.85	113.16
42	H	170	THR	N-CA-C	7.31	119.33	111.36
1	S2	1352	G	O5'-C5'-C4'	7.29	122.43	111.50
1	S2	1351	G	O3'-P-O5'	7.24	114.85	104.00
1	S2	1351	G	O4'-C1'-N9	6.85	118.78	108.50
2	SA	108	PHE	N-CA-C	6.73	118.70	111.36
1	S2	1006	C	O5'-C5'-C4'	6.71	121.57	111.50
15	ST	99	VAL	N-CA-C	-6.54	106.42	112.96
83	y	15	GLY	C-N-CD	-6.49	98.41	125.00
6	SF	60	ARG	N-CA-C	6.47	119.62	110.23
17	SV	80	SER	N-CA-C	6.39	119.55	111.69
29	SW	118	ARG	N-CA-C	-6.39	104.40	111.36
1	S2	1351	G	P-O3'-C3'	6.38	129.78	120.20
1	S2	1349	G	P-O3'-C3'	6.26	129.59	120.20
56	V	60	VAL	N-CA-C	6.24	116.36	110.30
6	SF	63	LYS	CB-CG-CD	6.22	125.60	111.30
1	S2	1351	G	O5'-C5'-C4'	6.02	120.54	111.50
58	X	44	ARG	CA-C-N	5.99	132.32	120.94
58	X	44	ARG	C-N-CA	5.99	132.32	120.94
6	SF	57	ALA	N-CA-C	5.87	118.45	110.06
76	p	103	VAL	CA-C-N	5.85	132.50	121.97
76	p	103	VAL	C-N-CA	5.85	132.50	121.97
14	SS	82	TRP	CA-CB-CG	5.82	124.66	113.60
54	T	27	LEU	CA-CB-CG	5.77	136.50	116.30
83	y	16	PRO	N-CA-C	5.68	124.17	112.47
1	S2	1351	G	C4'-C3'-O3'	5.64	121.46	113.00
2	SA	107	THR	N-CA-C	-5.62	105.05	111.07
25	SJ	71	LEU	CB-CG-CD1	-5.53	94.11	110.70
62	b	46	ASP	CA-C-N	5.52	132.08	121.54
62	b	46	ASP	C-N-CA	5.52	132.08	121.54
25	SJ	65	GLU	CA-C-N	5.48	132.00	121.54
25	SJ	65	GLU	C-N-CA	5.48	132.00	121.54
79	t	901	U	P-O3'-C3'	5.46	128.40	120.20
1	S2	1350	U	P-O5'-C5'	5.46	129.09	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	SJ	71	LEU	CA-CB-CG	5.45	135.37	116.30
1	S2	1813	A	C2'-C3'-O3'	5.42	117.62	109.50
45	K	10	ARG	N-CA-C	-5.41	99.27	110.80
37	C	57	LEU	N-CA-C	-5.39	99.31	110.80
68	h	60	ARG	CA-CB-CG	5.39	124.88	114.10
1	S2	1349	G	O3'-P-O5'	5.38	112.06	104.00
17	SV	81	LYS	N-CA-C	-5.35	104.51	111.74
83	y	4	LEU	CA-C-N	5.33	125.31	120.03
83	y	4	LEU	C-N-CA	5.33	125.31	120.03
45	K	10	ARG	CA-C-N	5.30	131.66	121.54
45	K	10	ARG	C-N-CA	5.30	131.66	121.54
46	L	170	TYR	CA-C-N	5.29	131.65	121.54
46	L	170	TYR	C-N-CA	5.29	131.65	121.54
3	SB	86	LEU	N-CA-C	5.27	117.07	110.91
2	SA	109	THR	N-CA-C	5.25	119.69	113.28
1	S2	1815	A	P-O3'-C3'	5.24	128.05	120.20
1	S2	1802	C	C2'-C3'-O3'	5.22	121.53	113.70
2	SA	140	VAL	CA-C-N	5.21	130.21	122.82
2	SA	140	VAL	C-N-CA	5.21	130.21	122.82
54	T	161	ARG	CA-C-N	5.21	131.49	121.54
54	T	161	ARG	C-N-CA	5.21	131.49	121.54
78	r	106	LEU	CA-CB-CG	5.20	134.48	116.30
76	p	104	ILE	N-CA-C	5.18	120.12	109.34
41	G	233	PHE	CA-C-N	5.18	131.43	121.54
41	G	233	PHE	C-N-CA	5.18	131.43	121.54
47	M	62	PRO	CA-C-N	5.17	131.41	121.54
47	M	62	PRO	C-N-CA	5.17	131.41	121.54
1	S2	1352	G	O5'-P-OP1	-5.15	92.55	108.00
79	t	4946	U	P-O3'-C3'	5.15	127.92	120.20
42	H	168	ALA	N-CA-C	-5.11	101.63	109.76
82	w	20	G	C2'-C3'-O3'	5.08	121.33	113.70
16	SU	46	LYS	CA-C-N	5.07	130.02	122.82
16	SU	46	LYS	C-N-CA	5.07	130.02	122.82
25	SJ	66	LYS	CA-CB-CG	5.05	124.20	114.10
1	S2	1813	A	P-O3'-C3'	5.04	127.76	120.20
81	v	50	U	P-O3'-C3'	5.03	127.74	120.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	B	296	GLY	Peptide

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Mol	Chain	Res	Type	Group
40	F	264	LYS	Peptide
47	M	62	PRO	Peptide
1	S2	1351	G	Sidechain
11	SP	14	LYS	Peptide
13	SR	67	ARG	Peptide
64	d	12	GLU	Peptide
76	p	103	VAL	Peptide
76	p	104	ILE	Peptide

5.2 Too-close contacts [i](#)

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	18415	244	0
2	SA	1741	0	1745	61	0
3	SB	1738	0	1809	25	0
4	SD	1757	0	1853	22	0
5	SE	2059	0	2162	37	0
6	SF	1495	0	1547	73	0
7	SH	1497	0	1590	44	0
8	SI	1673	0	1756	35	0
9	SK	827	0	854	13	0
10	SL	1247	0	1321	15	0
11	SP	1045	0	1095	12	0
12	SQ	1158	0	1232	19	0
13	SR	1082	0	1137	17	0
14	SS	1198	0	1261	24	0
15	ST	1112	0	1146	16	0
16	SU	821	0	883	12	0
17	SV	625	0	625	33	0
18	SX	1098	0	1167	29	0
19	Sa	821	0	870	15	0
20	Sc	506	0	536	16	0
21	Sd	459	0	452	11	0
22	Sg	2429	0	2386	36	0
23	SC	1715	0	1802	31	0
24	SG	1923	0	2089	25	0
25	SJ	1533	0	1653	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	SM	912	0	930	10	0
27	SN	1208	0	1294	14	0
28	SO	1024	0	1050	16	0
29	SW	1034	0	1080	24	0
30	SY	1073	0	1155	27	0
31	SZ	579	0	639	6	0
32	Sb	640	0	665	12	0
33	Se	452	0	498	3	0
34	Sf	548	0	552	5	0
35	A	1930	0	2030	24	0
36	B	3202	0	3343	48	0
37	C	2888	0	3063	59	0
38	D	3337	0	1692	16	0
39	E	2541	0	1285	11	0
40	F	2392	0	2425	24	0
41	G	1904	0	2055	35	0
42	H	1870	0	1996	46	0
43	I	1880	0	2018	17	0
44	J	1526	0	1605	24	0
45	K	1692	0	1744	19	0
46	L	1353	0	1386	15	0
47	M	1657	0	1764	28	0
48	N	1138	0	1204	22	0
49	O	1701	0	1749	34	0
50	P	1606	0	1745	20	0
51	Q	1242	0	1269	18	0
52	R	1513	0	1628	18	0
53	S	1517	0	1670	28	0
54	T	1449	0	1493	30	0
55	U	1284	0	1352	25	0
56	V	808	0	831	8	0
57	W	969	0	1031	12	0
58	X	511	0	521	4	0
59	Y	958	0	1029	9	0
60	Z	1115	0	1205	21	0
61	a	1103	0	1179	16	0
62	b	1162	0	1213	18	0
63	c	814	0	880	8	0
64	d	801	0	845	13	0
65	e	879	0	924	8	0
66	f	1064	0	1160	18	0
67	g	876	0	912	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	h	906	0	1002	10	0
69	i	1015	0	1148	16	0
70	j	794	0	870	7	0
71	k	689	0	717	10	0
72	l	569	0	637	6	0
73	m	444	0	483	8	0
74	n	411	0	443	6	0
75	o	240	0	289	3	0
76	p	863	0	930	16	0
77	q	708	0	756	6	0
78	r	980	0	1041	19	0
79	t	77332	0	39077	440	0
80	u	1613	0	821	8	0
81	v	1618	0	826	12	0
82	w	213	0	109	1	0
83	y	204	0	216	73	0
84	A	1	0	0	0	0
84	B	1	0	0	0	0
84	D	7	0	0	0	0
84	E	9	0	0	0	0
84	S2	2	0	0	0	0
84	b	1	0	0	0	0
84	o	1	0	0	0	0
84	t	9	0	0	0	0
85	S2	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sf	1	0	0	0	0
85	k	1	0	0	0	0
85	p	1	0	0	0	0
85	q	1	0	0	0	0
86	t	31	0	0	7	0
87	S2	6	0	0	1	0
87	SA	1	0	0	0	0
87	SC	1	0	0	0	0
87	SN	1	0	0	0	0
87	SP	1	0	0	0	0
87	SQ	1	0	0	0	0
87	SS	1	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	0	0
All	All	214893	0	158860	1851	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 5.

All (1851) 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	1.66
6:SF:60:ARG:NH1	17:SV:61:ARG:HH11	1.12	1.45
2:SA:139:TYR:HE1	6:SF:60:ARG:NE	1.06	1.42
6:SF:60:ARG:NH1	17:SV:61:ARG:NH1	1.68	1.40
2:SA:109:THR:CG2	6:SF:62:ARG:HB2	1.47	1.38
2:SA:139:TYR:CE1	6:SF:60:ARG:NE	1.94	1.35
6:SF:59:LYS:HZ1	23:SC:87:PRO:CB	1.40	1.33
2:SA:109:THR:CG2	6:SF:62:ARG:CB	1.88	1.32
86:t:5110:MVM:N5	83:y:18:GLY:HA2	1.48	1.28
6:SF:59:LYS:HZ1	23:SC:87:PRO:CA	1.49	1.25
86:t:5110:MVM:N6	83:y:18:GLY:HA2	1.52	1.24
2:SA:109:THR:HG21	6:SF:62:ARG:CB	0.92	1.24
6:SF:59:LYS:NZ	23:SC:87:PRO:HB3	1.54	1.20
37:C:83:GLY:O	83:y:8:LEU:CB	1.90	1.19
37:C:83:GLY:O	83:y:8:LEU:HB3	1.39	1.18
42:H:158:GLY:O	42:H:169:LEU:CD2	1.94	1.14
6:SF:60:ARG:HH12	17:SV:61:ARG:NH1	1.36	1.09
2:SA:109:THR:HG21	6:SF:62:ARG:HB3	1.19	1.07
6:SF:59:LYS:HZ1	23:SC:87:PRO:HB3	1.09	1.06
67:g:106:TYR:HB3	67:g:107:PRO:HD2	1.06	1.04
67:g:106:TYR:CB	67:g:107:PRO:HD2	1.83	1.04
79:t:3878:G:N2	83:y:23:GLU:CB	2.22	1.02
2:SA:139:TYR:HE1	6:SF:60:ARG:CZ	1.74	1.01
6:SF:59:LYS:NZ	23:SC:87:PRO:CB	2.14	1.00
7:SH:10:LYS:HZ3	7:SH:17:ASP:CB	1.75	0.99
7:SH:10:LYS:HZ3	7:SH:17:ASP:HB3	1.25	0.98
42:H:158:GLY:C	42:H:169:LEU:CD2	2.37	0.97
6:SF:59:LYS:NZ	23:SC:87:PRO:CA	2.28	0.96
20:Sc:20:ARG:HE	20:Sc:28:THR:HG22	1.26	0.95
2:SA:139:TYR:CE1	6:SF:60:ARG:CZ	2.48	0.94
7:SH:10:LYS:NZ	7:SH:17:ASP:CG	2.25	0.94
29:SW:114:GLU:O	29:SW:118:ARG:HG3	1.66	0.94
51:Q:117:ILE:HD12	51:Q:148:MET:HE2	1.49	0.93
2:SA:139:TYR:HE1	6:SF:60:ARG:HE	0.97	0.93
17:SV:74:LYS:HE3	17:SV:81:LYS:HA	1.49	0.93
79:t:1583:A:N6	86:t:5110:MVM:CL	2.39	0.92
86:t:5110:MVM:N6	83:y:18:GLY:CA	2.34	0.90
6:SF:60:ARG:HH11	17:SV:61:ARG:HH11	1.13	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SH:10:LYS:NZ	7:SH:17:ASP:HB3	1.86	0.90
1:S2:1495:G:H1	21:Sd:42:CYS:HG	1.11	0.89
41:G:153:LEU:HD13	67:g:105:LEU:O	1.73	0.88
79:t:4493:U:O4	83:y:24:ASP:OD1	1.91	0.88
30:SY:90:ARG:HA	30:SY:93:ARG:HG3	1.54	0.88
6:SF:59:LYS:HZ1	23:SC:87:PRO:HA	1.38	0.87
2:SA:139:TYR:CE1	6:SF:60:ARG:CG	2.58	0.87
7:SH:10:LYS:NZ	7:SH:17:ASP:CB	2.36	0.87
7:SH:10:LYS:NZ	7:SH:17:ASP:OD1	2.08	0.86
42:H:158:GLY:C	42:H:169:LEU:HD21	2.00	0.86
17:SV:79:VAL:HG23	17:SV:80:SER:H	1.39	0.86
79:t:3878:G:N2	83:y:23:GLU:HB3	1.91	0.84
42:H:158:GLY:C	42:H:169:LEU:HD22	2.01	0.84
1:S2:984:C:O2'	28:SO:138:ASP:O	1.94	0.84
7:SH:14:GLU:OE1	7:SH:14:GLU:N	2.11	0.84
42:H:158:GLY:O	42:H:169:LEU:HD22	1.77	0.83
83:y:12:LEU:CD1	83:y:13:LEU:O	2.26	0.83
6:SF:60:ARG:HH12	17:SV:61:ARG:HH11	0.93	0.83
18:SX:61:GLN:HG2	18:SX:62:PRO:HD3	1.60	0.82
37:C:83:GLY:O	83:y:8:LEU:HB2	1.78	0.82
17:SV:51:LYS:HZ2	17:SV:76:ASP:HB3	1.44	0.81
17:SV:79:VAL:HG23	17:SV:80:SER:N	1.93	0.81
1:S2:1748:G:H1	1:S2:1786:U:H3	1.27	0.80
2:SA:139:TYR:CE1	6:SF:60:ARG:HG3	2.15	0.79
6:SF:60:ARG:HH12	17:SV:61:ARG:CZ	1.94	0.79
79:t:3879:A:C6	83:y:21:ALA:O	2.36	0.79
1:S2:925:G:H1	1:S2:1017:U:H3	1.32	0.78
83:y:9:LEU:O	83:y:9:LEU:HD22	1.84	0.77
1:S2:1824:A:OP1	18:SX:61:GLN:NE2	2.17	0.77
20:Sc:20:ARG:HE	20:Sc:28:THR:CG2	1.98	0.77
83:y:14:LEU:H	83:y:14:LEU:HD22	1.50	0.77
2:SA:139:TYR:CD1	6:SF:60:ARG:HG2	2.20	0.76
79:t:3878:G:H22	83:y:23:GLU:HB3	1.47	0.76
2:SA:109:THR:HG21	6:SF:62:ARG:HB2	0.76	0.76
79:t:3878:G:C2	83:y:23:GLU:HG3	2.20	0.76
83:y:12:LEU:HD13	83:y:13:LEU:N	2.01	0.76
47:M:25:TRP:HE1	49:O:199:GLN:HE21	1.34	0.76
83:y:14:LEU:HD22	83:y:14:LEU:N	2.01	0.76
6:SF:59:LYS:HZ2	23:SC:87:PRO:HB3	1.51	0.75
79:t:3878:G:N2	83:y:23:GLU:HB2	2.01	0.75
83:y:12:LEU:HD13	83:y:13:LEU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:158:GLY:O	42:H:169:LEU:HD21	1.84	0.74
2:SA:139:TYR:CD1	6:SF:60:ARG:CG	2.70	0.74
1:S2:1351:G:C4	6:SF:63:LYS:HB3	2.22	0.74
6:SF:59:LYS:NZ	23:SC:87:PRO:HA	1.99	0.74
20:Sc:31:ARG:HA	20:Sc:43:ILE:HA	1.70	0.74
67:g:109:ARG:H	67:g:109:ARG:CD	2.01	0.74
7:SH:15:LYS:HD2	7:SH:15:LYS:C	2.13	0.73
17:SV:51:LYS:HZ3	17:SV:78:ILE:HD11	1.50	0.73
1:S2:1357:A:N6	25:SJ:64:ASP:OD1	2.21	0.73
36:B:300:LYS:HB3	36:B:313:SER:HB2	1.71	0.73
79:t:1060:C:H42	79:t:1217:G:H22	1.35	0.73
2:SA:139:TYR:CE1	6:SF:60:ARG:CD	2.71	0.73
51:Q:128:ARG:NH2	83:y:7:LEU:HD11	2.03	0.72
83:y:4:LEU:HD13	83:y:4:LEU:N	2.04	0.72
83:y:9:LEU:HD22	83:y:9:LEU:C	2.14	0.72
20:Sc:29:GLN:HE21	20:Sc:65:ALA:HB1	1.54	0.72
79:t:1411:U:H3	79:t:1438:G:H22	1.37	0.72
83:y:11:LEU:C	83:y:11:LEU:HD22	2.14	0.72
60:Z:52:ASP:HB2	60:Z:110:LYS:HD2	1.72	0.71
83:y:20:ARG:O	83:y:21:ALA:HB3	1.88	0.71
86:t:5110:MVM:N5	83:y:18:GLY:CA	2.42	0.71
79:t:708:U:H3	79:t:938:G:H1	1.39	0.71
67:g:5:LEU:O	67:g:105:LEU:HD23	1.91	0.70
7:SH:7:LYS:HE3	7:SH:17:ASP:OD2	1.92	0.70
74:n:106:ARG:HH22	79:t:4658:C:H4'	1.56	0.70
1:S2:681:U:O2'	18:SX:8:ARG:NH1	2.24	0.70
79:t:703:C:H42	79:t:943:A:H61	1.39	0.70
65:e:26:THR:HG23	65:e:85:ARG:HH11	1.57	0.70
79:t:465:A:H62	79:t:677:G:H21	1.39	0.70
1:S2:1723:G:H1	1:S2:1810:U:H3	1.37	0.70
22:Sg:87:LEU:HB2	22:Sg:101:PHE:HB2	1.74	0.70
37:C:323:ARG:HA	37:C:326:LEU:HB2	1.73	0.70
42:H:169:LEU:HD23	42:H:169:LEU:H	1.57	0.69
1:S2:928:G:H1	1:S2:1013:U:H3	1.40	0.69
79:t:4951:G:H1	79:t:5016:A:H61	1.40	0.69
41:G:53:GLY:HA3	79:t:1264:G:H22	1.56	0.69
1:S2:1351:G:H8	6:SF:56:TYR:HB2	1.58	0.69
69:i:89:ARG:HA	69:i:92:ARG:HE	1.57	0.69
83:y:4:LEU:O	83:y:4:LEU:HD22	1.92	0.69
83:y:23:GLU:OE1	83:y:23:GLU:HA	1.92	0.69
22:Sg:127:LYS:HE3	22:Sg:148:SER:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:y:7:LEU:N	83:y:7:LEU:HD23	2.08	0.68
25:SJ:37:LEU:HD23	25:SJ:42:GLU:HG3	1.76	0.68
83:y:10:LEU:O	83:y:10:LEU:HD13	1.94	0.68
5:SE:41:CYS:SG	5:SE:42:LEU:N	2.67	0.68
50:P:185:VAL:HG13	50:P:186:GLU:HG3	1.76	0.68
79:t:2499:C:H5	79:t:2514:G:H1	1.41	0.68
17:SV:51:LYS:NZ	17:SV:78:ILE:HD11	2.08	0.68
79:t:2372:C:OP2	79:t:2373:G:N2	2.26	0.68
2:SA:139:TYR:OH	6:SF:60:ARG:CZ	2.42	0.68
8:SI:57:ALA:H	8:SI:180:GLY:HA2	1.59	0.68
61:a:17:ARG:NH1	79:t:2557:G:N7	2.42	0.68
79:t:484:C:O2	79:t:658:G:N2	2.26	0.68
2:SA:77:ILE:HG22	2:SA:99:ILE:HB	1.77	0.67
54:T:81:TRP:HB3	54:T:127:MET:HE3	1.75	0.67
79:t:3879:A:N6	83:y:21:ALA:O	2.26	0.67
1:S2:1648:G:H5''	12:SQ:125:ARG:HB2	1.75	0.67
32:Sb:36:LYS:HB3	32:Sb:78:SER:HB3	1.77	0.67
37:C:94:ASN:HD22	37:C:102:PHE:HB2	1.60	0.67
13:SR:115:SER:HB3	13:SR:117:LEU:HD23	1.76	0.67
54:T:93:MET:HG3	79:t:1933:G:H4'	1.77	0.67
17:SV:51:LYS:NZ	17:SV:76:ASP:HB3	2.10	0.66
67:g:105:LEU:HD22	67:g:105:LEU:N	2.09	0.66
22:Sg:195:LEU:HA	22:Sg:211:GLY:HA3	1.78	0.66
40:F:4:VAL:N	79:t:1760:C:HO2'	1.93	0.66
83:y:12:LEU:HD13	83:y:12:LEU:C	2.21	0.66
22:Sg:157:SER:HB3	22:Sg:164:ILE:HG22	1.78	0.66
67:g:106:TYR:HB3	67:g:107:PRO:CD	2.02	0.66
67:g:100:ARG:HH21	67:g:102:ARG:HH21	1.44	0.65
2:SA:74:VAL:HG12	2:SA:121:LEU:HB3	1.79	0.65
7:SH:166:VAL:HG12	7:SH:169:LYS:HD2	1.79	0.65
8:SI:48:VAL:HG11	8:SI:54:LYS:HE3	1.78	0.65
37:C:198:ASN:HD22	60:Z:10:ASP:HB3	1.62	0.65
7:SH:17:ASP:O	7:SH:20:GLU:OE1	2.13	0.65
53:S:103:ARG:NH1	53:S:124:TYR:OH	2.30	0.65
53:S:133:LYS:H	53:S:137:ILE:HD11	1.62	0.65
2:SA:109:THR:O	6:SF:62:ARG:CD	2.44	0.65
42:H:245:ARG:NH2	79:t:930:A:OP1	2.29	0.65
5:SE:71:LYS:HB2	5:SE:91:SER:HB2	1.77	0.65
20:Sc:13:ARG:HB2	20:Sc:35:MET:HE2	1.79	0.65
28:SO:57:THR:HG22	28:SO:59:GLY:H	1.62	0.65
21:Sd:30:LEU:HA	21:Sd:39:CYS:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Sa:87:ARG:NH1	19:Sa:94:ASP:OD1	2.29	0.65
54:T:154:LEU:HB3	54:T:157:ARG:HD3	1.80	0.64
9:SK:3:MET:SD	9:SK:8:ARG:NE	2.67	0.64
35:A:192:LYS:HB3	35:A:193:ARG:HE	1.63	0.64
38:D:149:G:H21	43:I:64:GLN:HE22	1.44	0.64
49:O:93:LYS:NZ	79:t:281:U:O2	2.31	0.64
79:t:4493:U:O4	83:y:24:ASP:CG	2.40	0.64
5:SE:87:MET:HE2	5:SE:123:LEU:HB2	1.80	0.64
79:t:3878:G:N2	83:y:23:GLU:CG	2.61	0.64
51:Q:80:GLN:NE2	79:t:3863:U:O2'	2.30	0.64
79:t:1743:G:H1	79:t:1753:U:H3	1.45	0.64
8:SI:129:LEU:HB2	8:SI:133:GLU:HB3	1.79	0.64
79:t:4716:G:H22	79:t:4837:C:H1'	1.63	0.64
40:F:37:VAL:HG22	40:F:67:ALA:HB2	1.79	0.63
79:t:173:G:H22	79:t:255:G:H1	1.46	0.63
79:t:104:G:HO2'	79:t:1344:G:HO2'	1.44	0.63
1:S2:962:A:H5'	28:SO:66:ARG:HG3	1.79	0.63
79:t:289:A:N6	79:t:4323:U:O2'	2.32	0.63
41:G:188:ARG:NH1	41:G:214:ASP:OD1	2.32	0.63
28:SO:57:THR:HB	28:SO:60:MET:HG3	1.80	0.63
52:R:99:LYS:HE2	52:R:119:LYS:HD3	1.81	0.63
28:SO:103:ASN:HD21	28:SO:142:ARG:HA	1.63	0.63
46:L:15:LEU:HD21	46:L:157:ILE:HG21	1.80	0.63
79:t:200:U:H3	79:t:207:C:H42	1.47	0.63
67:g:106:TYR:CB	67:g:107:PRO:CD	2.72	0.63
1:S2:1495:G:N1	21:Sd:42:CYS:SG	2.64	0.62
60:Z:2:LYS:HD2	60:Z:7:VAL:HG13	1.80	0.62
67:g:104:MET:C	67:g:105:LEU:HD22	2.24	0.62
79:t:162:A:H61	79:t:265:C:H42	1.46	0.62
80:u:51:U:H3	80:u:63:G:H1	1.47	0.62
79:t:4710:U:H3	79:t:4909:G:H1	1.47	0.62
22:Sg:20:GLN:NE2	22:Sg:69:VAL:O	2.32	0.62
46:L:18:ARG:HB3	46:L:133:VAL:HG23	1.80	0.62
60:Z:8:THR:O	79:t:223:G:N2	2.31	0.62
70:j:70:LEU:HD11	70:j:84:LYS:HG2	1.81	0.62
36:B:224:LYS:HD3	36:B:340:THR:HG22	1.80	0.62
67:g:58:VAL:HG22	67:g:60:PRO:HD2	1.81	0.62
67:g:109:ARG:H	67:g:109:ARG:NE	1.97	0.62
79:t:2626:A:H62	79:t:2665:G:H8	1.47	0.62
13:SR:31:ASN:HD22	13:SR:55:THR:HG22	1.63	0.62
53:S:107:ARG:NH2	79:t:2645:U:OP1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:g:5:LEU:O	67:g:105:LEU:CD2	2.47	0.62
79:t:3878:G:N2	83:y:23:GLU:HG3	2.14	0.62
51:Q:146:ILE:O	51:Q:146:ILE:HD12	1.99	0.62
1:S2:955:A:N6	1:S2:971:G:O2'	2.33	0.62
42:H:158:GLY:O	42:H:169:LEU:HD23	1.97	0.62
56:V:81:ARG:NH2	79:t:2601:G:O6	2.33	0.62
79:t:2374:A:N3	79:t:2785:A:O2'	2.32	0.62
41:G:91:THR:HB	41:G:109:LEU:HD22	1.81	0.61
61:a:76:ASN:OD1	61:a:79:HIS:ND1	2.33	0.61
62:b:26:ARG:NH2	79:t:1638:U:OP2	2.33	0.61
22:Sg:104:HIS:H	22:Sg:106:LYS:HE3	1.65	0.61
37:C:190:ARG:HE	37:C:202:ILE:HG12	1.63	0.61
49:O:71:ARG:HD2	49:O:94:PHE:HB2	1.83	0.61
79:t:459:G:H1	79:t:683:U:H3	1.49	0.61
80:u:27:G:H1	80:u:43:C:H41	1.47	0.61
1:S2:1547:C:N4	1:S2:1586:U:O4	2.33	0.61
1:S2:1824:A:P	18:SX:61:GLN:NE2	2.73	0.61
53:S:39:GLN:NE2	79:t:2688:C:OP1	2.34	0.61
57:W:45:ILE:HG21	57:W:53:PRO:HB3	1.82	0.61
79:t:4732:U:H3	79:t:4820:G:H22	1.46	0.61
38:D:55:U:H3	38:D:62:A:H2	1.49	0.61
50:P:118:MET:HG2	54:T:169:THR:HG22	1.83	0.61
79:t:196:G:N2	79:t:206:U:OP1	2.32	0.61
9:SK:92:ALA:HA	9:SK:96:ARG:HG3	1.81	0.61
22:Sg:138:CYS:SG	22:Sg:139:LYS:N	2.73	0.61
61:a:5:MET:O	61:a:28:ASN:ND2	2.33	0.61
1:S2:322:C:O2'	1:S2:324:C:N4	2.32	0.61
42:H:151:ASN:HA	42:H:191:ILE:HD11	1.81	0.61
2:SA:177:MET:SD	2:SA:180:ARG:NH2	2.69	0.61
39:E:27:G:OP1	46:L:146:ARG:NH2	2.34	0.61
67:g:109:ARG:H	67:g:109:ARG:HD2	1.66	0.61
1:S2:1653:U:H3	1:S2:1671:G:H1	1.49	0.61
2:SA:109:THR:CG2	6:SF:62:ARG:HB3	1.94	0.61
6:SF:127:ARG:HH11	6:SF:137:GLN:HB2	1.64	0.61
22:Sg:85:GLY:HA2	22:Sg:107:ASP:HA	1.83	0.61
36:B:6:PHE:HB3	57:W:49:LEU:HD21	1.83	0.61
79:t:3878:G:H21	83:y:23:GLU:HB2	1.66	0.61
79:t:4730:G:H1	79:t:4822:U:H3	1.47	0.61
2:SA:139:TYR:CZ	6:SF:60:ARG:CZ	2.83	0.60
14:SS:3:LEU:HD12	14:SS:4:VAL:HG23	1.82	0.60
41:G:283:PRO:O	41:G:284:HIS:ND1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L:136:ARG:NH2	46:L:161:GLU:OE2	2.34	0.60
47:M:74:ARG:NH1	79:t:76:A:OP2	2.35	0.60
51:Q:23:ARG:NH2	51:Q:125:MET:SD	2.72	0.60
79:t:1921:G:H22	79:t:4396:C:H5''	1.66	0.60
7:SH:145:ARG:NH1	29:SW:51:GLU:OE2	2.34	0.60
23:SC:136:HIS:HB3	23:SC:162:ILE:HD11	1.83	0.60
37:C:178:ASN:OD1	79:t:2279:A:N6	2.34	0.60
64:d:8:LYS:HG3	64:d:9:LYS:HD3	1.83	0.60
79:t:1069:C:H42	79:t:1193:C:H42	1.47	0.60
78:r:107:ARG:NH2	79:t:2242:A:OP1	2.35	0.60
6:SF:122:ARG:HE	20:Sc:59:LEU:HD12	1.66	0.60
67:g:100:ARG:HH11	79:t:4713:G:H5''	1.65	0.60
1:S2:913:A:N6	7:SH:99:ARG:O	2.34	0.60
7:SH:154:ILE:HB	7:SH:185:VAL:HG12	1.83	0.60
83:y:20:ARG:O	83:y:21:ALA:CB	2.49	0.60
1:S2:573:U:C4	30:SY:93:ARG:NH1	2.69	0.60
3:SB:171:ILE:HG12	3:SB:174:ARG:HH21	1.67	0.60
9:SK:31:LYS:HE3	9:SK:36:ALA:HA	1.84	0.60
54:T:29:ARG:HB2	55:U:148:PRO:HB2	1.83	0.60
59:Y:107:HIS:O	59:Y:111:GLN:NE2	2.35	0.60
61:a:21:ARG:NH1	61:a:47:ASP:O	2.35	0.60
48:N:97:ALA:O	50:P:198:THR:OG1	2.18	0.59
52:R:112:ARG:HG2	52:R:115:ARG:HH21	1.67	0.59
76:p:65:LYS:HE3	76:p:87:ARG:HH21	1.66	0.59
1:S2:910:G:OP2	53:S:173:ARG:NH1	2.35	0.59
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	1.83	0.59
6:SF:100:ILE:HD11	6:SF:177:LEU:HD21	1.84	0.59
8:SI:124:LYS:HG2	8:SI:125:LYS:HG2	1.83	0.59
10:SL:11:GLN:HB3	10:SL:56:ILE:HG21	1.84	0.59
36:B:10:ARG:NH1	36:B:11:HIS:O	2.35	0.59
48:N:119:ARG:HH22	50:P:191:LYS:HD3	1.67	0.59
51:Q:116:HIS:HB3	51:Q:149:ILE:HB	1.85	0.59
28:SO:30:VAL:HG12	28:SO:94:HIS:HB2	1.83	0.59
44:J:31:ARG:NH1	44:J:149:ASN:OD1	2.35	0.59
56:V:28:PRO:HG3	56:V:100:LEU:HD21	1.82	0.59
20:Sc:29:GLN:HG2	20:Sc:43:ILE:HD11	1.84	0.59
2:SA:163:CYS:SG	2:SA:164:ASN:N	2.70	0.59
3:SB:226:GLY:HA3	79:t:4070:C:H4'	1.85	0.59
7:SH:10:LYS:HZ1	7:SH:17:ASP:CG	2.09	0.59
42:H:169:LEU:CD2	42:H:169:LEU:H	2.15	0.59
54:T:16:CYS:HA	54:T:59:GLY:HA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:174:G:H1	79:t:254:C:H41	1.50	0.59
79:t:1058:G:H1	79:t:1218:G:H1	1.49	0.59
37:C:250:CYS:SG	37:C:252:TRP:NE1	2.75	0.59
41:G:181:LEU:O	79:t:4841:C:N4	2.32	0.59
79:t:2536:G:H1	79:t:2549:U:H3	1.51	0.59
2:SA:118:GLU:HG3	23:SC:65:LYS:HG3	1.85	0.59
5:SE:90:ILE:HD11	5:SE:99:PHE:HD2	1.68	0.59
24:SG:159:ARG:HG2	24:SG:173:ALA:HB2	1.84	0.59
32:Sb:23:ARG:NH1	32:Sb:27:SER:OG	2.36	0.59
23:SC:64:THR:HG23	23:SC:67:GLY:H	1.68	0.59
36:B:315:ASN:ND2	36:B:325:GLU:OE2	2.36	0.59
83:y:11:LEU:O	83:y:11:LEU:HD13	2.02	0.59
15:ST:11:GLN:OE1	15:ST:62:ARG:NH2	2.35	0.58
17:SV:79:VAL:CG2	17:SV:80:SER:N	2.63	0.58
83:y:7:LEU:HD23	83:y:7:LEU:H	1.68	0.58
17:SV:77:GLY:HA2	17:SV:81:LYS:NZ	2.18	0.58
60:Z:70:VAL:HG12	60:Z:82:ILE:HG12	1.85	0.58
81:v:19:G:N3	81:v:57:G:N2	2.51	0.58
1:S2:573:U:O4	30:SY:93:ARG:NH1	2.35	0.58
60:Z:54:GLU:HA	60:Z:69:LYS:HA	1.83	0.58
79:t:1164:C:N4	79:t:1167:A:O2'	2.35	0.58
8:SI:6:ASP:HB3	8:SI:28:GLU:HG2	1.85	0.58
79:t:3731:A:N1	80:u:37:U:O2'	2.37	0.58
23:SC:267:GLN:HA	23:SC:270:THR:HG23	1.84	0.58
35:A:129:ALA:HB3	35:A:132:ASN:HD22	1.68	0.58
37:C:328:LEU:HD11	42:H:170:THR:O	2.03	0.58
79:t:658:G:O2'	79:t:662:A:N6	2.36	0.58
17:SV:77:GLY:C	17:SV:81:LYS:HZ3	2.11	0.58
36:B:224:LYS:NZ	79:t:4588:A:OP2	2.36	0.58
65:e:113:THR:HG22	65:e:115:LYS:H	1.68	0.58
79:t:4692:C:H1'	79:t:4693:G:H2'	1.85	0.58
1:S2:65:C:H4'	24:SG:172:LYS:HE2	1.85	0.58
1:S2:1351:G:C5	6:SF:63:LYS:HB3	2.39	0.58
1:S2:1658:G:OP2	1:S2:1660:C:N4	2.37	0.58
40:F:82:GLU:OE2	40:F:108:ARG:NH2	2.28	0.58
50:P:90:HIS:O	50:P:96:GLN:NE2	2.37	0.58
60:Z:11:ARG:HG3	79:t:225:C:H5''	1.85	0.58
1:S2:167:G:H21	24:SG:132:ARG:HH22	1.50	0.58
32:Sb:65:GLN:HG2	32:Sb:74:THR:HG22	1.86	0.58
36:B:170:LEU:O	36:B:328:ASN:ND2	2.36	0.58
43:I:73:ARG:NH1	79:t:4046:G:OP1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:162:GLN:HE21	79:t:1900:G:H4'	1.67	0.58
81:v:48:C:H2'	81:v:59:U:H1'	1.84	0.58
1:S2:681:U:O3'	18:SX:8:ARG:NE	2.29	0.58
26:SM:40:LYS:O	26:SM:44:LYS:NZ	2.36	0.58
67:g:33:VAL:HG23	67:g:38:GLU:HG3	1.85	0.58
79:t:1788:G:H1	79:t:1814:G:H1	1.51	0.58
6:SF:167:LYS:HD2	6:SF:171:GLU:HB3	1.84	0.58
47:M:62:PRO:HG3	79:t:74:G:H1'	1.86	0.58
58:X:51:TRP:O	79:t:4999:G:N2	2.36	0.58
66:f:100:ALA:O	66:f:108:ARG:NH2	2.36	0.58
1:S2:805:U:O3'	29:SW:120:HIS:HE1	1.85	0.57
28:SO:74:ALA:HB1	28:SO:115:ALA:HB2	1.85	0.57
36:B:174:ARG:HH22	79:t:4932:C:H1'	1.69	0.57
48:N:27:ILE:HA	48:N:38:VAL:HG12	1.86	0.57
73:m:40:LYS:NZ	79:t:359:U:O2'	2.34	0.57
79:t:197:U:H5	79:t:210:G:H1	1.52	0.57
79:t:1636:G:N2	79:t:1660:C:OP1	2.37	0.57
6:SF:140:ASP:HB2	20:Sc:46:VAL:HG12	1.86	0.57
14:SS:17:ASN:ND2	14:SS:101:ASN:OD1	2.36	0.57
53:S:39:GLN:NE2	79:t:2689:C:OP2	2.37	0.57
60:Z:2:LYS:NZ	60:Z:4:ASN:O	2.37	0.57
79:t:2030:G:HO2'	79:t:3855:U:HO2'	1.51	0.57
23:SC:108:LYS:HE3	23:SC:110:MET:HB3	1.84	0.57
40:F:28:THR:O	79:t:4242:A:N6	2.37	0.57
37:C:149:GLU:OE2	78:r:71:ARG:NH1	2.36	0.57
79:t:3590:G:O2'	79:t:3593:C:N4	2.37	0.57
18:SX:60:LYS:O	18:SX:63:ASN:O	2.23	0.57
43:I:164:ILE:HG22	49:O:22:LEU:HD13	1.87	0.57
79:t:2590:A:H5'	79:t:2667:G:H4'	1.87	0.57
68:h:38:VAL:O	68:h:60:ARG:NH2	2.37	0.57
79:t:3681:G:N2	79:t:3681:G:OP2	2.37	0.57
43:I:157:ILE:HD12	43:I:170:LEU:HD22	1.85	0.57
57:W:71:GLU:HG2	57:W:72:LEU:HD12	1.86	0.57
79:t:4885:G:OP2	79:t:4885:G:N2	2.36	0.57
1:S2:874:G:H21	7:SH:114:GLN:HE22	1.51	0.57
2:SA:106:GLY:HA2	2:SA:109:THR:HG22	1.86	0.57
3:SB:113:MET:HE3	3:SB:209:ASP:HB3	1.86	0.57
45:K:150:GLU:OE2	45:K:153:ARG:NH2	2.38	0.57
49:O:49:ARG:NH2	79:t:150:G:OP2	2.37	0.57
49:O:125:SER:HB2	79:t:3908:C:H1'	1.85	0.57
1:S2:1636:G:O2'	6:SF:164:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:167:ILE:HD13	42:H:174:LEU:HD23	1.87	0.57
46:L:90:ARG:NH2	46:L:108:GLY:O	2.38	0.57
1:S2:104:A:H62	1:S2:356:C:H5	1.51	0.57
1:S2:902:G:N2	1:S2:904:A:N1	2.53	0.57
1:S2:904:A:N6	87:S2:2001:HOH:O	2.37	0.57
1:S2:1644:C:H4'	12:SQ:140:ARG:HB2	1.86	0.57
7:SH:55:GLY:H	7:SH:57:ARG:HE	1.52	0.57
14:SS:24:ARG:HH21	14:SS:28:PHE:HB3	1.70	0.57
69:i:27:GLU:HG3	69:i:30:GLN:HE21	1.70	0.57
79:t:62:A:N3	79:t:77:U:O2'	2.36	0.57
1:S2:1147:C:OP1	19:Sa:6:ARG:NH1	2.38	0.56
14:SS:63:GLU:OE1	14:SS:66:ARG:NH2	2.35	0.56
65:e:64:ILE:HG22	65:e:106:VAL:HB	1.86	0.56
76:p:39:ARG:HD2	79:t:289:A:H5'	1.87	0.56
79:t:2001:U:H2'	79:t:2002:G:H8	1.69	0.56
83:y:4:LEU:HD22	83:y:4:LEU:C	2.29	0.56
75:o:14:LYS:HA	75:o:17:ARG:HG2	1.86	0.56
76:p:3:ASN:ND2	76:p:95:GLY:O	2.38	0.56
83:y:9:LEU:HD11	83:y:11:LEU:HB3	1.85	0.56
1:S2:943:U:OP1	3:SB:214:LYS:NZ	2.38	0.56
7:SH:144:ILE:HG23	29:SW:52:ILE:HB	1.87	0.56
8:SI:22:HIS:ND1	8:SI:23:LYS:O	2.37	0.56
18:SX:60:LYS:HG3	18:SX:114:ASP:HB2	1.86	0.56
35:A:138:SER:HB3	35:A:147:ARG:HG2	1.85	0.56
67:g:100:ARG:NH1	79:t:4713:G:OP2	2.38	0.56
79:t:2841:G:N3	79:t:3595:A:O2'	2.35	0.56
36:B:71:GLU:OE2	36:B:366:LYS:NZ	2.38	0.56
46:L:160:GLU:OE2	46:L:164:ARG:NH2	2.37	0.56
54:T:8:ARG:NH1	54:T:35:PRO:O	2.38	0.56
66:f:19:LYS:NZ	79:t:2301:G:O6	2.39	0.56
79:t:4707:G:H22	79:t:4912:G:H1	1.53	0.56
1:S2:197:U:O2'	1:S2:203:G:N2	2.34	0.56
37:C:222:ARG:NH1	79:t:221:U:OP1	2.38	0.56
40:F:21:ARG:HA	40:F:24:ARG:HH21	1.70	0.56
72:l:38:CYS:SG	72:l:39:SER:N	2.78	0.56
83:y:12:LEU:O	83:y:14:LEU:HD13	2.05	0.56
1:S2:693:A:N6	1:S2:738:C:O2'	2.39	0.56
76:p:61:LYS:HD3	76:p:87:ARG:HH12	1.70	0.56
79:t:463:C:N4	79:t:680:C:O2	2.38	0.56
79:t:1619:A:OP1	79:t:1622:C:N4	2.37	0.56
1:S2:326:C:O2	1:S2:327:G:N2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:354:U:OP1	10:SL:90:ARG:NH1	2.39	0.56
1:S2:533:A:H61	1:S2:550:C:H42	1.54	0.56
7:SH:13:GLY:C	7:SH:14:GLU:OE1	2.48	0.56
59:Y:129:ARG:NH2	59:Y:133:GLU:OE1	2.38	0.56
79:t:1380:A:HO2'	79:t:1449:C:HO2'	1.54	0.56
1:S2:1341:C:N4	1:S2:1486:A:N1	2.53	0.56
32:Sb:49:HIS:ND1	32:Sb:69:GLY:O	2.34	0.56
62:b:42:ARG:NH1	79:t:4338:A:O2'	2.39	0.56
63:c:116:LEU:HD21	79:t:1222:C:H5'	1.87	0.56
79:t:1716:G:N2	79:t:1717:U:O4	2.37	0.56
1:S2:334:C:OP2	24:SG:190:ARG:NH2	2.39	0.56
50:P:14:HIS:HE1	50:P:120:VAL:H	1.52	0.56
57:W:15:ARG:NH1	57:W:16:ILE:O	2.38	0.56
79:t:129:C:O2	79:t:139:G:N2	2.38	0.56
1:S2:1351:G:C8	6:SF:56:TYR:HB2	2.38	0.56
1:S2:1593:C:O2	15:ST:12:GLN:NE2	2.39	0.56
1:S2:1804:U:OP1	57:W:67:LYS:NZ	2.39	0.56
19:Sa:45:VAL:HG21	19:Sa:64:LEU:HD13	1.88	0.56
22:Sg:202:PRO:HG2	22:Sg:243:PRO:HA	1.87	0.56
38:D:150:C:N4	43:I:52:THR:O	2.39	0.56
79:t:4433:U:H3	79:t:4446:G:H1	1.53	0.56
8:SI:83:TYR:HB3	8:SI:101:ILE:HB	1.87	0.55
36:B:384:GLU:OE2	58:X:14:TYR:OH	2.22	0.55
37:C:44:LEU:HD21	37:C:120:LYS:HE2	1.87	0.55
44:J:7:ASN:HB3	44:J:58:ASP:HB3	1.87	0.55
67:g:56:ASN:HB3	67:g:64:PRO:HB2	1.87	0.55
76:p:12:CYS:SG	76:p:19:GLN:NE2	2.77	0.55
1:S2:155:G:H4'	24:SG:15:LEU:HD13	1.87	0.55
1:S2:1812:U:O4	1:S2:1813:A:N6	2.37	0.55
6:SF:127:ARG:O	6:SF:135:ARG:NE	2.38	0.55
36:B:4:ARG:NH1	36:B:6:PHE:O	2.39	0.55
36:B:59:GLU:HB2	36:B:366:LYS:HD2	1.88	0.55
67:g:59:THR:HG23	67:g:60:PRO:HD3	1.87	0.55
72:l:35:LYS:HE2	79:t:2675:A:H62	1.70	0.55
5:SE:31:PRO:HG2	5:SE:38:LEU:HB2	1.88	0.55
5:SE:51:ARG:NH2	5:SE:109:PHE:O	2.38	0.55
13:SR:36:GLU:OE1	13:SR:47:ARG:NH1	2.38	0.55
21:Sd:6:LEU:HA	21:Sd:9:SER:HB3	1.87	0.55
36:B:167:GLN:HE22	36:B:204:GLN:HE21	1.54	0.55
45:K:188:LYS:HD2	45:K:212:LEU:HD13	1.87	0.55
1:S2:1354:G:N2	1:S2:1357:A:OP2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Z:80:ILE:HD11	60:Z:104:VAL:HG21	1.89	0.55
77:q:51:ALA:HB3	77:q:54:ILE:HD12	1.88	0.55
79:t:193:C:O2	79:t:218:C:O2'	2.25	0.55
1:S2:672:A:N6	1:S2:1027:A:OP1	2.35	0.55
1:S2:678:U:OP1	27:SN:127:ARG:NH1	2.39	0.55
37:C:209:ILE:HG13	37:C:251:ILE:HB	1.89	0.55
76:p:81:ARG:HH22	79:t:4256:C:H5''	1.71	0.55
42:H:148:LYS:HG3	42:H:245:ARG:HH21	1.72	0.55
64:d:103:ASP:HB2	64:d:106:ARG:HB2	1.87	0.55
1:S2:1464:C:H4'	13:SR:60:ARG:HH22	1.72	0.55
10:SL:23:VAL:HG23	10:SL:25:LEU:H	1.72	0.55
36:B:223:THR:O	36:B:343:ARG:NH1	2.40	0.55
38:D:141:C:O2'	49:O:136:ASP:OD2	2.25	0.55
57:W:21:PRO:HA	57:W:54:ALA:HA	1.89	0.55
62:b:100:ILE:HG22	62:b:123:ILE:HD11	1.88	0.55
74:n:94:MET:HG2	74:n:105:PRO:HA	1.89	0.55
76:p:28:LYS:O	79:t:4306:U:O2'	2.23	0.55
1:S2:10:G:H21	23:SC:114:LYS:HA	1.71	0.55
1:S2:1222:G:H4'	1:S2:1676:U:H3	1.72	0.55
1:S2:1418:C:H3'	1:S2:1419:C:H2'	1.88	0.55
3:SB:219:LYS:HE2	77:q:90:LYS:HA	1.88	0.55
7:SH:20:GLU:HA	7:SH:23:ILE:HB	1.88	0.55
8:SI:76:THR:OG1	8:SI:105:ASP:OD1	2.25	0.55
28:SO:75:MET:SD	28:SO:79:GLN:NE2	2.80	0.55
28:SO:137:SER:O	28:SO:138:ASP:HB3	2.06	0.55
79:t:221:U:O3'	79:t:238:G:N2	2.39	0.55
86:t:5110:MVM:C21	83:y:15:GLY:HA3	2.36	0.55
83:y:11:LEU:HD22	83:y:11:LEU:O	2.07	0.55
1:S2:1512:C:O2'	21:Sd:7:TYR:O	2.21	0.55
1:S2:1285:G:OP2	1:S2:1286:G:N2	2.40	0.55
3:SB:40:ASN:ND2	3:SB:75:GLN:OE1	2.39	0.55
13:SR:23:ARG:NH2	22:Sg:149:GLU:OE2	2.40	0.55
30:SY:6:THR:HB	30:SY:28:LEU:HB3	1.89	0.55
49:O:12:ARG:NH2	79:t:302:G:O6	2.40	0.55
50:P:133:ARG:NH1	79:t:2036:G:OP2	2.37	0.55
51:Q:146:ILE:HD12	51:Q:146:ILE:C	2.32	0.55
54:T:51:LEU:HD12	55:U:151:LEU:HD13	1.89	0.55
13:SR:28:PHE:HA	13:SR:55:THR:HG21	1.88	0.54
36:B:220:ILE:HG12	36:B:278:THR:HG22	1.88	0.54
53:S:110:ARG:NH1	79:t:2643:G:OP1	2.40	0.54
54:T:159:LEU:O	54:T:161:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:g:21:GLN:NE2	67:g:23:GLU:OE2	2.40	0.54
71:k:52:LYS:NZ	79:t:369:G:OP2	2.35	0.54
1:S2:659:G:HO2'	1:S2:662:G:HO2'	1.52	0.54
7:SH:69:LEU:HD13	7:SH:96:ALA:HB2	1.88	0.54
10:SL:13:GLN:NE2	10:SL:63:THR:OG1	2.39	0.54
13:SR:98:VAL:HG23	13:SR:119:VAL:HG12	1.90	0.54
17:SV:43:THR:OG1	17:SV:45:ARG:NH1	2.40	0.54
18:SX:41:PHE:O	18:SX:76:LYS:NZ	2.40	0.54
45:K:33:ILE:O	45:K:69:ARG:NH1	2.36	0.54
70:j:62:LYS:HE3	70:j:94:LEU:HD11	1.89	0.54
1:S2:683:OMG:N1	1:S2:1022:U:OP2	2.31	0.54
5:SE:104:ASP:HB3	5:SE:110:ALA:HB2	1.89	0.54
86:t:5110:MVM:N7	83:y:15:GLY:HA3	2.22	0.54
83:y:4:LEU:HB2	83:y:5:PRO:HD2	1.89	0.54
20:Sc:14:VAL:CG1	20:Sc:30:VAL:HB	2.37	0.54
79:t:205:A:N6	79:t:229:G:N7	2.56	0.54
37:C:340:ILE:HD13	41:G:51:VAL:HG21	1.90	0.54
68:h:90:ARG:NH1	79:t:4091:G:O3'	2.41	0.54
79:t:1227:G:H21	79:t:1228:C:H41	1.55	0.54
79:t:1951:A:N6	79:t:1996:U:OP2	2.41	0.54
4:SD:105:LEU:HD22	4:SD:122:VAL:HG11	1.89	0.54
35:A:38:HIS:O	35:A:93:LYS:NZ	2.38	0.54
37:C:282:HIS:ND1	37:C:284:MET:O	2.40	0.54
47:M:129:ARG:HH22	69:i:115:PRO:HB2	1.71	0.54
70:j:28:ARG:NH2	79:t:320:C:OP2	2.40	0.54
1:S2:936:G:H1	1:S2:1006:C:N4	2.06	0.54
7:SH:146:VAL:HA	7:SH:152:ARG:HA	1.88	0.54
9:SK:13:GLU:OE2	9:SK:38:LYS:NZ	2.35	0.54
55:U:87:LYS:NZ	79:t:4262:U:OP1	2.40	0.54
55:U:127:GLN:OE1	79:t:1816:G:N2	2.39	0.54
76:p:26:TYR:HB3	76:p:67:VAL:HG23	1.90	0.54
79:t:1084:C:H42	79:t:1177:G:H1	1.54	0.54
8:SI:67:TRP:HD1	8:SI:70:GLU:H	1.55	0.54
13:SR:27:ASP:O	13:SR:31:ASN:ND2	2.40	0.54
29:SW:115:GLU:HA	29:SW:118:ARG:NH1	2.22	0.54
53:S:130:ASN:ND2	79:t:1553:G:O2'	2.41	0.54
79:t:167:C:H42	79:t:260:C:H42	1.55	0.54
79:t:1263:C:O2'	79:t:1265:G:N7	2.37	0.54
35:A:40:TYR:HA	35:A:91:GLY:HA3	1.89	0.54
48:N:113:MET:HG3	79:t:4838:C:C4	2.43	0.54
52:R:180:ARG:NH2	79:t:1479:A:N7	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:143:LYS:HA	54:T:146:HIS:HD1	1.73	0.54
63:c:25:ARG:NH2	79:t:1825:G:OP1	2.41	0.54
79:t:652:C:N4	79:t:653:G:O6	2.40	0.54
79:t:2072:G:O2'	79:t:2241:G:N2	2.41	0.54
79:t:4379:C:N4	79:t:4384:A:O2'	2.41	0.54
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.73	0.54
37:C:330:PRO:HG3	42:H:47:ARG:HH21	1.74	0.54
67:g:22:ARG:NH2	79:t:2051:U:OP1	2.40	0.54
1:S2:1349:G:H2'	1:S2:1350:U:C2	2.42	0.53
2:SA:137:ALA:HB1	2:SA:142:LEU:HD22	1.89	0.53
6:SF:49:LEU:HD22	12:SQ:49:TYR:HB2	1.89	0.53
6:SF:138:ALA:O	6:SF:204:ARG:NH2	2.41	0.53
35:A:207:VAL:HG23	35:A:208:GLU:HG3	1.88	0.53
37:C:83:GLY:C	83:y:8:LEU:HD13	2.26	0.53
48:N:16:SER:HB3	48:N:56:GLN:HE21	1.73	0.53
1:S2:1533:A:OP1	6:SF:164:ARG:NH1	2.42	0.53
10:SL:59:LYS:HD3	10:SL:134:LEU:HD23	1.90	0.53
30:SY:83:LYS:NZ	30:SY:96:LEU:HB3	2.23	0.53
57:W:85:ARG:HH21	57:W:100:ASP:HA	1.74	0.53
62:b:123:ILE:HG22	62:b:143:ALA:HB3	1.89	0.53
1:S2:326:C:O2'	1:S2:328:U:N3	2.40	0.53
19:Sa:10:ARG:HG2	19:Sa:34:LYS:HB2	1.89	0.53
24:SG:181:THR:HG22	24:SG:183:ARG:H	1.72	0.53
29:SW:3:ARG:NH2	29:SW:9:ASP:OD2	2.42	0.53
53:S:7:GLN:NE2	53:S:35:ALA:O	2.42	0.53
79:t:216:G:H1	79:t:233:G:H1	1.56	0.53
1:S2:1036:A:N3	1:S2:1844:U:O2'	2.40	0.53
5:SE:126:VAL:HG22	5:SE:158:ASP:H	1.74	0.53
6:SF:60:ARG:HH11	17:SV:61:ARG:NH1	1.79	0.53
10:SL:115:PRO:O	10:SL:118:ARG:NH1	2.42	0.53
36:B:264:PHE:N	50:P:64:THR:O	2.41	0.53
58:X:11:TYR:OH	79:t:4999:G:N2	2.42	0.53
79:t:192:C:H42	79:t:240:A:H61	1.57	0.53
1:S2:1091:C:OP1	27:SN:9:LYS:NZ	2.34	0.53
35:A:13:GLY:O	35:A:17:ARG:NH1	2.41	0.53
66:f:128:ARG:NH2	79:t:2285:G:OP1	2.42	0.53
79:t:2532:A:H2	79:t:2744:A:H62	1.55	0.53
1:S2:150:A:N6	1:S2:169:U:O2	2.42	0.53
2:SA:191:ARG:NH1	17:SV:44:GLY:O	2.39	0.53
8:SI:57:ALA:HB2	8:SI:183:GLY:HA2	1.90	0.53
14:SS:4:VAL:HG12	14:SS:5:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Sc:14:VAL:HG12	20:Sc:30:VAL:HB	1.90	0.53
30:SY:55:ILE:HG13	30:SY:75:ILE:HG12	1.90	0.53
36:B:128:LYS:NZ	79:t:4924:A:OP1	2.41	0.53
68:h:10:ARG:NH1	79:t:2382:A:OP1	2.39	0.53
78:r:84:LYS:HB2	78:r:89:THR:HB	1.90	0.53
79:t:256:C:H3'	79:t:257:G:H8	1.72	0.53
79:t:1912:C:N4	79:t:2021:A:O2'	2.35	0.53
79:t:1963:G:O2'	79:t:1991:A:O2'	2.25	0.53
1:S2:1286:G:N2	26:SM:35:ILE:O	2.42	0.53
6:SF:204:ARG:HD3	20:Sc:60:GLU:HG2	1.91	0.53
18:SX:68:LYS:HD2	18:SX:91:LEU:HD22	1.91	0.53
20:Sc:31:ARG:HG2	20:Sc:31:ARG:O	2.08	0.53
30:SY:110:ARG:NH1	30:SY:127:ALA:O	2.42	0.53
51:Q:117:ILE:HD12	51:Q:148:MET:CE	2.30	0.53
54:T:115:ALA:O	54:T:118:ARG:NH1	2.41	0.53
1:S2:936:G:H1	1:S2:1006:C:H42	1.57	0.53
36:B:19:ARG:NH2	79:t:4585:G:OP1	2.41	0.53
39:E:99:G:N7	54:T:55:LYS:NZ	2.56	0.53
41:G:246:ARG:HH12	79:t:4898:C:H1'	1.73	0.53
51:Q:32:THR:HG23	51:Q:91:LEU:HD21	1.91	0.53
79:t:698:C:H42	79:t:1273:G:H1	1.56	0.53
1:S2:127:C:O2	5:SE:134:LYS:NZ	2.42	0.53
5:SE:31:PRO:HB3	5:SE:43:PRO:HB3	1.91	0.53
45:K:162:ARG:NH2	79:t:2014:A:OP1	2.42	0.53
49:O:31:ARG:NH1	49:O:124:ASP:OD2	2.42	0.53
8:SI:42:ARG:HH21	8:SI:59:ARG:HD3	1.74	0.53
10:SL:101:ARG:HG2	18:SX:7:LEU:HA	1.91	0.53
27:SN:75:LEU:HB3	27:SN:81:ALA:HB2	1.91	0.53
43:I:37:LYS:NZ	79:t:4095:C:OP1	2.42	0.53
2:SA:80:ARG:HD3	2:SA:82:THR:HG23	1.91	0.52
17:SV:77:GLY:CA	17:SV:81:LYS:NZ	2.72	0.52
18:SX:87:ASN:HD21	18:SX:134:TYR:HB2	1.73	0.52
37:C:211:TYR:HE1	37:C:229:LEU:HB3	1.74	0.52
40:F:211:LEU:HB3	40:F:219:TYR:HB2	1.90	0.52
41:G:266:GLN:HE22	79:t:4888:C:H5''	1.73	0.52
48:N:119:ARG:NH1	50:P:194:GLU:OE1	2.42	0.52
54:T:15:ARG:HB3	54:T:27:LEU:HB3	1.90	0.52
1:S2:1156:U:O4	23:SC:194:ARG:NH1	2.39	0.52
37:C:234:LYS:HD2	79:t:1356:A:H2	1.74	0.52
42:H:159:TYR:CD1	42:H:168:ALA:HA	2.44	0.52
46:L:112:HIS:HD2	46:L:126:TYR:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:d:81:LEU:HD21	64:d:94:LEU:HD23	1.90	0.52
78:r:13:CYS:SG	79:t:2317:C:O2'	2.66	0.52
78:r:39:ARG:NH1	78:r:105:ASP:OD2	2.40	0.52
79:t:2766:A:H2	79:t:2780:U:H3	1.56	0.52
1:S2:1310:U:H5''	34:Sf:130:VAL:HB	1.92	0.52
31:SZ:76:ARG:HE	31:SZ:77:LEU:HD12	1.75	0.52
45:K:31:ILE:HD12	45:K:34:PHE:HE1	1.75	0.52
55:U:115:LYS:HD3	55:U:126:VAL:HG21	1.92	0.52
55:U:130:ARG:NH2	79:t:1784:A:N3	2.58	0.52
1:S2:1867:U:H4'	1:S2:1868:U:H5'	1.91	0.52
8:SI:177:SER:OG	8:SI:182:CYS:SG	2.66	0.52
20:Sc:29:GLN:NE2	20:Sc:65:ALA:HB1	2.24	0.52
44:J:186:THR:O	44:J:189:GLN:NE2	2.43	0.52
48:N:104:MET:O	48:N:109:ARG:NH2	2.43	0.52
52:R:172:ARG:HD2	62:b:57:GLY:HA3	1.90	0.52
79:t:4973:G:O2'	79:t:4992:A:N6	2.41	0.52
1:S2:123:G:O3'	5:SE:148:ARG:NH2	2.42	0.52
3:SB:83:LYS:HE3	3:SB:106:THR:HG22	1.91	0.52
7:SH:44:ASN:OD1	7:SH:68:GLN:NE2	2.42	0.52
10:SL:111:VAL:HG12	10:SL:140:PHE:HB2	1.91	0.52
17:SV:19:ALA:O	29:SW:23:ARG:NH2	2.42	0.52
28:SO:34:PHE:HB3	28:SO:41:PHE:HB2	1.91	0.52
44:J:95:VAL:HG22	74:n:82:LEU:HB3	1.91	0.52
49:O:116:LEU:HD22	49:O:135:ILE:HD11	1.91	0.52
79:t:1074:C:O2	79:t:1188:G:N2	2.42	0.52
79:t:2827:G:O2'	79:t:3809:U:O4	2.21	0.52
83:y:0:SER:O	83:y:2:TRP:N	2.43	0.52
22:Sg:42:MET:HB2	22:Sg:57:ARG:HB2	1.90	0.52
24:SG:5:ILE:HD11	24:SG:113:ILE:HG13	1.92	0.52
27:SN:5:HIS:HB3	27:SN:117:LEU:HD23	1.91	0.52
51:Q:127:ARG:NH1	79:t:2399:A:OP2	2.43	0.52
66:f:78:LEU:O	78:r:20:ARG:NH1	2.42	0.52
79:t:4265:C:H2'	79:t:4267:G:H8	1.74	0.52
1:S2:1357:A:N3	25:SJ:70:ARG:HB3	2.25	0.52
22:Sg:199:THR:HG21	22:Sg:240:CYS:HA	1.89	0.52
41:G:273:SER:OG	79:t:4839:U:O2'	2.23	0.52
83:y:13:LEU:N	83:y:13:LEU:HD23	2.25	0.52
5:SE:87:MET:HE1	5:SE:236:ILE:HG21	1.92	0.52
7:SH:160:LYS:HA	7:SH:163:GLN:HB2	1.92	0.52
29:SW:83:LEU:HD11	29:SW:120:HIS:C	2.35	0.52
74:n:100:TYR:OH	79:t:4387:G:OP1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:y:12:LEU:HD12	83:y:13:LEU:O	2.09	0.52
1:S2:433:A:OP1	8:SI:25:ARG:NH1	2.38	0.52
18:SX:87:ASN:ND2	18:SX:90:CYS:SG	2.83	0.52
35:A:30:ARG:O	35:A:163:ARG:NH2	2.43	0.52
38:D:112:G:OP1	79:t:2758:C:O2'	2.24	0.52
47:M:28:GLN:HA	47:M:31:ARG:HG2	1.92	0.52
79:t:2390:C:O2'	79:t:2505:C:O2	2.27	0.52
79:t:4048:C:O2'	79:t:4134:A:N1	2.43	0.52
79:t:4069:G:N2	79:t:4077:G:OP2	2.40	0.52
1:S2:54:A:OP2	30:SY:111:LYS:NZ	2.38	0.52
2:SA:77:ILE:HD11	2:SA:124:VAL:HG22	1.91	0.52
3:SB:87:ILE:HG13	3:SB:101:HIS:HB2	1.92	0.52
11:SP:87:PRO:HB3	11:SP:112:ILE:HD11	1.92	0.52
22:Sg:10:THR:HG22	22:Sg:308:ARG:HG2	1.90	0.52
37:C:85:HIS:HD2	83:y:8:LEU:HG	1.75	0.52
41:G:94:LYS:NZ	79:t:680:C:OP1	2.43	0.52
45:K:140:THR:HB	45:K:144:ASN:HD22	1.73	0.52
83:y:16:PRO:HG2	83:y:20:ARG:NH1	2.25	0.52
1:S2:1060:A:O2'	1:S2:1062:A:N7	2.36	0.51
30:SY:18:LEU:O	30:SY:85:ASN:ND2	2.44	0.51
44:J:41:ILE:HG21	44:J:73:ILE:HD11	1.92	0.51
59:Y:104:ALA:O	59:Y:134:LYS:NZ	2.36	0.51
1:S2:1868:U:N3	19:Sa:98:PRO:O	2.44	0.51
42:H:62:ARG:NH1	79:t:932:U:OP2	2.43	0.51
5:SE:35:PRO:HD2	5:SE:83:PRO:HG2	1.91	0.51
19:Sa:87:ARG:O	19:Sa:89:ARG:NH1	2.44	0.51
24:SG:194:LEU:HD13	24:SG:197:GLN:HE21	1.75	0.51
37:C:83:GLY:H	83:y:10:LEU:HG	1.74	0.51
49:O:161:MET:O	79:t:54:G:N2	2.36	0.51
52:R:184:ARG:HH12	62:b:56:VAL:HA	1.74	0.51
60:Z:45:ARG:NH2	79:t:234:G:OP2	2.42	0.51
79:t:113:A:H62	79:t:155:A:H2	1.59	0.51
83:y:7:LEU:N	83:y:7:LEU:CD2	2.73	0.51
1:S2:1175:G:OP1	75:o:21:ARG:NH2	2.44	0.51
1:S2:1236:G:O6	14:SS:137:LYS:NZ	2.44	0.51
30:SY:91:LEU:HD12	30:SY:96:LEU:HD12	1.93	0.51
68:h:62:LYS:NZ	79:t:2495:G:O2'	2.44	0.51
79:t:161:G:H1	79:t:266:U:H3	1.59	0.51
79:t:176:G:H1	79:t:252:C:H41	1.57	0.51
1:S2:748:C:O2'	1:S2:794:A:N6	2.43	0.51
3:SB:70:SER:HA	3:SB:83:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SL:73:LEU:HD12	10:SL:140:PHE:HE2	1.74	0.51
22:Sg:252:THR:HG21	22:Sg:257:LYS:HE2	1.93	0.51
50:P:119:VAL:HG11	54:T:171:ARG:HD3	1.91	0.51
67:g:105:LEU:N	67:g:105:LEU:CD2	2.73	0.51
26:SM:69:LEU:HD11	26:SM:76:LEU:HD23	1.92	0.51
41:G:152:ILE:O	41:G:159:GLY:N	2.43	0.51
42:H:232:ASP:HB2	42:H:236:ARG:NH2	2.26	0.51
46:L:112:HIS:CD2	46:L:126:TYR:H	2.28	0.51
50:P:77:SER:HB3	50:P:106:ASP:HB2	1.93	0.51
22:Sg:20:GLN:HG2	22:Sg:68:ASP:HA	1.93	0.51
22:Sg:175:LYS:HE2	22:Sg:177:TRP:HE1	1.75	0.51
79:t:2092:G:H1'	79:t:2229:C:H42	1.74	0.51
79:t:2417:A:O2'	79:t:2419:U:OP2	2.27	0.51
1:S2:1340:U:OP2	1:S2:1341:C:O2'	2.24	0.51
2:SA:76:VAL:HG23	2:SA:123:VAL:HG13	1.93	0.51
42:H:35:LYS:NZ	79:t:2079:G:OP1	2.40	0.51
59:Y:81:LEU:HD13	59:Y:99:ILE:HD11	1.92	0.51
78:r:51:VAL:HG12	78:r:62:VAL:HG22	1.92	0.51
79:t:1939:A:O2'	79:t:2006:A:N1	2.37	0.51
1:S2:591:U:O2	1:S2:593:C:N4	2.43	0.51
3:SB:121:ILE:HD11	3:SB:207:LEU:HD21	1.92	0.51
5:SE:183:VAL:HG13	5:SE:189:LEU:HA	1.93	0.51
48:N:11:ARG:HE	48:N:61:ILE:HG22	1.76	0.51
49:O:116:LEU:HD23	49:O:133:ILE:HD11	1.92	0.51
50:P:54:TYR:OH	50:P:73:PHE:O	2.28	0.51
50:P:179:LYS:HE3	79:t:4830:G:C8	2.46	0.51
79:t:1308:C:N4	79:t:3851:G:OP1	2.44	0.51
1:S2:1414:A:O2'	15:ST:128:GLN:NE2	2.44	0.51
1:S2:1424:G:H21	15:ST:3:GLY:HA3	1.76	0.51
29:SW:112:ASP:HB2	29:SW:115:GLU:H	1.75	0.51
47:M:77:SER:HB2	47:M:102:ARG:HD2	1.93	0.51
54:T:158:VAL:HG12	54:T:161:ARG:HH21	1.76	0.51
59:Y:48:ARG:HB3	79:t:2451:A:H1'	1.93	0.51
2:SA:57:LYS:HD3	17:SV:70:LEU:HD12	1.93	0.50
8:SI:67:TRP:NE1	8:SI:70:GLU:OE1	2.35	0.50
27:SN:3:ARG:HG2	27:SN:6:ALA:HB3	1.93	0.50
48:N:96:GLU:OE2	48:N:100:ARG:NH2	2.44	0.50
55:U:108:ARG:HA	55:U:111:GLU:HG3	1.92	0.50
83:y:4:LEU:N	83:y:4:LEU:CD1	2.73	0.50
14:SS:25:LYS:HA	14:SS:55:ARG:HA	1.93	0.50
24:SG:32:MET:HB2	24:SG:100:CYS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Sf:139:HIS:O	34:Sf:147:THR:OG1	2.26	0.50
48:N:46:ARG:NH2	79:t:924:U:OP1	2.44	0.50
1:S2:38:A:O3'	25:SJ:5:ARG:NH1	2.45	0.50
1:S2:1401:A:H4'	16:SU:52:GLY:HA3	1.93	0.50
23:SC:211:LYS:HG2	23:SC:215:MET:HE2	1.93	0.50
44:J:59:LYS:HE2	44:J:66:GLU:HB3	1.92	0.50
57:W:13:LYS:O	79:t:4579:G:O2'	2.27	0.50
62:b:25:HIS:CD2	79:t:1321:G:H22	2.29	0.50
71:k:30:GLN:NE2	79:t:1602:U:OP2	2.44	0.50
79:t:2524:U:OP2	79:t:2525:G:N2	2.45	0.50
1:S2:72:C:N4	24:SG:169:PRO:O	2.44	0.50
1:S2:917:U:H1'	7:SH:118:ARG:HD2	1.92	0.50
14:SS:15:VAL:HG12	14:SS:16:LEU:HD12	1.94	0.50
17:SV:16:LYS:HB3	17:SV:23:ILE:HD13	1.93	0.50
17:SV:74:LYS:O	17:SV:81:LYS:NZ	2.43	0.50
38:D:95:A:H5'	71:k:82:THR:HA	1.94	0.50
49:O:172:ARG:NH1	79:t:62:A:OP1	2.45	0.50
62:b:114:LYS:HE2	79:t:1380:A:H8	1.76	0.50
72:l:26:LYS:HE3	79:t:2674:A:H5''	1.93	0.50
79:t:1320:A:H62	79:t:2325:C:H5	1.58	0.50
79:t:1414:C:H42	79:t:1435:A:H61	1.58	0.50
79:t:4562:G:O2'	79:t:4571:G:O6	2.23	0.50
79:t:4726:A:H61	79:t:4826:G:H22	1.60	0.50
1:S2:17:C:O2'	1:S2:1194:A:N1	2.42	0.50
1:S2:1829:G:H1'	1:S2:1850:MA6:H2	1.92	0.50
2:SA:147:LEU:HA	2:SA:161:ILE:HB	1.93	0.50
12:SQ:19:ALA:HB2	12:SQ:75:GLY:HA3	1.93	0.50
18:SX:40:PRO:HA	18:SX:79:LYS:HD2	1.94	0.50
38:D:66:A:H5''	69:i:7:ARG:HH21	1.76	0.50
42:H:35:LYS:NZ	79:t:2077:U:OP1	2.44	0.50
79:t:742:G:N2	79:t:743:G:O6	2.44	0.50
83:y:10:LEU:C	83:y:10:LEU:HD22	2.36	0.50
2:SA:205:ARG:HE	2:SA:206:ASP:H	1.59	0.50
20:Sc:44:ARG:NH1	20:Sc:60:GLU:OE2	2.39	0.50
36:B:114:CYS:HG	36:B:165:HIS:CE1	2.29	0.50
48:N:7:VAL:HG12	48:N:57:LEU:HD21	1.94	0.50
52:R:91:ARG:HG3	62:b:76:ASP:HB3	1.94	0.50
54:T:85:ASP:HB2	54:T:123:SER:HB2	1.92	0.50
54:T:101:THR:HG23	54:T:104:GLY:H	1.76	0.50
57:W:48:ARG:HG2	57:W:51:ARG:HE	1.76	0.50
79:t:1078:A:H2	79:t:1183:G:H22	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:189:U:H3	1:S2:210:U:H3	1.59	0.50
4:SD:45:ARG:NH1	4:SD:84:VAL:O	2.43	0.50
49:O:113:LEU:HB3	49:O:134:LEU:HD12	1.94	0.50
61:a:136:PHE:O	79:t:4091:G:O2'	2.30	0.50
79:t:3879:A:N1	83:y:21:ALA:O	2.45	0.50
56:V:60:VAL:HG11	56:V:76:VAL:HG23	1.94	0.50
58:X:19:ARG:NH2	79:t:4592:G:O5'	2.45	0.50
62:b:114:LYS:HE2	79:t:1380:A:C8	2.47	0.50
79:t:457:A:H61	79:t:685:C:H42	1.59	0.50
83:y:9:LEU:HD13	83:y:11:LEU:H	1.76	0.50
1:S2:429:C:OP1	5:SE:10:LYS:NZ	2.42	0.50
1:S2:575:A:OP1	30:SY:93:ARG:NH2	2.44	0.50
1:S2:1240:A:N3	1:S2:1267:C:O2'	2.43	0.50
17:SV:17:CYS:HB2	17:SV:56:CYS:HB3	1.93	0.50
41:G:161:ARG:O	41:G:182:ASN:ND2	2.38	0.50
41:G:183:ARG:HD3	79:t:4894:G:C6	2.47	0.50
1:S2:656:G:O2'	23:SC:227:ARG:NH2	2.45	0.49
1:S2:1352:G:H5'	6:SF:62:ARG:H	1.77	0.49
4:SD:28:GLU:OE2	4:SD:65:ARG:NH2	2.42	0.49
7:SH:34:SER:HB2	7:SH:78:ARG:HD3	1.94	0.49
8:SI:6:ASP:OD2	8:SI:8:TRP:NE1	2.44	0.49
25:SJ:108:ARG:HH12	25:SJ:154:GLN:HG3	1.77	0.49
38:D:62:A:OP1	69:i:52:LYS:NZ	2.42	0.49
39:E:6:C:H4'	40:F:52:ILE:HD13	1.94	0.49
42:H:60:GLU:OE2	42:H:192:HIS:NE2	2.45	0.49
56:V:101:ARG:NH2	79:t:2602:A:OP1	2.45	0.49
1:S2:686:U:O2	7:SH:118:ARG:NH2	2.45	0.49
1:S2:1235:G:H21	11:SP:135:ALA:HB2	1.76	0.49
18:SX:90:CYS:HA	18:SX:93:PHE:HD2	1.77	0.49
36:B:292:LEU:HB2	36:B:299:ILE:HD11	1.92	0.49
40:F:166:ALA:HB1	40:F:171:LEU:HD12	1.95	0.49
60:Z:10:ASP:OD1	60:Z:10:ASP:N	2.34	0.49
64:d:47:ILE:HD12	64:d:94:LEU:HD11	1.94	0.49
80:u:27:G:H22	80:u:43:C:H5	1.60	0.49
1:S2:441:C:OP1	8:SI:2:GLY:N	2.45	0.49
1:S2:1272:C:H4'	21:Sd:2:GLY:HA3	1.93	0.49
4:SD:106:ARG:HH21	4:SD:174:HIS:H	1.59	0.49
11:SP:110:GLU:HB3	14:SS:117:ILE:HG21	1.95	0.49
15:ST:5:THR:HG23	15:ST:7:LYS:H	1.77	0.49
16:SU:63:ILE:HD11	21:Sd:31:ILE:HD13	1.94	0.49
38:D:60:G:O6	69:i:62:ASN:ND2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M:18:TRP:NE1	79:t:1498:G:O2'	2.45	0.49
47:M:114:VAL:HG12	47:M:118:LYS:HE3	1.94	0.49
79:t:2850:A:H62	79:t:2857:G:H21	1.58	0.49
79:t:4936:G:O2'	79:t:4939:G:N1	2.42	0.49
32:Sb:56:CYS:SG	32:Sb:57:VAL:N	2.84	0.49
36:B:50:LYS:HB3	36:B:345:LEU:HD21	1.95	0.49
37:C:235:LEU:HD23	37:C:240:LEU:HD11	1.93	0.49
42:H:95:ILE:HD12	42:H:96:ARG:HG2	1.94	0.49
47:M:21:ARG:HH12	49:O:196:ASN:HB3	1.77	0.49
51:Q:69:ARG:NH2	79:t:4938:C:N3	2.59	0.49
61:a:22:LYS:HE3	61:a:134:LEU:HB2	1.94	0.49
76:p:80:LYS:HE2	79:t:4308:U:H5''	1.94	0.49
17:SV:77:GLY:HA2	17:SV:81:LYS:CE	2.43	0.49
40:F:155:THR:HG22	40:F:179:ARG:HA	1.95	0.49
41:G:216:TYR:OH	41:G:249:ASP:OD2	2.31	0.49
41:G:244:GLU:HA	41:G:247:LYS:HZ1	1.77	0.49
79:t:198:C:H42	79:t:209:A:H61	1.60	0.49
79:t:1061:A:H2	79:t:1216:G:H22	1.59	0.49
1:S2:1084:A:OP1	1:S2:1858:G:O2'	2.30	0.49
2:SA:36:GLN:O	2:SA:53:ARG:NH1	2.45	0.49
3:SB:138:PHE:O	3:SB:213:ARG:N	2.44	0.49
42:H:158:GLY:CA	42:H:169:LEU:HD21	2.42	0.49
43:I:63:LEU:HD11	49:O:29:GLN:HG2	1.94	0.49
53:S:117:ARG:HH11	79:t:2642:G:H4'	1.77	0.49
56:V:48:LYS:NZ	79:t:2609:U:OP1	2.43	0.49
62:b:72:THR:HG22	62:b:110:LYS:HB3	1.93	0.49
78:r:63:VAL:HG12	78:r:79:ARG:HB3	1.94	0.49
79:t:1789:C:O2	79:t:1814:G:N2	2.46	0.49
1:S2:924:G:OP1	27:SN:3:ARG:NE	2.40	0.49
1:S2:1654:G:OP1	15:ST:82:ARG:NH2	2.45	0.49
2:SA:159:ILE:HD11	17:SV:34:MET:HE1	1.94	0.49
4:SD:28:GLU:HA	9:SK:61:GLN:HE22	1.77	0.49
10:SL:68:ILE:HD11	10:SL:129:GLY:HA3	1.95	0.49
13:SR:28:PHE:HZ	13:SR:48:ASN:HB2	1.77	0.49
25:SJ:114:VAL:HG21	25:SJ:135:ILE:HD13	1.92	0.49
37:C:165:LYS:NZ	79:t:219:C:O2	2.46	0.49
37:C:190:ARG:NH1	79:t:2274:C:OP1	2.46	0.49
37:C:343:GLN:HE22	79:t:934:C:H1'	1.76	0.49
41:G:206:VAL:HG13	41:G:207:LYS:H	1.76	0.49
53:S:139:MET:O	53:S:143:HIS:ND1	2.35	0.49
66:f:4:LEU:O	66:f:121:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:h:101:LYS:HA	68:h:104:VAL:HG12	1.93	0.49
69:i:109:ARG:HA	69:i:112:ARG:HG2	1.93	0.49
79:t:2373:G:N2	79:t:2798:U:OP2	2.46	0.49
79:t:2453:G:O2'	79:t:2481:G:N2	2.46	0.49
1:S2:1120:U:OP1	32:Sb:72:ARG:NE	2.46	0.49
12:SQ:31:LEU:HD11	12:SQ:33:LYS:HE3	1.93	0.49
18:SX:19:ASP:HA	18:SX:22:TRP:HD1	1.78	0.49
24:SG:63:MET:HG2	24:SG:98:ARG:HD2	1.93	0.49
37:C:83:GLY:O	83:y:8:LEU:HD13	2.12	0.49
47:M:28:GLN:HG3	47:M:29:PRO:HD3	1.95	0.49
55:U:129:LYS:HE2	79:t:1817:G:H4'	1.95	0.49
79:t:3878:G:N1	83:y:23:GLU:HG3	2.27	0.49
83:y:10:LEU:O	83:y:10:LEU:HD22	2.12	0.49
1:S2:346:C:H5''	5:SE:38:LEU:HD22	1.94	0.49
26:SM:26:LEU:HD22	26:SM:31:LEU:HD21	1.95	0.49
35:A:225:ILE:HD11	35:A:238:ILE:HG12	1.95	0.49
37:C:60:HIS:CE1	37:C:100:ARG:HE	2.31	0.49
41:G:110:ARG:NH2	79:t:955:C:O4'	2.46	0.49
49:O:60:VAL:HG13	49:O:134:LEU:HB2	1.94	0.49
51:Q:15:CYS:SG	51:Q:16:LYS:N	2.86	0.49
66:f:112:VAL:HG23	66:f:122:VAL:HG11	1.94	0.49
79:t:1846:G:N2	79:t:1849:A:OP2	2.35	0.49
83:y:12:LEU:CD1	83:y:12:LEU:C	2.86	0.49
4:SD:132:LYS:HE3	4:SD:156:LEU:HD11	1.95	0.49
6:SF:59:LYS:CE	23:SC:87:PRO:HB3	2.37	0.49
40:F:152:ARG:O	40:F:157:ASN:ND2	2.46	0.49
42:H:94:ARG:NH2	42:H:97:GLY:O	2.45	0.49
79:t:4493:U:C4	83:y:24:ASP:OD1	2.65	0.49
27:SN:46:THR:H	27:SN:49:GLN:HE21	1.61	0.48
29:SW:102:ILE:HG13	29:SW:113:HIS:HB3	1.94	0.48
47:M:59:VAL:HG13	79:t:74:G:H5'	1.93	0.48
66:f:89:LEU:HD13	66:f:118:LEU:HD22	1.94	0.48
68:h:66:ARG:NH1	79:t:2496:A:O2'	2.45	0.48
79:t:358:G:O2'	79:t:369:G:O6	2.28	0.48
79:t:1953:G:H1	79:t:1975:C:H42	1.59	0.48
79:t:4915:C:N3	79:t:4916:C:N4	2.61	0.48
1:S2:838:G:H1'	1:S2:839:C:H3'	1.96	0.48
1:S2:974:C:O2	28:SO:55:ARG:NH1	2.46	0.48
2:SA:107:THR:HG23	2:SA:115:ALA:O	2.13	0.48
37:C:318:PRO:HG3	37:C:324:ILE:HG22	1.94	0.48
47:M:77:SER:OG	47:M:102:ARG:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:h:41:ALA:HB3	68:h:52:ARG:HB3	1.94	0.48
79:t:1229:G:N2	79:t:1247:C:O2	2.46	0.48
79:t:1977:C:N4	79:t:1981:G:OP2	2.32	0.48
1:S2:193:C:O2'	1:S2:195:C:N4	2.39	0.48
6:SF:123:GLU:OE1	6:SF:204:ARG:NH1	2.43	0.48
15:ST:128:GLN:HA	15:ST:131:LEU:HD23	1.95	0.48
23:SC:105:GLU:HG2	23:SC:216:MET:HE1	1.95	0.48
24:SG:137:ARG:HD2	24:SG:178:ARG:HD3	1.95	0.48
43:I:104:PRO:HG2	43:I:194:VAL:HG23	1.96	0.48
44:J:5:LEU:HD22	44:J:60:TRP:CZ3	2.48	0.48
49:O:39:ALA:HB2	49:O:63:ARG:HE	1.78	0.48
2:SA:80:ARG:NH2	2:SA:126:ASP:OD2	2.42	0.48
26:SM:93:LYS:HG3	26:SM:102:LYS:H	1.77	0.48
35:A:117:GLU:HG2	35:A:124:GLY:H	1.78	0.48
42:H:159:TYR:N	42:H:169:LEU:HD22	2.28	0.48
45:K:37:GLY:HA3	45:K:86:HIS:HA	1.95	0.48
45:K:138:ILE:HD11	45:K:148:VAL:HG22	1.95	0.48
67:g:81:SER:O	67:g:81:SER:OG	2.30	0.48
1:S2:303:C:O2	8:SI:184:ARG:NH1	2.47	0.48
1:S2:990:A:OP1	3:SB:116:LYS:NZ	2.34	0.48
4:SD:5:ILE:HD13	4:SD:9:ARG:HG3	1.95	0.48
37:C:54:VAL:HG22	38:D:27:U:H4'	1.96	0.48
47:M:127:PHE:HB2	69:i:118:LYS:HG3	1.95	0.48
54:T:95:ARG:NH1	79:t:1932:G:O3'	2.46	0.48
65:e:97:ASP:OD1	65:e:97:ASP:N	2.45	0.48
79:t:123:C:H42	79:t:144:A:H61	1.59	0.48
1:S2:1350:U:H2'	6:SF:56:TYR:HD2	1.79	0.48
1:S2:1863:A:OP2	19:Sa:4:LYS:NZ	2.38	0.48
7:SH:144:ILE:HD11	7:SH:152:ARG:HD3	1.95	0.48
16:SU:38:ASP:OD1	16:SU:41:ARG:NH2	2.46	0.48
41:G:277:LEU:HB3	67:g:4:ARG:HH21	1.78	0.48
53:S:59:SER:HA	79:t:2613:C:H5'	1.95	0.48
54:T:98:ARG:HH22	79:t:737:A:N6	2.12	0.48
24:SG:217:MET:O	24:SG:221:LYS:NZ	2.43	0.48
28:SO:27:VAL:HG13	28:SO:90:ILE:HD12	1.96	0.48
36:B:114:CYS:HG	36:B:165:HIS:CG	2.31	0.48
41:G:243:THR:O	41:G:247:LYS:N	2.39	0.48
53:S:93:VAL:HG11	79:t:2704:A:H1'	1.94	0.48
60:Z:69:LYS:HG2	60:Z:83:GLU:HG2	1.96	0.48
79:t:4485:A:H5''	79:t:4486:G:H5'	1.96	0.48
1:S2:1528:G:O2'	1:S2:1666:C:OP1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:109:THR:O	6:SF:62:ARG:NE	2.47	0.48
2:SA:144:THR:OG1	2:SA:156:TYR:O	2.32	0.48
17:SV:59:ILE:HD11	32:Sb:3:LEU:HD11	1.95	0.48
24:SG:221:LYS:HA	24:SG:224:ARG:HB3	1.96	0.48
36:B:142:GLY:HA2	36:B:145:GLN:HE21	1.79	0.48
37:C:33:ARG:HG3	37:C:122:TYR:HE1	1.78	0.48
37:C:153:VAL:HG12	37:C:252:TRP:HB2	1.95	0.48
45:K:182:GLU:HA	45:K:185:VAL:HG12	1.96	0.48
61:a:11:VAL:HG12	61:a:82:PRO:HA	1.95	0.48
79:t:3625:G:O2'	79:t:3664:U:OP1	2.30	0.48
1:S2:1100:A:O3'	13:SR:132:ARG:NH1	2.47	0.48
1:S2:1299:A:O2'	1:S2:1301:A:OP1	2.30	0.48
1:S2:1527:C:H5'	12:SQ:142:GLN:HB3	1.96	0.48
2:SA:38:ILE:HD11	2:SA:47:TYR:HB3	1.96	0.48
8:SI:106:SER:HB3	8:SI:171:LEU:HD13	1.96	0.48
41:G:190:HIS:HD2	41:G:192:LYS:HG2	1.79	0.48
79:t:402:A:H4'	79:t:403:G:H3'	1.96	0.48
79:t:2398:C:H5	79:t:2406:G:H1	1.61	0.48
1:S2:496:C:H5'	5:SE:29:PRO:HA	1.95	0.48
3:SB:31:TYR:HD2	3:SB:62:LEU:HD11	1.78	0.48
16:SU:32:LEU:HD21	16:SU:85:HIS:HB2	1.96	0.48
53:S:42:ARG:HA	53:S:45:ILE:HD12	1.95	0.48
79:t:1982:G:O6	79:t:1984:G:N2	2.42	0.48
1:S2:96:C:H1'	1:S2:474:G:H5'	1.96	0.47
1:S2:308:G:OP2	8:SI:53:LYS:NZ	2.45	0.47
1:S2:529:A:N6	1:S2:555:A:N7	2.60	0.47
1:S2:944:A:H5''	28:SO:134:PRO:HB3	1.96	0.47
1:S2:1490:G:N2	16:SU:72:GLU:OE1	2.47	0.47
5:SE:129:ILE:HG22	5:SE:139:LEU:HB3	1.96	0.47
11:SP:41:GLN:HG3	11:SP:84:ILE:HD12	1.95	0.47
30:SY:56:PHE:CD1	30:SY:94:HIS:HE1	2.32	0.47
38:D:51:U:OP2	73:m:21:ARG:NH2	2.44	0.47
40:F:41:LYS:NZ	55:U:32:ARG:O	2.36	0.47
42:H:80:ASN:HD22	55:U:143:THR:H	1.60	0.47
44:J:58:ASP:OD1	44:J:58:ASP:N	2.44	0.47
48:N:14:TYR:HB3	48:N:56:GLN:HB3	1.95	0.47
49:O:22:LEU:HD12	49:O:26:ARG:HH21	1.79	0.47
66:f:99:ILE:HG23	66:f:111:ILE:HD11	1.95	0.47
72:l:23:VAL:HG22	72:l:36:VAL:HG22	1.96	0.47
79:t:1424:C:H42	79:t:2084:G:H1	1.62	0.47
79:t:2231:G:N2	79:t:2232:A:N7	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:830:A:OP2	1:S2:846:G:N2	2.47	0.47
62:b:92:LYS:HG3	62:b:94:LYS:HZ2	1.79	0.47
1:S2:1130:G:OP2	1:S2:1130:G:N2	2.36	0.47
1:S2:1352:G:N3	6:SF:64:ALA:HA	2.29	0.47
2:SA:3:GLY:HA3	2:SA:59:LEU:HD13	1.96	0.47
69:i:97:LYS:O	69:i:101:ASN:ND2	2.47	0.47
70:j:29:ARG:NH2	79:t:270:C:N3	2.57	0.47
79:t:3612:U:H5'	79:t:3613:A:H5''	1.95	0.47
1:S2:507:G:OP2	30:SY:104:ARG:NH2	2.47	0.47
1:S2:691:G:OP2	1:S2:691:G:N2	2.41	0.47
29:SW:89:TRP:HE3	29:SW:93:LEU:HD21	1.79	0.47
55:U:115:LYS:HE3	55:U:128:LEU:HB3	1.96	0.47
57:W:16:ILE:HB	57:W:88:TYR:HB2	1.96	0.47
70:j:34:THR:OG1	79:t:270:C:OP2	2.32	0.47
1:S2:921:G:C2	32:Sb:22:LYS:HG2	2.49	0.47
1:S2:1340:U:H3'	1:S2:1341:C:H2'	1.95	0.47
2:SA:42:LYS:HD3	2:SA:46:ILE:HB	1.95	0.47
13:SR:57:LEU:HA	13:SR:60:ARG:HB3	1.97	0.47
18:SX:68:LYS:HB3	18:SX:91:LEU:HD13	1.95	0.47
22:Sg:34:ALA:HB2	22:Sg:69:VAL:HG12	1.96	0.47
41:G:219:LYS:NZ	79:t:1275:C:OP1	2.40	0.47
1:S2:1597:C:OP2	31:SZ:85:ARG:NH2	2.41	0.47
5:SE:214:ASN:HA	23:SC:192:LEU:HG	1.94	0.47
37:C:83:GLY:O	83:y:8:LEU:CD1	2.62	0.47
40:F:22:ARG:HD2	40:F:27:LYS:HB2	1.96	0.47
52:R:108:ARG:NH1	79:t:1338:G:OP1	2.43	0.47
65:e:88:LEU:HG	65:e:106:VAL:HG22	1.97	0.47
1:S2:165:G:OP2	1:S2:165:G:N2	2.43	0.47
1:S2:682:U:P	18:SX:8:ARG:HE	2.37	0.47
1:S2:1242:U:O2	1:S2:1517:G:O2'	2.30	0.47
3:SB:123:ALA:HB2	3:SB:165:ARG:HG3	1.96	0.47
8:SI:124:LYS:HD2	8:SI:167:GLN:HE21	1.79	0.47
9:SK:26:ASP:O	9:SK:42:ASN:ND2	2.48	0.47
14:SS:98:VAL:HG11	14:SS:106:LYS:HD3	1.97	0.47
16:SU:21:ARG:HD3	16:SU:88:LEU:HD21	1.95	0.47
19:Sa:4:LYS:HG2	19:Sa:5:ARG:HG3	1.97	0.47
25:SJ:65:GLU:O	25:SJ:66:LYS:HG3	2.15	0.47
29:SW:2:VAL:HG13	29:SW:4:MET:HE2	1.97	0.47
37:C:94:ASN:HD21	79:t:1502:C:H4'	1.79	0.47
43:I:244:PRO:HA	43:I:247:VAL:HG12	1.97	0.47
49:O:135:ILE:HD12	49:O:151:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S:105:LEU:HD23	53:S:138:LEU:HD12	1.96	0.47
62:b:2:PRO:HG2	79:t:1491:C:H5''	1.96	0.47
66:f:108:ARG:NH1	79:t:2305:G:OP1	2.42	0.47
79:t:2693:G:H2'	79:t:2694:G:H8	1.79	0.47
79:t:4601:G:H1	79:t:4622:G:H22	1.63	0.47
1:S2:1824:A:P	18:SX:61:GLN:HE22	2.37	0.47
43:I:145:THR:O	43:I:149:ASN:ND2	2.48	0.47
45:K:91:LEU:HD21	45:K:135:ILE:HG12	1.97	0.47
47:M:81:LEU:HD23	47:M:117:LEU:HD21	1.97	0.47
68:h:24:ARG:HG3	79:t:2618:U:H5''	1.96	0.47
79:t:2314:C:H2'	79:t:2315:G:H8	1.79	0.47
80:u:54:U:H2'	80:u:55:U:H5	1.80	0.47
3:SB:229:MET:HB3	79:t:4071:C:H5'	1.97	0.47
12:SQ:94:ALA:HA	12:SQ:97:GLN:HG2	1.97	0.47
12:SQ:146:ARG:NH2	81:v:35:C:OP2	2.48	0.47
36:B:175:GLN:HG3	79:t:4943:U:H4'	1.97	0.47
62:b:6:ARG:HG3	62:b:8:THR:HG22	1.96	0.47
74:n:100:TYR:O	79:t:4434:G:O2'	2.32	0.47
79:t:131:C:H2'	79:t:132:G:C4	2.50	0.47
79:t:1304:G:OP1	79:t:1861:G:O2'	2.28	0.47
79:t:1928:U:O2	79:t:4655:C:N4	2.40	0.47
79:t:4832:A:H1'	79:t:4834:U:C2	2.49	0.47
1:S2:1228:A:H2'	1:S2:1229:G:C8	2.50	0.47
1:S2:1244:U:H2'	1:S2:1245:G:H8	1.79	0.47
2:SA:215:GLN:HA	2:SA:218:ALA:HB3	1.97	0.47
7:SH:49:LYS:HG3	7:SH:51:ILE:HG23	1.96	0.47
16:SU:99:LYS:NZ	16:SU:103:SER:OG	2.47	0.47
37:C:134:PRO:HG3	37:C:150:LEU:HG	1.97	0.47
2:SA:109:THR:O	6:SF:62:ARG:HD2	2.16	0.46
23:SC:229:CYS:SG	23:SC:232:THR:OG1	2.62	0.46
36:B:3:HIS:ND1	79:t:4478:G:OP2	2.46	0.46
39:E:23:A:N3	39:E:118:C:O2'	2.43	0.46
44:J:92:MET:HE2	44:J:181:VAL:HG12	1.96	0.46
49:O:64:ILE:HD11	49:O:102:ALA:HA	1.96	0.46
50:P:14:HIS:CE1	50:P:120:VAL:H	2.31	0.46
51:Q:84:PRO:HB2	51:Q:87:SER:HB3	1.97	0.46
52:R:67:ILE:HD11	52:R:92:VAL:HG21	1.96	0.46
61:a:84:ARG:NH1	68:h:99:GLU:OE1	2.34	0.46
79:t:4693:G:H1'	79:t:4694:G:H2'	1.96	0.46
1:S2:1398:G:H1'	22:Sg:63:SER:HB3	1.97	0.46
4:SD:101:GLN:HE22	4:SD:188:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SI:113:TYR:OH	8:SI:156:ALA:O	2.32	0.46
12:SQ:58:LEU:HD11	12:SQ:112:LEU:HD11	1.97	0.46
47:M:169:ILE:H	47:M:169:ILE:HG13	1.45	0.46
53:S:23:TRP:CD1	53:S:50:ILE:HG12	2.50	0.46
61:a:31:ASP:N	61:a:31:ASP:OD1	2.48	0.46
79:t:492:C:O2'	79:t:495:C:N4	2.46	0.46
79:t:1742:G:H2'	79:t:1743:G:H8	1.79	0.46
83:y:11:LEU:C	83:y:11:LEU:CD2	2.86	0.46
1:S2:368:U:OP1	1:S2:369:C:O2'	2.27	0.46
5:SE:216:ASN:HD21	23:SC:190:SER:HB2	1.80	0.46
11:SP:38:SER:OG	11:SP:41:GLN:OE1	2.33	0.46
11:SP:108:LYS:HG2	11:SP:111:MET:HE3	1.95	0.46
25:SJ:60:LEU:HD22	25:SJ:70:ARG:HG3	1.96	0.46
30:SY:4:THR:OG1	30:SY:32:LYS:NZ	2.48	0.46
47:M:49:ARG:HD2	69:i:118:LYS:HA	1.97	0.46
60:Z:14:ASN:ND2	79:t:224:A:O2'	2.48	0.46
71:k:20:ARG:NH1	71:k:39:TYR:OH	2.49	0.46
77:q:9:GLY:O	79:t:1535:A:O2'	2.28	0.46
79:t:1572:C:H3'	79:t:1573:U:H4'	1.97	0.46
79:t:1769:A:N3	79:t:4172:U:O2'	2.47	0.46
79:t:1853:G:O2'	79:t:4181:A:N3	2.37	0.46
79:t:4597:A:H2	79:t:4625:G:H21	1.63	0.46
83:y:4:LEU:C	83:y:4:LEU:CD2	2.88	0.46
1:S2:1648:G:N2	1:S2:1675:A:OP2	2.35	0.46
6:SF:68:ILE:H	6:SF:68:ILE:HG13	1.58	0.46
10:SL:103:GLU:HG3	18:SX:11:ARG:HB2	1.98	0.46
49:O:68:ARG:NH2	79:t:297:C:OP2	2.47	0.46
59:Y:51:THR:HG21	79:t:11:G:H1'	1.97	0.46
83:y:4:LEU:HD13	83:y:4:LEU:H	1.78	0.46
1:S2:396:U:HO2'	1:S2:401:A:HO2'	1.64	0.46
1:S2:579:C:H42	30:SY:61:ARG:HH22	1.64	0.46
1:S2:1016:U:O5'	27:SN:14:SER:OG	2.33	0.46
2:SA:37:TYR:OH	2:SA:57:LYS:NZ	2.47	0.46
4:SD:76:ARG:HB2	9:SK:22:VAL:HG11	1.98	0.46
5:SE:123:LEU:HD22	5:SE:228:ILE:HG22	1.98	0.46
5:SE:214:ASN:HD22	5:SE:244:ILE:HG21	1.80	0.46
37:C:134:PRO:HA	37:C:137:VAL:HG12	1.98	0.46
67:g:109:ARG:CD	67:g:109:ARG:N	2.73	0.46
73:m:27:ILE:O	73:m:33:ASN:ND2	2.47	0.46
79:t:457:A:H61	79:t:685:C:N4	2.13	0.46
1:S2:1001:A:N7	19:Sa:19:GLN:NE2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:137:LEU:HD11	3:SB:176:VAL:HG21	1.96	0.46
5:SE:193:GLY:HA3	5:SE:212:ASP:HA	1.98	0.46
6:SF:201:LYS:HA	6:SF:204:ARG:HB2	1.97	0.46
7:SH:10:LYS:HG3	7:SH:20:GLU:HG2	1.98	0.46
10:SL:4:ILE:HD11	10:SL:54:THR:HG23	1.97	0.46
22:Sg:210:GLY:HA3	22:Sg:236:ILE:HD11	1.98	0.46
25:SJ:84:ILE:HD12	25:SJ:150:ARG:HG2	1.97	0.46
54:T:112:ASP:OD1	54:T:116:ARG:NH1	2.48	0.46
57:W:18:LEU:HD23	57:W:54:ALA:HB3	1.97	0.46
79:t:189:G:H1	79:t:244:G:H1	1.63	0.46
79:t:2576:G:H2'	79:t:2577:A:H8	1.81	0.46
79:t:4413:G:N2	79:t:4414:U:O4	2.41	0.46
2:SA:139:TYR:O	6:SF:59:LYS:HD2	2.16	0.46
18:SX:63:ASN:ND2	18:SX:114:ASP:OD2	2.49	0.46
25:SJ:140:GLN:NE2	30:SY:64:PHE:O	2.49	0.46
28:SO:40:THR:HG21	28:SO:74:ALA:HB2	1.97	0.46
53:S:23:TRP:CH2	53:S:26:PRO:HA	2.51	0.46
76:p:12:CYS:HB3	76:p:21:HIS:HE1	1.80	0.46
79:t:35:U:O2'	79:t:1507:A:N1	2.48	0.46
79:t:376:G:N1	79:t:379:A:OP2	2.48	0.46
79:t:3893:G:OP2	79:t:4145:G:N2	2.42	0.46
1:S2:1013:U:OP1	1:S2:1129:G:O2'	2.32	0.46
1:S2:1386:A:OP2	4:SD:160:SER:OG	2.30	0.46
8:SI:130:THR:HA	8:SI:134:GLU:HB2	1.98	0.46
37:C:278:ASN:HD22	37:C:279:LEU:H	1.63	0.46
49:O:157:LYS:O	49:O:162:ARG:NH1	2.47	0.46
53:S:134:ASN:HD22	79:t:2875:G:H5'	1.80	0.46
2:SA:67:ALA:HB2	17:SV:37:ALA:HB2	1.97	0.46
8:SI:67:TRP:CD1	8:SI:70:GLU:H	2.33	0.46
23:SC:70:VAL:HG11	23:SC:93:ILE:HG13	1.98	0.46
29:SW:112:ASP:H	29:SW:115:GLU:HB3	1.80	0.46
35:A:227:ARG:HH22	79:t:3630:G:H4'	1.81	0.46
37:C:342:ARG:HA	37:C:345:ARG:HG2	1.97	0.46
41:G:141:ARG:HG3	41:G:191:GLN:HE21	1.81	0.46
46:L:100:SER:OG	46:L:104:ASN:OD1	2.28	0.46
47:M:188:ASN:ND2	79:t:1464:G:OP1	2.49	0.46
53:S:46:LYS:NZ	79:t:2684:G:O6	2.48	0.46
60:Z:4:ASN:HB3	60:Z:7:VAL:HG12	1.98	0.46
61:a:92:ASP:N	61:a:92:ASP:OD1	2.48	0.46
64:d:20:LEU:HD22	64:d:102:SER:HB3	1.98	0.46
71:k:22:CYS:SG	71:k:24:SER:OG	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:3848:A:N3	79:t:4363:G:O2'	2.47	0.46
1:S2:1152:U:H1'	29:SW:16:ASN:HD21	1.80	0.46
1:S2:1252:C:N4	12:SQ:146:ARG:O	2.45	0.46
10:SL:120:VAL:HG22	10:SL:145:VAL:HG21	1.97	0.46
30:SY:41:ARG:NH1	30:SY:52:PRO:O	2.49	0.46
36:B:372:SER:HB3	36:B:377:GLY:HA3	1.98	0.46
37:C:13:GLU:OE1	37:C:161:TYR:OH	2.27	0.46
46:L:103:GLY:HA3	46:L:157:ILE:HD12	1.98	0.46
47:M:19:GLN:HE22	79:t:1500:A:H61	1.63	0.46
49:O:50:ARG:HA	79:t:113:A:H1'	1.97	0.46
71:k:13:ASN:N	71:k:13:ASN:OD1	2.47	0.46
73:m:3:SER:HB2	79:t:2763:C:H41	1.80	0.46
79:t:951:A:H2'	79:t:952:G:H4'	1.98	0.46
1:S2:1846:G:O6	75:o:8:LYS:NZ	2.49	0.45
2:SA:51:LEU:HA	2:SA:54:THR:HG22	1.97	0.45
7:SH:145:ARG:HG3	29:SW:51:GLU:HG3	1.98	0.45
16:SU:79:ARG:H	21:Sd:54:LYS:NZ	2.13	0.45
18:SX:90:CYS:HB3	18:SX:130:LEU:HD11	1.98	0.45
22:Sg:70:VAL:HG22	22:Sg:111:VAL:HG23	1.98	0.45
31:SZ:99:LEU:HD21	31:SZ:102:LYS:HB2	1.98	0.45
36:B:189:THR:HG23	36:B:192:GLU:H	1.81	0.45
37:C:52:TYR:HB2	37:C:111:TRP:CH2	2.51	0.45
39:E:7:G:O5'	40:F:33:ARG:NH1	2.49	0.45
42:H:242:ARG:NH2	79:t:929:G:OP2	2.43	0.45
48:N:91:TRP:CE2	79:t:4827:U:H5'	2.51	0.45
62:b:32:ARG:HD2	79:t:37:U:H4'	1.97	0.45
79:t:655:A:H2'	79:t:656:C:C2	2.50	0.45
1:S2:1033:G:H1	1:S2:1080:A:HO2'	1.62	0.45
2:SA:140:VAL:HG23	23:SC:87:PRO:HG3	1.98	0.45
8:SI:139:LYS:HG3	8:SI:141:ARG:HH21	1.80	0.45
17:SV:77:GLY:CA	17:SV:81:LYS:HZ3	2.30	0.45
40:F:180:PHE:HB3	40:F:195:HIS:CD2	2.51	0.45
41:G:250:GLN:O	41:G:254:ASP:N	2.37	0.45
42:H:60:GLU:HA	42:H:63:GLN:HG2	1.98	0.45
42:H:159:TYR:HD1	42:H:168:ALA:HA	1.81	0.45
54:T:1:MET:HE3	54:T:3:ALA:HB2	1.97	0.45
79:t:925:C:H1'	79:t:926:G:H8	1.82	0.45
1:S2:695:C:H42	1:S2:736:C:H3'	1.80	0.45
1:S2:1098:C:H2'	1:S2:1099:G:C8	2.52	0.45
7:SH:14:GLU:N	7:SH:14:GLU:CD	2.73	0.45
18:SX:60:LYS:HG3	18:SX:114:ASP:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:190:ARG:HA	37:C:202:ILE:HD11	1.98	0.45
44:J:21:LYS:HB3	44:J:24:THR:HB	1.98	0.45
51:Q:67:VAL:HG22	51:Q:82:ARG:HH21	1.81	0.45
53:S:37:SER:HB3	53:S:40:GLN:HG2	1.97	0.45
54:T:170:LYS:HB2	79:t:4832:A:H5'	1.98	0.45
55:U:112:ASN:HD21	55:U:128:LEU:HD13	1.81	0.45
60:Z:87:ARG:NH2	79:t:398:U:O3'	2.49	0.45
79:t:47:A:H5'	79:t:49:U:H1'	1.98	0.45
79:t:2004:C:O2'	79:t:4656:G:N2	2.45	0.45
1:S2:304:C:O2'	1:S2:305:U:OP2	2.33	0.45
1:S2:373:G:H21	10:SL:83:GLN:HE21	1.65	0.45
7:SH:144:ILE:HD13	7:SH:154:ILE:HG13	1.98	0.45
37:C:266:THR:HG23	37:C:268:ARG:H	1.80	0.45
41:G:137:VAL:HG12	79:t:702:A:H5''	1.98	0.45
41:G:192:LYS:HD3	79:t:700:C:H5''	1.98	0.45
5:SE:124:CYS:HB3	5:SE:141:THR:HB	1.98	0.45
8:SI:81:VAL:HG12	8:SI:91:VAL:HG23	1.98	0.45
12:SQ:146:ARG:NH1	81:v:33:U:OP2	2.50	0.45
13:SR:94:GLU:O	13:SR:116:ASN:ND2	2.49	0.45
22:Sg:165:ILE:HB	22:Sg:177:TRP:HB2	1.98	0.45
26:SM:93:LYS:HD2	26:SM:103:VAL:HG22	1.99	0.45
37:C:53:ALA:HB3	79:t:344:C:H1'	1.99	0.45
43:I:166:LEU:HA	49:O:7:ILE:HD12	1.98	0.45
47:M:39:ARG:NH1	79:t:1345:G:OP1	2.48	0.45
73:m:21:ARG:HG2	73:m:22:PRO:HD2	1.98	0.45
76:p:36:GLN:NE2	79:t:4304:C:OP1	2.49	0.45
79:t:2824:A:H61	79:t:3814:C:H42	1.63	0.45
79:t:3832:A:H2'	79:t:3833:A:C8	2.52	0.45
81:v:7:G:N2	81:v:68:C:O2	2.50	0.45
1:S2:38:A:O2'	25:SJ:5:ARG:NH2	2.50	0.45
5:SE:74:GLY:HA3	5:SE:164:LEU:HD13	1.98	0.45
30:SY:92:ALA:HB2	30:SY:97:TYR:HB3	1.98	0.45
31:SZ:66:LYS:H	31:SZ:66:LYS:HD2	1.81	0.45
35:A:21:LYS:HD2	79:t:1523:C:H5''	1.98	0.45
35:A:68:ARG:NH2	79:t:4054:G:N7	2.64	0.45
42:H:169:LEU:HD23	42:H:169:LEU:N	2.27	0.45
79:t:729:C:H2'	79:t:730:G:C8	2.51	0.45
80:u:13:C:H2'	80:u:14:A:H8	1.82	0.45
1:S2:1006:C:H4'	64:d:11:LEU:HB2	1.98	0.45
2:SA:139:TYR:OH	6:SF:60:ARG:NH1	2.50	0.45
10:SL:4:ILE:HD12	10:SL:55:TYR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SP:103:ASN:ND2	11:SP:120:SER:OG	2.45	0.45
14:SS:38:ARG:HH21	15:ST:44:GLU:HG3	1.81	0.45
39:E:103:A:O2'	79:t:1723:G:O6	2.28	0.45
41:G:52:ARG:O	79:t:1264:G:N1	2.45	0.45
22:Sg:5:MET:HB3	22:Sg:310:TRP:HB3	1.99	0.45
23:SC:144:SER:HB3	23:SC:150:ALA:HB2	1.99	0.45
25:SJ:114:VAL:HG22	25:SJ:119:LEU:HB2	1.99	0.45
35:A:123:ARG:NH1	79:t:4053:U:OP1	2.49	0.45
36:B:168:MET:HA	36:B:171:LEU:HD12	1.98	0.45
39:E:12:U:O3'	39:E:109:U:O2'	2.32	0.45
42:H:166:ARG:HD2	42:H:209:TRP:CE2	2.52	0.45
43:I:121:LYS:HD2	43:I:125:LYS:HA	1.98	0.45
79:t:190:G:H1	79:t:243:G:H1	1.65	0.45
1:S2:396:U:H4'	8:SI:14:THR:HG22	1.98	0.45
1:S2:1033:G:N1	1:S2:1080:A:O2'	2.39	0.45
9:SK:8:ARG:HH12	9:SK:44:HIS:HB3	1.81	0.45
41:G:164:PHE:HA	41:G:175:VAL:HG23	1.99	0.45
48:N:82:ILE:O	48:N:86:TRP:N	2.42	0.45
54:T:28:TYR:OH	54:T:52:LYS:NZ	2.39	0.45
79:t:227:G:H21	79:t:234:G:H1	1.63	0.45
79:t:1088:C:H2'	79:t:1089:A:H8	1.82	0.45
5:SE:214:ASN:HB3	23:SC:191:VAL:HA	1.97	0.45
7:SH:25:GLN:HA	7:SH:28:LEU:HD12	1.98	0.45
14:SS:39:ARG:HH11	15:ST:38:LYS:HB2	1.83	0.45
24:SG:159:ARG:HH21	24:SG:171:THR:HG23	1.82	0.45
25:SJ:68:PRO:HA	25:SJ:71:LEU:HD12	1.98	0.45
38:D:146:U:O2	59:Y:51:THR:OG1	2.31	0.45
54:T:76:LYS:NZ	54:T:100:LEU:O	2.50	0.45
1:S2:85:A:H5'	30:SY:119:GLY:HA2	1.99	0.44
1:S2:1006:C:O5'	64:d:8:LYS:N	2.48	0.44
1:S2:1481:G:H1'	21:Sd:55:LEU:HD12	1.99	0.44
5:SE:43:PRO:HD2	5:SE:46:ILE:HD11	1.98	0.44
8:SI:123:ARG:HD2	8:SI:128:LYS:HD3	1.99	0.44
13:SR:25:GLY:O	13:SR:31:ASN:ND2	2.30	0.44
18:SX:105:PHE:HD1	18:SX:121:LYS:HB3	1.82	0.44
38:D:39:G:OP1	69:i:86:LYS:NZ	2.48	0.44
39:E:13:A:OP2	39:E:66:G:N2	2.48	0.44
47:M:3:PRO:HD2	62:b:41:HIS:CE1	2.52	0.44
47:M:49:ARG:HH12	69:i:116:LEU:HD21	1.81	0.44
67:g:54:LYS:HA	67:g:66:LYS:HE3	1.99	0.44
1:S2:1265:A:H2	1:S2:1517:G:H22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:169:ASP:N	4:SD:169:ASP:OD1	2.50	0.44
15:ST:18:LEU:HD12	15:ST:134:ILE:HD11	1.99	0.44
15:ST:44:GLU:HG2	15:ST:45:LEU:HD12	2.00	0.44
23:SC:187:ARG:HG2	23:SC:192:LEU:HB3	1.98	0.44
34:Sf:89:LYS:H	34:Sf:89:LYS:HD2	1.83	0.44
37:C:67:TRP:CZ3	83:y:13:LEU:HD21	2.53	0.44
37:C:159:GLU:HA	37:C:217:ILE:HB	1.98	0.44
37:C:242:PRO:HB2	79:t:2276:G:H4'	1.99	0.44
40:F:22:ARG:HA	40:F:22:ARG:HD3	1.78	0.44
53:S:105:LEU:HD22	53:S:135:LYS:HG3	1.98	0.44
78:r:37:SER:HB3	78:r:40:TYR:H	1.82	0.44
79:t:691:G:H2'	79:t:692:G:H8	1.82	0.44
79:t:2357:G:N2	79:t:2360:A:OP2	2.48	0.44
1:S2:126:G:H2'	24:SG:199:THR:HG21	1.99	0.44
1:S2:1378:A:N6	6:SF:62:ARG:HA	2.32	0.44
11:SP:121:ILE:HG22	14:SS:120:HIS:HD2	1.81	0.44
14:SS:98:VAL:HG23	14:SS:103:LEU:HD23	2.00	0.44
15:ST:113:VAL:HA	15:ST:123:LEU:HA	1.98	0.44
35:A:179:ILE:HG21	35:A:185:ALA:HB2	1.99	0.44
47:M:25:TRP:HB3	47:M:28:GLN:HG2	1.97	0.44
83:y:14:LEU:N	83:y:14:LEU:CD2	2.73	0.44
1:S2:1226:G:N1	1:S2:1639:G:OP2	2.40	0.44
6:SF:85:LYS:HB3	6:SF:88:MET:HG2	1.98	0.44
8:SI:171:LEU:HD23	8:SI:189:VAL:HG11	2.00	0.44
35:A:147:ARG:HA	35:A:157:VAL:HA	2.00	0.44
36:B:219:VAL:HG11	36:B:337:VAL:HG13	1.98	0.44
44:J:43:VAL:HG23	44:J:59:LYS:HB2	2.00	0.44
45:K:53:VAL:HG22	45:K:134:VAL:HG12	1.99	0.44
65:e:41:ARG:HD3	65:e:78:ARG:HA	2.00	0.44
78:r:13:CYS:HA	79:t:2317:C:H4'	1.99	0.44
79:t:1056:G:H22	79:t:1221:A:H2	1.65	0.44
79:t:3663:A:H62	79:t:3794:G:H21	1.64	0.44
1:S2:529:A:H62	1:S2:555:A:H62	1.66	0.44
1:S2:805:U:O3'	29:SW:120:HIS:CE1	2.68	0.44
5:SE:11:ARG:NH1	5:SE:27:PHE:O	2.50	0.44
7:SH:26:ALA:O	7:SH:86:LYS:NZ	2.50	0.44
12:SQ:97:GLN:HB3	12:SQ:105:LYS:HD3	2.00	0.44
22:Sg:257:LYS:HD2	22:Sg:266:ILE:HD12	1.99	0.44
24:SG:106:LEU:HD22	24:SG:109:LEU:HB3	1.99	0.44
25:SJ:142:VAL:HG12	25:SJ:144:ILE:H	1.83	0.44
27:SN:53:ILE:HG22	32:Sb:52:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:14:SER:OG	79:t:1610:C:OP1	2.25	0.44
35:A:54:ARG:NH2	79:t:3651:U:OP1	2.40	0.44
42:H:179:LEU:HD11	42:H:204:ALA:HA	2.00	0.44
49:O:114:ARG:NH1	49:O:151:ILE:O	2.51	0.44
61:a:107:LYS:NZ	79:t:2557:G:OP1	2.37	0.44
79:t:4964:U:H4'	79:t:4965:A:H5'	2.00	0.44
1:S2:84:A:O2'	30:SY:119:GLY:O	2.30	0.44
1:S2:122:G:OP1	5:SE:77:ARG:NH2	2.50	0.44
1:S2:887:U:O2'	1:S2:889:U:O4	2.34	0.44
1:S2:921:G:C6	32:Sb:22:LYS:HA	2.53	0.44
1:S2:1522:A:H5''	14:SS:144:ARG:HB3	1.99	0.44
1:S2:1591:C:H5'	6:SF:85:LYS:HE3	2.00	0.44
12:SQ:34:VAL:HG12	12:SQ:70:VAL:HB	2.00	0.44
25:SJ:46:VAL:HG23	25:SJ:102:ILE:HD11	1.99	0.44
33:Se:39:ASN:HA	33:Se:43:VAL:HG22	2.00	0.44
40:F:164:LYS:HD3	40:F:195:HIS:HE1	1.83	0.44
41:G:183:ARG:NH2	79:t:4896:A:OP1	2.45	0.44
42:H:184:ILE:HG21	42:H:193:GLU:HG3	2.00	0.44
52:R:65:ARG:NH2	79:t:1441:A:OP1	2.35	0.44
78:r:15:SER:OG	78:r:16:PHE:N	2.51	0.44
83:y:13:LEU:HD23	83:y:13:LEU:H	1.83	0.44
1:S2:1122:A:N3	3:SB:146:ARG:NH1	2.66	0.44
1:S2:1532:C:O2'	1:S2:1601:A:N1	2.50	0.44
1:S2:1581:C:H5'	1:S2:1582:C:H5	1.83	0.44
4:SD:70:THR:HG22	4:SD:86:LEU:HG	1.99	0.44
5:SE:126:VAL:HA	5:SE:141:THR:HA	1.99	0.44
6:SF:51:HIS:ND1	12:SQ:82:TYR:OH	2.35	0.44
16:SU:49:LYS:H	16:SU:92:HIS:HE1	1.65	0.44
17:SV:77:GLY:HA2	17:SV:81:LYS:HE2	2.00	0.44
27:SN:84:LEU:HD11	27:SN:149:LEU:HD23	2.00	0.44
28:SO:141:ARG:HG3	28:SO:142:ARG:N	2.33	0.44
37:C:32:ILE:HD12	37:C:130:ALA:HB2	2.00	0.44
41:G:120:ASP:OD2	78:r:112:ARG:NH2	2.51	0.44
43:I:88:ASP:OD1	43:I:88:ASP:N	2.50	0.44
44:J:12:ILE:HD13	44:J:18:ILE:HD12	1.98	0.44
44:J:79:ASN:ND2	79:t:4652:G:OP1	2.47	0.44
55:U:64:VAL:HG13	55:U:72:VAL:HG13	1.98	0.44
1:S2:1006:C:C6	64:d:8:LYS:HA	2.53	0.44
1:S2:1255:G:OP1	1:S2:1256:G:O2'	2.33	0.44
4:SD:50:ILE:HB	4:SD:88:ALA:HA	1.99	0.44
4:SD:106:ARG:HG3	4:SD:175:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:57:VAL:HB	36:B:367:PHE:HB3	1.99	0.44
49:O:15:GLN:NE2	79:t:299:A:OP2	2.46	0.44
52:R:151:HIS:ND1	52:R:164:LYS:O	2.49	0.44
63:c:36:ASP:HA	63:c:37:PRO:HD3	1.85	0.44
72:l:23:VAL:HG21	72:l:60:LEU:HD11	1.99	0.44
79:t:1964:A:H4'	79:t:1965:A:H5'	2.00	0.44
1:S2:379:C:O2	8:SI:31:ARG:NE	2.50	0.44
8:SI:178:ARG:HD3	8:SI:181:GLN:HG2	1.99	0.44
18:SX:105:PHE:CD1	18:SX:121:LYS:HB3	2.53	0.44
56:V:35:ASP:OD1	56:V:35:ASP:N	2.49	0.44
5:SE:212:ASP:OD1	5:SE:216:ASN:N	2.50	0.43
9:SK:8:ARG:HD3	9:SK:8:ARG:HA	1.81	0.43
12:SQ:13:PHE:HA	12:SQ:22:VAL:HA	2.00	0.43
26:SM:23:LYS:HE2	26:SM:88:TRP:CE2	2.53	0.43
36:B:161:ARG:HG2	36:B:184:GLN:HA	2.01	0.43
44:J:94:SER:HB3	44:J:142:ASP:HB2	1.99	0.43
53:S:115:ILE:HG12	53:S:142:ILE:HD11	1.99	0.43
54:T:1:MET:HG3	54:T:39:VAL:HG11	2.00	0.43
73:m:36:ARG:HG3	73:m:37:TYR:HD1	1.83	0.43
1:S2:560:A:H2'	25:SJ:164:PRO:HB3	2.00	0.43
2:SA:184:ARG:HD3	2:SA:191:ARG:HD3	2.00	0.43
7:SH:160:LYS:HD2	7:SH:189:PHE:HB3	1.99	0.43
22:Sg:191:HIS:CD2	22:Sg:195:LEU:HD22	2.54	0.43
24:SG:74:ARG:HA	24:SG:96:SER:HA	2.00	0.43
36:B:252:ALA:HB1	79:t:4486:G:N3	2.33	0.43
40:F:155:THR:HG22	40:F:179:ARG:HD3	2.00	0.43
50:P:27:VAL:O	50:P:101:ARG:NH2	2.51	0.43
51:Q:138:PRO:HB2	51:Q:140:MET:HG3	1.99	0.43
72:l:69:LEU:HD21	79:t:2675:A:C5	2.53	0.43
79:t:32:G:H1	79:t:48:G:HO2'	1.64	0.43
79:t:1838:C:H2'	79:t:1839:A:C8	2.53	0.43
79:t:2652:G:H5''	79:t:2653:A:H3'	2.00	0.43
1:S2:1232:U:H2'	1:S2:1233:G:H8	1.83	0.43
5:SE:137:PRO:HG2	5:SE:150:PRO:HD2	2.00	0.43
6:SF:39:ILE:HG22	6:SF:41:VAL:HG23	2.01	0.43
7:SH:7:LYS:HE3	7:SH:17:ASP:CG	2.43	0.43
36:B:53:MET:HG2	36:B:77:THR:HA	2.00	0.43
52:R:42:THR:HB	79:t:1411:U:H5''	2.00	0.43
53:S:21:LYS:O	53:S:53:LYS:HB3	2.18	0.43
64:d:28:VAL:HG23	64:d:34:THR:HG22	2.00	0.43
66:f:90:MET:HE3	78:r:113:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:r:28:GLU:HB2	78:r:31:ASN:HB2	2.00	0.43
4:SD:66:ILE:O	4:SD:70:THR:N	2.46	0.43
13:SR:60:ARG:HG2	13:SR:66:VAL:HG21	2.00	0.43
36:B:80:GLU:OE1	36:B:323:TYR:OH	2.27	0.43
42:H:81:PHE:HB2	55:U:141:VAL:HG22	2.01	0.43
47:M:127:PHE:HD2	69:i:118:LYS:HE2	1.84	0.43
48:N:16:SER:HB3	48:N:56:GLN:NE2	2.34	0.43
52:R:14:ARG:NH2	79:t:2064:C:OP2	2.51	0.43
52:R:86:ILE:HD12	52:R:105:VAL:HG22	2.01	0.43
71:k:27:TYR:HA	71:k:34:CYS:HA	2.00	0.43
79:t:190:G:H22	79:t:243:G:H1	1.64	0.43
79:t:1181:G:H2'	79:t:1182:G:H8	1.83	0.43
83:y:3:PRO:HB2	83:y:4:LEU:H	1.59	0.43
1:S2:39:A:H61	1:S2:515:G:H1'	1.83	0.43
1:S2:562:U:H2'	1:S2:563:G:C8	2.53	0.43
1:S2:641:A:O2'	1:S2:645:C:OP1	2.35	0.43
1:S2:1079:C:O2'	1:S2:1182:A:N1	2.50	0.43
11:SP:85:ILE:HA	11:SP:89:MET:HE2	2.00	0.43
25:SJ:83:ARG:HE	25:SJ:150:ARG:HD3	1.84	0.43
29:SW:114:GLU:O	29:SW:118:ARG:CG	2.53	0.43
37:C:326:LEU:HD21	37:C:333:LYS:HD3	2.00	0.43
41:G:150:LEU:HB2	41:G:162:VAL:HG23	1.99	0.43
79:t:1988:G:H21	79:t:1993:A:H62	1.67	0.43
81:v:68:C:N4	81:v:69:G:O6	2.52	0.43
1:S2:890:U:H5'	1:S2:896:U:H3	1.83	0.43
1:S2:1692:U:O3'	19:Sa:89:ARG:NH2	2.52	0.43
5:SE:208:VAL:HG21	5:SE:225:ILE:HG13	2.00	0.43
12:SQ:74:GLY:O	12:SQ:80:GLN:NE2	2.38	0.43
22:Sg:16:GLY:N	22:Sg:305:ASN:OD1	2.52	0.43
34:Sf:132:MET:HG2	34:Sf:139:HIS:HB3	2.01	0.43
36:B:248:LEU:N	79:t:2817:G:OP1	2.45	0.43
39:E:49:A:OP1	40:F:224:SER:N	2.52	0.43
42:H:87:PRO:HG2	42:H:144:TYR:CG	2.53	0.43
53:S:81:ARG:NH2	79:t:3579:A:OP2	2.41	0.43
79:t:2568:C:O2'	79:t:2746:U:O2'	2.28	0.43
20:Sc:37:ASP:OD1	20:Sc:37:ASP:N	2.52	0.43
36:B:229:LYS:HD3	36:B:272:LYS:HD3	2.01	0.43
36:B:321:VAL:HG12	36:B:322:HIS:CD2	2.54	0.43
42:H:69:ILE:H	42:H:69:ILE:HG13	1.73	0.43
43:I:67:ARG:HB3	49:O:28:TRP:HZ3	1.83	0.43
43:I:161:VAL:HG21	43:I:167:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:41:ASP:OD1	55:U:41:ASP:N	2.42	0.43
59:Y:150:ALA:HB1	59:Y:155:ILE:HD12	2.01	0.43
61:a:40:HIS:HA	61:a:76:ASN:HA	2.01	0.43
66:f:5:ARG:NH1	79:t:695:C:OP1	2.51	0.43
79:t:2254:G:H2'	79:t:2255:A:C8	2.54	0.43
81:v:71:G:H21	81:v:72:C:H41	1.65	0.43
1:S2:170:A:P	24:Sg:140:ARG:HH21	2.41	0.43
7:SH:96:ALA:HB3	7:SH:98:ARG:HE	1.83	0.43
12:SQ:51:LEU:HB2	12:SQ:84:ILE:HD11	2.00	0.43
20:Sc:31:ARG:HA	20:Sc:42:ILE:O	2.19	0.43
22:Sg:251:ALA:HB2	22:Sg:289:LEU:HD22	2.00	0.43
30:SY:74:MET:HE2	30:SY:74:MET:HB2	1.73	0.43
31:SZ:101:SER:OG	31:SZ:102:LYS:N	2.52	0.43
33:Se:8:ARG:HD2	33:Se:11:LYS:HG3	2.01	0.43
37:C:11:TYR:HE2	37:C:149:GLU:HB3	1.82	0.43
49:O:93:LYS:O	79:t:294:A:O2'	2.37	0.43
49:O:181:HIS:HB3	49:O:184:ILE:HD13	2.01	0.43
65:e:18:ASN:HA	65:e:102:LEU:HD11	2.00	0.43
1:S2:561:A:P	25:SJ:171:GLY:H	2.41	0.43
3:SB:87:ILE:HG13	3:SB:87:ILE:H	1.63	0.43
7:SH:54:GLY:HA3	7:SH:57:ARG:HH11	1.83	0.43
7:SH:80:VAL:HA	7:SH:83:LEU:HB2	2.01	0.43
7:SH:143:ARG:HB2	7:SH:155:LYS:HB2	2.01	0.43
16:SU:49:LYS:HG3	16:SU:92:HIS:CE1	2.54	0.43
25:SJ:136:ARG:HA	25:SJ:141:VAL:HA	2.00	0.43
27:SN:20:ARG:HH21	29:SW:56:HIS:HB3	1.83	0.43
42:H:80:ASN:HA	55:U:143:THR:HG22	2.00	0.43
44:J:41:ILE:HD13	44:J:73:ILE:HD11	2.00	0.43
52:R:9:LYS:O	52:R:11:ARG:N	2.52	0.43
60:Z:72:GLN:HB3	60:Z:81:TYR:HD2	1.84	0.43
79:t:1309:A:OP2	79:t:4407:U:O2'	2.33	0.43
79:t:4861:G:H2'	79:t:4862:G:H8	1.84	0.43
1:S2:636:C:H5''	33:Se:24:LYS:HE2	2.01	0.43
2:SA:77:ILE:HG12	2:SA:122:LEU:HD11	2.00	0.43
7:SH:160:LYS:NZ	7:SH:191:GLU:OE2	2.52	0.43
13:SR:103:LYS:HD2	13:SR:119:VAL:HG11	2.00	0.43
35:A:130:SER:OG	35:A:174:ARG:NH1	2.52	0.43
40:F:5:LYS:NZ	79:t:1737:C:O2	2.41	0.43
45:K:169:LYS:HE2	45:K:170:LYS:HE3	2.00	0.43
49:O:155:VAL:O	49:O:162:ARG:NH2	2.51	0.43
50:P:30:GLY:HA2	50:P:101:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:45:MET:HE2	55:U:94:GLU:HB3	2.01	0.43
70:j:50:PHE:HZ	70:j:93:VAL:HG11	1.84	0.43
76:p:23:VAL:HB	76:p:70:LEU:HD23	2.00	0.43
77:q:37:TYR:HB2	77:q:47:MET:HB2	2.00	0.43
79:t:474:C:N3	79:t:669:G:N2	2.67	0.43
79:t:1264:G:OP1	79:t:1264:G:N2	2.42	0.43
79:t:3661:U:O2'	79:t:3788:A:N3	2.38	0.43
1:S2:196:C:O2	1:S2:203:G:O2'	2.31	0.42
1:S2:1263:U:OP2	1:S2:1264:C:O2'	2.35	0.42
1:S2:1300:U:O2'	11:SP:51:ARG:NH1	2.51	0.42
3:SB:105:LEU:HD13	3:SB:213:ARG:HA	2.00	0.42
12:SQ:1:MET:HA	12:SQ:2:PRO:HD3	1.82	0.42
14:SS:35:GLY:O	14:SS:97:GLN:NE2	2.51	0.42
23:SC:196:ILE:HB	23:SC:223:TYR:HB2	2.01	0.42
29:SW:30:CYS:SG	29:SW:31:SER:N	2.92	0.42
29:SW:30:CYS:HA	29:SW:34:ILE:HD11	2.01	0.42
42:H:61:TYR:HA	42:H:64:MET:HG2	2.00	0.42
60:Z:82:ILE:HB	60:Z:85:VAL:HG12	2.01	0.42
68:h:82:MET:HE1	68:h:90:ARG:HE	1.81	0.42
71:k:59:THR:HG22	79:t:23:C:H4'	2.01	0.42
79:t:25:A:N3	79:t:333:C:O2'	2.47	0.42
79:t:1315:C:H2'	79:t:1316:A:C8	2.54	0.42
79:t:3754:A:H2	79:t:3761:U:H3	1.65	0.42
1:S2:194:C:H5''	1:S2:196:C:H41	1.85	0.42
1:S2:1006:C:H4'	64:d:11:LEU:HD13	2.01	0.42
1:S2:1006:C:C5	64:d:8:LYS:HA	2.54	0.42
1:S2:1398:G:OP1	22:Sg:60:ARG:NH1	2.51	0.42
1:S2:1866:A:C6	19:Sa:87:ARG:HD2	2.54	0.42
2:SA:158:ASP:HB2	2:SA:159:ILE:HD12	2.00	0.42
22:Sg:168:CYS:HB2	22:Sg:195:LEU:HD11	2.01	0.42
36:B:92:TYR:HB3	36:B:99:LEU:HD22	2.01	0.42
37:C:212:ASN:HB3	37:C:232:VAL:HG12	2.00	0.42
45:K:87:ILE:HB	45:K:138:ILE:HG22	1.99	0.42
50:P:49:ARG:NH1	79:t:1913:A:OP2	2.38	0.42
55:U:3:ASN:ND2	55:U:9:ARG:HH22	2.17	0.42
56:V:23:LEU:HD11	56:V:83:LEU:HB3	2.01	0.42
79:t:965:G:H22	79:t:1260:G:H1	1.66	0.42
79:t:1388:C:H2'	79:t:1389:G:C8	2.54	0.42
79:t:3762:C:N4	79:t:4465:A:N3	2.67	0.42
1:S2:1113:A:O2'	3:SB:202:GLN:NE2	2.52	0.42
1:S2:1752:C:N3	1:S2:1780:G:N1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1780:G:H3'	1:S2:1781:A:H4'	2.01	0.42
2:SA:110:ASN:O	2:SA:116:PHE:CD1	2.72	0.42
4:SD:220:THR:OG1	4:SD:221:THR:N	2.51	0.42
9:SK:32:HIS:CD2	9:SK:45:VAL:HG21	2.55	0.42
14:SS:20:ILE:HG22	14:SS:32:ALA:HB3	2.00	0.42
14:SS:25:LYS:O	14:SS:29:ALA:N	2.52	0.42
30:SY:90:ARG:HG2	30:SY:93:ARG:HD2	2.01	0.42
32:Sb:19:HIS:CD2	32:Sb:21:LYS:H	2.36	0.42
35:A:158:ILE:HD12	35:A:162:ASN:HD22	1.84	0.42
43:I:59:ARG:HA	43:I:62:ARG:HG2	2.00	0.42
44:J:123:ILE:H	44:J:123:ILE:HG13	1.63	0.42
66:f:26:ASP:OD1	66:f:26:ASP:N	2.52	0.42
78:r:7:TRP:O	78:r:11:ARG:N	2.51	0.42
79:t:955:C:O2'	79:t:956:C:O4'	2.34	0.42
79:t:3748:G:O2'	79:t:3786:G:O6	2.34	0.42
1:S2:121:OMU:HM23	5:SE:144:ALA:HB3	2.00	0.42
1:S2:644:OMG:HM23	1:S2:644:OMG:H1'	1.73	0.42
1:S2:1589:A:N3	1:S2:1653:U:O2'	2.44	0.42
3:SB:172:MET:HE2	3:SB:172:MET:HB3	1.73	0.42
24:SG:51:ARG:N	24:SG:112:VAL:O	2.50	0.42
42:H:71:MET:HA	42:H:74:MET:HE2	2.00	0.42
42:H:158:GLY:HA3	42:H:169:LEU:HD21	2.01	0.42
42:H:164:LYS:HE2	42:H:164:LYS:HB2	1.85	0.42
43:I:63:LEU:HD21	49:O:29:GLN:HE21	1.83	0.42
48:N:37:LEU:HD13	54:T:100:LEU:HD21	2.00	0.42
50:P:85:ARG:HG2	50:P:99:LEU:HD11	2.00	0.42
53:S:44:LEU:HD22	53:S:49:LEU:HD22	2.02	0.42
62:b:10:LYS:HA	62:b:10:LYS:HD3	1.89	0.42
79:t:725:G:H22	79:t:916:A:H8	1.67	0.42
79:t:735:G:N2	79:t:908:C:O2	2.52	0.42
79:t:896:A:H2'	79:t:897:G:C8	2.54	0.42
79:t:1523:C:O2'	79:t:2427:G:N3	2.53	0.42
79:t:2822:U:O2'	79:t:4594:U:OP1	2.35	0.42
81:v:50:U:H3	81:v:65:G:H1	1.67	0.42
81:v:55:U:H2'	81:v:56:C:H2'	2.01	0.42
1:S2:1337:4AC:H2'	1:S2:1338:G:C8	2.54	0.42
17:SV:1:MET:H1	17:SV:10:ASP:HB2	1.84	0.42
24:SG:5:ILE:HG12	24:SG:45:TRP:HH2	1.85	0.42
41:G:179:LEU:HB2	41:G:250:GLN:HE22	1.84	0.42
44:J:42:ASN:O	44:J:59:LYS:NZ	2.49	0.42
46:L:31:ASP:O	46:L:35:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O:18:VAL:HG11	70:j:48:CYS:HA	2.01	0.42
63:c:111:ARG:HG2	79:t:1253:A:H2	1.84	0.42
79:t:365:A:N3	79:t:1513:U:O2'	2.52	0.42
79:t:920:G:N3	79:t:925:C:O2'	2.52	0.42
79:t:4841:C:H2'	79:t:4842:G:C8	2.55	0.42
1:S2:382:C:H2'	1:S2:383:G:H8	1.85	0.42
1:S2:494:C:N4	1:S2:509:OMG:HN22	2.18	0.42
1:S2:1704:C:N4	82:w:18:G:OP1	2.46	0.42
2:SA:22:GLY:O	2:SA:24:HIS:ND1	2.52	0.42
14:SS:45:LEU:HD13	14:SS:50:ILE:HD11	2.01	0.42
18:SX:94:ILE:HG22	18:SX:125:VAL:HG21	2.00	0.42
25:SJ:120:ALA:HB2	25:SJ:129:LEU:HD12	2.02	0.42
26:SM:36:ARG:HE	26:SM:36:ARG:HB2	1.37	0.42
76:p:37:GLY:O	81:v:75:C:N4	2.49	0.42
79:t:1952:C:N4	79:t:1982:G:OP1	2.50	0.42
79:t:3688:A:H2'	79:t:3689:A:C8	2.54	0.42
5:SE:125:LYS:O	5:SE:142:HIS:N	2.52	0.42
14:SS:40:TYR:CZ	14:SS:97:GLN:HG2	2.54	0.42
16:SU:56:MET:HE3	16:SU:56:MET:HB3	1.89	0.42
36:B:55:HIS:NE2	36:B:369:ASP:OD2	2.53	0.42
36:B:301:ASN:ND2	36:B:304:SER:OG	2.52	0.42
37:C:192:GLY:O	37:C:195:LYS:NZ	2.44	0.42
40:F:83:LEU:HG	40:F:88:VAL:HB	2.01	0.42
40:F:229:ASN:OD1	40:F:229:ASN:N	2.52	0.42
42:H:167:ILE:H	42:H:167:ILE:HG13	1.46	0.42
52:R:7:HIS:CE1	63:c:18:ARG:HG3	2.55	0.42
53:S:22:VAL:HG22	53:S:23:TRP:HB2	2.02	0.42
61:a:73:LYS:NZ	79:t:2560:A:OP1	2.46	0.42
69:i:88:THR:O	69:i:90:ALA:N	2.53	0.42
78:r:20:ARG:O	78:r:22:LYS:N	2.53	0.42
79:t:466:C:H42	79:t:676:G:H1	1.68	0.42
79:t:4726:A:N6	79:t:4826:G:H22	2.17	0.42
80:u:76:A:O2'	83:y:25:GLU:CA	2.43	0.42
3:SB:87:ILE:H	3:SB:101:HIS:HB2	1.85	0.42
6:SF:25:THR:OG1	6:SF:41:VAL:O	2.37	0.42
15:ST:51:ASN:HB2	15:ST:54:TYR:HD2	1.84	0.42
26:SM:42:LEU:HD12	26:SM:68:LEU:HG	2.01	0.42
41:G:74:SER:HA	79:t:1256:G:H1'	2.02	0.42
61:a:47:ASP:N	61:a:69:LYS:O	2.47	0.42
77:q:4:ARG:NH2	79:t:1537:G:N7	2.67	0.42
79:t:1268:U:O2'	79:t:1269:C:O4'	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:3916:A:H2'	79:t:3917:G:H8	1.83	0.42
79:t:4436:A:OP2	79:t:4438:C:N4	2.53	0.42
79:t:4503:G:N2	79:t:4506:A:OP2	2.44	0.42
1:S2:561:A:N3	25:SJ:132:GLN:NE2	2.67	0.42
1:S2:628:A:H2	1:S2:1500:G:H21	1.68	0.42
18:SX:61:GLN:CD	18:SX:61:GLN:H	2.28	0.42
22:Sg:5:MET:N	22:Sg:5:MET:SD	2.93	0.42
22:Sg:129:ILE:HG13	22:Sg:142:VAL:HG11	2.02	0.42
24:SG:48:TYR:OH	24:SG:119:LYS:O	2.37	0.42
48:N:124:LYS:HA	48:N:127:VAL:HG12	2.01	0.42
55:U:144:ASN:OD1	55:U:144:ASN:N	2.53	0.42
79:t:201:U:H3	79:t:205:A:H2	1.66	0.42
79:t:2373:G:H8	79:t:2799:C:H41	1.67	0.42
79:t:2580:A:N6	79:t:2723:A:OP2	2.53	0.42
1:S2:66:G:OP1	24:SG:172:LYS:NZ	2.50	0.42
1:S2:1563:G:OP1	15:ST:121:ARG:NH2	2.52	0.42
37:C:53:ALA:HB2	79:t:342:G:N2	2.35	0.42
37:C:322:LEU:O	79:t:1264:G:O2'	2.30	0.42
38:D:52:A:H4'	73:m:19:GLN:HA	2.01	0.42
46:L:109:ILE:HG12	46:L:128:LEU:HB2	2.01	0.42
48:N:47:ARG:HB3	54:T:73:LEU:HD13	2.02	0.42
60:Z:26:ARG:HD3	60:Z:75:ARG:O	2.20	0.42
61:a:36:ARG:HH12	79:t:2559:U:H5'	1.84	0.42
61:a:60:LYS:O	61:a:64:LYS:N	2.44	0.42
64:d:33:GLN:HE22	79:t:2637:G:H2'	1.84	0.42
79:t:2728:C:H2'	79:t:2729:G:C8	2.55	0.42
1:S2:39:A:H5'	25:SJ:5:ARG:HH12	1.85	0.41
1:S2:604:A:H5'	25:SJ:22:LYS:HB2	2.02	0.41
9:SK:24:LYS:HA	9:SK:66:HIS:HA	2.02	0.41
13:SR:37:GLU:HG3	22:Sg:150:TRP:HE1	1.85	0.41
18:SX:60:LYS:HG3	18:SX:114:ASP:CA	2.50	0.41
25:SJ:63:LEU:O	25:SJ:70:ARG:NH1	2.52	0.41
26:SM:63:LYS:HG2	34:Sf:108:VAL:HG11	2.02	0.41
30:SY:83:LYS:HZ3	30:SY:96:LEU:HB3	1.84	0.41
38:D:102:G:OP2	38:D:104:A:O2'	2.28	0.41
42:H:238:ASP:N	42:H:238:ASP:OD1	2.53	0.41
44:J:17:ASP:OD1	44:J:17:ASP:N	2.53	0.41
45:K:34:PHE:HD2	79:t:1730:U:H4'	1.84	0.41
46:L:167:GLN:HE21	46:L:174:ILE:HG12	1.84	0.41
50:P:178:ARG:HA	50:P:181:ALA:HB3	2.02	0.41
55:U:106:LEU:HA	55:U:109:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:13:GLY:HA2	79:t:1642:U:H3'	2.02	0.41
63:c:50:ASN:HB3	79:t:1795:U:H1'	2.02	0.41
79:t:476:G:H1	79:t:666:G:H1	1.68	0.41
79:t:654:G:H2'	79:t:655:A:C8	2.54	0.41
79:t:1715:G:N3	79:t:4176:A:H2'	2.35	0.41
1:S2:159:A2M:HM'3	1:S2:159:A2M:H1'	1.82	0.41
1:S2:588:G:OP2	1:S2:588:G:N2	2.43	0.41
1:S2:1351:G:O3'	6:SF:62:ARG:HG3	2.20	0.41
2:SA:76:VAL:HG22	2:SA:87:VAL:HG23	2.01	0.41
3:SB:121:ILE:HG22	3:SB:161:VAL:HG13	2.02	0.41
4:SD:195:THR:HG23	4:SD:201:LYS:HG3	2.02	0.41
8:SI:117:TYR:HB3	8:SI:119:LEU:HD13	2.01	0.41
22:Sg:297:THR:HG22	22:Sg:311:GLN:HG3	2.01	0.41
30:SY:56:PHE:CD1	30:SY:94:HIS:CE1	3.08	0.41
47:M:149:GLN:HE21	69:i:122:LYS:HG2	1.85	0.41
47:M:198:ARG:NH2	79:t:1467:C:N3	2.68	0.41
52:R:10:ASP:O	79:t:2062:C:O2'	2.38	0.41
52:R:71:LYS:NZ	79:t:1402:G:OP1	2.43	0.41
74:n:93:LYS:HD3	74:n:102:ARG:HG2	2.02	0.41
78:r:31:ASN:O	78:r:113:ARG:NH1	2.51	0.41
79:t:715:C:H2'	79:t:716:G:C8	2.55	0.41
79:t:3753:C:H2'	79:t:3780:G:H1	1.85	0.41
6:SF:50:PRO:HG3	6:SF:69:VAL:HG12	2.02	0.41
16:SU:61:LEU:HB2	21:Sd:34:TYR:CZ	2.56	0.41
31:SZ:51:ASP:OD1	31:SZ:51:ASP:N	2.52	0.41
35:A:116:LEU:HG	35:A:126:LEU:HB2	2.02	0.41
37:C:27:VAL:HA	37:C:279:LEU:HD11	2.02	0.41
37:C:83:GLY:O	83:y:8:LEU:CG	2.63	0.41
44:J:23:ARG:HA	44:J:45:LEU:HD12	2.02	0.41
45:K:8:CYS:SG	79:t:4367:G:H5'	2.60	0.41
46:L:144:LYS:O	46:L:148:THR:OG1	2.36	0.41
56:V:48:LYS:HG3	56:V:53:ALA:HA	2.02	0.41
59:Y:149:VAL:HG13	59:Y:152:LYS:HE3	2.02	0.41
67:g:6:TRP:CD2	67:g:102:ARG:HG3	2.55	0.41
79:t:4861:G:H2'	79:t:4862:G:C8	2.56	0.41
1:S2:1025:U:H2'	1:S2:1026:C:O4'	2.20	0.41
6:SF:18:LYS:HE3	6:SF:22:LYS:HA	2.02	0.41
7:SH:140:VAL:HG12	27:SN:19:ARG:HD3	2.01	0.41
19:Sa:47:ALA:HA	19:Sa:50:VAL:HG23	2.02	0.41
38:D:93:C:OP1	71:k:76:HIS:NE2	2.36	0.41
44:J:5:LEU:HD12	44:J:58:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:K:61:SER:HA	45:K:126:VAL:HA	2.01	0.41
45:K:205:PRO:HD2	45:K:208:LYS:HE3	2.03	0.41
47:M:67:HIS:HD2	79:t:72:C:H5	1.69	0.41
48:N:60:PHE:HE1	48:N:85:LYS:HE3	1.85	0.41
66:f:38:PRO:HB2	66:f:43:ASN:ND2	2.35	0.41
79:t:1155:C:H42	79:t:1172:G:H1	1.67	0.41
79:t:1651:A:N3	79:t:1833:U:O2'	2.49	0.41
81:v:26:A:H61	81:v:44:G:H1	1.68	0.41
81:v:27:G:H2'	81:v:28:G:C8	2.56	0.41
1:S2:388:U:H2'	1:S2:389:A:C8	2.56	0.41
6:SF:51:HIS:O	12:SQ:50:LYS:NZ	2.34	0.41
9:SK:8:ARG:NH1	9:SK:44:HIS:HB3	2.36	0.41
14:SS:26:ILE:HG12	14:SS:56:ALA:HA	2.02	0.41
15:ST:9:VAL:HG11	15:ST:138:VAL:HG13	2.03	0.41
23:SC:180:VAL:HG23	23:SC:197:PRO:HG3	2.01	0.41
24:SG:5:ILE:HD13	24:SG:111:LEU:HD12	2.02	0.41
24:SG:64:LYS:NZ	24:SG:82:SER:OG	2.41	0.41
42:H:125:LEU:HA	42:H:125:LEU:HD23	1.81	0.41
57:W:16:ILE:HD11	57:W:57:VAL:H	1.84	0.41
66:f:99:ILE:HD13	66:f:108:ARG:HG3	2.02	0.41
76:p:105:GLN:OE1	76:p:105:GLN:N	2.54	0.41
79:t:321:U:H4'	79:t:322:A:H5'	2.03	0.41
79:t:463:C:H2'	79:t:464:A:O4'	2.20	0.41
79:t:1060:C:H42	79:t:1217:G:N2	2.11	0.41
79:t:1658:C:H41	79:t:4340:A:H2'	1.86	0.41
1:S2:86:C:OP1	30:SY:118:ARG:NH2	2.53	0.41
5:SE:174:LYS:O	5:SE:179:ASN:ND2	2.54	0.41
8:SI:177:SER:HB3	8:SI:186:ASP:H	1.86	0.41
18:SX:105:PHE:CE2	18:SX:112:VAL:HG22	2.56	0.41
22:Sg:166:VAL:HG12	22:Sg:176:VAL:HG22	2.02	0.41
30:SY:89:HIS:CD2	30:SY:90:ARG:HG3	2.56	0.41
36:B:114:CYS:SG	36:B:165:HIS:ND1	2.88	0.41
51:Q:48:LEU:HD23	51:Q:92:LEU:HB2	2.01	0.41
66:f:33:ARG:NH1	79:t:1286:A:OP2	2.51	0.41
76:p:9:ARG:HA	76:p:20:PRO:HA	2.02	0.41
79:t:4707:G:N2	79:t:4912:G:H22	2.18	0.41
83:y:9:LEU:C	83:y:9:LEU:CD2	2.86	0.41
1:S2:220:U:H2'	1:S2:221:A:C8	2.56	0.41
1:S2:1117:C:O2'	1:S2:1118:C:O4'	2.35	0.41
1:S2:1206:G:H1	1:S2:1692:U:H3	1.68	0.41
3:SB:113:MET:HE2	3:SB:142:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SH:13:GLY:C	7:SH:14:GLU:CD	2.89	0.41
27:SN:47:PRO:HG3	27:SN:72:LEU:HD12	2.03	0.41
36:B:92:TYR:HB2	36:B:159:VAL:HG23	2.03	0.41
36:B:265:SER:OG	79:t:4421:U:O3'	2.36	0.41
40:F:99:TYR:OH	40:F:168:ASP:OD2	2.28	0.41
49:O:73:ARG:HA	49:O:74:PRO:HD3	1.86	0.41
54:T:83:ARG:NH1	55:U:154:ILE:O	2.54	0.41
1:S2:159:A2M:H2	1:S2:468:A:H1'	2.02	0.41
1:S2:218:U:O2	8:SI:184:ARG:NH2	2.52	0.41
2:SA:30:LEU:HD22	2:SA:47:TYR:CZ	2.56	0.41
4:SD:5:ILE:H	4:SD:5:ILE:HG13	1.79	0.41
5:SE:46:ILE:H	5:SE:46:ILE:HG13	1.78	0.41
22:Sg:99:ARG:HH12	22:Sg:135:LEU:HD22	1.86	0.41
35:A:132:ASN:ND2	79:t:3653:A:H5''	2.36	0.41
36:B:49:TYR:HE1	36:B:344:VAL:HG13	1.85	0.41
51:Q:120:ASN:OD1	51:Q:145:HIS:HB2	2.21	0.41
54:T:173:ASN:HA	79:t:4724:A:H2	1.86	0.41
71:k:18:LEU:HA	71:k:25:LYS:H	1.86	0.41
76:p:23:VAL:HG21	76:p:68:LEU:HD13	2.02	0.41
79:t:2576:G:H1	79:t:2727:C:H5	1.69	0.41
79:t:4063:G:N1	79:t:4064:G:O6	2.53	0.41
80:u:20:U:H2'	80:u:21:A:H4'	2.02	0.41
1:S2:484:A2M:HM'3	1:S2:484:A2M:H1'	1.90	0.41
1:S2:579:C:N3	30:SY:61:ARG:NH2	2.68	0.41
1:S2:988:C:OP1	19:Sa:70:LYS:NZ	2.54	0.41
1:S2:1005:G:C4	64:d:8:LYS:HB2	2.56	0.41
1:S2:1024:A:OP2	27:SN:124:ARG:NH2	2.44	0.41
1:S2:1355:C:H3'	1:S2:1356:G:C8	2.56	0.41
2:SA:190:SER:HA	17:SV:45:ARG:HH21	1.86	0.41
3:SB:171:ILE:HD12	3:SB:197:ILE:HG22	2.03	0.41
11:SP:44:ARG:HG2	11:SP:84:ILE:HD11	2.03	0.41
23:SC:182:CYS:HB2	29:SW:95:PRO:HB2	2.02	0.41
29:SW:114:GLU:HA	29:SW:117:ARG:HG2	2.03	0.41
36:B:181:MET:HG2	36:B:182:GLU:H	1.86	0.41
37:C:199:ARG:HH22	79:t:343:A:H4'	1.86	0.41
37:C:221:PHE:HB2	37:C:229:LEU:HD11	2.03	0.41
41:G:227:HIS:O	79:t:447:G:N2	2.54	0.41
44:J:37:ASP:OD1	44:J:37:ASP:N	2.53	0.41
44:J:42:ASN:HD22	44:J:42:ASN:HA	1.63	0.41
48:N:31:ILE:HD11	48:N:35:ARG:HB2	2.02	0.41
48:N:65:PRO:HG2	79:t:907:C:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q:139:TYR:CD1	79:t:3830:G:H4'	2.55	0.41
53:S:153:LYS:HE2	53:S:153:LYS:HB3	1.91	0.41
55:U:25:VAL:HG11	55:U:45:MET:HE1	2.01	0.41
55:U:89:ILE:HD13	79:t:4262:U:H4'	2.03	0.41
66:f:81:ASN:OD1	66:f:81:ASN:N	2.54	0.41
67:g:27:LEU:HA	67:g:85:ARG:HA	2.02	0.41
79:t:159:A:H61	79:t:268:C:H42	1.69	0.41
79:t:502:G:O2'	79:t:504:U:OP1	2.32	0.41
79:t:732:C:H42	79:t:910:C:H42	1.68	0.41
1:S2:1101:U:H2'	1:S2:1102:G:C8	2.56	0.41
1:S2:1817:G:H2'	1:S2:1818:A:C8	2.56	0.41
6:SF:89:THR:HA	6:SF:92:ILE:HG12	2.03	0.41
14:SS:13:LEU:HD22	14:SS:20:ILE:HD11	2.04	0.41
19:Sa:44:ILE:HD11	28:SO:97:LEU:HD23	2.02	0.41
25:SJ:79:ARG:HH12	25:SJ:83:ARG:HH21	1.69	0.41
37:C:330:PRO:HG3	42:H:47:ARG:NH2	2.36	0.41
40:F:12:TYR:OH	79:t:4227:U:OP1	2.31	0.41
42:H:226:HIS:CD2	42:H:234:GLY:HA3	2.56	0.41
47:M:67:HIS:HD2	79:t:72:C:C5	2.39	0.41
79:t:85:G:O2'	79:t:97:G:O6	2.32	0.41
79:t:2484:C:H4'	79:t:2485:G:C2	2.56	0.41
79:t:4819:G:H2'	79:t:4820:G:C8	2.56	0.41
79:t:4948:C:H6	79:t:4948:C:H2'	1.69	0.41
1:S2:24:C:H4'	1:S2:415:A:H4'	2.04	0.40
1:S2:1010:G:H2'	1:S2:1011:A:H8	1.86	0.40
1:S2:1171:G:O2'	1:S2:1187:G:O6	2.32	0.40
1:S2:1352:G:N7	6:SF:63:LYS:HE3	2.36	0.40
1:S2:1610:G:N7	14:SS:132:ARG:NH2	2.69	0.40
4:SD:101:GLN:HE21	4:SD:186:VAL:HG11	1.87	0.40
8:SI:79:ILE:HG21	8:SI:170:LYS:HD2	2.02	0.40
36:B:19:ARG:HB2	36:B:234:ARG:HH21	1.86	0.40
36:B:367:PHE:HZ	36:B:380:GLN:HE22	1.69	0.40
40:F:118:ILE:HG21	40:F:138:GLN:HG2	2.03	0.40
50:P:179:LYS:HB2	50:P:179:LYS:HE2	1.85	0.40
55:U:54:HIS:CD2	79:t:4263:U:H4'	2.57	0.40
63:c:58:GLN:HE22	79:t:1793:G:H21	1.69	0.40
66:f:23:HIS:CD2	66:f:24:GLN:HG2	2.56	0.40
73:m:37:TYR:O	79:t:356:A:N6	2.52	0.40
79:t:1437:G:H2'	79:t:1438:G:C8	2.57	0.40
1:S2:1356:G:O2'	25:SJ:71:LEU:HD11	2.21	0.40
4:SD:96:LEU:HD23	4:SD:198:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:222:PRO:HG2	22:Sg:226:HIS:CE1	2.56	0.40
8:SI:67:TRP:CD1	8:SI:70:GLU:HB2	2.56	0.40
9:SK:1:MET:N	9:SK:3:MET:HE2	2.37	0.40
11:SP:13:ARG:HG3	11:SP:14:LYS:H	1.85	0.40
18:SX:8:ARG:HH22	18:SX:9:THR:HB	1.86	0.40
22:Sg:11:LEU:HD22	22:Sg:53:GLY:HA3	2.03	0.40
29:SW:60:LYS:NZ	32:Sb:23:ARG:O	2.52	0.40
29:SW:101:PHE:HA	29:SW:113:HIS:CE1	2.56	0.40
37:C:326:LEU:HD21	37:C:333:LYS:HB2	2.03	0.40
39:E:79:U:O2'	79:t:1777:A:N3	2.52	0.40
45:K:188:LYS:HE3	45:K:213:HIS:CE1	2.56	0.40
52:R:87:THR:HG22	52:R:106:THR:HG21	2.04	0.40
53:S:67:THR:HA	53:S:70:ARG:HG2	2.03	0.40
60:Z:87:ARG:NH1	79:t:380:A:O2'	2.54	0.40
69:i:99:GLU:HA	69:i:102:LEU:HG	2.03	0.40
78:r:108:MET:HA	78:r:111:ILE:HG12	2.03	0.40
79:t:1430:C:H2'	79:t:1431:G:C4	2.56	0.40
79:t:1505:A:N3	79:t:4351:C:O2'	2.45	0.40
79:t:3765:C:H2'	79:t:3766:A:C8	2.56	0.40
79:t:4647:U:H2'	79:t:4648:G:C8	2.56	0.40
1:S2:1864:U:H3'	19:Sa:5:ARG:HH21	1.86	0.40
35:A:55:GLY:HA3	35:A:174:ARG:NH1	2.36	0.40
47:M:87:HIS:CD2	47:M:89:LYS:H	2.39	0.40
55:U:7:LYS:O	79:t:4296:U:O2'	2.23	0.40
65:e:28:ASN:HB3	65:e:83:ARG:HE	1.86	0.40
66:f:75:ARG:HB2	66:f:95:TYR:HD1	1.86	0.40
77:q:50:ARG:HG2	77:q:51:ALA:H	1.85	0.40
79:t:4735:C:O2'	79:t:4736:C:O2	2.39	0.40
1:S2:1505:U:H4'	1:S2:1508:A:H1'	2.04	0.40
2:SA:21:ALA:HB2	13:SR:91:LEU:HD11	2.02	0.40
2:SA:85:ARG:HD3	2:SA:203:PHE:O	2.22	0.40
14:SS:117:ILE:H	14:SS:117:ILE:HG13	1.79	0.40
21:Sd:40:ARG:HE	21:Sd:41:GLN:NE2	2.19	0.40
39:E:82:G:H2'	39:E:83:A:C8	2.57	0.40
44:J:12:ILE:HG12	44:J:81:ILE:HD11	2.03	0.40
44:J:155:SER:OG	79:t:4650:C:O3'	2.35	0.40
46:L:37:ALA:HB2	46:L:70:VAL:HG11	2.03	0.40
48:N:46:ARG:HH12	79:t:925:C:P	2.45	0.40
60:Z:18:HIS:O	60:Z:78:TYR:OH	2.28	0.40
63:c:36:ASP:OD1	63:c:36:ASP:N	2.53	0.40
79:t:2576:G:H2'	79:t:2577:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:101:GLN:HA	4:SD:104:SER:HB3	2.03	0.40
15:ST:37:VAL:HG22	15:ST:39:LEU:H	1.86	0.40
35:A:208:GLU:OE2	79:t:1611:G:N2	2.41	0.40
36:B:115:LYS:HA	36:B:118:PHE:HD2	1.86	0.40
41:G:115:TYR:CE1	78:r:119:ARG:HD2	2.55	0.40
45:K:67:ALA:HB1	45:K:158:LYS:HD3	2.04	0.40
60:Z:34:LEU:HD23	60:Z:106:ILE:HB	2.03	0.40
79:t:1305:A:N6	79:t:4408:U:OP1	2.48	0.40
79:t:4973:G:H21	79:t:4992:A:H2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	193 (88%)	25 (11%)	1 (0%)	24	57
3	SB	212/214 (99%)	189 (89%)	23 (11%)	0	100	100
4	SD	224/226 (99%)	194 (87%)	30 (13%)	0	100	100
5	SE	253/259 (98%)	232 (92%)	21 (8%)	0	100	100
6	SF	183/189 (97%)	163 (89%)	20 (11%)	0	100	100
7	SH	180/189 (95%)	158 (88%)	22 (12%)	0	100	100
8	SI	202/204 (99%)	183 (91%)	19 (9%)	0	100	100
9	SK	96/98 (98%)	84 (88%)	12 (12%)	0	100	100
10	SL	147/153 (96%)	130 (88%)	17 (12%)	0	100	100
11	SP	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
12	SQ	144/146 (99%)	119 (83%)	23 (16%)	2 (1%)	9	34
13	SR	132/134 (98%)	115 (87%)	16 (12%)	1 (1%)	16	47
14	SS	143/145 (99%)	128 (90%)	15 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	ST	141/143 (99%)	133 (94%)	6 (4%)	2 (1%)	9	34
16	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
17	SV	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	9	35
18	SX	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	49
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	12	41
20	Sc	62/64 (97%)	51 (82%)	10 (16%)	1 (2%)	7	30
21	Sd	53/55 (96%)	43 (81%)	9 (17%)	1 (2%)	6	27
22	Sg	310/312 (99%)	259 (84%)	51 (16%)	0	100	100
23	SC	215/220 (98%)	198 (92%)	16 (7%)	1 (0%)	24	57
24	SG	235/237 (99%)	215 (92%)	20 (8%)	0	100	100
25	SJ	184/185 (100%)	167 (91%)	16 (9%)	1 (0%)	24	57
26	SM	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
27	SN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
28	SO	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
29	SW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
30	SY	130/131 (99%)	124 (95%)	6 (5%)	0	100	100
31	SZ	71/73 (97%)	61 (86%)	10 (14%)	0	100	100
32	Sb	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
33	Se	55/57 (96%)	47 (86%)	8 (14%)	0	100	100
34	Sf	65/67 (97%)	50 (77%)	15 (23%)	0	100	100
35	A	250/252 (99%)	226 (90%)	22 (9%)	2 (1%)	16	47
36	B	395/397 (100%)	358 (91%)	34 (9%)	3 (1%)	16	47
37	C	361/363 (99%)	326 (90%)	33 (9%)	2 (1%)	21	52
40	F	292/294 (99%)	269 (92%)	22 (8%)	1 (0%)	36	67
41	G	232/247 (94%)	197 (85%)	32 (14%)	3 (1%)	9	35
42	H	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	14	44
43	I	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	30	61
44	J	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
45	K	204/211 (97%)	185 (91%)	18 (9%)	1 (0%)	24	57
46	L	167/169 (99%)	152 (91%)	15 (9%)	0	100	100
47	M	203/205 (99%)	172 (85%)	30 (15%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	N	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
49	O	201/203 (99%)	179 (89%)	21 (10%)	1 (0%)	24	57
50	P	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	57
51	Q	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
52	R	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	11	39
53	S	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
54	T	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
55	U	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	9	35
56	V	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
57	W	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
58	X	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
59	Y	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
60	Z	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
61	a	132/134 (98%)	119 (90%)	13 (10%)	0	100	100
62	b	145/147 (99%)	125 (86%)	20 (14%)	0	100	100
63	c	94/121 (78%)	80 (85%)	14 (15%)	0	100	100
64	d	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
65	e	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
66	f	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
67	g	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	14	44
68	h	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
69	i	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	3	17
70	j	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	5	25
71	k	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
72	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
73	m	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
74	n	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
75	o	23/25 (92%)	23 (100%)	0	0	100	100
76	p	103/105 (98%)	95 (92%)	6 (6%)	2 (2%)	6	27
77	q	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
78	r	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	y	24/26 (92%)	17 (71%)	3 (12%)	4 (17%)	0	0
All	All	11201/11416 (98%)	10107 (90%)	1043 (9%)	51 (0%)	26	57

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	SV	79	VAL
23	SC	78	LEU
52	R	10	ASP
67	g	107	PRO
69	i	89	ARG
76	p	104	ILE
76	p	105	GLN
15	ST	41	LYS
36	B	4	ARG
40	F	260	GLU
70	j	35	LYS
83	y	1	TRP
83	y	3	PRO
83	y	16	PRO
12	SQ	117	ARG
13	SR	67	ARG
18	SX	8	ARG
19	Sa	47	ALA
37	C	69	THR
41	G	127	SER
41	G	136	HIS
42	H	238	ASP
45	K	11	TYR
52	R	9	LYS
55	U	53	PRO
78	r	21	ASN
83	y	21	ALA
2	SA	12	GLU
42	H	223	LYS
47	M	145	LYS
49	O	95	ALA
69	i	41	ALA
78	r	22	LYS
78	r	23	GLN
15	ST	39	LEU
21	Sd	4	GLN

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Mol	Chain	Res	Type
35	A	251	THR
36	B	356	LYS
50	P	184	ASN
69	i	88	THR
69	i	95	LEU
12	SQ	116	ASP
35	A	144	LYS
36	B	3	HIS
41	G	128	HIS
55	U	18	PRO
70	j	34	THR
25	SJ	123	ILE
37	C	70	GLY
43	I	30	PRO
20	Sc	32	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	181 (99%)	2 (1%)	65	78
3	SB	195/195 (100%)	194 (100%)	1 (0%)	81	85
4	SD	189/189 (100%)	186 (98%)	3 (2%)	55	75
5	SE	222/222 (100%)	219 (99%)	3 (1%)	59	76
6	SF	159/159 (100%)	155 (98%)	4 (2%)	42	69
7	SH	166/169 (98%)	166 (100%)	0	100	100
8	SI	177/177 (100%)	175 (99%)	2 (1%)	65	78
9	SK	89/89 (100%)	89 (100%)	0	100	100
10	SL	137/137 (100%)	137 (100%)	0	100	100
11	SP	113/113 (100%)	112 (99%)	1 (1%)	70	80
12	SQ	121/121 (100%)	119 (98%)	2 (2%)	53	74
13	SR	121/121 (100%)	119 (98%)	2 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	SS	126/126 (100%)	126 (100%)	0	100	100
15	ST	113/113 (100%)	110 (97%)	3 (3%)	39	67
16	SU	94/94 (100%)	94 (100%)	0	100	100
17	SV	66/66 (100%)	65 (98%)	1 (2%)	57	75
18	SX	113/113 (100%)	111 (98%)	2 (2%)	51	73
19	Sa	89/89 (100%)	88 (99%)	1 (1%)	65	78
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	47 (98%)	1 (2%)	47	71
22	Sg	271/271 (100%)	269 (99%)	2 (1%)	76	82
23	SC	187/186 (100%)	183 (98%)	4 (2%)	47	71
24	SG	207/207 (100%)	206 (100%)	1 (0%)	81	85
25	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	78
26	SM	98/100 (98%)	96 (98%)	2 (2%)	48	72
27	SN	130/130 (100%)	130 (100%)	0	100	100
28	SO	107/107 (100%)	105 (98%)	2 (2%)	50	73
29	SW	112/112 (100%)	111 (99%)	1 (1%)	70	80
30	SY	114/113 (101%)	114 (100%)	0	100	100
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	35	64
32	Sb	74/74 (100%)	73 (99%)	1 (1%)	59	76
33	Se	46/46 (100%)	45 (98%)	1 (2%)	45	71
34	Sf	60/60 (100%)	60 (100%)	0	100	100
35	A	194/194 (100%)	189 (97%)	5 (3%)	40	68
36	B	345/345 (100%)	338 (98%)	7 (2%)	48	72
37	C	302/302 (100%)	297 (98%)	5 (2%)	53	74
40	F	248/248 (100%)	246 (99%)	2 (1%)	73	81
41	G	209/220 (95%)	207 (99%)	2 (1%)	68	79
42	H	194/194 (100%)	191 (98%)	3 (2%)	57	75
43	I	199/199 (100%)	197 (99%)	2 (1%)	68	79
44	J	170/170 (100%)	166 (98%)	4 (2%)	43	69
45	K	178/179 (99%)	177 (99%)	1 (1%)	78	83
46	L	142/142 (100%)	141 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M	171/171 (100%)	168 (98%)	3 (2%)	51	73
48	N	118/118 (100%)	116 (98%)	2 (2%)	53	74
49	O	171/171 (100%)	166 (97%)	5 (3%)	37	66
50	P	168/168 (100%)	167 (99%)	1 (1%)	78	83
51	Q	134/134 (100%)	132 (98%)	2 (2%)	57	75
52	R	164/164 (100%)	162 (99%)	2 (1%)	63	78
53	S	160/160 (100%)	160 (100%)	0	100	100
54	T	156/156 (100%)	155 (99%)	1 (1%)	78	83
55	U	138/138 (100%)	135 (98%)	3 (2%)	45	71
56	V	89/89 (100%)	88 (99%)	1 (1%)	65	78
57	W	100/100 (100%)	99 (99%)	1 (1%)	68	79
58	X	53/53 (100%)	52 (98%)	1 (2%)	50	73
59	Y	105/105 (100%)	103 (98%)	2 (2%)	50	73
60	Z	124/124 (100%)	122 (98%)	2 (2%)	55	75
61	a	117/117 (100%)	116 (99%)	1 (1%)	70	80
62	b	120/120 (100%)	119 (99%)	1 (1%)	73	81
63	c	82/101 (81%)	80 (98%)	2 (2%)	43	69
64	d	88/88 (100%)	86 (98%)	2 (2%)	44	70
65	e	97/97 (100%)	96 (99%)	1 (1%)	68	79
66	f	115/115 (100%)	115 (100%)	0	100	100
67	g	88/88 (100%)	82 (93%)	6 (7%)	14	42
68	h	98/98 (100%)	98 (100%)	0	100	100
69	i	109/109 (100%)	109 (100%)	0	100	100
70	j	83/83 (100%)	83 (100%)	0	100	100
71	k	71/71 (100%)	71 (100%)	0	100	100
72	l	64/64 (100%)	63 (98%)	1 (2%)	55	75
73	m	47/47 (100%)	46 (98%)	1 (2%)	47	71
74	n	46/46 (100%)	46 (100%)	0	100	100
75	o	24/24 (100%)	24 (100%)	0	100	100
76	p	93/93 (100%)	90 (97%)	3 (3%)	34	64
77	q	74/74 (100%)	73 (99%)	1 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	r	106/106 (100%)	105 (99%)	1 (1%)	70	80
83	y	21/21 (100%)	12 (57%)	9 (43%)	0	0
All	All	9785/9818 (100%)	9652 (99%)	133 (1%)	59	76

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	82	THR
2	SA	122	LEU
3	SB	87	ILE
4	SD	5	ILE
4	SD	105	LEU
4	SD	126	ILE
5	SE	90	ILE
5	SE	228	ILE
5	SE	238	LEU
6	SF	61	PHE
6	SF	63	LYS
6	SF	68	ILE
6	SF	83	ASN
8	SI	60	LEU
8	SI	128	LYS
11	SP	121	ILE
12	SQ	22	VAL
12	SQ	111	ILE
13	SR	83	ASN
13	SR	85	VAL
15	ST	4	VAL
15	ST	37	VAL
15	ST	131	LEU
17	SV	79	VAL
18	SX	61	GLN
18	SX	112	VAL
19	Sa	75	VAL
21	Sd	26	ASN
22	Sg	195	LEU
22	Sg	252	THR
23	SC	155	ILE
23	SC	156	ILE
23	SC	200[A]	ARG
23	SC	200[B]	ARG

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Mol	Chain	Res	Type
24	SG	111	LEU
25	SJ	138[A]	ARG
25	SJ	138[B]	ARG
26	SM	35	ILE
26	SM	89	VAL
28	SO	129	ILE
28	SO	140	THR
29	SW	103	VAL
31	SZ	62	VAL
31	SZ	67	LEU
32	Sb	24	LEU
33	Se	6	LEU
35	A	20	VAL
35	A	45	VAL
35	A	101	VAL
35	A	116	LEU
35	A	207	VAL
36	B	60	VAL
36	B	67	VAL
36	B	85	VAL
36	B	254	ILE
36	B	299	ILE
36	B	301	ASN
36	B	345	LEU
37	C	150	LEU
37	C	193	LYS
37	C	199	ARG
37	C	223	ASN
37	C	263	LEU
40	F	6	VAL
40	F	37	VAL
41	G	50	LEU
41	G	279	ASN
42	H	41	MET
42	H	167	ILE
42	H	169	LEU
43	I	45	ILE
43	I	55	VAL
44	J	42	ASN
44	J	57	VAL
44	J	63	ASN
44	J	111	LEU

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Mol	Chain	Res	Type
45	K	26	VAL
46	L	33	LEU
47	M	63	THR
47	M	125	ILE
47	M	169	ILE
48	N	5	ARG
48	N	45	VAL
49	O	64	ILE
49	O	133	ILE
49	O	183	THR
49	O	200	LEU
49	O	204	ARG
50	P	36	VAL
51	Q	24	VAL
51	Q	127	ARG
52	R	14	ARG
52	R	138	LEU
54	T	67	VAL
55	U	75	VAL
55	U	128	LEU
55	U	154	ILE
56	V	103	VAL
57	W	132	ILE
58	X	43	LYS
59	Y	96	LEU
59	Y	119	ILE
60	Z	79	VAL
60	Z	104	VAL
61	a	13	VAL
62	b	63	LEU
63	c	54	LEU
63	c	116	LEU
64	d	35	LEU
64	d	77	ASN
65	e	93	ASN
67	g	33	VAL
67	g	58	VAL
67	g	59	THR
67	g	105	LEU
67	g	109	ARG
67	g	110	ILE
72	l	46	VAL

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Mol	Chain	Res	Type
73	m	27	ILE
76	p	10	THR
76	p	23	VAL
76	p	58	LYS
77	q	29	ILE
78	r	78	VAL
83	y	2	TRP
83	y	4	LEU
83	y	7	LEU
83	y	9	LEU
83	y	10	LEU
83	y	11	LEU
83	y	13	LEU
83	y	14	LEU
83	y	23	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (192) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	9	GLN
2	SA	50	ASN
3	SB	40	ASN
3	SB	92	GLN
3	SB	101	HIS
3	SB	158	HIS
3	SB	186	ASN
3	SB	202	GLN
4	SD	226	GLN
5	SE	36	HIS
5	SE	98	ASN
5	SE	112	HIS
5	SE	142	HIS
5	SE	179	ASN
6	SF	79	HIS
6	SF	137	GLN
7	SH	25	GLN
7	SH	39	GLN
7	SH	73	GLN
7	SH	114	GLN
7	SH	168	HIS
8	SI	7	ASN
8	SI	167	GLN

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Mol	Chain	Res	Type
8	SI	181	GLN
9	SK	61	GLN
10	SL	19	ASN
10	SL	65	ASN
10	SL	83	GLN
10	SL	154	GLN
11	SP	54	HIS
11	SP	103	ASN
11	SP	114	HIS
13	SR	83	ASN
14	SS	85	ASN
14	SS	120	HIS
15	ST	128	GLN
17	SV	2	GLN
17	SV	21	ASN
17	SV	35	ASN
18	SX	61	GLN
18	SX	87	ASN
20	Sc	7	GLN
20	Sc	29	GLN
22	Sg	64	HIS
22	Sg	104	HIS
22	Sg	147	HIS
22	Sg	162	ASN
22	Sg	222	ASN
23	SC	115	GLN
24	SG	59	GLN
24	SG	81	HIS
24	SG	163	ASN
24	SG	197	GLN
25	SJ	154	GLN
26	SM	55	ASN
27	SN	5	HIS
27	SN	49	GLN
27	SN	123	HIS
28	SO	103	ASN
29	SW	15	ASN
29	SW	16	ASN
29	SW	98	GLN
29	SW	120	HIS
30	SY	2	ASN
30	SY	94	HIS

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Mol	Chain	Res	Type
31	SZ	89	GLN
31	SZ	106	GLN
32	Sb	19	HIS
32	Sb	83	GLN
34	Sf	91	ASN
34	Sf	135	HIS
35	A	50	HIS
35	A	97	ASN
35	A	132	ASN
35	A	162	ASN
35	A	209	HIS
35	A	218	HIS
36	B	55	HIS
36	B	121	ASN
36	B	145	GLN
36	B	167	GLN
36	B	213	GLN
36	B	245	HIS
36	B	301	ASN
36	B	322	HIS
36	B	376	HIS
37	C	21	ASN
37	C	38	ASN
37	C	85	HIS
37	C	94	ASN
37	C	198	ASN
37	C	223	ASN
37	C	236	ASN
37	C	278	ASN
37	C	343	GLN
37	C	347	HIS
40	F	39	GLN
40	F	198	HIS
40	F	202	GLN
40	F	244	HIS
40	F	275	GLN
41	G	101	ASN
41	G	167	GLN
41	G	190	HIS
41	G	250	GLN
41	G	266	GLN
41	G	279	ASN

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Mol	Chain	Res	Type
42	H	24	ASN
42	H	80	ASN
42	H	151	ASN
42	H	226	HIS
43	I	64	GLN
43	I	149	ASN
43	I	159	HIS
43	I	206	GLN
44	J	42	ASN
44	J	63	ASN
44	J	108	ASN
44	J	140	GLN
44	J	189	GLN
45	K	14	ASN
45	K	86	HIS
45	K	92	HIS
45	K	144	ASN
45	K	213	HIS
46	L	71	HIS
46	L	112	HIS
46	L	155	HIS
46	L	167	GLN
47	M	19	GLN
47	M	87	HIS
47	M	104	ASN
48	N	44	GLN
48	N	48	GLN
48	N	56	GLN
48	N	120	ASN
48	N	125	ASN
49	O	86	HIS
49	O	158	HIS
49	O	199	GLN
50	P	14	HIS
50	P	50	ASN
50	P	63	ASN
50	P	96	GLN
50	P	167	HIS
50	P	184	ASN
51	Q	34	GLN
51	Q	80	GLN
51	Q	133	HIS

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Mol	Chain	Res	Type
51	Q	145	HIS
52	R	7	HIS
52	R	160	HIS
53	S	130	ASN
54	T	91	HIS
54	T	162	GLN
57	W	77	HIS
57	W	101	ASN
59	Y	107	HIS
59	Y	111	GLN
60	Z	14	ASN
60	Z	20	ASN
60	Z	61	HIS
62	b	28	HIS
62	b	49	HIS
62	b	89	ASN
63	c	6	ASN
63	c	19	ASN
63	c	58	GLN
64	d	40	GLN
64	d	77	ASN
65	e	34	HIS
65	e	93	ASN
65	e	100	ASN
66	f	107	ASN
67	g	55	ASN
67	g	56	ASN
69	i	20	GLN
69	i	30	GLN
69	i	107	GLN
70	j	26	HIS
70	j	80	HIS
71	k	57	ASN
73	m	43	HIS
74	n	104	HIS
74	n	109	ASN
76	p	21	HIS
76	p	102	GLN
77	q	56	HIS
78	r	6	GLN
78	r	41	ASN
78	r	83	ASN

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Mol	Chain	Res	Type
83	y	22	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1687/1714 (98%)	544 (32%)	34 (2%)
38	D	156/157 (99%)	39 (25%)	0
39	E	118/119 (99%)	13 (11%)	0
79	t	3592/3607 (99%)	880 (24%)	0
80	u	74/76 (97%)	28 (37%)	0
81	v	73/76 (96%)	29 (39%)	0
82	w	9/10 (90%)	2 (22%)	0
All	All	5709/5759 (99%)	1535 (26%)	34 (0%)

All (1535) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	7	G
1	S2	16	G
1	S2	23	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	36	U
1	S2	37	C
1	S2	38	A
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	44	U
1	S2	46	A
1	S2	53	C
1	S2	54	A
1	S2	55	U
1	S2	56	G
1	S2	60	A
1	S2	61	A
1	S2	64	A
1	S2	65	C
1	S2	66	G

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Mol	Chain	Res	Type
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	77	A
1	S2	78	C
1	S2	79	A
1	S2	80	G
1	S2	83	A
1	S2	90	G
1	S2	99	A
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	119	PSU
1	S2	123	G
1	S2	125	C
1	S2	126	G
1	S2	143	U
1	S2	155	G
1	S2	159	A2M
1	S2	160	U
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	176	U
1	S2	182	C
1	S2	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
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G

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Mol	Chain	Res	Type
1	S2	204	G
1	S2	206	G
1	S2	208	G
1	S2	209	A
1	S2	210	U
1	S2	214	U
1	S2	215	G
1	S2	290	U
1	S2	291	G
1	S2	292	A
1	S2	293	C
1	S2	294	U
1	S2	295	C
1	S2	302	A
1	S2	305	U
1	S2	308	G
1	S2	311	C
1	S2	312	G
1	S2	316	G
1	S2	318	A
1	S2	319	C
1	S2	320	G
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	330	G
1	S2	335	G
1	S2	338	G
1	S2	340	C
1	S2	347	G
1	S2	360	A
1	S2	364	A
1	S2	368	U
1	S2	369	C
1	S2	377	G
1	S2	379	C
1	S2	380	G
1	S2	385	G

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Mol	Chain	Res	Type
1	S2	386	C
1	S2	387	C
1	S2	394	G
1	S2	395	G
1	S2	398	A
1	S2	399	C
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	417	C
1	S2	418	A
1	S2	419	G
1	S2	429	C
1	S2	438	G
1	S2	446	G
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	470	G
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	481	C
1	S2	482	G
1	S2	484	A2M
1	S2	485	A
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	525	A
1	S2	528	A
1	S2	530	U
1	S2	531	A
1	S2	532	C

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Mol	Chain	Res	Type
1	S2	534	G
1	S2	535	G
1	S2	536	A
1	S2	537	C
1	S2	538	U
1	S2	541	U
1	S2	542	U
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	548	C
1	S2	549	C
1	S2	550	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	576	A
1	S2	578	C
1	S2	580	U
1	S2	583	C
1	S2	585	C
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	594	A
1	S2	597	G
1	S2	607	U
1	S2	608	C
1	S2	610	G
1	S2	614	C
1	S2	625	G
1	S2	627	U
1	S2	628	A
1	S2	629	A

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Mol	Chain	Res	Type
1	S2	631	U
1	S2	632	C
1	S2	643	A
1	S2	655	A
1	S2	659	G
1	S2	660	C
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	683	OMG
1	S2	687	C
1	S2	689	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	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	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	794	A

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Mol	Chain	Res	Type
1	S2	797	C
1	S2	807	G
1	S2	810	A
1	S2	815	U
1	S2	821	G
1	S2	822	PSU
1	S2	830	A
1	S2	831	G
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	840	C
1	S2	841	G
1	S2	847	A
1	S2	851	C
1	S2	855	G
1	S2	856	C
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	870	A
1	S2	871	U
1	S2	872	A
1	S2	873	G
1	S2	878	G
1	S2	880	G
1	S2	885	U
1	S2	886	A
1	S2	887	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	894	G
1	S2	895	G
1	S2	896	U
1	S2	897	U

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Mol	Chain	Res	Type
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	903	A
1	S2	904	A
1	S2	905	C
1	S2	906	U
1	S2	907	G
1	S2	909	G
1	S2	910	G
1	S2	913	A
1	S2	914	U
1	S2	915	G
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	924	G
1	S2	933	G
1	S2	943	U
1	S2	956	G
1	S2	963	A
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	986	G
1	S2	990	A
1	S2	992	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1003	U
1	S2	1005	G
1	S2	1006	C
1	S2	1007	C
1	S2	1009	A
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

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Mol	Chain	Res	Type
1	S2	1045	U
1	S2	1049	A
1	S2	1058	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1064	C
1	S2	1072	U
1	S2	1078	C
1	S2	1083	A
1	S2	1085	C
1	S2	1089	G
1	S2	1109	C
1	S2	1113	A
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1117	C
1	S2	1118	C
1	S2	1119	A
1	S2	1121	G
1	S2	1133	A
1	S2	1138	C
1	S2	1146	C
1	S2	1149	A
1	S2	1150	A
1	S2	1154	U
1	S2	1155	U
1	S2	1159	G
1	S2	1166	G
1	S2	1170	A
1	S2	1180	C
1	S2	1195	A
1	S2	1207	G
1	S2	1208	A
1	S2	1209	A
1	S2	1212	G
1	S2	1215	C
1	S2	1217	A
1	S2	1224	G
1	S2	1233	G
1	S2	1242	U

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Mol	Chain	Res	Type
1	S2	1251	A
1	S2	1253	A
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	1265	A
1	S2	1271	C
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1289	U
1	S2	1294	G
1	S2	1295	A
1	S2	1296	U
1	S2	1297	U
1	S2	1298	G
1	S2	1300	U
1	S2	1302	G
1	S2	1304	U
1	S2	1313	A
1	S2	1320	G
1	S2	1322	G
1	S2	1328	G
1	S2	1330	G
1	S2	1331	C
1	S2	1340	U
1	S2	1341	C
1	S2	1348	G
1	S2	1350	U
1	S2	1351	G
1	S2	1352	G
1	S2	1353	A
1	S2	1355	C
1	S2	1356	G
1	S2	1357	A

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Mol	Chain	Res	Type
1	S2	1364	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1375	G
1	S2	1376	A
1	S2	1378	A
1	S2	1379	A
1	S2	1397	U
1	S2	1403	C
1	S2	1411	G
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G
1	S2	1454	A
1	S2	1455	A
1	S2	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1464	C
1	S2	1466	G
1	S2	1477	U
1	S2	1480	A
1	S2	1481	G
1	S2	1482	C
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1495	G
1	S2	1496	U
1	S2	1497	G

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Mol	Chain	Res	Type
1	S2	1498	A
1	S2	1505	U
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1523	C
1	S2	1528	G
1	S2	1533	A
1	S2	1550	G
1	S2	1551	U
1	S2	1552	G
1	S2	1553	C
1	S2	1555	U
1	S2	1556	A
1	S2	1557	C
1	S2	1558	C
1	S2	1560	U
1	S2	1568	C
1	S2	1570	G
1	S2	1573	G
1	S2	1578	U
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1586	U
1	S2	1588	A
1	S2	1594	A
1	S2	1598	G
1	S2	1599	U
1	S2	1601	A
1	S2	1621	U
1	S2	1623	A
1	S2	1647	A
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A
1	S2	1665	G
1	S2	1671	G
1	S2	1674	G

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Mol	Chain	Res	Type
1	S2	1675	A
1	S2	1676	U
1	S2	1677	U
1	S2	1680	G
1	S2	1682	C
1	S2	1683	C
1	S2	1686	G
1	S2	1687	C
1	S2	1693	G
1	S2	1695	A
1	S2	1698	C
1	S2	1699	A
1	S2	1720	U
1	S2	1721	U
1	S2	1722	G
1	S2	1728	U
1	S2	1729	U
1	S2	1744	G
1	S2	1749	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
1	S2	1784	G
1	S2	1785	C
1	S2	1786	U
1	S2	1803	U
1	S2	1805	G
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	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	UR3
1	S2	1831	A

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Mol	Chain	Res	Type
1	S2	1835	A
1	S2	1836	G
1	S2	1838	U
1	S2	1841	C
1	S2	1849	G
1	S2	1850	MA6
1	S2	1851	MA6
1	S2	1852	C
1	S2	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	1869	A
38	D	2	G
38	D	13	G
38	D	34	U
38	D	35	C
38	D	39	G
38	D	49	G
38	D	51	U
38	D	52	A
38	D	59	A
38	D	61	A
38	D	63	U
38	D	72	A
38	D	80	A
38	D	81	C
38	D	82	A
38	D	83	C
38	D	87	G
38	D	94	G
38	D	96	C
38	D	103	A
38	D	104	A
38	D	105	C
38	D	109	C
38	D	110	U
38	D	111	U
38	D	112	G

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Mol	Chain	Res	Type
38	D	114	G
38	D	121	G
38	D	122	G
38	D	123	U
38	D	124	U
38	D	125	C
38	D	126	C
38	D	127	U
38	D	128	C
38	D	129	C
38	D	130	C
38	D	148	A
38	D	150	C
39	E	7	G
39	E	11	A
39	E	22	A
39	E	23	A
39	E	33	U
39	E	35	U
39	E	40	U
39	E	48	G
39	E	49	A
39	E	53	U
39	E	64	G
39	E	96	U
39	E	110	G
79	t	6	C
79	t	9	C
79	t	11	G
79	t	17	A
79	t	18	C
79	t	25	A
79	t	30	C
79	t	32	G
79	t	39	A
79	t	42	A
79	t	48	G
79	t	49	U
79	t	58	G
79	t	59	A
79	t	64	A
79	t	65	A

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Mol	Chain	Res	Type
79	t	66	A
79	t	70	A
79	t	71	C
79	t	72	C
79	t	74	G
79	t	75	G
79	t	91	G
79	t	93	G
79	t	101	A
79	t	108	A
79	t	110	C
79	t	116	G
79	t	118	C
79	t	119	G
79	t	120	A
79	t	129	C
79	t	130	C
79	t	131	C
79	t	132	G
79	t	133	C
79	t	134	G
79	t	135	G
79	t	137	G
79	t	138	C
79	t	143	G
79	t	144	A
79	t	148	G
79	t	149	U
79	t	156	C
79	t	157	G
79	t	169	C
79	t	173	G
79	t	174	G
79	t	176	G
79	t	181	U
79	t	182	C
79	t	183	G
79	t	184	U
79	t	185	G
79	t	193	C
79	t	196	G
79	t	205	A

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Mol	Chain	Res	Type
79	t	206	U
79	t	212	C
79	t	213	C
79	t	214	C
79	t	215	A
79	t	228	U
79	t	229	G
79	t	230	U
79	t	233	G
79	t	237	G
79	t	249	C
79	t	250	G
79	t	253	G
79	t	256	C
79	t	258	C
79	t	260	C
79	t	272	G
79	t	289	A
79	t	291	U
79	t	300	A
79	t	309	G
79	t	310	U
79	t	311	A
79	t	323	A
79	t	334	C
79	t	339	C
79	t	343	A
79	t	367	G
79	t	370	A
79	t	379	A
79	t	380	A
79	t	381	G
79	t	404	A
79	t	405	G
79	t	406	G
79	t	407	G
79	t	408	C
79	t	409	G
79	t	425	G
79	t	426	U
79	t	434	U
79	t	444	G

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Mol	Chain	Res	Type
79	t	447	G
79	t	448	U
79	t	449	C
79	t	451	G
79	t	456	G
79	t	458	G
79	t	463	C
79	t	466	C
79	t	474	C
79	t	479	C
79	t	480	C
79	t	482	G
79	t	484	C
79	t	485	G
79	t	486	U
79	t	487	G
79	t	489	C
79	t	492	C
79	t	494	G
79	t	496	C
79	t	497	C
79	t	498	G
79	t	504	U
79	t	507	U
79	t	509	C
79	t	511	C
79	t	512	G
79	t	514	C
79	t	633	U
79	t	634	C
79	t	635	G
79	t	636	G
79	t	643	A
79	t	648	C
79	t	649	C
79	t	650	C
79	t	651	C
79	t	654	G
79	t	657	C
79	t	658	G
79	t	659	G
79	t	660	C

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Mol	Chain	Res	Type
79	t	661	G
79	t	674	C
79	t	676	G
79	t	677	G
79	t	678	C
79	t	679	G
79	t	680	C
79	t	690	C
79	t	692	G
79	t	693	U
79	t	695	C
79	t	696	G
79	t	698	C
79	t	703	C
79	t	709	C
79	t	714	A
79	t	719	U
79	t	720	G
79	t	721	G
79	t	724	A
79	t	727	C
79	t	728	C
79	t	730	G
79	t	736	G
79	t	737	A
79	t	738	A
79	t	739	G
79	t	741	U
79	t	743	G
79	t	900	U
79	t	901	U
79	t	902	A
79	t	903	C
79	t	904	A
79	t	905	G
79	t	906	C
79	t	914	G
79	t	917	G
79	t	919	A
79	t	920	G
79	t	921	C
79	t	922	A

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Mol	Chain	Res	Type
79	t	923	C
79	t	924	U
79	t	925	C
79	t	926	G
79	t	927	C
79	t	931	A
79	t	932	U
79	t	933	C
79	t	934	C
79	t	938	G
79	t	944	G
79	t	947	A
79	t	948	G
79	t	949	C
79	t	950	G
79	t	952	G
79	t	953	A
79	t	957	G
79	t	959	C
79	t	964	C
79	t	969	U
79	t	1055	C
79	t	1059	C
79	t	1061	A
79	t	1063	C
79	t	1065	C
79	t	1069	C
79	t	1070	A
79	t	1075	G
79	t	1084	C
79	t	1087	C
79	t	1149	G
79	t	1150	C
79	t	1152	G
79	t	1154	G
79	t	1156	G
79	t	1162	U
79	t	1163	C
79	t	1165	C
79	t	1167	A
79	t	1172	G
79	t	1174	C

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Mol	Chain	Res	Type
79	t	1179	G
79	t	1180	C
79	t	1190	C
79	t	1192	U
79	t	1193	C
79	t	1196	G
79	t	1197	C
79	t	1198	C
79	t	1199	C
79	t	1201	G
79	t	1218	G
79	t	1220	C
79	t	1221	A
79	t	1222	C
79	t	1223	G
79	t	1225	G
79	t	1226	C
79	t	1228	C
79	t	1234	C
79	t	1237	A
79	t	1238	A
79	t	1239	G
79	t	1240	G
79	t	1248	G
79	t	1250	C
79	t	1251	G
79	t	1258	G
79	t	1259	C
79	t	1260	G
79	t	1261	C
79	t	1268	U
79	t	1269	C
79	t	1271	G
79	t	1277	A
79	t	1279	G
79	t	1285	U
79	t	1296	C
79	t	1301	C
79	t	1309	A
79	t	1337	A
79	t	1341	G
79	t	1342	G

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Mol	Chain	Res	Type
79	t	1348	C
79	t	1349	G
79	t	1350	C
79	t	1351	A
79	t	1353	G
79	t	1354	A
79	t	1361	C
79	t	1362	C
79	t	1364	U
79	t	1370	A
79	t	1377	G
79	t	1380	A
79	t	1381	A
79	t	1391	G
79	t	1392	C
79	t	1393	U
79	t	1394	C
79	t	1395	G
79	t	1396	C
79	t	1401	C
79	t	1403	A
79	t	1420	C
79	t	1421	U
79	t	1423	U
79	t	1424	C
79	t	1426	A
79	t	1427	G
79	t	1428	U
79	t	1430	C
79	t	1431	G
79	t	1439	G
79	t	1463	C
79	t	1464	G
79	t	1465	C
79	t	1466	G
79	t	1467	C
79	t	1468	C
79	t	1469	G
79	t	1473	A
79	t	1480	G
79	t	1500	A
79	t	1507	A

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Mol	Chain	Res	Type
79	t	1516	A
79	t	1521	G
79	t	1531	G
79	t	1548	C
79	t	1560	U
79	t	1564	U
79	t	1573	U
79	t	1578	U
79	t	1583	A
79	t	1587	G
79	t	1593	C
79	t	1606	G
79	t	1607	G
79	t	1613	A
79	t	1614	A
79	t	1615	G
79	t	1616	A
79	t	1619	A
79	t	1620	A
79	t	1622	C
79	t	1624	A
79	t	1632	A
79	t	1636	G
79	t	1638	U
79	t	1643	C
79	t	1652	G
79	t	1658	C
79	t	1659	U
79	t	1660	C
79	t	1663	G
79	t	1676	C
79	t	1680	C
79	t	1700	C
79	t	1701	A
79	t	1713	C
79	t	1723	G
79	t	1732	G
79	t	1736	U
79	t	1746	G
79	t	1747	A
79	t	1750	C
79	t	1757	A

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Mol	Chain	Res	Type
79	t	1769	A
79	t	1776	A
79	t	1779	G
79	t	1785	G
79	t	1786	A
79	t	1794	C
79	t	1797	G
79	t	1803	G
79	t	1814	G
79	t	1816	G
79	t	1818	A
79	t	1823	G
79	t	1836	G
79	t	1850	G
79	t	1869	A
79	t	1870	U
79	t	1871	G
79	t	1872	A
79	t	1879	C
79	t	1887	U
79	t	1891	G
79	t	1896	C
79	t	1898	A
79	t	1900	G
79	t	1902	C
79	t	1903	G
79	t	1906	G
79	t	1909	C
79	t	1911	U
79	t	1912	C
79	t	1913	A
79	t	1916	C
79	t	1920	A
79	t	1921	G
79	t	1928	U
79	t	1929	G
79	t	1933	G
79	t	1938	U
79	t	1939	A
79	t	1940	U
79	t	1941	A
79	t	1942	G

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Mol	Chain	Res	Type
79	t	1943	A
79	t	1955	U
79	t	1956	G
79	t	1957	G
79	t	1958	C
79	t	1961	U
79	t	1963	G
79	t	1964	A
79	t	1967	U
79	t	1968	C
79	t	1972	A
79	t	1973	U
79	t	1974	C
79	t	1978	U
79	t	1980	A
79	t	1982	G
79	t	1983	A
79	t	1984	G
79	t	1985	U
79	t	1988	G
79	t	1989	U
79	t	1991	A
79	t	1994	A
79	t	2007	A
79	t	2025	U
79	t	2027	G
79	t	2029	U
79	t	2036	G
79	t	2037	G
79	t	2043	C
79	t	2050	A
79	t	2051	U
79	t	2065	C
79	t	2069	G
79	t	2072	G
79	t	2073	A
79	t	2074	G
79	t	2075	A
79	t	2076	G
79	t	2078	G
79	t	2079	G
79	t	2081	C

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Mol	Chain	Res	Type
79	t	2082	G
79	t	2084	G
79	t	2087	C
79	t	2090	C
79	t	2091	G
79	t	2092	G
79	t	2229	C
79	t	2232	A
79	t	2233	G
79	t	2234	C
79	t	2235	C
79	t	2241	G
79	t	2246	U
79	t	2247	A
79	t	2249	G
79	t	2268	C
79	t	2269	C
79	t	2278	G
79	t	2279	A
79	t	2280	G
79	t	2282	C
79	t	2284	U
79	t	2285	G
79	t	2292	A
79	t	2301	G
79	t	2310	G
79	t	2326	A
79	t	2327	G
79	t	2330	C
79	t	2336	G
79	t	2340	G
79	t	2343	G
79	t	2357	G
79	t	2358	A
79	t	2374	A
79	t	2375	A
79	t	2377	U
79	t	2381	G
79	t	2387	U
79	t	2388	U
79	t	2396	A
79	t	2400	G

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Mol	Chain	Res	Type
79	t	2401	C
79	t	2404	U
79	t	2416	C
79	t	2421	G
79	t	2426	U
79	t	2429	G
79	t	2431	G
79	t	2442	G
79	t	2446	U
79	t	2447	U
79	t	2449	C
79	t	2453	G
79	t	2457	C
79	t	2458	G
79	t	2467	C
79	t	2468	C
79	t	2469	U
79	t	2472	G
79	t	2473	U
79	t	2474	U
79	t	2475	G
79	t	2482	G
79	t	2483	C
79	t	2484	C
79	t	2485	G
79	t	2492	A
79	t	2499	C
79	t	2516	A
79	t	2523	G
79	t	2524	U
79	t	2525	G
79	t	2526	G
79	t	2532	A
79	t	2533	U
79	t	2545	G
79	t	2565	G
79	t	2566	A
79	t	2568	C
79	t	2570	A
79	t	2579	A
79	t	2580	A
79	t	2585	G

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Mol	Chain	Res	Type
79	t	2595	C
79	t	2599	G
79	t	2617	G
79	t	2618	U
79	t	2632	C
79	t	2645	U
79	t	2648	C
79	t	2652	G
79	t	2665	G
79	t	2666	U
79	t	2673	G
79	t	2675	A
79	t	2686	U
79	t	2689	C
79	t	2690	G
79	t	2691	G
79	t	2700	G
79	t	2705	G
79	t	2714	G
79	t	2719	U
79	t	2722	A
79	t	2723	A
79	t	2732	G
79	t	2733	G
79	t	2739	G
79	t	2741	G
79	t	2742	U
79	t	2745	A
79	t	2746	U
79	t	2748	U
79	t	2751	C
79	t	2766	A
79	t	2767	U
79	t	2769	U
79	t	2776	C
79	t	2778	G
79	t	2785	A
79	t	2794	A
79	t	2798	U
79	t	2805	U
79	t	2806	G
79	t	2817	G

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Mol	Chain	Res	Type
79	t	2829	A
79	t	2834	G
79	t	2835	C
79	t	2846	C
79	t	2858	A
79	t	2860	A
79	t	2870	U
79	t	2871	C
79	t	2876	G
79	t	2880	G
79	t	3570	A
79	t	3571	G
79	t	3572	C
79	t	3574	G
79	t	3577	U
79	t	3587	U
79	t	3589	C
79	t	3591	G
79	t	3596	G
79	t	3597	G
79	t	3601	A
79	t	3606	A
79	t	3607	C
79	t	3612	U
79	t	3615	U
79	t	3616	U
79	t	3617	A
79	t	3619	A
79	t	3635	G
79	t	3643	G
79	t	3644	C
79	t	3651	U
79	t	3662	G
79	t	3667	C
79	t	3670	C
79	t	3675	U
79	t	3683	A
79	t	3697	A
79	t	3700	U
79	t	3707	A
79	t	3719	A
79	t	3728	G

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Mol	Chain	Res	Type
79	t	3730	A
79	t	3731	A
79	t	3741	U
79	t	3745	A
79	t	3747	G
79	t	3748	G
79	t	3751	G
79	t	3754	A
79	t	3755	A
79	t	3759	C
79	t	3781	C
79	t	3782	G
79	t	3784	A
79	t	3785	U
79	t	3788	A
79	t	3789	U
79	t	3790	G
79	t	3795	A
79	t	3798	G
79	t	3799	A
79	t	3809	U
79	t	3811	U
79	t	3838	A
79	t	3848	A
79	t	3849	C
79	t	3850	G
79	t	3851	G
79	t	3852	G
79	t	3860	G
79	t	3861	A
79	t	3863	U
79	t	3866	G
79	t	3868	G
79	t	3872	A
79	t	3876	A
79	t	3877	A
79	t	3878	G
79	t	3879	A
79	t	3886	U
79	t	3887	G
79	t	3890	C
79	t	3897	C

Continued on next page...

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Mol	Chain	Res	Type
79	t	3908	C
79	t	3909	G
79	t	3918	A
79	t	4046	G
79	t	4049	C
79	t	4054	G
79	t	4060	G
79	t	4062	G
79	t	4064	G
79	t	4065	G
79	t	4066	C
79	t	4067	G
79	t	4068	A
79	t	4069	G
79	t	4070	C
79	t	4071	C
79	t	4072	C
79	t	4074	A
79	t	4076	G
79	t	4078	G
79	t	4079	C
79	t	4080	U
79	t	4083	C
79	t	4084	G
79	t	4086	U
79	t	4088	C
79	t	4097	A
79	t	4104	G
79	t	4105	C
79	t	4107	C
79	t	4108	G
79	t	4109	G
79	t	4110	C
79	t	4124	C
79	t	4125	U
79	t	4126	C
79	t	4130	G
79	t	4132	A
79	t	4145	G
79	t	4146	G
79	t	4153	G
79	t	4158	G

Continued on next page...

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Mol	Chain	Res	Type
79	t	4165	A
79	t	4167	A
79	t	4168	C
79	t	4174	A
79	t	4176	A
79	t	4187	G
79	t	4190	G
79	t	4191	U
79	t	4195	A
79	t	4199	C
79	t	4205	C
79	t	4213	A
79	t	4215	A
79	t	4216	G
79	t	4220	C
79	t	4228	G
79	t	4229	G
79	t	4230	A
79	t	4235	A
79	t	4242	A
79	t	4243	A
79	t	4253	G
79	t	4260	A
79	t	4266	A
79	t	4267	G
79	t	4268	U
79	t	4276	C
79	t	4288	G
79	t	4291	G
79	t	4292	G
79	t	4294	C
79	t	4299	C
79	t	4300	G
79	t	4301	A
79	t	4311	C
79	t	4316	U
79	t	4320	U
79	t	4326	G
79	t	4327	C
79	t	4333	G
79	t	4334	U
79	t	4335	G

Continued on next page...

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Mol	Chain	Res	Type
79	t	4338	A
79	t	4339	G
79	t	4340	A
79	t	4341	A
79	t	4343	A
79	t	4349	C
79	t	4353	G
79	t	4356	A
79	t	4358	A
79	t	4360	C
79	t	4367	G
79	t	4372	G
79	t	4373	G
79	t	4384	A
79	t	4388	C
79	t	4402	G
79	t	4414	U
79	t	4426	A
79	t	4437	G
79	t	4455	U
79	t	4459	U
79	t	4465	A
79	t	4474	U
79	t	4475	A
79	t	4477	G
79	t	4480	A
79	t	4481	C
79	t	4485	A
79	t	4486	G
79	t	4490	G
79	t	4510	A
79	t	4517	U
79	t	4518	U
79	t	4522	C
79	t	4529	G
79	t	4532	G
79	t	4537	G
79	t	4551	A
79	t	4552	A
79	t	4559	U
79	t	4561	A
79	t	4562	G

Continued on next page...

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Mol	Chain	Res	Type
79	t	4578	A
79	t	4579	G
79	t	4586	A
79	t	4593	G
79	t	4595	G
79	t	4598	U
79	t	4599	G
79	t	4601	G
79	t	4611	G
79	t	4618	A
79	t	4619	U
79	t	4626	A
79	t	4632	C
79	t	4634	A
79	t	4649	A
79	t	4656	G
79	t	4657	C
79	t	4662	A
79	t	4671	U
79	t	4674	C
79	t	4681	G
79	t	4684	G
79	t	4692	C
79	t	4693	G
79	t	4694	G
79	t	4695	C
79	t	4696	A
79	t	4699	G
79	t	4703	C
79	t	4704	G
79	t	4712	G
79	t	4715	U
79	t	4718	C
79	t	4720	U
79	t	4722	G
79	t	4726	A
79	t	4727	G
79	t	4732	U
79	t	4734	C
79	t	4736	C
79	t	4737	G
79	t	4824	C

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Mol	Chain	Res	Type
79	t	4827	U
79	t	4828	G
79	t	4831	G
79	t	4832	A
79	t	4833	G
79	t	4834	U
79	t	4838	C
79	t	4839	U
79	t	4840	U
79	t	4841	C
79	t	4852	A
79	t	4853	C
79	t	4854	G
79	t	4855	G
79	t	4858	C
79	t	4859	G
79	t	4860	C
79	t	4864	C
79	t	4865	G
79	t	4866	G
79	t	4868	A
79	t	4870	G
79	t	4871	G
79	t	4880	C
79	t	4882	C
79	t	4883	U
79	t	4885	G
79	t	4886	C
79	t	4894	G
79	t	4895	C
79	t	4896	A
79	t	4898	C
79	t	4901	A
79	t	4902	C
79	t	4907	G
79	t	4908	U
79	t	4909	G
79	t	4917	U
79	t	4924	A
79	t	4933	G
79	t	4934	U
79	t	4937	A

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Mol	Chain	Res	Type
79	t	4943	U
79	t	4946	U
79	t	4947	U
79	t	4949	U
79	t	4950	G
79	t	4957	G
79	t	4971	C
79	t	4972	A
79	t	4975	G
79	t	4982	C
79	t	4984	U
79	t	4985	C
79	t	4986	G
79	t	4998	U
79	t	4999	G
79	t	5005	C
79	t	5007	G
79	t	5008	C
79	t	5011	U
79	t	5012	C
79	t	5015	C
79	t	5016	A
79	t	5020	G
79	t	5024	U
80	u	4	C
80	u	8	U
80	u	15	G
80	u	17	C
80	u	18	G
80	u	19	G
80	u	20	U
80	u	21	A
80	u	23	A
80	u	24	G
80	u	44	G
80	u	46	G
80	u	47	U
80	u	48	C
80	u	50	U
80	u	52	G
80	u	56	C
80	u	57	G

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Mol	Chain	Res	Type
80	u	59	U
80	u	60	U
80	u	61	C
80	u	64	A
80	u	69	G
80	u	71	G
80	u	72	C
80	u	73	A
80	u	74	C
80	u	76	A
81	v	8	U
81	v	11	C
81	v	12	C
81	v	13	C
81	v	15	G
81	v	16	A
81	v	17	A
81	v	19	G
81	v	20	U
81	v	21	A
81	v	30	G
81	v	44	G
81	v	47	U
81	v	48	C
81	v	49	C
81	v	51	U
81	v	54	U
81	v	55	U
81	v	56	C
81	v	58	A
81	v	61	C
81	v	62	C
81	v	68	C
81	v	69	G
81	v	71	G
81	v	72	C
81	v	73	A
81	v	75	C
81	v	76	A
82	w	17	G
82	w	21	G

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	42	A
1	S2	53	C
1	S2	60	A
1	S2	79	A
1	S2	196	C
1	S2	205	G
1	S2	292	A
1	S2	304	C
1	S2	315	C
1	S2	317	C
1	S2	386	C
1	S2	417	C
1	S2	445	A
1	S2	536	A
1	S2	559	G
1	S2	563	G
1	S2	670	A
1	S2	814	5MU
1	S2	866	U
1	S2	872	A
1	S2	1261	C
1	S2	1265	A
1	S2	1375	G
1	S2	1378	A
1	S2	1396	A
1	S2	1567	G
1	S2	1572	C
1	S2	1600	G
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	OMC	S2	174	1	19,22,23	3.56	8 (42%)	25,31,34	0.80	0
1	OMC	S2	517	1	19,22,23	3.57	8 (42%)	25,31,34	0.84	1 (4%)
1	OMU	S2	116	1	19,22,23	3.17	6 (31%)	25,31,34	1.84	5 (20%)
1	OMC	S2	1703	1	19,22,23	3.47	7 (36%)	25,31,34	0.89	1 (4%)
1	B8Q	S2	1219	1	18,22,23	4.72	7 (38%)	21,32,35	1.80	4 (19%)
1	E3C	S2	568	1	19,23,24	3.52	7 (36%)	21,33,36	2.67	6 (28%)
1	4AC	S2	1842	1	21,24,25	3.27	9 (42%)	28,34,37	1.34	4 (14%)
1	MA6	S2	1851	1	23,26,27	1.49	5 (21%)	33,38,41	3.59	14 (42%)
1	A2M	S2	159	1	22,25,26	4.08	8 (36%)	30,36,39	2.92	13 (43%)
1	PSU	S2	1243	1	18,21,22	4.39	7 (38%)	21,30,33	2.03	5 (23%)
1	A2M	S2	1678	1	22,25,26	4.12	12 (54%)	30,36,39	2.96	17 (56%)
1	6MZ	S2	1832	1	22,25,26	2.73	6 (27%)	29,36,39	2.53	11 (37%)
1	A2M	S2	668	1	22,25,26	4.10	10 (45%)	30,36,39	3.11	14 (46%)
1	5MC	S2	1374	1	19,22,23	3.59	8 (42%)	26,32,35	1.08	2 (7%)
1	A2M	S2	166	1	22,25,26	4.15	9 (40%)	30,36,39	2.91	14 (46%)
1	OMU	S2	121	1	19,22,23	3.11	6 (31%)	25,31,34	1.82	5 (20%)
1	MA6	S2	1850	1	23,26,27	1.49	5 (21%)	33,38,41	3.64	15 (45%)
1	UR3	S2	1830	1	19,22,23	2.95	7 (36%)	26,32,35	3.17	7 (26%)
1	OMG	S2	683	1	23,26,27	2.41	8 (34%)	32,38,41	2.07	9 (28%)
1	PSU	S2	612	1	18,21,22	4.42	8 (44%)	21,30,33	2.21	6 (28%)
1	PSU	S2	1081	1	18,21,22	4.24	8 (44%)	21,30,33	1.84	4 (19%)
1	4AC	S2	1337	1	21,24,25	3.29	9 (42%)	28,34,37	1.02	2 (7%)
1	OMG	S2	509	1	23,26,27	2.37	8 (34%)	32,38,41	2.08	9 (28%)
1	B8N	S2	1248	1	25,29,30	3.18	6 (24%)	28,42,45	2.17	9 (32%)
1	PSU	S2	823	1	18,21,22	4.42	8 (44%)	21,30,33	2.61	6 (28%)
1	5MU	S2	814	1	19,22,23	7.69	8 (42%)	27,32,35	3.45	12 (44%)
1	M7A	S2	1806	1	19,25,26	1.64	3 (15%)	25,37,40	3.81	8 (32%)
1	OMG	S2	644	1	23,26,27	2.42	8 (34%)	32,38,41	2.07	10 (31%)
1	A2M	S2	1031	1	22,25,26	4.10	9 (40%)	30,36,39	2.96	12 (40%)
1	A2M	S2	27	1	22,25,26	4.06	9 (40%)	30,36,39	2.98	13 (43%)
1	A2M	S2	484	1	22,25,26	4.13	9 (40%)	30,36,39	3.06	13 (43%)
1	PSU	S2	822	1	18,21,22	4.49	7 (38%)	21,30,33	1.93	5 (23%)
1	OMC	S2	1710	1	19,22,23	3.52	8 (42%)	25,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	119	1	18,21,22	4.57	7 (38%)	21,30,33	2.01	5 (23%)

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	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	MA6	S2	1851	1	-	4/11/29/30	0/3/3/3
1	A2M	S2	159	1	-	4/9/27/28	0/3/3/3
1	PSU	S2	1243	1	-	1/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	2/9/27/28	0/3/3/3
1	6MZ	S2	1832	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	668	1	-	3/9/27/28	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	2/11/29/30	0/3/3/3
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	612	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
1	OMG	S2	509	1	-	0/9/27/28	0/3/3/3
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2
1	PSU	S2	823	1	-	0/7/25/26	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	M7A	S2	1806	1	-	1/7/37/38	0/3/3/3
1	OMG	S2	644	1	-	3/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	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	22.80	1.81	1.44
1	S2	814	5MU	C6-N1	17.01	1.66	1.38
1	S2	119	PSU	C6-C5	11.84	1.48	1.35
1	S2	814	5MU	C6-C5	-11.66	1.15	1.34
1	S2	823	PSU	C6-C5	11.62	1.48	1.35
1	S2	822	PSU	C6-C5	11.50	1.48	1.35
1	S2	612	PSU	C6-C5	11.31	1.47	1.35
1	S2	1243	PSU	C6-C5	11.22	1.47	1.35
1	S2	1219	B8Q	C4-N3	11.13	1.65	1.48
1	S2	814	5MU	C4-N3	-10.92	1.18	1.38
1	S2	1219	B8Q	C6-C5	10.72	1.55	1.33
1	S2	1081	PSU	C6-C5	10.64	1.47	1.35
1	S2	484	A2M	C2'-C1'	-10.60	1.27	1.53
1	S2	166	A2M	C2'-C1'	-10.57	1.27	1.53
1	S2	1031	A2M	C2'-C1'	-10.44	1.27	1.53
1	S2	668	A2M	C2'-C1'	-10.37	1.27	1.53
1	S2	159	A2M	C2'-C1'	-10.35	1.27	1.53
1	S2	166	A2M	C3'-C4'	-10.33	1.26	1.53
1	S2	1832	6MZ	C6-N6	10.30	1.46	1.34
1	S2	27	A2M	C2'-C1'	-10.28	1.27	1.53
1	S2	668	A2M	C3'-C4'	-10.27	1.26	1.53
1	S2	1031	A2M	C3'-C4'	-10.15	1.27	1.53
1	S2	484	A2M	C3'-C4'	-10.04	1.27	1.53
1	S2	119	PSU	C2-N1	10.02	1.49	1.36
1	S2	27	A2M	C3'-C4'	-10.00	1.27	1.53
1	S2	159	A2M	C3'-C4'	-9.87	1.27	1.53
1	S2	822	PSU	C2-N1	9.85	1.49	1.36
1	S2	1678	A2M	C2'-C1'	-9.75	1.29	1.53
1	S2	1219	B8Q	C2-N1	9.68	1.51	1.38
1	S2	1243	PSU	C2-N1	9.44	1.49	1.36
1	S2	612	PSU	C2-N1	9.41	1.48	1.36
1	S2	823	PSU	C2-N1	9.33	1.48	1.36
1	S2	1081	PSU	C2-N1	9.20	1.48	1.36
1	S2	1374	5MC	C6-C5	9.14	1.49	1.34
1	S2	1678	A2M	C3'-C4'	-8.93	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1710	OMC	C4-N4	8.41	1.54	1.33
1	S2	517	OMC	C4-N4	8.36	1.54	1.33
1	S2	116	OMU	C2-N1	8.35	1.51	1.38
1	S2	174	OMC	C4-N4	8.32	1.54	1.33
1	S2	1703	OMC	C4-N4	8.28	1.54	1.33
1	S2	568	E3C	C6-C5	7.93	1.49	1.33
1	S2	121	OMU	C2-N1	7.88	1.50	1.38
1	S2	823	PSU	C2-N3	7.87	1.50	1.37
1	S2	1830	UR3	C2-N1	7.86	1.49	1.38
1	S2	1248	B8N	C4-N3	-7.84	1.26	1.40
1	S2	568	E3C	C2-N1	7.75	1.49	1.38
1	S2	1842	4AC	C4-N3	7.61	1.45	1.32
1	S2	1337	4AC	C4-N3	7.53	1.45	1.32
1	S2	568	E3C	C2-N3	7.53	1.46	1.37
1	S2	1248	B8N	C6-N1	7.46	1.54	1.36
1	S2	1248	B8N	C4-C5	7.40	1.64	1.47
1	S2	1243	PSU	C2-N3	7.28	1.49	1.37
1	S2	612	PSU	C2-N3	7.17	1.49	1.37
1	S2	822	PSU	C2-N3	7.16	1.49	1.37
1	S2	119	PSU	C2-N3	7.04	1.49	1.37
1	S2	174	OMC	C2-N3	6.95	1.50	1.36
1	S2	517	OMC	C2-N3	6.83	1.49	1.36
1	S2	1710	OMC	C2-N3	6.72	1.49	1.36
1	S2	121	OMU	C2-N3	6.71	1.49	1.38
1	S2	517	OMC	C6-C5	6.69	1.50	1.35
1	S2	1703	OMC	C2-N3	6.64	1.49	1.36
1	S2	174	OMC	C6-C5	6.62	1.50	1.35
1	S2	1678	A2M	C6-N6	6.61	1.51	1.34
1	S2	644	OMG	C4-N3	6.59	1.49	1.34
1	S2	116	OMU	C2-N3	6.57	1.49	1.38
1	S2	1703	OMC	C6-C5	6.56	1.50	1.35
1	S2	1678	A2M	C3'-C2'	6.56	1.67	1.53
1	S2	683	OMG	C4-N3	6.53	1.49	1.34
1	S2	1710	OMC	C6-C5	6.48	1.50	1.35
1	S2	1678	A2M	O4'-C1'	6.47	1.57	1.42
1	S2	1081	PSU	C2-N3	6.35	1.47	1.37
1	S2	166	A2M	O4'-C1'	6.34	1.56	1.42
1	S2	509	OMG	C4-N3	6.31	1.48	1.34
1	S2	1337	4AC	C6-C5	6.21	1.49	1.35
1	S2	1374	5MC	C4-N3	6.18	1.44	1.34
1	S2	1830	UR3	C6-C5	6.08	1.49	1.35
1	S2	116	OMU	C6-C5	6.08	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	121	OMU	C6-C5	6.07	1.49	1.35
1	S2	1710	OMC	C4-N3	6.03	1.46	1.34
1	S2	174	OMC	C4-N3	6.00	1.46	1.34
1	S2	517	OMC	C4-N3	6.00	1.46	1.34
1	S2	668	A2M	C3'-C2'	5.99	1.66	1.53
1	S2	159	A2M	O4'-C1'	5.97	1.55	1.42
1	S2	27	A2M	O4'-C1'	5.85	1.55	1.42
1	S2	1248	B8N	C2-N1	5.84	1.56	1.39
1	S2	484	A2M	O4'-C1'	5.83	1.55	1.42
1	S2	1842	4AC	C2-N3	5.82	1.47	1.36
1	S2	1031	A2M	O4'-C1'	5.81	1.55	1.42
1	S2	159	A2M	C3'-C2'	5.80	1.65	1.53
1	S2	1703	OMC	C4-N3	5.78	1.45	1.34
1	S2	1842	4AC	C6-C5	5.76	1.48	1.35
1	S2	484	A2M	C3'-C2'	5.74	1.65	1.53
1	S2	1337	4AC	C2-N3	5.71	1.47	1.36
1	S2	1031	A2M	C3'-C2'	5.67	1.65	1.53
1	S2	1374	5MC	C2-N3	5.67	1.47	1.36
1	S2	484	A2M	C6-N6	5.66	1.48	1.34
1	S2	668	A2M	O4'-C1'	5.59	1.54	1.42
1	S2	166	A2M	C6-N6	5.58	1.48	1.34
1	S2	644	OMG	C2-N3	5.51	1.46	1.33
1	S2	27	A2M	C3'-C2'	5.50	1.65	1.53
1	S2	27	A2M	C6-N6	5.45	1.48	1.34
1	S2	159	A2M	C6-N6	5.45	1.48	1.34
1	S2	1374	5MC	C5-C4	5.42	1.48	1.44
1	S2	568	E3C	C4-N3	5.42	1.56	1.48
1	S2	1031	A2M	C6-N6	5.38	1.47	1.34
1	S2	814	5MU	C2-N3	5.37	1.47	1.38
1	S2	1219	B8Q	C2-N3	-5.36	1.25	1.35
1	S2	668	A2M	C6-N6	5.36	1.47	1.34
1	S2	683	OMG	C2-N3	5.32	1.46	1.33
1	S2	166	A2M	C3'-C2'	5.31	1.64	1.53
1	S2	509	OMG	C2-N3	5.26	1.45	1.33
1	S2	1081	PSU	O2-C2	-5.18	1.12	1.23
1	S2	612	PSU	O2-C2	-5.16	1.12	1.23
1	S2	823	PSU	O2-C2	-5.09	1.12	1.23
1	S2	119	PSU	O2-C2	-5.06	1.12	1.23
1	S2	159	A2M	O4'-C4'	5.01	1.56	1.45
1	S2	1678	A2M	O4'-C4'	5.00	1.56	1.45
1	S2	1830	UR3	C2-N3	4.93	1.48	1.39
1	S2	119	PSU	O4-C4	-4.92	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1248	B8N	C6-C5	4.92	1.42	1.35
1	S2	1081	PSU	O4-C4	-4.89	1.14	1.23
1	S2	822	PSU	O4-C4	-4.87	1.14	1.23
1	S2	822	PSU	O2-C2	-4.86	1.13	1.23
1	S2	1243	PSU	O2-C2	-4.86	1.13	1.23
1	S2	166	A2M	O4'-C4'	4.81	1.55	1.45
1	S2	1806	M7A	C6-N6	4.76	1.46	1.34
1	S2	1243	PSU	O4-C4	-4.75	1.14	1.23
1	S2	1031	A2M	O4'-C4'	4.73	1.55	1.45
1	S2	612	PSU	O4-C4	-4.71	1.14	1.23
1	S2	121	OMU	C4-N3	4.71	1.46	1.38
1	S2	683	OMG	C2-N2	4.70	1.45	1.34
1	S2	1219	B8Q	C4-C5	-4.69	1.39	1.49
1	S2	116	OMU	C4-N3	4.69	1.46	1.38
1	S2	644	OMG	C2-N2	4.65	1.45	1.34
1	S2	27	A2M	O4'-C4'	4.62	1.55	1.45
1	S2	509	OMG	C2-N2	4.61	1.45	1.34
1	S2	484	A2M	O4'-C4'	4.60	1.55	1.45
1	S2	1337	4AC	C7-N4	4.55	1.46	1.37
1	S2	1842	4AC	C2-N1	4.51	1.49	1.40
1	S2	1337	4AC	C2-N1	4.48	1.49	1.40
1	S2	1842	4AC	C7-N4	4.48	1.46	1.37
1	S2	814	5MU	C2-N1	4.42	1.45	1.38
1	S2	1842	4AC	C4-N4	4.40	1.46	1.39
1	S2	1374	5MC	C6-N1	4.39	1.45	1.38
1	S2	1374	5MC	C4-N4	4.38	1.45	1.34
1	S2	174	OMC	C2-N1	4.38	1.49	1.40
1	S2	119	PSU	C6-N1	4.37	1.43	1.36
1	S2	517	OMC	C2-N1	4.34	1.49	1.40
1	S2	1832	6MZ	C5-C4	-4.27	1.31	1.39
1	S2	1337	4AC	C5-C4	4.23	1.50	1.41
1	S2	822	PSU	C6-N1	4.19	1.43	1.36
1	S2	612	PSU	C6-N1	4.18	1.43	1.36
1	S2	1337	4AC	C4-N4	4.16	1.46	1.39
1	S2	668	A2M	O4'-C4'	4.01	1.53	1.45
1	S2	1337	4AC	C6-N1	4.00	1.47	1.38
1	S2	1243	PSU	C6-N1	4.00	1.42	1.36
1	S2	1703	OMC	C2-N1	3.98	1.48	1.40
1	S2	1710	OMC	C2-N1	3.96	1.48	1.40
1	S2	1842	4AC	C5-C4	3.95	1.49	1.41
1	S2	1842	4AC	C6-N1	3.92	1.47	1.38
1	S2	517	OMC	C6-N1	3.89	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1806	M7A	C5-N7	3.88	1.48	1.39
1	S2	1081	PSU	C6-N1	3.85	1.42	1.36
1	S2	1374	5MC	C2-N1	3.76	1.47	1.40
1	S2	1832	6MZ	C8-N9	-3.75	1.31	1.37
1	S2	174	OMC	C6-N1	3.75	1.47	1.38
1	S2	1710	OMC	C6-N1	3.69	1.46	1.38
1	S2	1830	UR3	C5-C4	3.64	1.52	1.43
1	S2	823	PSU	C6-N1	3.61	1.42	1.36
1	S2	1703	OMC	C6-N1	3.56	1.46	1.38
1	S2	1850	MA6	C6-N6	3.48	1.46	1.36
1	S2	1851	MA6	C5-C4	-3.46	1.32	1.39
1	S2	1850	MA6	C5-C4	-3.36	1.33	1.39
1	S2	683	OMG	C5-N7	-3.35	1.32	1.39
1	S2	668	A2M	C5-C4	-3.32	1.33	1.39
1	S2	509	OMG	C5-N7	-3.31	1.32	1.39
1	S2	823	PSU	C4-N3	3.30	1.45	1.38
1	S2	1851	MA6	C6-N6	3.23	1.45	1.36
1	S2	1830	UR3	O2-C2	-3.17	1.16	1.22
1	S2	823	PSU	O4-C4	-3.16	1.17	1.23
1	S2	1031	A2M	C5-C4	-3.14	1.33	1.39
1	S2	27	A2M	C5-C4	-3.13	1.33	1.39
1	S2	1830	UR3	C4-N3	3.12	1.46	1.40
1	S2	484	A2M	C5-C4	-3.09	1.33	1.39
1	S2	644	OMG	C5-N7	-3.08	1.32	1.39
1	S2	484	A2M	C5-N7	-3.04	1.33	1.39
1	S2	1031	A2M	C5-N7	-3.03	1.33	1.39
1	S2	612	PSU	C4-N3	3.01	1.44	1.38
1	S2	159	A2M	C5-N7	-3.01	1.33	1.39
1	S2	1243	PSU	C4-N3	3.01	1.44	1.38
1	S2	568	E3C	C31-N3	2.93	1.55	1.47
1	S2	668	A2M	C5-N7	-2.92	1.33	1.39
1	S2	1850	MA6	C5-N7	-2.92	1.33	1.39
1	S2	119	PSU	C4-N3	2.91	1.44	1.38
1	S2	568	E3C	C6-N1	2.90	1.45	1.38
1	S2	1219	B8Q	C31-N3	2.89	1.52	1.46
1	S2	166	A2M	C5-N7	-2.89	1.33	1.39
1	S2	27	A2M	C5-N7	-2.86	1.33	1.39
1	S2	822	PSU	C4-N3	2.84	1.44	1.38
1	S2	1678	A2M	O3'-C3'	2.79	1.49	1.43
1	S2	1851	MA6	C5-N7	-2.75	1.34	1.39
1	S2	116	OMU	C6-N1	2.75	1.44	1.38
1	S2	1851	MA6	C8-N9	-2.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1832	6MZ	C5-N7	-2.73	1.34	1.39
1	S2	166	A2M	C5-C4	-2.71	1.34	1.39
1	S2	1850	MA6	C8-N9	-2.70	1.33	1.37
1	S2	1374	5MC	O2-C2	-2.66	1.18	1.23
1	S2	1081	PSU	O4'-C1'	-2.63	1.40	1.43
1	S2	568	E3C	C4-C5	-2.60	1.44	1.49
1	S2	1851	MA6	C4-N9	-2.59	1.32	1.37
1	S2	159	A2M	C5-C4	-2.58	1.34	1.39
1	S2	1703	OMC	O2-C2	-2.56	1.18	1.23
1	S2	509	OMG	O6-C6	-2.56	1.18	1.23
1	S2	1830	UR3	C6-N1	2.55	1.44	1.38
1	S2	683	OMG	O6-C6	-2.55	1.18	1.23
1	S2	644	OMG	O6-C6	-2.54	1.18	1.23
1	S2	1219	B8Q	C6-N1	-2.51	1.32	1.38
1	S2	121	OMU	C6-N1	2.50	1.44	1.38
1	S2	27	A2M	C8-N9	-2.45	1.33	1.37
1	S2	1832	6MZ	C9-N6	2.43	1.49	1.45
1	S2	668	A2M	C8-N9	-2.42	1.33	1.37
1	S2	683	OMG	C2-N1	2.41	1.43	1.37
1	S2	1081	PSU	C4-N3	2.40	1.43	1.38
1	S2	644	OMG	C2-N1	2.39	1.43	1.37
1	S2	484	A2M	C8-N9	-2.39	1.33	1.37
1	S2	644	OMG	C5-C6	2.36	1.53	1.44
1	S2	1678	A2M	C8-N9	-2.36	1.33	1.37
1	S2	509	OMG	C5-C6	2.32	1.53	1.44
1	S2	814	5MU	O4-C4	-2.31	1.19	1.23
1	S2	814	5MU	O2-C2	-2.29	1.19	1.23
1	S2	509	OMG	C2-N1	2.29	1.43	1.37
1	S2	1678	A2M	C5-N7	-2.26	1.35	1.39
1	S2	174	OMC	O2-C2	-2.23	1.19	1.23
1	S2	1031	A2M	C8-N9	-2.23	1.33	1.37
1	S2	517	OMC	O2-C2	-2.22	1.19	1.23
1	S2	1710	OMC	O2-C2	-2.21	1.19	1.23
1	S2	166	A2M	C8-N9	-2.21	1.33	1.37
1	S2	1850	MA6	C4-N9	-2.20	1.33	1.37
1	S2	121	OMU	O4-C4	-2.19	1.20	1.24
1	S2	1248	B8N	O4-C4	-2.19	1.18	1.23
1	S2	683	OMG	C5-C6	2.19	1.52	1.44
1	S2	1710	OMC	C5-C4	2.17	1.48	1.42
1	S2	116	OMU	O4-C4	-2.13	1.20	1.24
1	S2	1832	6MZ	C4-N9	-2.13	1.33	1.37
1	S2	823	PSU	O4'-C1'	-2.13	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1678	A2M	C5'-C4'	2.12	1.57	1.51
1	S2	174	OMC	C5-C4	2.11	1.47	1.42
1	S2	1337	4AC	O2-C2	-2.11	1.19	1.23
1	S2	644	OMG	C6-N1	2.09	1.42	1.38
1	S2	668	A2M	C4-N9	-2.08	1.33	1.37
1	S2	1842	4AC	O2-C2	-2.08	1.19	1.23
1	S2	517	OMC	C5-C4	2.06	1.47	1.42
1	S2	1806	M7A	C5-C6	-2.06	1.35	1.40
1	S2	1678	A2M	C2-N1	2.06	1.37	1.33
1	S2	1678	A2M	C8-N7	2.06	1.35	1.31
1	S2	612	PSU	O4'-C1'	-2.05	1.41	1.43
1	S2	683	OMG	C6-N1	2.03	1.42	1.38
1	S2	509	OMG	C4-N9	-2.02	1.32	1.38

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1850	MA6	N1-C6-N6	-12.92	101.11	116.86
1	S2	1851	MA6	N1-C6-N6	-12.74	101.33	116.86
1	S2	1806	M7A	C5-C6-N6	10.96	142.38	123.75
1	S2	1806	M7A	N6-C6-N1	-9.46	97.30	118.38
1	S2	814	5MU	C5-C4-N3	9.31	123.42	115.32
1	S2	1850	MA6	C5-C6-N6	9.24	139.96	125.33
1	S2	1851	MA6	C5-C6-N6	8.99	139.57	125.33
1	S2	1830	UR3	C6-N1-C2	-8.12	115.16	121.80
1	S2	814	5MU	C5-C6-N1	-7.65	115.00	123.31
1	S2	1830	UR3	C1'-N1-C2	7.61	129.49	117.04
1	S2	668	A2M	C4-N9-C1'	-7.55	108.97	126.63
1	S2	1806	M7A	C4-N9-C1'	-7.44	109.30	126.63
1	S2	484	A2M	C4-N9-C1'	-7.16	109.89	126.63
1	S2	1830	UR3	O2-C2-N3	-7.06	111.57	121.33
1	S2	568	E3C	C1'-N1-C2	7.05	128.57	117.04
1	S2	668	A2M	C1'-N9-C8	6.98	142.58	127.09
1	S2	814	5MU	C4-N3-C2	-6.91	118.29	127.34
1	S2	484	A2M	C1'-N9-C8	6.79	142.17	127.09
1	S2	27	A2M	C4-N9-C1'	-6.77	110.79	126.63
1	S2	1031	A2M	C4-N9-C1'	-6.65	111.09	126.63
1	S2	568	E3C	O2-C2-N3	-6.42	113.89	122.10
1	S2	1806	M7A	N3-C2-N1	-6.38	118.92	128.58
1	S2	1850	MA6	N1-C2-N3	-6.32	119.02	128.58
1	S2	27	A2M	C1'-N9-C8	6.26	141.00	127.09
1	S2	1832	6MZ	N1-C2-N3	-6.26	119.10	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1031	A2M	C1'-N9-C8	6.20	140.86	127.09
1	S2	1678	A2M	C5-C4-N3	-6.16	118.23	126.72
1	S2	27	A2M	N3-C2-N1	-6.08	119.38	128.58
1	S2	668	A2M	N3-C2-N1	-6.04	119.44	128.58
1	S2	166	A2M	C4-N9-C1'	-5.99	112.61	126.63
1	S2	1031	A2M	N3-C2-N1	-5.97	119.55	128.58
1	S2	484	A2M	N3-C2-N1	-5.85	119.72	128.58
1	S2	823	PSU	C6-C5-C4	5.80	122.09	118.17
1	S2	1832	6MZ	C9-N6-C6	5.79	128.22	122.85
1	S2	159	A2M	C5-C4-N3	-5.78	118.76	126.72
1	S2	683	OMG	C5-C4-N3	-5.77	119.21	128.39
1	S2	166	A2M	C1'-N9-C8	5.68	139.70	127.09
1	S2	509	OMG	C5-C4-N3	-5.67	119.36	128.39
1	S2	1851	MA6	N1-C2-N3	-5.61	120.08	128.58
1	S2	644	OMG	C5-C4-N3	-5.56	119.53	128.39
1	S2	166	A2M	N3-C2-N1	-5.51	120.25	128.58
1	S2	823	PSU	N1-C2-N3	5.48	120.95	115.17
1	S2	1678	A2M	N3-C2-N1	-5.47	120.31	128.58
1	S2	159	A2M	N6-C6-N1	-5.46	106.21	118.38
1	S2	166	A2M	C5-C4-N3	-5.44	119.22	126.72
1	S2	159	A2M	C4-N9-C1'	-5.44	113.92	126.63
1	S2	814	5MU	N3-C2-N1	5.42	121.94	114.89
1	S2	159	A2M	C1'-N9-C8	5.41	139.10	127.09
1	S2	823	PSU	C6-N1-C2	-5.29	117.78	122.69
1	S2	1031	A2M	N6-C6-N1	-5.21	106.76	118.38
1	S2	1830	UR3	C4-N3-C2	-5.19	120.41	124.58
1	S2	1830	UR3	C3U-N3-C4	5.19	125.06	117.87
1	S2	159	A2M	N3-C2-N1	-5.16	120.77	128.58
1	S2	484	A2M	N6-C6-N1	-5.16	106.89	118.38
1	S2	116	OMU	C4-N3-C2	-5.16	120.21	126.61
1	S2	27	A2M	N6-C6-N1	-5.13	106.96	118.38
1	S2	1248	B8N	C1'-C5-C4	5.09	125.33	117.61
1	S2	1678	A2M	N6-C6-N1	-5.08	107.06	118.38
1	S2	668	A2M	N6-C6-N1	-5.08	107.07	118.38
1	S2	166	A2M	N6-C6-N1	-5.07	107.09	118.38
1	S2	612	PSU	N1-C2-N3	5.00	120.44	115.17
1	S2	1851	MA6	N9-C8-N7	-5.00	106.85	113.94
1	S2	1248	B8N	C5-C4-N3	4.97	125.18	116.15
1	S2	612	PSU	C4-N3-C2	-4.96	119.54	126.37
1	S2	823	PSU	O2-C2-N1	-4.95	117.68	122.79
1	S2	814	5MU	C5M-C5-C6	-4.94	116.17	122.85
1	S2	1832	6MZ	N9-C8-N7	-4.88	107.01	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1031	A2M	C5-C4-N3	-4.88	120.00	126.72
1	S2	484	A2M	C5-C4-N3	-4.86	120.02	126.72
1	S2	121	OMU	C4-N3-C2	-4.80	120.66	126.61
1	S2	683	OMG	C2-N3-C4	4.74	120.47	112.30
1	S2	119	PSU	N1-C2-N3	4.72	120.14	115.17
1	S2	27	A2M	C5-C4-N3	-4.69	120.25	126.72
1	S2	119	PSU	C4-N3-C2	-4.69	119.91	126.37
1	S2	822	PSU	C4-N3-C2	-4.68	119.92	126.37
1	S2	1248	B8N	C4-N3-C2	-4.68	119.86	125.62
1	S2	1243	PSU	N1-C2-N3	4.61	120.03	115.17
1	S2	1243	PSU	C4-N3-C2	-4.58	120.06	126.37
1	S2	1081	PSU	C4-N3-C2	-4.56	120.09	126.37
1	S2	1850	MA6	C5-C4-N3	-4.56	120.44	126.72
1	S2	1678	A2M	C1'-N9-C8	4.55	137.20	127.09
1	S2	644	OMG	C2-N3-C4	4.47	119.99	112.30
1	S2	668	A2M	N9-C8-N7	-4.44	107.64	113.94
1	S2	1851	MA6	C1'-N9-C8	-4.41	117.31	127.09
1	S2	1806	M7A	N3-C4-N9	4.40	132.39	126.88
1	S2	1678	A2M	C5-C6-N6	4.39	134.15	123.29
1	S2	509	OMG	C2-N3-C4	4.39	119.85	112.30
1	S2	668	A2M	C5-C4-N3	-4.36	120.71	126.72
1	S2	1678	A2M	C4-N9-C1'	-4.34	116.49	126.63
1	S2	1219	B8Q	N3-C2-N1	4.32	123.18	117.16
1	S2	1219	B8Q	C31-N3-C4	4.31	122.23	114.76
1	S2	822	PSU	N1-C2-N3	4.31	119.71	115.17
1	S2	1081	PSU	N1-C2-N3	4.27	119.68	115.17
1	S2	1031	A2M	N9-C8-N7	-4.22	107.95	113.94
1	S2	484	A2M	N9-C8-N7	-4.15	108.06	113.94
1	S2	116	OMU	N3-C2-N1	4.14	120.28	114.89
1	S2	568	E3C	C6-N1-C2	-4.14	118.42	121.80
1	S2	1850	MA6	N9-C8-N7	-4.12	108.09	113.94
1	S2	121	OMU	N3-C2-N1	4.12	120.25	114.89
1	S2	159	A2M	C5-C6-N6	4.11	133.46	123.29
1	S2	1851	MA6	C5-C4-N3	-4.09	121.09	126.72
1	S2	814	5MU	C6-C5-C4	4.08	121.39	118.02
1	S2	27	A2M	N9-C8-N7	-4.04	108.20	113.94
1	S2	823	PSU	C4-N3-C2	-4.03	120.82	126.37
1	S2	1832	6MZ	C5-C4-N3	-4.02	121.18	126.72
1	S2	1850	MA6	C1'-N9-C8	-3.99	118.25	127.09
1	S2	668	A2M	C5-C6-N6	3.92	133.00	123.29
1	S2	27	A2M	C5-C6-N6	3.91	132.98	123.29
1	S2	568	E3C	C4-N3-C2	-3.90	114.97	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	484	A2M	C5-C6-N6	3.88	132.89	123.29
1	S2	1850	MA6	C2-N1-C6	3.88	121.30	111.83
1	S2	1031	A2M	C5-C6-N6	3.88	132.88	123.29
1	S2	166	A2M	N9-C8-N7	-3.87	108.45	113.94
1	S2	1248	B8N	N3-C2-N1	3.86	121.44	116.72
1	S2	509	OMG	C1'-N9-C4	-3.84	115.15	126.49
1	S2	683	OMG	N9-C4-N3	3.81	133.58	125.95
1	S2	1678	A2M	C2-N3-C4	3.80	121.10	111.83
1	S2	166	A2M	C5-C6-N6	3.78	132.64	123.29
1	S2	644	OMG	C1'-N9-C4	-3.77	115.34	126.49
1	S2	1678	A2M	C3'-C2'-C1'	3.76	110.02	102.81
1	S2	119	PSU	C6-N1-C2	-3.75	119.21	122.69
1	S2	612	PSU	C6-C5-C4	3.72	120.69	118.17
1	S2	1851	MA6	C2-N1-C6	3.69	120.84	111.83
1	S2	1832	6MZ	C5-N7-C8	3.68	109.23	103.45
1	S2	1243	PSU	C6-N1-C2	-3.68	119.28	122.69
1	S2	1850	MA6	C2-N3-C4	3.67	120.79	111.83
1	S2	509	OMG	N9-C4-N3	3.67	133.29	125.95
1	S2	159	A2M	N3-C4-N9	3.67	133.40	127.17
1	S2	568	E3C	C1'-N1-C6	-3.65	112.98	120.78
1	S2	612	PSU	O2-C2-N1	-3.63	119.05	122.79
1	S2	612	PSU	C6-N1-C2	-3.63	119.33	122.69
1	S2	644	OMG	N9-C4-N3	3.63	133.20	125.95
1	S2	1851	MA6	C4-N9-C8	3.57	109.49	105.74
1	S2	814	5MU	O4-C4-C5	-3.55	120.86	124.92
1	S2	1832	6MZ	C4-C5-N7	-3.55	106.53	110.58
1	S2	509	OMG	C1'-N9-C8	3.54	136.78	126.73
1	S2	1248	B8N	C31-N3-C4	3.53	122.17	117.18
1	S2	1850	MA6	C4-C5-C6	3.50	119.52	115.91
1	S2	1219	B8Q	O2-C2-N3	-3.49	118.06	122.95
1	S2	159	A2M	C2-N3-C4	3.47	120.31	111.83
1	S2	116	OMU	C5-C4-N3	3.46	119.64	114.80
1	S2	1851	MA6	C4-C5-C6	3.45	119.47	115.91
1	S2	814	5MU	C5M-C5-C4	3.43	122.44	118.78
1	S2	1832	6MZ	C2-N3-C4	3.42	120.18	111.83
1	S2	484	A2M	C2-N3-C4	3.42	120.18	111.83
1	S2	166	A2M	C2-N3-C4	3.42	120.17	111.83
1	S2	166	A2M	N3-C4-N9	3.41	132.97	127.17
1	S2	1031	A2M	C2-N3-C4	3.41	120.15	111.83
1	S2	159	A2M	O4'-C1'-C2'	-3.40	100.74	106.59
1	S2	1243	PSU	C6-C5-C4	3.40	120.47	118.17
1	S2	27	A2M	C2-N3-C4	3.39	120.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	159	A2M	N9-C8-N7	-3.38	109.14	113.94
1	S2	1806	M7A	C2-N3-C4	3.37	120.06	111.83
1	S2	644	OMG	C1'-N9-C8	3.34	136.22	126.73
1	S2	509	OMG	C2-N1-C6	-3.33	119.07	125.11
1	S2	1678	A2M	O2'-C2'-C1'	3.31	115.27	108.99
1	S2	822	PSU	C6-N1-C2	-3.26	119.67	122.69
1	S2	683	OMG	C1'-N9-C4	-3.24	116.92	126.49
1	S2	668	A2M	C2-N3-C4	3.23	119.72	111.83
1	S2	1806	M7A	C71-N7-C5	-3.23	109.98	123.44
1	S2	1678	A2M	N3-C4-N9	3.20	132.60	127.17
1	S2	1081	PSU	C6-N1-C2	-3.19	119.73	122.69
1	S2	1678	A2M	C6-C5-C4	3.16	121.50	117.18
1	S2	644	OMG	C2-N1-C6	-3.13	119.43	125.11
1	S2	1851	MA6	C2-N3-C4	3.11	119.43	111.83
1	S2	1678	A2M	C5-C4-N9	3.08	109.17	105.81
1	S2	1850	MA6	C4-N9-C1'	3.07	133.81	126.63
1	S2	683	OMG	C2-N1-C6	-3.05	119.58	125.11
1	S2	1851	MA6	C5-N7-C8	3.05	108.24	103.45
1	S2	1678	A2M	C4-C5-N7	-3.03	107.12	110.58
1	S2	1219	B8Q	C31-N3-C2	3.01	122.43	117.70
1	S2	121	OMU	O4-C4-C5	-3.00	119.99	125.16
1	S2	1031	A2M	N3-C4-N9	2.96	132.19	127.17
1	S2	116	OMU	O4-C4-C5	-2.95	120.08	125.16
1	S2	27	A2M	N3-C4-N9	2.95	132.18	127.17
1	S2	1832	6MZ	C4-N9-C8	2.94	108.83	105.74
1	S2	121	OMU	C5-C4-N3	2.92	118.89	114.80
1	S2	683	OMG	C1'-N9-C8	2.92	135.03	126.73
1	S2	1850	MA6	C5-N7-C8	2.90	108.01	103.45
1	S2	1678	A2M	N9-C8-N7	-2.89	109.83	113.94
1	S2	484	A2M	N3-C4-N9	2.89	132.08	127.17
1	S2	1842	4AC	C5-C4-N3	-2.88	118.09	122.60
1	S2	644	OMG	N9-C8-N7	-2.87	108.08	113.40
1	S2	1842	4AC	C6-C5-C4	2.84	120.42	117.00
1	S2	814	5MU	O3'-C3'-C2'	2.83	120.89	111.82
1	S2	1830	UR3	C1'-N1-C6	-2.82	114.76	120.78
1	S2	1031	A2M	C5-N7-C8	2.80	107.84	103.45
1	S2	1851	MA6	C4-N9-C1'	2.78	133.13	126.63
1	S2	166	A2M	C5-N7-C8	2.78	107.81	103.45
1	S2	484	A2M	C5-N7-C8	2.77	107.81	103.45
1	S2	668	A2M	C3'-C2'-C1'	2.76	108.09	102.81
1	S2	1243	PSU	O2-C2-N1	-2.76	119.94	122.79
1	S2	1374	5MC	C5-C6-N1	-2.76	120.32	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	121	OMU	C6-N1-C2	-2.74	117.66	121.00
1	S2	1374	5MC	C5-C4-N3	-2.74	118.95	121.75
1	S2	668	A2M	C5-N7-C8	2.73	107.75	103.45
1	S2	668	A2M	C4'-O4'-C1'	-2.73	103.45	109.47
1	S2	683	OMG	N9-C8-N7	-2.72	108.36	113.40
1	S2	1842	4AC	O7-C7-CM7	-2.71	117.23	122.05
1	S2	644	OMG	C5-C6-N1	2.66	120.03	113.25
1	S2	683	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	119	PSU	C6-C5-C4	2.65	119.96	118.17
1	S2	484	A2M	C3'-C2'-C1'	2.64	107.87	102.81
1	S2	822	PSU	C6-C5-C4	2.64	119.95	118.17
1	S2	509	OMG	N9-C8-N7	-2.63	108.53	113.40
1	S2	1678	A2M	C5-N7-C8	2.62	107.58	103.45
1	S2	1850	MA6	C4-C5-N7	-2.62	107.59	110.58
1	S2	27	A2M	C5-N7-C8	2.61	107.55	103.45
1	S2	509	OMG	C5-C6-N1	2.61	119.89	113.25
1	S2	1842	4AC	CM7-C7-N4	2.59	119.45	115.27
1	S2	668	A2M	C4-N9-C8	2.58	108.44	105.74
1	S2	683	OMG	O6-C6-C5	-2.55	119.80	126.53
1	S2	166	A2M	C4'-O4'-C1'	-2.54	103.87	109.47
1	S2	116	OMU	C6-N1-C2	-2.52	117.93	121.00
1	S2	166	A2M	O4'-C1'-C2'	-2.50	102.29	106.59
1	S2	1678	A2M	C2'-C3'-C4'	2.50	107.36	101.99
1	S2	1806	M7A	C5-C4-N3	-2.50	120.79	126.56
1	S2	159	A2M	C6-C5-C4	2.48	120.57	117.18
1	S2	668	A2M	N3-C4-N9	2.48	131.39	127.17
1	S2	166	A2M	C6-C5-C4	2.44	120.51	117.18
1	S2	1851	MA6	N3-C4-N9	2.44	131.32	127.17
1	S2	1830	UR3	C6-C5-C4	2.44	125.40	120.73
1	S2	1337	4AC	C6-C5-C4	2.41	119.91	117.00
1	S2	1851	MA6	C4-C5-N7	-2.41	107.83	110.58
1	S2	1248	B8N	O4-C4-N3	-2.38	116.12	119.99
1	S2	644	OMG	O6-C6-C5	-2.38	120.26	126.53
1	S2	1832	6MZ	C5-C4-N9	2.38	108.40	105.81
1	S2	509	OMG	O6-C6-C5	-2.37	120.29	126.53
1	S2	1850	MA6	N3-C4-N9	2.36	131.18	127.17
1	S2	1031	A2M	O4'-C1'-C2'	-2.36	102.53	106.59
1	S2	1850	MA6	C5-C4-N9	2.36	108.38	105.81
1	S2	27	A2M	C4-N9-C8	2.35	108.21	105.74
1	S2	517	OMC	O2-C2-N3	-2.34	118.63	122.33
1	S2	119	PSU	O2-C2-N1	-2.34	120.38	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	814	5MU	O4-C4-N3	-2.33	115.73	120.11
1	S2	1678	A2M	CM'-O2'-C2'	2.32	120.43	114.47
1	S2	1703	OMC	O2-C2-N3	-2.31	118.69	122.33
1	S2	822	PSU	O2-C2-N1	-2.29	120.42	122.79
1	S2	568	E3C	C31-N3-C2	2.26	120.33	117.49
1	S2	1832	6MZ	C4-C5-C6	2.25	118.65	116.78
1	S2	1248	B8N	O4-C4-C5	-2.24	118.70	122.58
1	S2	1248	B8N	O2-C2-N3	-2.20	119.02	121.98
1	S2	823	PSU	O4'-C1'-C2'	2.20	108.20	105.15
1	S2	1031	A2M	C4-N9-C8	2.20	108.05	105.74
1	S2	1832	6MZ	C6-C5-N7	2.20	134.82	132.43
1	S2	1248	B8N	O4'-C1'-C2'	2.12	108.08	105.15
1	S2	159	A2M	C3'-C2'-C1'	2.11	106.86	102.81
1	S2	1850	MA6	C4-N9-C8	2.10	107.94	105.74
1	S2	484	A2M	C4-N9-C8	2.08	107.93	105.74
1	S2	814	5MU	O3'-C3'-C4'	2.08	117.07	111.08
1	S2	1337	4AC	C5-C4-N3	-2.07	119.36	122.60
1	S2	1081	PSU	O4-C4-N3	-2.06	116.25	120.11
1	S2	644	OMG	C8-N7-C5	2.05	107.91	104.26
1	S2	814	5MU	O2-C2-N3	-2.04	117.72	121.49
1	S2	166	A2M	C4-C5-N7	-2.04	108.25	110.58
1	S2	484	A2M	C2'-C3'-C4'	2.04	106.38	101.99
1	S2	27	A2M	C4'-O4'-C1'	-2.03	104.97	109.47
1	S2	668	A2M	C4-C5-N7	-2.02	108.27	110.58
1	S2	27	A2M	O2'-C2'-C1'	2.02	112.83	108.99
1	S2	612	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	568	E3C	O4'-C1'-N1-C2
1	S2	568	E3C	O4'-C1'-N1-C6
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	644	OMG	C1'-C2'-O2'-CM2
1	S2	1248	B8N	C31-C32-C33-C34
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1830	UR3	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	S2	1830	UR3	O4'-C1'-N1-C2
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1850	MA6	O4'-C4'-C5'-O5'
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	119	PSU	O4'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	568	E3C	O4'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	1337	4AC	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	119	PSU	C3'-C4'-C5'-O5'
1	S2	1703	OMC	C3'-C4'-C5'-O5'
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	1851	MA6	C5-C6-N6-C10
1	S2	1031	A2M	C3'-C4'-C5'-O5'
1	S2	1248	B8N	N3-C31-C32-C33
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	1031	A2M	O4'-C4'-C5'-O5'
1	S2	1678	A2M	C4'-C5'-O5'-P
1	S2	1806	M7A	C2'-C1'-N9-C8
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	1337	4AC	C3'-C4'-C5'-O5'
1	S2	1081	PSU	C4'-C5'-O5'-P
1	S2	1243	PSU	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	159	A2M	2	0
1	S2	121	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1850	MA6	1	0
1	S2	683	OMG	1	0
1	S2	1337	4AC	1	0
1	S2	509	OMG	1	0
1	S2	814	5MU	1	0
1	S2	644	OMG	1	0
1	S2	484	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	MVM	t	5110	-	35,35,35	1.01	2 (5%)	44,49,49	1.34	6 (13%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	C5-N1	2.87	1.41	1.37
86	t	5110	MVM	C1-N2	2.20	1.52	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5110	MVM	C22-N4-N5	-3.56	108.54	110.25
86	t	5110	MVM	N7-C22-N4	3.14	129.40	125.88
86	t	5110	MVM	C1-C9-N1	-3.12	108.33	116.16
86	t	5110	MVM	C9-N1-C5	-2.42	115.00	118.64
86	t	5110	MVM	O1-C5-N1	-2.41	118.43	121.51
86	t	5110	MVM	N4-N5-N6	2.17	109.99	108.77

There are no chirality outliers.

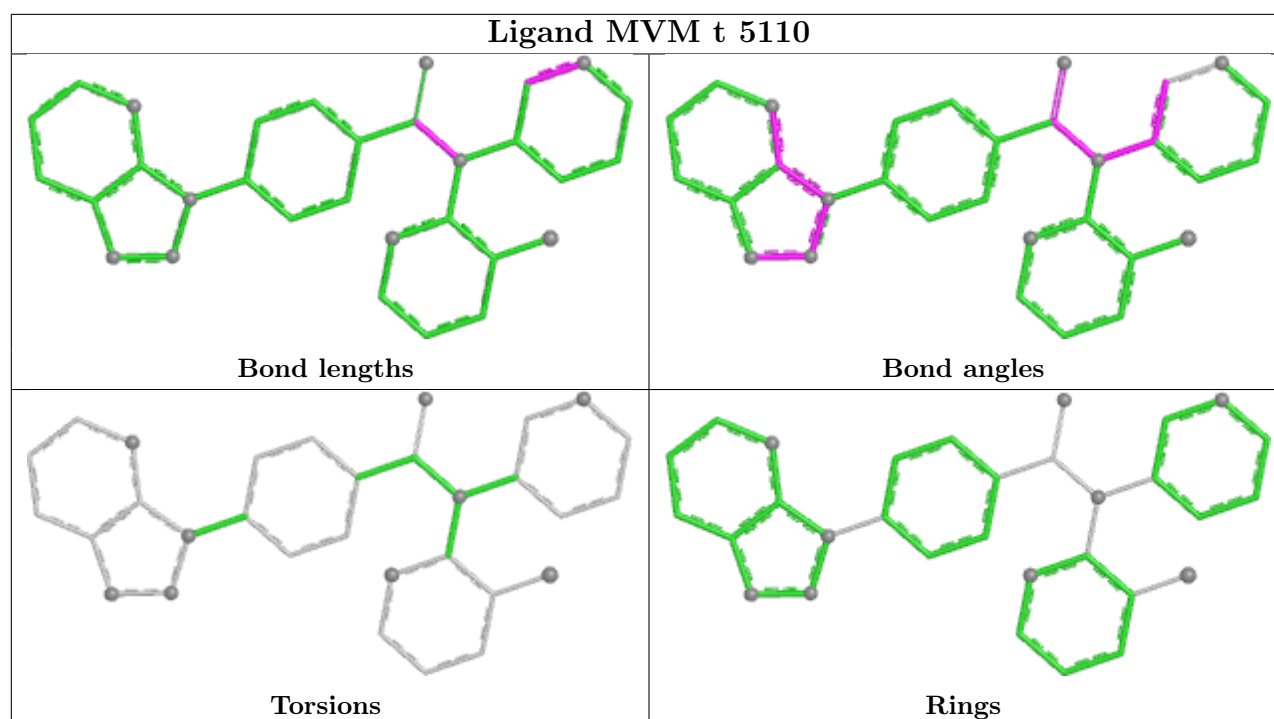
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	t	5110	MVM	7	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
1	S2	17
79	t	16
81	v	4
6	SF	2
23	SC	2
5	SE	2
10	SL	2
7	SH	1
63	c	1
80	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1677:U	O3'	1678:A2M	P	60.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1353:A	O3'	1354:G	P	60.47
1	S2	1357:A	O3'	1358:U	P	59.69
1	SF	55:ARG	C	56:TYR	N	59.69
1	S2	503:C	O3'	504:G	P	59.61
1	SF	64:ALA	C	65:GLN	N	59.48
1	S2	798:A	O3'	799:U	P	59.13
1	S2	110:U	O3'	111:A	P	58.91
1	SH	103:LYS	C	104:PRO	N	58.86
1	SC	192:LEU	C	193:VAL	N	58.85
1	S2	863:U	O3'	864:A	P	58.84
1	S2	1680:G	O3'	1681:U	P	58.79
1	SC	185:THR	C	186:GLY	N	58.65
1	S2	859:G	O3'	860:G	P	58.28
1	SE	67:GLN	C	68:ARG	N	58.15
1	SE	65:CYS	C	66:MET	N	57.86
1	S2	797:C	O3'	798:A	P	57.78
1	S2	500:A	O3'	501:C	P	57.65
1	SL	37:TYR	C	38:LYS	N	57.16
1	SL	47:PRO	C	48:LYS	N	56.76
1	S2	115:U	O3'	116:OMU	P	56.57
1	S2	753:C	O3'	785:C	P	27.35
1	t	750:G	O3'	890:C	P	20.71
1	t	3919:C	O3'	4035:G	P	18.97
1	t	517:C	O3'	629:G	P	18.72
1	t	976:U	O3'	1047:G	P	17.38
1	t	1680:C	O3'	1699:C	P	16.85
1	S2	1752:C	O3'	1779:G	P	16.14
1	t	2093:C	O3'	2228:C	P	16.13
1	t	4737:G	O3'	4815:C	P	15.62
1	t	2881:G	O3'	3569:C	P	15.22
1	t	1202:G	O3'	1216:G	P	15.08
1	t	1089:A	O3'	1145:G	P	14.75
1	S2	739:C	O3'	746:C	P	12.31
1	t	1253:A	O3'	1256:G	P	12.14
1	S2	698:G	O3'	730:C	P	11.42
1	S2	225:G	O3'	287:U	P	7.30
1	c	119:CYS	C	120:ARG	N	7.11
1	t	945:G	O3'	946:G	P	6.09
1	v	17:A	O3'	18:G	P	5.92
1	t	4734:C	O3'	4735:C	P	5.26
1	u	54:U	O3'	55:U	P	4.22
1	v	21:A	O3'	22:G	P	4.22

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	4817:G	O3'	4818:G	P	4.20
1	v	10:G	O3'	11:C	P	3.33
1	t	964:C	O3'	965:G	P	3.26
1	v	41:C	O3'	42:C	P	3.25
1	t	1938:U	O3'	1939:A	P	3.22

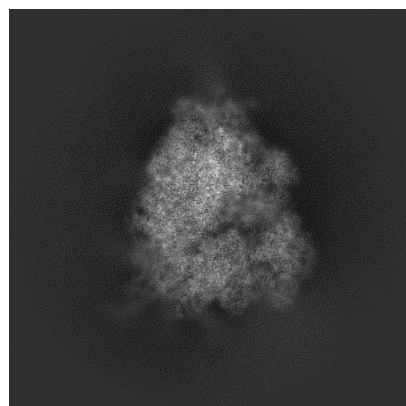
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0596. These allow visual inspection of the internal detail of the map and identification of artifacts.

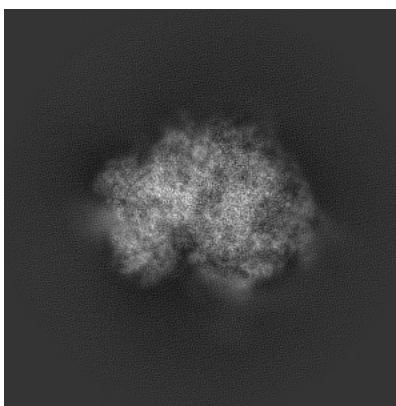
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

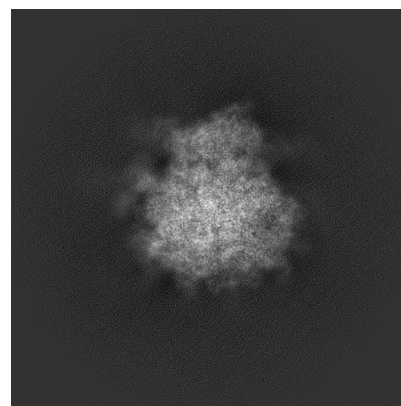
6.1.1 Primary map



X

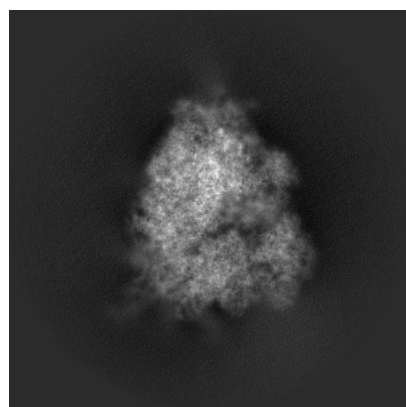


Y

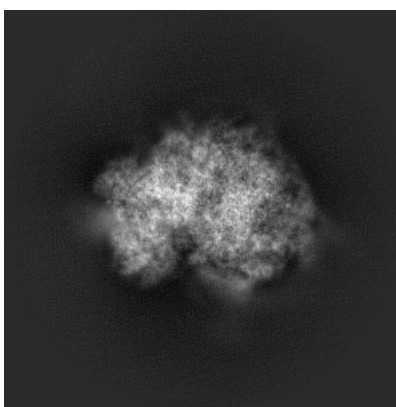


Z

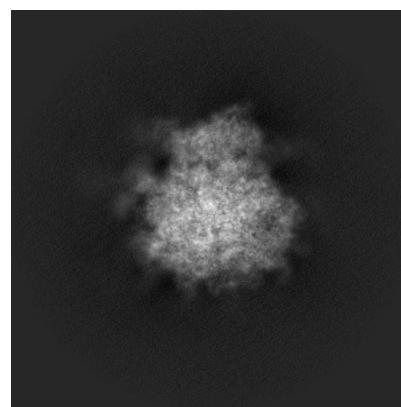
6.1.2 Raw map



X



Y

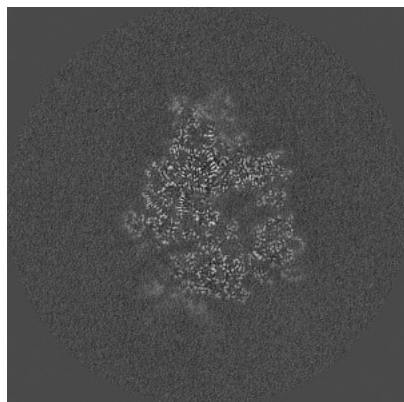


Z

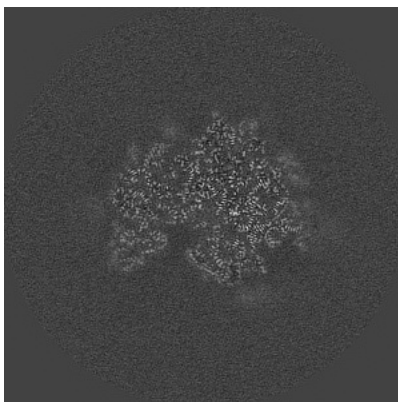
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

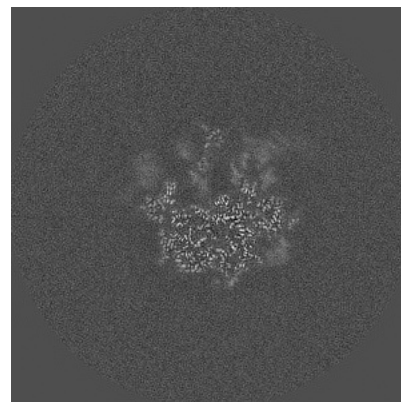
6.2.1 Primary map



X Index: 215

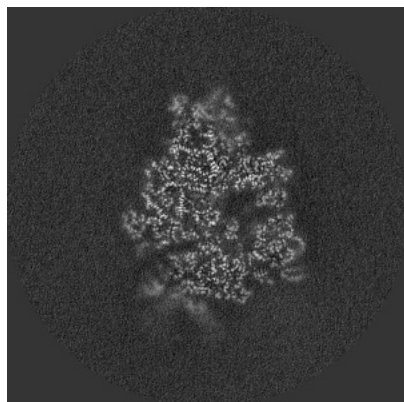


Y Index: 215

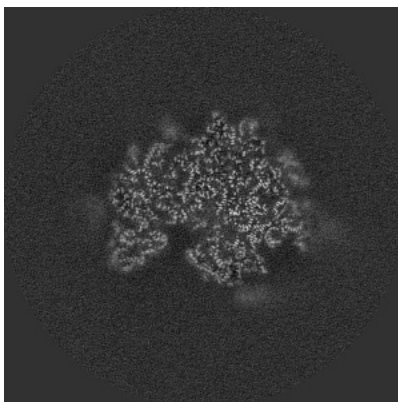


Z Index: 215

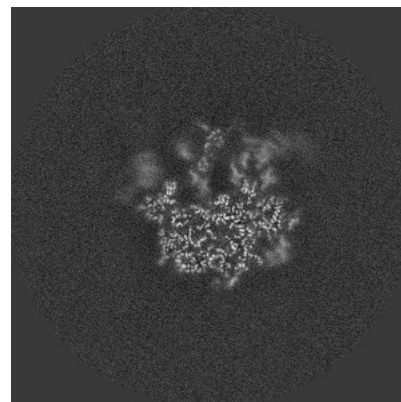
6.2.2 Raw map



X Index: 215



Y Index: 215

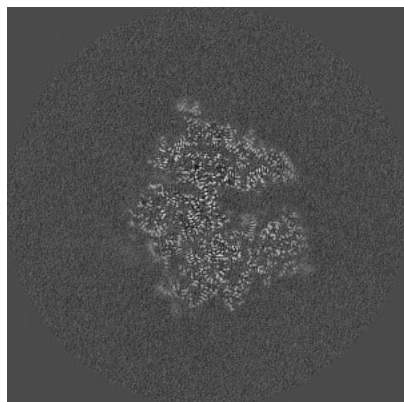


Z Index: 215

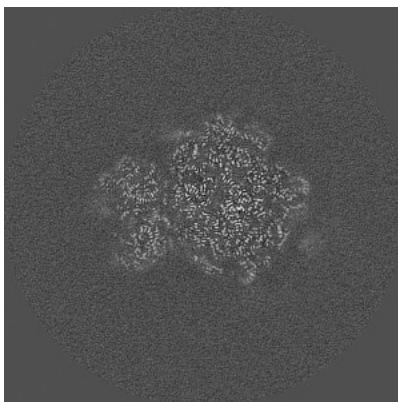
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

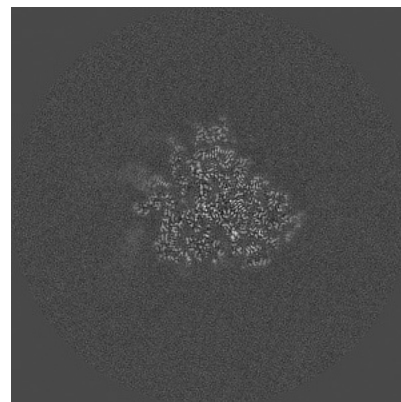
6.3.1 Primary map



X Index: 231

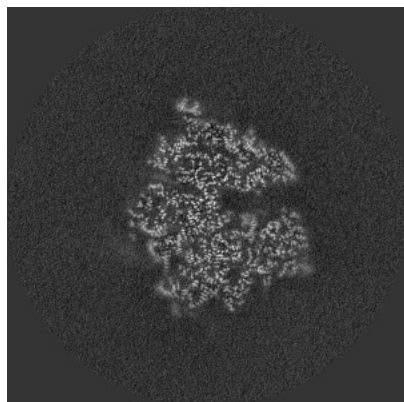


Y Index: 204

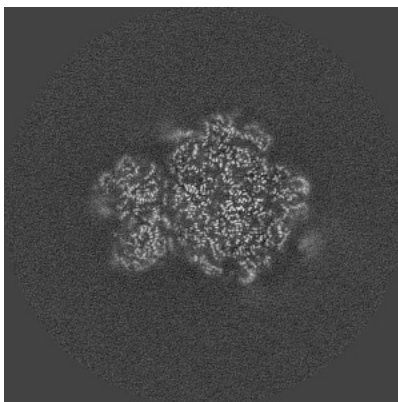


Z Index: 243

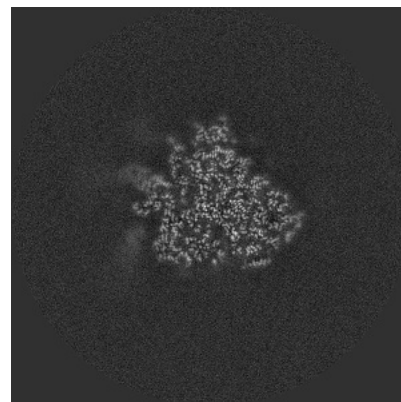
6.3.2 Raw map



X Index: 231



Y Index: 204

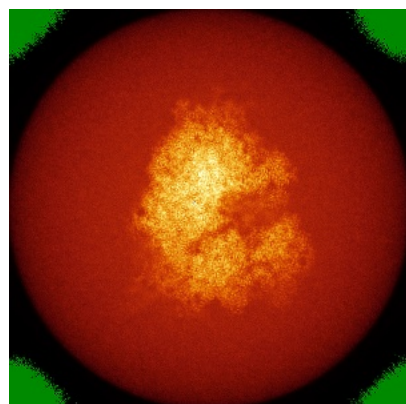


Z Index: 243

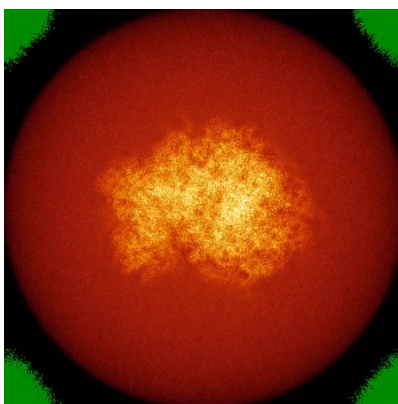
The images above show the largest variance slices of the map in three orthogonal directions.

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

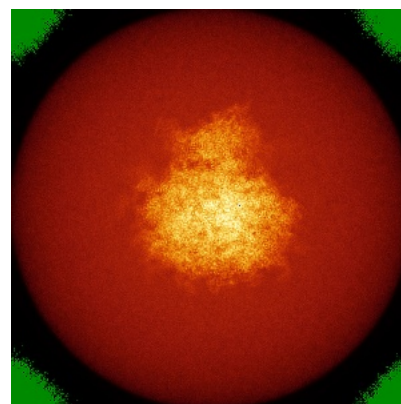
6.4.1 Primary map



X

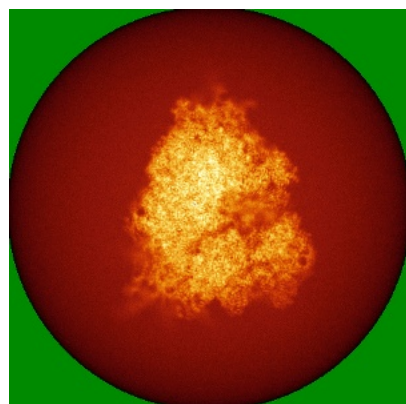


Y

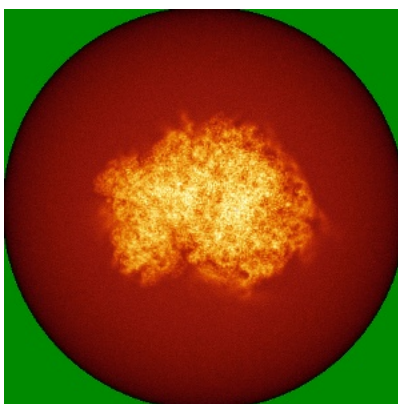


Z

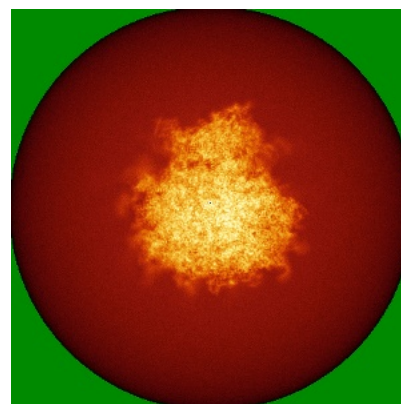
6.4.2 Raw map



X



Y

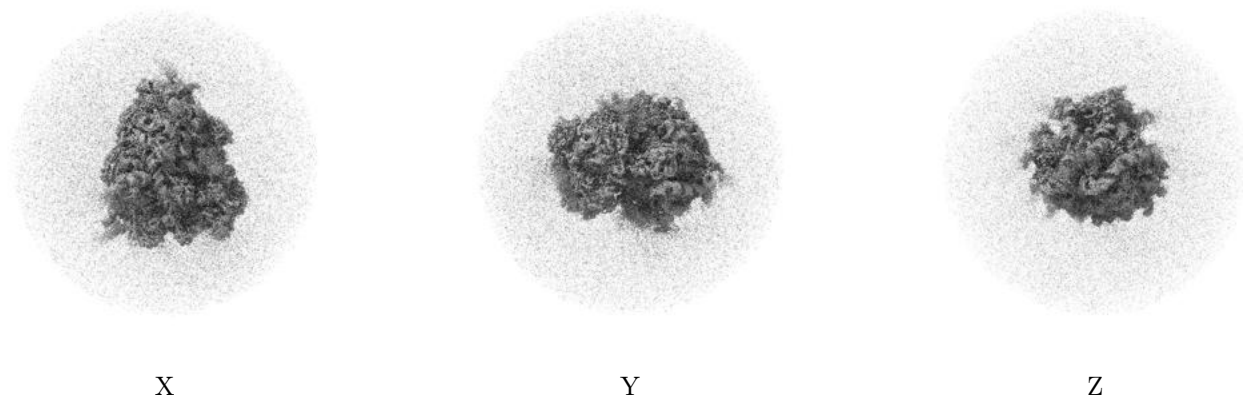


Z

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.

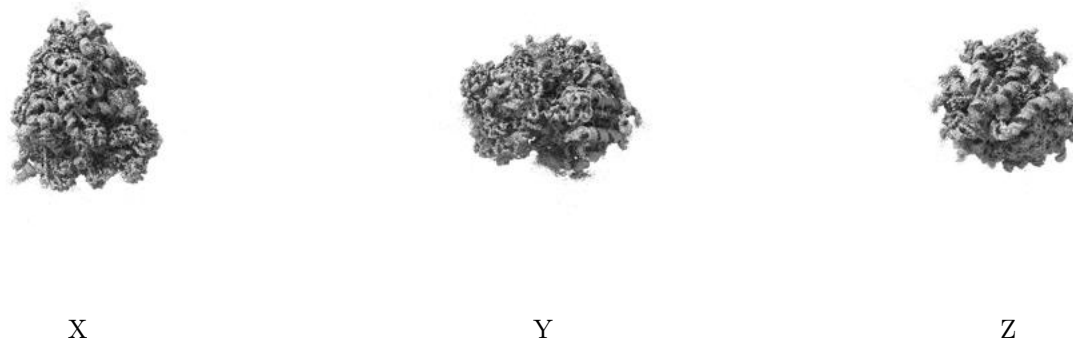
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

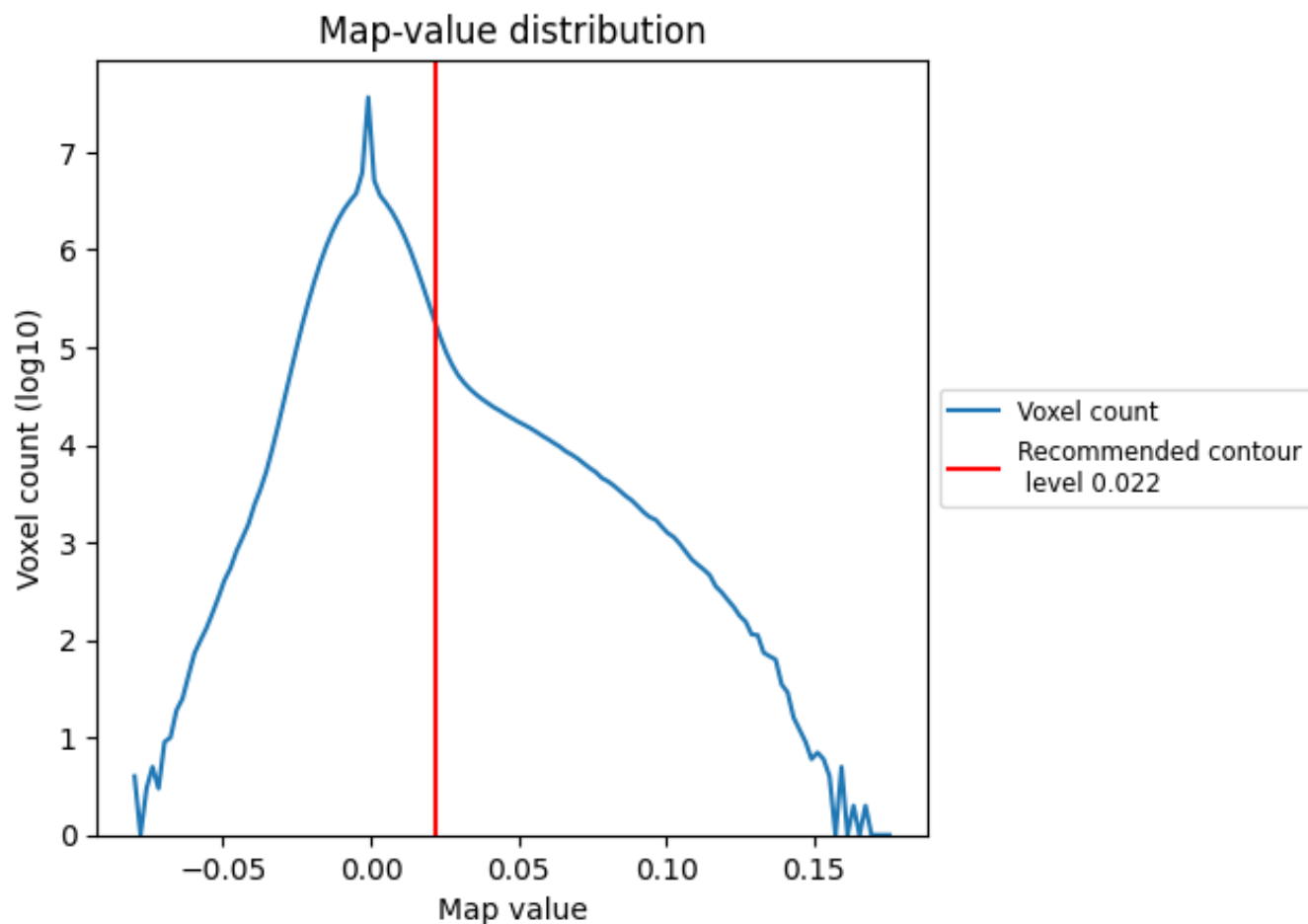
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

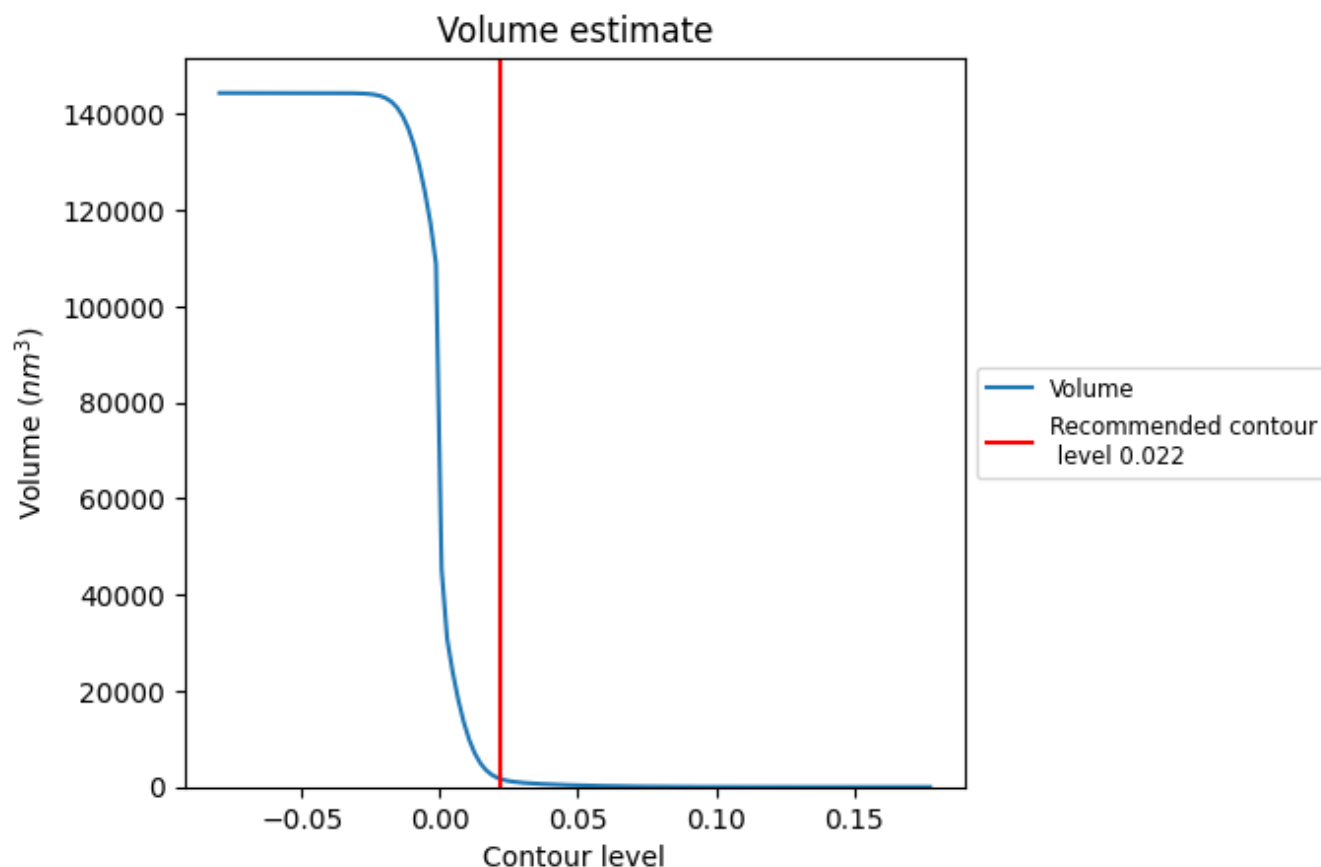
This section contains the results of statistical analysis of the map.

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.

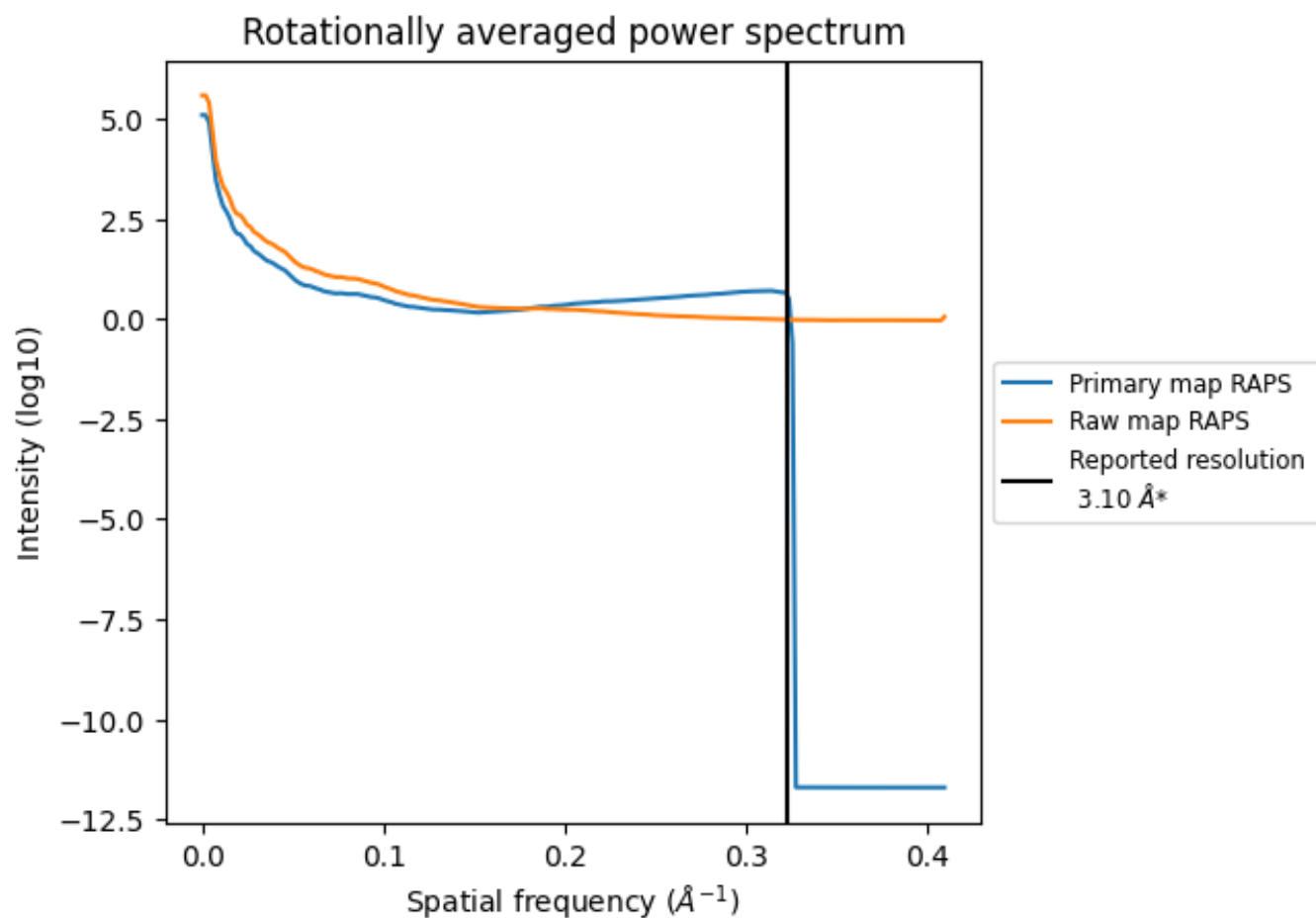
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1680 nm^3 ; this corresponds to an approximate mass of 1518 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 ⓘ

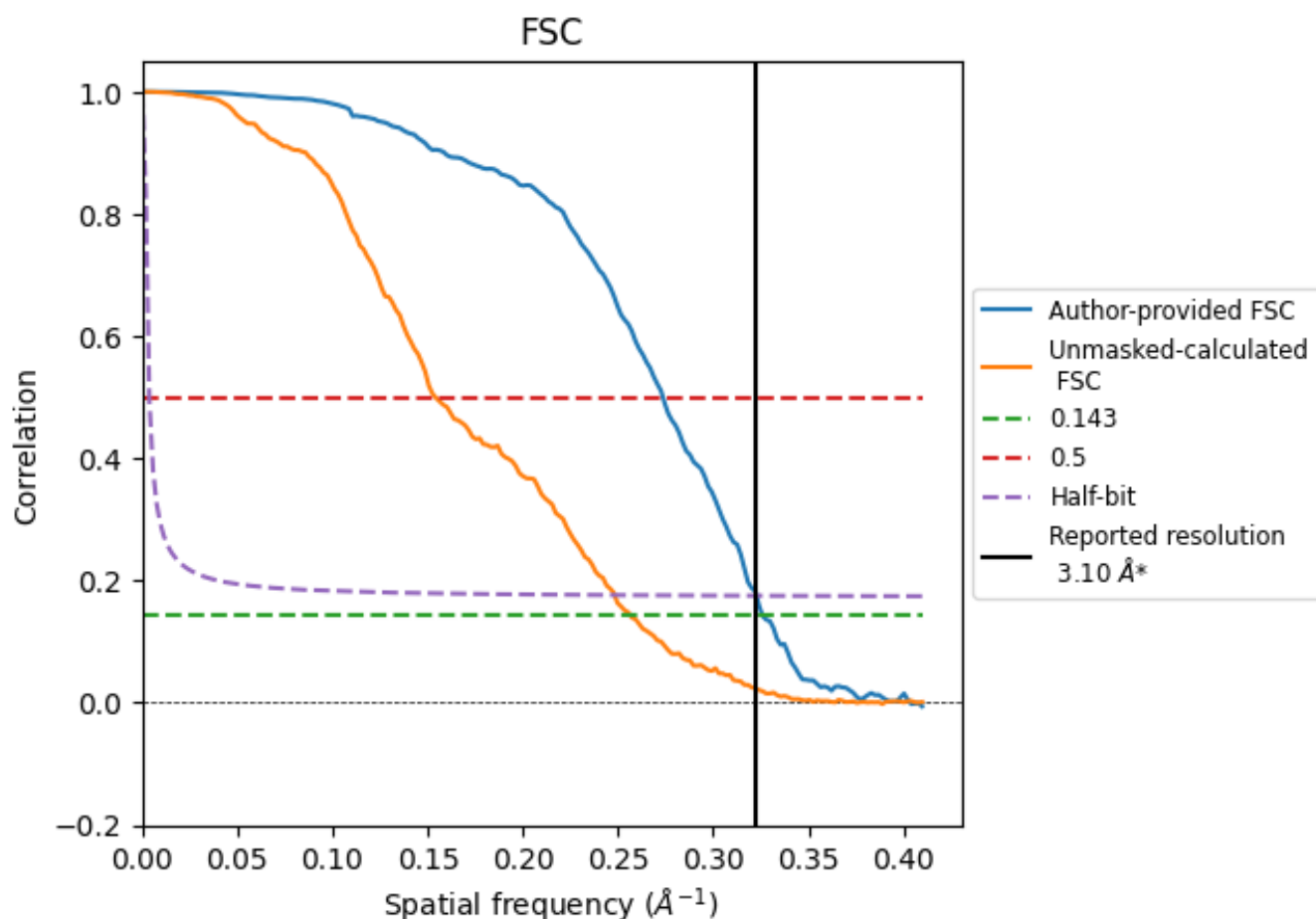


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

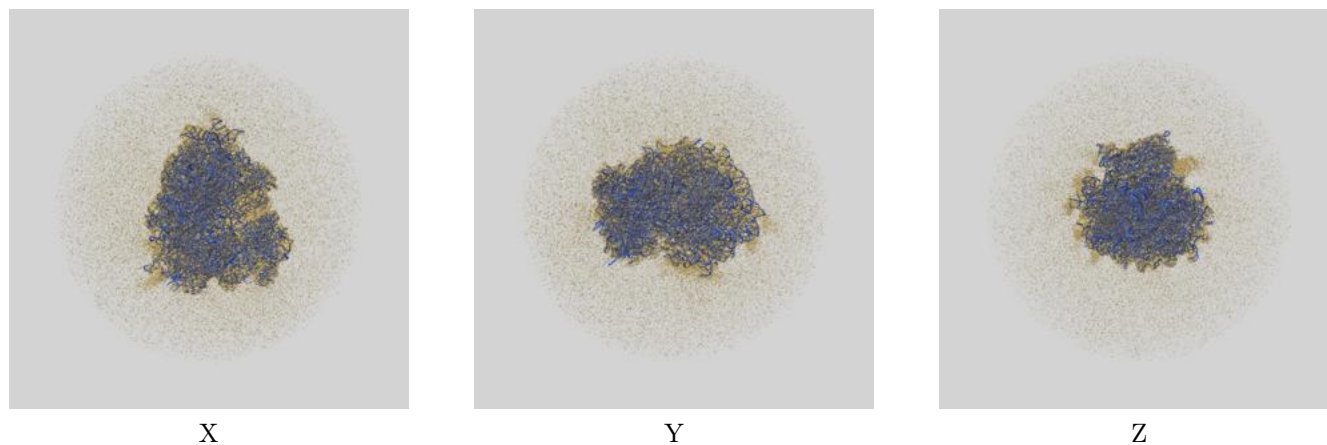
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.65	3.10
Unmasked-calculated*	3.90	6.49	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

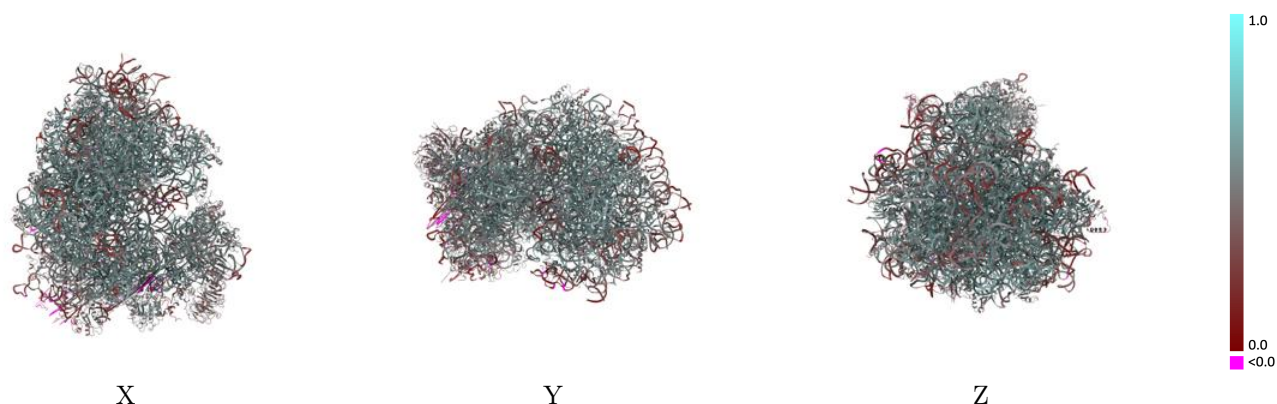
This section contains information regarding the fit between EMDB map EMD-0596 and PDB model 6OM0. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



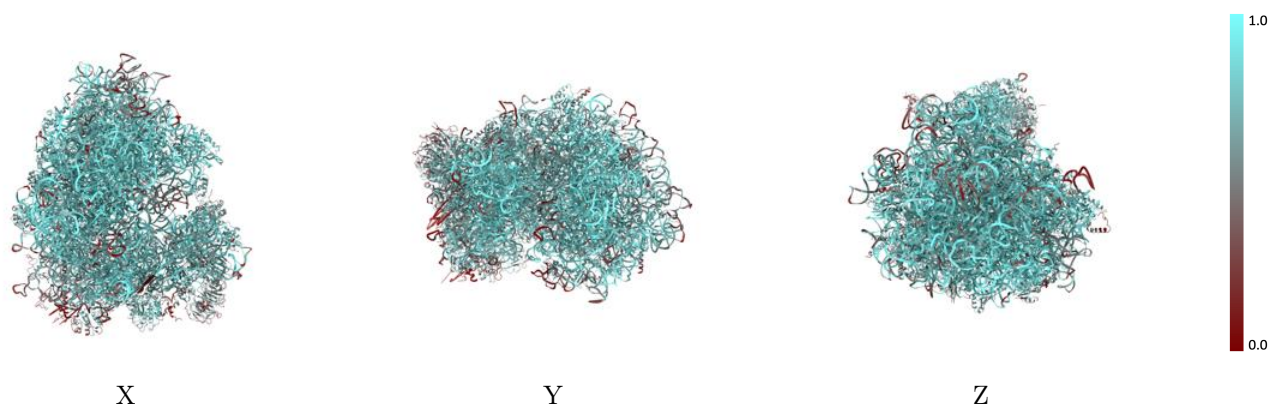
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



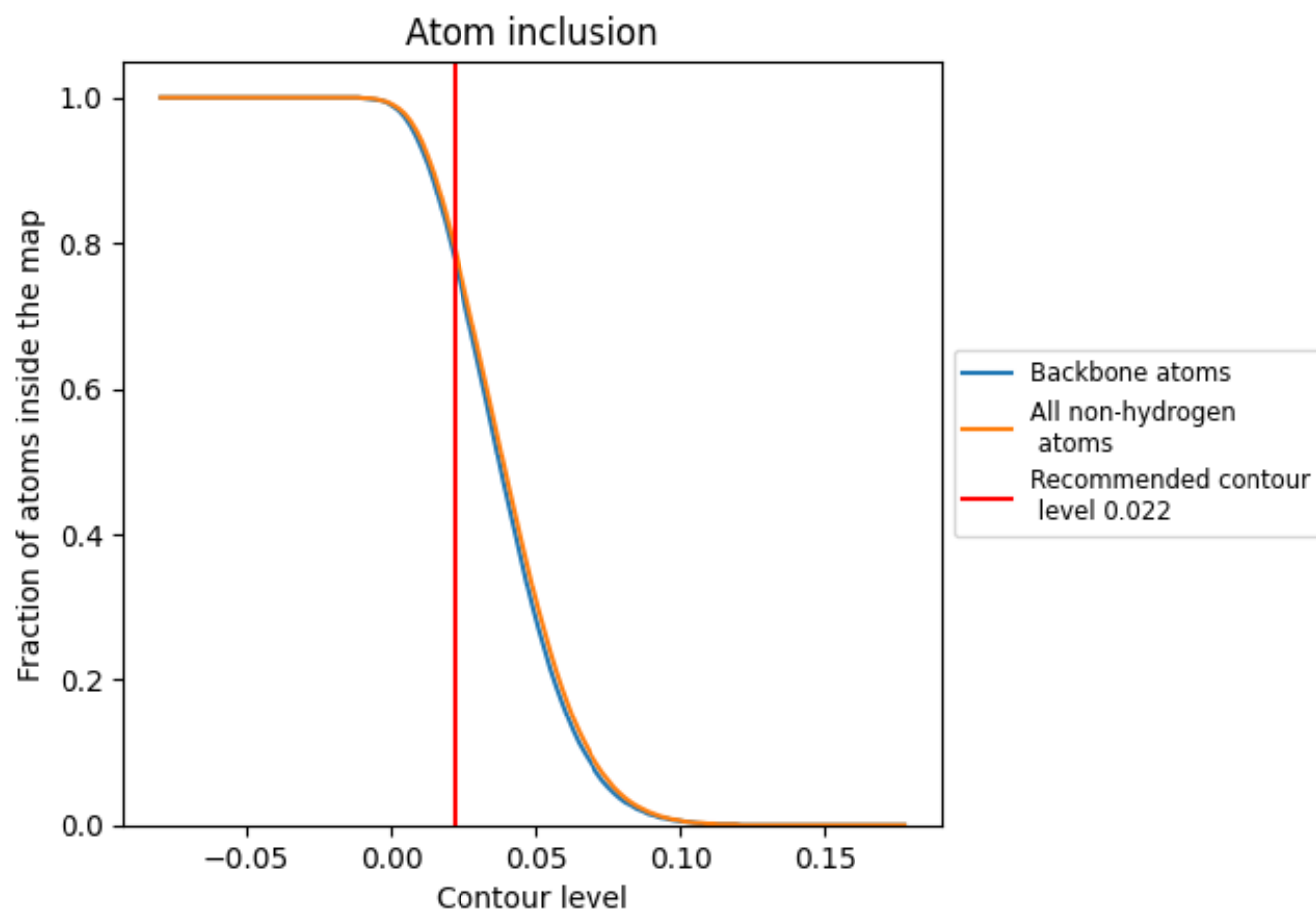
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.5110
A	 0.8440	 0.5700
B	 0.7950	 0.5320
C	 0.8140	 0.5430
D	 0.8720	 0.5480
E	 0.9550	 0.5870
F	 0.7710	 0.4980
G	 0.6920	 0.4610
H	 0.8160	 0.5450
I	 0.7130	 0.4920
J	 0.7430	 0.5130
K	 0.7770	 0.5310
L	 0.7380	 0.4980
M	 0.7520	 0.5070
N	 0.7890	 0.5220
O	 0.8780	 0.5710
P	 0.8250	 0.5430
Q	 0.8330	 0.5520
R	 0.8230	 0.5440
S	 0.7140	 0.4920
S2	 0.8410	 0.5160
SA	 0.6690	 0.4770
SB	 0.7230	 0.5040
SC	 0.7100	 0.5020
SD	 0.6020	 0.4500
SE	 0.7060	 0.4920
SF	 0.6180	 0.4400
SG	 0.5740	 0.4160
SH	 0.5200	 0.4010
SI	 0.6620	 0.4590
SJ	 0.6960	 0.4650
SK	 0.5990	 0.4320
SL	 0.6500	 0.4680
SM	 0.2370	 0.2420
SN	 0.7420	 0.5160



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Chain	Atom inclusion	Q-score
SO	 0.7090	 0.4980
SP	 0.6790	 0.4650
SQ	 0.6630	 0.4730
SR	 0.5890	 0.4430
SS	 0.6960	 0.4690
ST	 0.7060	 0.4800
SU	 0.5590	 0.4160
SV	 0.7010	 0.4850
SW	 0.8030	 0.5390
SX	 0.7670	 0.5220
SY	 0.6360	 0.4440
SZ	 0.6110	 0.4440
Sa	 0.7390	 0.5060
Sb	 0.6810	 0.4770
Sc	 0.5180	 0.4230
Sd	 0.8000	 0.5170
Se	 0.6200	 0.4420
Sf	 0.2960	 0.2930
Sg	 0.4820	 0.3750
T	 0.8150	 0.5370
U	 0.7870	 0.5230
V	 0.6750	 0.4470
W	 0.7940	 0.5560
X	 0.8210	 0.5500
Y	 0.7830	 0.5250
Z	 0.7980	 0.5320
a	 0.7640	 0.5040
b	 0.8390	 0.5580
c	 0.7010	 0.4870
d	 0.7110	 0.4850
e	 0.7640	 0.5250
f	 0.8310	 0.5620
g	 0.8270	 0.5470
h	 0.7840	 0.5410
i	 0.7570	 0.5070
j	 0.7400	 0.4920
k	 0.8630	 0.5660
l	 0.6640	 0.4710
m	 0.8110	 0.5510
n	 0.7810	 0.5350
o	 0.7590	 0.5130
p	 0.7530	 0.5150

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Chain	Atom inclusion	Q-score
q	 0.7940	 0.5560
r	 0.8160	 0.5320
t	 0.8650	 0.5290
u	 0.5910	 0.3780
v	 0.6790	 0.3970
w	 0.8870	 0.5610
y	 0.1600	 0.1540